

In Silico Mass Spectrometric Fragmentation and Liquid Chromatography with Tandem Mass Spectrometry (LC-MS/MS) Betalainic fingerprinting: Identification of Betalains in Red Pitaya

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Table S1. *In silico* analysis of betalains, using MassFrontier (Thermo Scientific) software.

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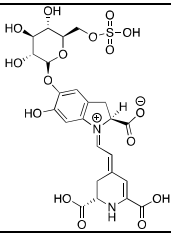
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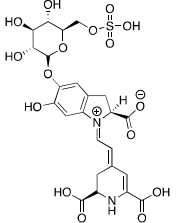
Betacyanins

Betainin-type

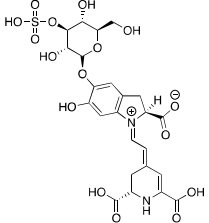
Prebetanin

Chemical structure										
Name:	Prebetanin									
Chemical Formula	C ₂₄ H ₂₆ N ₂ O ₁₆ S									
Molecular weight	630.53									
Monoisotopic mass	630.1003									
m/z [M+H]	631.1076									
Theoretical fragments (m/z)	631.11	630.1	629.09	628.08	615.11	614.1	613.1	612.09	611.08	603.11
		602.1	601.1	599.12	598.11	597.1	596.09	595.09	594.08	593.07
		591.11	589.1	588.09	587.12	586.11	585.1	584.09	583.09	581.11
		580.1	579.09	578.08	577.08	575.06	573.1	571.12	570.12	569.11
		568.1	567.09	566.08	565.08	563.1	561.1	559.09	558.08	557.11
		556.1	555.09	553.11	552.1	551.1	550.09	549.08	545.11	543.09
		542.08	541.08	540.07	539.1	538.09	537.08	533.14	532.13	531.12
		527.1	525.08	523.07	517.15	516.14	515.13	514.12	513.11	509.09
		507.07	505.15	504.14	503.13	501.15	499.13	498.13	497.12	495.1
		493.15	491.13	489.15	488.14	487.13	486.13	485.12	483.14	481.12
		479.11	475.13	473.16	471.14	470.13	469.12	463.13	462.07	461.12
		460.11	459.14	458.13	457.12	449.06	448.05	447.14	446.08	445.12
		444.06	443.11	438.07	437.06	436.05	435.05	432.06	431.05	429.13
		427.11	425.1	423.06	422.05	421.04	420.06	419.05	418.04	417.04
		410.08	408.06	405.05	404.04	403.03	402.05	400.03	393.05	392.06
		391.06	390.05	389.1	388.09	387.08	386.03	380.06	379.03	378.05
		377.05	376.05	375.12	374.05	373.1	372.1	371.09	370.08	369.07
		368.06	366.05	365.05	364.1	361.1	360.05	359.12	357.11	356.1
		355.09	354.08	353.05	351.04	350.03	349.1	348.05	347.04	345.11
		344.1	343.13	342.08	341.11	340.1	339.1	338.09	337.08	335.04
		334.04	333.03	332.02	331.09	330.04	329.11	327.1	326.09	325.08
		324.08	323.08	322.09	320.08	319.09	317.08	316.07	315.1	314.09
		313.08	307.08	306.07	303.1	301.08	300.07	299.07	298.06	297.09
		294.1	287.1	285.09	284.08	283.07	282.06	281.08	280.07	279.09
		271.11	269.09	268.08	267.06	265.08	264.07	263.07	262.06	259.01
		255.09	253.08	252.06	251.07	250.08	249.05	247.07	245.06	243.02
		237.09	235.07	233.06	231.04	225.01	223.07	222.06	220.06	211.07
		209.06	208.05	207.08	205.06	196.06	195.05	194.04	193.04	192.03
		191.05	182.08	181.05	180.04	179.03	178.05	177.04	176.03	167.07
		166.09	165.05	164.05	163.04	150.05	147.04	146.04	145.05	135.04
		134.04	130.04	124.04	123.04	119.05	111.04	110.06	109.03	108.02
		107.05	106.04							
References	<p>Wyler, H.; Rösler, H.; Mercier, M.; Dreiding, A.S. Präbetanin, ein Schwefelsäure-halbesther des Betanins. Ein Beitrag zur Kenntnis der Betacyane. <i>Helvetica Chimica Acta</i> 1967, 50, 545–561.</p> <p>Schliemann, W.; Joy, R.W.; Komamine, A.; Metzger, J.W.; Nimtz, M.; Wray, V.; Strack, D. Betacyanins from plants and cell cultures of <i>Phytolacca americana</i>. <i>Phytochemistry</i> 1996, 42, 1039–1046.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

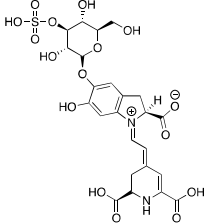
Isoprebetanin

Chemical structure										
Name:	Isoprebetanin									
Chemical Formula	C ₂₄ H ₂₆ N ₂ O ₁₆ S									
Molecular weight	630.53									
Monoisotopic mass	630.1003									
m/z [M+H]	631.1076									
Theoretical fragments (m/z)	631.11	630.1	629.09	628.08	615.11	614.1	613.1	612.09	611.08	603.11
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		591.11	589.1	588.09	587.12	586.11	585.1	584.09	583.09	581.11
		580.1	579.09	578.08	577.08	575.06	573.1	571.12	570.12	569.11
		568.1	567.09	566.08	565.08	563.1	561.1	559.09	558.08	557.11
		556.1	555.09	553.11	552.1	551.1	550.09	549.08	545.11	543.09
		542.08	541.08	540.07	539.1	538.09	537.08	533.14	532.13	531.12
		527.1	525.08	523.07	517.15	516.14	515.13	514.12	513.11	509.09
		507.07	505.15	504.14	503.13	501.15	499.13	498.13	497.12	495.1
		493.15	491.13	489.15	488.14	487.13	486.13	485.12	483.14	481.12
		479.11	475.13	473.16	471.14	470.13	469.12	463.13	462.07	461.12
		460.11	459.14	458.13	457.12	449.06	448.05	447.14	446.08	445.12
		444.06	443.11	438.07	437.06	436.05	435.05	432.06	431.05	429.13
		427.11	425.1	423.06	422.05	421.04	420.06	419.05	418.04	417.04
		410.08	408.06	405.05	404.04	403.03	402.05	400.03	393.05	392.06
		391.06	390.05	389.1	388.09	387.08	386.03	380.06	379.03	378.05
		377.05	376.05	375.12	374.05	373.1	372.1	371.09	370.08	369.07
		368.06	366.05	365.05	364.1	361.1	360.05	359.12	357.11	356.1
		355.09	354.08	353.05	351.04	350.03	349.1	348.05	347.04	345.11
		344.1	343.13	342.08	341.11	340.1	339.1	338.09	337.08	335.04
		334.04	333.03	332.02	331.09	330.04	329.11	327.1	326.09	325.08
		324.08	323.08	322.09	320.08	319.09	317.08	316.07	315.1	314.09
		313.08	307.08	306.07	303.1	301.08	300.07	299.07	298.06	297.09
		294.1	287.1	285.09	284.08	283.07	282.06	281.08	280.07	279.09
		271.11	269.09	268.08	267.06	265.08	264.07	263.07	262.06	259.01
		255.09	253.08	252.06	251.07	250.08	249.05	247.07	245.06	243.02
		237.09	235.07	233.06	231.04	225.01	223.07	222.06	220.06	211.07
		209.06	208.05	207.08	205.06	196.06	195.05	194.04	193.04	192.03
		191.05	182.08	181.05	180.04	179.03	178.05	177.04	176.03	167.07
		166.09	165.05	164.05	163.04	150.05	147.04	146.04	145.05	135.04
		134.04	130.04	124.04	123.04	119.05	111.04	110.06	109.03	108.02
		107.05	106.04							
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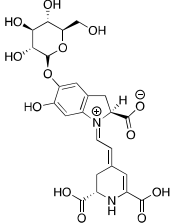
Rivinianin

Chemical structure										
Name:	Rivinianin									
Chemical Formula	C ₂₄ H ₂₆ N ₂ O ₁₆ S									
Molecular weight	630.53									
Monoisotopic mass	630.1003									
m/z [M+H]	631.1076									
Theoretical fragments (m/z)	631.11	630.1	629.09	628.08	615.11	614.1	613.1	612.09	611.08	603.11
		602.1	601.1	599.12	598.11	597.1	596.09	595.09	594.08	593.07
		591.11	589.1	588.09	587.12	586.11	585.1	584.09	583.09	581.11
		580.1	579.09	578.08	577.08	575.06	573.1	571.12	570.12	569.11
		568.1	567.09	566.08	565.08	563.1	561.1	559.09	558.08	557.11
		556.1	555.09	553.11	552.1	551.1	550.09	549.08	545.11	543.09
		542.08	541.08	540.07	539.1	538.09	537.08	533.14	532.13	531.12
		527.1	525.08	523.07	517.15	516.14	515.13	514.12	513.11	509.09
		507.07	505.15	504.14	503.13	501.15	499.13	498.13	497.12	495.1
		493.15	491.13	489.15	488.14	487.13	486.13	485.12	483.14	481.12
		479.11	475.13	473.16	471.14	470.13	469.12	463.13	462.07	461.12
		460.11	459.14	458.13	457.12	449.06	448.05	447.14	446.08	445.12
		444.06	443.11	438.07	437.06	436.05	435.05	432.06	431.05	429.13
		427.11	425.1	423.06	422.05	421.04	420.06	419.05	418.04	417.04
		410.08	408.06	405.05	404.04	403.03	402.05	400.03	393.05	392.06
		391.06	390.05	389.1	388.09	387.08	386.03	380.06	379.03	378.05
		377.05	376.05	375.12	374.05	373.1	372.1	371.09	370.08	369.07
		368.06	366.05	365.05	364.1	361.1	360.05	359.12	357.11	356.1
		355.09	354.08	353.05	351.04	350.03	349.1	348.05	347.04	345.11
		344.1	343.13	342.08	341.11	340.1	339.1	338.09	337.08	335.04
		334.04	333.03	332.02	331.09	330.04	329.11	327.1	326.09	325.08
		324.08	323.08	322.09	320.08	319.09	317.08	316.07	315.1	314.09
		313.08	307.08	306.07	303.1	301.08	300.07	299.07	298.06	297.09
		294.1	287.1	285.09	284.08	283.07	282.06	281.08	280.07	279.09
		271.11	269.09	268.08	267.06	265.08	264.07	263.07	262.06	259.01
		255.09	253.08	252.06	251.07	250.08	249.05	247.07	245.06	243.02
		237.09	235.07	233.06	231.04	225.01	223.07	222.06	220.06	211.07
		209.06	208.05	207.08	205.06	196.06	195.05	194.04	193.04	192.03
		191.05	182.08	181.05	180.04	179.03	178.05	177.04	176.03	167.07
		166.09	165.05	164.05	163.04	150.05	147.04	146.04	145.05	135.04
		134.04	130.04	124.04	123.04	119.05	111.04	110.06	109.03	108.02
		107.05	106.04							
References	<p>Imperato, F. <i>Phytochemistry</i> 1975, 14, 2526–2527.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spóma-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

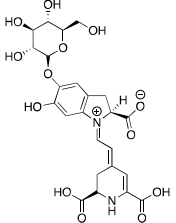
Isorivininianin

Chemical structure										
Name:	Isorivininianin									
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Molecular weight	630.53									
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		602.1	601.1	599.12	598.11	597.1	596.09	595.09	594.08	593.07
		591.11	589.1	588.09	587.12	586.11	585.1	584.09	583.09	581.11
		580.1	579.09	578.08	577.08	575.06	573.1	571.12	570.12	569.11
		568.1	567.09	566.08	565.08	563.1	561.1	559.09	558.08	557.11
		556.1	555.09	553.11	552.1	551.1	550.09	549.08	545.11	543.09
		542.08	541.08	540.07	539.1	538.09	537.08	533.14	532.13	531.12
		527.1	525.08	523.07	517.15	516.14	515.13	514.12	513.11	509.09
		507.07	505.15	504.14	503.13	501.15	499.13	498.13	497.12	495.1
		493.15	491.13	489.15	488.14	487.13	486.13	485.12	483.14	481.12
		479.11	475.13	473.16	471.14	470.13	469.12	463.13	462.07	461.12
		460.11	459.14	458.13	457.12	449.06	448.05	447.14	446.08	445.12
		444.06	443.11	438.07	437.06	436.05	435.05	432.06	431.05	429.13
		427.11	425.1	423.06	422.05	421.04	420.06	419.05	418.04	417.04
		410.08	408.06	405.05	404.04	403.03	402.05	400.03	393.05	392.06
		391.06	390.05	389.1	388.09	387.08	386.03	380.06	379.03	378.05
		377.05	376.05	375.12	374.05	373.1	372.1	371.09	370.08	369.07
		368.06	366.05	365.05	364.1	361.1	360.05	359.12	357.11	356.1
		355.09	354.08	353.05	351.04	350.03	349.1	348.05	347.04	345.11
		344.1	343.13	342.08	341.11	340.1	339.1	338.09	337.08	335.04
		334.04	333.03	332.02	331.09	330.04	329.11	327.1	326.09	325.08
		324.08	323.08	322.09	320.08	319.09	317.08	316.07	315.1	314.09
		313.08	307.08	306.07	303.1	301.08	300.07	299.07	298.06	297.09
		294.1	287.1	285.09	284.08	283.07	282.06	281.08	280.07	279.09
		271.11	269.09	268.08	267.06	265.08	264.07	263.07	262.06	259.01
		255.09	253.08	252.06	251.07	250.08	249.05	247.07	245.06	243.02
		237.09	235.07	233.06	231.04	225.01	223.07	222.06	220.06	211.07
		209.06	208.05	207.08	205.06	196.06	195.05	194.04	193.04	192.03
		191.05	182.08	181.05	180.04	179.03	178.05	177.04	176.03	167.07
		166.09	165.05	164.05	163.04	150.05	147.04	146.04	145.05	135.04
		134.04	130.04	124.04	123.04	119.05	111.04	110.06	109.03	108.02
		107.05	106.04							
References	<p>Imperato, F. <i>Phytochemistry</i> 1975, 14, 2526–2527.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spóma-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

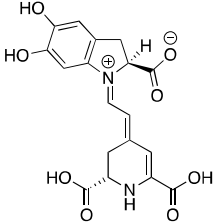
Betanin

Chemical structure										
Name:	Betanin									
Chemical Formula	C ₂₄ H ₂₆ N ₂ O ₁₃									
Molecular weight	550.47 g/mol									
Monoisotopic mass	550.1435 Da									
m/z [M+H]	551.1508 Da									
Theoretical fragments (m/z)	551.15	550.14	549.14	548.13	535.16	534.15	533.14	532.13	531.12	523.16
		522.15	521.14	519.16	518.15	517.15	516.14	515.13	514.12	513.11
		511.16	509.14	508.13	507.16	506.15	505.15	504.14	503.13	501.15
		500.14	499.13	498.13	497.12	495.1	493.15	491.17	490.16	489.15
		488.14	487.13	486.13	485.12	483.14	481.15	479.13	478.12	477.15
		476.14	475.13	473.16	472.15	471.14	470.13	469.12	465.15	463.13
		462.13	461.12	460.11	459.14	458.13	457.12	447.14	445.12	443.11
		429.13	427.11	425.1	419.11	417.09	389.1	388.09	387.08	386.07
		382.11	375.12	373.1	372.1	371.09	370.08	369.07	368.1	366.12
		364.1	361.1	360.1	359.12	358.11	357.11	356.1	355.09	354.08
		353.08	352.1	351.06	349.1	347.09	345.11	344.1	343.13	342.09
		341.09	340.1	339.1	338.09	337.08	335.09	331.09	330.12	329.11
		328.1	327.1	326.09	325.09	324.08	323.08	322.09	320.08	319.09
		317.08	316.07	315.1	314.09	313.09	312.11	311.1	310.09	307.08
		306.07	303.1	301.08	300.07	299.07	298.06	297.1	296.09	294.1
		288.11	287.1	286.09	285.1	284.08	283.07	282.06	281.08	280.07
		279.09	273.1	271.08	270.07	269.09	268.09	267.06	265.08	264.07
		263.07	262.06	255.09	254.08	253.08	252.06	251.07	250.08	249.05
		247.07	245.06	237.09	235.07	233.06	231.04	223.07	222.06	220.06
		211.07	209.06	208.05	207.08	205.06	196.06	195.05	194.04	193.04
		192.03	191.05	182.08	181.05	180.04	179.03	178.05	177.04	176.03
		167.07	166.09	165.05	164.05	163.04	150.05	147.04	146.04	145.05
		135.04	134.04	130.04	124.04	123.04	119.05	111.04	110.06	109.03
		108.02	107.05	106.04						
References	<p>Wyler, H.; Dreiding, A.S. Kristallisiertes Betanin. Vorläufige Mitteilung. <i>Helvetica Chimica Acta</i>. 1957, 40, 191-192.</p> <p>Piattelli, M.; Minale, L. Pigments of centrospermae—I. <i>Phytochemistry</i>, 1964, 3, 307-311.</p> <p>Heuer, S.; Wray, V.; Metzger, J.W.; Strack, D. Betacyanins from flowers of <i>Gomphrena globosa</i>. <i>Phytochemistry</i> 1992, 31, 1801–1807.</p> <p>Slimen, I.B.; Najjar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

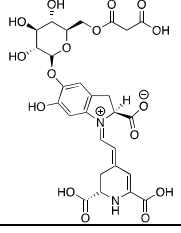
Isobetanin

Chemical structure										
Name:	Isobetanin									
Chemical Formula	C ₂₄ H ₂₆ N ₂ O ₁₃									
Molecular weight	550.47 g/mol									
Monoisotopic mass	550.1435 Da									
m/z [M+H]	551.1508 Da									
Theoretical fragments (m/z)	551.15	550.14	549.14	548.13	535.16	534.15	533.14	532.13	531.12	523.16
		522.15	521.14	519.16	518.15	517.15	516.14	515.13	514.12	513.11
		511.16	509.14	508.13	507.16	506.15	505.15	504.14	503.13	501.15
		500.14	499.13	498.13	497.12	495.1	493.15	491.17	490.16	489.15
		488.14	487.13	486.13	485.12	483.14	481.15	479.13	478.12	477.15
		476.14	475.13	473.16	472.15	471.14	470.13	469.12	465.15	463.13
		462.13	461.12	460.11	459.14	458.13	457.12	447.14	445.12	443.11
		429.13	427.11	425.1	419.11	417.09	389.1	388.09	387.08	386.07
		382.11	375.12	373.1	372.1	371.09	370.08	369.07	368.1	366.12
		364.1	361.1	360.1	359.12	358.11	357.11	356.1	355.09	354.08
		353.08	352.1	351.06	349.1	347.09	345.11	344.1	343.13	342.09
		341.09	340.1	339.1	338.09	337.08	335.09	331.09	330.12	329.11
		328.1	327.1	326.09	325.09	324.08	323.08	322.09	320.08	319.09
		317.08	316.07	315.1	314.09	313.09	312.11	311.1	310.09	307.08
		306.07	303.1	301.08	300.07	299.07	298.06	297.1	296.09	294.1
		288.11	287.1	286.09	285.1	284.08	283.07	282.06	281.08	280.07
		279.09	273.1	271.08	270.07	269.09	268.09	267.06	265.08	264.07
		263.07	262.06	255.09	254.08	253.08	252.06	251.07	250.08	249.05
		247.07	245.06	237.09	235.07	233.06	231.04	223.07	222.06	220.06
		211.07	209.06	208.05	207.08	205.06	196.06	195.05	194.04	193.04
		192.03	191.05	182.08	181.05	180.04	179.03	178.05	177.04	176.03
		167.07	166.09	165.05	164.05	163.04	150.05	147.04	146.04	145.05
		135.04	134.04	130.04	124.04	123.04	119.05	111.04	110.06	109.03
		108.02	107.05	106.04						
References	<p>Wyler, H.; Dreiding, A.S. Kristallisiertes Betanin. Vorläufige Mitteilung. <i>Helvetica Chimica Acta</i>. 1957, 40, 191-192.</p> <p>Piattelli, M.; Minale, L. Pigments of centrospermae—I. <i>Phytochemistry</i>, 1964, 3, 307-311.</p> <p>Heuer, S.; Wray, V.; Metzger, J.W.; Strack, D. Betacyanins from flowers of <i>Gomphrena globosa</i>. <i>Phytochemistry</i> 1992, 31, 1801–1807.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

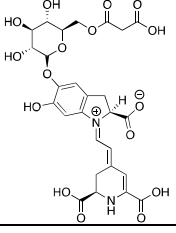
Betanidin

Chemical structure										
Name:	Betanidin									
Chemical Formula	C ₁₈ H ₁₆ N ₂ O ₈									
Molecular weight	388.33 g/mol									
Monoisotopic mass	388.0907 Da									
m/z [M+H]	389.0979									
Theoretical fragments (m/z)	389.1	388.09	387.08	386.07	374.09	373.1	372.1	371.09	370.08	369.07
		361.1	360.1	359.09	358.08	357.11	356.1	355.09	354.08	353.08
		352.07	351.06	349.1	347.09	346.08	345.11	344.1	343.09	342.08
		341.08	340.08	339.1	338.09	337.08	336.07	335.09	333.11	331.09
		330.08	329.11	328.11	327.1	326.09	325.08	324.07	323.07	319.09
		318.1	317.08	316.07	315.1	314.09	313.08	312.07	311.1	310.09
		309.09	308.08	307.07	305.11	304.08	303.1	302.1	301.08	300.07
		299.07	298.09	297.06	296.08	291.1	288.09	287.1	286.09	285.09
		284.12	283.07	282.1	281.09	280.07	279.06	275.1	274.09	273.09
		272.08	271.07	270.08	269.09	267.06	266.05	265.08	264.07	263.07
		262.06	260.09	259.08	258.08	257.09	256.1	255.08	254.08	253.08
		252.07	251.07	250.06	249.09	248.04	247.07	246.08	245.06	244.06
		242.08	240.07	235.07	234.08	233.06	232.06	230.08	228.07	223.07
		222.06	220.06	218.08	216.07	211.07	209.06	208.05	207.05	206.04
		205.06	204.07	202.05	196.06	195.05	194.04	193.04	192.05	191.05
		190.05	182.04	181.05	180.04	179.03	178.05	177.04	176.03	174.05
		169.04	168.07	167.08	166.05	165.05	164.05	163.04	162.03	152.07
		151.04	150.05	149.05	148.04	147.04	146.04	144.03	142.01	138.05
		137.02	136.04	135.04	134.04	132.04	126.05	124.04	123.04	119.05
		118.04	114.02	111.04	110.02	109.03	108.02	107.05	106.04	100.04
References	<p>Wyler, H.; Dreiding, A.S. Darstellung und Abbauprodukte des Betanidins. 3. Über die Konstitution des Randenfarbstoffes Betanin. <i>Helv. Chim. Acta</i> 1959, 42, 1699–702.</p> <p>Wyler, H.; Dreiding, A.S. Deuterierung von Betanidin und Indicaxanthin. (E/Z)-stereoisomerie in Betalainen. <i>Helv. Chim. Acta</i> 1984, 67, 1793–1800.</p> <p>Slimen, I.B.; Najjar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

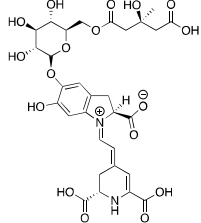
Phyllocactin

Chemical structure										
Name:	Phyllocactin									
Chemical Formula	C ₂₇ H ₂₈ N ₂ O ₁₆									
Molecular weight	636.52									
Monoisotopic mass	636.1439									
m/z [M+H]	637.1512									
Theoretical fragments (m/z)	637.15	636.14	635.14	634.13	621.16	620.15	619.14	618.13	617.12	609.16
		608.15	607.14	605.16	604.15	603.15	602.14	601.13	600.12	599.11
		597.16	595.14	594.13	593.16	592.15	591.15	590.14	589.13	587.15
		586.14	585.14	584.13	583.12	581.1	579.15	577.17	575.15	574.14
		573.14	572.13	571.12	569.14	567.15	565.13	564.12	563.15	562.14
		561.14	559.16	558.15	557.14	556.13	555.12	551.15	550.14	549.14
		548.13	547.12	546.11	545.14	544.13	543.12	535.16	534.15	533.14
		532.13	531.12	529.11	523.16	522.15	521.14	519.16	517.15	516.14
		515.13	514.12	513.11	511.1	509.14	507.16	505.15	504.14	503.13
		501.15	499.13	498.13	497.12	495.1	493.15	491.13	489.15	488.14
		487.13	486.13	485.12	481.15	479.13	478.12	477.15	476.14	475.13
		473.16	471.14	470.13	469.12	468.11	465.15	463.13	461.12	460.11
		459.14	458.13	457.12	455.11	447.14	445.12	444.11	443.11	442.1
		441.09	429.1	428.09	427.09	426.1	425.1	424.09	423.08	412.1
		411.09	410.08	409.08	408.09	406.08	399.09	398.11	397.1	396.09
		395.1	394.09	393.08	392.07	389.1	388.09	387.08	386.07	385.08
		383.1	382.09	380.1	375.12	373.1	372.09	371.1	370.08	369.07
		367.1	366.09	365.09	361.1	360.1	359.12	358.11	357.11	356.07
		355.09	354.09	353.09	351.06	349.1	347.09	345.11	343.13	342.09
		341.11	340.1	339.1	338.09	337.08	336.08	335.08	331.09	329.11
		327.1	326.09	325.09	324.08	323.08	321.06	320.08	319.09	317.08
		316.07	315.1	314.09	313.08	312.11	307.08	306.07	303.1	301.08
		300.07	299.07	298.06	297.1	294.1	287.1	285.1	284.08	283.07
		282.06	281.08	280.07	279.09	273.1	271.08	270.07	269.09	268.09
		267.06	265.08	264.07	263.07	262.06	255.09	253.08	252.06	251.07
		250.08	249.05	247.07	245.06	237.09	235.07	233.06	231.04	223.07
		222.06	211.07	207.08	205.06	196.06	194.04	193.04	192.03	182.08
		180.04	179.03	178.05	177.04	165.05	164.05	163.04	150.05	147.04
		146.04	135.04	134.04	130.04	123.04	119.05	111.04	109.03	108.02
		107.05	106.04							
References	<p>Piattelli, M.; Minale, L. Pigments of centrospermae—I. <i>Phytochemistry</i>, 1964, 3, 307-311.</p> <p>Kobayashi, N.; Schmidt, J.; Nimtz, M.; Wray, V.; Schliemann, W. Betalains from Christmas cactus. <i>Phytochemistry</i> 2000, 54, 419-426.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675-689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315-2346.</p>									

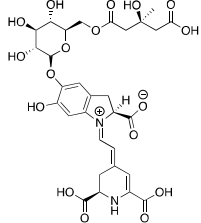
Isophyllocactin

Chemical structure										
Name:	Isophyllocactin									
Chemical Formula	C ₂₇ H ₂₈ N ₂ O ₁₆									
Molecular weight	636.52									
Monoisotopic mass	636.1439									
m/z [M+H]	637.1512									
Theoretical fragments (m/z)	637.15	636.14	635.14	634.13	621.16	620.15	619.14	618.13	617.12	609.16
		608.15	607.14	605.16	604.15	603.15	602.14	601.13	600.12	599.11
		597.16	595.14	594.13	593.16	592.15	591.15	590.14	589.13	587.15
		586.14	585.14	584.13	583.12	581.1	579.15	577.17	575.15	574.14
		573.14	572.13	571.12	569.14	567.15	565.13	564.12	563.15	562.14
		561.14	559.16	558.15	557.14	556.13	555.12	551.15	550.14	549.14
		548.13	547.12	546.11	545.14	544.13	543.12	535.16	534.15	533.14
		532.13	531.12	529.11	523.16	522.15	521.14	519.16	517.15	516.14
		515.13	514.12	513.11	511.1	509.14	507.16	505.15	504.14	503.13
		501.15	499.13	498.13	497.12	495.1	493.15	491.13	489.15	488.14
		487.13	486.13	485.12	481.15	479.13	478.12	477.15	476.14	475.13
		473.16	471.14	470.13	469.12	468.11	465.15	463.13	461.12	460.11
		459.14	458.13	457.12	455.11	447.14	445.12	444.11	443.11	442.1
		441.09	429.1	428.09	427.09	426.1	425.1	424.09	423.08	412.1
		411.09	410.08	409.08	408.09	406.08	399.09	398.11	397.1	396.09
		395.1	394.09	393.08	392.07	389.1	388.09	387.08	386.07	385.08
		383.1	382.09	380.1	375.12	373.1	372.09	371.1	370.08	369.07
		367.1	366.09	365.09	361.1	360.1	359.12	358.11	357.11	356.07
		355.09	354.09	353.09	351.06	349.1	347.09	345.11	343.13	342.09
		341.11	340.1	339.1	338.09	337.08	336.08	335.08	331.09	329.11
		327.1	326.09	325.09	324.08	323.08	321.06	320.08	319.09	317.08
		316.07	315.1	314.09	313.08	312.11	307.08	306.07	303.1	301.08
		300.07	299.07	298.06	297.1	294.1	287.1	285.1	284.08	283.07
		282.06	281.08	280.07	279.09	273.1	271.08	270.07	269.09	268.09
		267.06	265.08	264.07	263.07	262.06	255.09	253.08	252.06	251.07
		250.08	249.05	247.07	245.06	237.09	235.07	233.06	231.04	223.07
		222.06	211.07	207.08	205.06	196.06	194.04	193.04	192.03	182.08
		180.04	179.03	178.05	177.04	165.05	164.05	163.04	150.05	147.04
		146.04	135.04	134.04	130.04	123.04	119.05	111.04	109.03	108.02
		107.05	106.04							
References	<p>Piattelli, M.; Minale, L. Pigments of centrospermae—I. <i>Phytochemistry</i>, 1964, 3, 307-311.</p> <p>Kobayashi, N.; Schmidt, J.; Nimtz, M.; Wray, V.; Schliemann, W. Betalains from Christmas cactus. <i>Phytochemistry</i> 2000, 54, 419-426.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675-689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315-2346.</p>									

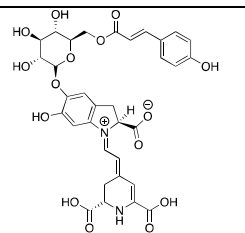
Hylocerenin

Chemical structure										
Name:	Hylocerenin									
Chemical Formula	C ₃₀ H ₃₄ N ₂ O ₁₇									
Molecular weight	694.60									
Monoisotopic mass	694.1857									
m/z [M+H]	695.1930									
Theoretical fragments (m/z)	695.19	694.19	693.18	692.17	679.2	678.19	677.18	676.17	675.17	667.2
		666.19	665.18	663.2	662.2	661.19	660.18	659.17	658.16	657.16
		655.2	653.18	652.17	651.2	650.2	649.19	648.18	647.17	645.19
		644.18	643.18	642.17	641.16	639.15	637.19	635.21	633.19	632.18
		631.18	630.17	629.16	627.18	625.19	623.17	622.16	621.19	620.18
		619.18	617.2	616.19	615.18	614.17	613.17	609.19	607.18	606.17
		605.16	604.15	603.18	602.17	601.17	593.2	591.18	589.17	587.15
		575.19	573.17	571.16	569.14	551.15	550.14	549.14	535.16	534.15
		533.14	532.13	531.12	526.16	523.16	522.15	521.14	519.16	517.15
		516.14	515.13	514.12	513.11	511.16	509.14	507.16	505.15	504.14
		503.13	502.16	501.15	500.14	499.13	498.13	497.12	495.1	493.15
		491.13	489.15	488.14	487.13	486.14	485.13	484.14	483.14	482.13
		481.15	479.13	478.12	477.15	476.14	475.13	471.14	470.14	469.13
		468.13	467.12	465.15	463.13	461.12	460.11	459.14	458.13	457.13
		456.15	455.14	454.13	453.14	452.13	451.12	450.12	447.14	445.12
		443.11	441.14	440.13	430.13	429.14	427.11	425.14	424.14	423.13
		417.14	415.12	414.12	413.14	412.14	411.13	401.14	399.13	398.12
		397.11	396.11	395.13	394.13	393.12	389.1	388.09	387.08	386.07
		385.15	383.13	381.12	379.1	375.12	373.1	372.1	371.09	370.08
		369.07	361.1	360.1	359.12	358.11	357.11	356.1	355.09	354.08
		353.08	351.06	349.1	347.09	345.11	343.13	342.09	341.11	340.1
		339.1	338.09	337.08	335.09	331.09	329.11	327.1	326.09	325.09
		324.08	323.08	319.09	317.08	316.07	315.1	314.09	313.08	307.08
		306.07	303.1	301.08	300.07	299.07	298.06	297.1	287.1	285.1
		284.08	283.07	282.06	281.08	280.07	279.09	273.1	271.08	270.07
		269.09	268.09	267.06	265.08	264.07	263.07	262.06	255.09	253.08
		252.06	251.07	250.08	249.05	247.07	245.06	237.09	235.07	233.06
		231.04	223.07	211.07	207.08	205.06	196.06	194.04	193.04	182.08
		180.04	179.03	178.05	177.04	165.05	164.05	163.04	147.04	146.04
		135.04	134.04	130.04	123.04	119.05	111.04	109.03	108.02	107.05
		106.04								
References	<p>Wybraniec, S.; Platzner, I.; Geresch, S.; Gottlieb, H.E.; Haimberg, M.; Mogilnitzki, M.; Mizrahi, Y. Betacyanins from vine cactus <i>Hylocereus polyrhizus</i>. <i>Phytochemistry</i> 2001, 58, 1209–1212.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

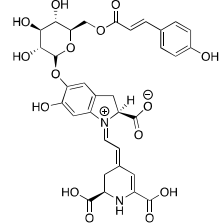
Isohylocerenin

Chemical structure										
Name:	Isohylocerenin									
Chemical Formula	C ₃₀ H ₃₄ N ₂ O ₁₇									
Molecular weight	694.60									
Monoisotopic mass	694.1857									
m/z [M+H]	695.1930									
Theoretical fragments (m/z)	695.19	694.19	693.18	692.17	679.2	678.19	677.18	676.17	675.17	667.2
		666.19	665.18	663.2	662.2	661.19	660.18	659.17	658.16	657.16
		655.2	653.18	652.17	651.2	650.2	649.19	648.18	647.17	645.19
		644.18	643.18	642.17	641.16	639.15	637.19	635.21	633.19	632.18
		631.18	630.17	629.16	627.18	625.19	623.17	622.16	621.19	620.18
		619.18	617.2	616.19	615.18	614.17	613.17	609.19	607.18	606.17
		605.16	604.15	603.18	602.17	601.17	593.2	591.18	589.17	587.15
		575.19	573.17	571.16	569.14	551.15	550.14	549.14	535.16	534.15
		533.14	532.13	531.12	526.16	523.16	522.15	521.14	519.16	517.15
		516.14	515.13	514.12	513.11	511.16	509.14	507.16	505.15	504.14
		503.13	502.16	501.15	500.14	499.13	498.13	497.12	495.1	493.15
		491.13	489.15	488.14	487.13	486.14	485.13	484.14	483.14	482.13
		481.15	479.13	478.12	477.15	476.14	475.13	471.14	470.14	469.13
		468.13	467.12	465.15	463.13	461.12	460.11	459.14	458.13	457.13
		456.15	455.14	454.13	453.14	452.13	451.12	450.12	447.14	445.12
		443.11	441.14	440.13	430.13	429.14	427.11	425.14	424.14	423.13
		417.14	415.12	414.12	413.14	412.14	411.13	401.14	399.13	398.12
		397.11	396.11	395.13	394.13	393.12	389.1	388.09	387.08	386.07
		385.15	383.13	381.12	379.1	375.12	373.1	372.1	371.09	370.08
		369.07	361.1	360.1	359.12	358.11	357.11	356.1	355.09	354.08
		353.08	351.06	349.1	347.09	345.11	343.13	342.09	341.11	340.1
		339.1	338.09	337.08	335.09	331.09	329.11	327.1	326.09	325.09
		324.08	323.08	319.09	317.08	316.07	315.1	314.09	313.08	307.08
		306.07	303.1	301.08	300.07	299.07	298.06	297.1	287.1	285.1
		284.08	283.07	282.06	281.08	280.07	279.09	273.1	271.08	270.07
		269.09	268.09	267.06	265.08	264.07	263.07	262.06	255.09	253.08
		252.06	251.07	250.08	249.05	247.07	245.06	237.09	235.07	233.06
		231.04	223.07	211.07	207.08	205.06	196.06	194.04	193.04	182.08
		180.04	179.03	178.05	177.04	165.05	164.05	163.04	147.04	146.04
		135.04	134.04	130.04	123.04	119.05	111.04	109.03	108.02	107.05
		106.04								
References	<p>Wybraniec, S.; Platzner, I.; Geresch, S.; Gottlieb, H.E.; Haimberg, M.; Mogilnitzki, M.; Mizrahi, Y. Betacyanins from vine cactus <i>Hylocereus polyrhizus</i>. <i>Phytochemistry</i> 2001, 58, 1209–1212.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

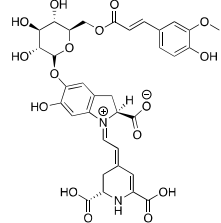
Lampranthin I

Chemical structure										
Name:	Lampranthin I									
Chemical Formula	C ₃₃ H ₃₂ N ₂ O ₁₅									
Molecular weight	696.62									
Monoisotopic mass	696.1803									
m/z [M+H]	697.1875									
Theoretical fragments (m/z)	697.19	696.18	695.17	694.16	681.19	680.18	679.18	678.17	677.16	669.19
		668.18	667.18	665.2	664.19	663.18	662.17	661.17	660.16	659.15
		657.19	655.18	654.17	653.2	652.19	651.18	650.17	649.17	647.19
		646.18	645.17	644.16	643.16	641.14	639.18	637.2	636.19	635.19
		634.18	633.17	632.16	631.16	629.18	627.18	625.17	624.16	623.19
		622.18	621.17	619.19	618.18	617.18	616.17	615.16	611.19	609.17
		608.16	607.16	606.15	605.18	604.17	603.16	593.18	591.16	589.15
		575.17	573.15	571.13	533.14	532.13	531.12	528.15	517.15	516.14
		515.13	514.12	513.11	512.16	510.14	505.15	504.15	503.13	502.13
		501.13	499.13	498.13	497.12	495.1	493.15	491.13	489.15	488.13
		487.12	486.14	485.12	484.12	483.12	481.12	479.11	476.16	475.13
		474.14	473.16	471.13	470.12	469.11	468.13	466.11	463.13	461.12
		460.11	459.13	458.14	457.14	456.13	453.12	452.11	447.14	446.14
		445.12	444.13	443.13	442.13	440.13	434.14	432.13	431.13	429.13
		427.11	426.13	425.12	419.13	417.12	416.11	414.13	413.12	401.12
		400.12	399.11	398.1	396.12	395.11	389.1	388.09	387.08	386.07
		383.11	381.1	375.12	373.1	372.1	371.09	370.08	369.07	364.1
		361.1	360.1	359.12	357.11	356.1	355.09	354.08	353.08	351.06
		349.1	347.09	345.11	344.1	343.13	342.08	341.11	340.1	339.1
		338.09	337.08	335.09	331.09	329.11	327.1	326.09	325.08	324.08
		323.08	322.09	320.08	319.09	317.08	316.07	315.1	314.09	313.08
		309.1	307.08	306.07	303.1	301.08	300.07	299.07	298.06	297.09
		294.1	291.09	287.1	285.09	284.08	283.07	282.06	281.08	280.07
		279.09	271.11	269.09	268.08	267.06	265.08	264.07	263.07	262.06
		255.09	253.08	252.06	251.07	250.08	249.05	247.07	245.06	237.09
		235.07	233.06	231.04	223.07	222.06	220.06	211.07	209.06	208.05
		207.08	205.06	196.06	195.05	194.04	193.04	192.03	191.05	182.08
		181.05	180.04	179.03	178.05	177.04	176.03	167.07	166.09	165.05
		164.05	163.04	150.05	147.04	146.04	145.05	135.04	134.04	130.04
		124.04	123.04	119.05	111.04	110.06	109.03	108.02	107.05	106.04
References	<p>Piattelli, M.; Impellizzeri, G. Betacyanins from <i>Lampranthus</i> sp. (aizoaceae). <i>Phytochemistry</i> 1969, 8, 1595–1596.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

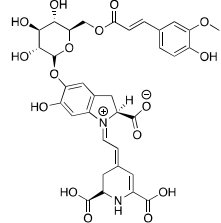
Isoampranthin I

Chemical structure										
Name:	Isolampranthin I									
Chemical Formula	C ₃₃ H ₃₂ N ₂ O ₁₅									
Molecular weight	696.62									
Monoisotopic mass	696.1803									
m/z [M+H]	697.1875									
Theoretical fragments (m/z)	697.19	696.18	695.17	694.16	681.19	680.18	679.18	678.17	677.16	669.19
		668.18	667.18	665.2	664.19	663.18	662.17	661.17	660.16	659.15
		657.19	655.18	654.17	653.2	652.19	651.18	650.17	649.17	647.19
		646.18	645.17	644.16	643.16	641.14	639.18	637.2	636.19	635.19
		634.18	633.17	632.16	631.16	629.18	627.18	625.17	624.16	623.19
		622.18	621.17	619.19	618.18	617.18	616.17	615.16	611.19	609.17
		608.16	607.16	606.15	605.18	604.17	603.16	593.18	591.16	589.15
		575.17	573.15	571.13	533.14	532.13	531.12	528.15	517.15	516.14
		515.13	514.12	513.11	512.16	510.14	505.15	504.15	503.13	502.13
		501.13	499.13	498.13	497.12	495.1	493.15	491.13	489.15	488.13
		487.12	486.14	485.12	484.12	483.12	481.12	479.11	476.16	475.13
		474.14	473.16	471.13	470.12	469.11	468.13	466.11	463.13	461.12
		460.11	459.13	458.14	457.14	456.13	453.12	452.11	447.14	446.14
		445.12	444.13	443.13	442.13	440.13	434.14	432.13	431.13	429.13
		427.11	426.13	425.12	419.13	417.12	416.11	414.13	413.12	401.12
		400.12	399.11	398.1	396.12	395.11	389.1	388.09	387.08	386.07
		383.11	381.1	375.12	373.1	372.1	371.09	370.08	369.07	364.1
		361.1	360.1	359.12	357.11	356.1	355.09	354.08	353.08	351.06
		349.1	347.09	345.11	344.1	343.13	342.08	341.11	340.1	339.1
		338.09	337.08	335.09	331.09	329.11	327.1	326.09	325.08	324.08
		323.08	322.09	320.08	319.09	317.08	316.07	315.1	314.09	313.08
		309.1	307.08	306.07	303.1	301.08	300.07	299.07	298.06	297.09
		294.1	291.09	287.1	285.09	284.08	283.07	282.06	281.08	280.07
		279.09	271.11	269.09	268.08	267.06	265.08	264.07	263.07	262.06
		255.09	253.08	252.06	251.07	250.08	249.05	247.07	245.06	237.09
		235.07	233.06	231.04	223.07	222.06	220.06	211.07	209.06	208.05
		207.08	205.06	196.06	195.05	194.04	193.04	192.03	191.05	182.08
		181.05	180.04	179.03	178.05	177.04	176.03	167.07	166.09	165.05
		164.05	163.04	150.05	147.04	146.04	145.05	135.04	134.04	130.04
		124.04	123.04	119.05	111.04	110.06	109.03	108.02	107.05	106.04
References	<p>Piattelli, M.; Impellizzeri, G. Betacyanins from Lampranthus sp. (aizoaceae). <i>Phytochemistry</i> 1969, 8, 1595–1596.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

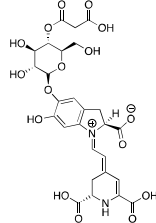
Lampranthin II

Chemical structure										
Name:	Lampranthin II									
Chemical Formula	C ₃₄ H ₃₄ N ₂ O ₁₆									
Molecular weight	726.64									
Monoisotopic mass	726.1908									
m/z [M+H]	727.1981									
Theoretical fragments (m/z)	727.2	726.19	725.18	724.17	711.2	710.2	709.19	708.18	707.17	699.2
		698.2	697.19	695.21	694.2	693.19	692.18	691.18	690.17	689.16
		687.2	685.19	684.18	683.21	682.2	681.19	680.18	679.18	677.2
		676.19	675.18	674.17	673.17	671.15	669.19	667.21	666.21	665.2
		664.19	663.18	662.17	661.17	659.19	657.19	655.18	654.17	653.2
		652.19	651.18	649.2	648.19	647.19	646.18	645.17	641.2	639.18
		638.17	637.17	636.16	635.19	634.18	633.17	623.19	621.17	619.16
		605.18	603.16	601.15	558.16	545.15	544.14	542.17	540.15	534.16
		533.14	532.14	531.14	528.15	527.14	519.15	518.14	517.15	516.15
		515.13	514.13	513.11	506.17	505.15	504.14	503.13	501.14	500.13
		499.13	498.13	497.12	496.12	495.1	493.15	491.13	489.15	488.16
		487.13	486.14	485.12	483.13	482.12	481.12	479.11	476.16	475.13
		474.14	473.14	472.14	471.14	470.13	469.12	464.16	463.13	462.14
		461.14	460.11	459.14	458.13	457.12	456.14	455.13	449.14	447.13
		446.12	445.12	444.14	443.13	431.13	430.13	429.12	428.11	427.11
		426.13	425.12	419.11	417.09	413.12	411.11	389.1	388.09	387.08
		386.07	375.12	373.1	372.1	371.09	370.08	369.07	364.1	361.1
		360.1	359.12	357.11	356.1	355.09	354.08	353.08	351.06	349.1
		347.09	345.11	344.1	343.13	342.08	341.11	340.1	339.1	338.09
		337.08	335.09	331.09	329.11	327.1	326.09	325.08	324.08	323.08
		322.09	321.1	320.08	319.09	317.08	316.07	315.1	314.09	313.08
		307.08	306.07	303.1	301.08	300.07	299.07	298.06	297.09	294.1
		287.1	285.09	284.08	283.07	282.06	281.08	280.07	279.09	271.11
		269.09	268.08	267.06	265.08	264.07	263.07	262.06	255.09	253.08
		252.06	251.07	250.08	249.05	247.07	245.06	237.09	235.07	233.06
		231.04	223.07	222.06	220.06	211.07	209.06	208.05	207.08	205.06
		196.06	195.05	194.04	193.04	192.03	191.05	182.08	181.05	180.04
		179.03	178.05	177.04	176.03	167.07	166.09	165.05	164.05	163.04
		150.05	147.04	146.04	145.05	135.04	134.04	130.04	124.04	123.04
		119.05	111.04	110.06	109.03	108.02	107.05	106.04		
References	<p>Strack, D.; Bokern, M.; Marxen, N.; Wray, V. Feruloylbetainin from petals of <i>Lampranthus</i> and feruloylamaranthin from cell suspension cultures of <i>Chenopodium rubrum</i>. <i>Phytochemistry</i> 1988, 27, 3529–3531.</p> <p>Heuer, S.; Wray, V.; Metzger, J.W.; Strack, D. Betacyanins from flowers of <i>Gomphrena globosa</i>. <i>Phytochemistry</i> 1992, 31, 1801–1807.</p> <p>Piattelli, M.; Impellizzeri, G. Betacyanins from <i>Lampranthus</i> sp. (aizoaceae). <i>Phytochemistry</i> 1969, 8, 1595–1596.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

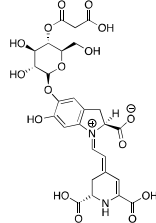
Isolampranthin II

Chemical structure										
Name:	Isolampranthin II									
Chemical Formula	C ₃₄ H ₃₄ N ₂ O ₁₆									
Molecular weight	726.64									
Monoisotopic mass	726.1908									
m/z [M+H]	727.1981									
Theoretical fragments (m/z)	727.2	726.19	725.18	724.17	711.2	710.2	709.19	708.18	707.17	699.2
		698.2	697.19	695.21	694.2	693.19	692.18	691.18	690.17	689.16
		687.2	685.19	684.18	683.21	682.2	681.19	680.18	679.18	677.2
		676.19	675.18	674.17	673.17	671.15	669.19	667.21	666.21	665.2
		664.19	663.18	662.17	661.17	659.19	657.19	655.18	654.17	653.2
		652.19	651.18	649.2	648.19	647.19	646.18	645.17	641.2	639.18
		638.17	637.17	636.16	635.19	634.18	633.17	623.19	621.17	619.16
		605.18	603.16	601.15	558.16	545.15	544.14	542.17	540.15	534.16
		533.14	532.14	531.14	528.15	527.14	519.15	518.14	517.15	516.15
		515.13	514.13	513.11	506.17	505.15	504.14	503.13	501.14	500.13
		499.13	498.13	497.12	496.12	495.1	493.15	491.13	489.15	488.16
		487.13	486.14	485.12	483.13	482.12	481.12	479.11	476.16	475.13
		474.14	473.14	472.14	471.14	470.13	469.12	464.16	463.13	462.14
		461.14	460.11	459.14	458.13	457.12	456.14	455.13	449.14	447.13
		446.12	445.12	444.14	443.13	431.13	430.13	429.12	428.11	427.11
		426.13	425.12	419.11	417.09	413.12	411.11	389.1	388.09	387.08
		386.07	375.12	373.1	372.1	371.09	370.08	369.07	364.1	361.1
		360.1	359.12	357.11	356.1	355.09	354.08	353.08	351.06	349.1
		347.09	345.11	344.1	343.13	342.08	341.11	340.1	339.1	338.09
		337.08	335.09	331.09	329.11	327.1	326.09	325.08	324.08	323.08
		322.09	321.1	320.08	319.09	317.08	316.07	315.1	314.09	313.08
		307.08	306.07	303.1	301.08	300.07	299.07	298.06	297.09	294.1
		287.1	285.09	284.08	283.07	282.06	281.08	280.07	279.09	271.11
		269.09	268.08	267.06	265.08	264.07	263.07	262.06	255.09	253.08
		252.06	251.07	250.08	249.05	247.07	245.06	237.09	235.07	233.06
		231.04	223.07	222.06	220.06	211.07	209.06	208.05	207.08	205.06
		196.06	195.05	194.04	193.04	192.03	191.05	182.08	181.05	180.04
		179.03	178.05	177.04	176.03	167.07	166.09	165.05	164.05	163.04
		150.05	147.04	146.04	145.05	135.04	134.04	130.04	124.04	123.04
		119.05	111.04	110.06	109.03	108.02	107.05	106.04		
References	<p>Strack, D.; Bokern, M.; Marxen, N.; Wray, V. Feruloylbetainin from petals of Lampranthus and feruloylamaranthin from cell suspension cultures of Chenopodium rubrum. <i>Phytochemistry</i> 1988, 27, 3529–3531.</p> <p>Heuer, S.; Wray, V.; Metzger, J.W.; Strack, D. Betacyanins from flowers of Gomphrena globosa. <i>Phytochemistry</i> 1992, 31, 1801–1807.</p> <p>Piattelli, M.; Impellizzeri, G. Betacyanins from Lampranthus sp. (aizoaceae). <i>Phytochemistry</i> 1969, 8, 1595–1596.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

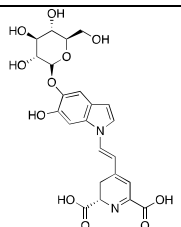
4'-O-malonyl-betainin

Chemical structure										
Name:	4'-O-malonyl-betainin									
Chemical Formula	C ₂₇ H ₂₈ N ₂ O ₁₆									
Molecular weight	636.52									
Monoisotopic mass	636.1439									
m/z [M+H]	637.1512									
Theoretical fragments (m/z)	637.15	636.14	635.14	634.13	621.16	620.15	619.14	618.13	617.12	
		609.16	608.15	607.14	605.16	604.15	603.15	602.14	601.13	
		600.12	599.11	597.16	595.14	594.13	593.16	592.15	591.15	
		590.14	589.13	587.15	586.14	585.14	584.13	583.12	581.1	
		579.15	577.17	575.15	574.14	573.14	572.13	571.12	569.14	
		567.15	565.13	564.12	563.15	562.14	561.14	559.16	558.15	
		557.14	556.13	555.12	551.15	550.14	549.14	548.13	547.12	
		546.11	545.14	544.13	543.12	535.16	534.15	533.14	532.13	
		531.12	529.11	523.16	522.15	521.14	519.16	517.15	516.14	
		515.13	514.12	513.11	511.1	509.14	507.16	505.15	504.14	
		503.13	501.15	499.13	498.13	497.12	495.1	493.15	491.13	
		489.15	488.14	487.13	486.13	485.12	481.15	479.13	478.12	
		477.15	476.14	475.13	473.16	471.14	470.13	469.12	468.11	
		465.15	463.13	461.12	460.11	459.14	458.13	457.12	455.11	
		447.14	445.12	444.11	443.11	442.1	441.09	429.1	428.09	
		427.09	426.1	425.1	424.09	423.08	412.1	411.09	410.08	
		409.08	408.09	406.08	399.09	398.11	397.1	396.09	395.1	
		394.09	393.08	392.07	389.1	388.09	387.08	386.07	385.08	
		383.1	382.09	380.1	375.12	373.1	372.09	371.1	370.08	
		369.07	367.1	366.09	365.09	361.1	360.1	359.12	358.11	
		357.11	356.07	355.09	354.09	353.09	351.06	349.1	347.09	
		345.11	343.13	342.09	341.11	340.1	339.1	338.09	337.08	
		336.08	335.08	331.09	329.11	327.1	326.09	325.09	324.08	
		323.08	321.06	320.08	319.09	317.08	316.07	315.1	314.09	
		313.08	312.11	307.08	306.07	303.1	301.08	300.07	299.07	
		298.06	297.1	294.1	287.1	285.1	284.08	283.07	282.06	
		281.08	280.07	279.09	273.1	271.08	270.07	269.09	268.09	
		267.06	265.08	264.07	263.07	262.06	255.09	253.08	252.06	
		251.07	250.08	249.05	247.07	245.06	237.09	235.07	233.06	
		231.04	223.07	222.06	211.07	207.08	205.06	196.06	194.04	
		193.04	192.03	182.08	180.04	179.03	178.05	177.04	165.05	
		164.05	163.04	150.05	147.04	146.04	135.04	134.04	130.04	
		123.04	119.05	111.04	109.03	108.02	107.05	106.04		
References	<p>Wybraniec, S.; Nowak-Wydra, B.; Mitka, K.; Kowalski, P.; Mizrahi, Y. Minor betalains in fruits of <i>Hylocereus</i> species. <i>Phytochemistry</i> 2007, 68, 251–259.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

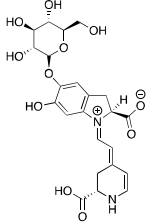
4'-O-malonyl-isobetanin

Chemical structure										
Name:	4'-O-malonyl-isobetanin									
Chemical Formula	C ₂₇ H ₂₈ N ₂ O ₁₆									
Molecular weight	636.52									
Monoisotopic mass	636.1439									
m/z [M+H]	637.1512									
Theoretical fragments (m/z)	637.15	636.14	635.14	634.13	621.16	620.15	619.14	618.13	617.12	609.16
		608.15	607.14	605.16	604.15	603.15	602.14	601.13	600.12	599.11
		597.16	595.14	594.13	593.16	592.15	591.15	590.14	589.13	587.15
		586.14	585.14	584.13	583.12	581.1	579.15	577.17	575.15	574.14
		573.14	572.13	571.12	569.14	567.15	565.13	564.12	563.15	562.14
		561.14	559.16	558.15	557.14	556.13	555.12	551.15	550.14	549.14
		548.13	547.12	546.11	545.14	544.13	543.12	535.16	534.15	533.14
		532.13	531.12	529.11	523.16	522.15	521.14	519.16	517.15	516.14
		515.13	514.12	513.11	511.1	509.14	507.16	505.15	504.14	503.13
		501.15	499.13	498.13	497.12	495.1	493.15	491.13	489.15	488.14
		487.13	486.13	485.12	481.15	479.13	478.12	477.15	476.14	475.13
		473.16	471.14	470.13	469.12	468.11	465.15	463.13	461.12	460.11
		459.14	458.13	457.12	455.11	447.14	445.12	444.11	443.11	442.1
		441.09	429.1	428.09	427.09	426.1	425.1	424.09	423.08	412.1
		411.09	410.08	409.08	408.09	406.08	399.09	398.11	397.1	396.09
		395.1	394.09	393.08	392.07	389.1	388.09	387.08	386.07	385.08
		383.1	382.09	380.1	375.12	373.1	372.09	371.1	370.08	369.07
		367.1	366.09	365.09	361.1	360.1	359.12	358.11	357.11	356.07
		355.09	354.09	353.09	351.06	349.1	347.09	345.11	343.13	342.09
		341.11	340.1	339.1	338.09	337.08	336.08	335.08	331.09	329.11
		327.1	326.09	325.09	324.08	323.08	321.06	320.08	319.09	317.08
		316.07	315.1	314.09	313.08	312.11	307.08	306.07	303.1	301.08
		300.07	299.07	298.06	297.1	294.1	287.1	285.1	284.08	283.07
		282.06	281.08	280.07	279.09	273.1	271.08	270.07	269.09	268.09
		267.06	265.08	264.07	263.07	262.06	255.09	253.08	252.06	251.07
		250.08	249.05	247.07	245.06	237.09	235.07	233.06	231.04	223.07
		222.06	211.07	207.08	205.06	196.06	194.04	193.04	192.03	182.08
		180.04	179.03	178.05	177.04	165.05	164.05	163.04	150.05	147.04
		146.04	135.04	134.04	130.04	123.04	119.05	111.04	109.03	108.02
		107.05	106.04							
References	<p>Wybraniec, S.; Nowak-Wydra, B.; Mitka, K.; Kowalski, P.; Mizrahi, Y. Minor betalains in fruits of <i>Hylocereus</i> species. <i>Phytochemistry</i> 2007, 68, 251–259.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

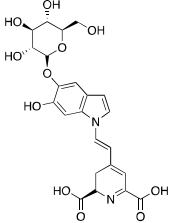
2-decarboxy-2,3-dehydro-betanin

Chemical structure										
Name:	2-decarboxy-2,3-dehydro-betanin (2-decarboxy-xanbetanin)									
Chemical Formula	C ₂₃ H ₂₄ N ₂ O ₁₁									
Molecular weight	504.45									
Monoisotopic mass	504.1380									
m/z [M+H]	505.1453									
Theoretical fragments (m/z)	505.15	504.14	503.13	502.12	501.11	500.11	489.15	488.14	487.13	486.13
		485.12	484.11	483.1	479.13	478.12	477.15	475.13	474.13	473.12
		472.11	471.14	470.13	469.12	468.12	467.11	465.15	463.13	461.16
		460.11	459.14	458.1	457.12	456.12	455.11	454.1	453.13	451.11
		449.12	447.14	445.16	444.12	443.14	442.1	441.13	440.12	439.11
		438.11	437.1	435.12	434.14	433.12	432.13	431.11	430.1	429.09
		428.12	427.11	426.11	425.1	424.09	423.12	419.12	417.13	415.11
		414.11	413.1	411.12	410.11	409.1	408.1	407.09	403.11	401.1
		400.09	399.08	398.11	397.1	396.1	395.09	389.1	385.1	384.1
		383.09	382.08	381.07	376.14	374.12	373.1	371.09	369.07	368.1
		367.09	366.08	362.12	357.11	355.09	354.08	353.08	343.09	342.08
		341.08	339.1	338.09	337.08	336.11	329.11	327.1	326.09	325.08
		324.07	323.07	318.1	317.08	316.07	315.1	313.12	312.11	311.1
		309.09	307.07	303.1	301.08	300.09	299.1	297.09	295.11	294.1
		293.09	287.1	286.09	285.09	283.11	281.09	276.09	271.08	270.07
		255.09	253.07	235.07	222.06	194.04	180.06	179.06	178.05	177.04
		176.03	175.02	174.05	168.03	165.08	164.07	163.06	162.05	161.04
		160.04	159.03	152.03	151.06	150.02	149.05	148.04	147.07	146.06
		145.05	144.04	143.03	139.06	137.08	136.08	135.07	134.06	133.05
		132.04	131.03	130.03	129.05	128.03	127.04	126.02	121.05	120.04
		119.03	118.03	117.02	116.05	115.04	114.02	113.02	110.06	109.03
		108.02	107.07	105.05	104.05	103.04	102.03	101.02	100.04	
References	<p>Amaya-Cruz Iz, D.M.; Pérez-Ramírez, I.F.; Delgado-García, J.; Mondragón-Jacobo, C.; Dector-Espinoza, A.; Reynoso-Camacho, R. An integral profile of bioactive compounds and functional properties of prickly pear (<i>Opuntia ficus indica</i> L.) peel with different tonalities. <i>Food Chem.</i> 2019, 278, 568–578.</p> <p>Xie, G.R.; Chen, H.J. Comprehensive Betalain Profiling of Djulis (<i>Chenopodium formosanum</i>) Cultivars Using HPLC-Q-Orbitrap High-Resolution Mass Spectrometry. <i>J. Agric. Food Chem.</i> 2021, 69, 15699–15715.</p> <p>Slimen, I.B.; Najjar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

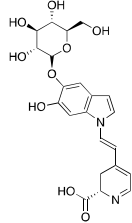
17-decarboxy-betanin

Chemical structure										
Name:	17-decarboxy-betanin									
Chemical Formula	C ₂₃ H ₂₆ N ₂ O ₁₁									
Molecular weight	506.46									
Monoisotopic mass	506.1537									
m/z [M+H]	507.1609									
Theoretical fragments (m/z)	507.16	506.15	505.15	504.14	491.17	490.16	489.15	488.14	487.13	479.17
	478.16	477.15	475.17	474.16	473.16	472.15	471.14	470.13	469.12	
	467.17	465.15	464.14	463.17	462.16	461.16	460.15	459.14	457.16	
	456.15	455.14	454.14	453.13	451.11	449.16	447.18	446.17	445.16	
	444.15	443.14	442.14	441.13	439.15	437.16	435.14	434.13	433.16	
	432.15	431.14	429.17	428.16	427.15	426.14	425.13	421.16	419.14	
	418.14	417.13	416.12	415.15	414.14	413.13	403.15	401.13	399.12	
	385.14	383.12	382.11	381.11	375.12	373.1	369.11	368.1	366.12	
	364.1	358.11	357.11	356.1	355.09	352.1	351.09	345.11	344.1	
	343.09	342.09	341.09	340.1	339.09	338.09	337.08	331.13	330.12	
	329.11	328.11	327.1	326.09	325.09	324.08	323.08	322.09	320.08	
	317.11	316.11	315.13	313.12	312.11	311.1	310.09	309.09	307.08	
	306.07	305.11	303.1	301.12	300.11	299.14	298.09	297.12	296.09	
	295.11	294.1	293.09	291.1	288.11	287.1	286.09	285.1	283.11	
	282.1	281.09	280.09	279.09	275.1	273.1	272.08	271.08	270.07	
	269.09	268.09	267.09	259.11	257.09	256.08	255.09	254.08	253.07	
	252.06	250.08	249.08	243.11	241.1	240.09	239.08	238.07	237.09	
	236.08	235.06	227.12	225.1	223.07	221.09	220.08	219.08	218.07	
	209.09	207.08	205.06	203.08	201.07	196.06	195.05	194.04	193.1	
	192.03	191.08	189.07	187.05	182.08	181.05	180.04	179.08	178.05	
	177.04	167.08	166.09	165.05	164.05	163.09	161.07	152.07	151.09	
	150.05	149.07	147.04	146.04	145.05	136.08	135.04	134.04	132.04	
	130.04	124.04	123.04	119.05	111.04	110.06	109.03	108.02	107.05	
	106.04									
References	<p>Amaya-Cruz Iz, D.M.; Pérez-Ramírez, I.F.; Delgado-García, J.; Mondragón-Jacobo, C.; Dector-Espinoza, A.; Reynoso-Camacho, R. An integral profile of bioactive compounds and functional properties of prickly pear (<i>Opuntia ficus indica</i> L.) peel with different tonalities. <i>Food Chem.</i> 2019, 278, 568–578.</p> <p>Xie, G.R.; Chen, H.J. Comprehensive Betalain Profiling of Djulis (<i>Chenopodium formosanum</i>) Cultivars Using HPLC-Q-Orbitrap High-Resolution Mass Spectrometry. <i>J. Agric. Food Chem.</i> 2021, 69, 15699–15715.</p> <p>Slimen, I.B.; Najjar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

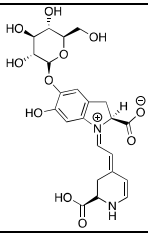
2-decarboxy-2,3-dehydro-isobetanim

Chemical structure										
Name:	2-decarboxy-2,3-dehydro-isobetanim (2-decarboxy-isoxanbetanim)									
Chemical Formula	C ₂₃ H ₂₄ N ₂ O ₁₁									
Molecular weight	504.45									
Monoisotopic mass	504.1380									
m/z [M+H]	505.1453									
Theoretical fragments (m/z)	505.15	504.14	503.13	502.12	501.11	500.11	489.15	488.14	487.13	486.13
	485.12	484.11	483.1	479.13	478.12	477.15	475.13	474.13	473.12	
	472.11	471.14	470.13	469.12	468.12	467.11	465.15	463.13	461.16	
	460.11	459.14	458.1	457.12	456.12	455.11	454.1	453.13	451.11	
	449.12	447.14	445.16	444.12	443.14	442.1	441.13	440.12	439.11	
	438.11	437.1	435.12	434.14	433.12	432.13	431.11	430.1	429.09	
	428.12	427.11	426.11	425.1	424.09	423.12	419.12	417.13	415.11	
	414.11	413.1	411.12	410.11	409.1	408.1	407.09	403.11	401.1	
	400.09	399.08	398.11	397.1	396.1	395.09	389.1	385.1	384.1	
	383.09	382.08	381.07	376.14	374.12	373.1	371.09	369.07	368.1	
	367.09	366.08	362.12	357.11	355.09	354.08	353.08	343.09	342.08	
	341.08	339.1	338.09	337.08	336.11	329.11	327.1	326.09	325.08	
	324.07	323.07	318.1	317.08	316.07	315.1	313.12	312.11	311.1	
	309.09	307.07	303.1	301.08	300.09	299.1	297.09	295.11	294.1	
	293.09	287.1	286.09	285.09	283.11	281.09	276.09	271.08	270.07	
	255.09	253.07	235.07	222.06	194.04	180.06	179.06	178.05	177.04	
	176.03	175.02	174.05	168.03	165.08	164.07	163.06	162.05	161.04	
	160.04	159.03	152.03	151.06	150.02	149.05	148.04	147.07	146.06	
	145.05	144.04	143.03	139.06	137.08	136.08	135.07	134.06	133.05	
	132.04	131.03	130.03	129.05	128.03	127.04	126.02	121.05	120.04	
	119.03	118.03	117.02	116.05	115.04	114.02	113.02	110.06	109.03	
	108.02	107.07	105.05	104.05	103.04	102.03	101.02	100.04		
References	<p>Amaya-Cruz Iz, D.M.; Pérez-Ramírez, I.F.; Delgado-García, J.; Mondragón-Jacobo, C.; Dector-Espinoza, A.; Reynoso-Camacho, R. An integral profile of bioactive compounds and functional properties of prickly pear (<i>Opuntia ficus indica</i> L.) peel with different tonalities. <i>Food Chem.</i> 2019, 278, 568–578.</p> <p>Xie, G.R.; Chen, H.J. Comprehensive Betalain Profiling of Djulis (<i>Chenopodium formosanum</i>) Cultivars Using HPLC-Q-Orbitrap High-Resolution Mass Spectrometry. <i>J. Agric. Food Chem.</i> 2021, 69, 15699–15715.</p> <p>Slimen, I.B.; Najjar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

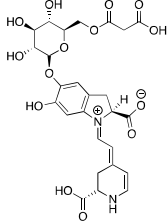
2,17-bidecarboxy-2,3-dehydro-isobetanim

Chemical structure										
Name:	2,17-bidecarboxy-2,3-dehydro-betanin (2,17-bidecarboxy-xanbetanim)									
Chemical Formula	C ₂₂ H ₂₄ N ₂ O ₉									
Molecular weight	460.44									
Monoisotopic mass	460.1482									
m/z [M+H]	461.1555									
Theoretical fragments (m/z)	461.16	460.15	459.14	458.13	457.12	456.12	445.16	444.15	443.14	442.14
	441.13	440.12	439.11	435.14	434.14	433.16	431.14	430.14	429.13	
	428.12	427.15	426.14	425.13	424.13	423.12	421.16	420.13	419.14	
	417.17	416.12	415.15	414.11	413.13	412.13	411.12	410.11	409.14	
	407.12	405.13	403.15	401.13	400.13	399.12	398.11	397.14	396.13	
	395.12	394.12	393.11	391.13	389.13	388.13	387.12	386.11	385.1	
	384.13	383.12	382.12	381.11	380.1	379.13	376.14	375.12	373.14	
	371.12	370.12	369.11	367.13	366.12	365.11	364.11	363.1	362.12	
	359.12	358.12	357.11	356.1	355.09	354.12	353.11	352.11	351.1	
	350.12	345.11	341.11	340.11	339.1	338.09	337.08	336.11	329.11	
	327.1	326.09	325.08	324.11	323.1	322.09	318.1	313.12	312.11	
	311.1	310.09	309.09	300.09	299.1	298.09	297.09	295.11	294.1	
	293.09	292.08	286.09	285.12	283.11	282.1	281.09	280.08	279.08	
	276.09	273.09	272.08	271.08	270.07	269.13	267.11	265.1	263.08	
	259.11	257.09	256.08	255.11	253.1	243.11	241.1	227.08	191.08	
	180.06	179.06	178.07	177.04	175.02	174.05	165.08	164.07	163.06	
	162.05	161.04	160.04	159.03	151.06	150.05	149.05	148.04	147.07	
	146.06	145.05	144.04	143.03	139.06	137.08	136.08	135.07	134.06	
	133.05	132.04	131.03	130.03	129.05	127.04	124.04	121.05	120.04	
	119.03	118.03	117.02	116.05	115.04	114.03	113.02	110.06	109.03	
	108.04	107.07	106.03	105.05	104.05	103.04	102.03	101.02	100.02	
References	<p>Amaya-CruzIz, D.M.; Pérez-Ramírez, I.F.; Delgado-García, J.; Mondragón-Jacobo, C.; Dector-Espinoza, A.; Reynoso-Camacho, R. An integral profile of bioactive compounds and functional properties of prickly pear (<i>Opuntia ficus indica</i> L.) peel with different tonalities. <i>Food Chem.</i> 2019, 278, 568–578.</p> <p>Xie, G.R.; Chen, H.J. Comprehensive Betalain Profiling of Djulis (<i>Chenopodium formosanum</i>) Cultivars Using HPLC-Q-Orbitrap High-Resolution Mass Spectrometry. <i>J. Agric. Food Chem.</i> 2021, 69, 15699–15715.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

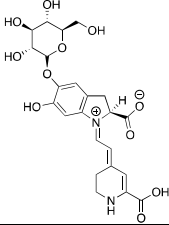
17-decarboxy-isobetanim

Chemical structure										
Name:	17-decarboxy-isobetanim									
Chemical Formula	C ₂₃ H ₂₆ N ₂ O ₁₁									
Molecular weight	506.46									
Monoisotopic mass	506.1537									
m/z [M+H]	507.1609									
Theoretical fragments (m/z)	507.16	506.15	505.15	504.14	491.17	490.16	489.15	488.14	487.13	479.17
		478.16	477.15	475.17	474.16	473.16	472.15	471.14	470.13	469.12
		467.17	465.15	464.14	463.17	462.16	461.16	460.15	459.14	457.16
		456.15	455.14	454.14	453.13	451.11	449.16	447.18	446.17	445.16
		444.15	443.14	442.14	441.13	439.15	437.16	435.14	434.13	433.16
		432.15	431.14	429.17	428.16	427.15	426.14	425.13	421.16	419.14
		418.14	417.13	416.12	415.15	414.14	413.13	403.15	401.13	399.12
		385.14	383.12	382.11	381.11	375.12	373.1	369.11	368.1	366.12
		364.1	358.11	357.11	356.1	355.09	352.1	351.09	345.11	344.1
		343.09	342.09	341.09	340.1	339.09	338.09	337.08	331.13	330.12
		329.11	328.11	327.1	326.09	325.09	324.08	323.08	322.09	320.08
		317.11	316.11	315.13	313.12	312.11	311.1	310.09	309.09	307.08
		306.07	305.11	303.1	301.12	300.11	299.14	298.09	297.12	296.09
		295.11	294.1	293.09	291.1	288.11	287.1	286.09	285.1	283.11
		282.1	281.09	280.09	279.09	275.1	273.1	272.08	271.08	270.07
		269.09	268.09	267.09	259.11	257.09	256.08	255.09	254.08	253.07
		252.06	250.08	249.08	243.11	241.1	240.09	239.08	238.07	237.09
		236.08	235.06	227.12	225.1	223.07	221.09	220.08	219.08	218.07
		209.09	207.08	205.06	203.08	201.07	196.06	195.05	194.04	193.1
		192.03	191.08	189.07	187.05	182.08	181.05	180.04	179.08	178.05
		177.04	167.08	166.09	165.05	164.05	163.09	161.07	152.07	151.09
		150.05	149.07	147.04	146.04	145.05	136.08	135.04	134.04	132.04
		130.04	124.04	123.04	119.05	111.04	110.06	109.03	108.02	107.05
		106.04								
References	<p>Amaya-CruzIz, D.M.; Pérez-Ramírez, I.F.; Delgado-García, J.; Mondragón-Jacobo, C.; Dector-Espinoza, A.; Reynoso-Camacho, R. An integral profile of bioactive compounds and functional properties of prickly pear (<i>Opuntia ficus indica</i> L.) peel with different tonalities. <i>Food Chem.</i> 2019, 278, 568–578.</p> <p>Xie, G.R.; Chen, H.J. Comprehensive Betalain Profiling of Djulis (<i>Chenopodium formosanum</i>) Cultivars Using HPLC-Q-Orbitrap High-Resolution Mass Spectrometry. <i>J. Agric. Food Chem.</i> 2021, 69, 15699–15715.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

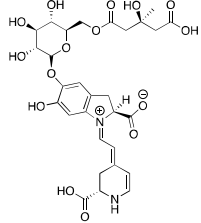
17-decarboxy-phyllactin

Chemical structure										
Name:	17-decarboxy-phyllactin									
Chemical Formula	C ₂₆ H ₂₈ N ₂ O ₁₄									
Molecular weight	592.51									
Monoisotopic mass	592.1541									
m/z [M+H]	593.1613									
Theoretical fragments (m/z)	593.16	592.15	591.15	590.14	577.17	576.16	575.15	574.14	573.14	565.17
		564.16	563.15	561.17	560.16	559.16	558.15	557.14	556.13	555.12
		553.17	551.15	550.14	549.17	548.16	547.16	546.15	545.14	543.16
		542.15	541.15	540.14	539.13	537.11	535.16	533.18	531.16	530.15
		529.15	528.14	527.13	525.15	523.16	521.14	520.13	519.16	518.15
		517.15	515.17	514.16	513.15	512.14	511.13	507.16	506.15	505.15
		504.14	503.13	502.12	501.15	500.14	499.13	491.17	490.16	489.15
		488.14	487.13	485.12	479.17	478.16	477.15	475.17	473.16	472.15
		471.14	470.13	469.12	468.11	467.11	465.15	463.17	461.16	460.15
		459.14	457.16	455.14	454.14	453.13	451.11	449.16	447.14	445.16
		444.11	443.14	442.1	441.09	437.16	435.14	434.13	433.16	432.15
		431.14	429.1	428.09	427.09	426.1	425.1	424.09	423.08	421.16
		419.14	417.13	416.12	415.15	414.14	413.13	412.1	411.09	410.08
		409.08	408.09	406.08	403.15	401.13	399.12	398.11	397.1	396.09
		395.1	394.09	393.08	392.07	385.14	383.1	382.09	381.11	380.1
		372.09	371.1	367.1	366.09	365.09	359.1	358.11	357.08	356.07
		355.1	354.09	353.09	345.11	344.1	343.09	342.09	341.09	340.1
		339.07	338.09	337.09	336.08	335.08	331.13	329.11	328.11	327.1
		326.09	325.08	324.08	323.08	321.06	320.08	317.11	316.11	315.13
		313.12	312.11	311.1	310.09	309.09	307.08	306.07	305.11	303.1
		301.12	299.14	298.09	297.12	295.11	294.1	293.09	291.1	287.1
		285.1	283.11	282.1	281.09	280.08	279.09	275.1	273.09	272.08
		271.08	270.07	269.09	268.09	267.09	265.06	259.11	257.09	256.08
		255.09	254.07	253.07	252.06	250.08	249.08	243.11	241.1	240.09
		239.08	238.07	237.09	236.08	235.06	227.12	225.1	223.07	221.09
		220.08	219.08	218.07	209.09	207.08	205.06	203.08	201.07	196.06
		194.04	193.1	192.03	191.08	189.07	187.05	182.08	180.04	179.08
		178.05	177.04	167.08	165.05	164.05	163.09	161.07	152.07	150.05
		147.04	146.04	136.08	135.04	134.04	130.04	123.04	119.05	111.04
		109.03	108.02	107.05	106.04					
References	<p>Amaya-Cruz Iz, D.M.; Pérez-Ramírez, I.F.; Delgado-García, J.; Mondragón-Jacobo, C.; Dector-Espinoza, A.; Reynoso-Camacho, R. An integral profile of bioactive compounds and functional properties of prickly pear (<i>Opuntia ficus indica</i> L.) peel with different tonalities. <i>Food Chem.</i> 2019, 278, 568–578.</p> <p>Xie, G.R.; Chen, H.J. Comprehensive Betalain Profiling of Djulis (<i>Chenopodium formosanum</i>) Cultivars Using HPLC-Q-Orbitrap High-Resolution Mass Spectrometry. <i>J. Agric. Food Chem.</i> 2021, 69, 15699–15715.</p> <p>Slimen, I.B.; Najjar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

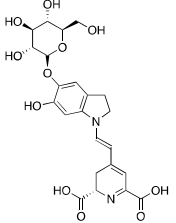
15-decarboxy-betanin

Chemical structure											
Name:	15-decarboxy-betanin										
Chemical Formula	C ₂₃ H ₂₆ N ₂ O ₁₁										
Molecular weight	506.46										
Monoisotopic mass	506.1537										
m/z [M+H]	507.1609										
Theoretical fragments (m/z)	507.16	506.15	505.15	504.14	492.15	491.17	490.16	489.15	488.14	487.13	
	479.17	478.16	477.15	475.17	473.16	472.15	471.14	470.13	469.12		
	467.17	465.15	464.14	463.17	462.16	461.16	460.15	459.14	455.14		
	454.14	453.13	451.11	449.16	448.15	447.14	445.16	444.15	443.14		
	442.14	441.13	437.16	435.14	434.13	432.15	431.14	429.17	427.15		
	426.14	425.13	419.14	418.14	417.13	416.12	414.14	413.13	409.14		
	408.13	401.13	399.12	396.13	383.12	382.11	381.11	375.12	373.1		
	369.11	368.1	366.12	364.1	358.11	357.11	356.1	355.09	352.1		
	351.09	348.11	346.09	345.11	344.1	343.09	342.09	341.09	340.1		
	339.09	338.09	337.08	334.09	331.13	330.12	329.11	328.11	327.1		
	326.09	325.09	324.08	323.08	322.09	321.08	320.08	319.07	317.11		
	316.11	315.13	314.13	313.12	312.11	311.1	310.09	307.08	306.07		
	305.11	303.1	302.07	301.12	300.11	299.1	298.09	297.1	296.09		
	295.11	294.1	293.09	291.1	288.11	287.1	286.09	285.1	284.12		
	283.11	282.1	281.09	280.09	279.09	276.09	275.1	273.1	272.08		
	271.08	270.07	269.13	268.09	267.09	259.11	257.09	256.08	255.09		
	254.08	253.07	252.06	250.08	249.08	243.11	241.1	240.09	237.09		
	236.08	235.06	223.07	221.09	220.06	219.08	209.09	207.08	205.06		
	204.07	202.05	196.06	195.05	194.04	193.1	192.03	191.08	190.05		
	189.07	182.08	181.05	180.04	179.08	178.05	177.04	176.03	167.08		
	166.09	165.05	164.05	163.04	162.05	152.07	150.05	149.05	148.04		
	147.04	146.04	145.05	136.08	135.04	134.04	132.04	130.04	124.04		
	123.04	119.05	111.04	110.06	109.03	108.02	107.05	106.04			
References	<p>Amaya-CruzIz, D.M.; Pérez-Ramírez, I.F.; Delgado-García, J.; Mondragón-Jacobo, C.; Dector-Espinoza, A.; Reynoso-Camacho, R. An integral profile of bioactive compounds and functional properties of prickly pear (<i>Opuntia ficus indica</i> L.) peel with different tonalities. <i>Food Chem.</i> 2019, 278, 568–578.</p> <p>Xie, G.R.; Chen, H.J. Comprehensive Betalain Profiling of Djulis (<i>Chenopodium formosanum</i>) Cultivars Using HPLC-Q-Orbitrap High-Resolution Mass Spectrometry. <i>J. Agric. Food Chem.</i> 2021, 69, 15699–15715.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>										

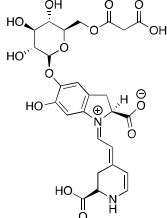
17-decarboxy-hylocerenin

Chemical structure										
Name:	17-decarboxy-hylocerenin									
Chemical Formula	C ₂₉ H ₃₄ N ₂ O ₁₅									
Molecular weight	650.59									
Monoisotopic mass	650.1959									
m/z [M+H]	651.2032									
heorical fragments (m/z)	651.2	650.2	649.19	648.18	635.21	634.2	633.19	632.18	631.18	623.21
		622.2	621.19	619.21	618.21	617.2	616.19	615.18	614.17	613.17
		611.21	609.19	608.18	607.21	606.21	605.2	604.19	603.18	601.2
		600.19	599.19	598.18	597.17	595.16	593.2	591.22	589.2	588.19
		587.19	586.18	585.17	583.19	581.2	579.18	578.17	577.2	576.19
		575.19	573.21	572.2	571.19	570.18	569.18	565.2	563.19	562.18
		561.17	560.16	559.19	558.18	557.18	549.21	547.19	545.18	543.16
		531.2	529.18	527.17	526.16	525.15	513.15	507.16	506.15	505.15
		502.16	500.14	499.13	491.17	490.16	489.15	488.14	487.13	486.14
		485.13	484.14	483.14	482.13	481.12	479.17	478.16	477.15	475.17
		473.16	472.15	471.14	470.14	469.13	468.13	467.12	465.15	463.17
		461.16	460.15	459.14	457.16	456.15	455.14	454.13	453.13	452.13
		451.12	450.12	449.16	447.14	445.16	444.15	443.14	442.14	441.14
		440.13	437.16	435.14	434.13	433.16	432.15	431.14	430.13	429.14
		427.15	426.14	425.14	424.14	423.13	421.16	419.14	417.14	416.12
		415.12	414.12	413.14	412.14	411.13	403.15	401.14	399.13	398.12
		397.11	396.11	395.13	394.13	393.12	385.15	383.13	381.12	379.1
		358.11	356.1	355.09	345.11	344.1	343.09	342.09	341.09	340.1
		338.09	337.08	331.13	329.11	328.11	327.1	326.09	325.08	324.08
		323.08	317.11	316.11	315.13	313.12	312.11	311.1	310.09	309.09
		307.08	306.07	305.11	303.1	301.12	299.14	298.09	297.12	295.11
		293.09	291.1	287.1	285.1	283.11	282.1	281.09	280.08	279.09
		275.1	273.09	272.08	271.08	270.07	269.09	268.09	267.09	259.11
		257.09	256.08	255.09	254.07	253.07	252.06	250.08	249.08	243.11
		241.1	240.09	239.08	238.07	237.09	236.08	235.06	227.12	225.1
		223.07	221.09	220.08	219.08	218.07	209.09	207.08	205.06	203.08
		201.07	196.06	194.04	193.1	191.08	189.07	187.05	182.08	180.04
		179.08	178.05	177.04	167.08	165.05	164.05	163.09	161.07	152.07
		150.05	147.04	146.04	136.08	135.04	134.04	130.04	123.04	119.05
		111.04	109.03	108.02	107.05	106.04				
References	<p>Amaya-CruzIz, D.M.; Pérez-Ramírez, I.F.; Delgado-García, J.; Mondragón-Jacobo, C.; Dector-Espinoza, A.; Reynoso-Camacho, R. An integral profile of bioactive compounds and functional properties of prickly pear (<i>Opuntia ficus indica</i> L.) peel with different tonalities. <i>Food Chem.</i> 2019, 278, 568–578.</p> <p>Xie, G.R.; Chen, H.J. Comprehensive Betalain Profiling of Djulis (<i>Chenopodium formosanum</i>) Cultivars Using HPLC-Q-Orbitrap High-Resolution Mass Spectrometry. <i>J. Agric. Food Chem.</i> 2021, 69, 15699–15715.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

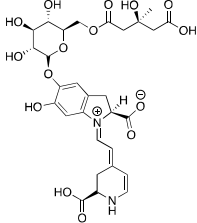
2-decarboxy-betanin

Chemical structure										
Name:	2-decarboxy-betanin									
Chemical Formula	C ₂₃ H ₂₆ N ₂ O ₁₁									
Molecular weight	506.46									
Monoisotopic mass	506.1537									
m/z [M+H]	507.1609									
Theoretical fragments (m/z)	507.16	506.15	505.15	504.14	503.13	502.12	493.15	492.14	491.17	490.16
	489.15	488.14	487.13	486.13	485.12	481.15	479.17	478.12	477.15	
	476.14	475.13	474.13	473.16	472.15	471.14	470.13	469.12	467.17	
	465.15	463.17	462.13	461.16	460.15	459.14	458.13	457.12	456.12	
	455.14	453.13	451.13	449.16	447.18	446.13	445.16	444.12	443.14	
	441.13	439.11	437.13	436.16	435.14	434.13	433.12	432.12	431.11	
	430.14	429.13	428.12	427.11	426.11	425.13	421.14	419.14	417.13	
	416.12	415.11	413.13	412.13	411.12	410.11	409.1	405.13	403.11	
	402.11	401.1	400.13	399.12	398.11	397.1	391.11	387.12	386.11	
	385.1	384.1	383.09	376.14	375.12	373.1	371.09	370.12	369.11	
	368.1	364.14	359.12	357.11	356.1	355.09	345.11	344.1	343.09	
	341.11	340.11	339.1	338.12	331.13	329.11	328.11	327.1	326.09	
	325.08	320.11	319.09	317.08	316.07	315.13	314.12	313.12	312.11	
	311.1	310.09	309.09	303.1	302.1	301.12	300.11	299.1	297.1	
	296.11	294.1	288.11	287.1	286.09	285.1	283.11	282.1	279.09	
	278.1	276.09	273.09	271.08	270.07	268.09	267.09	255.11	237.09	
	236.08	235.07	223.07	222.06	211.07	207.08	205.06	196.06	194.04	
	180.06	179.06	178.05	177.04	176.07	175.02	168.03	165.08	164.07	
	163.06	162.05	161.04	160.04	159.03	152.03	151.06	150.02	149.04	
	148.04	147.07	146.06	145.05	144.04	143.03	139.06	138.09	137.08	
	136.08	135.04	134.06	133.05	132.04	131.03	130.03	129.05	127.04	
	124.04	123.04	122.06	121.05	120.04	119.03	118.03	117.02	116.05	
	115.04	113.02	111.04	110.06	108.04	107.07	105.05	104.05	103.04	
	102.03	101.02	100.04							
References	<p>Amaya-CruzIz, D.M.; Pérez-Ramírez, I.F.; Delgado-García, J.; Mondragón-Jacobo, C.; Dector-Espinoza, A.; Reynoso-Camacho, R. An integral profile of bioactive compounds and functional properties of prickly pear (<i>Opuntia ficus indica</i> L.) peel with different tonalities. <i>Food Chem.</i> 2019, 278, 568–578.</p> <p>Xie, G.R.; Chen, H.J. Comprehensive Betalain Profiling of Djulis (<i>Chenopodium formosanum</i>) Cultivars Using HPLC-Q-Orbitrap High-Resolution Mass Spectrometry. <i>J. Agric. Food Chem.</i> 2021, 69, 15699–15715.</p> <p>Slimen, I.B.; Najjar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

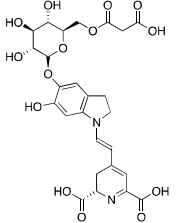
17-decarboxy-isophyllocactin

Chemical structure										
Name:	17-decarboxy-isophyllocactin									
Chemical Formula	C ₂₆ H ₂₈ N ₂ O ₁₄									
Molecular weight	592.51									
Monoisotopic mass	592.1541									
m/z [M+H]	593.1613									
Theoretical fragments (m/z)	593.16	592.15	591.15	590.14	577.17	576.16	575.15	574.14	573.14	565.17
		564.16	563.15	561.17	560.16	559.16	558.15	557.14	556.13	555.12
		553.17	551.15	550.14	549.17	548.16	547.16	546.15	545.14	543.16
		542.15	541.15	540.14	539.13	537.11	535.16	533.18	531.16	530.15
		529.15	528.14	527.13	525.15	523.16	521.14	520.13	519.16	518.15
		517.15	515.17	514.16	513.15	512.14	511.13	507.16	506.15	505.15
		504.14	503.13	502.12	501.15	500.14	499.13	491.17	490.16	489.15
		488.14	487.13	485.12	479.17	478.16	477.15	475.17	473.16	472.15
		471.14	470.13	469.12	468.11	467.11	465.15	463.17	461.16	460.15
		459.14	457.16	455.14	454.14	453.13	451.11	449.16	447.14	445.16
		444.11	443.14	442.1	441.09	437.16	435.14	434.13	433.16	432.15
		431.14	429.1	428.09	427.09	426.1	425.1	424.09	423.08	421.16
		419.14	417.13	416.12	415.15	414.14	413.13	412.1	411.09	410.08
		409.08	408.09	406.08	403.15	401.13	399.12	398.11	397.1	396.09
		395.1	394.09	393.08	392.07	385.14	383.1	382.09	381.11	380.1
		372.09	371.1	367.1	366.09	365.09	359.1	358.11	357.08	356.07
		355.1	354.09	353.09	345.11	344.1	343.09	342.09	341.09	340.1
		339.07	338.09	337.09	336.08	335.08	331.13	329.11	328.11	327.1
		326.09	325.08	324.08	323.08	321.06	320.08	317.11	316.11	315.13
		313.12	312.11	311.1	310.09	309.09	307.08	306.07	305.11	303.1
		301.12	299.14	298.09	297.12	295.11	294.1	293.09	291.1	287.1
		285.1	283.11	282.1	281.09	280.08	279.09	275.1	273.09	272.08
		271.08	270.07	269.09	268.09	267.09	265.06	259.11	257.09	256.08
		255.09	254.07	253.07	252.06	250.08	249.08	243.11	241.1	240.09
		239.08	238.07	237.09	236.08	235.06	227.12	225.1	223.07	221.09
		220.08	219.08	218.07	209.09	207.08	205.06	203.08	201.07	196.06
		194.04	193.1	192.03	191.08	189.07	187.05	182.08	180.04	179.08
		178.05	177.04	167.08	165.05	164.05	163.09	161.07	152.07	150.05
		147.04	146.04	136.08	135.04	134.04	130.04	123.04	119.05	111.04
		109.03	108.02	107.05	106.04					
References	<p>Amaya-Cruz Iz, D.M.; Pérez-Ramírez, I.F.; Delgado-García, J.; Mondragón-Jacobo, C.; Dector-Espinoza, A.; Reynoso-Camacho, R. An integral profile of bioactive compounds and functional properties of prickly pear (<i>Opuntia ficus indica</i> L.) peel with different tonalities. <i>Food Chem.</i> 2019, 278, 568–578.</p> <p>Xie, G.R.; Chen, H.J. Comprehensive Betalain Profiling of Djulis (<i>Chenopodium formosanum</i>) Cultivars Using HPLC-Q-Orbitrap High-Resolution Mass Spectrometry. <i>J. Agric. Food Chem.</i> 2021, 69, 15699–15715.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

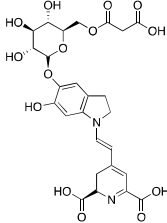
17-decarboxy-isohydrocerenin

Chemical structure										
Name:	17-decarboxy-isohydrocerenin									
Chemical Formula	C ₂₉ H ₃₄ N ₂ O ₁₅									
Molecular weight	650.59									
Monoisotopic mass	650.1959									
m/z [M+H]	651.2032									
Theoretical fragments (m/z)	651.2	650.2	649.19	648.18	635.21	634.2	633.19	632.18	631.18	623.21
			622.2	621.19	619.21	618.21	617.2	616.19	615.18	614.17
			613.17	611.21	609.19	608.18	607.21	606.21	605.2	604.19
			603.18	601.2	600.19	599.19	598.18	597.17	595.16	593.2
			591.22	589.2	588.19	587.19	586.18	585.17	583.19	581.2
			579.18	578.17	577.2	576.19	575.19	573.21	572.2	571.19
			570.18	569.18	565.2	563.19	562.18	561.17	560.16	559.19
			558.18	557.18	549.21	547.19	545.18	543.16	531.2	529.18
			527.17	526.16	525.15	513.15	507.16	506.15	505.15	502.16
			500.14	499.13	491.17	490.16	489.15	488.14	487.13	486.14
			485.13	484.14	483.14	482.13	481.12	479.17	478.16	477.15
			475.17	473.16	472.15	471.14	470.14	469.13	468.13	467.12
			465.15	463.17	461.16	460.15	459.14	457.16	456.15	455.14
			454.13	453.13	452.13	451.12	450.12	449.16	447.14	445.16
			444.15	443.14	442.14	441.14	440.13	437.16	435.14	434.13
			433.16	432.15	431.14	430.13	429.14	427.15	426.14	425.14
			424.14	423.13	421.16	419.14	417.14	416.12	415.12	414.12
			413.14	412.14	411.13	403.15	401.14	399.13	398.12	397.11
			396.11	395.13	394.13	393.12	385.15	383.13	381.12	379.1
			358.11	356.1	355.09	345.11	344.1	343.09	342.09	341.09
			340.1	338.09	337.08	331.13	329.11	328.11	327.1	326.09
			325.08	324.08	323.08	317.11	316.11	315.13	313.12	312.11
			311.1	310.09	309.09	307.08	306.07	305.11	303.1	301.12
			299.14	298.09	297.12	295.11	293.09	291.1	287.1	285.1
			283.11	282.1	281.09	280.08	279.09	275.1	273.09	272.08
			271.08	270.07	269.09	268.09	267.09	259.11	257.09	256.08
			255.09	254.07	253.07	252.06	250.08	249.08	243.11	241.1
			240.09	239.08	238.07	237.09	236.08	235.06	227.12	225.1
			223.07	221.09	220.08	219.08	218.07	209.09	207.08	205.06
			203.08	201.07	196.06	194.04	193.1	191.08	189.07	187.05
			182.08	180.04	179.08	178.05	177.04	167.08	165.05	164.05
			163.09	161.07	152.07	150.05	147.04	146.04	136.08	135.04
			134.04	130.04	123.04	119.05	111.04	109.03	108.02	107.05
			106.04							
References	<p>Amaya-CruzIz, D.M.; Pérez-Ramírez, I.F.; Delgado-García, J.; Mondragón-Jacobo, C.; Dector-Espinoza, A.; Reynoso-Camacho, R. An integral profile of bioactive compounds and functional properties of prickly pear (<i>Opuntia ficus indica</i> L.) peel with different tonalities. <i>Food Chem.</i> 2019, 278, 568–578.</p> <p>Xie, G.R.; Chen, H.J. Comprehensive Betalain Profiling of Djulis (<i>Chenopodium formosanum</i>) Cultivars Using HPLC-Q-Orbitrap High-Resolution Mass Spectrometry. <i>J. Agric. Food Chem.</i> 2021, 69, 15699–15715.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

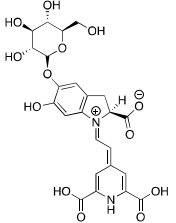
2-decarboxy-phylllocactin

Chemical structure										
Name:	2-decarboxy-phylllocactin									
Chemical Formula	C ₂₆ H ₂₈ N ₂ O ₁₄									
Molecular weight	592.51									
Monoisotopic mass	592.1541									
m/z [M+H]	593.1613									
Theoretical fragments (m/z)	593.16	592.15	591.15	590.14	579.15	577.17	576.16	575.15	574.14	573.14
			567.15	565.13	564.12	563.15	562.14	561.14	559.16	557.14
			555.12	551.15	549.14	548.13	547.12	546.15	545.14	544.13
			543.12	541.15	539.13	535.16	533.14	532.17	531.12	530.12
			529.11	528.14	527.13	526.12	525.15	523.13	521.12	520.14
			517.15	515.13	513.11	511.1	507.16	505.15	493.15	491.17
			489.15	487.13	481.15	479.13	478.12	477.15	476.14	475.13
			473.16	471.14	469.12	465.15	463.13	462.13	461.12	460.11
			459.14	458.13	457.12	455.14	453.13	447.14	445.12	444.12
			443.11	442.14	441.13	440.12	439.11	437.13	435.12	429.13
			427.11	425.1	424.12	411.12	408.13	406.11	400.12	399.12
			398.11	397.1	396.09	395.12	393.11	386.11	384.13	383.1
			382.11	381.11	380.1	379.09	375.12	374.11	373.1	372.09
			371.1	370.11	369.11	368.1	367.1	366.12	365.09	364.1
			362.09	359.1	357.08	356.07	355.1	354.09	353.09	349.09
			347.08	345.11	344.1	343.09	342.08	341.09	340.08	339.07
			338.06	337.09	336.08	335.08	331.13	329.11	328.11	327.1
			326.09	325.08	323.08	321.06	320.11	319.09	317.08	316.07
			315.13	314.09	313.12	312.11	311.1	309.09	307.11	303.1
			301.08	300.07	299.07	298.09	297.1	296.11	295.11	294.1
			293.09	287.1	286.09	285.1	284.08	283.07	282.06	279.09
			278.1	276.09	273.1	271.08	270.07	269.09	268.09	267.09
			261.08	255.09	253.07	252.06	250.08	249.08	237.09	236.08
			235.06	233.07	231.05	223.07	222.06	221.09	220.08	219.08
			218.07	211.07	207.08	205.06	196.06	195.08	194.04	193.06
			191.05	180.07	178.05	176.07	163.06	161.04	152.07	151.06
			150.05	149.05	148.04	147.07	145.05	138.09	136.08	135.04
			134.06	133.05	124.04	123.04	122.06	121.06	119.05	111.04
			110.06	109.03	108.02	107.05	106.04	103.05		
References	<p>Amaya-Cruz Iz, D.M.; Pérez-Ramírez, I.F.; Delgado-García, J.; Mondragón-Jacobo, C.; Dector-Espinoza, A.; Reynoso-Camacho, R. An integral profile of bioactive compounds and functional properties of prickly pear (<i>Opuntia ficus indica</i> L.) peel with different tonalities. <i>Food Chem.</i> 2019, 278, 568–578.</p> <p>Xie, G.R.; Chen, H.J. Comprehensive Betalain Profiling of Djulis (<i>Chenopodium formosanum</i>) Cultivars Using HPLC-Q-Orbitrap High-Resolution Mass Spectrometry. <i>J. Agric. Food Chem.</i> 2021, 69, 15699–15715.</p> <p>Slimen, I.B.; Najjar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

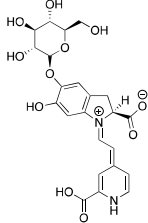
2-decarboxy-isophyllocactin

Chemical structure										
Name:	2-decarboxy-isophyllocactin									
Chemical Formula	C ₂₆ H ₂₈ N ₂ O ₁₄									
Molecular weight	592.51									
Monoisotopic mass	592.1541									
m/z [M+H]	593.1613									
Theoretical fragments (m/z)	593.16	592.15	591.15	590.14	579.15	577.17	576.16	575.15	574.14	573.14
			567.15	565.13	564.12	563.15	562.14	561.14	559.16	557.14
			555.12	551.15	549.14	548.13	547.12	546.15	545.14	544.13
			543.12	541.15	539.13	535.16	533.14	532.17	531.12	530.12
			529.11	528.14	527.13	526.12	525.15	523.13	521.12	520.14
			517.15	515.13	513.11	511.1	507.16	505.15	493.15	491.17
			489.15	487.13	481.15	479.13	478.12	477.15	476.14	475.13
			473.16	471.14	469.12	465.15	463.13	462.13	461.12	460.11
			459.14	458.13	457.12	455.14	453.13	447.14	445.12	444.12
			443.11	442.14	441.13	440.12	439.11	437.13	435.12	429.13
			427.11	425.1	424.12	411.12	408.13	406.11	400.12	399.12
			398.11	397.1	396.09	395.12	393.11	386.11	384.13	383.1
			382.11	381.11	380.1	379.09	375.12	374.11	373.1	372.09
			371.1	370.11	369.11	368.1	367.1	366.12	365.09	364.1
			362.09	359.1	357.08	356.07	355.1	354.09	353.09	349.09
			347.08	345.11	344.1	343.09	342.08	341.09	340.08	339.07
			338.06	337.09	336.08	335.08	331.13	329.11	328.11	327.1
			326.09	325.08	323.08	321.06	320.11	319.09	317.08	316.07
			315.13	314.09	313.12	312.11	311.1	309.09	307.11	303.1
			301.08	300.07	299.07	298.09	297.1	296.11	295.11	294.1
			293.09	287.1	286.09	285.1	284.08	283.07	282.06	279.09
			278.1	276.09	273.1	271.08	270.07	269.09	268.09	267.09
			261.08	255.09	253.07	252.06	250.08	249.08	237.09	236.08
			235.06	233.07	231.05	223.07	222.06	221.09	220.08	219.08
			218.07	211.07	207.08	205.06	196.06	195.08	194.04	193.06
			191.05	180.07	178.05	176.07	163.06	161.04	152.07	151.06
			150.05	149.05	148.04	147.07	145.05	138.09	136.08	135.04
			134.06	133.05	124.04	123.04	122.06	121.06	119.05	111.04
			110.06	109.03	108.02	107.05	106.04	103.05		
References	<p>Amaya-Cruz Iz, D.M.; Pérez-Ramírez, I.F.; Delgado-García, J.; Mondragón-Jacobo, C.; Dector-Espinoza, A.; Reynoso-Camacho, R. An integral profile of bioactive compounds and functional properties of prickly pear (<i>Opuntia ficus indica</i> L.) peel with different tonalities. <i>Food Chem.</i> 2019, 278, 568–578.</p> <p>Xie, G.R.; Chen, H.J. Comprehensive Betalain Profiling of Djulis (<i>Chenopodium formosanum</i>) Cultivars Using HPLC-Q-Orbitrap High-Resolution Mass Spectrometry. <i>J. Agric. Food Chem.</i> 2021, 69, 15699–15715.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

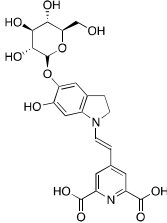
Neobetanin

Chemical structure										
Name:	Neobetanin									
Chemical Formula	C ₂₄ H ₂₄ N ₂ O ₁₃									
Molecular weight	548.46									
Monoisotopic mass	548.1278									
m/z [M+H]	549.1351									
Theoretical fragments (m/z)	549.14	548.13	547.12	546.11	533.14	532.13	531.12	530.12	529.11	521.14
		520.13	519.12	517.15	516.14	515.13	514.12	513.11	512.11	511.1
		509.14	507.12	506.12	505.15	504.14	503.13	502.12	501.11	497.12
		496.11	495.1	493.09	491.13	490.12	489.11	488.14	487.13	486.13
		485.12	484.11	483.1	479.13	477.11	476.11	474.13	473.12	471.14
		469.12	468.12	467.11	461.12	460.11	459.1	458.1	456.12	455.11
		451.11	443.11	441.09	433.12	425.1	423.08	417.09	415.08	387.08
		386.07	385.07	384.06	373.1	371.09	370.08	369.07	368.06	367.06
		359.09	358.08	357.11	356.1	355.09	354.08	353.08	352.07	351.09
		350.09	347.09	345.07	343.09	342.09	341.09	340.07	339.1	338.09
		337.08	336.07	334.09	333.07	329.08	327.1	326.09	325.09	324.08
		323.08	322.09	321.08	320.08	319.07	317.08	315.06	314.05	313.08
		312.11	311.1	310.09	308.09	307.08	306.07	302.07	301.08	299.07
		298.06	297.1	296.09	294.1	293.09	285.1	283.07	282.06	280.09
		279.06	278.05	277.05	276.09	273.1	271.08	270.07	268.09	267.09
		265.05	264.04	263.07	262.06	261.05	255.09	254.08	253.07	252.06
		251.07	250.08	249.05	247.03	237.08	235.07	233.06	231.04	221.06
		209.06	207.05	206.03	194.04	193.04	192.03	191.06	190.05	181.05
		180.04	179.03	178.05	177.04	176.03	167.07	165.05	164.05	163.04
		162.05	150.05	149.05	148.04	147.04	146.04	145.05	136.08	135.04
		134.04	132.04	130.04	123.04	119.05	111.04	109.03	108.02	107.05
		106.04								
References	<p>Amaya-Cruz Iz, D.M.; Pérez-Ramírez, I.F.; Delgado-García, J.; Mondragón-Jacobo, C.; Dector-Espinoza, A.; Reynoso-Camacho, R. An integral profile of bioactive compounds and functional properties of prickly pear (<i>Opuntia ficus indica</i> L.) peel with different tonalities. <i>Food Chem.</i> 2019, 278, 568–578.</p> <p>Xie, G.R.; Chen, H.J. Comprehensive Betalain Profiling of Djulis (<i>Chenopodium formosanum</i>) Cultivars Using HPLC-Q-Orbitrap High-Resolution Mass Spectrometry. <i>J. Agric. Food Chem.</i> 2021, 69, 15699–15715.</p> <p>Slimen, I.B.; Najjar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

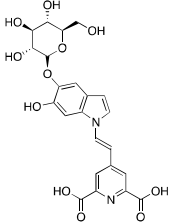
17-decarboxy-neobetainin

Chemical structure										
Name:	17-decarboxy-neobetainin									
Chemical Formula	C ₂₃ H ₂₄ N ₂ O ₁₁									
Molecular weight	504.45									
Monoisotopic mass	504.1380									
m/z [M+H]	505.1453									
Theoretical fragments (m/z)	505.15	504.14	503.13	502.12	501.11	500.11	491.13	490.12	489.15	488.14
			487.13	486.13	485.12	484.11	483.1	479.13	477.15	476.14
			475.13	474.13	473.12	472.11	471.14	470.13	469.12	468.12
			467.11	465.15	463.13	461.16	460.15	459.14	458.13	457.12
			456.12	455.11	454.1	453.13	452.12	451.11	449.12	448.15
			447.14	446.13	445.16	444.12	443.14	442.1	441.13	439.11
			437.1	435.14	433.12	432.12	431.11	430.14	429.09	428.12
			427.11	426.11	425.1	424.09	423.12	419.11	417.13	415.11
			414.11	413.1	411.12	410.11	409.1	408.1	403.11	401.1
			400.09	399.08	398.11	397.1	396.1	395.09	389.1	385.1
			384.1	383.09	382.11	381.07	373.1	371.09	369.07	368.1
			367.09	366.12	364.1	358.11	357.11	356.1	355.09	354.08
			353.08	348.11	346.09	343.09	342.08	341.08	340.1	339.1
			338.09	337.08	336.07	330.12	329.11	328.1	327.1	326.09
			325.08	324.07	323.07	322.09	320.08	315.1	313.12	312.11
			311.1	310.09	309.09	308.08	307.07	301.12	300.11	299.1
			298.09	297.09	296.08	295.07	294.1	288.11	286.09	285.1
			283.11	281.09	279.08	273.1	271.07	270.07	269.09	268.09
			267.09	257.09	255.08	254.07	241.1	239.08	235.07	234.06
			233.06	221.06	220.06	219.08	217.06	207.08	205.06	204.07
			203.05	202.05	196.06	195.05	194.04	193.06	192.05	191.05
			182.08	180.07	179.06	178.05	177.04	176.06	175.02	166.09
			165.08	164.07	163.06	162.05	161.04	160.04	159.03	151.06
			150.05	149.04	148.04	147.07	146.06	145.05	144.04	143.03
			139.06	136.04	135.07	134.06	133.05	132.04	131.03	130.03
			129.05	127.04	124.04	123.04	122.02	121.05	120.04	119.03
			118.03	117.02	116.05	115.04	113.02	111.04	110.06	108.04
			107.07	105.05	104.05	103.04	102.03	101.02	100.02	
References	<p>Amaya-CruzIz, D.M.; Pérez-Ramírez, I.F.; Delgado-García, J.; Mondragón-Jacobo, C.; Dector-Espinoza, A.; Reynoso-Camacho, R. An integral profile of bioactive compounds and functional properties of prickly pear (<i>Opuntia ficus indica</i> L.) peel with different tonalities. <i>Food Chem.</i> 2019, 278, 568–578.</p> <p>Xie, G.R.; Chen, H.J. Comprehensive Betalain Profiling of Djulis (<i>Chenopodium formosanum</i>) Cultivars Using HPLC-Q-Orbitrap High-Resolution Mass Spectrometry. <i>J. Agric. Food Chem.</i> 2021, 69, 15699–15715.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

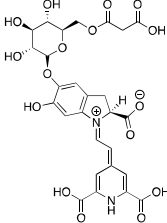
2-decarboxy-neobetanim

Chemical structure										
Name:	2-decarboxy-neobetanim									
Chemical Formula	C ₂₃ H ₂₄ N ₂ O ₁₁									
Molecular weight	504.45									
Monoisotopic mass	504.1380									
m/z [M+H]	505.1453									
Theoretical fragments (m/z)	505.15	504.14	503.13	502.12	491.13	490.12	489.15	488.14	487.13	486.13
		485.12	479.13	477.11	476.11	474.13	473.12	472.15	471.14	470.13
		469.12	468.12	467.11	461.12	460.11	459.1	458.1	457.12	456.12
		455.11	454.14	453.13	452.12	451.11	450.11	447.14	444.15	443.11
		442.14	441.09	438.11	437.1	435.14	434.11	433.12	432.12	431.11
		430.14	429.13	426.14	425.1	424.13	423.08	417.17	416.16	415.15
		413.1	408.13	407.12	399.16	398.15	397.14	373.1	371.09	355.09
		354.08	343.09	342.08	341.08	340.07	329.11	328.11	327.1	326.09
		325.08	324.07	323.1	317.08	315.06	314.05	313.08	312.11	311.1
		310.09	307.11	306.1	303.1	301.08	299.07	298.06	297.1	296.11
		294.1	293.09	285.1	283.07	282.06	281.1	280.08	279.09	278.1
		276.09	275.08	273.1	271.08	270.07	269.09	268.09	267.09	261.08
		258.08	257.07	255.09	254.08	253.07	252.06	251.08	250.08	249.08
		237.08	235.07	234.06	233.06	221.06	220.05	209.06	208.05	207.04
		206.03	204.05	194.04	193.04	192.05	180.03	178.05	177.07	176.06
		175.05	165.05	163.06	162.05	161.04	160.06	150.05	149.05	148.04
		147.07	145.05	143.03	136.08	135.04	134.06	133.05	132.04	127.04
		123.04	121.06	120.08	119.05	118.07	111.04	109.03	108.02	107.05
		106.04	103.05	101.02						
References	<p>Amaya-Cruz Iz, D.M.; Pérez-Ramírez, I.F.; Delgado-García, J.; Mondragón-Jacobo, C.; Dector-Espinoza, A.; Reynoso-Camacho, R. An integral profile of bioactive compounds and functional properties of prickly pear (<i>Opuntia ficus indica</i> L.) peel with different tonalities. <i>Food Chem.</i> 2019, 278, 568–578.</p> <p>Xie, G.R.; Chen, H.J. Comprehensive Betalain Profiling of Djulis (<i>Chenopodium formosanum</i>) Cultivars Using HPLC-Q-Orbitrap High-Resolution Mass Spectrometry. <i>J. Agric. Food Chem.</i> 2021, 69, 15699–15715.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

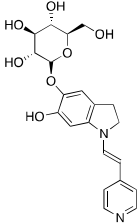
2-decarboxy-2,3-dehydro-neobetanin

Chemical structure										
Name:	2-Decarboxy-2,3-dehydro-neobetanin									
Chemical Formula	C ₂₃ H ₂₂ N ₂ O ₁₁									
Molecular weight	502.43									
Monoisotopic mass	502.1224									
m/z [M+H]	503.1296									
Theoretical fragments (m/z)	503.13	502.12	487.13	486.13	485.12	484.11	477.11	476.11	475.13	470.13
		469.12	468.12	467.11	466.1	461.12	460.11	459.14	458.13	457.12
		455.11	452.12	451.11	450.11	449.1	448.09	444.12	443.11	442.1
		441.13	440.12	439.11	437.1	434.11	433.12	432.1	431.11	428.09
		426.11	425.1	424.13	423.12	422.11	421.1	417.13	416.12	415.15
		414.14	413.1	412.09	411.12	406.12	405.11	404.1	403.09	399.08
		397.14	396.13	395.12	389.13	388.11	387.12	379.13	378.12	377.11
		370.08	369.07	361.12	353.08	341.08	340.07	339.06	327.1	326.09
		325.08	324.07	323.07	315.06	314.05	313.08	310.09	309.09	308.08
		307.07	301.08	300.07	299.07	298.06	297.09	296.08	295.07	294.1
		292.08	285.09	284.08	283.07	282.06	281.09	280.08	279.08	277.06
		271.08	270.07	268.08	266.1	265.1	262.08	257.09	256.08	255.09
		254.08	253.07	252.06	251.08	241.1	240.09	239.12	238.11	237.08
		235.06	234.05	233.06	220.05	216.04	213.1	209.06	208.05	207.04
		206.03	203.05	194.04	193.04	192.05	190.04	189.07	180.03	176.03
		175.05	166.01	165.07	163.06	162.04	150.02	148.04	147.07	146.06
		136.04	134.06	132.04	122.02	119.05	118.04	109.03	108.02	107.05
		106.03	102.05							
References	<p>Amaya-Cruz Iz, D.M.; Pérez-Ramírez, I.F.; Delgado-García, J.; Mondragón-Jacobo, C.; Dector-Espinoza, A.; Reynoso-Camacho, R. An integral profile of bioactive compounds and functional properties of prickly pear (<i>Opuntia ficus indica</i> L.) peel with different tonalities. <i>Food Chem.</i> 2019, 278, 568–578.</p> <p>Xie, G.R.; Chen, H.J. Comprehensive Betalain Profiling of Djulis (<i>Chenopodium formosanum</i>) Cultivars Using HPLC-Q-Orbitrap High-Resolution Mass Spectrometry. <i>J. Agric. Food Chem.</i> 2021, 69, 15699–15715.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

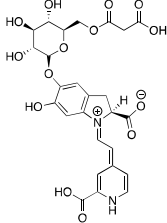
Neophyllocactin

Chemical structure										
Name:	Neophyllocactin									
Chemical Formula	C ₂₇ H ₂₆ N ₂ O ₁₆									
Molecular weight	634.50									
Monoisotopic mass	634.1282									
m/z [M+H]	635.1355									
Theoretical fragments (m/z)	635.14	634.13	633.12	632.11	619.14	618.13	617.12	616.12	615.11	607.14
		606.13	605.12	603.15	602.14	601.13	600.12	599.11	598.11	597.1
		595.14	593.12	592.12	591.15	590.14	589.13	588.12	587.11	585.14
		584.13	583.12	582.11	581.1	579.09	577.13	575.15	573.14	572.13
		571.12	570.11	569.1	567.12	565.13	563.11	562.11	561.14	560.13
		559.12	557.14	556.13	555.12	554.12	553.11	549.14	548.13	547.12
		546.11	545.1	544.1	543.12	542.12	541.11	533.14	532.13	531.12
		530.12	529.11	527.09	521.14	520.13	519.12	515.13	514.12	513.11
		512.11	511.1	509.08	507.12	505.15	503.13	502.12	501.11	497.12
		496.11	495.1	493.09	491.13	489.11	487.13	486.13	485.12	484.11
		483.1	479.13	477.11	476.11	474.13	473.12	469.12	468.12	467.11
		461.12	459.1	458.1	456.12	455.11	454.1	443.11	442.1	441.09
		439.11	438.1	437.1	429.1	428.09	427.09	426.1	425.1	424.09
		423.08	417.09	415.08	413.11	412.1	411.09	410.08	409.08	408.09
		406.08	399.09	398.11	397.1	396.09	395.1	394.09	393.08	392.07
		387.08	386.07	385.07	384.06	383.1	382.09	380.1	373.1	371.09
		370.08	369.07	368.06	367.06	366.09	365.09	359.1	358.08	357.11
		356.07	355.09	354.09	353.08	352.07	351.09	347.09	345.07	343.1
		342.09	341.09	340.07	339.07	338.09	337.08	336.08	335.08	333.07
		329.08	327.1	325.08	324.08	323.08	321.06	320.08	317.08	315.06
		314.05	313.08	312.07	307.08	306.07	301.08	299.07	298.06	297.1
		294.1	285.1	283.07	282.06	279.06	278.05	277.05	273.1	271.08
		270.07	268.09	267.09	265.05	263.07	261.05	255.09	253.07	252.06
		251.07	250.08	249.05	247.03	237.08	235.07	233.06	231.04	221.06
		209.06	207.05	206.03	194.04	193.04	192.03	191.06	181.05	180.04
		179.03	178.05	177.04	167.07	165.05	164.05	163.04	150.05	147.04
		146.04	145.05	135.04	134.04	130.04	123.04	119.05	111.04	109.03
		108.02	107.05	106.04						
References	<p>Amaya-CruzIz, D.M.; Pérez-Ramírez, I.F.; Delgado-García, J.; Mondragón-Jacobo, C.; Dector-Espinoza, A.; Reynoso-Camacho, R. An integral profile of bioactive compounds and functional properties of prickly pear (<i>Opuntia ficus indica</i> L.) peel with different tonalities. <i>Food Chem.</i> 2019, 278, 568–578.</p> <p>Xie, G.R.; Chen, H.J. Comprehensive Betalain Profiling of Djulis (<i>Chenopodium formosanum</i>) Cultivars Using HPLC-Q-Orbitrap High-Resolution Mass Spectrometry. <i>J. Agric. Food Chem.</i> 2021, 69, 15699–15715.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

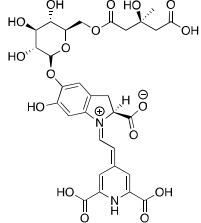
2,15,17-tridecarboxy-neobetainin

Chemical structure										
Name:	2,15,17-tridecarboxy-neobetainin									
Chemical Formula	C ₂₁ H ₂₄ N ₂ O ₇									
Molecular weight	416.43									
Monoisotopic mass	416.1584									
m/z [M+H]	417.1656									
Theoretical fragments (m/z)	417.17	416.16	415.15	414.14	413.13	412.13	403.15	402.14	401.13	400.16
		399.16	398.15	397.14	396.13	395.12	391.15	390.14	389.13	388.13
		387.16	386.15	385.14	384.13	383.12	382.15	381.14	380.14	379.13
		375.16	373.14	372.13	371.12	370.12	369.14	368.14	367.13	366.12
		365.11	363.13	361.14	359.12	357.14	356.14	355.13	354.12	353.11
		351.13	350.13	349.12	345.14	344.14	343.13	342.12	341.11	340.11
		339.13	338.12	337.12	331.13	329.15	327.13	326.13	325.12	324.11
		323.1	321.12	320.11	319.11	315.13	314.12	313.12	312.11	311.1
		310.09	309.12	308.12	307.11	302.1	301.12	300.11	299.11	298.09
		297.12	296.11	295.11	294.1	293.09	288.11	286.09	285.1	284.09
		283.11	282.1	281.09	279.09	278.1	276.09	273.1	271.08	270.07
		269.13	268.09	267.11	266.1	255.11	254.1	253.1	241.13	240.09
		239.12	237.1	236.09	229.1	227.08	226.07	225.1	224.09	223.12
		213.1	211.09	210.08	197.11	195.09	180.06	179.06	178.05	177.04
		176.07	175.02	165.08	164.07	163.06	162.05	161.04	160.04	159.03
		152.07	151.06	150.05	149.04	148.04	147.07	146.08	145.05	144.04
		143.03	139.06	138.09	137.08	136.08	135.04	134.06	133.08	132.07
		131.03	130.03	129.05	127.04	124.04	123.04	122.06	121.05	120.04
		119.03	118.03	117.02	116.05	115.04	114.03	113.02	111.04	110.06
		109.03	108.04	107.07	106.07	105.05	104.05	103.04	102.03	101.02
		100.02	99.01	97.03	95.05	93.03	92.03	91.04	90.03	89.02
		88.02	87.01	86.04	85.03	83.01	78.03	77.06	76.02	75.04
		74.04	73.03	72.02	71.01	69	67.02	63.04	62.04	61.03
		60.02	59.01	58	57.03	56.03	55.02	53	51.02	49.03
		47.01	46	45	44.03	43.02	42.03	41.03	33.03	31.02
		30.01								
References	<p>Amaya-CruzIz, D.M.; Pérez-Ramírez, I.F.; Delgado-García, J.; Mondragón-Jacobo, C.; Dector-Espinoza, A.; Reynoso-Camacho, R. An integral profile of bioactive compounds and functional properties of prickly pear (<i>Opuntia ficus indica</i> L.) peel with different tonalities. <i>Food Chem.</i> 2019, 278, 568–578.</p> <p>Xie, G.R.; Chen, H.J. Comprehensive Betalain Profiling of Djulis (<i>Chenopodium formosanum</i>) Cultivars Using HPLC-Q-Orbitrap High-Resolution Mass Spectrometry. <i>J. Agric. Food Chem.</i> 2021, 69, 15699–15715.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

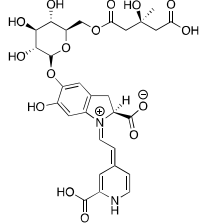
17-decarboxy-neophyllocactin

Chemical structure										
Name:	17-decarboxy-neophyllocactin									
Chemical Formula	C ₂₆ H ₂₆ N ₂ O ₁₄									
Molecular weight	590.49									
Monoisotopic mass	590.1384									
m/z [M+H]	591.1457									
Theoretical fragments (m/z)	591.15	590.14	589.13	588.12	587.11	577.13	576.12	575.15	574.14	573.14
		572.13	571.12	563.15	562.14	561.14	560.13	559.16	558.11	557.14
		556.13	555.12	547.16	546.15	545.14	543.12	541.15	539.13	537.11
		533.14	532.13	531.12	530.15	529.15	528.14	527.13	521.14	519.12
		515.13	513.11	511.13	505.15	504.14	503.13	501.11	489.15	488.14
		487.13	486.13	485.12	477.15	475.13	474.13	473.12	472.11	471.14
		470.13	469.12	468.11	461.16	460.11	459.14	457.12	456.12	455.11
		453.13	452.12	451.11	450.1	445.12	444.11	443.14	442.1	441.09
		440.12	436.12	434.11	433.12	432.09	431.11	429.09	428.12	427.11
		426.1	425.1	424.09	415.11	414.11	413.1	403.11	401.1	400.09
		399.08	398.11	397.1	385.1	384.1	383.09	382.11	373.1	372.09
		371.09	369.07	366.12	364.1	359.1	358.11	357.08	356.1	355.09
		354.08	348.11	346.09	343.09	342.08	341.08	340.1	339.1	338.09
		337.08	336.07	329.11	327.1	326.09	325.08	323.07	315.1	313.12
		311.1	309.09	307.07	299.1	298.09	297.09	283.11	281.09	271.07
		266.06	265.06	263.04	261.02	257.09	255.08	251.08	250.07	249.06
		248.05	247.04	245.03	236.05	235.04	234.06	233.07	231.05	221.06
		220.06	219.05	217.03	215.06	213.04	207.05	206.04	205.06	204.07
		203.02	202.05	201.04	196.06	194.04	193.07	191.06	190.05	189.04
		188.03	187.02	182.08	180.07	179.06	178.05	177.04	175.05	173.04
		171.03	165.05	163.06	161.04	159.03	158.02	157.01	150.05	148.04
		147.03	145.05	143.03	141.02	133.01	131.03	130.03	129.02	127.04
		122.02	121.05	120.04	119.03	117.02	116.01	113.02	105.02	104.01
		103	101.02							
References	<p>Amaya-Cruz Iz, D.M.; Pérez-Ramírez, I.F.; Delgado-García, J.; Mondragón-Jacobo, C.; Dector-Espinoza, A.; Reynoso-Camacho, R. An integral profile of bioactive compounds and functional properties of prickly pear (<i>Opuntia ficus indica</i> L.) peel with different tonalities. <i>Food Chem.</i> 2019, 278, 568–578.</p> <p>Xie, G.R.; Chen, H.J. Comprehensive Betalain Profiling of Djulis (<i>Chenopodium formosanum</i>) Cultivars Using HPLC-Q-Orbitrap High-Resolution Mass Spectrometry. <i>J. Agric. Food Chem.</i> 2021, 69, 15699–15715.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

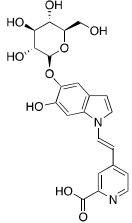
Neohylocerenin

Chemical structure										
Name:	Neohylocerenin									
Chemical Formula	C ₃₀ H ₃₂ N ₂ O ₁₇									
Molecular weight	692.58									
Monoisotopic mass	692.1701									
m/z [M+H]	693.1774									
Theoretical fragments (m/z)	693.18	692.17	691.16	690.15	677.18	676.17	675.17	674.16	673.15	665.18
		664.17	663.17	661.19	660.18	659.17	658.16	657.16	656.15	655.14
		653.18	651.17	650.16	649.19	648.18	647.17	646.16	645.16	643.18
		642.17	641.16	640.15	639.15	637.13	635.17	633.19	631.18	630.17
		629.16	628.15	627.15	625.17	623.17	621.16	620.15	619.18	618.17
		617.16	615.18	614.17	613.17	612.16	611.15	607.18	605.16	604.15
		603.15	602.14	601.17	600.16	599.15	591.18	589.17	587.15	585.14
		573.17	571.16	569.14	567.12	549.14	548.13	547.12	533.14	532.13
		531.12	530.12	529.11	521.14	520.13	519.12	515.13	514.12	513.11
		512.11	511.1	509.14	507.12	505.15	503.13	502.12	501.11	500.14
		499.13	497.12	496.11	495.1	493.09	491.13	489.11	487.13	486.14
		485.13	484.14	483.14	482.13	481.12	479.13	477.11	476.11	474.13
		473.12	471.15	470.14	469.13	468.13	467.12	466.13	464.12	461.12
		459.1	458.1	457.13	456.15	455.14	454.13	453.14	452.13	451.12
		450.12	443.11	441.14	440.13	438.14	429.14	425.14	424.14	423.13
		417.14	415.12	414.12	413.14	412.14	411.13	401.14	399.13	398.12
		397.11	396.11	395.13	394.13	393.12	387.08	386.07	385.07	384.06
		383.13	381.12	379.1	373.1	371.09	370.08	369.07	368.06	367.06
		359.09	358.08	357.11	356.1	355.09	354.08	353.08	352.07	351.09
		347.09	345.07	343.09	342.09	341.08	340.07	339.1	338.09	337.08
		333.07	329.08	327.1	325.08	324.08	323.08	320.08	317.08	315.06
		314.05	313.08	312.07	307.08	306.07	301.08	299.07	298.06	297.1
		294.1	291.11	289.09	285.1	283.07	282.06	279.06	278.05	273.1
		271.08	270.07	268.09	267.09	265.05	263.07	261.05	255.09	253.07
		252.06	251.07	250.08	249.05	247.03	237.08	235.07	233.06	231.04
		221.06	209.06	207.05	206.03	194.04	193.04	192.03	191.06	181.05
		180.04	179.03	178.05	177.04	167.07	165.05	164.05	163.04	150.05
		147.04	146.04	145.05	135.04	134.04	130.04	123.04	119.05	111.04
		109.03	108.02	107.05	106.04					
References	<p>Amaya-Cruz Iz, D.M.; Pérez-Ramírez, I.F.; Delgado-García, J.; Mondragón-Jacobo, C.; Dector-Espinoza, A.; Reynoso-Camacho, R. An integral profile of bioactive compounds and functional properties of prickly pear (<i>Opuntia ficus indica</i> L.) peel with different tonalities. <i>Food Chem.</i> 2019, 278, 568–578.</p> <p>Xie, G.R.; Chen, H.J. Comprehensive Betalain Profiling of Djulis (<i>Chenopodium formosanum</i>) Cultivars Using HPLC-Q-Orbitrap High-Resolution Mass Spectrometry. <i>J. Agric. Food Chem.</i> 2021, 69, 15699–15715.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

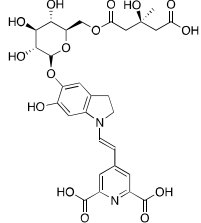
17-decarboxy-neohylocerenin

Chemical structure										
Name:	17-decarboxy-neohylocerenin									
Chemical Formula	C ₂₉ H ₃₂ N ₂ O ₁₅									
Molecular weight	648.57									
Monoisotopic mass	648.1803									
m/z [M+H]	649.1875									
Theoretical fragments (m/z)	649.19	648.18	647.17	646.16	645.16	635.17	634.16	633.16	632.18	631.18
		630.17	629.16	621.19	620.18	619.18	618.17	617.2	616.15	615.18
		614.17	613.17	605.2	604.19	603.18	602.17	601.17	599.19	597.17
		595.16	591.15	590.17	589.17	588.16	587.19	586.18	585.17	583.16
		579.18	577.17	575.15	573.14	571.16	570.15	569.18	567.16	563.15
		561.17	559.16	558.15	556.13	547.16	546.15	545.14	543.16	541.15
		531.12	529.15	527.13	526.16	517.15	515.13	513.11	510.16	508.14
		505.15	504.14	503.13	502.16	501.15	500.14	499.13	498.16	494.17
		492.15	490.13	489.15	487.13	486.16	485.12	484.14	482.13	477.15
		475.13	474.13	473.12	472.11	471.14	469.12	461.16	460.11	459.14
		457.12	456.15	455.11	453.13	451.11	445.12	444.12	443.14	442.1
		441.13	433.12	431.11	430.13	429.14	428.12	427.11	426.11	425.1
		417.14	415.11	414.11	413.1	403.11	401.1	400.09	399.08	397.1
		385.1	384.1	383.09	382.11	373.1	371.09	369.07	366.12	364.1
		358.11	356.1	355.09	354.08	348.11	346.09	343.09	342.08	341.08
		340.1	339.1	338.09	337.08	336.07	329.11	327.1	325.08	324.11
		323.1	321.08	319.07	315.1	313.12	311.1	309.12	308.11	307.1
		306.09	305.09	303.07	299.1	298.09	297.09	294.09	293.09	291.11
		289.09	283.11	281.09	278.1	277.09	275.11	273.1	271.07	265.09
		264.08	263.08	261.06	259.08	257.09	255.08	251.11	249.1	248.09
		247.08	246.07	245.07	243.09	235.08	234.06	233.06	231.09	229.07
		221.06	220.06	219.09	217.07	216.06	215.06	205.06	204.07	203.06
		202.05	201.08	199.06	196.06	194.04	191.06	189.08	188.07	187.06
		182.08	180.07	179.06	178.05	177.08	175.06	174.05	173.04	165.05
		163.06	162.05	161.04	159.07	157.05	150.05	148.04	147.07	146.02
		145.05	144.04	143.03	135.07	134.06	133.05	131.03	129.05	128.05
		127.04	122.02	121.05	120.04	119.03	118.06	117.05	116.05	115.04
		113.02	111.04	109.03	105.02	104.05	103.04	102.03	101.06	100.05
References	<p>Amaya-CruzIz, D.M.; Pérez-Ramírez, I.F.; Delgado-García, J.; Mondragón-Jacobo, C.; Dector-Espinoza, A.; Reynoso-Camacho, R. An integral profile of bioactive compounds and functional properties of prickly pear (<i>Opuntia ficus indica</i> L.) peel with different tonalities. <i>Food Chem.</i> 2019, 278, 568–578.</p> <p>Xie, G.R.; Chen, H.J. Comprehensive Betalain Profiling of Djulis (<i>Chenopodium formosanum</i>) Cultivars Using HPLC-Q-Orbitrap High-Resolution Mass Spectrometry. <i>J. Agric. Food Chem.</i> 2021, 69, 15699–15715.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

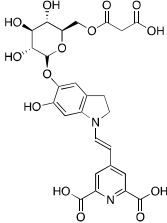
2,17-bidecarboxy-2,3-dehydro-neobetatin

Chemical structure										
Name:	2,17-bidecarboxy-2,3-dehydro-neobetatin									
Chemical Formula	C ₂₂ H ₂₂ N ₂ O ₉									
Molecular weight	458.42									
Monoisotopic mass	458.1325									
m/z [M+H]	459.1398									
Theoretical fragments (m/z)	459.14	458.13	443.14	442.14	441.13	440.12	433.12	432.12	431.14	425.13
		424.13	423.12	422.11	417.13	416.12	415.15	414.14	413.13	411.12
		407.12	406.12	405.11	404.1	400.13	399.12	398.11	397.14	396.13
		395.12	393.11	389.13	388.11	387.12	384.1	382.12	381.11	380.14
		379.13	378.12	377.11	373.14	371.12	369.11	368.1	362.13	361.12
		360.11	359.1	355.09	353.11	326.09	325.08	323.1	310.09	309.09
		298.09	297.09	296.08	295.07	292.08	283.11	282.1	281.09	280.08
		279.08	271.08	270.07	269.09	266.1	265.1	264.09	263.08	262.08
		257.09	256.08	255.08	254.07	253.1	252.06	251.08	241.1	240.09
		239.08	238.07	237.08	236.09	235.06	234.05	227.08	226.07	225.07
		224.09	221.11	216.04	213.1	212.09	211.09	210.08	197.11	195.09
		189.07	176.06	165.07	164.06	163.05	162.04	159.06	150.05	149.05
		148.04	147.07	146.06	145.08	136.04	134.06	132.04	122.02	121.08
		120.06	119.05	118.04	109.03	108.02	107.05	106.03	105.02	104.05
		102.05								
References	<p>Amaya-Cruz Iz, D.M.; Pérez-Ramírez, I.F.; Delgado-García, J.; Mondragón-Jacobo, C.; Dector-Espinoza, A.; Reynoso-Camacho, R. An integral profile of bioactive compounds and functional properties of prickly pear (<i>Opuntia ficus indica</i> L.) peel with different tonalities. <i>Food Chem.</i> 2019, 278, 568–578.</p> <p>Xie, G.R.; Chen, H.J. Comprehensive Betalain Profiling of Djulis (<i>Chenopodium formosanum</i>) Cultivars Using HPLC-Q-Orbitrap High-Resolution Mass Spectrometry. <i>J. Agric. Food Chem.</i> 2021, 69, 15699–15715.</p> <p>Slimen, I.B.; Najjar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

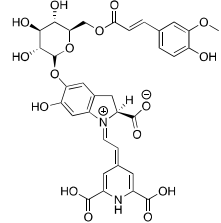
2-decarboxy-neohylocerenin

Chemical structure										
Name:	2-decarboxy-neohylocerenin									
Chemical Formula	C ₂₉ H ₃₂ N ₂ O ₁₅									
Molecular weight	648.57									
Monoisotopic mass	648.1803									
m/z [M+H]	649.1875									
Theoretical fragments (m/z)	649.19	648.18	647.17	646.16	645.16	635.17	634.16	633.16	632.18	631.18
		630.17	629.16	623.17	621.19	620.15	619.18	618.17	617.2	616.19
		615.18	614.17	613.17	607.18	605.2	604.19	603.18	602.17	601.17
		600.16	599.19	597.17	595.16	591.15	589.17	588.16	587.19	585.17
		583.16	575.15	573.14	571.16	570.15	569.18	567.16	563.15	561.14
		559.16	558.15	556.13	547.16	546.15	545.14	543.16	541.15	531.12
		529.15	527.13	517.15	513.11	505.15	504.14	503.13	491.13	489.15
		488.14	487.13	486.13	485.12	482.17	479.13	477.11	475.13	474.13
		473.12	472.11	471.14	470.13	469.12	467.11	466.17	464.16	461.16
		460.11	459.1	458.17	457.12	456.15	455.14	454.13	453.13	451.11
		450.18	448.16	446.14	445.12	444.12	443.14	442.17	441.14	440.16
		438.14	432.15	431.11	430.13	429.14	428.16	427.11	426.11	425.1
		424.16	423.13	422.14	420.13	417.14	415.11	414.11	413.1	412.14
		411.13	409.1	403.11	401.1	400.09	399.08	397.1	385.1	384.1
		383.09	373.1	371.09	369.07	355.09	354.08	343.09	342.08	341.08
		338.12	329.11	327.1	326.09	325.08	324.11	323.1	322.09	321.08
		320.11	319.07	317.08	315.06	314.12	313.08	312.11	311.1	309.12
		308.11	307.1	306.09	305.09	303.07	302.1	301.08	300.11	299.1
		298.06	297.1	296.11	295.1	294.1	293.09	291.11	289.09	287.08
		286.09	285.1	283.07	282.1	279.09	278.1	277.09	276.09	275.11
		273.1	271.08	268.08	267.09	265.09	264.08	263.08	261.06	259.08
		257.1	255.09	253.07	251.11	249.1	248.09	247.08	246.07	245.07
		243.09	235.08	234.06	233.06	231.09	229.07	221.06	220.05	219.09
		217.07	216.06	215.06	209.06	205.07	203.06	201.08	199.06	194.04
		192.03	191.06	189.08	188.07	187.06	179.06	177.08	176.07	175.06
		174.05	173.04	166.01	165.08	163.06	162.05	161.04	159.07	157.05
		152.07	151.06	150.05	149.04	147.07	146.02	145.05	144.04	143.03
		138.09	136.08	135.07	134.06	133.05	132.04	131.03	129.05	128.05
		127.04	126.03	124.04	123.04	122.06	121.06	120.04	119.03	118.06
		117.05	116.05	115.04	113.02	111.04	110.06	109.03	108.04	107.05
		105.02	104.05	103.04	102.03	101.06	100.05			
References	<p>Amaya-Cruz Iz, D.M.; Pérez-Ramírez, I.F.; Delgado-García, J.; Mondragón-Jacobo, C.; Dector-Espinoza, A.; Reynoso-Camacho, R. An integral profile of bioactive compounds and functional properties of prickly pear (<i>Opuntia ficus indica</i> L.) peel with different tonalities. <i>Food Chem.</i> 2019, 278, 568–578.</p> <p>Xie, G.R.; Chen, H.J. Comprehensive Betalain Profiling of Djulis (<i>Chenopodium formosanum</i>) Cultivars Using HPLC-Q-Orbitrap High-Resolution Mass Spectrometry. <i>J. Agric. Food Chem.</i> 2021, 69, 15699–15715.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

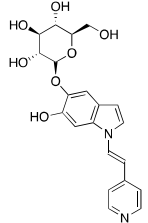
2-decarboxy-neophyllocactin

Chemical structure										
Name:	2-decarboxy-neophyllocactin									
Chemical Formula	C ₂₆ H ₂₆ N ₂ O ₁₄									
Molecular weight	590.49									
Monoisotopic mass	590.1384									
m/z [M+H]	591.1457									
Theoretical fragments (m/z)	591.15	590.14	589.13	588.12	587.11	577.13	576.12	575.15	574.14	573.14
		572.13	571.12	565.13	563.15	562.11	561.14	560.13	559.16	558.15
		557.14	556.13	555.12	554.12	553.11	549.14	547.16	546.15	545.14
		544.13	543.12	542.12	541.15	539.13	537.11	531.12	530.15	529.15
		528.14	527.13	517.11	513.11	511.13	505.15	504.14	503.13	502.12
		501.11	491.13	489.15	488.14	487.13	486.13	485.12	484.11	479.13
		477.11	475.13	474.13	473.12	472.11	471.14	470.13	469.12	467.11
		463.13	461.16	460.11	459.1	458.1	457.12	456.12	455.11	453.13
		451.11	449.12	447.1	445.12	444.12	443.14	442.1	441.09	439.11
		433.12	431.11	430.1	429.09	427.11	426.11	425.1	424.12	419.11
		415.11	414.11	413.1	411.12	409.1	408.13	406.11	403.11	401.1
		400.12	399.08	398.11	397.1	396.09	395.09	390.12	389.1	388.1
		386.11	385.1	384.13	383.09	382.11	380.1	379.09	374.11	373.1
		372.09	371.09	370.11	369.07	368.1	367.1	366.12	365.09	364.1
		362.09	359.1	357.08	356.07	355.09	354.08	353.09	343.09	342.08
		341.08	338.12	329.11	327.1	326.09	325.08	324.07	320.11	317.08
		315.06	314.12	313.08	312.11	311.1	302.1	301.08	300.11	299.1
		298.06	297.1	296.11	294.1	286.09	285.1	283.07	282.1	279.09
		278.1	276.09	273.1	268.08	267.09	266.06	265.06	264.05	263.04
		261.02	255.09	251.08	250.07	249.06	248.05	247.04	245.03	237.06
		236.05	235.04	234.06	233.07	232.06	231.05	230.04	229.03	225.06
		221.06	220.06	219.05	218.04	217.03	215.06	213.04	209.06	207.05
		206.04	205.03	204.06	203.02	202.05	201.04	197.04	195.03	194.04
		193.07	192.03	191.06	190.05	189.04	188.03	187.02	180.06	179.06
		177.04	176.07	175.06	174.05	173.04	172.04	171.03	170.02	169.01
		166.01	165.08	163.06	162.05	161.04	160.04	159.03	158.02	157.01
		155.03	153.02	152.07	151.06	150.05	149.04	147.03	145.05	143.03
		141.02	138.09	136.08	135.04	134.06	133.01	132.04	131.03	130.03
		129.02	127.04	125.02	124.04	123.04	122.06	121.06	120.04	119.03
		118.03	117.02	116.01	115	113.02	111.04	110.06	108.04	107.05
		105.02	104.01	103	102.03	101.02	100.02			
References	<p>Amaya-Cruz Iz, D.M.; Pérez-Ramírez, I.F.; Delgado-García, J.; Mondragón-Jacobo, C.; Dector-Espinoza, A.; Reynoso-Camacho, R. An integral profile of bioactive compounds and functional properties of prickly pear (<i>Opuntia ficus indica</i> L.) peel with different tonalities. <i>Food Chem.</i> 2019, 278, 568–578.</p> <p>Xie, G.R.; Chen, H.J. Comprehensive Betalain Profiling of Djulis (<i>Chenopodium formosanum</i>) Cultivars Using HPLC-Q-Orbitrap High-Resolution Mass Spectrometry. <i>J. Agric. Food Chem.</i> 2021, 69, 15699–15715.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

Neolampranthin II

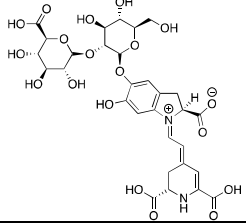
Chemical structure										
Name:	Neolampranthin II									
Chemical Formula	C ₃₄ H ₃₂ N ₂ O ₁₆									
Molecular weight	724.63									
Monoisotopic mass	724.1752									
m/z [M+H]	725.1825									
Theoretical fragments (m/z)	725.18	724.17	723.17	722.16	709.19	708.18	707.17	706.16	705.16	697.19
	696.18	695.17	693.19	692.18	691.18	690.17	689.16	688.15	687.15	
	685.19	683.17	682.16	681.19	680.18	679.18	678.17	677.16	673.17	
	672.16	671.15	669.14	667.18	666.17	665.16	664.19	663.18	662.17	
	661.17	660.16	659.15	655.18	653.16	652.15	650.17	649.17	647.19	
	645.17	644.16	643.16	637.17	636.16	635.15	634.14	632.16	631.16	
	619.16	617.14	609.17	601.15	545.15	544.14	543.14	532.14	531.12	
	530.12	529.11	528.15	527.14	526.13	519.15	518.14	517.13	516.15	
	515.13	514.13	513.11	512.11	511.1	510.14	503.13	502.12	501.14	
	500.13	499.12	498.14	497.12	496.11	495.1	493.09	491.13	489.14	
	488.16	487.15	486.14	485.12	484.11	483.13	482.12	479.11	477.09	
	475.12	474.14	473.14	472.14	471.14	470.14	469.12	468.12	467.11	
	461.14	459.1	458.1	456.14	455.13	452.13	451.11	449.14	447.13	
	446.12	444.14	443.13	441.09	431.13	430.13	429.12	428.11	426.13	
	425.12	423.08	417.09	415.08	413.12	411.11	387.08	386.07	385.07	
	384.06	373.1	371.09	370.08	369.07	368.06	367.06	359.09	358.08	
	357.11	356.1	355.09	354.08	353.08	352.07	351.09	350.09	347.09	
	345.07	343.09	342.08	341.08	340.07	339.1	338.09	337.08	336.07	
	334.09	333.07	329.08	327.1	326.09	325.08	324.08	323.08	322.09	
	321.1	320.08	319.07	317.08	315.06	314.05	313.08	312.07	311.1	
	307.08	306.07	302.07	301.08	299.07	298.06	294.1	293.09	285.09	
	283.07	282.06	279.06	278.05	277.05	276.09	267.09	265.05	264.04	
	263.07	262.06	261.05	255.09	253.07	252.06	251.07	250.08	249.05	
	247.03	237.08	235.07	233.06	231.04	221.06	209.06	207.05	206.03	
	194.04	193.04	192.03	191.06	190.05	181.05	180.04	179.03	178.05	
	177.04	176.03	167.07	165.05	164.05	163.04	162.05	150.05	149.05	
	148.04	147.04	146.04	145.05	136.08	135.04	134.04	132.04	130.04	
	123.04	119.05	111.04	109.03	108.02	107.05	106.04			
References	<p>Amaya-CruzIz, D.M.; Pérez-Ramírez, I.F.; Delgado-García, J.; Mondragón-Jacobo, C.; Dector-Espinoza, A.; Reynoso-Camacho, R. An integral profile of bioactive compounds and functional properties of prickly pear (<i>Opuntia ficus indica</i> L.) peel with different tonalities. <i>Food Chem.</i> 2019, 278, 568–578.</p> <p>Xie, G.R.; Chen, H.J. Comprehensive Betalain Profiling of Djulis (<i>Chenopodium formosanum</i>) Cultivars Using HPLC-Q-Orbitrap High-Resolution Mass Spectrometry. <i>J. Agric. Food Chem.</i> 2021, 69, 15699–15715.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

Dehydrogenated tridecarboxy-neobetanin

Chemical structure										
Name:	Dehydrogenated tridecarboxy-neobetanin									
Chemical Formula	C ₂₁ H ₂₂ N ₂ O ₇									
Molecular weight	414.41									
Monoisotopic mass	414.1427									
m/z [M+H]	415.1499									
Theoretical fragments (m/z)	415.15	414.14	413.13	412.13	411.12	410.11	399.16	398.15	397.14	396.13
	395.12	394.12	393.11	389.13	388.13	387.16	385.14	384.13	383.12	
	382.12	381.11	380.14	379.13	378.12	377.11	373.14	371.12	370.12	
	369.14	368.1	367.13	366.12	365.11	364.11	363.1	361.12	359.12	
	357.11	355.13	354.12	353.11	352.11	351.1	349.12	348.11	347.1	
	343.13	342.12	341.11	340.11	339.1	338.09	337.12	336.11	335.1	
	329.11	327.13	325.12	324.11	323.1	322.09	321.09	319.11	318.1	
	317.09	313.12	312.11	311.1	310.09	309.09	308.08	307.11	306.1	
	305.09	300.09	299.1	296.09	295.11	294.1	293.09	292.08	291.08	
	286.09	285.1	283.11	282.08	281.09	280.08	279.08	277.1	276.09	
	275.08	273.1	271.08	270.07	267.11	265.1	264.09	255.09	254.08	
	253.1	252.09	251.08	239.12	237.1	236.09	235.09	234.08	227.08	
	226.07	223.12	221.11	220.1	213.1	211.09	210.08	197.11	195.09	
	180.06	179.06	178.05	177.04	175.02	174.05	165.08	164.07	163.06	
	162.05	161.04	160.04	159.03	151.06	150.05	149.05	148.04	147.07	
	146.06	145.05	144.04	143.03	139.06	137.08	136.08	135.07	134.06	
	133.05	132.07	131.03	130.03	129.05	127.04	122.06	121.05	120.04	
	119.03	118.03	117.02	116.05	115.04	114.03	113.02	110.06	109.03	
	108.02	107.07	105.05	104.05	103.04	102.03	101.02	100.02		
References	<p>Amaya-CruzIz, D.M.; Pérez-Ramírez, I.F.; Delgado-García, J.; Mondragón-Jacobo, C.; Dector-Espinoza, A.; Reynoso-Camacho, R. An integral profile of bioactive compounds and functional properties of prickly pear (<i>Opuntia ficus indica</i> L.) peel with different tonalities. <i>Food Chem.</i> 2019, 278, 568–578.</p> <p>Xie, G.R.; Chen, H.J. Comprehensive Betalain Profiling of Djulis (<i>Chenopodium formosanum</i>) Cultivars Using HPLC-Q-Orbitrap High-Resolution Mass Spectrometry. <i>J. Agric. Food Chem.</i> 2021, 69, 15699–15715.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

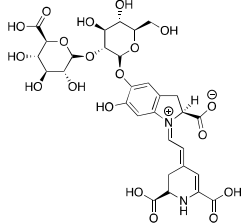
Amaranthin-type

Amaranthin

Chemical structure										
Name:	Amaranthin									
Chemical Formula	C ₃₀ H ₃₄ N ₂ O ₁₉									
Molecular weight	726.60									
Monoisotopic mass	726.1756									
m/z [M+H]	727.1829									
Theoretical fragments (m/z)	727.18	726.18	725.17	724.16	711.19	710.18	709.17	708.16	707.16	699.19
		698.18	697.17	695.19	694.19	693.18	692.17	691.16	690.15	689.15
		687.19	685.17	683.19	682.19	681.18	680.17	679.16	677.18	676.17
		675.17	674.16	673.15	671.14	669.18	667.2	665.18	664.17	663.17
		662.16	661.15	659.17	657.18	655.16	654.15	653.18	652.17	651.17
		649.19	648.18	647.17	646.16	645.16	641.18	639.17	638.16	637.15
		636.14	635.17	634.16	633.16	625.19	623.17	621.16	619.14	607.18
		605.16	603.15	601.13	558.15	551.15	550.14	549.14	545.14	535.16
		534.15	533.14	532.13	531.12	523.16	522.15	521.14	519.16	518.13
		517.15	516.13	515.13	514.12	513.11	511.16	509.14	507.16	505.15
		504.14	503.13	502.13	501.12	500.12	499.13	498.13	497.12	495.1
		493.15	491.13	489.15	488.14	487.13	486.12	485.13	484.12	483.11
		482.11	481.15	479.13	478.12	477.15	476.14	475.13	473.13	472.12
		471.14	470.13	469.12	465.15	463.13	462.12	461.13	460.11	459.14
		458.13	457.13	456.13	455.12	449.13	447.11	446.11	445.13	444.13
		443.12	433.13	431.12	430.11	429.1	428.09	427.12	426.12	425.11
		415.12	413.11	411.09	389.1	388.09	387.08	386.07	375.12	373.1
		372.1	371.09	370.08	369.07	361.1	360.1	359.12	358.11	357.11
		356.1	355.09	354.08	353.08	351.06	349.1	347.09	345.11	343.13
		342.09	341.11	340.1	339.1	338.09	337.08	335.09	331.09	329.11
		327.1	326.09	325.09	324.08	323.08	319.09	317.08	316.07	315.1
		314.09	313.08	307.08	306.07	303.1	301.08	300.07	299.07	298.06
		297.1	287.1	285.1	284.08	283.07	282.06	281.08	280.07	279.09
		273.1	271.08	270.07	269.09	268.09	267.06	265.08	264.07	263.07
		262.06	255.09	253.08	252.06	251.07	250.08	249.05	247.07	245.06
		237.09	235.07	233.06	231.04	223.07	211.07	207.08	205.06	196.06
		194.04	193.04	182.08	180.04	179.03	178.05	177.04	165.05	164.05
		163.04	147.04	146.04	135.04	134.04	130.04	123.04	119.05	111.04
		109.03	108.02	107.05	106.04					
References	<p>Piattelli, M.; Minale, L. Pigments of centrospermae—I. <i>Phytochemistry</i>, 1964, 3, 307-311.</p> <p>Minale, L.; Piattelli, M.; de Stefano, S.; Nicolaus, R.A. Pigments of Centrospermae VI. Acylated betacyanins. <i>Phytochemistry</i> 1966, 5, 1037–1052.</p> <p>Cai, Y.; Sun, M.; Corke, H. Identification and Distribution of Simple and Acylated Betacyanins in the Amaranthaceae. <i>J. Agric. Food Chem.</i> 2001, 49, 1971–1978.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p> <p>Miguel, M.G. Betalains in Some Species of the Amaranthaceae Family: A Review. <i>Antioxidants</i> 2018, 7, 53.</p> <p>Xie, G.R.; Chen, H.J. Comprehensive Betalain Profiling of Djulis (<i>Chenopodium formosanum</i>) Cultivars Using HPLC-Q-Orbitrap High-Resolution Mass Spectrometry. <i>J. Agric. Food Chem.</i> 2021, 69, 15699–15715.</p>									

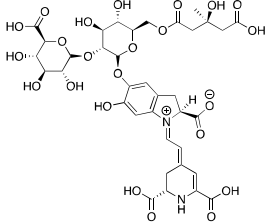
	Araujo-León, J.A.; Aguilar-Hernández, V.; Sánchez-del Pino, I.; Brito-Argáez, L.; Peraza-Sánchez, S.R.; Xingú-López, A.; Ortiz-Andrade, R. Analysis of Red Amaranth (<i>Amaranthus cruentus</i> L.) Betalains by LC-MS. <i>J. Mex. Chem. Soc.</i> 2023 , 67, 227–239.
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Isoamaranthin

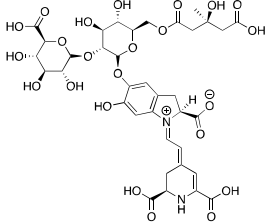
Chemical structure										
Name:	Isoamaranthin									
Chemical Formula	C ₃₀ H ₃₄ N ₂ O ₁₉									
Molecular weight	726.60									
Monoisotopic mass	726.1756									
m/z [M+H]	727.1829									
Theoretical fragments (m/z)	727.18	726.18	725.17	724.16	711.19	710.18	709.17	708.16	707.16	699.19
		698.18	697.17	695.19	694.19	693.18	692.17	691.16	690.15	689.15
		687.19	685.17	683.19	682.19	681.18	680.17	679.16	677.18	676.17
		675.17	674.16	673.15	671.14	669.18	667.2	665.18	664.17	663.17
		662.16	661.15	659.17	657.18	655.16	654.15	653.18	652.17	651.17
		649.19	648.18	647.17	646.16	645.16	641.18	639.17	638.16	637.15
		636.14	635.17	634.16	633.16	625.19	623.17	621.16	619.14	607.18
		605.16	603.15	601.13	558.15	551.15	550.14	549.14	545.14	535.16
		534.15	533.14	532.13	531.12	523.16	522.15	521.14	519.16	518.13
		517.15	516.13	515.13	514.12	513.11	511.16	509.14	507.16	505.15
		504.14	503.13	502.13	501.12	500.12	499.13	498.13	497.12	495.1
		493.15	491.13	489.15	488.14	487.13	486.12	485.13	484.12	483.11
		482.11	481.15	479.13	478.12	477.15	476.14	475.13	473.13	472.12
		471.14	470.13	469.12	465.15	463.13	462.12	461.13	460.11	459.14
		458.13	457.13	456.13	455.12	449.13	447.11	446.11	445.13	444.13
		443.12	433.13	431.12	430.11	429.1	428.09	427.12	426.12	425.11
		415.12	413.11	411.09	389.1	388.09	387.08	386.07	375.12	373.1
		372.1	371.09	370.08	369.07	361.1	360.1	359.12	358.11	357.11
		356.1	355.09	354.08	353.08	351.06	349.1	347.09	345.11	343.13
		342.09	341.11	340.1	339.1	338.09	337.08	335.09	331.09	329.11
		327.1	326.09	325.09	324.08	323.08	319.09	317.08	316.07	315.1
		314.09	313.08	307.08	306.07	303.1	301.08	300.07	299.07	298.06
		297.1	287.1	285.1	284.08	283.07	282.06	281.08	280.07	279.09
		273.1	271.08	270.07	269.09	268.09	267.06	265.08	264.07	263.07
		262.06	255.09	253.08	252.06	251.07	250.08	249.05	247.07	245.06
		237.09	235.07	233.06	231.04	223.07	211.07	207.08	205.06	196.06
		194.04	193.04	182.08	180.04	179.03	178.05	177.04	165.05	164.05
		163.04	147.04	146.04	135.04	134.04	130.04	123.04	119.05	111.04
		109.03	108.02	107.05	106.04					
References	<p>Piattelli, M.; Minale, L. Pigments of centrospermae—I. <i>Phytochemistry</i>, 1964, 3, 307-311.</p> <p>Minale, L.; Piattelli, M.; de Stefano, S.; Nicolaus, R.A. Pigments of Centrospermae VI. Acylated betacyanins. <i>Phytochemistry</i> 1966, 5, 1037-1052.</p> <p>Cai, Y.; Sun, M.; Corke, H. Identification and Distribution of Simple and Acylated Betacyanins in the Amaranthaceae. <i>J. Agric. Food Chem.</i> 2001, 49, 1971-1978.</p> <p>Slimen, I.B.; Najjar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675-689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315-2346.</p> <p>Miguel, M.G. Betalains in Some Species of the Amaranthaceae Family: A Review. <i>Antioxidants</i> 2018, 7, 53.</p> <p>Xie, G.R.; Chen, H.J. Comprehensive Betalain Profiling of Djulis (<i>Chenopodium formosanum</i>) Cultivars Using HPLC-Q-Orbitrap High-Resolution Mass Spectrometry. <i>J. Agric. Food Chem.</i> 2021, 69, 15699-15715.</p> <p>Araujo-León, J.A.; Aguilar-Hernández, V.; Sánchez-del Pino, I.; Brito-Argáez, L.; Peraza-Sánchez, S.R.; Xingú-López, A.; Ortiz-Andrade, R. Analysis of Red Amaranth (<i>Amaranthus</i></p>									

	<i>cruentus</i> L.) Betalains by LC-MS. <i>J. Mex. Chem. Soc.</i> 2023 , 67, 227–239.
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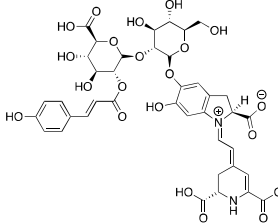
Iresinin I

Chemical structure										
Name:	Iresinin I									
Chemical Formula	C ₃₆ H ₄₂ N ₂ O ₂₃									
Molecular weight	870.72									
Monoisotopic mass	870.2178									
m/z [M+H]	871.2251									
Theoretical fragments (m/z)	871.23	870.22	869.21	868.2	855.23	854.22	853.21	852.21	851.2	843.23
		842.22	841.21	839.24	837.22	836.21	835.2	833.19	831.23	829.21
		827.24	826.23	825.22	824.21	823.2	821.22	819.21	817.19	813.22
		811.24	809.22	808.22	807.21	801.22	799.2	798.2	797.22	796.22
		795.21	785.22	783.21	782.2	781.19	767.21	765.2	763.18	727.18
		726.18	725.17	711.19	709.17	708.16	707.16	702.19	699.19	697.17
		695.19	694.19	693.18	691.16	689.15	683.19	681.18	679.2	678.19
		677.18	676.17	675.16	673.15	669.18	667.2	665.18	663.2	662.17
		661.19	660.18	659.17	658.16	657.16	655.16	651.17	649.19	647.17
		646.17	645.17	644.16	643.18	641.16	639.17	637.15	633.19	632.18
		631.18	630.17	629.17	628.16	627.16	626.15	625.19	623.17	621.16
		619.18	617.17	616.16	607.18	606.17	605.17	601.18	600.17	599.16
		593.17	591.16	590.15	589.18	588.17	587.16	577.18	575.16	574.15
		573.15	572.14	571.17	570.16	569.15	561.18	559.17	557.15	551.15
		549.14	535.16	534.15	533.14	532.13	531.12	518.13	517.15	516.13
		515.13	514.12	513.11	502.16	501.12	500.12	499.13	497.12	486.14
		485.13	484.14	483.11	482.13	481.12	479.13	473.13	470.14	469.13
		468.13	467.12	461.13	455.12	452.13	451.12	450.12	449.13	447.11
		446.11	445.13	444.13	443.12	441.14	433.13	431.12	429.14	428.09
		427.12	426.12	425.11	423.13	417.14	415.12	414.12	413.14	412.14
		411.13	401.14	399.13	397.11	396.11	395.13	394.13	393.12	389.1
		388.09	387.08	386.07	383.13	381.12	375.12	373.1	372.1	371.09
		370.08	369.07	361.1	360.1	359.12	357.11	356.1	355.09	354.08
		353.08	351.06	349.1	347.09	345.11	343.13	342.08	341.11	339.1
		337.08	335.09	331.09	329.11	327.1	326.09	325.08	324.08	319.09
		317.08	316.07	315.1	314.09	313.08	306.07	303.1	301.08	300.07
		299.07	287.1	285.09	284.08	283.07	281.08	280.07	273.1	271.11
		269.09	267.06	265.08	264.07	263.07	262.06	255.09	253.08	251.07
		249.05	247.07	245.06	237.09	235.07	233.06	231.04	223.07	211.07
		207.08	205.06	196.06	194.04	193.04	182.08	180.04	179.03	178.05
		177.04	165.05	164.05	163.04	147.04	146.04	135.04	134.04	130.04
		123.04	119.05	111.04	109.03	108.02	107.05	106.04		
References	<p>Minale, L.; Piattelli, M.; de Stefano, S.; Nicolaus, R.A. Pigments of Centrospermae VI. Acylated betacyanins. <i>Phytochemistry</i> 1966, 5, 1037–1052.</p> <p>Cai, Y.; Sun, M.; Corke, H. Identification and Distribution of Simple and Acylated Betacyanins in the Amaranthaceae. <i>J. Agric. Food Chem.</i> 2001, 49, 1971–1978.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

Isoiresinin I

Chemical structure										
Name:	Isoiresinin I									
Chemical Formula	C ₃₆ H ₄₂ N ₂ O ₂₃									
Molecular weight	870.72									
Monoisotopic mass	870.2178									
m/z [M+H]	871.2251									
Theoretical fragments (m/z)	871.23	870.22	869.21	868.2	855.23	854.22	853.21	852.21	851.2	843.23
		842.22	841.21	839.24	837.22	836.21	835.2	833.19	831.23	829.21
		827.24	826.23	825.22	824.21	823.2	821.22	819.21	817.19	813.22
		811.24	809.22	808.22	807.21	801.22	799.2	798.2	797.22	796.22
		795.21	785.22	783.21	782.2	781.19	767.21	765.2	763.18	727.18
		726.18	725.17	711.19	709.17	708.16	707.16	702.19	699.19	697.17
		695.19	694.19	693.18	691.16	689.15	683.19	681.18	679.2	678.19
		677.18	676.17	675.16	673.15	669.18	667.2	665.18	663.2	662.17
		661.19	660.18	659.17	658.16	657.16	655.16	651.17	649.19	647.17
		646.17	645.17	644.16	643.18	641.16	639.17	637.15	633.19	632.18
		631.18	630.17	629.17	628.16	627.16	626.15	625.19	623.17	621.16
		619.18	617.17	616.16	607.18	606.17	605.17	601.18	600.17	599.16
		593.17	591.16	590.15	589.18	588.17	587.16	577.18	575.16	574.15
		573.15	572.14	571.17	570.16	569.15	561.18	559.17	557.15	551.15
		549.14	535.16	534.15	533.14	532.13	531.12	518.13	517.15	516.13
		515.13	514.12	513.11	502.16	501.12	500.12	499.13	497.12	486.14
		485.13	484.14	483.11	482.13	481.12	479.13	473.13	470.14	469.13
		468.13	467.12	461.13	455.12	452.13	451.12	450.12	449.13	447.11
		446.11	445.13	444.13	443.12	441.14	433.13	431.12	429.14	428.09
		427.12	426.12	425.11	423.13	417.14	415.12	414.12	413.14	412.14
		411.13	401.14	399.13	397.11	396.11	395.13	394.13	393.12	389.1
		388.09	387.08	386.07	383.13	381.12	375.12	373.1	372.1	371.09
		370.08	369.07	361.1	360.1	359.12	357.11	356.1	355.09	354.08
		353.08	351.06	349.1	347.09	345.11	343.13	342.08	341.11	339.1
		337.08	335.09	331.09	329.11	327.1	326.09	325.08	324.08	319.09
		317.08	316.07	315.1	314.09	313.08	306.07	303.1	301.08	300.07
		299.07	287.1	285.09	284.08	283.07	281.08	280.07	273.1	271.11
		269.09	267.06	265.08	264.07	263.07	262.06	255.09	253.08	251.07
		249.05	247.07	245.06	237.09	235.07	233.06	231.04	223.07	211.07
		207.08	205.06	196.06	194.04	193.04	182.08	180.04	179.03	178.05
		177.04	165.05	164.05	163.04	147.04	146.04	135.04	134.04	130.04
		123.04	119.05	111.04	109.03	108.02	107.05	106.04		
References	<p>Minale, L.; Piattelli, M.; de Stefano, S.; Nicolaus, R.A. Pigments of Centrospermae VI. Acylated betacyanins. <i>Phytochemistry</i> 1966, 5, 1037–1052.</p> <p>Cai, Y.; Sun, M.; Corke, H. Identification and Distribution of Simple and Acylated Betacyanins in the Amaranthaceae. <i>J. Agric. Food Chem.</i> 2001, 49, 1971–1978.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

Celosianin I

Chemical structure										
Name:	Celosianin I (argentianin)									
Chemical Formula	C ₃₉ H ₄₀ N ₂ O ₂₁									
Molecular weight	872.74									
Monoisotopic mass	872.2129									
m/z [M+H]	873.2196									
Theoretical fragments (m/z)	873.22	872.21	871.2	870.2	857.22	856.22	855.21	854.2	853.19	845.22
		844.22	843.21	841.23	840.22	839.21	838.21	837.2	836.19	835.18
		833.22	831.21	829.23	828.22	827.21	826.21	825.2	823.22	822.21
		821.2	820.2	819.19	817.17	815.21	813.23	811.22	810.21	809.2
		808.2	807.19	805.21	803.21	801.2	800.19	799.22	798.21	797.2
		795.22	794.22	793.21	792.2	791.19	787.22	785.2	784.2	783.19
		782.18	781.21	780.2	779.19	771.22	769.21	767.19	765.18	753.21
		751.2	749.18	747.17	709.17	708.16	707.16	704.18	693.18	692.17
		691.16	690.15	689.15	681.18	680.18	679.16	678.17	677.16	675.17
		673.15	671.14	665.18	664.16	663.16	662.17	661.16	660.16	659.15
		657.16	655.14	651.17	648.17	647.16	646.15	645.15	639.17	637.15
		635.16	634.18	633.17	632.16	631.17	630.16	629.15	628.14	623.17
		621.16	619.17	618.16	608.16	607.17	605.16	603.17	602.16	601.16
		595.17	593.15	592.14	591.17	590.16	589.16	579.17	577.16	576.15
		575.14	574.13	573.16	572.15	571.14	561.16	559.14	557.13	551.15
		550.14	549.14	535.16	534.15	533.14	532.13	531.12	523.16	522.15
		521.14	519.16	517.15	516.13	515.13	514.12	513.11	511.16	509.14
		507.16	505.15	504.14	503.13	501.15	500.12	499.13	498.13	497.12
		495.1	493.15	491.13	489.15	488.14	487.13	486.13	485.12	484.12
		483.11	482.11	481.15	479.13	478.12	477.15	476.14	475.13	471.14
		470.13	469.12	465.15	463.13	461.12	460.11	459.14	458.13	457.12
		455.12	447.14	445.12	443.12	431.12	429.1	428.09	427.12	426.12
		425.11	415.12	413.11	411.09	389.1	388.09	387.08	386.07	375.12
		373.1	372.1	371.09	370.08	369.07	361.1	360.1	359.12	358.11
		357.11	356.1	355.09	354.08	353.08	351.06	349.1	347.09	345.11
		343.13	342.09	341.11	340.1	339.1	338.09	337.08	335.09	331.09
		329.11	327.1	326.09	325.09	324.08	323.08	319.09	317.08	316.07
		315.1	314.09	313.08	307.08	306.07	303.1	301.08	300.07	299.07
		298.06	297.1	287.1	285.1	284.08	283.07	282.06	281.08	280.07
		279.09	273.1	271.08	270.07	269.09	268.09	267.06	265.08	264.07
		263.07	262.06	255.09	253.08	252.06	251.07	250.08	249.05	247.07
		245.06	237.09	235.07	233.06	231.04	223.07	211.07	207.08	205.06
		196.06	194.04	193.04	182.08	180.04	179.03	178.05	177.04	165.05
		164.05	163.04	147.04	146.04	135.04	134.04	130.04	123.04	119.05
		111.04	109.03	108.02	107.05	106.04				
References	<p>Cai, Y.; Sun, M.; Corke, H. Identification and Distribution of Simple and Acylated Betacyanins in the Amaranthaceae. <i>J. Agric. Food Chem.</i> 2001, 49, 1971–1978.</p> <p>Spórna-Kucab, A.; Wróbel, N.; Kumorkiewicz-Jamro, A.; Wybraniec, S. Separation of betacyanins from <i>Iresine herbstii</i> Hook. ex Lindl. leaves by high-speed countercurrent chromatography in a polar solvent system. <i>J. Chromatogr. A</i> 2020, 1626, 461370.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

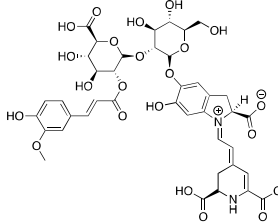
Isocelosianin I

Chemical structure										
Name:	Isocelosianin I (isoargentianin)									
Chemical Formula	C ₃₉ H ₄₀ N ₂ O ₂₁									
Molecular weight	872.74									
Monoisotopic mass	872.2124									
m/z [M+H]	873.2196									
Theoretical fragments (m/z)	873.22	872.21	871.2	870.2	857.22	856.22	855.21	854.2	853.19	845.22
		844.22	843.21	841.23	840.22	839.21	838.21	837.2	836.19	835.18
		833.22	831.21	829.23	828.22	827.21	826.21	825.2	823.22	822.21
		821.2	820.2	819.19	817.17	815.21	813.23	811.22	810.21	809.2
		808.2	807.19	805.21	803.21	801.2	800.19	799.22	798.21	797.2
		795.22	794.22	793.21	792.2	791.19	787.22	785.2	784.2	783.19
		782.18	781.21	780.2	779.19	771.22	769.21	767.19	765.18	753.21
		751.2	749.18	747.17	709.17	708.16	707.16	704.18	693.18	692.17
		691.16	690.15	689.15	681.18	680.18	679.16	678.17	677.16	675.17
		673.15	671.14	665.18	664.16	663.16	662.17	661.16	660.16	659.15
		657.16	655.14	651.17	648.17	647.16	646.15	645.15	639.17	637.15
		635.16	634.18	633.17	632.16	631.17	630.16	629.15	628.14	623.17
		621.16	619.17	618.16	608.16	607.17	605.16	603.17	602.16	601.16
		595.17	593.15	592.14	591.17	590.16	589.16	579.17	577.16	576.15
		575.14	574.13	573.16	572.15	571.14	561.16	559.14	557.13	551.15
		550.14	549.14	535.16	534.15	533.14	532.13	531.12	523.16	522.15
		521.14	519.16	517.15	516.13	515.13	514.12	513.11	511.16	509.14
		507.16	505.15	504.14	503.13	501.15	500.12	499.13	498.13	497.12
		495.1	493.15	491.13	489.15	488.14	487.13	486.13	485.12	484.12
		483.11	482.11	481.15	479.13	478.12	477.15	476.14	475.13	471.14
		470.13	469.12	465.15	463.13	461.12	460.11	459.14	458.13	457.12
		455.12	447.14	445.12	443.12	431.12	429.1	428.09	427.12	426.12
		425.11	415.12	413.11	411.09	389.1	388.09	387.08	386.07	375.12
		373.1	372.1	371.09	370.08	369.07	361.1	360.1	359.12	358.11
		357.11	356.1	355.09	354.08	353.08	351.06	349.1	347.09	345.11
		343.13	342.09	341.11	340.1	339.1	338.09	337.08	335.09	331.09
		329.11	327.1	326.09	325.09	324.08	323.08	319.09	317.08	316.07
		315.1	314.09	313.08	307.08	306.07	303.1	301.08	300.07	299.07
		298.06	297.1	287.1	285.1	284.08	283.07	282.06	281.08	280.07
		279.09	273.1	271.08	270.07	269.09	268.09	267.06	265.08	264.07
		263.07	262.06	255.09	253.08	252.06	251.07	250.08	249.05	247.07
		245.06	237.09	235.07	233.06	231.04	223.07	211.07	207.08	205.06
	196.06	194.04	193.04	182.08	180.04	179.03	178.05	177.04	165.05	
	164.05	163.04	147.04	146.04	135.04	134.04	130.04	123.04	119.05	
	111.04	109.03	108.02	107.05	106.04					
References	<p>Cai, Y.; Sun, M.; Corke, H. Identification and Distribution of Simple and Acylated Betacyanins in the Amaranthaceae. <i>J. Agric. Food Chem.</i> 2001, 49, 1971–1978.</p> <p>Spórna-Kucab, A.; Wróbel, N.; Kumorkiewicz-Jamro, A.; Wybraniec, S. Separation of betacyanins from <i>Iresine herbstii</i> Hook. ex Lindl. leaves by high-speed countercurrent chromatography in a polar solvent system. <i>J. Chromatogr. A</i> 2020, 1626, 461370.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

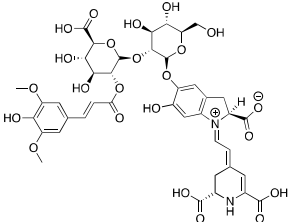
Celosianin II

Chemical structure										
Name:	Celosianin II									
Chemical Formula	C ₄₀ H ₄₂ N ₂ O ₂₂									
Molecular weight	902.77									
Monoisotopic mass	902.2229									
m/z [M+H]	903.2302									
Theoretical fragments (m/z)	903.23	902.22	901.21	900.21	887.24	886.23	885.22	884.21	883.2	875.24
		874.23	873.22	871.24	870.23	869.22	868.22	867.21	866.2	865.19
		863.24	861.22	859.24	858.23	857.22	856.22	855.21	853.23	852.22
		851.21	850.21	849.2	847.18	845.22	843.25	841.23	840.22	839.21
		838.21	837.2	835.22	833.22	831.21	830.2	829.23	828.22	827.21
		825.23	824.23	823.22	822.21	821.2	817.23	815.21	814.21	813.2
		812.19	811.22	810.21	809.2	801.23	799.22	797.2	795.19	783.22
		781.21	779.19	777.18	734.19	721.18	710.19	709.17	708.18	707.17
		695.18	694.17	693.18	692.18	691.16	690.17	689.15	681.18	679.16
		678.18	677.17	676.16	675.17	673.15	671.14	665.18	664.19	663.17
		662.17	661.18	660.17	659.16	658.15	657.16	655.14	651.17	649.18
		648.17	647.17	645.16	639.17	638.17	637.18	635.17	633.18	632.17
		631.17	625.18	623.16	622.15	621.18	620.17	619.17	609.18	607.17
		606.16	605.15	604.14	603.17	602.16	601.16	591.17	589.16	587.14
		551.15	550.14	549.14	535.16	534.15	533.14	532.13	531.12	523.16
		522.15	521.14	519.16	517.15	516.13	515.13	514.12	513.11	511.16
		509.14	507.16	505.15	504.14	503.13	501.15	500.12	499.13	498.13
		497.12	495.1	493.15	491.13	489.15	488.14	487.13	486.13	485.12
		484.12	483.11	482.11	481.15	479.13	478.12	477.15	476.14	475.13
		471.14	470.13	469.12	465.15	463.13	461.12	460.11	459.14	458.13
		457.12	455.12	447.14	445.12	443.12	431.12	429.1	428.09	427.12
		426.12	425.11	415.12	413.11	411.09	389.1	388.09	387.08	386.07
		375.12	373.1	372.1	371.09	370.08	369.07	361.1	360.1	359.12
		358.11	357.11	356.1	355.09	354.08	353.08	351.06	349.1	347.09
		345.11	343.13	342.09	341.11	340.1	339.1	338.09	337.08	335.09
		331.09	329.11	327.1	326.09	325.09	324.08	323.08	319.09	317.08
		316.07	315.1	314.09	313.08	307.08	306.07	303.1	301.08	300.07
		299.07	298.06	297.1	287.1	285.1	284.08	283.07	282.06	281.08
		280.07	279.09	273.1	271.08	270.07	269.09	268.09	267.06	265.08
		264.07	263.07	262.06	255.09	253.08	252.06	251.07	250.08	249.05
		247.07	245.06	237.09	235.07	233.06	231.04	223.07	211.07	207.08
		205.06	196.06	194.04	193.04	182.08	180.04	179.03	178.05	177.04
		165.05	164.05	163.04	147.04	146.04	135.04	134.04	130.04	123.04
		119.05	111.04	109.03	108.02	107.05	106.04			
References	<p>Strack, D.; Bokern, M.; Marxen, N.; Wray, V. Feruloylbetanin from petals of <i>Lampranthus</i> and feruloylamaranthin from cell suspension cultures of <i>Chenopodium rubrum</i>. <i>Phytochemistry</i> 1988, 27, 3529–3531.</p> <p>Cai, Y.; Sun, M.; Corke, H. Identification and Distribution of Simple and Acylated Betacyanins in the Amaranthaceae. <i>J. Agric. Food Chem.</i> 2001, 49, 1971–1978.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

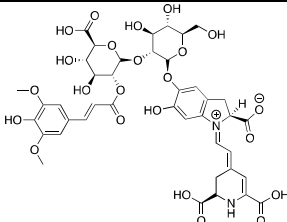
Isocelosianin II

Chemical structure										
Name:	Isocelosianin II									
Chemical Formula	C ₄₀ H ₄₂ N ₂ O ₂₂									
Molecular weight	902.77									
Monoisotopic mass	902.2229									
m/z [M+H]	903.2302									
Theoretical fragments (m/z)	903.23	902.22	901.21	900.21	887.24	886.23	885.22	884.21	883.2	875.24
		874.23	873.22	871.24	870.23	869.22	868.22	867.21	866.2	865.19
		863.24	861.22	859.24	858.23	857.22	856.22	855.21	853.23	852.22
		851.21	850.21	849.2	847.18	845.22	843.25	841.23	840.22	839.21
		838.21	837.2	835.22	833.22	831.21	830.2	829.23	828.22	827.21
		825.23	824.23	823.22	822.21	821.2	817.23	815.21	814.21	813.2
		812.19	811.22	810.21	809.2	801.23	799.22	797.2	795.19	783.22
		781.21	779.19	777.18	734.19	721.18	710.19	709.17	708.18	707.17
		695.18	694.17	693.18	692.18	691.16	690.17	689.15	681.18	679.16
		678.18	677.17	676.16	675.17	673.15	671.14	665.18	664.19	663.17
		662.17	661.18	660.17	659.16	658.15	657.16	655.14	651.17	649.18
		648.17	647.17	645.16	639.17	638.17	637.18	635.17	633.18	632.17
		631.17	625.18	623.16	622.15	621.18	620.17	619.17	609.18	607.17
		606.16	605.15	604.14	603.17	602.16	601.16	591.17	589.16	587.14
		551.15	550.14	549.14	535.16	534.15	533.14	532.13	531.12	523.16
		522.15	521.14	519.16	517.15	516.13	515.13	514.12	513.11	511.16
		509.14	507.16	505.15	504.14	503.13	501.15	500.12	499.13	498.13
		497.12	495.1	493.15	491.13	489.15	488.14	487.13	486.13	485.12
		484.12	483.11	482.11	481.15	479.13	478.12	477.15	476.14	475.13
		471.14	470.13	469.12	465.15	463.13	461.12	460.11	459.14	458.13
		457.12	455.12	447.14	445.12	443.12	431.12	429.1	428.09	427.12
		426.12	425.11	415.12	413.11	411.09	389.1	388.09	387.08	386.07
		375.12	373.1	372.1	371.09	370.08	369.07	361.1	360.1	359.12
		358.11	357.11	356.1	355.09	354.08	353.08	351.06	349.1	347.09
		345.11	343.13	342.09	341.11	340.1	339.1	338.09	337.08	335.09
		331.09	329.11	327.1	326.09	325.09	324.08	323.08	319.09	317.08
		316.07	315.1	314.09	313.08	307.08	306.07	303.1	301.08	300.07
		299.07	298.06	297.1	287.1	285.1	284.08	283.07	282.06	281.08
		280.07	279.09	273.1	271.08	270.07	269.09	268.09	267.06	265.08
		264.07	263.07	262.06	255.09	253.08	252.06	251.07	250.08	249.05
		247.07	245.06	237.09	235.07	233.06	231.04	223.07	211.07	207.08
		205.06	196.06	194.04	193.04	182.08	180.04	179.03	178.05	177.04
		165.05	164.05	163.04	147.04	146.04	135.04	134.04	130.04	123.04
		119.05	111.04	109.03	108.02	107.05	106.04			
References	<p>Strack, D.; Bokern, M.; Marxen, N.; Wray, V. Feruloylbetainin from petals of <i>Lampranthus</i> and feruloylamaranthin from cell suspension cultures of <i>Chenopodium rubrum</i>. <i>Phytochemistry</i> 1988, 27, 3529–3531.</p> <p>Cai, Y.; Sun, M.; Corke, H. Identification and Distribution of Simple and Acylated Betacyanins in the Amaranthaceae. <i>J. Agric. Food Chem.</i> 2001, 49, 1971–1978.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

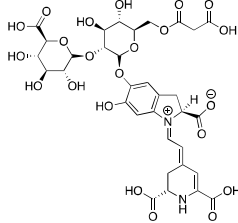
Sinapoyl-amaranthin

Chemical structure										
Name:	Sinapoyl-amaranthin									
Chemical Formula	C ₄₁ H ₄₄ N ₂ O ₂₃									
Molecular weight	932.79									
Monoisotopic mass	932.2335									
m/z [M+H]	933.2408									
Theoretical fragments (m/z)	933.24	932.23	931.23	930.22	917.25	916.24	915.23	914.22	913.21	905.25
		904.24	903.23	901.25	900.24	899.24	898.23	897.22	896.21	895.2
		893.25	891.23	889.25	888.24	887.24	886.23	885.22	883.24	882.23
		881.22	880.22	879.21	877.19	875.24	873.26	871.24	870.23	869.22
		868.22	867.21	865.23	863.24	861.22	860.21	859.24	858.23	857.22
		855.25	854.24	853.23	852.22	851.21	847.24	845.22	844.22	843.21
		842.2	841.23	840.22	839.21	831.25	829.23	827.21	825.2	813.23
		811.22	809.2	807.19	764.2	751.2	740.2	738.19	737.18	725.19
		724.18	723.18	722.19	721.18	720.18	719.17	709.17	708.19	707.16
		706.17	705.17	695.18	694.2	693.18	692.18	691.16	690.18	689.15
		688.16	681.18	679.19	678.18	677.18	675.17	673.15	671.14	668.18
		667.19	665.18	663.17	662.18	661.18	659.17	657.16	655.19	653.17
		652.16	651.19	650.18	649.18	647.17	645.16	639.19	637.15	636.17
		635.16	634.15	633.18	632.17	631.17	623.17	621.16	619.14	617.15
		605.16	603.15	601.13	551.15	550.14	549.14	535.16	534.15	533.14
		532.13	531.12	523.16	522.15	521.14	519.16	517.15	516.13	515.13
		514.12	513.11	511.16	509.14	507.16	505.15	504.14	503.13	501.15
		500.12	499.13	498.13	497.12	495.1	493.15	491.13	489.15	488.14
		487.13	486.13	485.12	484.12	483.11	482.11	481.15	479.13	478.12
		477.15	476.14	475.13	471.14	470.13	469.12	465.15	463.13	461.12
		460.11	459.14	458.13	457.12	455.12	447.14	445.12	443.12	431.12
		429.1	428.09	427.12	426.12	425.11	415.12	413.11	411.09	389.1
		388.09	387.08	386.07	375.12	373.1	372.1	371.09	370.08	369.07
		361.1	360.1	359.12	358.11	357.11	356.1	355.09	354.08	353.08
		351.06	349.1	347.09	345.11	343.13	342.09	341.11	340.1	339.1
		338.09	337.08	335.09	331.09	329.11	327.1	326.09	325.09	324.08
		323.08	319.09	317.08	316.07	315.1	314.09	313.08	307.08	306.07
		303.1	301.08	300.07	299.07	298.06	297.1	287.1	285.1	284.08
		283.07	282.06	281.08	280.07	279.09	273.1	271.08	270.07	269.09
		268.09	267.06	265.08	264.07	263.07	262.06	255.09	253.08	252.06
		251.07	250.08	249.05	247.07	245.06	237.09	235.07	233.06	231.04
		223.07	211.07	207.08	205.06	196.06	194.04	193.04	182.08	180.04
		179.03	178.05	177.04	165.05	164.05	163.04	147.04	146.04	135.04
		134.04	130.04	123.04	119.05	111.04	109.03	108.02	107.05	106.04
References	Cai, Y.; Sun, M.; Corke, H. Identification and Distribution of Simple and Acylated Betacyanins in the Amaranthaceae. <i>J. Agric. Food Chem.</i> 2001 , 49, 1971–1978									

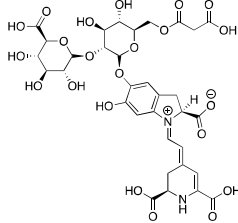
Sinapoyl-isoamaranthin

Chemical structure										
Name:	Sinapoyl-isoamaranthin									
Chemical Formula	C ₄₁ H ₄₄ N ₂ O ₂₃									
Molecular weight	932.79									
Monoisotopic mass	932.2335									
m/z [M+H]	933.2408									
Theoretical fragments (m/z)	933.24	932.23	931.23	930.22	917.25	916.24	915.23	914.22	913.21	905.25
		904.24	903.23	901.25	900.24	899.24	898.23	897.22	896.21	895.2
		893.25	891.23	889.25	888.24	887.24	886.23	885.22	883.24	882.23
		881.22	880.22	879.21	877.19	875.24	873.26	871.24	870.23	869.22
		868.22	867.21	865.23	863.24	861.22	860.21	859.24	858.23	857.22
		855.25	854.24	853.23	852.22	851.21	847.24	845.22	844.22	843.21
		842.2	841.23	840.22	839.21	831.25	829.23	827.21	825.2	813.23
		811.22	809.2	807.19	764.2	751.2	740.2	738.19	737.18	725.19
		724.18	723.18	722.19	721.18	720.18	719.17	709.17	708.19	707.16
		706.17	705.17	695.18	694.2	693.18	692.18	691.16	690.18	689.15
		688.16	681.18	679.19	678.18	677.18	675.17	673.15	671.14	668.18
		667.19	665.18	663.17	662.18	661.18	659.17	657.16	655.19	653.17
		652.16	651.19	650.18	649.18	647.17	645.16	639.19	637.15	636.17
		635.16	634.15	633.18	632.17	631.17	623.17	621.16	619.14	617.15
		605.16	603.15	601.13	551.15	550.14	549.14	535.16	534.15	533.14
		532.13	531.12	523.16	522.15	521.14	519.16	517.15	516.13	515.13
		514.12	513.11	511.16	509.14	507.16	505.15	504.14	503.13	501.15
		500.12	499.13	498.13	497.12	495.1	493.15	491.13	489.15	488.14
		487.13	486.13	485.12	484.12	483.11	482.11	481.15	479.13	478.12
		477.15	476.14	475.13	471.14	470.13	469.12	465.15	463.13	461.12
		460.11	459.14	458.13	457.12	455.12	447.14	445.12	443.12	431.12
		429.1	428.09	427.12	426.12	425.11	415.12	413.11	411.09	389.1
		388.09	387.08	386.07	375.12	373.1	372.1	371.09	370.08	369.07
		361.1	360.1	359.12	358.11	357.11	356.1	355.09	354.08	353.08
		351.06	349.1	347.09	345.11	343.13	342.09	341.11	340.1	339.1
		338.09	337.08	335.09	331.09	329.11	327.1	326.09	325.09	324.08
		323.08	319.09	317.08	316.07	315.1	314.09	313.08	307.08	306.07
	303.1	301.08	300.07	299.07	298.06	297.1	287.1	285.1	284.08	
	283.07	282.06	281.08	280.07	279.09	273.1	271.08	270.07	269.09	
	268.09	267.06	265.08	264.07	263.07	262.06	255.09	253.08	252.06	
	251.07	250.08	249.05	247.07	245.06	237.09	235.07	233.06	231.04	
	223.07	211.07	207.08	205.06	196.06	194.04	193.04	182.08	180.04	
	179.03	178.05	177.04	165.05	164.05	163.04	147.04	146.04	135.04	
	134.04	130.04	123.04	119.05	111.04	109.03	108.02	107.05	106.04	
References	Cai, Y.; Sun, M.; Corke, H. Identification and Distribution of Simple and Acylated Betacyanins in the Amaranthaceae. <i>J. Agric. Food Chem.</i> 2001 , 49, 1971–1978. Sliemen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017 , 65, 675–689. Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021 , 38, 2315–2346.									

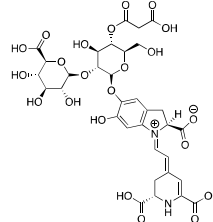
6'-O-malonyl-amaranthin

Chemical structure										
Name:	6'-O-malonyl-amaranthin (Celoscristatin)									
Chemical Formula	C ₃₃ H ₃₆ N ₂ O ₂₂									
Molecular weight	812.64									
Monoisotopic mass	812.1760									
m/z [M+H]	813.1832									
Theoretical fragments (m/z)	813.18	812.18	811.17	810.16	797.19	796.18	795.17	794.16	793.16	785.19
		784.18	783.17	781.19	779.18	778.17	777.16	775.15	773.19	771.17
		769.19	768.19	767.18	766.17	765.16	763.18	761.17	759.15	755.18
		753.2	751.18	750.18	749.17	743.18	741.16	740.15	739.18	738.18
		737.17	727.18	726.18	725.17	724.16	723.15	711.19	709.17	708.16
		707.16	705.14	699.19	697.17	695.19	693.18	691.16	689.15	683.19
		681.18	679.16	677.18	675.17	673.15	669.18	665.18	663.17	657.18
		655.16	651.17	644.15	639.17	637.15	636.14	635.14	631.14	621.16
		620.15	619.14	618.13	617.12	609.16	607.14	605.16	604.13	603.15
		602.14	601.13	600.12	599.11	593.16	591.15	589.13	588.13	587.12
		586.12	585.14	583.12	579.15	575.15	574.14	573.14	572.12	571.13
		570.12	569.11	568.11	567.15	565.13	561.14	559.13	558.12	551.15
		549.14	548.12	547.13	543.13	542.13	541.12	535.13	534.15	533.11
		532.11	531.13	530.13	529.12	519.13	518.13	517.12	516.13	515.13
		514.12	513.11	512.12	511.11	503.14	502.13	501.12	500.12	499.13
		497.12	484.12	483.11	482.11	479.13	473.13	461.13	455.12	449.13
		447.11	446.11	445.13	444.11	443.12	442.1	441.09	433.13	431.12
		429.1	428.09	427.09	426.1	425.11	424.09	423.08	415.12	413.11
		412.1	411.09	410.08	409.08	394.09	393.08	392.07	389.1	388.09
		387.08	386.07	383.1	375.12	373.1	372.1	371.09	370.08	369.07
		365.09	361.1	360.1	359.12	357.11	356.1	355.09	354.09	353.09
		351.06	349.1	347.09	345.11	343.13	342.08	341.11	339.1	338.06
		337.08	336.08	335.08	331.09	329.11	327.1	326.09	325.09	324.08
		323.08	319.09	317.08	316.07	315.1	314.09	313.08	306.07	303.1
		301.08	300.07	299.07	287.1	285.09	284.08	283.07	281.08	280.07
		273.1	271.11	269.09	267.06	265.08	264.07	263.07	262.06	255.09
		253.08	251.07	249.05	247.07	245.06	237.09	235.07	233.06	231.04
		223.07	211.07	207.08	205.06	196.06	194.04	193.04	182.08	180.04
		179.03	178.05	177.04	165.05	164.05	163.04	147.04	146.04	135.04
		134.04	130.04	123.04	119.05	111.04	109.03	108.02	107.05	106.04
References	<p>Lystvan, K.; Kumorkiewicz, A.; Szneler, E.; Wybraniec, S. Study on Betalains in Celosia Cristata Linn. Callus Culture and Identification of New Malonylated Amaranthins. <i>J. Agric. Food Chem.</i> 2018, 66, 3870–3879.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

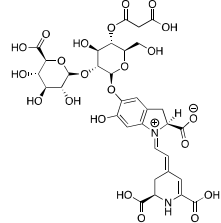
6'-O-malonyl-isoamaranthin

Chemical structure										
Name:	6'-O-malonyl-isoamaranthin (isoceloscrustin)									
Chemical Formula	C ₃₃ H ₃₆ N ₂ O ₂₂									
Molecular weight	812.64									
Monoisotopic mass	812.1760									
m/z [M+H]	813.1832									
Theoretical fragments (m/z)	813.18	812.18	811.17	810.16	797.19	796.18	795.17	794.16	793.16	785.19
		784.18	783.17	781.19	779.18	778.17	777.16	775.15	773.19	771.17
		769.19	768.19	767.18	766.17	765.16	763.18	761.17	759.15	755.18
		753.2	751.18	750.18	749.17	743.18	741.16	740.15	739.18	738.18
		737.17	727.18	726.18	725.17	724.16	723.15	711.19	709.17	708.16
		707.16	705.14	699.19	697.17	695.19	693.18	691.16	689.15	683.19
		681.18	679.16	677.18	675.17	673.15	669.18	665.18	663.17	657.18
		655.16	651.17	644.15	639.17	637.15	636.14	635.14	631.14	621.16
		620.15	619.14	618.13	617.12	609.16	607.14	605.16	604.13	603.15
		602.14	601.13	600.12	599.11	593.16	591.15	589.13	588.13	587.12
		586.12	585.14	583.12	579.15	575.15	574.14	573.14	572.12	571.13
		570.12	569.11	568.11	567.15	565.13	561.14	559.13	558.12	551.15
		549.14	548.12	547.13	543.13	542.13	541.12	535.13	534.15	533.11
		532.11	531.13	530.13	529.12	519.13	518.13	517.12	516.13	515.13
		514.12	513.11	512.12	511.11	503.14	502.13	501.12	500.12	499.13
		497.12	484.12	483.11	482.11	479.13	473.13	461.13	455.12	449.13
		447.11	446.11	445.13	444.11	443.12	442.1	441.09	433.13	431.12
		429.1	428.09	427.09	426.1	425.11	424.09	423.08	415.12	413.11
		412.1	411.09	410.08	409.08	394.09	393.08	392.07	389.1	388.09
		387.08	386.07	383.1	375.12	373.1	372.1	371.09	370.08	369.07
		365.09	361.1	360.1	359.12	357.11	356.1	355.09	354.09	353.09
		351.06	349.1	347.09	345.11	343.13	342.08	341.11	339.1	338.06
		337.08	336.08	335.08	331.09	329.11	327.1	326.09	325.09	324.08
		323.08	319.09	317.08	316.07	315.1	314.09	313.08	306.07	303.1
		301.08	300.07	299.07	287.1	285.09	284.08	283.07	281.08	280.07
		273.1	271.11	269.09	267.06	265.08	264.07	263.07	262.06	255.09
		253.08	251.07	249.05	247.07	245.06	237.09	235.07	233.06	231.04
		223.07	211.07	207.08	205.06	196.06	194.04	193.04	182.08	180.04
		179.03	178.05	177.04	165.05	164.05	163.04	147.04	146.04	135.04
		134.04	130.04	123.04	119.05	111.04	109.03	108.02	107.05	106.04
References	<p>Lystvan, K.; Kumorkiewicz, A.; Szneler, E.; Wybraniec, S. Study on Betalains in Celosia Cristata Linn. Callus Culture and Identification of New Malonylated Amarantins. <i>J. Agric. Food Chem.</i> 2018, 66, 3870–3879.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

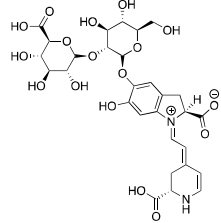
4'-O-malonyl-amaranthin

Chemical structure										
Name:	4'-O-malonyl-amaranthin									
Chemical Formula	C ₃₃ H ₃₆ N ₂ O ₂₂									
Molecular weight	812.64									
Monoisotopic mass	812.1760									
m/z [M+H]	813.1832									
Theoretical fragments (m/z)	813.18	812.18	811.17	810.16	797.19	796.18	795.17	794.16	793.16	785.19
		784.18	783.17	781.19	779.18	778.17	777.16	775.15	773.19	771.17
		769.19	768.19	767.18	766.17	765.16	763.18	761.17	759.15	755.18
		753.2	751.18	750.18	749.17	743.18	741.16	740.15	739.18	738.18
		737.17	727.18	726.18	725.17	724.16	723.15	711.19	709.17	708.16
		707.16	705.14	699.19	697.17	695.19	693.18	691.16	689.15	683.19
		681.18	679.16	677.18	675.17	673.15	669.18	665.18	663.17	657.18
		655.16	651.17	644.15	639.17	637.15	636.14	635.14	631.14	621.16
		620.15	619.14	618.13	617.12	609.16	607.14	605.16	604.13	603.15
		602.14	601.13	600.12	599.11	593.16	591.15	589.13	588.13	587.12
		586.12	585.14	583.12	579.15	575.15	574.14	573.14	572.12	571.13
		570.12	569.11	568.11	567.15	565.13	561.14	559.13	558.12	551.15
		549.14	548.12	547.13	543.13	542.13	541.12	535.13	534.15	533.11
		532.11	531.13	530.13	529.12	519.13	518.13	517.12	516.13	515.13
		514.12	513.11	512.12	511.11	503.14	502.13	501.12	500.12	499.13
		497.12	484.12	483.11	482.11	479.13	473.13	461.13	455.12	449.13
		447.11	446.11	445.13	444.11	443.12	442.1	441.09	433.13	431.12
		429.1	428.09	427.09	426.1	425.11	424.09	423.08	415.12	413.11
		412.1	411.09	410.08	409.08	394.09	393.08	392.07	389.1	388.09
		387.08	386.07	383.1	375.12	373.1	372.1	371.09	370.08	369.07
		365.09	361.1	360.1	359.12	357.11	356.1	355.09	354.09	353.09
		351.06	349.1	347.09	345.11	343.13	342.08	341.11	339.1	338.06
		337.08	336.08	335.08	331.09	329.11	327.1	326.09	325.09	324.08
		323.08	319.09	317.08	316.07	315.1	314.09	313.08	306.07	303.1
		301.08	300.07	299.07	287.1	285.09	284.08	283.07	281.08	280.07
		273.1	271.11	269.09	267.06	265.08	264.07	263.07	262.06	255.09
		253.08	251.07	249.05	247.07	245.06	237.09	235.07	233.06	231.04
		223.07	211.07	207.08	205.06	196.06	194.04	193.04	182.08	180.04
		179.03	178.05	177.04	165.05	164.05	163.04	147.04	146.04	135.04
		134.04	130.04	123.04	119.05	111.04	109.03	108.02	107.05	106.04
References	<p>Lystvan, K.; Kumorkiewicz, A.; Szneler, E.; Wybraniec, S. Study on Betalains in Celosia Cristata Linn. Callus Culture and Identification of New Malonylated Amaranthins. <i>J. Agric. Food Chem.</i> 2018, 66, 3870–3879.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

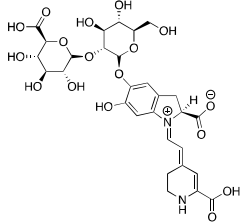
4'-O-malonyl-isoamaranthin

Chemical structure										
Name:	4'-O-malonyl-amaranthin									
Chemical Formula	C ₃₃ H ₃₆ N ₂ O ₂₂									
Molecular weight	812.64									
Monoisotopic mass	812.1760									
m/z [M+H]	813.1832									
Theoretical fragments (m/z)	813.18	812.18	811.17	810.16	797.19	796.18	795.17	794.16	793.16	785.19
		784.18	783.17	781.19	779.18	778.17	777.16	775.15	773.19	771.17
		769.19	768.19	767.18	766.17	765.16	763.18	761.17	759.15	755.18
		753.2	751.18	750.18	749.17	743.18	741.16	740.15	739.18	738.18
		737.17	727.18	726.18	725.17	724.16	723.15	711.19	709.17	708.16
		707.16	705.14	699.19	697.17	695.19	693.18	691.16	689.15	683.19
		681.18	679.16	677.18	675.17	673.15	669.18	665.18	663.17	657.18
		655.16	651.17	644.15	639.17	637.15	636.14	635.14	631.14	621.16
		620.15	619.14	618.13	617.12	609.16	607.14	605.16	604.13	603.15
		602.14	601.13	600.12	599.11	593.16	591.15	589.13	588.13	587.12
		586.12	585.14	583.12	579.15	575.15	574.14	573.14	572.12	571.13
		570.12	569.11	568.11	567.15	565.13	561.14	559.13	558.12	551.15
		549.14	548.12	547.13	543.13	542.13	541.12	535.13	534.15	533.11
		532.11	531.13	530.13	529.12	519.13	518.13	517.12	516.13	515.13
		514.12	513.11	512.12	511.11	503.14	502.13	501.12	500.12	499.13
		497.12	484.12	483.11	482.11	479.13	473.13	461.13	455.12	449.13
		447.11	446.11	445.13	444.11	443.12	442.1	441.09	433.13	431.12
		429.1	428.09	427.09	426.1	425.11	424.09	423.08	415.12	413.11
		412.1	411.09	410.08	409.08	394.09	393.08	392.07	389.1	388.09
		387.08	386.07	383.1	375.12	373.1	372.1	371.09	370.08	369.07
		365.09	361.1	360.1	359.12	357.11	356.1	355.09	354.09	353.09
		351.06	349.1	347.09	345.11	343.13	342.08	341.11	339.1	338.06
		337.08	336.08	335.08	331.09	329.11	327.1	326.09	325.09	324.08
		323.08	319.09	317.08	316.07	315.1	314.09	313.08	306.07	303.1
		301.08	300.07	299.07	287.1	285.09	284.08	283.07	281.08	280.07
		273.1	271.11	269.09	267.06	265.08	264.07	263.07	262.06	255.09
		253.08	251.07	249.05	247.07	245.06	237.09	235.07	233.06	231.04
		223.07	211.07	207.08	205.06	196.06	194.04	193.04	182.08	180.04
		179.03	178.05	177.04	165.05	164.05	163.04	147.04	146.04	135.04
		134.04	130.04	123.04	119.05	111.04	109.03	108.02	107.05	106.04
References	<p>Lystvan, K.; Kumorkiewicz, A.; Szneler, E.; Wybraniec, S. Study on Betalains in Celosia Cristata Linn. Callus Culture and Identification of New Malonylated Amaranthins. <i>J. Agric. Food Chem.</i> 2018, 66, 3870–3879.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

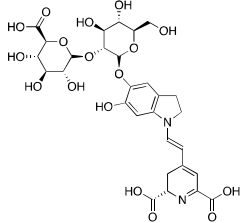
17-decarboxy-amaranthin

Chemical structure										
Name:	17-decarboxy-amaranthin									
Chemical Formula	C ₂₉ H ₃₄ N ₂ O ₁₇									
Molecular weight	682.59									
Monoisotopic mass	682.1857									
m/z [M+H]	683.1930									
Theoretical fragments (m/z)	683.19	682.19	681.18	680.17	667.2	666.19	665.18	664.17	663.17	655.2
		654.19	653.18	651.2	650.2	649.19	648.18	647.17	646.16	645.16
		643.2	641.18	639.2	638.2	637.19	636.18	635.17	633.19	632.18
		631.18	630.17	629.16	627.15	625.19	623.21	621.19	620.18	619.18
		618.17	617.16	615.18	613.19	611.17	610.16	609.19	608.18	607.18
		605.2	604.19	603.18	602.17	601.17	597.19	595.18	594.17	593.16
		592.15	591.18	590.17	589.17	581.2	579.18	577.17	575.15	563.19
		561.17	559.16	558.15	557.14	545.14	534.15	532.13	531.12	519.13
		518.13	517.12	516.13	515.13	514.12	513.11	507.16	506.15	505.15
		502.13	501.12	500.12	499.11	491.17	490.16	489.15	488.14	487.13
		486.12	485.13	484.12	483.11	482.11	479.17	478.16	477.15	475.17
		473.16	472.12	471.14	470.13	469.12	467.17	465.15	463.17	462.12
		461.13	460.15	459.14	457.16	456.13	455.14	454.14	453.13	451.11
		449.13	447.11	446.11	445.13	444.13	443.12	442.14	441.13	437.16
		435.14	434.13	433.13	432.15	431.12	430.11	429.1	428.09	427.12
		426.12	425.11	421.16	419.14	417.13	416.12	415.12	414.14	413.11
		411.09	403.15	401.13	399.12	385.14	383.12	381.11	358.11	356.1
		355.09	345.11	344.1	343.09	342.09	341.09	340.1	338.09	337.08
		331.13	329.11	328.11	327.1	326.09	325.08	324.08	323.08	317.11
		316.11	315.13	313.12	312.11	311.1	310.09	309.09	307.08	306.07
		305.11	303.1	301.12	299.14	298.09	297.12	295.11	293.09	291.1
		287.1	285.1	283.11	282.1	281.09	279.09	275.1	273.09	272.08
		271.08	270.07	269.09	268.09	267.09	259.11	257.09	256.08	255.09
		254.07	253.07	252.06	250.08	249.08	243.11	241.1	240.09	239.08
		238.07	237.09	236.08	235.06	227.12	225.1	223.07	221.09	220.08
		219.08	218.07	209.09	207.08	205.06	203.08	201.07	196.06	194.04
		193.1	191.08	189.07	187.05	182.08	180.04	179.08	178.05	177.04
		167.08	165.05	164.05	163.09	161.07	152.07	150.05	147.04	146.04
		135.04	134.04	130.04	123.04	119.05	111.04	109.03	108.02	107.05
		106.04								
References	<p>Miguel, M.G. Betalains in Some Species of the Amaranthaceae Family: A Review. <i>Antioxidants</i> 2018, <i>7</i>, 53.</p> <p>Xie, G.R.; Chen, H.J. Comprehensive Betalain Profiling of Djulis (<i>Chenopodium formosanum</i>) Cultivars Using HPLC-Q-Orbitrap High-Resolution Mass Spectrometry. <i>J. Agric. Food Chem.</i> 2021, <i>69</i>, 15699–15715.</p> <p>Araujo-León, J.A.; Aguilar-Hernández, V.; Sánchez-del Pino, I.; Brito-Argáez, L.; Peraza-Sánchez, S.R.; Xingú-López, A.; Ortiz-Andrade, R. Analysis of Red Amaranth (<i>Amaranthus cruentus</i> L.) Betalains by LC-MS. <i>J. Mex. Chem. Soc.</i> 2023, <i>67</i>, 227–239.</p>									

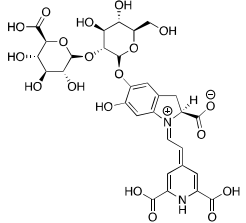
15-decarboxy-amaranthin

Chemical structure										
Name:	15-decarboxy-amaranthin									
Chemical Formula	C ₂₉ H ₃₄ N ₂ O ₁₇									
Molecular weight	682.59									
Monoisotopic mass	682.1857									
m/z [M+H]	683.1930									
Theoretical fragments (m/z)	683.19	682.19	681.18	680.17	667.2	666.19	665.18	664.17	663.17	655.2
		654.19	653.18	651.2	650.2	649.19	648.18	647.17	646.16	645.16
		643.2	641.18	639.2	638.2	637.19	636.18	635.17	633.19	632.18
		631.18	630.17	629.16	627.15	625.19	623.21	621.19	620.18	619.18
		618.17	617.16	615.18	613.19	611.17	610.16	609.19	608.18	607.18
		605.2	604.19	603.18	602.17	601.17	597.19	595.18	594.17	593.16
		592.15	591.18	590.17	589.17	581.2	579.18	577.17	575.15	563.19
		561.17	559.16	558.15	557.14	545.14	534.15	532.13	531.12	519.13
		518.13	517.12	516.13	515.13	514.12	513.11	507.16	506.15	505.15
		502.13	501.12	500.12	499.11	491.17	490.16	489.15	488.14	487.13
		486.12	485.13	484.12	483.11	482.11	479.17	478.16	477.15	475.17
		473.16	472.12	471.14	470.13	469.12	467.17	465.15	463.17	462.12
		461.13	460.15	459.14	457.16	456.13	455.14	454.14	453.13	451.11
		449.13	447.11	446.11	445.13	444.13	443.12	442.14	441.13	437.16
		435.14	434.13	433.13	432.15	431.12	430.11	429.1	428.09	427.12
		426.12	425.11	421.16	419.14	417.13	416.12	415.12	414.14	413.11
		411.09	403.15	401.13	399.12	385.14	383.12	381.11	358.11	356.1
		355.09	345.11	344.1	343.09	342.09	341.09	340.1	338.09	337.08
		331.13	329.11	328.11	327.1	326.09	325.08	324.08	323.08	317.11
		316.11	315.13	313.12	312.11	311.1	310.09	309.09	307.08	306.07
		305.11	303.1	301.12	299.14	298.09	297.12	295.11	293.09	291.1
		287.1	285.1	283.11	282.1	281.09	279.09	275.1	273.09	272.08
		271.08	270.07	269.09	268.09	267.09	259.11	257.09	256.08	255.09
		254.07	253.07	252.06	250.08	249.08	243.11	241.1	240.09	239.08
		238.07	237.09	236.08	235.06	227.12	225.1	223.07	221.09	220.08
		219.08	218.07	209.09	207.08	205.06	203.08	201.07	196.06	194.04
		193.1	191.08	189.07	187.05	182.08	180.04	179.08	178.05	177.04
		167.08	165.05	164.05	163.09	161.07	152.07	150.05	147.04	146.04
		135.04	134.04	130.04	123.04	119.05	111.04	109.03	108.02	107.05
		106.04								
References	<p>Miguel, M.G. Betalains in Some Species of the Amaranthaceae Family: A Review. <i>Antioxidants</i> 2018, <i>7</i>, 53.</p> <p>Xie, G.R.; Chen, H.J. Comprehensive Betalain Profiling of Djulis (<i>Chenopodium formosanum</i>) Cultivars Using HPLC-Q-Orbitrap High-Resolution Mass Spectrometry. <i>J. Agric. Food Chem.</i> 2021, <i>69</i>, 15699–15715.</p> <p>Araujo-León, J.A.; Aguilar-Hernández, V.; Sánchez-del Pino, I.; Brito-Argáez, L.; Peraza-Sánchez, S.R.; Xingú-López, A.; Ortiz-Andrade, R. Analysis of Red Amaranth (<i>Amaranthus cruentus</i> L.) Betalains by LC-MS. <i>J. Mex. Chem. Soc.</i> 2023, <i>67</i>, 227–239.</p>									

2-decarboxy-amaranthin

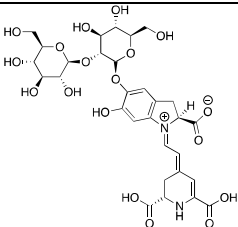
Chemical structure										
Name:	2-decarboxy-amaranthin									
Chemical Formula	C ₂₉ H ₃₄ N ₂ O ₁₇									
Molecular weight	682.59									
Monoisotopic mass	682.1857									
m/z [M+H]	683.1930									
Theoretical fragments (m/z)	683.19	682.19	681.18	680.17	667.2	666.19	665.18	664.17	663.17	655.2
		654.19	653.18	651.2	650.2	649.19	648.18	647.17	646.16	645.16
		643.2	641.18	639.2	638.2	637.19	636.18	635.17	633.19	632.18
		631.18	630.17	629.16	627.15	625.19	623.21	621.19	620.18	619.18
		618.17	617.16	615.18	613.19	611.17	610.16	609.19	608.18	607.18
		605.2	604.19	603.18	602.17	601.17	597.19	595.18	594.17	593.16
		592.15	591.18	590.17	589.17	581.2	579.18	577.17	575.15	563.19
		561.17	559.16	558.15	557.14	545.14	534.15	532.13	531.12	519.13
		518.13	517.12	516.13	515.13	514.12	513.11	507.16	506.15	505.15
		502.13	501.12	500.12	499.11	491.17	490.16	489.15	488.14	487.13
		486.12	485.13	484.12	483.11	482.11	479.17	478.16	477.15	475.17
		473.16	472.12	471.14	470.13	469.12	467.17	465.15	463.17	462.12
		461.13	460.15	459.14	457.16	456.13	455.14	454.14	453.13	451.11
		449.13	447.11	446.11	445.13	444.13	443.12	442.14	441.13	437.16
		435.14	434.13	433.13	432.15	431.12	430.11	429.1	428.09	427.12
		426.12	425.11	421.16	419.14	417.13	416.12	415.12	414.14	413.11
		411.09	403.15	401.13	399.12	385.14	383.12	381.11	358.11	356.1
		355.09	345.11	344.1	343.09	342.09	341.09	340.1	338.09	337.08
		331.13	329.11	328.11	327.1	326.09	325.08	324.08	323.08	317.11
		316.11	315.13	313.12	312.11	311.1	310.09	309.09	307.08	306.07
		305.11	303.1	301.12	299.14	298.09	297.12	295.11	293.09	291.1
		287.1	285.1	283.11	282.1	281.09	279.09	275.1	273.09	272.08
		271.08	270.07	269.09	268.09	267.09	259.11	257.09	256.08	255.09
		254.07	253.07	252.06	250.08	249.08	243.11	241.1	240.09	239.08
		238.07	237.09	236.08	235.06	227.12	225.1	223.07	221.09	220.08
		219.08	218.07	209.09	207.08	205.06	203.08	201.07	196.06	194.04
		193.1	191.08	189.07	187.05	182.08	180.04	179.08	178.05	177.04
		167.08	165.05	164.05	163.09	161.07	152.07	150.05	147.04	146.04
		135.04	134.04	130.04	123.04	119.05	111.04	109.03	108.02	107.05
		106.04								
References	<p>Miguel, M.G. Betalains in Some Species of the Amaranthaceae Family: A Review. <i>Antioxidants</i> 2018, <i>7</i>, 53.</p> <p>Xie, G.R.; Chen, H.J. Comprehensive Betalain Profiling of Djulis (<i>Chenopodium formosanum</i>) Cultivars Using HPLC-Q-Orbitrap High-Resolution Mass Spectrometry. <i>J. Agric. Food Chem.</i> 2021, <i>69</i>, 15699–15715.</p> <p>Araujo-León, J.A.; Aguilar-Hernández, V.; Sánchez-del Pino, I.; Brito-Argáez, L.; Peraza-Sánchez, S.R.; Xingú-López, A.; Ortiz-Andrade, R. Analysis of Red Amaranth (<i>Amaranthus cruentus</i> L.) Betalains by LC-MS. <i>J. Mex. Chem. Soc.</i> 2023, <i>67</i>, 227–239.</p>									

Neoamaranthin

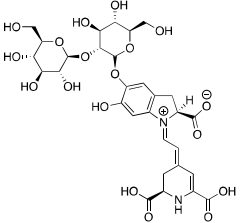
Chemical structure										
Name:	Neoamaranthin									
Chemical Formula	C ₃₀ H ₃₂ N ₂ O ₁₉									
Molecular weight	724.58									
Monoisotopic mass	724.1599									
m/z [M+H]	725.1672									
Theoretical fragments (m/z)	725.17	724.16	723.15	722.14	709.17	708.16	707.16	706.15	705.14	697.17
		696.16	695.16	693.18	692.17	691.16	690.15	689.15	688.14	687.13
		685.17	683.16	682.15	681.18	680.17	679.16	678.15	677.15	675.17
		674.16	673.15	672.14	671.14	669.12	667.16	665.18	663.17	662.16
		661.15	660.14	659.14	657.16	655.16	653.15	652.14	651.17	650.16
		649.15	647.17	646.16	645.16	644.15	643.14	639.17	637.15	636.14
		635.14	634.13	633.16	632.15	631.14	621.16	619.14	617.12	603.15
		601.13	599.11	549.14	548.13	547.12	545.14	533.14	532.13	531.12
		530.12	529.11	528.13	521.14	520.13	519.12	518.13	517.12	516.13
		515.13	514.12	513.11	512.11	511.1	509.14	507.12	505.15	503.13
		502.13	501.12	500.12	499.11	498.12	497.12	496.11	495.1	493.09
		491.13	489.12	488.14	487.13	486.12	485.12	484.12	483.11	482.11
		479.13	477.11	476.11	475.11	474.13	473.13	472.12	470.13	469.12
		468.12	467.11	461.13	459.1	458.1	457.13	456.13	455.12	449.13
		447.11	446.11	445.13	444.13	443.12	441.09	433.13	431.12	430.11
		429.1	428.09	427.12	426.12	425.11	423.08	415.12	413.11	411.09
		387.08	386.07	385.07	384.06	373.1	371.09	370.08	369.07	368.06
		367.06	359.09	358.08	357.11	356.1	355.09	354.08	353.08	352.07
		347.09	345.07	343.09	342.09	341.08	340.07	339.1	338.09	337.08
		333.07	329.08	327.1	325.08	324.08	323.08	320.08	317.08	315.06
		314.05	313.08	312.07	307.08	306.07	301.08	299.07	298.06	297.1
		294.1	285.1	283.07	282.06	279.06	278.05	273.1	271.08	270.07
		268.09	267.09	265.05	263.07	261.05	255.09	253.07	252.06	251.07
		250.08	249.05	247.03	237.08	235.07	233.06	231.04	221.06	209.06
		207.05	194.04	193.04	192.03	191.06	181.05	180.04	179.03	178.05
		177.04	167.07	165.05	164.05	163.04	150.05	147.04	146.04	135.04
		134.04	130.04	123.04	119.05	111.04	109.03	108.02	107.05	106.04
References	<p>Miguel, M.G. Betalains in Some Species of the Amaranthaceae Family: A Review. <i>Antioxidants</i> 2018, 7, 53.</p> <p>Xie, G.R.; Chen, H.J. Comprehensive Betalain Profiling of Djulis (<i>Chenopodium formosanum</i>) Cultivars Using HPLC-Q-Orbitrap High-Resolution Mass Spectrometry. <i>J. Agric. Food Chem.</i> 2021, 69, 15699–15715.</p> <p>Araujo-León, J.A.; Aguilar-Hernández, V.; Sánchez-del Pino, I.; Brito-Argáez, L.; Peraza-Sánchez, S.R.; Xingú-López, A.; Ortiz-Andrade, R. Analysis of Red Amaranth (<i>Amaranthus cruentus</i> L.) Betalains by LC-MS. <i>J. Mex. Chem. Soc.</i> 2023, 67, 227–239.</p>									

Melocactin-type

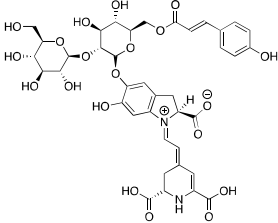
Melocactin

Chemical structure										
Name:	Melocactin (2'-O-glycosyl- betanin / Bougainvillein-r)									
Chemical Formula	C ₃₀ H ₃₆ N ₂ O ₁₈									
Molecular weight	712.61									
Monoisotopic mass	712.1963									
m/z [M+H]	713.2036									
Theoretical fragments (m/z)	713.2	712.2	711.19	710.18	697.21	696.2	695.19	694.19	693.18	685.21
		684.2	683.19	681.21	679.2	678.19	677.18	676.17	675.17	673.21
		671.19	669.21	668.21	667.2	666.19	665.18	663.2	661.19	660.18
		659.17	657.16	655.2	653.22	651.2	650.2	649.19	648.18	647.17
		643.2	641.18	640.17	639.2	638.2	637.19	633.19	632.18	631.18
		627.2	625.19	624.18	623.17	622.16	621.19	620.18	619.18	609.19
		607.18	605.16	591.18	589.17	587.15	551.15	550.14	549.14	544.17
		535.16	534.15	533.14	532.13	531.12	523.16	522.15	521.14	520.17
		519.16	518.15	517.14	516.14	515.13	514.12	513.11	511.16	509.14
		507.16	505.15	504.15	503.14	502.16	501.15	500.14	499.13	498.13
		497.12	495.1	493.15	491.13	489.15	488.14	487.14	486.14	485.13
		481.15	479.13	478.12	477.15	476.14	475.13	474.16	473.15	472.14
		471.14	470.13	469.13	468.13	465.15	463.13	461.12	460.11	459.15
		458.14	457.12	448.14	447.15	445.12	443.11	442.15	441.14	435.15
		433.13	432.13	430.15	429.14	427.11	425.1	417.14	416.13	415.12
		414.12	412.14	411.13	399.13	397.11	389.1	388.09	387.08	386.07
		375.12	373.1	372.1	371.09	370.08	369.07	361.1	360.1	359.12
		358.11	357.11	356.1	355.09	354.08	353.08	351.06	349.1	347.09
		345.11	343.13	342.09	341.11	340.1	339.1	338.09	337.08	335.09
		331.09	329.11	327.1	326.09	325.09	324.08	323.08	319.09	317.08
		316.07	315.1	314.09	313.08	307.08	306.07	303.1	301.08	300.07
		299.07	297.1	287.1	285.1	284.08	283.07	281.08	280.07	279.09
		273.1	271.08	270.07	269.09	268.09	267.06	265.08	264.07	263.07
		262.06	255.09	253.08	252.06	251.07	250.08	249.05	247.07	245.06
		237.09	235.07	233.06	231.04	223.07	211.07	207.08	205.06	196.06
		194.04	193.04	182.08	180.04	179.03	178.05	177.04	165.05	164.05
		163.04	147.04	146.04	135.04	134.04	130.04	123.04	119.05	111.04
		109.03	108.02	107.05	106.04					
References	<p>Piattelli, M; Imperato, F. Betacyanins from Bougainvillea. <i>Phytochemistry</i> 1970, 9, 455–458.</p> <p>Wybraniec, S.; Nowak-Wydra, B.; Mitka, K.; Kowalski, P.; Mizrahi, Y. Minor betalains in fruits of <i>Hylocereus</i> species. <i>Phytochemistry</i> 2007, 68, 251–259.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

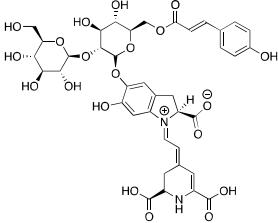
Isomelocactin

Chemical structure										
Name:	Isomelocactin (2'-O-glycosyl- isobetanan / isobougainvillein-r)									
Chemical Formula	C ₃₀ H ₃₆ N ₂ O ₁₈									
Molecular weight	712.61									
Monoisotopic mass	712.1963									
m/z [M+H]	713.2036									
Theoretical fragments (m/z)	713.2	712.2	711.19	710.18	697.21	696.2	695.19	694.19	693.18	685.21
		684.2	683.19	681.21	679.2	678.19	677.18	676.17	675.17	673.21
		671.19	669.21	668.21	667.2	666.19	665.18	663.2	661.19	660.18
		659.17	657.16	655.2	653.22	651.2	650.2	649.19	648.18	647.17
		643.2	641.18	640.17	639.2	638.2	637.19	633.19	632.18	631.18
		627.2	625.19	624.18	623.17	622.16	621.19	620.18	619.18	609.19
		607.18	605.16	591.18	589.17	587.15	551.15	550.14	549.14	544.17
		535.16	534.15	533.14	532.13	531.12	523.16	522.15	521.14	520.17
		519.16	518.15	517.14	516.14	515.13	514.12	513.11	511.16	509.14
		507.16	505.15	504.15	503.14	502.16	501.15	500.14	499.13	498.13
		497.12	495.1	493.15	491.13	489.15	488.14	487.14	486.14	485.13
		481.15	479.13	478.12	477.15	476.14	475.13	474.16	473.15	472.14
		471.14	470.13	469.13	468.13	465.15	463.13	461.12	460.11	459.15
		458.14	457.12	448.14	447.15	445.12	443.11	442.15	441.14	435.15
		433.13	432.13	430.15	429.14	427.11	425.1	417.14	416.13	415.12
		414.12	412.14	411.13	399.13	397.11	389.1	388.09	387.08	386.07
		375.12	373.1	372.1	371.09	370.08	369.07	361.1	360.1	359.12
		358.11	357.11	356.1	355.09	354.08	353.08	351.06	349.1	347.09
		345.11	343.13	342.09	341.11	340.1	339.1	338.09	337.08	335.09
		331.09	329.11	327.1	326.09	325.09	324.08	323.08	319.09	317.08
		316.07	315.1	314.09	313.08	307.08	306.07	303.1	301.08	300.07
		299.07	297.1	287.1	285.1	284.08	283.07	281.08	280.07	279.09
		273.1	271.08	270.07	269.09	268.09	267.06	265.08	264.07	263.07
		262.06	255.09	253.08	252.06	251.07	250.08	249.05	247.07	245.06
		237.09	235.07	233.06	231.04	223.07	211.07	207.08	205.06	196.06
		194.04	193.04	182.08	180.04	179.03	178.05	177.04	165.05	164.05
		163.04	147.04	146.04	135.04	134.04	130.04	123.04	119.05	111.04
		109.03	108.02	107.05	106.04					
References	<p>Piattelli, M; Imperato, F. Betacyanins from Bougainvillea. <i>Phytochemistry</i> 1970, 9, 455–458.</p> <p>Wybraniec, S.; Nowak-Wydra, B.; Mitka, K.; Kowalski, P.; Mizrahi, Y. Minor betalains in fruits of <i>Hylocereus</i> species. <i>Phytochemistry</i> 2007, 68, 251–259.</p> <p>Slimen, I.B.; Najjar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

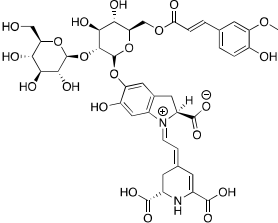
Bougainvillein-r III

Chemical structure										
Name:	Bougainvillein-r III									
Chemical Formula	C ₃₉ H ₄₂ N ₂ O ₂₀									
Molecular weight	858.76									
Monoisotopic mass	858.2331									
m/z [M+H]	859.2404									
Theoretical fragments (m/z)	859.24	858.23	857.22	856.22	843.25	842.24	841.23	840.22	839.21	831.25
		830.24	829.23	827.25	825.23	824.23	823.22	822.21	821.2	819.25
		817.23	815.25	814.24	813.23	812.23	811.22	809.24	807.22	806.22
		805.21	803.19	801.23	799.26	797.24	796.23	795.22	794.22	793.21
		789.23	787.22	786.21	785.24	784.23	783.22	779.23	778.22	777.21
		773.24	771.22	770.22	769.21	768.2	767.23	766.22	765.21	755.23
		753.21	751.2	737.22	735.2	733.19	697.19	696.18	695.19	694.19
		693.18	690.2	681.19	680.18	679.18	678.17	677.16	676.17	675.17
		669.19	668.18	667.18	666.2	665.18	664.19	663.18	662.17	661.17
		660.16	659.15	657.19	655.18	653.2	651.18	650.18	649.18	648.19
		647.19	646.18	645.17	644.16	643.16	641.14	639.18	637.19	635.19
		634.18	633.18	632.17	631.17	627.18	625.17	624.16	623.17	622.18
		621.17	620.2	619.19	618.18	617.18	616.17	615.17	614.16	611.19
		609.17	607.16	606.15	605.19	604.18	603.16	594.18	593.19	591.16
		589.15	588.18	587.18	581.19	579.17	578.16	576.18	575.18	573.15
		571.13	563.18	562.17	561.16	560.15	558.17	557.17	545.17	543.15
		533.14	532.13	531.12	517.15	515.13	514.12	513.11	505.15	504.15
		503.13	502.13	501.13	500.14	499.13	497.12	495.1	488.13	487.12
		486.14	485.13	484.12	483.12	481.12	479.11	475.13	471.13	470.12
		469.11	468.13	463.13	461.12	457.12	453.12	452.11	445.12	443.11
		441.14	431.13	429.14	427.11	425.12	419.13	417.14	416.11	415.12
		414.13	413.12	412.14	411.13	401.12	399.11	398.1	397.11	396.12
		395.11	389.1	388.09	387.08	386.07	383.11	381.1	375.12	373.1
		372.1	371.09	370.08	369.07	361.1	360.1	359.12	357.11	356.1
		355.09	354.08	353.08	351.06	349.1	347.09	345.11	343.13	342.08
		341.11	339.1	337.08	335.09	331.09	329.11	327.1	326.09	325.08
		324.08	319.09	317.08	316.07	315.1	314.09	313.08	306.07	303.1
		301.08	300.07	299.07	287.1	285.09	284.08	283.07	281.08	280.07
		271.11	269.09	267.06	265.08	264.07	263.07	262.06	255.09	253.08
		251.07	249.05	247.07	245.06	237.09	235.07	233.06	231.04	223.07
		211.07	207.08	205.06	196.06	194.04	193.04	182.08	180.04	179.03
		178.05	177.04	165.05	164.05	163.04	147.04	146.04	135.04	134.04
		130.04	123.04	119.05	111.04	109.03	108.02	107.05	106.04	
References	<p>Piattelli, M; Imperato, F. Betacyanins from Bougainvillea. <i>Phytochemistry</i> 1970, 9, 455–458.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

Isobougainvillein-r III

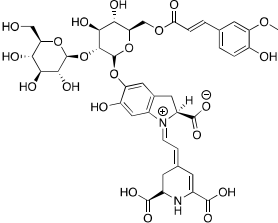
Chemical structure										
Name:	Isobougainvillein-r III									
Chemical Formula	C ₃₉ H ₄₂ N ₂ O ₂₀									
Molecular weight	858.76									
Monoisotopic mass	858.2331									
m/z [M+H]	859.2404									
Theoretical fragments (m/z)	859.24	858.23	857.22	856.22	843.25	842.24	841.23	840.22	839.21	831.25
		830.24	829.23	827.25	825.23	824.23	823.22	822.21	821.2	819.25
		817.23	815.25	814.24	813.23	812.23	811.22	809.24	807.22	806.22
		805.21	803.19	801.23	799.26	797.24	796.23	795.22	794.22	793.21
		789.23	787.22	786.21	785.24	784.23	783.22	779.23	778.22	777.21
		773.24	771.22	770.22	769.21	768.2	767.23	766.22	765.21	755.23
		753.21	751.2	737.22	735.2	733.19	697.19	696.18	695.19	694.19
		693.18	690.2	681.19	680.18	679.18	678.17	677.16	676.17	675.17
		669.19	668.18	667.18	666.2	665.18	664.19	663.18	662.17	661.17
		660.16	659.15	657.19	655.18	653.2	651.18	650.18	649.18	648.19
		647.19	646.18	645.17	644.16	643.16	641.14	639.18	637.19	635.19
		634.18	633.18	632.17	631.17	627.18	625.17	624.16	623.17	622.18
		621.17	620.2	619.19	618.18	617.18	616.17	615.17	614.16	611.19
		609.17	607.16	606.15	605.19	604.18	603.16	594.18	593.19	591.16
		589.15	588.18	587.18	581.19	579.17	578.16	576.18	575.18	573.15
		571.13	563.18	562.17	561.16	560.15	558.17	557.17	545.17	543.15
		533.14	532.13	531.12	517.15	515.13	514.12	513.11	505.15	504.15
		503.13	502.13	501.13	500.14	499.13	497.12	495.1	488.13	487.12
		486.14	485.13	484.12	483.12	481.12	479.11	475.13	471.13	470.12
		469.11	468.13	463.13	461.12	457.12	453.12	452.11	445.12	443.11
		441.14	431.13	429.14	427.11	425.12	419.13	417.14	416.11	415.12
		414.13	413.12	412.14	411.13	401.12	399.11	398.1	397.11	396.12
		395.11	389.1	388.09	387.08	386.07	383.11	381.1	375.12	373.1
		372.1	371.09	370.08	369.07	361.1	360.1	359.12	357.11	356.1
		355.09	354.08	353.08	351.06	349.1	347.09	345.11	343.13	342.08
		341.11	339.1	337.08	335.09	331.09	329.11	327.1	326.09	325.08
		324.08	319.09	317.08	316.07	315.1	314.09	313.08	306.07	303.1
		301.08	300.07	299.07	287.1	285.09	284.08	283.07	281.08	280.07
		271.11	269.09	267.06	265.08	264.07	263.07	262.06	255.09	253.08
		251.07	249.05	247.07	245.06	237.09	235.07	233.06	231.04	223.07
		211.07	207.08	205.06	196.06	194.04	193.04	182.08	180.04	179.03
		178.05	177.04	165.05	164.05	163.04	147.04	146.04	135.04	134.04
		130.04	123.04	119.05	111.04	109.03	108.02	107.05	106.04	
References	<p>Piattelli, M; Imperato, F. Betacyanins from Bougainvillea. <i>Phytochemistry</i> 1970, 9, 455–458.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

Feruloyl-bougainvillein-r I

Chemical structure										
Name:	Feruloyl-bougainvillein-r I									
Chemical Formula	C ₄₀ H ₄₄ N ₂ O ₂₁									
Molecular weight	888.79									
Monoisotopic mass	888.2437									
m/z [M+H]	889.2509									
Theoretical fragments (m/z)	889.25	888.24	887.24	886.23	873.26	872.25	871.24	870.23	869.22	861.26
		860.25	859.24	857.26	855.25	854.24	853.23	852.22	851.21	849.26
		847.24	845.26	844.25	843.25	842.24	841.23	839.25	837.23	836.23
		835.22	833.2	831.25	829.27	827.25	826.24	825.23	824.23	823.22
		819.25	817.23	816.22	815.25	814.24	813.23	809.24	808.23	807.22
		803.25	801.23	800.23	799.22	798.21	797.24	796.23	795.22	785.24
		783.22	781.21	767.23	765.21	763.2	727.2	726.19	725.18	720.21
		711.2	710.2	709.19	708.18	707.17	699.2	698.2	697.19	696.21
		695.19	694.2	693.19	692.18	691.18	690.17	689.16	687.2	685.19
		683.21	681.19	680.19	679.2	678.2	677.18	676.19	675.18	674.17
		673.17	671.15	669.19	667.2	666.19	665.18	664.19	663.19	662.18
		661.19	660.18	659.17	657.19	655.18	654.17	653.2	652.19	651.18
		650.21	649.19	648.19	647.19	646.18	645.18	644.17	643.18	641.2
		639.18	637.17	636.16	635.2	634.19	633.17	632.18	631.18	625.19
		624.19	623.2	622.16	621.17	620.18	619.16	618.19	617.19	611.2
		609.18	608.17	607.18	606.19	605.19	603.16	601.15	593.19	592.18
		591.17	590.16	589.17	588.18	587.18	575.18	573.16	534.16	533.14
		532.14	531.12	518.14	517.15	516.15	515.13	514.13	513.11	505.15
		503.13	502.16	501.14	500.13	499.13	497.12	495.1	487.13	486.14
		485.13	483.13	482.12	481.12	479.11	475.13	473.14	469.13	468.13
		463.13	461.14	457.12	455.13	449.14	447.13	446.12	445.12	444.14
		443.13	441.14	431.13	429.14	428.11	427.11	426.13	425.12	417.14
		415.12	414.12	413.12	412.14	411.13	399.13	397.11	389.1	388.09
		387.08	386.07	375.12	373.1	372.1	371.09	370.08	369.07	361.1
		360.1	359.12	357.11	356.1	355.09	354.08	353.08	351.06	349.1
		347.09	345.11	343.13	342.08	341.11	339.1	337.08	335.09	331.09
		329.11	327.1	326.09	325.08	324.08	319.09	317.08	316.07	315.1
		314.09	313.08	306.07	303.1	301.08	300.07	299.07	287.1	285.09
		284.08	283.07	281.08	280.07	271.11	269.09	267.06	265.08	264.07
		263.07	262.06	255.09	253.08	251.07	249.05	247.07	245.06	237.09
		235.07	233.06	231.04	223.07	211.07	207.08	205.06	196.06	194.04
		193.04	182.08	180.04	179.03	178.05	177.04	165.05	164.05	163.04
		147.04	146.04	135.04	134.04	130.04	123.04	119.05	111.04	109.03
		108.02	107.05	106.04						
References	<p>Vogt, T.; Ibdah, M.; Schmidt, J.; Wray, V.; Nimtz, M.; Strack, D. Light-induced betacyanin and flavonol accumulation in bladder cells of <i>Mesembryanthemum crystallinum</i>. <i>Phytochemistry</i> 1999, 52, 583–592.</p> <p>Kugler, F.; Stintzing, F.C.; Carle, R. Identification of betalains from petioles of differently colored Swiss chard (<i>Beta vulgaris</i> L. ssp. <i>cicla</i> Alef. Cv. Bright Lights) by high-performance liquid chromatography-electrospray ionization mass spectrometry. <i>J. Agric. Food Chem.</i> 2004, 52, 2975–2981.</p> <p>Svenson, J.; Smallfield, B.M.; Joyce, N.I.; Sanson, C.E.; Perry, N.B. Betalains in red and yellow varieties of the Andean tuber crop ulluco (<i>Ullucus tuberosus</i>). <i>J. Agric. Food Chem.</i> 2008, 56, 7730–7737.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p>									

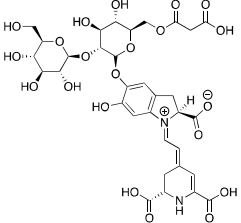
	Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021 , 38, 2315–2346.
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Feruloyl-isobougainvillein-r I

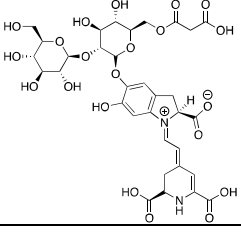
Chemical structure										
Name:	Feruloyl-isobougainvillein-r I									
Chemical Formula	C ₄₀ H ₄₄ N ₂ O ₂₁									
Molecular weight	888.79									
Monoisotopic mass	888.2437									
m/z [M+H]	889.2509									
Theoretical fragments (m/z)	889.25	888.24	887.24	886.23	873.26	872.25	871.24	870.23	869.22	861.26
		860.25	859.24	857.26	855.25	854.24	853.23	852.22	851.21	849.26
		847.24	845.26	844.25	843.25	842.24	841.23	839.25	837.23	836.23
		835.22	833.2	831.25	829.27	827.25	826.24	825.23	824.23	823.22
		819.25	817.23	816.22	815.25	814.24	813.23	809.24	808.23	807.22
		803.25	801.23	800.23	799.22	798.21	797.24	796.23	795.22	785.24
		783.22	781.21	767.23	765.21	763.2	727.2	726.19	725.18	720.21
		711.2	710.2	709.19	708.18	707.17	699.2	698.2	697.19	696.21
		695.19	694.2	693.19	692.18	691.18	690.17	689.16	687.2	685.19
		683.21	681.19	680.19	679.2	678.2	677.18	676.19	675.18	674.17
		673.17	671.15	669.19	667.2	666.19	665.18	664.19	663.19	662.18
		661.19	660.18	659.17	657.19	655.18	654.17	653.2	652.19	651.18
		650.21	649.19	648.19	647.19	646.18	645.18	644.17	643.18	641.2
		639.18	637.17	636.16	635.2	634.19	633.17	632.18	631.18	625.19
		624.19	623.2	622.16	621.17	620.18	619.16	618.19	617.19	611.2
		609.18	608.17	607.18	606.19	605.19	603.16	601.15	593.19	592.18
		591.17	590.16	589.17	588.18	587.18	575.18	573.16	534.16	533.14
		532.14	531.12	518.14	517.15	516.15	515.13	514.13	513.11	505.15
		503.13	502.16	501.14	500.13	499.13	497.12	495.1	487.13	486.14
		485.13	483.13	482.12	481.12	479.11	475.13	473.14	469.13	468.13
		463.13	461.14	457.12	455.13	449.14	447.13	446.12	445.12	444.14
		443.13	441.14	431.13	429.14	428.11	427.11	426.13	425.12	417.14
		415.12	414.12	413.12	412.14	411.13	399.13	397.11	389.1	388.09
		387.08	386.07	375.12	373.1	372.1	371.09	370.08	369.07	361.1
		360.1	359.12	357.11	356.1	355.09	354.08	353.08	351.06	349.1
		347.09	345.11	343.13	342.08	341.11	339.1	337.08	335.09	331.09
		329.11	327.1	326.09	325.08	324.08	319.09	317.08	316.07	315.1
		314.09	313.08	306.07	303.1	301.08	300.07	299.07	287.1	285.09
		284.08	283.07	281.08	280.07	271.11	269.09	267.06	265.08	264.07
		263.07	262.06	255.09	253.08	251.07	249.05	247.07	245.06	237.09
		235.07	233.06	231.04	223.07	211.07	207.08	205.06	196.06	194.04
		193.04	182.08	180.04	179.03	178.05	177.04	165.05	164.05	163.04
		147.04	146.04	135.04	134.04	130.04	123.04	119.05	111.04	109.03
		108.02	107.05	106.04						
References	<p>Vogt, T.; Ibdah, M.; Schmidt, J.; Wray, V.; Nimtz, M.; Strack, D. Light-induced betacyanin and flavonol accumulation in bladder cells of <i>Mesembryanthemum crystallinum</i>. <i>Phytochemistry</i> 1999, 52, 583–592.</p> <p>Kugler, F.; Stintzing, F.C.; Carle, R. Identification of betalains from petioles of differently colored Swiss chard (<i>Beta vulgaris</i> L. ssp. <i>cicla</i> Alef. Cv. Bright Lights) by high-performance liquid chromatography-electrospray ionization mass spectrometry. <i>J. Agric. Food Chem.</i> 2004, 52, 2975–2981.</p> <p>Svenson, J.; Smallfield, B.M.; Joyce, N.I.; Sanson, C.E.; Perry, N.B. Betalains in red and yellow varieties of the Andean tuber crop ulluco (<i>Ullucus tuberosus</i>). <i>J. Agric. Food Chem.</i> 2008, 56, 7730–7737.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p>									

	Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021 , 38, 2315–2346.
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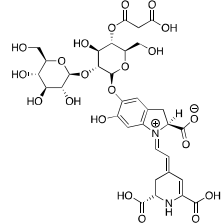
Mammillarinin

Chemical structure										
Name:	Mammillarinin									
Chemical Formula	C ₃₃ H ₃₈ N ₂ O ₂₁									
Molecular weight	798.66									
Monoisotopic mass	798.1967									
m/z [M+H]	799.2040									
Theoretical fragments (m/z)	799.2	798.2	797.19	796.18	783.21	782.2	781.19	780.19	779.18	771.21
		770.2	769.19	767.21	765.2	764.19	763.18	761.17	759.21	757.19
		755.21	754.21	753.2	752.19	751.18	749.2	747.19	745.17	741.2
		739.22	737.2	736.2	735.19	729.2	727.18	726.18	725.2	724.2
		723.19	713.2	712.2	711.19	710.18	709.17	697.21	695.19	694.19
		693.18	691.16	685.21	683.19	681.21	679.2	677.18	675.17	669.21
		667.2	665.18	663.2	661.19	659.17	655.2	651.2	649.19	643.2
		641.18	637.15	636.14	635.14	630.17	625.19	623.17	621.16	619.14
		618.13	617.12	609.16	607.14	606.17	605.16	604.15	603.14	601.13
		599.11	593.16	591.15	590.15	589.14	588.16	587.15	586.14	585.14
		583.12	579.15	575.15	574.15	573.15	572.14	571.13	567.15	565.13
		561.14	560.16	559.15	558.15	557.15	556.14	555.13	554.13	551.15
		549.14	547.12	545.15	544.14	535.16	534.15	533.15	531.12	529.11
		528.15	527.14	521.15	520.17	519.13	518.13	517.16	516.15	515.13
		513.11	505.16	504.15	503.14	502.16	501.12	500.14	499.13	498.14
		497.12	487.14	486.14	485.13	479.13	469.13	468.13	461.12	459.15
		447.15	444.11	443.11	442.1	441.09	435.15	433.13	432.13	430.15
		429.14	428.09	427.09	426.1	424.09	423.08	417.14	415.12	414.12
		412.1	411.09	410.08	409.08	399.13	394.09	393.08	392.07	389.1
		388.09	387.08	386.07	383.1	375.12	373.1	372.1	371.09	370.08
		369.07	365.09	361.1	360.1	359.12	357.11	356.1	355.09	354.09
		353.09	351.06	349.1	347.09	345.11	343.13	342.08	341.11	339.1
		338.06	337.08	336.08	335.08	331.09	329.11	327.1	326.09	325.09
		324.08	323.08	319.09	317.08	316.07	315.1	314.09	313.08	306.07
		303.1	301.08	300.07	299.07	287.1	285.09	284.08	283.07	281.08
		280.07	273.1	271.11	269.09	267.06	265.08	264.07	263.07	262.06
		255.09	253.08	251.07	249.05	247.07	245.06	237.09	235.07	233.06
		231.04	223.07	211.07	207.08	205.06	196.06	194.04	193.04	182.08
		180.04	179.03	178.05	177.04	165.05	164.05	163.04	147.04	146.04
		135.04	134.04	130.04	123.04	119.05	111.04	109.03	108.02	107.05
		106.04								
References	<p>Wybraniec, S.; Nowak-Wydra, B. Mammillarinin—A new malonylated betacyanin in fruits of Mammillaria. <i>J. Agric. Food Chem.</i> 2007, 55, 8138–8143.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

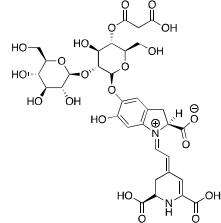
Isomammillarinin

Chemical structure										
Name:	Isomammillarinin									
Chemical Formula	C ₃₃ H ₃₈ N ₂ O ₂₁									
Molecular weight	798.66									
Monoisotopic mass	798.1967									
m/z [M+H]	799.2040									
Theoretical fragments (m/z)	799.2	798.2	797.19	796.18	783.21	782.2	781.19	780.19	779.18	771.21
		770.2	769.19	767.21	765.2	764.19	763.18	761.17	759.21	757.19
		755.21	754.21	753.2	752.19	751.18	749.2	747.19	745.17	741.2
		739.22	737.2	736.2	735.19	729.2	727.18	726.18	725.2	724.2
		723.19	713.2	712.2	711.19	710.18	709.17	697.21	695.19	694.19
		693.18	691.16	685.21	683.19	681.21	679.2	677.18	675.17	669.21
		667.2	665.18	663.2	661.19	659.17	655.2	651.2	649.19	643.2
		641.18	637.15	636.14	635.14	630.17	625.19	623.17	621.16	619.14
		618.13	617.12	609.16	607.14	606.17	605.16	604.15	603.14	601.13
		599.11	593.16	591.15	590.15	589.14	588.16	587.15	586.14	585.14
		583.12	579.15	575.15	574.15	573.15	572.14	571.13	567.15	565.13
		561.14	560.16	559.15	558.15	557.15	556.14	555.13	554.13	551.15
		549.14	547.12	545.15	544.14	535.16	534.15	533.15	531.12	529.11
		528.15	527.14	521.15	520.17	519.13	518.13	517.16	516.15	515.13
		513.11	505.16	504.15	503.14	502.16	501.12	500.14	499.13	498.14
		497.12	487.14	486.14	485.13	479.13	469.13	468.13	461.12	459.15
		447.15	444.11	443.11	442.1	441.09	435.15	433.13	432.13	430.15
		429.14	428.09	427.09	426.1	424.09	423.08	417.14	415.12	414.12
		412.1	411.09	410.08	409.08	399.13	394.09	393.08	392.07	389.1
		388.09	387.08	386.07	383.1	375.12	373.1	372.1	371.09	370.08
		369.07	365.09	361.1	360.1	359.12	357.11	356.1	355.09	354.09
		353.09	351.06	349.1	347.09	345.11	343.13	342.08	341.11	339.1
		338.06	337.08	336.08	335.08	331.09	329.11	327.1	326.09	325.09
		324.08	323.08	319.09	317.08	316.07	315.1	314.09	313.08	306.07
		303.1	301.08	300.07	299.07	287.1	285.09	284.08	283.07	281.08
		280.07	273.1	271.11	269.09	267.06	265.08	264.07	263.07	262.06
		255.09	253.08	251.07	249.05	247.07	245.06	237.09	235.07	233.06
		231.04	223.07	211.07	207.08	205.06	196.06	194.04	193.04	182.08
		180.04	179.03	178.05	177.04	165.05	164.05	163.04	147.04	146.04
		135.04	134.04	130.04	123.04	119.05	111.04	109.03	108.02	107.05
		106.04								
References	<p>Wybraniec, S.; Nowak-Wydra, B. Mammillarinin—A new malonylated betacyanin in fruits of Mammillaria. <i>J. Agric. Food Chem.</i> 2007, 55, 8138–8143.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

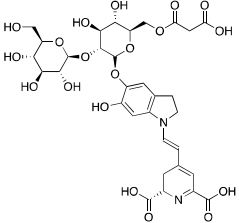
4'-O-Malonyl-bougainvillein-r I

Chemical structure										
Name:	4'-O-Malonyl-bougainvillein-r I									
Chemical Formula	C ₃₃ H ₃₈ N ₂ O ₂₁									
Molecular weight	798.66									
Monoisotopic mass	798.1967									
m/z [M+H]	799.2040									
Theoretical fragments (m/z)	799.2	798.2	797.19	796.18	783.21	782.2	781.19	780.19	779.18	771.21
		770.2	769.19	767.21	765.2	764.19	763.18	761.17	759.21	757.19
		755.21	754.21	753.2	752.19	751.18	749.2	747.19	745.17	741.2
		739.22	737.2	736.2	735.19	729.2	727.18	726.18	725.2	724.2
		723.19	713.2	712.2	711.19	710.18	709.17	697.21	695.19	694.19
		693.18	691.16	685.21	683.19	681.21	679.2	677.18	675.17	669.21
		667.2	665.18	663.2	661.19	659.17	655.2	651.2	649.19	643.2
		641.18	637.15	636.14	635.14	630.17	625.19	623.17	621.16	619.14
		618.13	617.12	609.16	607.14	606.17	605.16	604.15	603.14	601.13
		599.11	593.16	591.15	590.15	589.14	588.16	587.15	586.14	585.14
		583.12	579.15	575.15	574.15	573.15	572.14	571.13	567.15	565.13
		561.14	560.16	559.15	558.15	557.15	556.14	555.13	554.13	551.15
		549.14	547.12	545.15	544.14	535.16	534.15	533.15	531.12	529.11
		528.15	527.14	521.15	520.17	519.13	518.13	517.16	516.15	515.13
		513.11	505.16	504.15	503.14	502.16	501.12	500.14	499.13	498.14
		497.12	487.14	486.14	485.13	479.13	469.13	468.13	461.12	459.15
		447.15	444.11	443.11	442.1	441.09	435.15	433.13	432.13	430.15
		429.14	428.09	427.09	426.1	424.09	423.08	417.14	415.12	414.12
		412.1	411.09	410.08	409.08	399.13	394.09	393.08	392.07	389.1
		388.09	387.08	386.07	383.1	375.12	373.1	372.1	371.09	370.08
		369.07	365.09	361.1	360.1	359.12	357.11	356.1	355.09	354.09
		353.09	351.06	349.1	347.09	345.11	343.13	342.08	341.11	339.1
		338.06	337.08	336.08	335.08	331.09	329.11	327.1	326.09	325.09
		324.08	323.08	319.09	317.08	316.07	315.1	314.09	313.08	306.07
		303.1	301.08	300.07	299.07	287.1	285.09	284.08	283.07	281.08
		280.07	273.1	271.11	269.09	267.06	265.08	264.07	263.07	262.06
		255.09	253.08	251.07	249.05	247.07	245.06	237.09	235.07	233.06
		231.04	223.07	211.07	207.08	205.06	196.06	194.04	193.04	182.08
		180.04	179.03	178.05	177.04	165.05	164.05	163.04	147.04	146.04
		135.04	134.04	130.04	123.04	119.05	111.04	109.03	108.02	107.05
		106.04								
References	<p>Wybraniec, S.; Nowak-Wydra, B. Mammillarinin—A new malonylated betacyanin in fruits of Mammillaria. <i>J. Agric. Food Chem.</i> 2007, 55, 8138–8143.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

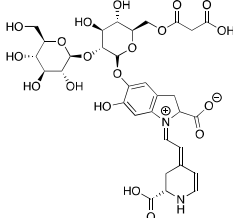
4'-O-Malonyl-isobougainvillein-r I

Chemical structure										
Name:	4'-O-Malonyl-isobougainvillein-r I									
Chemical Formula	C ₃₃ H ₃₈ N ₂ O ₂₁									
Molecular weight	798.66									
Monoisotopic mass	798.1967									
m/z [M+H]	799.2040									
Theoretical fragments (m/z)	799.2	798.2	797.19	796.18	783.21	782.2	781.19	780.19	779.18	771.21
		770.2	769.19	767.21	765.2	764.19	763.18	761.17	759.21	757.19
		755.21	754.21	753.2	752.19	751.18	749.2	747.19	745.17	741.2
		739.22	737.2	736.2	735.19	729.2	727.18	726.18	725.2	724.2
		723.19	713.2	712.2	711.19	710.18	709.17	697.21	695.19	694.19
		693.18	691.16	685.21	683.19	681.21	679.2	677.18	675.17	669.21
		667.2	665.18	663.2	661.19	659.17	655.2	651.2	649.19	643.2
		641.18	637.15	636.14	635.14	630.17	625.19	623.17	621.16	619.14
		618.13	617.12	609.16	607.14	606.17	605.16	604.15	603.14	601.13
		599.11	593.16	591.15	590.15	589.14	588.16	587.15	586.14	585.14
		583.12	579.15	575.15	574.15	573.15	572.14	571.13	567.15	565.13
		561.14	560.16	559.15	558.15	557.15	556.14	555.13	554.13	551.15
		549.14	547.12	545.15	544.14	535.16	534.15	533.15	531.12	529.11
		528.15	527.14	521.15	520.17	519.13	518.13	517.16	516.15	515.13
		513.11	505.16	504.15	503.14	502.16	501.12	500.14	499.13	498.14
		497.12	487.14	486.14	485.13	479.13	469.13	468.13	461.12	459.15
		447.15	444.11	443.11	442.1	441.09	435.15	433.13	432.13	430.15
		429.14	428.09	427.09	426.1	424.09	423.08	417.14	415.12	414.12
		412.1	411.09	410.08	409.08	399.13	394.09	393.08	392.07	389.1
		388.09	387.08	386.07	383.1	375.12	373.1	372.1	371.09	370.08
		369.07	365.09	361.1	360.1	359.12	357.11	356.1	355.09	354.09
		353.09	351.06	349.1	347.09	345.11	343.13	342.08	341.11	339.1
		338.06	337.08	336.08	335.08	331.09	329.11	327.1	326.09	325.09
		324.08	323.08	319.09	317.08	316.07	315.1	314.09	313.08	306.07
		303.1	301.08	300.07	299.07	287.1	285.09	284.08	283.07	281.08
		280.07	273.1	271.11	269.09	267.06	265.08	264.07	263.07	262.06
		255.09	253.08	251.07	249.05	247.07	245.06	237.09	235.07	233.06
		231.04	223.07	211.07	207.08	205.06	196.06	194.04	193.04	182.08
		180.04	179.03	178.05	177.04	165.05	164.05	163.04	147.04	146.04
		135.04	134.04	130.04	123.04	119.05	111.04	109.03	108.02	107.05
		106.04								
References	<p>Wybraniec, S.; Nowak-Wydra, B. Mammillarinin—A new malonylated betacyanin in fruits of Mammillaria. <i>J. Agric. Food Chem.</i> 2007, 55, 8138–8143.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

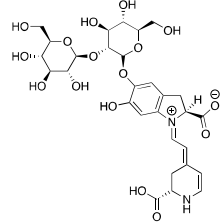
2-decarboxy-mammillarinin

Chemical structure										
Name:	2-decarboxy-mammillarinin									
Chemical Formula	C ₃₂ H ₃₈ N ₂ O ₁₉									
Molecular weight	754.65									
Monoisotopic mass	754.2069									
m/z [M+H]	755.2142									
Theoretical fragments (m/z)	755.21	754.21	753.2	752.19	741.2	739.22	738.21	737.2	735.19	729.2
		727.18	726.18	725.2	724.2	723.19	721.21	719.19	717.18	713.2
		711.19	710.18	709.17	708.2	707.19	706.19	705.18	703.2	701.18
		695.19	693.18	692.17	691.16	690.19	689.18	688.17	687.2	685.19
		683.17	677.18	675.17	673.15	669.21	667.2	655.2	653.22	651.2
		649.19	643.2	641.18	639.2	638.2	637.19	635.21	633.19	631.18
		625.19	623.17	621.19	620.18	619.18	617.2	615.18	607.18	605.16
		603.18	602.17	601.17	599.19	597.17	593.16	591.15	589.17	587.15
		586.18	579.15	577.17	575.15	573.14	567.15	565.13	564.12	563.15
		562.18	561.14	560.16	559.15	557.14	555.12	551.15	549.14	548.16
		547.12	546.18	545.15	544.13	543.12	542.15	541.15	539.13	534.15
		533.15	531.12	530.12	529.11	528.14	527.14	526.12	525.15	523.13
		521.15	519.13	518.13	517.16	516.15	515.14	513.11	511.1	509.13
		507.16	505.16	503.14	502.13	501.12	500.12	499.14	498.14	497.13
		493.15	491.17	489.15	487.13	485.13	483.11	481.15	479.13	477.15
		476.18	475.13	474.16	473.16	471.14	469.12	463.13	461.12	459.15
		458.17	457.12	456.15	455.14	453.13	447.15	445.12	443.11	441.14
		440.12	439.11	437.13	435.15	433.13	432.13	430.15	429.14	427.11
		425.1	423.13	417.14	415.12	414.12	412.14	411.13	400.12	399.13
		398.11	397.1	383.1	382.11	380.1	379.09	371.1	367.1	365.09
		359.1	357.08	356.07	355.1	354.09	353.09	349.09	347.08	345.11
		344.1	343.09	342.08	341.09	339.07	338.06	337.09	336.08	335.08
		331.13	329.11	328.11	327.1	326.09	325.08	323.08	321.06	319.09
		317.08	316.07	315.13	314.09	313.12	312.11	311.1	309.09	303.1
		301.08	300.07	299.07	298.09	297.09	296.08	295.11	287.1	285.09
		284.08	283.07	279.09	273.1	271.11	269.09	267.09	261.08	255.09
		253.07	249.08	237.09	236.08	235.06	223.07	221.09	220.08	219.08
		218.07	211.07	207.08	205.06	196.06	194.04	152.07	150.05	149.05
		138.09	136.08	135.04	134.06	133.05	123.04	121.06	119.05	111.04
		109.03	108.02	107.05	106.04					
References	<p>Wybraniec, S.; Nowak-Wydra, B. Mammillarinin—A new malonylated betacyanin in fruits of Mammillaria. <i>J. Agric. Food Chem.</i> 2007, 55, 8138–8143.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

17-decarboxy-mammillarinin

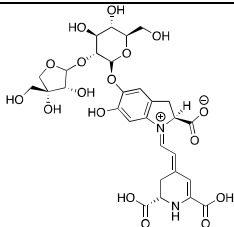
Chemical structure										
Name:	17-decarboxy-mammillarinin									
Chemical Formula	C ₃₂ H ₃₈ N ₂ O ₁₉									
Molecular weight	754.65									
Monoisotopic mass	754.2069									
m/z [M+H]	755.2142									
Theoretical fragments (m/z)	755.21	754.21	753.2	752.19	741.2	739.22	738.21	737.2	735.19	729.2
		727.18	726.18	725.2	724.2	723.19	721.21	719.19	717.18	713.2
		711.19	710.18	709.17	708.2	707.19	706.19	705.18	703.2	701.18
		695.19	693.18	692.17	691.16	690.19	689.18	688.17	687.2	685.19
		683.17	677.18	675.17	673.15	669.21	667.2	655.2	653.22	651.2
		649.19	643.2	641.18	639.2	638.2	637.19	635.21	633.19	631.18
		625.19	623.17	621.19	620.18	619.18	617.2	615.18	607.18	605.16
		603.18	602.17	601.17	599.19	597.17	593.16	591.15	589.17	587.15
		586.18	579.15	577.17	575.15	573.14	567.15	565.13	564.12	563.15
		562.18	561.14	560.16	559.15	557.14	555.12	551.15	549.14	548.16
		547.12	546.18	545.15	544.13	543.12	542.15	541.15	539.13	534.15
		533.15	531.12	530.12	529.11	528.14	527.14	526.12	525.15	523.13
		521.15	519.13	518.13	517.16	516.15	515.14	513.11	511.1	509.13
		507.16	505.16	503.14	502.13	501.12	500.12	499.14	498.14	497.13
		493.15	491.17	489.15	487.13	485.13	483.11	481.15	479.13	477.15
		476.18	475.13	474.16	473.16	471.14	469.12	463.13	461.12	459.15
		458.17	457.12	456.15	455.14	453.13	447.15	445.12	443.11	441.14
		440.12	439.11	437.13	435.15	433.13	432.13	430.15	429.14	427.11
		425.1	423.13	417.14	415.12	414.12	412.14	411.13	400.12	399.13
		398.11	397.1	383.1	382.11	380.1	379.09	371.1	367.1	365.09
		359.1	357.08	356.07	355.1	354.09	353.09	349.09	347.08	345.11
		344.1	343.09	342.08	341.09	339.07	338.06	337.09	336.08	335.08
		331.13	329.11	328.11	327.1	326.09	325.08	323.08	321.06	319.09
		317.08	316.07	315.13	314.09	313.12	312.11	311.1	309.09	303.1
		301.08	300.07	299.07	298.09	297.09	296.08	295.11	287.1	285.09
		284.08	283.07	279.09	273.1	271.11	269.09	267.09	261.08	255.09
		253.07	249.08	237.09	236.08	235.06	223.07	221.09	220.08	219.08
		218.07	211.07	207.08	205.06	196.06	194.04	152.07	150.05	149.05
		138.09	136.08	135.04	134.06	133.05	123.04	121.06	119.05	111.04
		109.03	108.02	107.05	106.04					
References	<p>Wybraniec, S.; Nowak-Wydra, B. Mammillarinin—A new malonylated betacyanin in fruits of Mammillaria. <i>J. Agric. Food Chem.</i> 2007, 55, 8138–8143.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

17-decarboxy-melocactin

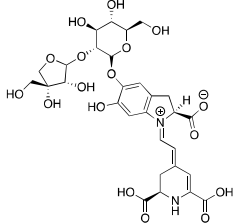
Chemical structure										
Name:	17-decarboxy-melocactin (17-decarboxy-bougainvillein-r)									
Chemical Formula	C ₂₉ H ₃₆ N ₂ O ₁₆									
Molecular weight	668.61									
Monoisotopic mass	668.2065									
m/z [M+H]	669.2138									
Theoretical fragments (m/z)	669.21	668.21	667.2	666.19	653.22	652.21	651.2	650.2	649.19	641.22
		640.21	639.2	637.22	635.21	634.2	633.19	632.18	631.18	629.22
		627.2	625.22	624.22	623.21	622.2	621.19	619.21	617.2	616.19
		615.18	613.17	611.21	609.23	607.21	606.21	605.2	604.19	603.18
		599.21	597.19	596.18	595.21	594.21	593.2	589.2	588.19	587.19
		583.21	581.2	580.19	579.18	578.17	577.2	576.19	575.19	565.2
		563.19	561.17	547.19	545.18	544.17	543.16	531.16	520.17	518.15
		517.14	507.16	506.15	505.15	504.15	503.14	502.16	500.14	499.13
		491.17	490.16	489.15	488.14	487.13	486.14	485.13	479.17	478.16
		477.15	475.17	474.16	473.16	472.14	471.14	470.13	469.12	468.13
		467.17	465.15	463.17	461.16	460.15	459.15	458.14	457.16	455.14
		454.14	453.13	451.11	449.16	448.14	447.15	445.16	444.15	443.14
		442.15	441.14	437.16	435.15	434.13	433.13	432.13	431.14	430.15
		429.14	427.15	426.14	425.13	421.16	419.14	417.13	416.13	415.12
		414.12	413.13	412.14	411.13	403.15	401.13	399.12	397.11	385.14
		383.12	381.11	358.11	356.1	355.09	345.11	344.1	343.09	342.09
		341.09	340.1	338.09	337.08	331.13	329.11	328.11	327.1	326.09
		325.08	324.08	323.08	317.11	316.11	315.13	313.12	312.11	311.1
		310.09	309.09	307.08	306.07	305.11	303.1	301.12	299.14	298.09
		297.12	295.11	293.09	291.1	287.1	285.1	283.11	282.1	281.09
		279.09	275.1	273.09	272.08	271.08	270.07	269.09	268.09	267.09
		259.11	257.09	256.08	255.09	253.07	252.06	250.08	249.08	243.11
		241.1	240.09	239.08	237.09	236.08	235.06	227.12	225.1	223.07
		221.09	220.08	219.08	218.07	209.09	207.08	205.06	203.08	201.07
		196.06	194.04	193.1	191.08	189.07	187.05	182.08	180.04	179.08
		178.05	177.04	167.08	165.05	164.05	163.09	161.07	152.07	150.05
		147.04	146.04	135.04	134.04	130.04	123.04	119.05	111.04	109.03
		108.02	107.05	106.04						
References	<p>Wybraniec, S.; Nowak-Wydra, B. Mammillarinin—A new malonylated betacyanin in fruits of Mammillaria. <i>J. Agric. Food Chem.</i> 2007, 55, 8138–8143.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

Apiocactin-type

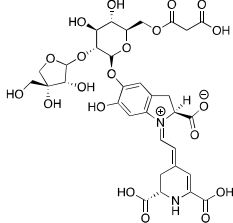
Apiocactin

Chemical structure										
Name:	Apiocactin (2'-O-Apiosyl- betanin)									
Chemical Formula	C ₂₉ H ₃₄ N ₂ O ₁₇									
Molecular weight	682.59									
Monoisotopic mass	682.1857									
m/z [M+H]	683.1930									
Theoretical fragments (m/z)	683.19	682.19	681.18	680.17	667.2	666.19	665.18	664.17	663.17	655.2
		654.19	653.18	651.2	650.2	649.19	648.18	647.17	646.16	645.16
		643.2	641.18	640.17	639.2	638.2	637.19	636.18	635.17	633.19
		632.18	631.18	630.17	629.16	627.15	625.19	623.21	621.19	620.18
		619.18	618.17	617.16	615.18	613.19	611.17	610.16	609.19	608.18
		607.18	605.2	604.19	603.18	602.17	601.17	597.19	595.18	594.17
		593.16	592.15	591.18	590.17	589.17	579.18	577.17	575.15	561.17
		559.16	557.14	551.15	550.14	549.14	535.16	534.15	533.14	532.13
		531.12	523.16	522.15	521.14	519.16	517.15	516.14	515.13	514.16
		513.11	511.16	509.14	507.16	505.15	504.14	503.13	501.15	499.13
		498.13	497.12	496.14	495.1	493.15	491.13	490.16	489.15	488.14
		487.13	486.13	485.12	483.14	481.15	479.13	478.12	477.15	476.14
		475.13	474.14	473.13	472.14	471.14	470.13	469.12	465.15	463.13
		462.16	461.12	460.11	459.14	458.13	457.13	456.13	455.12	454.13
		452.12	447.14	445.12	444.15	443.11	442.13	439.12	438.12	432.15
		431.12	429.14	428.13	427.11	426.14	425.1	420.15	418.13	417.14
		412.14	411.13	405.14	403.12	402.12	400.14	399.13	389.1	388.09
		387.08	386.07	385.11	384.11	382.13	381.12	375.12	373.1	372.1
		371.09	370.08	369.07	367.1	361.1	360.1	359.12	358.11	357.11
		356.1	355.09	354.08	353.08	351.06	349.1	347.09	345.11	344.1
		343.13	342.09	341.11	340.1	339.1	338.09	337.08	335.09	331.09
		329.11	327.1	326.09	325.09	324.08	323.08	322.09	320.08	319.09
		317.08	316.07	315.1	314.09	313.08	312.11	311.1	307.08	306.07
		303.1	301.08	300.07	299.07	298.06	297.1	295.1	294.1	287.1
		286.09	285.1	284.08	283.07	282.06	281.08	280.07	279.09	273.1
		271.08	270.07	269.09	268.09	267.06	265.08	264.07	263.07	262.06
		255.09	253.08	252.06	251.07	250.08	249.05	247.07	245.06	237.09
		235.07	233.06	231.04	223.07	222.06	220.06	211.07	207.08	205.06
		196.06	195.05	194.04	193.04	192.03	182.08	180.04	179.03	178.05
		177.04	166.09	165.05	164.05	163.04	150.05	147.04	146.04	135.04
		134.04	130.04	124.04	123.04	119.05	111.04	110.06	109.03	108.02
		107.05	106.04							
References	<p>Kobayashi, N.; Schmidt, J.; Nimtz, M.; Wray, V.; Schliemann, W. Betalains from <i>Christmas cactus</i>. <i>Phytochemistry</i> 2000, 54, 419–426.</p> <p>Wybraniec, S.; Nowak-Wydra, B.; Mitka, K.; Kowalski, P.; Mizrahi, Y. Minor betalains in fruits of <i>Hylocereus</i> species. <i>Phytochemistry</i> 2007, 68, 251–259.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

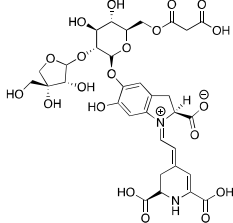
Isoapiocactin

Chemical structure										
Name:	Isoapiocactin (2'-O-Apiosyl- betanin)									
Chemical Formula	C ₂₉ H ₃₄ N ₂ O ₁₇									
Molecular weight	682.59									
Monoisotopic mass	682.1857									
m/z [M+H]	683.1930									
Theoretical fragments (m/z)	683.19	682.19	681.18	680.17	667.2	666.19	665.18	664.17	663.17	655.2
		654.19	653.18	651.2	650.2	649.19	648.18	647.17	646.16	645.16
		643.2	641.18	640.17	639.2	638.2	637.19	636.18	635.17	633.19
		632.18	631.18	630.17	629.16	627.15	625.19	623.21	621.19	620.18
		619.18	618.17	617.16	615.18	613.19	611.17	610.16	609.19	608.18
		607.18	605.2	604.19	603.18	602.17	601.17	597.19	595.18	594.17
		593.16	592.15	591.18	590.17	589.17	579.18	577.17	575.15	561.17
		559.16	557.14	551.15	550.14	549.14	535.16	534.15	533.14	532.13
		531.12	523.16	522.15	521.14	519.16	517.15	516.14	515.13	514.16
		513.11	511.16	509.14	507.16	505.15	504.14	503.13	501.15	499.13
		498.13	497.12	496.14	495.1	493.15	491.13	490.16	489.15	488.14
		487.13	486.13	485.12	483.14	481.15	479.13	478.12	477.15	476.14
		475.13	474.14	473.13	472.14	471.14	470.13	469.12	465.15	463.13
		462.16	461.12	460.11	459.14	458.13	457.13	456.13	455.12	454.13
		452.12	447.14	445.12	444.15	443.11	442.13	439.12	438.12	432.15
		431.12	429.14	428.13	427.11	426.14	425.1	420.15	418.13	417.14
		412.14	411.13	405.14	403.12	402.12	400.14	399.13	389.1	388.09
		387.08	386.07	385.11	384.11	382.13	381.12	375.12	373.1	372.1
		371.09	370.08	369.07	367.1	361.1	360.1	359.12	358.11	357.11
		356.1	355.09	354.08	353.08	351.06	349.1	347.09	345.11	344.1
		343.13	342.09	341.11	340.1	339.1	338.09	337.08	335.09	331.09
		329.11	327.1	326.09	325.09	324.08	323.08	322.09	320.08	319.09
		317.08	316.07	315.1	314.09	313.08	312.11	311.1	307.08	306.07
		303.1	301.08	300.07	299.07	298.06	297.1	295.1	294.1	287.1
		286.09	285.1	284.08	283.07	282.06	281.08	280.07	279.09	273.1
		271.08	270.07	269.09	268.09	267.06	265.08	264.07	263.07	262.06
		255.09	253.08	252.06	251.07	250.08	249.05	247.07	245.06	237.09
		235.07	233.06	231.04	223.07	222.06	220.06	211.07	207.08	205.06
		196.06	195.05	194.04	193.04	192.03	182.08	180.04	179.03	178.05
		177.04	166.09	165.05	164.05	163.04	150.05	147.04	146.04	135.04
		134.04	130.04	124.04	123.04	119.05	111.04	110.06	109.03	108.02
		107.05	106.04							
References	<p>Kobayashi, N.; Schmidt, J.; Nimtz, M.; Wray, V.; Schliemann, W. Betalains from <i>Christmas cactus</i>. <i>Phytochemistry</i> 2000, 54, 419–426.</p> <p>Wybraniec, S.; Nowak-Wydra, B.; Mitka, K.; Kowalski, P.; Mizrahi, Y. Minor betalains in fruits of <i>Hylocereus</i> species. <i>Phytochemistry</i> 2007, 68, 251–259.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

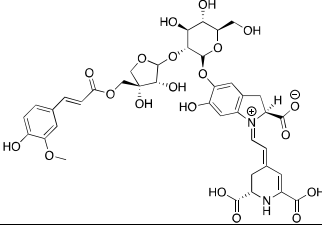
2'-O-apiosyl-phyllocactin

Chemical structure										
Name:	2'-O-apiosyl- phyllocactin									
Chemical Formula	C ₃₂ H ₃₆ N ₂ O ₂₀									
Molecular weight	768.63									
Monoisotopic mass	768.1861									
m/z [M+H]	769.1934									
Theoretical fragments (m/z)	769.19	768.19	767.18	766.17	753.2	752.19	751.18	750.18	749.17	741.2
		740.19	739.18	737.2	735.19	734.18	733.17	732.16	731.16	729.2
		727.18	725.2	724.2	723.19	722.18	721.17	719.19	717.18	716.17
		715.16	713.15	711.19	709.21	707.19	706.19	705.18	704.17	703.16
		701.18	699.19	697.17	696.16	695.19	694.19	693.18	689.18	688.17
		687.17	683.19	682.19	681.18	680.17	679.16	678.15	677.18	676.17
		675.17	667.2	665.18	664.17	663.17	661.15	655.2	653.18	651.2
		649.19	647.17	646.16	645.16	643.14	639.2	637.15	636.14	635.14
		633.19	631.18	629.16	627.15	625.19	621.16	620.15	619.14	618.13
		617.12	613.19	611.17	609.16	608.15	607.14	605.16	603.15	602.14
		601.13	600.16	599.11	597.16	595.18	593.16	591.15	590.14	589.13
		587.15	585.14	584.13	583.12	581.1	579.15	577.17	576.16	575.15
		574.14	573.13	572.13	571.12	569.14	567.15	565.13	564.12	563.15
		562.14	561.14	560.14	559.13	558.15	557.14	556.13	555.12	551.15
		550.14	549.14	547.12	546.11	545.14	544.14	543.13	542.13	541.12
		535.16	533.14	532.13	531.12	530.15	529.11	528.13	527.14	526.13
		525.12	524.12	523.16	521.14	517.15	515.13	514.13	513.11	511.1
		505.15	504.13	503.14	499.13	498.14	497.12	495.1	493.15	491.14
		490.16	489.12	488.12	487.14	486.14	485.13	481.12	479.13	475.14
		474.14	473.13	472.14	471.11	470.13	469.13	468.13	467.12	463.13
		461.12	457.13	456.13	455.12	453.1	445.12	444.11	443.11	442.1
		441.09	439.12	438.12	429.14	428.09	427.09	426.1	425.1	424.09
		423.08	417.14	412.1	411.09	410.08	409.08	405.14	403.12	402.12
		400.14	399.13	394.09	393.08	392.07	389.1	388.09	387.08	386.07
		385.11	384.11	383.1	382.13	381.12	375.12	373.1	372.1	371.09
		370.08	369.07	367.1	365.09	361.1	360.1	359.12	357.11	356.1
		355.09	354.09	353.09	351.06	349.1	347.09	345.11	343.13	342.08
		341.11	339.1	338.06	337.08	336.08	335.08	331.09	329.11	327.1
		326.09	325.09	324.08	323.08	321.06	319.09	317.08	316.07	315.1
		314.09	313.08	306.07	303.1	301.08	300.07	299.07	287.1	285.09
		284.08	283.07	281.08	280.07	273.1	271.11	269.09	267.06	265.08
		264.07	263.07	262.06	255.09	253.08	251.07	249.05	247.07	245.06
		237.09	235.07	233.06	231.04	223.07	211.07	207.08	205.06	196.06
		194.04	193.04	182.08	180.04	179.03	178.05	177.04	165.05	164.05
		163.04	147.04	146.04	135.04	134.04	130.04	123.04	119.05	111.04
		109.03	108.02	107.05	106.04					
References	<p>Kobayashi, N.; Schmidt, J.; Nimtz, M.; Wray, V.; Schliemann, W. Betalains from <i>Christmas cactus</i>. <i>Phytochemistry</i> 2000, 54, 419–426.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

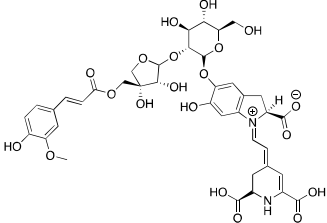
2'-O-apiosyl-isophyllocactin

Chemical structure										
Name:	2'-O-apiosyl-isophyllocactin									
Chemical Formula	C ₃₂ H ₃₆ N ₂ O ₂₀									
Molecular weight	768.63									
Monoisotopic mass	768.1861									
m/z [M+H]	769.1934									
Theoretical fragments (m/z)	769.19	768.19	767.18	766.17	753.2	752.19	751.18	750.18	749.17	741.2
		740.19	739.18	737.2	735.19	734.18	733.17	732.16	731.16	729.2
		727.18	725.2	724.2	723.19	722.18	721.17	719.19	717.18	716.17
		715.16	713.15	711.19	709.21	707.19	706.19	705.18	704.17	703.16
		701.18	699.19	697.17	696.16	695.19	694.19	693.18	689.18	688.17
		687.17	683.19	682.19	681.18	680.17	679.16	678.15	677.18	676.17
		675.17	667.2	665.18	664.17	663.17	661.15	655.2	653.18	651.2
		649.19	647.17	646.16	645.16	643.14	639.2	637.15	636.14	635.14
		633.19	631.18	629.16	627.15	625.19	621.16	620.15	619.14	618.13
		617.12	613.19	611.17	609.16	608.15	607.14	605.16	603.15	602.14
		601.13	600.16	599.11	597.16	595.18	593.16	591.15	590.14	589.13
		587.15	585.14	584.13	583.12	581.1	579.15	577.17	576.16	575.15
		574.14	573.13	572.13	571.12	569.14	567.15	565.13	564.12	563.15
		562.14	561.14	560.14	559.13	558.15	557.14	556.13	555.12	551.15
		550.14	549.14	547.12	546.11	545.14	544.14	543.13	542.13	541.12
		535.16	533.14	532.13	531.12	530.15	529.11	528.13	527.14	526.13
		525.12	524.12	523.16	521.14	517.15	515.13	514.13	513.11	511.1
		505.15	504.13	503.14	499.13	498.14	497.12	495.1	493.15	491.14
		490.16	489.12	488.12	487.14	486.14	485.13	481.12	479.13	475.14
		474.14	473.13	472.14	471.11	470.13	469.13	468.13	467.12	463.13
		461.12	457.13	456.13	455.12	453.1	445.12	444.11	443.11	442.1
		441.09	439.12	438.12	429.14	428.09	427.09	426.1	425.1	424.09
		423.08	417.14	412.1	411.09	410.08	409.08	405.14	403.12	402.12
		400.14	399.13	394.09	393.08	392.07	389.1	388.09	387.08	386.07
		385.11	384.11	383.1	382.13	381.12	375.12	373.1	372.1	371.09
		370.08	369.07	367.1	365.09	361.1	360.1	359.12	357.11	356.1
		355.09	354.09	353.09	351.06	349.1	347.09	345.11	343.13	342.08
		341.11	339.1	338.06	337.08	336.08	335.08	331.09	329.11	327.1
		326.09	325.09	324.08	323.08	321.06	319.09	317.08	316.07	315.1
		314.09	313.08	306.07	303.1	301.08	300.07	299.07	287.1	285.09
		284.08	283.07	281.08	280.07	273.1	271.11	269.09	267.06	265.08
		264.07	263.07	262.06	255.09	253.08	251.07	249.05	247.07	245.06
		237.09	235.07	233.06	231.04	223.07	211.07	207.08	205.06	196.06
		194.04	193.04	182.08	180.04	179.03	178.05	177.04	165.05	164.05
		163.04	147.04	146.04	135.04	134.04	130.04	123.04	119.05	111.04
		109.03	108.02	107.05	106.04					
References	<p>Kobayashi, N.; Schmidt, J.; Nimtz, M.; Wray, V.; Schliemann, W. Betalains from <i>Christmas cactus</i>. <i>Phytochemistry</i> 2000, 54, 419–426.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

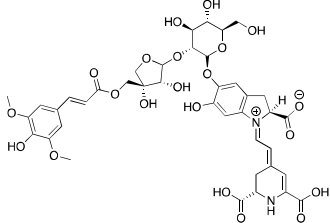
5''-O-E-Feruloyl-apiocactin

Chemical structure										
Name:	5''-O-E-Feruloyl-apiocactin									
Chemical Formula	C ₃₉ H ₄₂ N ₂ O ₂₀									
Molecular weight	858.76									
Monoisotopic mass	858.2331									
m/z [M+H]	859.2404									
Theoretical fragments (m/z)	859.24	858.23	857.22	856.22	843.25	842.24	841.23	840.22	839.21	831.25
		830.24	829.23	827.25	826.24	825.23	824.23	823.22	822.21	821.2
		819.25	817.23	816.22	815.25	814.24	813.23	812.23	811.22	809.24
		808.23	807.22	806.22	805.21	803.19	801.23	799.26	797.24	796.23
		795.22	794.22	793.21	789.23	787.22	786.21	785.24	784.23	783.22
		781.25	780.24	779.23	778.22	777.21	773.24	771.22	770.22	769.21
		768.2	767.23	766.22	765.21	755.23	753.21	751.2	737.22	735.2
		733.19	690.2	677.2	666.2	665.2	664.19	663.18	651.19	650.18
		649.18	648.19	646.18	645.17	638.21	636.19	633.18	632.17	631.17
		630.18	628.17	621.18	620.2	619.19	618.18	615.17	614.16	608.2
		607.17	605.19	604.18	602.19	596.2	594.18	593.19	588.18	587.18
		581.19	579.17	578.16	576.18	575.18	563.18	562.17	561.16	560.15
		558.17	557.17	551.15	550.14	549.14	545.17	543.15	535.16	534.15
		533.14	532.13	531.12	523.16	522.15	521.14	519.16	517.15	516.14
		515.13	514.12	513.11	511.16	509.14	507.16	505.15	504.14	503.13
		501.15	499.13	498.13	497.12	495.1	493.15	491.13	489.15	488.14
		487.13	486.13	485.12	483.14	481.15	479.13	478.12	477.15	476.14
		475.13	473.16	471.14	470.13	469.12	465.15	463.13	461.12	460.11
		459.14	458.13	457.12	447.14	445.12	443.11	429.13	427.11	425.1
		389.1	388.09	387.08	386.07	375.12	373.1	371.09	371.09	370.08
		369.07	361.1	360.1	359.12	358.11	357.11	356.1	355.09	354.08
		353.08	351.06	349.1	347.09	345.11	344.1	343.13	342.09	341.11
		340.1	339.1	338.09	337.08	335.09	331.09	329.11	327.1	326.09
		325.09	324.08	323.08	322.09	320.08	319.09	317.08	316.07	315.1
		314.09	313.08	312.11	307.08	306.07	303.1	301.08	300.07	299.07
		298.06	297.1	294.1	287.1	286.09	285.1	284.08	283.07	282.06
		281.08	280.07	279.09	273.1	271.08	270.07	269.09	268.09	267.06
		265.08	264.07	263.07	262.06	255.09	253.08	252.06	251.07	250.08
		249.05	247.07	245.06	237.09	235.07	233.06	231.04	223.07	222.06
		220.06	211.07	207.08	205.06	196.06	195.05	194.04	193.04	192.03
		182.08	180.04	179.03	178.05	177.04	166.09	165.05	164.05	163.04
		150.05	147.04	146.04	135.04	134.04	130.04	124.04	123.04	119.05
		111.04	110.06	109.03	108.02	107.05	106.04			
References	<p>Schliemann, W.; Joy, R.W.; Komamine, A.; Metzger, J.W.; Nimtz, M.; Wray, V.; Strack, D. Betacyanins from plants and cell cultures of <i>Phytolacca americana</i>. <i>Phytochemistry</i> 1996, 42, 1039–1046.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

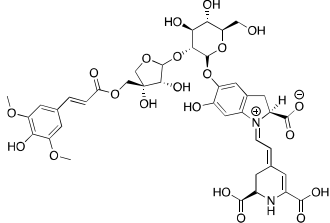
5''-O-E-Feruloyl-isoapiocactin

Chemical structure										
Name:	5''-O-E-Feruloyl-isoapiocactin									
Chemical Formula	C ₃₉ H ₄₂ N ₂ O ₂₀									
Molecular weight	858.76									
Monoisotopic mass	858.2331									
m/z [M+H]	859.2404									
Theoretical fragments (m/z)	859.24	858.23	857.22	856.22	843.25	842.24	841.23	840.22	839.21	831.25
		830.24	829.23	827.25	826.24	825.23	824.23	823.22	822.21	821.2
		819.25	817.23	816.22	815.25	814.24	813.23	812.23	811.22	809.24
		808.23	807.22	806.22	805.21	803.19	801.23	799.26	797.24	796.23
		795.22	794.22	793.21	789.23	787.22	786.21	785.24	784.23	783.22
		781.25	780.24	779.23	778.22	777.21	773.24	771.22	770.22	769.21
		768.2	767.23	766.22	765.21	755.23	753.21	751.2	737.22	735.2
		733.19	690.2	677.2	666.2	665.2	664.19	663.18	651.19	650.18
		649.18	648.19	646.18	645.17	638.21	636.19	633.18	632.17	631.17
		630.18	628.17	621.18	620.2	619.19	618.18	615.17	614.16	608.2
		607.17	605.19	604.18	602.19	596.2	594.18	593.19	588.18	587.18
		581.19	579.17	578.16	576.18	575.18	563.18	562.17	561.16	560.15
		558.17	557.17	551.15	550.14	549.14	545.17	543.15	535.16	534.15
		533.14	532.13	531.12	523.16	522.15	521.14	519.16	517.15	516.14
		515.13	514.12	513.11	511.16	509.14	507.16	505.15	504.14	503.13
		501.15	499.13	498.13	497.12	495.1	493.15	491.13	489.15	488.14
		487.13	486.13	485.12	483.14	481.15	479.13	478.12	477.15	476.14
		475.13	473.16	471.14	470.13	469.12	465.15	463.13	461.12	460.11
		459.14	458.13	457.12	447.14	445.12	443.11	429.13	427.11	425.1
		389.1	388.09	387.08	386.07	375.12	373.1	371.09	371.09	370.08
		369.07	361.1	360.1	359.12	358.11	357.11	356.1	355.09	354.08
		353.08	351.06	349.1	347.09	345.11	344.1	343.13	342.09	341.11
		340.1	339.1	338.09	337.08	335.09	331.09	329.11	327.1	326.09
		325.09	324.08	323.08	322.09	320.08	319.09	317.08	316.07	315.1
		314.09	313.08	312.11	307.08	306.07	303.1	301.08	300.07	299.07
		298.06	297.1	294.1	287.1	286.09	285.1	284.08	283.07	282.06
		281.08	280.07	279.09	273.1	271.08	270.07	269.09	268.09	267.06
		265.08	264.07	263.07	262.06	255.09	253.08	252.06	251.07	250.08
		249.05	247.07	245.06	237.09	235.07	233.06	231.04	223.07	222.06
		220.06	211.07	207.08	205.06	196.06	195.05	194.04	193.04	192.03
		182.08	180.04	179.03	178.05	177.04	166.09	165.05	164.05	163.04
		150.05	147.04	146.04	135.04	134.04	130.04	124.04	123.04	119.05
		111.04	110.06	109.03	108.02	107.05	106.04			
References	<p>Schliemann, W.; Joy, R.W.; Komamine, A.; Metzger, J.W.; Nimtz, M.; Wray, V.; Strack, D. Betacyanins from plants and cell cultures of <i>Phytolacca americana</i>. <i>Phytochemistry</i> 1996, 42, 1039–1046.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

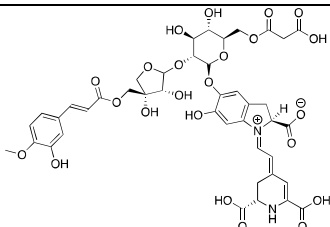
5''-O-E-Sinapoyl-apiocactin

Chemical structure										
Name:	5''-O-E-Sinapoyl-apiocactin									
Chemical Formula	C ₄₀ H ₄₄ N ₂ O ₂₁									
Molecular weight	888.79									
Monoisotopic mass	888.2437									
m/z [M+H]	889.2509									
Theoretical fragments (m/z)	889.25	888.24	887.24	886.23	873.26	872.25	871.24	870.23	869.22	861.26
		860.25	859.24	857.26	856.25	855.25	854.24	853.23	852.22	851.21
		849.26	847.24	846.23	845.26	844.25	843.25	842.24	841.23	839.25
		838.24	837.23	836.23	835.22	833.2	831.25	829.27	827.25	826.24
		825.23	824.23	823.22	819.25	817.23	816.22	815.25	814.24	813.23
		811.26	810.25	809.24	808.23	807.22	803.25	801.23	800.23	799.22
		798.21	797.24	796.23	795.22	785.24	783.22	781.21	767.23	765.21
		763.2	720.21	707.21	696.21	695.21	694.2	693.19	681.2	680.19
		679.19	678.2	676.19	675.18	668.22	666.2	663.19	662.18	661.18
		660.19	658.18	651.19	650.21	649.2	648.19	645.18	644.17	638.21
		637.18	635.2	634.19	632.2	626.21	624.19	623.2	618.19	617.19
		611.2	609.18	608.17	606.19	605.19	593.19	592.18	591.17	590.16
		588.18	587.18	575.18	573.16	551.15	550.14	549.14	535.16	534.15
		533.14	532.13	531.12	523.16	522.15	521.14	519.16	517.15	516.14
		515.13	514.12	513.11	511.16	509.14	507.16	505.15	504.14	503.13
		501.15	499.13	498.13	497.12	495.1	493.15	491.13	489.15	488.14
		487.13	486.13	485.12	483.14	481.15	479.13	478.12	477.15	476.14
		475.13	473.16	471.14	470.13	469.12	465.15	463.13	461.12	460.11
		459.14	458.13	457.12	447.14	445.12	443.11	429.13	427.11	425.1
		389.1	388.09	387.08	386.07	375.12	373.1	371.09	371.09	370.08
		369.07	361.1	360.1	359.12	358.11	357.11	356.1	355.09	354.08
		353.08	351.06	349.1	347.09	345.11	344.1	343.13	342.09	341.11
		340.1	339.1	338.09	337.08	335.09	331.09	329.11	327.1	326.09
		325.09	324.08	323.08	322.09	320.08	319.09	317.08	316.07	315.1
		314.09	313.08	312.11	307.08	306.07	303.1	301.08	300.07	299.07
		298.06	297.1	294.1	287.1	286.09	285.1	284.08	283.07	282.06
		281.08	280.07	279.09	273.1	271.08	270.07	269.09	268.09	267.06
		265.08	264.07	263.07	262.06	255.09	253.08	252.06	251.07	250.08
		249.05	247.07	245.06	237.09	235.07	233.06	231.04	223.07	222.06
		220.06	211.07	207.08	205.06	196.06	195.05	194.04	193.04	192.03
		182.08	180.04	179.03	178.05	177.04	166.09	165.05	164.05	163.04
		150.05	147.04	146.04	135.04	134.04	130.04	124.04	123.04	119.05
		111.04	110.06	109.03	108.02	107.05	106.04			
References	<p>Wybraniec, S.; Nowak-Wydra, B.; Mitka, K.; Kowalski, P.; Mizrahi, Y. Minor betalains in fruits of <i>Hylocereus</i> species. <i>Phytochemistry</i> 2007, 68, 251–259.</p> <p>Sutor, K.; Wybraniec, S. Identification and determination of betacyanins in fruit extracts of <i>Melocactus</i> species. <i>J. Agric. Food Chem.</i> 2020, 68, 11459–11467.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

5''-O-E-Sinapoyl-isoapiocactin

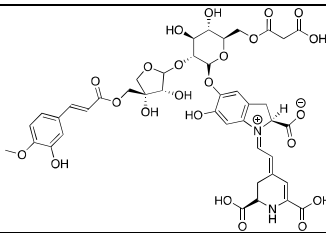
Chemical structure										
Name:	5''-O-E-Sinapoyl-isoapiocactin									
Chemical Formula	C ₄₀ H ₄₄ N ₂ O ₂₁									
Molecular weight	888.79									
Monoisotopic mass	888.2437									
m/z [M+H]	889.2509									
Theoretical fragments (m/z)	889.25	888.24	887.24	886.23	873.26	872.25	871.24	870.23	869.22	861.26
		860.25	859.24	857.26	856.25	855.25	854.24	853.23	852.22	851.21
		849.26	847.24	846.23	845.26	844.25	843.25	842.24	841.23	839.25
		838.24	837.23	836.23	835.22	833.2	831.25	829.27	827.25	826.24
		825.23	824.23	823.22	819.25	817.23	816.22	815.25	814.24	813.23
		811.26	810.25	809.24	808.23	807.22	803.25	801.23	800.23	799.22
		798.21	797.24	796.23	795.22	785.24	783.22	781.21	767.23	765.21
		763.2	720.21	707.21	696.21	695.21	694.2	693.19	681.2	680.19
		679.19	678.2	676.19	675.18	668.22	666.2	663.19	662.18	661.18
		660.19	658.18	651.19	650.21	649.2	648.19	645.18	644.17	638.21
		637.18	635.2	634.19	632.2	626.21	624.19	623.2	618.19	617.19
		611.2	609.18	608.17	606.19	605.19	593.19	592.18	591.17	590.16
		588.18	587.18	575.18	573.16	551.15	550.14	549.14	535.16	534.15
		533.14	532.13	531.12	523.16	522.15	521.14	519.16	517.15	516.14
		515.13	514.12	513.11	511.16	509.14	507.16	505.15	504.14	503.13
		501.15	499.13	498.13	497.12	495.1	493.15	491.13	489.15	488.14
		487.13	486.13	485.12	483.14	481.15	479.13	478.12	477.15	476.14
		475.13	473.16	471.14	470.13	469.12	465.15	463.13	461.12	460.11
		459.14	458.13	457.12	447.14	445.12	443.11	429.13	427.11	425.1
		389.1	388.09	387.08	386.07	375.12	373.1	371.09	371.09	370.08
		369.07	361.1	360.1	359.12	358.11	357.11	356.1	355.09	354.08
		353.08	351.06	349.1	347.09	345.11	344.1	343.13	342.09	341.11
		340.1	339.1	338.09	337.08	335.09	331.09	329.11	327.1	326.09
		325.09	324.08	323.08	322.09	320.08	319.09	317.08	316.07	315.1
		314.09	313.08	312.11	307.08	306.07	303.1	301.08	300.07	299.07
		298.06	297.1	294.1	287.1	286.09	285.1	284.08	283.07	282.06
		281.08	280.07	279.09	273.1	271.08	270.07	269.09	268.09	267.06
		265.08	264.07	263.07	262.06	255.09	253.08	252.06	251.07	250.08
		249.05	247.07	245.06	237.09	235.07	233.06	231.04	223.07	222.06
		220.06	211.07	207.08	205.06	196.06	195.05	194.04	193.04	192.03
		182.08	180.04	179.03	178.05	177.04	166.09	165.05	164.05	163.04
		150.05	147.04	146.04	135.04	134.04	130.04	124.04	123.04	119.05
		111.04	110.06	109.03	108.02	107.05	106.04			
References	<p>Wybraniec, S.; Nowak-Wydra, B.; Mitka, K.; Kowalski, P.; Mizrahi, Y. Minor betalains in fruits of <i>Hylocereus</i> species. <i>Phytochemistry</i> 2007, 68, 251–259.</p> <p>Sutor, K.; Wybraniec, S. Identification and determination of betacyanins in fruit extracts of <i>Melocactus</i> species. <i>J. Agric. Food Chem.</i> 2020, 68, 11459–11467.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

2'-O-β-(5''-O-E-Feruloyl)-apiosyl-phyllactin

Chemical structure										
Name:	2'-O-b-(5''-O-E-Feruloyl)-apiosyl-phyllactin									
Chemical Formula	C ₄₂ H ₄₄ N ₂ O ₂₃									
Molecular weight	944.81									
Monoisotopic mass	944.2335									
m/z [M+H]	945.2408									
Theoretical fragments (m/z)	945.24	944.23	943.23	942.22	929.25	928.24	927.23	926.22	925.21	917.25
		916.24	915.23	913.25	911.24	910.23	909.22	908.21	907.2	905.25
		903.23	901.25	900.24	899.24	898.23	897.22	895.24	893.22	892.22
		891.21	889.19	887.24	885.26	883.24	882.23	881.22	880.22	879.21
		877.23	875.24	873.22	872.21	871.24	870.23	869.22	865.23	864.22
		863.21	859.24	858.23	857.22	856.22	855.21	854.2	853.23	852.22
		851.21	843.25	841.23	840.22	839.21	837.2	831.25	829.23	827.25
		825.23	823.22	822.21	821.2	819.19	815.25	813.23	811.22	809.24
		807.22	805.21	803.19	801.23	797.24	795.22	793.21	789.23	787.22
		783.22	777.21	776.2	771.22	769.21	765.21	763.2	753.21	752.2
		751.2	750.19	749.18	737.19	736.18	735.18	734.19	733.18	732.18
		731.17	720.19	719.18	718.17	717.17	707.18	706.2	705.19	704.18
		703.19	702.18	701.17	700.16	691.19	690.18	680.18	679.19	675.19
		674.18	673.18	667.19	666.2	665.17	664.16	663.19	662.18	661.18
		651.19	650.18	649.18	648.19	647.16	646.18	645.18	644.17	643.17
		637.15	636.14	635.14	633.18	632.17	631.17	629.15	621.16	620.15
		619.14	618.13	617.12	615.17	614.16	609.16	608.15	607.14	605.16
		603.15	602.14	601.13	600.12	599.11	597.16	595.14	593.19	591.15
		590.14	589.13	587.15	585.14	584.13	583.12	581.19	579.15	578.16
		577.13	576.18	575.18	574.14	573.14	572.13	571.12	569.14	567.15
		565.13	564.12	563.18	562.14	561.14	560.15	558.17	557.17	556.13
		555.12	551.15	550.14	549.14	547.12	546.11	545.17	544.13	543.12
		535.16	533.14	532.13	531.12	529.11	523.16	521.14	517.15	515.13
		514.12	513.11	511.1	505.15	503.13	499.13	497.12	495.1	493.15
		487.13	485.12	481.12	479.13	475.13	469.12	463.13	461.12	457.12
		445.12	444.11	443.11	442.1	441.09	428.09	427.09	426.1	425.1
		424.09	423.08	412.1	411.09	410.08	409.08	394.09	393.08	392.07
		389.1	388.09	387.08	386.07	383.1	375.12	373.1	372.1	371.09
		370.08	369.07	365.09	361.1	360.1	359.12	357.11	356.1	355.09
		354.09	353.09	351.06	349.1	347.09	345.11	343.13	342.08	341.11
		339.1	338.06	337.08	336.08	335.08	331.09	329.11	327.1	326.09
		325.09	324.08	323.08	321.06	319.09	317.08	316.07	315.1	314.09
		313.08	306.07	303.1	301.08	300.07	299.07	287.1	285.09	284.08
		283.07	281.08	280.07	273.1	271.11	269.09	267.06	265.08	264.07
		263.07	262.06	255.09	253.08	251.07	249.05	247.07	245.06	237.09
		235.07	233.06	231.04	223.07	211.07	207.08	205.06	196.06	194.04
		193.04	182.08	180.04	179.03	178.05	177.04	165.05	164.05	163.04
		147.04	146.04	135.04	134.04	130.04	123.04	119.05	111.04	109.03
		108.02	107.05	106.04						
References	<p>Kobayashi, N.; Schmidt, J.; Nimtz, M.; Wray, V.; Schliemann, W. Betalains from <i>Christmas cactus</i>. <i>Phytochemistry</i> 2000, 54, 419–426.</p> <p>Schliemann, W.; Joy, R.W.; Komamine, A.; Metzger, J.W.; Nimtz, M.; Wray, V.; Strack, D. Betacyanins from plants and cell cultures of <i>Phytolacca americana</i>. <i>Phytochemistry</i> 1996, 42, 1039–1046.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-</p>									

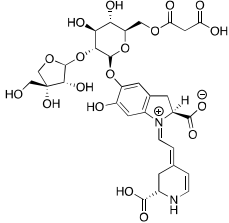
	colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021 , 38, 2315–2346.
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2'-O-β-(5''-O-E-Feruloyl)-apiosyl-isophyllocactin

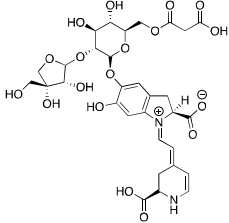
Chemical structure										
Name:	2'-O-β-(5''-O-E-Feruloyl)-apiosyl-isophyllocactin									
Chemical Formula	C ₄₂ H ₄₄ N ₂ O ₂₃									
Molecular weight	944.81									
Monoisotopic mass	944.2335									
m/z [M+H]	945.2408									
Theoretical fragments (m/z)	945.24	944.23	943.23	942.22	929.25	928.24	927.23	926.22	925.21	917.25
		916.24	915.23	913.25	911.24	910.23	909.22	908.21	907.2	905.25
		903.23	901.25	900.24	899.24	898.23	897.22	895.24	893.22	892.22
		891.21	889.19	887.24	885.26	883.24	882.23	881.22	880.22	879.21
		877.23	875.24	873.22	872.21	871.24	870.23	869.22	865.23	864.22
		863.21	859.24	858.23	857.22	856.22	855.21	854.2	853.23	852.22
		851.21	843.25	841.23	840.22	839.21	837.2	831.25	829.23	827.25
		825.23	823.22	822.21	821.2	819.19	815.25	813.23	811.22	809.24
		807.22	805.21	803.19	801.23	797.24	795.22	793.21	789.23	787.22
		783.22	777.21	776.2	771.22	769.21	765.21	763.2	753.21	752.2
		751.2	750.19	749.18	737.19	736.18	735.18	734.19	733.18	732.18
		731.17	720.19	719.18	718.17	717.17	707.18	706.2	705.19	704.18
		703.19	702.18	701.17	700.16	691.19	690.18	680.18	679.19	675.19
		674.18	673.18	667.19	666.2	665.17	664.16	663.19	662.18	661.18
		651.19	650.18	649.18	648.19	647.16	646.18	645.18	644.17	643.17
		637.15	636.14	635.14	633.18	632.17	631.17	629.15	621.16	620.15
		619.14	618.13	617.12	615.17	614.16	609.16	608.15	607.14	605.16
		603.15	602.14	601.13	600.12	599.11	597.16	595.14	593.19	591.15
		590.14	589.13	587.15	585.14	584.13	583.12	581.19	579.15	578.16
		577.13	576.18	575.18	574.14	573.14	572.13	571.12	569.14	567.15
		565.13	564.12	563.18	562.14	561.14	560.15	558.17	557.17	556.13
		555.12	551.15	550.14	549.14	547.12	546.11	545.17	544.13	543.12
		535.16	533.14	532.13	531.12	529.11	523.16	521.14	517.15	515.13
		514.12	513.11	511.1	505.15	503.13	499.13	497.12	495.1	493.15
		487.13	485.12	481.12	479.13	475.13	469.12	463.13	461.12	457.12
		445.12	444.11	443.11	442.1	441.09	428.09	427.09	426.1	425.1
		424.09	423.08	412.1	411.09	410.08	409.08	394.09	393.08	392.07
		389.1	388.09	387.08	386.07	383.1	375.12	373.1	372.1	371.09
		370.08	369.07	365.09	361.1	360.1	359.12	357.11	356.1	355.09
		354.09	353.09	351.06	349.1	347.09	345.11	343.13	342.08	341.11
		339.1	338.06	337.08	336.08	335.08	331.09	329.11	327.1	326.09
		325.09	324.08	323.08	321.06	319.09	317.08	316.07	315.1	314.09
		313.08	306.07	303.1	301.08	300.07	299.07	287.1	285.09	284.08
		283.07	281.08	280.07	273.1	271.11	269.09	267.06	265.08	264.07
		263.07	262.06	255.09	253.08	251.07	249.05	247.07	245.06	237.09
		235.07	233.06	231.04	223.07	211.07	207.08	205.06	196.06	194.04
		193.04	182.08	180.04	179.03	178.05	177.04	165.05	164.05	163.04
		147.04	146.04	135.04	134.04	130.04	123.04	119.05	111.04	109.03
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References	<p>Kobayashi, N.; Schmidt, J.; Nimtz, M.; Wray, V.; Schliemann, W. Betalains from <i>Christmas cactus</i>. <i>Phytochemistry</i> 2000, 54, 419–426.</p> <p>Schliemann, W.; Joy, R.W.; Komamine, A.; Metzger, J.W.; Nimtz, M.; Wray, V.; Strack, D. Betacyanins from plants and cell cultures of <i>Phytolacca americana</i>. <i>Phytochemistry</i> 1996, 42, 1039–1046.</p> <p>Slimen, I.B.; Najjar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-</p>									

	colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021 , 38, 2315–2346.
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17-decarboxy-2'-O-apiosyl-phyllocactin

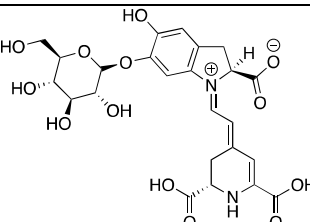
Chemical structure										
Name:	17-decarboxy-2'-O-apiosyl-phyllocactin									
Chemical Formula	C ₃₁ H ₃₆ N ₂ O ₁₈									
Molecular weight	724.62									
Monoisotopic mass	724.1963									
m/z [M+H]	725.2036									
Theoretical fragments (m/z)	725.2	724.2	723.19	722.18	709.21	708.2	707.19	706.19	705.18	697.21
			696.2	695.19	693.21	691.2	690.19	689.18	688.17	687.17
			685.21	683.19	681.21	680.21	679.2	678.19	677.18	675.2
			673.19	672.18	671.17	669.16	667.2	665.22	663.2	662.2
			661.19	660.18	659.17	657.19	655.2	653.18	652.17	651.2
			650.2	649.19	645.19	644.18	643.18	639.2	638.2	637.19
			636.18	635.17	634.16	633.19	632.18	631.18	623.21	621.19
			620.18	619.18	617.16	611.21	609.19	607.21	605.2	603.18
			602.17	601.17	600.16	599.15	595.21	593.16	592.15	591.15
			589.2	587.19	585.17	583.16	581.2	577.17	576.16	575.15
			574.14	573.13	569.2	567.18	565.17	564.16	563.15	561.17
			560.14	559.16	558.15	557.14	556.13	555.12	553.17	551.19
			549.17	547.16	546.15	545.14	544.14	543.13	542.13	541.15
			540.14	539.13	537.11	535.16	533.18	531.16	530.15	529.15
			528.13	527.14	526.13	525.12	524.12	523.16	521.14	520.13
			519.16	518.15	517.15	515.14	514.13	513.15	512.14	511.13
			507.16	506.15	505.15	504.13	503.14	502.12	501.15	500.14
			499.14	498.14	497.13	491.14	490.16	489.12	488.12	487.14
			486.14	485.13	479.17	477.15	475.14	474.14	473.13	472.14
			471.14	470.13	469.12	468.13	467.12	461.16	459.14	457.13
			456.13	455.14	453.13	451.11	449.16	444.11	443.14	442.1
			441.09	439.12	438.12	437.13	435.14	431.14	429.14	428.09
			427.09	426.1	425.13	424.09	423.08	419.14	417.14	413.13
			412.1	411.09	410.08	409.08	405.14	403.12	402.12	401.13
			400.14	399.13	394.09	393.08	392.07	387.13	385.11	384.11
			383.1	382.13	381.12	371.1	369.12	367.1	365.09	359.1
			357.08	356.07	355.1	354.09	353.09	345.11	344.1	343.09
			342.09	341.09	339.07	338.06	337.09	336.08	335.08	331.13
			329.11	328.11	327.1	326.09	325.08	324.08	323.08	321.06
			317.11	316.11	315.13	313.12	312.11	311.1	310.09	309.09
			307.07	306.07	305.11	303.1	301.12	299.14	298.09	297.12
			295.11	293.09	291.1	287.1	285.12	283.11	282.1	281.09
			275.1	273.09	272.08	271.11	270.1	269.09	267.09	259.11
			257.09	256.08	255.08	253.07	249.08	243.11	241.1	240.09
			239.08	237.09	236.08	235.06	227.12	225.1	223.07	221.09
			220.08	219.08	218.07	209.09	207.08	205.06	203.08	201.07
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			179.08	178.05	177.04	167.08	165.05	164.05	163.09	161.07
			152.07	150.05	147.04	146.04	135.04	134.04	130.04	123.04
			119.05	111.04	109.03	108.02	107.05	106.04		
References	<p>Kobayashi, N.; Schmidt, J.; Nimtz, M.; Wray, V.; Schliemann, W. Betalains from <i>Christmas cactus</i>. <i>Phytochemistry</i> 2000, 54, 419–426.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

17-decarboxy-2'-O-apiosyl-isophyllocactin

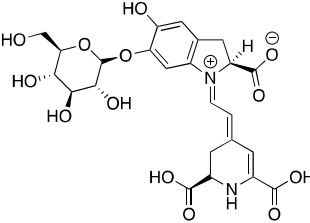
Chemical structure										
Name:	17-decarboxy-2'-O-apiosyl-isophyllocactin									
Chemical Formula	C ₃₁ H ₃₆ N ₂ O ₁₈									
Molecular weight	724.62									
Monoisotopic mass	724.1963									
m/z [M+H]	725.2036									
Theoretical fragments (m/z)	725.2	724.2	723.19	722.18	709.21	708.2	707.19	706.19	705.18	697.21
			696.2	695.19	693.21	691.2	690.19	689.18	688.17	687.17
			685.21	683.19	681.21	680.21	679.2	678.19	677.18	675.2
			673.19	672.18	671.17	669.16	667.2	665.22	663.2	662.2
			661.19	660.18	659.17	657.19	655.2	653.18	652.17	651.2
			650.2	649.19	645.19	644.18	643.18	639.2	638.2	637.19
			636.18	635.17	634.16	633.19	632.18	631.18	623.21	621.19
			620.18	619.18	617.16	611.21	609.19	607.21	605.2	603.18
			602.17	601.17	600.16	599.15	595.21	593.16	592.15	591.15
			589.2	587.19	585.17	583.16	581.2	577.17	576.16	575.15
			574.14	573.13	569.2	567.18	565.17	564.16	563.15	561.17
			560.14	559.16	558.15	557.14	556.13	555.12	553.17	551.19
			549.17	547.16	546.15	545.14	544.14	543.13	542.13	541.15
			540.14	539.13	537.11	535.16	533.18	531.16	530.15	529.15
			528.13	527.14	526.13	525.12	524.12	523.16	521.14	520.13
			519.16	518.15	517.15	515.14	514.13	513.15	512.14	511.13
			507.16	506.15	505.15	504.13	503.14	502.12	501.15	500.14
			499.14	498.14	497.13	491.14	490.16	489.12	488.12	487.14
			486.14	485.13	479.17	477.15	475.14	474.14	473.13	472.14
			471.14	470.13	469.12	468.13	467.12	461.16	459.14	457.13
			456.13	455.14	453.13	451.11	449.16	444.11	443.14	442.1
			441.09	439.12	438.12	437.13	435.14	431.14	429.14	428.09
			427.09	426.1	425.13	424.09	423.08	419.14	417.14	413.13
			412.1	411.09	410.08	409.08	405.14	403.12	402.12	401.13
			400.14	399.13	394.09	393.08	392.07	387.13	385.11	384.11
			383.1	382.13	381.12	371.1	369.12	367.1	365.09	359.1
			357.08	356.07	355.1	354.09	353.09	345.11	344.1	343.09
			342.09	341.09	339.07	338.06	337.09	336.08	335.08	331.13
			329.11	328.11	327.1	326.09	325.08	324.08	323.08	321.06
			317.11	316.11	315.13	313.12	312.11	311.1	310.09	309.09
			307.07	306.07	305.11	303.1	301.12	299.14	298.09	297.12
			295.11	293.09	291.1	287.1	285.12	283.11	282.1	281.09
			275.1	273.09	272.08	271.11	270.1	269.09	267.09	259.11
			257.09	256.08	255.08	253.07	249.08	243.11	241.1	240.09
			239.08	237.09	236.08	235.06	227.12	225.1	223.07	221.09
			220.08	219.08	218.07	209.09	207.08	205.06	203.08	201.07
			196.06	194.04	193.1	191.08	189.07	187.05	182.08	180.04
			179.08	178.05	177.04	167.08	165.05	164.05	163.09	161.07
			152.07	150.05	147.04	146.04	135.04	134.04	130.04	123.04
			119.05	111.04	109.03	108.02	107.05	106.04		
References	<p>Kobayashi, N.; Schmidt, J.; Nimtz, M.; Wray, V.; Schliemann, W. Betalains from <i>Christmas cactus</i>. <i>Phytochemistry</i> 2000, 54, 419–426.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

Gomphrenin-type

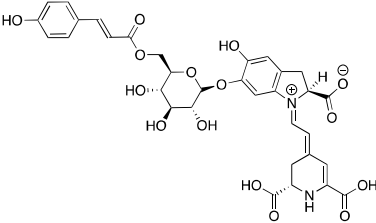
Gomphrenin I

Chemical structure										
Name:	Gomphrenin-I									
Chemical Formula	C ₂₄ H ₂₆ N ₂ O ₁₃									
Molecular weight	550.47									
Monoisotopic mass	550.1435									
m/z [M+H]	551.1508									
Theoretical fragments (m/z)	551.15	550.14	549.14	548.13	535.16	534.15	533.14	532.13	531.12	523.16
		522.15	521.14	519.16	518.15	517.15	516.14	515.13	514.12	513.11
		511.16	509.14	508.13	507.16	506.15	505.15	504.14	503.13	501.15
		499.13	497.12	495.1	493.15	491.17	490.16	489.15	488.14	487.13
		486.13	485.12	483.14	481.15	479.13	478.12	477.15	475.13	473.16
		471.14	469.12	465.15	463.13	462.13	461.12	460.11	459.14	457.12
		447.14	445.12	443.11	427.11	425.1	389.1	388.09	387.08	386.07
		382.11	375.12	374.11	373.1	372.1	371.09	370.08	369.07	368.1
		366.12	364.1	361.1	360.1	359.12	358.11	357.11	356.1	355.09
		354.08	353.08	352.1	351.06	349.1	347.09	345.11	344.1	343.13
		342.09	341.11	340.1	339.1	338.09	337.08	336.07	335.09	334.08
		331.09	330.08	329.11	328.1	327.1	326.1	325.09	324.08	323.1
		322.09	320.08	319.09	317.08	316.07	315.1	314.09	313.09	312.11
		311.1	310.09	309.1	308.09	307.08	306.07	303.1	301.08	300.07
		299.07	298.06	297.1	296.09	294.1	288.11	287.1	286.09	285.1
		283.07	281.08	280.07	279.09	273.1	271.08	270.07	269.1	268.08
		267.09	265.08	264.07	263.07	262.06	257.1	255.09	254.08	253.07
		252.06	251.07	249.08	247.07	245.06	239.09	237.08	235.07	233.06
		223.07	220.06	211.07	209.06	208.05	207.05	205.06	196.06	195.05
		194.04	193.04	191.06	182.08	181.05	180.04	179.03	178.05	177.04
		176.03	175.06	166.09	165.05	164.05	163.04	162.03	150.05	149.06
		148.05	147.04	139.04	135.04	124.04	123.04	122.04	121.03	119.05
		118.04	111.04	110.06	109.03	108.02	107.05	106.04		
References	<p>Minale, L.; Piattelli, M.; de Stefano, S. Pigments of Centrospermae VII. Betacyanins from <i>Gomphrena globosa</i> L. <i>Phytochemistry</i> 1967, 6, 703–708.</p> <p>Heuer, S.; Wray, V.; Metzger, J.W.; Strack, D. Betacyanins from flowers of <i>Gomphrena globosa</i>. <i>Phytochemistry</i> 1992, 31, 1801–1807.</p> <p>Wu, J.Y.; Chen, W.C.; Wu, Y.Y.; Chen, J.T.; Chen, L.G.; Chiou, R.Y.Y. NMR-based elucidation of the positional C6-<i>O</i>-glucopyranosyl substitution of gomphrenin I isolated from <i>Basella alba</i> fruits. <i>J. Sci. Food Agric.</i> 2013, 2, 8–11.</p> <p>Spórna-Kucab, A.; Wróbel, N.; Kumorkiewicz-Jamro, A.; Wybraniec, S. Separation of betacyanins from <i>Iresine herbstii</i> Hook. ex Lindl. leaves by high-speed countercurrent chromatography in a polar solvent system. <i>J. Chromatogr. A</i> 2020, 1626, 461370.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

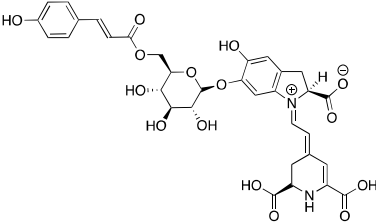
Isogomphrenin I

Chemical structure										
Name:	Isogomphrenin-I									
Chemical Formula	C ₂₄ H ₂₆ N ₂ O ₁₃									
Molecular weight	550.47									
Monoisotopic mass	550.1435									
m/z [M+H]	551.1508									
Theoretical fragments (m/z)	551.15	550.14	549.14	548.13	535.16	534.15	533.14	532.13	531.12	523.16
		522.15	521.14	519.16	518.15	517.15	516.14	515.13	514.12	513.11
		511.16	509.14	508.13	507.16	506.15	505.15	504.14	503.13	501.15
		499.13	497.12	495.1	493.15	491.17	490.16	489.15	488.14	487.13
		486.13	485.12	483.14	481.15	479.13	478.12	477.15	475.13	473.16
		471.14	469.12	465.15	463.13	462.13	461.12	460.11	459.14	457.12
		447.14	445.12	443.11	427.11	425.1	389.1	388.09	387.08	386.07
		382.11	375.12	374.11	373.1	372.1	371.09	370.08	369.07	368.1
		366.12	364.1	361.1	360.1	359.12	358.11	357.11	356.1	355.09
		354.08	353.08	352.1	351.06	349.1	347.09	345.11	344.1	343.13
		342.09	341.11	340.1	339.1	338.09	337.08	336.07	335.09	334.08
		331.09	330.08	329.11	328.1	327.1	326.1	325.09	324.08	323.1
		322.09	320.08	319.09	317.08	316.07	315.1	314.09	313.09	312.11
		311.1	310.09	309.1	308.09	307.08	306.07	303.1	301.08	300.07
		299.07	298.06	297.1	296.09	294.1	288.11	287.1	286.09	285.1
		283.07	281.08	280.07	279.09	273.1	271.08	270.07	269.1	268.08
		267.09	265.08	264.07	263.07	262.06	257.1	255.09	254.08	253.07
		252.06	251.07	249.08	247.07	245.06	239.09	237.08	235.07	233.06
		223.07	220.06	211.07	209.06	208.05	207.05	205.06	196.06	195.05
		194.04	193.04	191.06	182.08	181.05	180.04	179.03	178.05	177.04
		176.03	175.06	166.09	165.05	164.05	163.04	162.03	150.05	149.06
		148.05	147.04	139.04	135.04	124.04	123.04	122.04	121.03	119.05
		118.04	111.04	110.06	109.03	108.02	107.05	106.04		
References	<p>Minale, L.; Piattelli, M.; de Stefano, S. Pigments of Centrospermae VII. Betacyanins from <i>Gomphrena globosa</i> L. <i>Phytochemistry</i> 1967, 6, 703–708.</p> <p>Heuer, S.; Wray, V.; Metzger, J.W.; Strack, D. Betacyanins from flowers of <i>Gomphrena globosa</i>. <i>Phytochemistry</i> 1992, 31, 1801–1807.</p> <p>Wu, J.Y.; Chen, W.C.; Wu, Y.Y.; Chen, J.T.; Chen, L.G.; Chiou, R.Y.Y. NMR-based elucidation of the positional C6-<i>O</i>-glucopyranosyl substitution of gomphrenin I isolated from <i>Basella alba</i> fruits. <i>J. Sci. Food Agric.</i> 2013, 2, 8–11.</p> <p>Spórna-Kucab, A.; Wróbel, N.; Kumorkiewicz-Jamro, A.; Wybraniec, S. Separation of betacyanins from <i>Iresine herbstii</i> Hook. ex Lindl. leaves by high-speed countercurrent chromatography in a polar solvent system. <i>J. Chromatogr. A</i> 2020, 1626, 461370.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

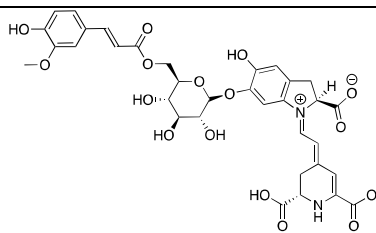
Gomphrenin II

Chemical structure										
Name:	Gomphrenin II									
Chemical Formula	C ₃₃ H ₃₂ N ₂ O ₁₅									
Molecular weight	696.62									
Monoisotopic mass	696.1803									
m/z [M+H]	697.1875									
Theoretical fragments (m/z)	697.19	696.18	695.17	694.16	681.19	680.18	679.18	678.17	677.16	669.19
		668.18	667.18	665.2	664.19	663.18	662.17	661.17	660.16	659.15
		657.19	655.18	654.17	653.2	652.19	651.18	650.17	649.17	647.19
		645.17	643.16	641.14	639.18	637.2	636.19	635.19	634.18	633.17
		632.16	631.16	629.18	627.18	625.17	624.16	623.19	621.17	619.19
		617.18	615.16	611.19	609.17	608.16	607.16	606.15	605.18	603.16
		593.18	591.16	589.15	573.15	571.13	533.14	532.13	531.12	528.15
		517.15	516.14	515.13	514.12	513.11	512.16	510.14	505.15	504.15
		503.13	502.13	501.13	499.13	498.14	497.12	495.1	493.15	491.13
		489.15	488.13	487.13	486.14	485.13	484.12	483.12	481.12	479.11
		476.16	475.13	474.14	473.16	472.14	471.13	470.12	469.12	468.13
		466.11	463.13	461.12	460.11	459.13	458.14	457.14	456.13	455.13
		454.13	453.12	452.11	447.14	446.14	445.12	444.13	443.13	442.13
		440.13	434.14	432.13	431.13	427.14	425.12	419.13	417.12	416.11
		415.14	414.12	413.12	403.14	401.12	400.12	399.11	398.1	397.13
		395.11	389.1	388.09	387.08	386.07	385.13	383.11	381.1	375.12
		374.11	373.1	372.1	371.09	370.08	369.07	364.1	361.1	360.1
		359.12	358.12	357.11	356.1	355.09	354.08	353.08	351.06	349.1
		347.09	345.11	344.1	343.13	342.08	341.11	340.1	339.1	338.09
		337.08	336.07	335.09	334.08	331.09	330.08	329.11	327.1	326.09
		325.12	324.08	323.1	322.09	320.08	319.09	317.08	316.07	315.1
		314.09	313.08	312.07	310.09	309.1	308.09	307.08	306.07	303.1
		301.08	300.07	299.07	298.06	296.08	294.1	287.1	285.09	283.07
		281.08	280.07	279.09	268.08	267.09	265.08	264.07	263.07	262.06
		255.09	253.07	252.06	251.07	249.08	247.07	245.06	239.09	237.08
		235.07	233.06	223.07	220.06	211.07	209.06	208.05	207.05	205.06
		196.06	195.05	194.04	193.04	191.06	182.08	181.05	180.04	179.03
		178.05	177.04	176.03	175.06	166.09	165.05	164.05	163.04	162.03
		150.05	149.06	148.05	147.04	139.04	135.04	124.04	123.04	122.04
		121.03	119.05	118.04	111.04	110.06	109.03	108.02	107.05	106.04
References	<p>Minale, L.; Piattelli, M.; de Stefano, S. Pigments of Centrospermae VII. Betacyanins from <i>Gomphrena globosa</i> L. <i>Phytochemistry</i> 1967, 6, 703–708.</p> <p>Heuer, S.; Wray, V.; Metzger, J.W.; Strack, D. Betacyanins from flowers of <i>Gomphrena globosa</i>. <i>Phytochemistry</i> 1992, 31, 1801–1807.</p> <p>Wu, J.Y.; Chen, W.C.; Wu, Y.Y.; Chen, J.T.; Chen, L.G.; Chiou, R.Y.Y. NMR-based elucidation of the positional C6-<i>O</i>-glucopyranosyl substitution of gomphrenin I isolated from <i>Basella alba</i> fruits. <i>J. Sci. Food Agric.</i> 2013, 2, 8–11.</p> <p>Spórna-Kucab, A.; Wróbel, N.; Kumorkiewicz-Jamro, A.; Wybraniec, S. Separation of betacyanins from <i>Iresine herbstii</i> Hook. ex Lindl. leaves by high-speed countercurrent chromatography in a polar solvent system. <i>J. Chromatogr. A</i> 2020, 1626, 461370.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

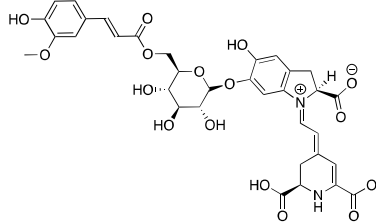
Isogomphrenin-II

Chemical structure										
Name:	Isogomphrenin-II									
Chemical Formula	C ₃₃ H ₃₂ N ₂ O ₁₅									
Molecular weight	696.62									
Monoisotopic mass	696.1803									
m/z [M+H]	697.1875									
Theoretical fragments (m/z)	697.19	696.18	695.17	694.16	681.19	680.18	679.18	678.17	677.16	669.19
		668.18	667.18	665.2	664.19	663.18	662.17	661.17	660.16	659.15
		657.19	655.18	654.17	653.2	652.19	651.18	650.17	649.17	647.19
		645.17	643.16	641.14	639.18	637.2	636.19	635.19	634.18	633.17
		632.16	631.16	629.18	627.18	625.17	624.16	623.19	621.17	619.19
		617.18	615.16	611.19	609.17	608.16	607.16	606.15	605.18	603.16
		593.18	591.16	589.15	573.15	571.13	533.14	532.13	531.12	528.15
		517.15	516.14	515.13	514.12	513.11	512.16	510.14	505.15	504.15
		503.13	502.13	501.13	499.13	498.14	497.12	495.1	493.15	491.13
		489.15	488.13	487.13	486.14	485.13	484.12	483.12	481.12	479.11
		476.16	475.13	474.14	473.16	472.14	471.13	470.12	469.12	468.13
		466.11	463.13	461.12	460.11	459.13	458.14	457.14	456.13	455.13
		454.13	453.12	452.11	447.14	446.14	445.12	444.13	443.13	442.13
		440.13	434.14	432.13	431.13	427.14	425.12	419.13	417.12	416.11
		415.14	414.12	413.12	403.14	401.12	400.12	399.11	398.1	397.13
		395.11	389.1	388.09	387.08	386.07	385.13	383.11	381.1	375.12
		374.11	373.1	372.1	371.09	370.08	369.07	364.1	361.1	360.1
		359.12	358.12	357.11	356.1	355.09	354.08	353.08	351.06	349.1
		347.09	345.11	344.1	343.13	342.08	341.11	340.1	339.1	338.09
		337.08	336.07	335.09	334.08	331.09	330.08	329.11	327.1	326.09
		325.12	324.08	323.1	322.09	320.08	319.09	317.08	316.07	315.1
		314.09	313.08	312.07	310.09	309.1	308.09	307.08	306.07	303.1
		301.08	300.07	299.07	298.06	296.08	294.1	287.1	285.09	283.07
		281.08	280.07	279.09	268.08	267.09	265.08	264.07	263.07	262.06
		255.09	253.07	252.06	251.07	249.08	247.07	245.06	239.09	237.08
		235.07	233.06	223.07	220.06	211.07	209.06	208.05	207.05	205.06
		196.06	195.05	194.04	193.04	191.06	182.08	181.05	180.04	179.03
		178.05	177.04	176.03	175.06	166.09	165.05	164.05	163.04	162.03
		150.05	149.06	148.05	147.04	139.04	135.04	124.04	123.04	122.04
		121.03	119.05	118.04	111.04	110.06	109.03	108.02	107.05	106.04
References	<p>Minale, L.; Piattelli, M.; de Stefano, S. Pigments of Centrospermae VII. Betacyanins from <i>Gomphrena globosa</i> L. <i>Phytochemistry</i> 1967, 6, 703–708.</p> <p>Heuer, S.; Wray, V.; Metzger, J.W.; Strack, D. Betacyanins from flowers of <i>Gomphrena globosa</i>. <i>Phytochemistry</i> 1992, 31, 1801–1807.</p> <p>Wu, J.Y.; Chen, W.C.; Wu, Y.Y.; Chen, J.T.; Chen, L.G.; Chiou, R.Y.Y. NMR-based elucidation of the positional C6-<i>O</i>-glucopyranosyl substitution of gomphrenin I isolated from <i>Basella alba</i> fruits. <i>J. Sci. Food Agric.</i> 2013, 2, 8–11.</p> <p>Spórna-Kucab, A.; Wróbel, N.; Kumorkiewicz-Jamro, A.; Wybraniec, S. Separation of betacyanins from <i>Iresine herbstii</i> Hook. ex Lindl. leaves by high-speed countercurrent chromatography in a polar solvent system. <i>J. Chromatogr. A</i> 2020, 1626, 461370.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

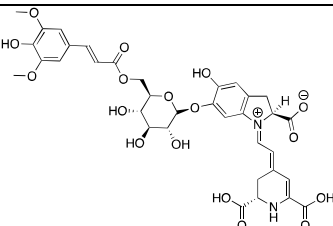
Gomphrenin-III

Chemical structure										
Name:	Gomphrenin-III									
Chemical Formula	C ₃₄ H ₃₄ N ₂ O ₁₆									
Molecular weight	726.64									
Monoisotopic mass	726.1908									
m/z [M+H]	727.1981									
Theoretical fragments (m/z)	727.2	726.19	725.18	724.17	711.2	710.2	709.19	708.18	707.17	699.2
	698.2	697.19	695.21	694.2	693.19	692.18	691.18	690.17	689.16	
	687.2	685.19	684.18	683.21	682.2	681.19	680.18	679.18	677.2	
	675.18	673.17	671.15	669.19	667.21	666.21	665.2	664.19	663.18	
	662.17	661.17	659.19	657.19	655.18	654.17	653.2	651.18	649.2	
	647.19	645.17	641.2	639.18	638.17	637.17	636.16	635.19	633.17	
	623.19	621.17	619.16	603.16	601.15	558.16	545.15	544.14	542.17	
	540.15	534.16	533.14	532.14	531.14	529.16	528.15	527.14	519.15	
	518.14	517.15	516.15	515.13	514.13	513.11	506.17	505.15	504.14	
	503.13	502.15	501.14	500.13	499.13	498.14	497.12	496.12	495.1	
	493.15	491.13	489.15	488.16	487.13	486.14	485.14	484.14	483.13	
	482.12	481.12	479.11	476.16	475.13	474.14	473.14	472.14	471.14	
	470.14	469.12	464.16	463.13	462.14	461.14	460.11	459.14	457.15	
	455.13	449.14	447.13	446.12	445.15	444.13	443.13	433.15	431.13	
	430.13	429.12	428.11	427.14	425.12	415.14	413.12	411.11	389.1	
	388.09	387.08	386.07	375.12	374.11	373.1	372.1	371.09	370.08	
	369.07	364.1	361.1	360.1	359.12	358.12	357.11	356.1	355.09	
	354.08	353.08	351.06	349.1	347.09	345.11	344.1	343.13	342.08	
	341.11	340.1	339.1	338.09	337.08	336.07	335.09	334.08	331.09	
	330.08	329.11	327.1	326.09	325.12	324.08	323.1	322.09	320.08	
	319.09	317.08	316.07	315.1	314.09	313.08	312.07	310.09	308.09	
	307.08	306.07	303.1	301.08	300.07	299.07	298.06	296.08	294.1	
	287.1	285.09	283.07	281.08	280.07	279.09	268.08	267.09	265.08	
	264.07	263.07	262.06	255.09	253.07	252.06	251.07	249.08	247.07	
	245.06	239.09	237.08	235.07	233.06	223.07	220.06	211.07	209.06	
	208.05	207.05	205.06	196.06	195.05	194.04	193.04	191.06	182.08	
	181.05	180.04	179.03	178.05	177.04	176.03	175.06	166.09	165.05	
	164.05	163.04	162.03	150.05	149.06	148.05	147.04	139.04	135.04	
	124.04	123.04	122.04	121.03	119.05	118.04	111.04	110.06	109.03	
	108.02	107.05	106.04							
References	<p>Minale, L.; Piattelli, M.; de Stefano, S. Pigments of Centrospermae VII. Betacyanins from <i>Gomphrena globosa</i> L. <i>Phytochemistry</i> 1967, 6, 703–708.</p> <p>Heuer, S.; Wray, V.; Metzger, J.W.; Strack, D. Betacyanins from flowers of <i>Gomphrena globosa</i>. <i>Phytochemistry</i> 1992, 31, 1801–1807.</p> <p>Wu, J.Y.; Chen, W.C.; Wu, Y.Y.; Chen, J.T.; Chen, L.G.; Chiou, R.Y.Y. NMR-based elucidation of the positional C6-<i>O</i>-glucopyranosyl substitution of gomphrenin I isolated from <i>Basella alba</i> fruits. <i>J. Sci. Food Agric.</i> 2013, 2, 8–11.</p> <p>Spórna-Kucab, A.; Wróbel, N.; Kumorkiewicz-Jamro, A.; Wybraniec, S. Separation of betacyanins from <i>Iresine herbstii</i> Hook. ex Lindl. leaves by high-speed countercurrent chromatography in a polar solvent system. <i>J. Chromatogr. A</i> 2020, 1626, 461370.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

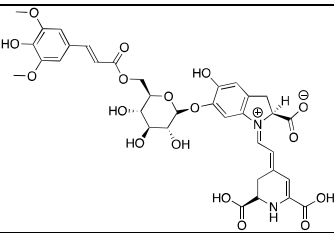
Isogomphrenin-III

Chemical structure										
Name:	Isogomphrenin-III									
Chemical Formula	C ₃₄ H ₃₄ N ₂ O ₁₆									
Molecular weight	726.64									
Monoisotopic mass	726.1908									
m/z [M+H]	727.1981									
Theoretical fragments (m/z)	727.2	726.19	725.18	724.17	711.2	710.2	709.19	708.18	707.17	699.2
		698.2	697.19	695.21	694.2	693.19	692.18	691.18	690.17	689.16
		687.2	685.19	684.18	683.21	682.2	681.19	680.18	679.18	677.2
		675.18	673.17	671.15	669.19	667.21	666.21	665.2	664.19	663.18
		662.17	661.17	659.19	657.19	655.18	654.17	653.2	651.18	649.2
		647.19	645.17	641.2	639.18	638.17	637.17	636.16	635.19	633.17
		623.19	621.17	619.16	603.16	601.15	558.16	545.15	544.14	542.17
		540.15	534.16	533.14	532.14	531.14	529.16	528.15	527.14	519.15
		518.14	517.15	516.15	515.13	514.13	513.11	506.17	505.15	504.14
		503.13	502.15	501.14	500.13	499.13	498.14	497.12	496.12	495.1
		493.15	491.13	489.15	488.16	487.13	486.14	485.14	484.14	483.13
		482.12	481.12	479.11	476.16	475.13	474.14	473.14	472.14	471.14
		470.14	469.12	464.16	463.13	462.14	461.14	460.11	459.14	457.15
		455.13	449.14	447.13	446.12	445.15	444.13	443.13	433.15	431.13
		430.13	429.12	428.11	427.14	425.12	415.14	413.12	411.11	389.1
		388.09	387.08	386.07	375.12	374.11	373.1	372.1	371.09	370.08
		369.07	364.1	361.1	360.1	359.12	358.12	357.11	356.1	355.09
		354.08	353.08	351.06	349.1	347.09	345.11	344.1	343.13	342.08
		341.11	340.1	339.1	338.09	337.08	336.07	335.09	334.08	331.09
		330.08	329.11	327.1	326.09	325.12	324.08	323.1	322.09	320.08
		319.09	317.08	316.07	315.1	314.09	313.08	312.07	310.09	308.09
		307.08	306.07	303.1	301.08	300.07	299.07	298.06	296.08	294.1
		287.1	285.09	283.07	281.08	280.07	279.09	268.08	267.09	265.08
		264.07	263.07	262.06	255.09	253.07	252.06	251.07	249.08	247.07
		245.06	239.09	237.08	235.07	233.06	223.07	220.06	211.07	209.06
		208.05	207.05	205.06	196.06	195.05	194.04	193.04	191.06	182.08
		181.05	180.04	179.03	178.05	177.04	176.03	175.06	166.09	165.05
		164.05	163.04	162.03	150.05	149.06	148.05	147.04	139.04	135.04
		124.04	123.04	122.04	121.03	119.05	118.04	111.04	110.06	109.03
		108.02	107.05	106.04						
References	<p>Minale, L.; Piattelli, M.; de Stefano, S. Pigments of Centrospermae VII. Betacyanins from <i>Gomphrena globosa</i> L. <i>Phytochemistry</i> 1967, 6, 703–708.</p> <p>Heuer, S.; Wray, V.; Metzger, J.W.; Strack, D. Betacyanins from flowers of <i>Gomphrena globosa</i>. <i>Phytochemistry</i> 1992, 31, 1801–1807.</p> <p>Wu, J.Y.; Chen, W.C.; Wu, Y.Y.; Chen, J.T.; Chen, L.G.; Chiou, R.Y.Y. NMR-based elucidation of the positional C6-<i>O</i>-glucopyranosyl substitution of gomphrenin I isolated from <i>Basella alba</i> fruits. <i>J. Sci. Food Agric.</i> 2013, 2, 8–11.</p> <p>Spórna-Kucab, A.; Wróbel, N.; Kumorkiewicz-Jamro, A.; Wybraniec, S. Separation of betacyanins from <i>Iresine herbstii</i> Hook. ex Lindl. leaves by high-speed countercurrent chromatography in a polar solvent system. <i>J. Chromatogr. A</i> 2020, 1626, 461370.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

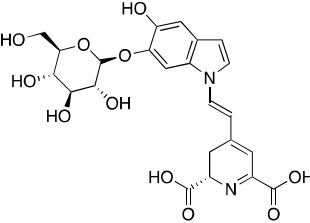
Gomphrenin-IV

Chemical structure										
Name:	Gomphrenin-IV									
Chemical Formula	C ₃₅ H ₃₆ N ₂ O ₁₇									
Molecular weight	756.67									
Monoisotopic mass	756.2014									
m/z [M+H]	757.2087									
Theoretical fragments (m/z)	757.21	756.2	755.19	754.19	741.21	740.21	739.2	738.19	737.18	729.21
	728.21	727.2	725.22	724.21	723.2	722.2	721.19	720.18	719.17	
	717.21	715.2	714.19	713.22	712.21	711.2	710.2	709.19	707.21	
	705.19	703.18	701.16	699.2	697.22	696.22	695.21	694.2	693.19	
	692.18	691.18	689.2	687.2	685.19	684.18	683.21	681.19	679.21	
	677.2	675.18	671.21	669.19	668.18	667.18	666.17	665.2	663.18	
	653.2	651.18	649.17	633.17	631.16	588.17	575.16	574.16	572.18	
	570.16	564.17	563.16	562.16	561.15	559.17	558.16	557.15	549.16	
	548.15	547.14	546.16	545.15	544.14	543.14	536.18	534.16	533.14	
	532.16	531.12	530.14	528.15	526.13	519.15	518.17	517.15	516.15	
	515.13	514.15	513.11	512.13	506.17	505.15	504.14	503.15	502.15	
	501.15	500.16	499.13	497.12	495.1	494.17	493.15	492.15	491.15	
	489.15	488.14	487.13	486.13	485.14	483.14	481.12	479.15	477.14	
	476.13	475.16	474.14	473.14	471.14	469.12	463.16	461.12	460.14	
	459.13	458.12	457.15	455.13	447.14	445.12	443.11	441.12	427.11	
	425.1	389.1	388.09	387.08	386.07	375.12	374.11	373.1	372.1	
	371.09	370.08	369.07	364.1	361.1	360.1	359.12	358.12	357.11	
	356.1	355.09	354.08	353.08	351.06	349.1	347.09	345.11	344.1	
	343.13	342.08	341.11	340.1	339.1	338.09	337.08	336.07	335.09	
	334.08	331.09	330.08	329.11	327.1	326.09	325.12	324.08	323.1	
	322.09	320.08	319.09	317.08	316.07	315.1	314.09	313.08	312.07	
	310.09	308.09	307.08	306.07	303.1	301.08	300.07	299.07	298.06	
	296.08	294.1	287.1	285.09	283.07	281.08	280.07	279.09	268.08	
	267.09	265.08	264.07	263.07	262.06	255.09	253.07	252.06	251.07	
	249.08	247.07	245.06	239.09	237.08	235.07	233.06	223.07	220.06	
	211.07	209.06	208.05	207.05	205.06	196.06	195.05	194.04	193.04	
	191.06	182.08	181.05	180.04	179.03	178.05	177.04	176.03	175.06	
	166.09	165.05	164.05	163.04	162.03	150.05	149.06	148.05	147.04	
	139.04	135.04	124.04	123.04	122.04	121.03	119.05	118.04	111.04	
	110.06	109.03	108.02	107.05	106.04					
References	<p>Minale, L.; Piattelli, M.; de Stefano, S. Pigments of Centrospermae VII. Betacyanins from <i>Gomphrena globosa</i> L. <i>Phytochemistry</i> 1967, 6, 703–708.</p> <p>Heuer, S.; Wray, V.; Metzger, J.W.; Strack, D. Betacyanins from flowers of <i>Gomphrena globosa</i>. <i>Phytochemistry</i> 1992, 31, 1801–1807.</p> <p>Wu, J.Y.; Chen, W.C.; Wu, Y.Y.; Chen, J.T.; Chen, L.G.; Chiou, R.Y.Y. NMR-based elucidation of the positional C6-<i>O</i>-glucopyranosyl substitution of gomphrenin I isolated from <i>Basella alba</i> fruits. <i>J. Sci. Food Agric.</i> 2013, 2, 8–11.</p> <p>Spórna-Kucab, A.; Wróbel, N.; Kumorkiewicz-Jamro, A.; Wybraniec, S. Separation of betacyanins from <i>Iresine herbstii</i> Hook. ex Lindl. leaves by high-speed countercurrent chromatography in a polar solvent system. <i>J. Chromatogr. A</i> 2020, 1626, 461370.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

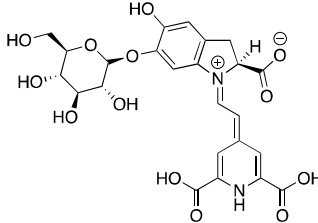
Isogomphrenin-IV

Chemical structure										
Name:	Isogomphrenin-IV									
Chemical Formula	C ₃₅ H ₃₆ N ₂ O ₁₇									
Molecular weight	756.67									
Monoisotopic mass	756.2014									
m/z [M+H]	757.2087									
Theoretical fragments (m/z)	757.21	756.2	755.19	754.19	741.21	740.21	739.2	738.19	737.18	729.21
	728.21	727.2	725.22	724.21	723.2	722.2	721.19	720.18	719.17	
	717.21	715.2	714.19	713.22	712.21	711.2	710.2	709.19	707.21	
	705.19	703.18	701.16	699.2	697.22	696.22	695.21	694.2	693.19	
	692.18	691.18	689.2	687.2	685.19	684.18	683.21	681.19	679.21	
	677.2	675.18	671.21	669.19	668.18	667.18	666.17	665.2	663.18	
	653.2	651.18	649.17	633.17	631.16	588.17	575.16	574.16	572.18	
	570.16	564.17	563.16	562.16	561.15	559.17	558.16	557.15	549.16	
	548.15	547.14	546.16	545.15	544.14	543.14	536.18	534.16	533.14	
	532.16	531.12	530.14	528.15	526.13	519.15	518.17	517.15	516.15	
	515.13	514.15	513.11	512.13	506.17	505.15	504.14	503.15	502.15	
	501.15	500.16	499.13	497.12	495.1	494.17	493.15	492.15	491.15	
	489.15	488.14	487.13	486.13	485.14	483.14	481.12	479.15	477.14	
	476.13	475.16	474.14	473.14	471.14	469.12	463.16	461.12	460.14	
	459.13	458.12	457.15	455.13	447.14	445.12	443.11	441.12	427.11	
	425.1	389.1	388.09	387.08	386.07	375.12	374.11	373.1	372.1	
	371.09	370.08	369.07	364.1	361.1	360.1	359.12	358.12	357.11	
	356.1	355.09	354.08	353.08	351.06	349.1	347.09	345.11	344.1	
	343.13	342.08	341.11	340.1	339.1	338.09	337.08	336.07	335.09	
	334.08	331.09	330.08	329.11	327.1	326.09	325.12	324.08	323.1	
	322.09	320.08	319.09	317.08	316.07	315.1	314.09	313.08	312.07	
	310.09	308.09	307.08	306.07	303.1	301.08	300.07	299.07	298.06	
	296.08	294.1	287.1	285.09	283.07	281.08	280.07	279.09	268.08	
	267.09	265.08	264.07	263.07	262.06	255.09	253.07	252.06	251.07	
	249.08	247.07	245.06	239.09	237.08	235.07	233.06	223.07	220.06	
	211.07	209.06	208.05	207.05	205.06	196.06	195.05	194.04	193.04	
	191.06	182.08	181.05	180.04	179.03	178.05	177.04	176.03	175.06	
	166.09	165.05	164.05	163.04	162.03	150.05	149.06	148.05	147.04	
	139.04	135.04	124.04	123.04	122.04	121.03	119.05	118.04	111.04	
	110.06	109.03	108.02	107.05	106.04					
References	<p>Minale, L.; Piattelli, M.; de Stefano, S. Pigments of Centrospermae VII. Betacyanins from <i>Gomphrena globosa</i> L. <i>Phytochemistry</i> 1967, 6, 703–708.</p> <p>Heuer, S.; Wray, V.; Metzger, J.W.; Strack, D. Betacyanins from flowers of <i>Gomphrena globosa</i>. <i>Phytochemistry</i> 1992, 31, 1801–1807.</p> <p>Wu, J.Y.; Chen, W.C.; Wu, Y.Y.; Chen, J.T.; Chen, L.G.; Chiou, R.Y.Y. NMR-based elucidation of the positional C6-<i>O</i>-glucopyranosyl substitution of gomphrenin I isolated from <i>Basella alba</i> fruits. <i>J. Sci. Food Agric.</i> 2013, 2, 8–11.</p> <p>Spórna-Kucab, A.; Wróbel, N.; Kumorkiewicz-Jamro, A.; Wybraniec, S. Separation of betacyanins from <i>Iresine herbstii</i> Hook. ex Lindl. leaves by high-speed countercurrent chromatography in a polar solvent system. <i>J. Chromatogr. A</i> 2020, 1626, 461370.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

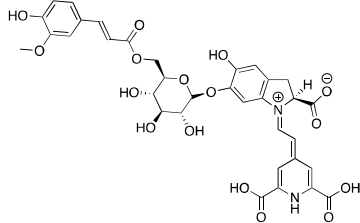
2-decarboxy-2,3-dehydro-gomphrenin

Chemical structure										
Name:	2-decarboxy-2,3-dehydro-gomphrenin (2-decarboxy-xangomphrenin)									
Chemical Formula	C ₂₃ H ₂₄ N ₂ O ₁₁									
Molecular weight	504.45									
Monoisotopic mass	504.1380									
m/z [M+H]	505.1453									
Theoretical fragments (m/z)	505.15	504.14	503.13	502.12	501.11	500.11	489.15	488.14	487.13	486.13
	485.12	484.11	483.1	479.13	478.12	477.15	475.13	474.13	473.12	
	472.11	471.14	470.13	469.12	468.12	467.11	465.15	463.13	461.16	
	460.11	459.14	458.1	457.12	456.12	455.11	454.1	453.13	451.11	
	449.12	447.14	445.16	444.12	443.14	442.1	441.13	440.12	439.11	
	438.11	437.1	435.12	434.14	433.12	432.13	431.11	430.1	429.09	
	428.12	427.11	426.11	425.1	424.09	423.12	419.12	415.11	414.11	
	413.1	412.09	411.08	410.11	409.1	408.1	403.11	401.1	400.09	
	399.08	398.11	397.1	396.1	395.09	389.1	385.1	384.1	383.09	
	382.08	381.07	376.14	374.12	373.1	371.09	369.07	368.1	367.09	
	366.08	362.12	357.11	355.09	354.08	353.08	343.09	342.08	341.08	
	339.1	338.09	337.08	336.11	329.11	327.1	326.09	325.08	324.07	
	323.07	318.1	317.08	315.1	313.12	312.11	311.1	310.09	309.09	
	307.07	303.1	301.08	300.09	299.1	297.09	296.11	295.11	294.1	
	293.09	287.1	286.09	285.09	283.11	281.09	276.09	271.08	270.07	
	254.08	253.07	194.04	180.06	179.06	178.05	177.04	176.03	175.02	
	174.05	168.03	165.08	163.06	162.05	161.04	160.04	159.03	152.03	
	151.06	150.02	149.04	148.04	147.07	146.06	145.05	144.04	143.03	
	139.06	136.08	135.07	134.06	133.05	132.04	131.04	130.03	129.05	
	128.03	127.04	126.02	124.04	122.06	121.05	120.04	119.03	118.07	
	117.02	116.05	115.04	114.02	113.02	110.06	109.03	108.04	107.07	
	105.05	104.05	103.04	102.03	101.02	100.04				
References	Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021 , 38, 2315–2346.									

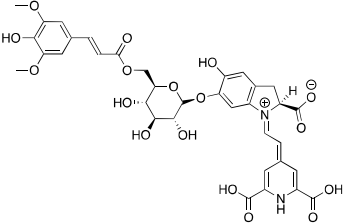
Neogomphrenin

Chemical structure										
Name:	Neogomphrenin									
Chemical Formula	C ₂₄ H ₂₄ N ₂ O ₁₃									
Molecular weight	548.46									
Monoisotopic mass	548.1278									
m/z [M+H]	549.1351									
Theoretical fragments (m/z)	549.14	548.13	547.12	546.11	533.14	532.13	531.12	530.12	529.11	521.14
			520.13	519.12	517.15	516.14	515.13	514.12	513.11	512.11
			511.1	509.14	507.12	506.12	505.15	504.14	503.13	502.12
			501.11	499.13	497.12	495.1	493.09	491.13	490.12	489.15
			488.14	487.13	485.12	484.11	483.1	479.13	477.11	476.11
			473.12	471.14	469.12	467.11	461.12	459.1	458.1	455.11
			451.11	443.11	441.09	433.12	423.08	417.09	387.08	386.07
			385.07	384.06	373.1	372.1	371.09	370.08	369.07	368.06
			367.06	359.09	358.08	357.11	356.1	355.09	354.08	353.08
			352.07	351.09	350.09	347.09	345.07	343.09	342.09	341.11
			340.1	339.1	338.09	337.08	336.07	334.09	333.07	332.06
			329.08	328.07	327.1	326.1	325.09	324.08	323.08	322.09
			321.08	320.08	319.07	317.08	315.06	314.05	313.09	312.07
			311.1	310.09	309.1	308.09	307.08	306.07	303.1	302.07
			301.08	299.07	298.09	297.1	296.09	295.07	294.1	293.09
			285.1	283.07	281.1	279.06	278.05	277.05	276.09	273.1
			271.08	270.07	269.1	267.09	265.05	264.04	263.07	262.06
			261.05	257.1	255.09	254.08	253.07	252.06	251.09	249.05
			247.03	239.09	237.08	235.06	233.06	221.06	209.06	207.05
			206.03	194.04	193.04	192.03	191.06	190.05	181.05	180.04
			179.03	178.05	177.04	176.03	175.06	165.05	164.05	163.04
			162.03	150.05	149.06	148.05	147.04	146.04	145.05	141.05
			139.04	136.08	135.04	134.06	132.04	123.04	122.04	121.03
			119.05	118.04	111.04	110.06	109.03	108.02	107.05	106.04
			105.03							
References	Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021 , 38, 2315–2346.									

Neogomphrenin III

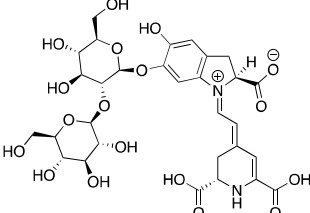
Chemical structure										
Name:	Neogomphrenin III									
Chemical Formula	C ₃₄ H ₃₂ N ₂ O ₁₆									
Molecular weight	724.63									
Monoisotopic mass	724.1752									
m/z [M+H]	725.1825									
Theoretical fragments (m/z)	725.18	724.17	723.17	722.16	709.19	708.18	707.17	706.16	705.16	697.19
	696.18	695.17	693.19	692.18	691.18	690.17	689.16	688.15	687.15	
	685.19	683.17	682.16	681.19	680.18	679.18	678.17	677.16	675.18	
	673.17	671.15	669.14	667.18	666.17	665.2	664.19	663.18	661.17	
	660.16	659.15	655.18	653.16	652.15	649.17	647.19	645.17	643.16	
	637.17	635.15	634.14	631.16	619.16	617.14	609.17	545.15	544.14	
	543.14	532.14	531.12	530.12	529.11	528.15	527.14	526.13	519.15	
	518.14	517.13	516.15	515.13	514.13	513.11	512.11	511.1	510.14	
	503.13	502.15	501.14	500.13	499.13	498.14	497.12	496.12	495.1	
	493.09	491.13	489.14	488.16	487.15	486.14	485.12	484.14	483.13	
	482.12	479.11	477.09	475.12	474.14	473.14	472.14	471.14	470.14	
	469.12	467.11	461.14	459.1	458.1	457.15	455.13	452.13	451.11	
	449.14	447.13	446.12	445.15	443.13	441.09	433.15	431.13	430.13	
	429.12	428.11	427.14	425.12	423.08	417.09	415.14	413.12	411.11	
	387.08	386.07	385.07	384.06	373.1	372.1	371.09	370.08	369.07	
	368.06	367.06	359.09	358.08	357.11	356.1	355.09	354.08	353.08	
	352.07	351.09	350.09	347.09	345.07	343.09	342.08	341.11	340.07	
	339.1	338.09	337.08	336.07	334.09	333.07	332.06	329.08	328.07	
	327.1	325.08	324.08	323.08	322.09	321.08	320.08	319.07	317.08	
	315.06	314.05	312.07	308.09	307.08	306.07	303.1	302.07	301.08	
	299.07	295.07	294.1	293.09	283.07	281.05	279.06	278.05	277.05	
	276.09	267.09	265.05	264.04	263.07	262.06	261.05	257.09	255.09	
	253.07	252.06	251.09	249.05	247.03	239.09	237.08	235.06	233.06	
	221.06	209.06	207.05	206.03	194.04	193.04	192.03	191.06	190.05	
	181.05	180.04	179.03	178.05	177.04	176.03	175.06	165.05	164.05	
	163.04	162.03	150.05	149.06	148.05	147.04	146.04	145.05	141.05	
	139.04	136.08	135.04	134.06	132.04	123.04	122.04	121.03	119.05	
	118.04	111.04	110.06	109.03	108.02	107.05	106.04	105.03		
References	Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021 , 38, 2315–2346.									

Neogomphrenin IV

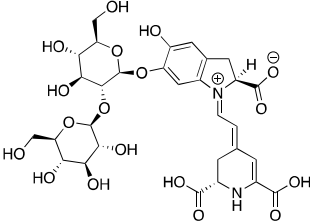
Chemical structure										
Name:	Neogomphrenin IV									
Chemical Formula	C ₃₅ H ₃₄ N ₂ O ₁₇									
Molecular weight	754.65									
Monoisotopic mass	754.1857									
m/z [M+H]	755.1930									
Theoretical fragments (m/z)	755.19	754.19	753.18	752.17	739.2	738.19	737.18	736.17	735.17	727.2
		726.19	725.18	723.2	722.2	721.19	720.18	719.17	718.16	717.16
		715.2	713.18	712.17	711.2	710.2	709.19	708.18	707.17	705.19
		703.18	701.16	699.15	697.19	696.18	695.21	694.2	693.19	691.18
		690.17	689.16	685.19	683.17	682.16	679.18	677.2	675.18	673.17
		667.18	665.16	664.15	661.17	649.17	647.15	639.18	575.16	574.16
		573.15	562.16	561.15	559.17	558.16	557.15	556.14	549.16	548.15
		547.14	546.16	545.15	544.14	543.14	540.15	533.17	532.16	531.12
		530.14	529.11	528.15	527.14	526.13	525.13	519.15	518.17	517.16
		516.15	515.13	514.15	513.11	512.13	511.1	505.13	504.15	503.15
		502.15	501.11	500.16	499.13	497.12	495.1	493.09	491.15	489.11
		487.13	485.12	484.11	483.1	482.14	479.15	477.14	476.13	475.16
		473.14	471.14	469.12	467.11	463.16	461.14	460.14	459.1	458.12
		457.15	455.13	451.11	445.15	443.13	441.09	423.08	417.09	387.08
		386.07	385.07	384.06	373.1	372.1	371.09	370.08	369.07	368.06
		367.06	359.09	358.08	357.11	356.1	355.09	354.08	353.08	352.07
		351.09	350.09	347.09	345.07	343.09	342.08	341.11	340.07	339.1
		338.09	337.08	336.07	334.09	333.07	332.06	329.08	328.07	327.1
		325.08	324.08	323.08	322.09	321.08	320.08	319.07	317.08	315.06
		314.05	312.07	308.09	307.08	306.07	303.1	302.07	301.08	299.07
		295.07	294.1	293.09	283.07	281.05	279.06	278.05	277.05	276.09
		267.09	265.05	264.04	263.07	262.06	261.05	257.09	255.09	253.07
		252.06	251.09	249.05	247.03	239.09	237.08	235.06	233.06	221.06
		209.06	207.05	206.03	194.04	193.04	192.03	191.06	190.05	181.05
		180.04	179.03	178.05	177.04	176.03	175.06	165.05	164.05	163.04
		162.03	150.05	149.06	148.05	147.04	146.04	145.05	141.05	139.04
		136.08	135.04	134.06	132.04	123.04	122.04	121.03	119.05	118.04
		111.04	110.06	109.03	108.02	107.05	106.04	105.03		
References	Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021 , 38, 2315–2346.									

Glabranin-type

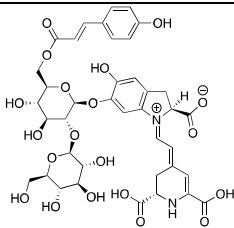
Glabranin

Chemical structure										
Name:	Glabranin (Betanidin 6'-O-β-D-sophoroside)									
Chemical Formula	C ₃₀ H ₃₆ N ₂ O ₁₈									
Molecular weight	712.61									
Monoisotopic mass	712.1963									
m/z [M+H]	713.2036									
Theoretical fragments (m/z)	713.2	712.2	711.19	710.18	697.21	696.2	695.19	694.19	693.18	685.21
		684.2	683.19	681.21	680.21	679.2	678.19	677.18	676.17	675.17
		673.21	671.19	669.21	668.21	667.2	666.19	665.18	663.2	661.19
		659.17	657.16	655.2	653.22	651.2	650.2	649.19	648.18	647.17
		643.2	641.18	640.17	639.2	637.19	633.19	631.18	627.2	625.19
		624.18	623.17	622.16	621.19	619.18	609.19	607.18	605.16	589.17
		587.15	551.15	550.14	549.14	544.17	535.16	534.15	533.14	532.13
		531.12	523.16	522.15	521.14	520.17	519.16	518.15	517.14	516.14
		515.13	514.12	513.11	511.16	509.14	507.16	505.15	504.15	503.13
		502.16	501.15	500.14	499.13	497.12	495.1	493.15	491.13	489.15
		488.15	487.14	486.14	485.12	481.15	479.13	478.12	477.15	475.13
		474.16	473.15	472.14	471.15	470.14	469.13	468.13	465.15	463.13
		461.12	460.11	459.15	458.14	457.12	448.14	447.15	445.12	443.11
		441.14	435.15	433.13	432.13	431.15	429.14	427.11	425.1	419.15
		417.14	416.13	415.12	414.12	413.14	411.13	401.14	399.13	397.11
		389.1	388.09	387.08	386.07	375.12	374.11	373.1	372.1	371.09
		370.08	369.07	361.1	360.1	359.12	358.11	357.11	356.1	355.09
		354.08	353.08	351.06	349.1	347.09	345.11	343.13	342.09	341.11
		340.1	339.1	338.09	337.08	336.07	335.09	331.09	330.08	329.11
		327.1	326.09	325.09	324.08	323.1	319.09	317.08	316.07	315.1
		314.09	313.08	312.07	310.09	308.09	307.08	306.07	303.1	301.08
		300.07	299.07	298.06	297.1	296.08	287.1	285.1	283.07	281.08
		280.07	279.09	273.1	271.08	270.07	269.1	267.09	265.08	264.07
		263.07	262.06	257.1	255.09	253.07	252.06	251.07	249.08	247.07
		245.06	239.09	237.08	235.07	233.06	223.07	211.07	196.06	195.05
		194.04	193.04	182.08	180.04	179.03	178.05	177.04	165.05	164.05
		163.04	162.03	149.06	148.05	147.04	139.04	135.04	123.04	122.04
		119.05	118.04	111.04	109.03	108.02	107.05	106.04		
References	<p>Piattelli, M; Imperato, F. Pigments of <i>Bougainvillea glabra</i>. <i>Phytochemistry</i> 1970, 9, 2557–2560.</p> <p>Heuer, S.; Richter, S.; Metzger, J.W.; Wray, V.; Nimtz, M.; Strack, D. Betacyanins from bracts of <i>Bougainvillea glabra</i>. <i>Phytochemistry</i> 1994, 37, 761–767.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

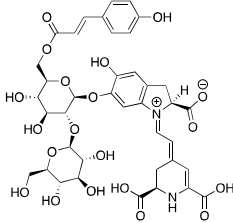
Isoglabranin

Chemical structure										
Name:	Isoglabranin (Isobetanidin 6'-O-β-D-sophoroside)									
Chemical Formula	C ₃₀ H ₃₆ N ₂ O ₁₈									
Molecular weight	712.61									
Monoisotopic mass	712.1963									
m/z [M+H]	713.2036									
Theoretical fragments (m/z)	713.2	712.2	711.19	710.18	697.21	696.2	695.19	694.19	693.18	685.21
		684.2	683.19	681.21	680.21	679.2	678.19	677.18	676.17	675.17
		673.21	671.19	669.21	668.21	667.2	666.19	665.18	663.2	661.19
		659.17	657.16	655.2	653.22	651.2	650.2	649.19	648.18	647.17
		643.2	641.18	640.17	639.2	637.19	633.19	631.18	627.2	625.19
		624.18	623.17	622.16	621.19	619.18	609.19	607.18	605.16	589.17
		587.15	551.15	550.14	549.14	544.17	535.16	534.15	533.14	532.13
		531.12	523.16	522.15	521.14	520.17	519.16	518.15	517.14	516.14
		515.13	514.12	513.11	511.16	509.14	507.16	505.15	504.15	503.13
		502.16	501.15	500.14	499.13	497.12	495.1	493.15	491.13	489.15
		488.15	487.14	486.14	485.12	481.15	479.13	478.12	477.15	475.13
		474.16	473.15	472.14	471.15	470.14	469.13	468.13	465.15	463.13
		461.12	460.11	459.15	458.14	457.12	448.14	447.15	445.12	443.11
		441.14	435.15	433.13	432.13	431.15	429.14	427.11	425.1	419.15
		417.14	416.13	415.12	414.12	413.14	411.13	401.14	399.13	397.11
		389.1	388.09	387.08	386.07	375.12	374.11	373.1	372.1	371.09
		370.08	369.07	361.1	360.1	359.12	358.11	357.11	356.1	355.09
		354.08	353.08	351.06	349.1	347.09	345.11	343.13	342.09	341.11
		340.1	339.1	338.09	337.08	336.07	335.09	331.09	330.08	329.11
		327.1	326.09	325.09	324.08	323.1	319.09	317.08	316.07	315.1
		314.09	313.08	312.07	310.09	308.09	307.08	306.07	303.1	301.08
		300.07	299.07	298.06	297.1	296.08	287.1	285.1	283.07	281.08
		280.07	279.09	273.1	271.08	270.07	269.1	267.09	265.08	264.07
		263.07	262.06	257.1	255.09	253.07	252.06	251.07	249.08	247.07
		245.06	239.09	237.08	235.07	233.06	223.07	211.07	196.06	195.05
		194.04	193.04	182.08	180.04	179.03	178.05	177.04	165.05	164.05
		163.04	162.03	149.06	148.05	147.04	139.04	135.04	123.04	122.04
		119.05	118.04	111.04	109.03	108.02	107.05	106.04		
References	<p>Piattelli, M; Imperato, F. Pigments of <i>Bougainvillea glabra</i>. <i>Phytochemistry</i> 1970, 9, 2557–2560.</p> <p>Heuer, S.; Richter, S.; Metzger, J.W.; Wray, V.; Nimtz, M.; Strack, D. Betacyanins from bracts of <i>Bougainvillea glabra</i>. <i>Phytochemistry</i> 1994, 37, 761–767.</p> <p>Slimen, I.B.; Najjar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

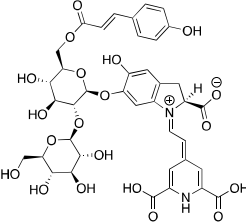
Coumglabranin

Chemical structure										
Name:	Coumglabranin (6'-O-E-4-Coumaroyl-glabranin)									
Chemical Formula	C ₃₉ H ₄₂ N ₂ O ₂₀									
Molecular weight	858.76									
Monoisotopic mass	858.2331									
m/z [M+H]	859.2403									
Theoretical fragments (m/z)	859.24	858.23	857.22	856.22	843.25	842.24	841.23	840.22	839.21	831.25
		830.24	829.23	827.25	826.24	825.23	824.23	823.22	822.21	821.2
		819.25	817.23	815.25	814.24	813.23	812.23	811.22	809.24	807.22
		805.21	803.19	801.23	799.26	797.24	796.23	795.22	794.22	793.21
		789.23	787.22	786.21	785.24	783.22	779.23	777.21	773.24	771.22
		770.22	769.21	768.2	767.23	765.21	755.23	753.21	751.2	735.2
		733.19	697.19	696.18	695.19	694.19	693.18	690.2	681.19	680.18
		679.18	678.17	677.16	676.17	675.17	669.19	668.18	667.18	666.2
		665.18	664.19	663.18	662.17	661.17	660.16	659.15	657.19	655.18
		653.2	651.18	650.18	649.17	648.19	647.19	646.18	645.17	643.16
		641.14	639.18	637.19	635.19	634.19	633.18	632.17	631.16	627.18
		625.17	624.16	623.17	621.17	620.2	619.19	618.18	617.19	616.18
		615.17	614.16	611.19	609.17	607.16	606.15	605.19	604.18	603.16
		594.18	593.19	591.16	589.15	587.18	581.19	579.17	578.16	577.19
		575.18	573.15	571.13	565.19	563.18	562.17	561.16	560.15	559.18
		557.17	547.18	545.17	543.15	533.14	532.13	531.12	517.15	515.13
		514.12	513.11	505.15	504.15	503.13	502.13	501.13	500.14	499.13
		497.12	495.1	488.13	487.13	486.14	485.12	484.12	483.12	481.12
		479.11	475.13	472.14	471.13	470.12	469.13	468.13	463.13	461.12
		457.12	454.13	453.12	452.11	445.12	443.11	441.14	431.13	429.14
		427.11	425.12	419.13	417.14	416.11	415.12	414.12	413.12	411.13
		403.14	401.12	399.11	398.1	397.13	395.11	389.1	388.09	387.08
		386.07	385.13	383.11	381.1	375.12	374.11	373.1	372.1	371.09
		370.08	369.07	361.1	360.1	359.12	358.12	357.11	356.1	355.09
		354.08	353.08	351.06	349.1	347.09	345.11	343.13	342.08	341.11
		339.1	338.09	337.08	336.07	335.09	331.09	330.08	329.11	327.1
		326.09	325.12	324.08	323.1	319.09	317.08	316.07	315.1	314.09
		313.08	312.07	310.09	308.08	306.07	303.1	301.08	300.07	299.07
		298.06	296.08	287.1	285.09	283.07	281.08	280.07	267.06	265.08
		264.07	263.07	262.06	255.09	253.07	251.07	249.08	247.07	245.06
		237.08	235.07	233.06	223.07	211.07	196.06	195.05	194.04	193.04
		182.08	180.04	179.03	178.05	177.04	165.05	164.05	163.04	162.03
		149.06	148.05	147.04	139.04	135.04	123.04	122.04	119.05	118.04
		111.04	109.03	108.02	107.05	106.04				
References	<p>Heuer, S.; Richter, S.; Metzger, J.W.; Wray, V.; Nimtz, M.; Strack, D. Betacyanins from bracts of <i>Bougainvillea glabra</i>. <i>Phytochemistry</i> 1994, 37, 761–767.</p> <p>Slimen, I.B.; Najjar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

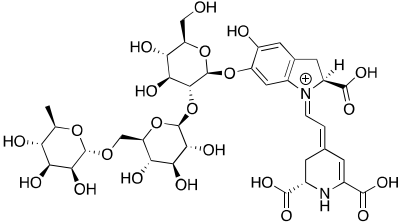
Isocoumglabranin

Chemical structure										
Name:	6'-O-E-4-Coumaroyl-isoglabranin (isocoumglabranin)									
Chemical Formula	C ₃₉ H ₄₂ N ₂ O ₂₀									
Molecular weight	858.76									
Monoisotopic mass	858.2331									
m/z [M+H]	859.2403									
Theoretical fragments (m/z)	859.24	858.23	857.22	856.22	843.25	842.24	841.23	840.22	839.21	831.25
		830.24	829.23	827.25	826.24	825.23	824.23	823.22	822.21	821.2
		819.25	817.23	815.25	814.24	813.23	812.23	811.22	809.24	807.22
		805.21	803.19	801.23	799.26	797.24	796.23	795.22	794.22	793.21
		789.23	787.22	786.21	785.24	783.22	779.23	777.21	773.24	771.22
		770.22	769.21	768.2	767.23	765.21	755.23	753.21	751.2	735.2
		733.19	697.19	696.18	695.19	694.19	693.18	690.2	681.19	680.18
		679.18	678.17	677.16	676.17	675.17	669.19	668.18	667.18	666.2
		665.18	664.19	663.18	662.17	661.17	660.16	659.15	657.19	655.18
		653.2	651.18	650.18	649.17	648.19	647.19	646.18	645.17	643.16
		641.14	639.18	637.19	635.19	634.19	633.18	632.17	631.16	627.18
		625.17	624.16	623.17	621.17	620.2	619.19	618.18	617.19	616.18
		615.17	614.16	611.19	609.17	607.16	606.15	605.19	604.18	603.16
		594.18	593.19	591.16	589.15	587.18	581.19	579.17	578.16	577.19
		575.18	573.15	571.13	565.19	563.18	562.17	561.16	560.15	559.18
		557.17	547.18	545.17	543.15	533.14	532.13	531.12	517.15	515.13
		514.12	513.11	505.15	504.15	503.13	502.13	501.13	500.14	499.13
		497.12	495.1	488.13	487.13	486.14	485.12	484.12	483.12	481.12
		479.11	475.13	472.14	471.13	470.12	469.13	468.13	463.13	461.12
		457.12	454.13	453.12	452.11	445.12	443.11	441.14	431.13	429.14
		427.11	425.12	419.13	417.14	416.11	415.12	414.12	413.12	411.13
		403.14	401.12	399.11	398.1	397.13	395.11	389.1	388.09	387.08
		386.07	385.13	383.11	381.1	375.12	374.11	373.1	372.1	371.09
		370.08	369.07	361.1	360.1	359.12	358.12	357.11	356.1	355.09
		354.08	353.08	351.06	349.1	347.09	345.11	343.13	342.08	341.11
		339.1	338.09	337.08	336.07	335.09	331.09	330.08	329.11	327.1
		326.09	325.12	324.08	323.1	319.09	317.08	316.07	315.1	314.09
		313.08	312.07	310.09	308.08	306.07	303.1	301.08	300.07	299.07
		298.06	296.08	287.1	285.09	283.07	281.08	280.07	267.06	265.08
		264.07	263.07	262.06	255.09	253.07	251.07	249.08	247.07	245.06
		237.08	235.07	233.06	223.07	211.07	196.06	195.05	194.04	193.04
		182.08	180.04	179.03	178.05	177.04	165.05	164.05	163.04	162.03
		149.06	148.05	147.04	139.04	135.04	123.04	122.04	119.05	118.04
		111.04	109.03	108.02	107.05	106.04				
References	<p>Heuer, S.; Richter, S.; Metzger, J.W.; Wray, V.; Nimtz, M.; Strack, D. Betacyanins from bracts of <i>Bougainvillea glabra</i>. <i>Phytochemistry</i> 1994, 37, 761–767.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

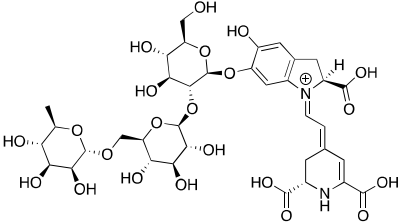
Neocoumglabranin

Chemical structure										
Name:	Neocoumglabranin									
Chemical Formula	C ₃₉ H ₄₀ N ₂ O ₂₀									
Molecular weight	856.74									
Monoisotopic mass	856.2174									
m/z [M+H]	857.2247									
Theoretical fragments (m/z)	857.22	856.22	855.21	854.2	841.23	840.22	839.21	838.21	837.2	829.23
	828.22	827.21	825.23	823.22	822.21	821.2	820.2	819.19	817.23	
	815.21	814.21	813.23	811.22	810.21	809.2	807.22	805.21	803.19	
	801.18	799.22	797.24	795.22	793.21	792.2	791.19	787.22	785.2	
	784.2	781.21	777.21	775.2	769.21	767.19	766.19	763.2	751.2	
	749.18	731.17	695.17	694.16	693.18	692.17	691.16	679.18	678.17	
	677.16	676.15	675.15	674.16	673.15	667.18	666.17	665.16	664.19	
	663.18	661.17	660.16	659.15	658.14	657.14	655.18	653.16	651.18	
	650.18	649.17	648.19	647.15	646.18	645.17	643.16	641.14	639.12	
	637.17	635.17	634.19	633.18	632.17	631.16	630.15	629.14	628.17	
	625.17	623.15	622.14	621.16	620.2	619.16	618.18	617.19	616.18	
	615.17	614.16	613.15	607.16	605.14	604.18	603.15	602.19	601.15	
	593.19	589.19	587.13	585.14	581.19	579.17	578.16	577.19	575.18	
	565.19	563.18	562.17	561.16	560.15	559.18	557.17	547.18	545.17	
	543.15	531.12	530.12	529.11	515.13	513.11	512.11	511.1	503.13	
	502.13	501.13	500.14	499.13	497.12	495.1	493.09	488.13	487.13	
	486.14	485.12	484.12	483.12	482.13	479.11	477.09	473.12	472.14	
	471.13	470.12	469.13	468.13	467.11	466.11	461.12	459.1	458.14	
	456.15	455.11	454.13	453.12	452.11	443.13	441.09	440.13	431.13	
	429.14	425.12	423.08	419.13	417.14	416.11	415.12	414.12	413.12	
	411.13	403.14	401.12	399.11	398.1	397.13	395.11	387.08	386.07	
	385.07	384.06	383.11	381.1	373.1	372.1	371.09	370.08	369.07	
	368.06	367.06	359.09	358.08	357.11	356.1	355.09	354.08	353.08	
	352.07	347.09	345.07	343.09	341.11	340.07	339.1	338.09	337.08	
	333.07	332.06	329.08	328.07	327.1	325.08	324.07	320.08	317.08	
	315.06	314.05	312.07	306.07	301.08	299.07	283.07	279.06	278.05	
	267.09	265.05	263.07	261.05	255.09	253.07	251.07	249.05	247.03	
	237.08	235.06	233.06	221.06	209.06	207.05	194.04	193.04	191.06	
	181.05	180.04	179.03	178.05	177.04	175.06	165.05	164.05	163.04	
	162.03	150.05	149.06	148.05	147.04	139.04	135.04	123.04	122.04	
	121.03	119.05	118.04	111.04	109.03	108.02	107.05	106.04		
References	<p>Heuer, S.; Richter, S.; Metzger, J.W.; Wray, V.; Nimtz, M.; Strack, D. Betacyanins from bracts of <i>Bougainvillea glabra</i>. <i>Phytochemistry</i> 1994, 37, 761–767.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

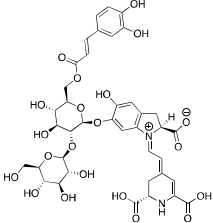
6''-O-Rhamnosy-glabranin

Chemical structure										
Name:	6''-O-Rhamnosyl-glabranin									
Chemical Formula	C ₃₆ H ₄₆ N ₂ O ₂₂									
Molecular weight	858.76									
Monoisotopic mass	858.2542									
m/z [M+H]	859.2615									
Theoretical fragments (m/z)	859.26	858.25	857.25	856.24	843.27	842.26	841.25	840.24	839.24	831.27
		830.26	829.25	827.27	825.26	823.24	821.22	819.27	817.25	815.27
		814.26	813.26	812.25	811.24	809.26	807.25	805.23	801.26	799.28
		797.26	795.25	789.26	787.24	786.23	785.26	783.25	773.26	771.25
		769.23	753.23	751.22	713.2	712.2	711.19	697.21	695.19	694.19
		693.18	690.22	685.21	683.19	681.21	679.2	677.18	675.17	669.21
		667.2	666.22	665.18	664.21	663.2	661.19	659.17	655.2	651.2
		650.21	649.19	648.21	647.21	646.2	645.19	643.2	641.18	637.19
		634.21	633.2	632.19	625.19	623.17	621.2	620.22	619.21	618.2
		617.21	616.2	615.19	614.18	607.18	605.21	604.2	594.2	593.21
		589.21	587.2	581.21	579.19	578.18	577.21	575.2	565.21	563.2
		562.19	561.18	560.17	559.2	557.19	551.15	550.14	549.14	547.2
		545.19	535.16	533.14	532.13	531.12	523.16	521.14	520.17	519.16
		518.15	517.15	515.13	513.11	507.16	505.15	504.15	503.13	502.16
		501.15	500.14	499.13	497.12	493.15	489.15	488.15	487.13	486.14
		481.15	479.13	475.13	471.17	470.14	469.13	468.13	463.13	461.12
		459.15	447.15	445.12	443.11	441.14	435.15	433.13	432.13	431.15
		429.14	419.15	417.14	415.12	414.12	413.14	411.13	401.14	399.13
		389.1	388.09	387.08	386.07	375.12	374.11	373.1	372.1	371.09
		370.08	369.07	361.1	360.1	359.12	358.11	357.11	356.1	355.09
		354.08	353.08	351.06	349.1	347.09	345.11	343.13	342.09	341.11
		340.1	339.1	338.09	337.08	335.09	331.09	330.08	329.11	327.1
		326.09	325.09	324.08	323.1	319.09	317.08	316.07	315.1	314.09
		313.08	308.09	307.08	306.07	303.1	301.08	300.07	299.07	298.06
		297.1	287.1	285.1	283.07	281.08	280.07	279.09	273.1	271.08
		270.07	269.1	267.09	265.08	264.07	263.07	262.06	257.1	255.09
		253.07	252.06	251.07	249.08	247.07	245.06	239.09	237.08	235.07
		233.06	223.07	211.07	196.06	195.05	194.04	193.04	182.08	180.04
		179.03	178.05	177.04	165.05	164.05	163.04	162.03	149.06	148.05
		147.04	139.04	135.04	123.04	122.04	119.05	118.04	111.04	109.03
		108.02	107.05	106.04						
References	Imperato, F. <i>Phytochemistry</i> 1975 , 14, 2526–2527. Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017 , 65, 675–689. Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021 , 38, 2315–2346.									

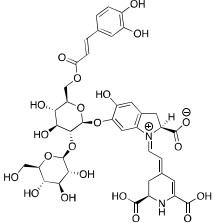
6''-O-Rhamnosy-isoglabranin

Chemical structure										
Name:	6''-O-Rhamnosyl-isoglabranin									
Chemical Formula	C ₃₆ H ₄₆ N ₂ O ₂₂									
Molecular weight	858.76									
Monoisotopic mass	858.2542									
m/z [M+H]	859.2615									
Theoretical fragments (m/z)	859.26	858.25	857.25	856.24	843.27	842.26	841.25	840.24	839.24	831.27
		830.26	829.25	827.27	825.26	823.24	821.22	819.27	817.25	815.27
		814.26	813.26	812.25	811.24	809.26	807.25	805.23	801.26	799.28
		797.26	795.25	789.26	787.24	786.23	785.26	783.25	773.26	771.25
		769.23	753.23	751.22	713.2	712.2	711.19	697.21	695.19	694.19
		693.18	690.22	685.21	683.19	681.21	679.2	677.18	675.17	669.21
		667.2	666.22	665.18	664.21	663.2	661.19	659.17	655.2	651.2
		650.21	649.19	648.21	647.21	646.2	645.19	643.2	641.18	637.19
		634.21	633.2	632.19	625.19	623.17	621.2	620.22	619.21	618.2
		617.21	616.2	615.19	614.18	607.18	605.21	604.2	594.2	593.21
		589.21	587.2	581.21	579.19	578.18	577.21	575.2	565.21	563.2
		562.19	561.18	560.17	559.2	557.19	551.15	550.14	549.14	547.2
		545.19	535.16	533.14	532.13	531.12	523.16	521.14	520.17	519.16
		518.15	517.15	515.13	513.11	507.16	505.15	504.15	503.13	502.16
		501.15	500.14	499.13	497.12	493.15	489.15	488.15	487.13	486.14
		481.15	479.13	475.13	471.17	470.14	469.13	468.13	463.13	461.12
		459.15	447.15	445.12	443.11	441.14	435.15	433.13	432.13	431.15
		429.14	419.15	417.14	415.12	414.12	413.14	411.13	401.14	399.13
		389.1	388.09	387.08	386.07	375.12	374.11	373.1	372.1	371.09
		370.08	369.07	361.1	360.1	359.12	358.11	357.11	356.1	355.09
		354.08	353.08	351.06	349.1	347.09	345.11	343.13	342.09	341.11
		340.1	339.1	338.09	337.08	335.09	331.09	330.08	329.11	327.1
		326.09	325.09	324.08	323.1	319.09	317.08	316.07	315.1	314.09
		313.08	308.09	307.08	306.07	303.1	301.08	300.07	299.07	298.06
		297.1	287.1	285.1	283.07	281.08	280.07	279.09	273.1	271.08
		270.07	269.1	267.09	265.08	264.07	263.07	262.06	257.1	255.09
		253.07	252.06	251.07	249.08	247.07	245.06	239.09	237.08	235.07
		233.06	223.07	211.07	196.06	195.05	194.04	193.04	182.08	180.04
		179.03	178.05	177.04	165.05	164.05	163.04	162.03	149.06	148.05
		147.04	139.04	135.04	123.04	122.04	119.05	118.04	111.04	109.03
		108.02	107.05	106.04						
References	<p>Imperato, F. <i>Phytochemistry</i> 1975, 14, 2526–2527.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

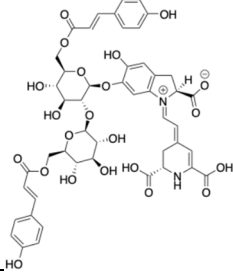
Cafglabranin

Chemical structure										
Name:	Cafglabranin (6'-O-E-Caffeoyl-glabranin)									
Chemical Formula	C ₃₉ H ₄₂ N ₂ O ₂₁									
Molecular weight	874.76									
Monoisotopic mass	874.2280									
m/z [M+H]	875.2353									
Theoretical fragments (m/z)	875.24	874.23	873.22	872.21	859.24	858.23	857.22	856.22	855.21	847.24
		846.23	845.22	843.25	842.24	841.23	840.22	839.21	838.21	837.2
		835.24	833.22	831.25	830.24	829.23	828.22	827.21	825.23	823.22
		821.2	819.19	817.23	815.25	813.23	812.23	811.22	810.21	809.2
		805.23	803.21	802.21	801.23	799.22	795.22	793.21	789.23	787.22
		786.21	785.2	784.2	783.22	781.21	771.22	769.21	767.19	751.2
		749.18	713.18	712.17	711.17	706.2	697.19	696.18	695.17	694.16
		693.16	685.19	684.18	683.17	682.2	681.19	680.18	679.17	678.17
		677.16	676.15	675.15	673.19	671.17	669.19	667.18	666.18	665.16
		664.19	663.18	662.17	661.17	659.15	657.14	655.18	653.16	651.18
		650.18	649.18	648.17	647.15	643.18	641.16	640.15	639.18	637.17
		636.19	635.18	634.18	633.18	632.17	631.17	630.16	627.18	625.17
		623.15	622.14	621.18	620.17	619.16	610.18	609.18	607.16	605.14
		603.17	597.18	595.17	594.16	593.19	591.17	589.15	587.13	581.19
		579.17	578.16	577.16	576.15	575.18	573.16	563.18	561.16	559.14
		533.14	532.13	531.12	520.14	518.13	517.15	515.13	514.12	513.11
		505.15	504.13	503.13	502.13	500.12	499.13	497.12	495.1	488.13
		487.12	486.12	485.12	481.12	479.11	475.13	470.12	469.11	468.11
		463.13	461.12	459.13	457.12	447.13	445.12	443.11	441.12	435.13
		433.11	432.11	431.13	429.12	427.11	425.1	419.13	417.12	415.1
		414.09	413.12	411.11	401.12	399.11	397.09	389.1	388.09	387.08
		386.07	375.12	374.11	373.1	372.1	371.09	370.08	369.07	361.1
		360.1	359.12	358.12	357.11	356.1	355.09	354.08	353.08	351.06
		349.1	347.09	345.11	343.13	342.08	341.11	339.1	338.09	337.08
		336.07	335.09	331.09	330.08	329.11	327.1	326.09	325.12	324.08
		323.1	319.09	317.08	316.07	315.1	314.09	313.08	312.07	310.09
		308.08	306.07	303.1	301.08	300.07	299.07	298.06	296.08	287.1
		285.09	283.07	281.08	280.07	267.06	265.08	264.07	263.07	262.06
		255.09	253.07	251.07	249.08	247.07	245.06	237.08	235.07	233.06
		223.07	211.07	196.06	195.05	194.04	193.04	182.08	180.04	179.03
		178.05	177.04	165.05	164.05	163.04	162.03	149.06	148.05	147.04
		139.04	135.04	123.04	122.04	119.05	118.04	111.04	109.03	108.02
		107.05	106.04							
References	<p>Heuer, S.; Richter, S.; Metzger, J.W.; Wray, V.; Nimtz, M.; Strack, D. Betacyanins from bracts of <i>Bougainvillea glabra</i>. <i>Phytochemistry</i> 1994, 37, 761–767.</p> <p>Slimen, I.B.; Najjar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

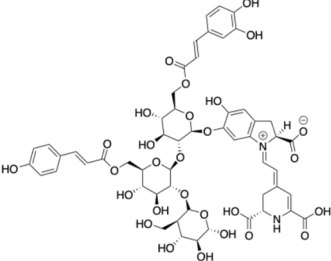
Isocafglabranin

Chemical structure										
Name:	Isocafglabranin (6'-O-E-Caffeoyl-isoglabranin)									
Chemical Formula	C ₃₉ H ₄₂ N ₂ O ₂₁									
Molecular weight	874.76									
Monoisotopic mass	874.2280									
m/z [M+H]	875.2353									
Theoretical fragments (m/z)	875.24	874.23	873.22	872.21	859.24	858.23	857.22	856.22	855.21	847.24
		846.23	845.22	843.25	842.24	841.23	840.22	839.21	838.21	837.2
		835.24	833.22	831.25	830.24	829.23	828.22	827.21	825.23	823.22
		821.2	819.19	817.23	815.25	813.23	812.23	811.22	810.21	809.2
		805.23	803.21	802.21	801.23	799.22	795.22	793.21	789.23	787.22
		786.21	785.2	784.2	783.22	781.21	771.22	769.21	767.19	751.2
		749.18	713.18	712.17	711.17	706.2	697.19	696.18	695.17	694.16
		693.16	685.19	684.18	683.17	682.2	681.19	680.18	679.17	678.17
		677.16	676.15	675.15	673.19	671.17	669.19	667.18	666.18	665.16
		664.19	663.18	662.17	661.17	659.15	657.14	655.18	653.16	651.18
		650.18	649.18	648.17	647.15	643.18	641.16	640.15	639.18	637.17
		636.19	635.18	634.18	633.18	632.17	631.17	630.16	627.18	625.17
		623.15	622.14	621.18	620.17	619.16	610.18	609.18	607.16	605.14
		603.17	597.18	595.17	594.16	593.19	591.17	589.15	587.13	581.19
		579.17	578.16	577.16	576.15	575.18	573.16	563.18	561.16	559.14
		533.14	532.13	531.12	520.14	518.13	517.15	515.13	514.12	513.11
		505.15	504.13	503.13	502.13	500.12	499.13	497.12	495.1	488.13
		487.12	486.12	485.12	481.12	479.11	475.13	470.12	469.11	468.11
		463.13	461.12	459.13	457.12	447.13	445.12	443.11	441.12	435.13
		433.11	432.11	431.13	429.12	427.11	425.1	419.13	417.12	415.1
		414.09	413.12	411.11	401.12	399.11	397.09	389.1	388.09	387.08
		386.07	375.12	374.11	373.1	372.1	371.09	370.08	369.07	361.1
		360.1	359.12	358.12	357.11	356.1	355.09	354.08	353.08	351.06
		349.1	347.09	345.11	343.13	342.08	341.11	339.1	338.09	337.08
		336.07	335.09	331.09	330.08	329.11	327.1	326.09	325.12	324.08
		323.1	319.09	317.08	316.07	315.1	314.09	313.08	312.07	310.09
		308.08	306.07	303.1	301.08	300.07	299.07	298.06	296.08	287.1
		285.09	283.07	281.08	280.07	267.06	265.08	264.07	263.07	262.06
		255.09	253.07	251.07	249.08	247.07	245.06	237.08	235.07	233.06
		223.07	211.07	196.06	195.05	194.04	193.04	182.08	180.04	179.03
		178.05	177.04	165.05	164.05	163.04	162.03	149.06	148.05	147.04
		139.04	135.04	123.04	122.04	119.05	118.04	111.04	109.03	108.02
		107.05	106.04							
References	<p>Heuer, S.; Richter, S.; Metzger, J.W.; Wray, V.; Nimtz, M.; Strack, D. Betacyanins from bracts of <i>Bougainvillea glabra</i>. <i>Phytochemistry</i> 1994, 37, 761–767.</p> <p>Slimen, I.B.; Najjar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021, 38, 2315–2346.</p>									

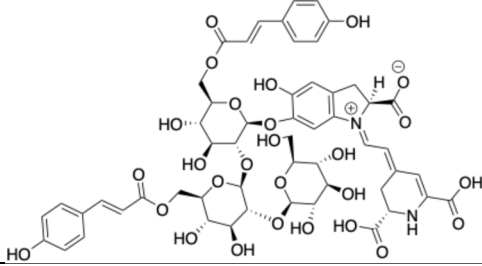
Bicoumglabranin

Chemical structure										
Name:	Bicoumglabranin (6',6''-Di-O-E-4-coumaroyl-glabranin)									
Chemical Formula	C ₄₈ H ₄₈ N ₂ O ₂₂									
Molecular weight	1004.90									
Monoisotopic mass	1004.2699									
m/z [M+H]	1005.2772									
Theoretical fragments (m/z)	1005.28	1004.27	1003.26	1002.25	989.28	988.27	987.27	986.26	985.25	977.28
	976.27	975.27	973.29	972.28	971.27	970.26	969.26	968.25	967.24	
	965.28	963.27	961.29	960.28	959.27	958.26	957.26	955.28	953.26	
	951.25	949.23	947.27	945.29	943.28	942.27	941.26	940.25	939.25	
	935.27	933.26	932.25	931.28	929.26	925.27	923.25	919.28	917.26	
	916.25	915.25	914.24	913.27	911.25	901.27	899.25	897.23	881.24	
	879.22	841.23	840.22	839.21	836.24	825.23	824.23	823.22	822.21	
	821.2	813.23	812.24	811.22	810.22	809.22	807.22	805.21	803.19	
	797.24	796.22	795.22	794.23	793.22	792.21	791.21	789.21	787.2	
	783.22	780.23	779.22	778.21	777.21	771.22	769.21	767.22	766.23	
	765.23	764.22	763.22	762.22	761.21	760.2	755.23	753.21	751.22	
	750.22	740.22	739.22	735.23	733.21	727.22	725.21	724.2	723.23	
	721.21	711.23	709.21	708.2	707.2	706.19	705.22	703.2	697.19	
	696.18	695.17	693.22	691.2	689.19	681.19	680.18	679.18	678.17	
	677.16	675.17	669.19	668.18	667.18	665.2	663.18	662.17	661.17	
	660.16	659.15	657.19	655.18	653.2	651.18	650.17	649.17	648.19	
	647.19	646.18	645.17	643.16	641.14	639.18	637.17	635.19	633.17	
	632.17	631.16	627.18	625.17	624.16	623.19	621.17	617.19	616.18	
	615.17	614.16	611.19	609.17	607.16	606.15	605.16	603.16	593.18	
	591.16	589.15	587.18	575.18	573.15	571.13	563.18	561.16	560.15	
	559.18	557.17	547.18	545.17	543.15	533.14	532.13	531.12	517.15	
	515.13	514.12	513.11	505.15	504.15	503.13	502.13	501.13	499.13	
	497.12	495.1	488.13	487.13	486.14	485.12	484.12	483.12	481.12	
	479.11	475.13	472.14	471.13	470.12	469.12	468.13	463.13	461.12	
	457.12	454.13	453.12	452.11	445.12	443.11	431.13	427.11	425.12	
	419.13	417.12	416.11	415.14	413.12	411.13	403.14	401.12	399.11	
	398.1	397.13	395.11	389.1	388.09	387.08	386.07	385.13	383.11	
	381.1	375.12	374.11	373.1	372.1	371.09	370.08	369.07	361.1	
	360.1	359.12	358.12	357.11	356.1	355.09	354.08	353.08	351.06	
	349.1	347.09	345.11	343.13	342.08	341.11	339.1	338.09	337.08	
	336.07	335.09	331.09	330.08	329.11	327.1	326.09	325.12	324.08	
	323.1	319.09	317.08	316.07	315.1	314.09	313.08	312.07	310.09	
	308.08	306.07	303.1	301.08	300.07	299.07	298.06	296.08	287.1	
	285.09	283.07	281.08	280.07	267.06	265.08	264.07	263.07	262.06	
	255.09	253.07	251.07	249.08	247.07	245.06	237.08	235.07	233.06	
	223.07	211.07	196.06	195.05	194.04	193.04	182.08	180.04	179.03	
	178.05	177.04	165.05	164.05	163.04	162.03	149.06	148.05	147.04	
	139.04	135.04	123.04	122.04	119.05	118.04	111.04	109.03	108.02	
	107.05	106.04								
References	Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021 , 38, 2315–2346.									

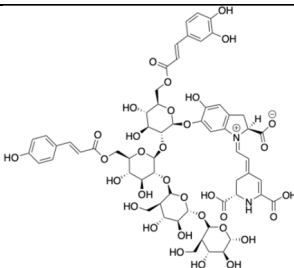
2''-O-[(6''-O-E-4-coumaroyl)]-glucosyl-cafglabranin

Chemical structure										
Name:	2''-O-[(6''-O-E-4-coumaroyl)]-glucosyl-cafglabranin									
Chemical Formula	C ₅₄ H ₅₈ N ₂ O ₂₈									
Molecular weight	1183.04									
Monoisotopic mass	1182.3176									
m/z [M+H]	1183.3289									
Theoretical fragments (m/z)	1183.32	1182.32	1181.31	1180.3	1167.33	1166.32	1165.31	1164.31	1163.3	1155.33
		1154.32	1153.31	1151.34	1149.32	1147.3	1145.29	1143.33	1141.31	1139.34
		1138.33	1137.32	1136.31	1135.3	1133.32	1131.31	1129.29	1125.32	1123.34
		1121.32	1119.31	1113.32	1111.3	1110.3	1109.32	1107.31	1097.32	1095.31
		1093.29	1077.3	1075.28	1021.27	1020.26	1019.28	1018.27	1017.26	1014.29
		1005.28	1003.28	1002.27	1001.27	999.25	993.28	991.26	990.29	989.27
		988.27	987.26	985.27	983.26	977.28	975.29	974.27	973.27	972.28
		971.29	970.26	969.28	967.24	963.27	961.27	959.29	958.27	957.27
		956.26	951.27	949.25	947.26	945.28	944.28	943.27	942.27	941.27
		940.26	939.26	938.25	933.26	931.26	929.27	928.26	918.27	917.27
		915.27	913.25	911.26	905.27	903.26	902.25	901.28	899.26	889.28
		887.26	886.25	885.24	884.24	883.27	881.25	871.27	869.25	857.22
		855.21	841.23	839.24	837.22	828.23	826.22	825.23	824.22	823.22
		821.22	812.22	810.22	808.23	807.22	805.21	796.22	795.21	794.23
		793.22	792.21	785.2	778.23	777.22	776.22	769.21	767.21	765.22
		755.22	753.22	751.2	749.23	743.22	741.22	740.19	739.21	738.2
		737.23	735.21	727.22	725.23	723.21	722.21	721.23	719.22	713.18
		712.17	711.17	709.23	707.22	697.19	695.17	694.16	693.16	685.19
		683.17	681.19	679.18	677.16	675.15	669.19	667.18	665.16	663.18
		661.17	659.15	655.18	651.18	649.17	648.17	643.18	641.16	637.17
		632.17	630.18	625.17	623.15	614.16	607.16	605.14	591.17	579.17
		575.18	573.18	563.18	561.18	557.17	545.17	533.14	531.12	520.14
		518.13	517.15	515.13	513.11	504.13	502.13	500.12	499.13	497.12
		488.13	487.12	486.12	470.12	469.11	468.11	461.12	459.13	447.13
		443.11	441.12	435.13	433.11	432.11	431.13	429.12	419.13	417.12
		415.1	414.09	413.12	411.11	401.12	399.11	389.1	388.09	387.08
		386.07	375.12	374.11	373.1	372.1	371.09	370.08	369.07	361.1
		360.1	359.12	358.12	357.11	356.1	355.09	354.08	353.08	351.06
		349.1	347.09	345.11	343.13	342.08	341.11	339.1	337.08	335.09
		331.09	330.08	329.11	327.1	326.09	325.12	324.08	323.1	319.09
		317.08	316.07	315.1	314.09	313.08	306.07	303.1	301.08	300.07
		299.07	298.06	287.1	285.09	283.07	281.08	280.07	267.06	265.08
		264.07	263.07	262.06	255.09	251.07	249.08	247.07	245.06	237.08
		235.07	233.06	223.07	211.07	196.06	195.05	194.04	193.04	182.08
		180.04	179.03	178.05	177.04	165.05	164.05	163.04	162.03	149.06
		148.05	147.04	139.04	135.04	123.04	122.04	119.05	118.04	111.04
		109.03	108.02	107.05	106.04					
References	Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021 , 38, 2315–2346.									

2''-O-glucosyl-bicoumglabranin

Chemical structure										
Name:	2''-O-glucosyl-bicoumglabranin									
Chemical Formula	C ₅₄ H ₅₈ N ₂ O ₂₇									
Molecular weight	1167.04									
Monoisotopic mass	1166.3227									
m/z [M+H]	1167.3300									
Theoretical fragments (m/z)	1167.33	1166.32	1165.31	1164.31	1151.34	1150.33	1149.32	1148.31	1147.3	1139.34
		1138.33	1137.32	1135.34	1133.32	1131.31	1129.29	1127.34	1125.32	1123.34
		1122.33	1121.32	1120.32	1119.31	1117.33	1115.31	1113.3	1109.32	1107.35
		1105.33	1103.31	1097.32	1095.31	1094.3	1093.33	1091.31	1081.33	1079.31
		1077.3	1061.3	1059.29	1005.28	1004.27	1003.28	1002.27	1001.27	998.29
		989.28	987.27	986.26	985.27	983.26	977.28	975.29	974.29	973.27
		972.28	971.27	969.26	967.26	961.29	959.27	958.27	957.28	956.28
		955.28	954.27	953.26	951.25	947.27	945.28	943.28	942.28	941.27
		940.26	935.27	933.26	931.26	929.26	928.29	927.28	926.27	925.28
		924.27	923.26	922.25	917.26	915.25	913.28	912.27	902.27	901.28
		899.25	897.23	895.27	889.28	887.26	886.25	885.28	883.27	873.28
		871.27	870.26	869.25	868.24	867.27	865.25	855.27	853.25	841.23
		839.24	837.22	825.23	823.22	821.22	812.24	810.22	809.22	808.23
		807.22	805.21	796.22	794.23	792.21	791.21	780.23	779.22	778.21
		777.22	776.22	769.21	767.21	762.22	761.21	760.2	751.2	749.23
		739.22	737.23	733.21	727.22	725.23	724.2	723.21	722.21	721.21
		719.22	711.23	709.21	707.2	706.19	705.22	703.2	697.19	696.18
		695.17	693.22	691.2	681.19	679.18	678.17	677.16	669.19	667.18
		665.2	663.18	661.17	659.15	653.2	651.18	649.17	647.19	645.17
		643.16	639.18	635.19	633.17	632.17	630.18	627.18	625.17	621.17
		614.16	609.17	607.16	591.16	589.15	575.18	573.18	563.18	561.18
		557.17	545.17	533.14	531.12	517.15	515.13	513.11	504.15	502.13
		501.13	499.13	497.12	488.13	486.14	484.12	483.12	472.14	471.13
		470.12	461.12	454.13	453.12	452.11	443.11	431.13	425.12	419.13
		417.12	416.11	415.14	413.12	403.14	401.12	399.11	398.1	397.13
		395.11	389.1	388.09	387.08	386.07	385.13	383.11	375.12	374.11
		373.1	372.1	371.09	370.08	369.07	361.1	360.1	359.12	358.12
		357.11	356.1	355.09	354.08	353.08	351.06	349.1	347.09	345.11
		343.13	342.08	341.11	339.1	337.08	335.09	331.09	330.08	329.11
		327.1	326.09	325.12	324.08	323.1	319.09	317.08	316.07	315.1
		314.09	313.08	306.07	303.1	301.08	300.07	299.07	298.06	287.1
		285.09	283.07	281.08	280.07	267.06	265.08	264.07	263.07	262.06
		255.09	251.07	249.08	247.07	245.06	237.08	235.07	233.06	223.07
		211.07	196.06	195.05	194.04	193.04	182.08	180.04	179.03	178.05
		177.04	165.05	164.05	163.04	162.03	149.06	148.05	147.04	139.04
		135.04	123.04	122.04	119.05	118.04	111.04	109.03	108.02	107.05
		106.04	98.02							
References	Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021 , 38, 2315–2346.									

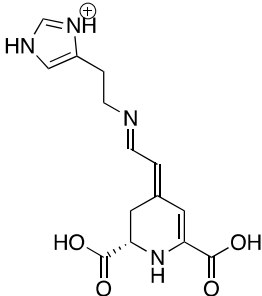
2''-O-[(6''-O-E-4-coumaroyl)]-sophorosyl-cafglabranin

Chemical structure										
Name:	2''-O-[(6''-O-E-4-coumaroyl)]-sophorosyl-cafglabranin									
Chemical Formula	C ₆₀ H ₆₈ N ₂ O ₃₃									
Molecular weight	1345.19									
Monoisotopic mass	1344.3704									
m/z [M+H]	1345.3777									
Theoretical fragments (m/z)	1345.38	1344.37	1343.36	1329.38	1328.37	1327.37	1326.36	1325.35	1317.38	1316.37
		1315.37	1313.39	1311.37	1309.36	1307.34	1305.38	1303.37	1301.39	1300.38
		1299.37	1298.36	1297.36	1295.38	1293.36	1291.35	1287.37	1285.39	1283.38
		1281.36	1275.37	1273.36	1272.35	1271.38	1269.36	1259.38	1257.36	1255.35
		1239.35	1237.34	1183.32	1182.32	1181.33	1180.32	1179.31	1176.34	1167.33
		1165.34	1164.33	1163.32	1161.3	1155.33	1153.34	1152.34	1151.32	1150.32
		1149.32	1147.32	1145.31	1139.34	1137.34	1136.32	1135.32	1134.33	1133.35
		1132.31	1131.33	1129.29	1125.32	1123.32	1121.35	1120.33	1119.32	1118.31
		1113.32	1111.3	1109.31	1107.33	1106.33	1105.33	1104.32	1095.31	1093.31
		1091.32	1080.32	1079.32	1077.32	1075.3	1067.32	1065.31	1064.3	1063.33
		1061.31	1051.33	1049.31	1047.3	1021.27	1020.26	1019.26	1017.26	1005.28
		1003.26	1002.25	1001.29	999.27	993.28	991.26	990.29	989.28	988.27
		987.27	986.28	985.25	983.28	977.28	975.27	974.27	973.25	972.27
		971.27	970.28	969.26	967.24	963.27	959.27	957.26	956.28	951.27
		949.25	947.26	945.26	933.26	931.24	929.27	917.27	915.28	913.23
		905.27	903.28	901.26	899.28	887.28	885.27	857.22	855.21	841.23
		839.21	837.2	828.23	826.22	825.23	823.22	821.2	812.22	810.22
		808.21	807.22	805.21	794.21	785.2	769.21	767.19	755.22	751.2
		743.22	741.2	737.21	725.21	723.19	713.18	712.17	711.17	697.19
		695.17	694.16	693.16	685.19	683.17	681.19	679.18	677.16	675.15
		669.19	667.18	665.16	663.18	661.17	659.15	655.18	651.18	649.17
		643.18	641.16	637.17	625.17	623.15	607.16	605.14	533.14	531.12
		520.14	518.13	517.15	515.13	513.11	504.13	502.13	500.12	499.13
		497.12	486.12	469.11	468.11	461.12	447.13	443.11	441.12	435.13
		433.11	429.12	417.12	415.1	414.09	411.11	399.11	389.1	388.09
		387.08	375.12	374.11	373.1	372.1	371.09	370.08	369.07	361.1
		359.12	358.12	357.11	356.1	355.09	354.08	353.08	345.11	343.13
		341.11	339.1	337.08	331.09	330.08	329.11	327.1	326.09	319.09
		317.08	316.07	314.09	306.07	303.1	301.08	300.07	299.07	298.06
		287.1	285.09	283.07	281.08	280.07	267.06	265.08	263.07	251.07
		249.08	237.08	235.07	233.06	196.06	195.05	194.04	193.04	182.08
		180.04	179.03	178.05	177.04	165.05	164.05	163.04	162.03	149.06
		148.05	147.04	139.04	135.04	123.04	122.04	119.05	111.04	109.03
		108.02	107.05	106.04						
References	Kumorkiewicz-Jamro, A.; Świergosz, T.; Sutor, K.; Spórna-Kucab, A.; Wybraniec, S. Multi-colored shades of betalains: Recent advances in betacyanin chemistry. <i>Nat. Prod. Rep.</i> 2021 , 38, 2315–2346.									

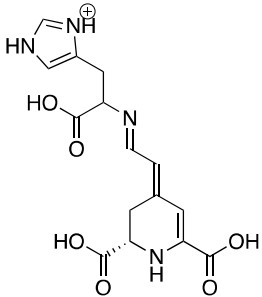
Betaxanthins

Positively charged-type

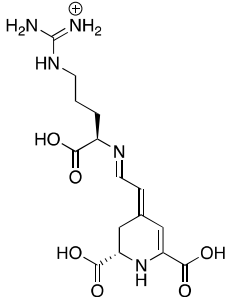
Histamine-bx

Chemical structure										
Name:	Histamine-bx									
Chemical Formula	C ₁₄ H ₁₆ N ₄ O ₄									
Molecular weight	304.31									
Monoisotopic mass	304.1172									
m/z [M+H]	305.1244									
Theoretical fragments (m/z)	305.12	304.12	303.11	302.1	301.09	290.11	289.13	288.12	287.11	286.11
		285.1	284.09	279.12	278.11	277.13	276.12	275.11	274.12	273.13
		272.1	271.12	270.09	269.1	268.1	266.11	265.13	264.1	263.11
		262.12	261.13	260.13	259.12	258.09	257.1	251.11	249.13	248.13
		247.12	246.11	245.14	244.11	243.12	242.12	241.11	239.09	237.09
		236.08	235.12	234.11	233.1	232.11	231.09	230.09	229.06	228.11
		227.09	224.08	223.07	222.06	221.09	220.11	219.08	218.09	217.14
		216.14	215.13	214.1	213.09	212.08	211.07	210.06	209.06	208.08
		207.08	206.07	205.06	204.11	203.13	202.1	201.11	200.08	199.1
		198.09	197.09	196.06	195.08	194.04	193.06	192.05	191.05	190.04
		189.11	188.12	187.1	186.1	184.06	183.05	182.04	181.06	180.07
		179.08	178.05	177.07	176.03	175.05	174.1	170.04	169.05	168.03
		167.08	166.07	165.07	164.03	163.05	162.1	161.09	160.09	158.04
		157.04	156.03	154.05	153.07	152.07	151.09	150.1	149.07	148.09
		147.08	146.07	145.04	144.03	143.02	142.05	141.07	140.03	139.05
		138.05	137.03	136.09	135.08	134.06	133.08	132.03	130.05	129.04
		128.03	126.02	125.05	124.09	123.08	122.07	121.06	120.06	119.06
		116.03	115.03	114.05	113.05	112.09	111.03	110.07	109.06	108.06
		107.05	106.07	105.03	102.02	100				
References	<p>F. Kugler, F. C. Stintzing, R. Carle, <i>J. Agric. Food Chem.</i> 2004, 52, 2975–2981. M. Piattelli, L. Minale, R. A. Nicolaus, <i>Phytochemistry</i> 1965, 4, 817–823. I. Belhadj Slimen, T. Najar, M. Abderrabba, <i>J. Agric. Food Chem.</i> 2017, 65, 675–689. L. C. Esteves, C. O. Machado, L. C. P. Gonçalves, V. F. Cavalcante, G. Obeid, T. C. Correra, E. L. Bastos, <i>Antioxidants</i> 2022, 11, 2259.</p>									

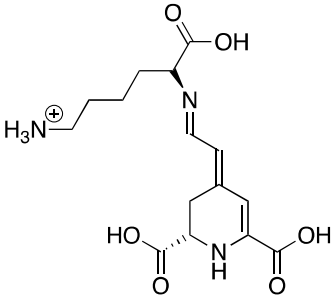
Histidine-bx

Chemical structure										
Name:	Histidine-bx (Muscaaurin VII)									
Chemical Formula	C ₁₅ H ₁₆ N ₄ O ₆									
Molecular weight	348.32									
Monoisotopic mass	348.1070									
m/z [M+H]	349.1143									
Theoretical fragments (m/z)	349.11	348.11	347.1	346.09	345.08	334.1	333.12	332.11	331.1	330.1
		329.09	322.1	321.12	320.11	319.1	318.11	317.12	316.09	315.11
		314.1	313.09	312.09	311.08	309.12	307.1	306.11	305.12	304.12
		303.11	302.1	301.09	300.1	299.11	298.08	297.1	295.08	293.12
		292.12	291.11	290.1	289.13	288.12	287.11	286.11	285.1	284.07
		283.08	282.08	281.08	280.07	279.11	278.1	277.09	276.1	275.11
		274.11	273.13	272.09	271.12	269.1	268.07	267.06	266.09	265.08
		264.07	263.07	262.08	261.1	260.1	259.08	258.09	257.07	253.08
		252.07	251.07	250.06	249.05	248.08	247.07	246.09	245.06	244.07
		243.09	242.09	241.11	240.08	239.07	238.09	237.09	236.08	235.07
		234.06	233.06	232.05	231.04	230.09	225.09	224.08	223.07	222.06
		221.09	219.08	218.09	217.06	215.09	213.09	212.08	211.07	210.06
		209.06	208.05	207.08	206.09	205.06	204.08	197.09	196.06	195.08
		194.04	193.06	192.05	191.07	190.06	189.09	188.08	187.07	186.07
		184.06	183.05	182.04	181.06	180.07	179.07	178.05	177.07	176.03
		175.05	174.07	173.06	172.05	170.04	169.05	168.03	167.07	166.06
		165.07	164.05	163.05	162.07	158.04	157.04	156.08	155.07	154.06
		153.05	152.07	151.07	150.07	149.06	148.05	147.06	144.03	142.05
		141.07	140.03	139.05	138.04	137.03	136.05	134.07	132.03	130.05
		129.04	128.08	126.07	125.05	124.04	123.06	122.05	121.04	120.04
		119.02	118.04	116.03	115.03	114.05	113.05	112.09	111.06	110.07
		109.04	108.06	107.05	106.07	105.03				
	<p>Musso, H. Pigments of fly agaric, <i>Amanita muscaria</i>. <i>Tetrahedron</i> 1979, 35, 2843–2853.</p> <p>Kugler, F.; Stintzing, F.C.; Carle, R. Identification of betalains from petioles of differently colored Swiss chard (<i>Beta vulgaris</i> L. ssp. <i>cicla</i> Alef. Cv. Bright Lights) by high-performance liquid chromatography-electrospray ionization mass spectrometry. <i>J. Agric. Food Chem.</i> 2004, 52, 2975–2981.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Esteves, L.C.; Machado, C.O.; Gonçalves, L.C.P.; Cavalcante, V.F.; Obeid, G.; Correra, T.C.; Bastos, E.L. Structural Effects on the Antioxidant Properties of Amino Acid Betaxanthins. <i>Antioxidants</i> 2022, 11, 2259.</p>									

Arginine-bx

Chemical structure										
Name:	Arginine-bx									
Chemical Formula	C ₁₅ H ₂₁ N ₅ O ₆									
Molecular weight	367.36									
Monoisotopic mass	367.1492									
m/z [M+H]	368.1565									
Theoretical fragments (m/z)	368.16	367.15	366.14	365.13	364.13	353.15	352.16	351.13	350.15	349.14
	348.13	347.12	346.11	340.16	339.15	338.15	337.14	336.17	335.12	
	334.1	333.14	332.14	331.13	330.12	328.16	326.13	325.13	324.17	
	323.16	322.15	321.14	320.14	319.13	318.16	317.12	316.14	315.11	
	314.12	312.17	311.16	310.15	309.11	308.1	307.09	306.16	305.08	
	304.14	303.13	302.12	298.15	297.14	296.14	295.09	294.16	293.11	
	292.11	291.1	290.09	289.08	288.15	287.07	283.09	282.08	281.08	
	280.13	279.12	278.12	277.11	276.11	275.1	274.09	273.09	272.08	
	271.07	270.08	269.08	268.07	267.06	266.16	265.12	264.11	263.1	
	262.06	261.09	260.08	259.11	257.09	255.1	253.08	252.05	251.07	
	250.06	249.05	248.08	247.11	246.1	245.09	241.08	239.07	238.08	
	237.09	236.09	235.07	234.06	233.06	232.05	231.11	229.1	225.09	
	224.08	223.07	222.06	221.09	220.07	219.08	218.08	217.06	213.09	
	212.08	211.07	210.06	209.1	208.05	207.08	206.07	205.06	204.05	
	199.12	198.11	197.09	196.06	195.08	194.04	193.06	192.05	191.09	
	190.04	187.12	186.11	185.1	184.06	183.05	182.04	181.11	180.07	
	179.08	178.05	177.07	176.03	175.12	174.11	173.1	172.1	171.09	
	170.04	169.11	168.1	167.08	166.07	165.07	164.03	163.05	160.11	
	159.12	158.09	157.08	156.08	155.09	154.05	153.11	152.07	151.09	
	150.05	149.07	147.12	145.11	144.09	143.08	142.1	141.07	140.08	
	139.06	138.07	137.08	136.08	134.06	132.04	131.08	130.1	129.11	
	128.08	127.1	126.05	125.05	124.09	123.07	122.06	121.05	120.04	
	118.1	116.07	115.03	114.1	113.05	112.09	111.08	110.07	109.05	
	108.04	105.03								
	<p>Kugler, F.; Graneis, S.; Stintzing, F.C.; Carle, R. Studies on betaxanthin profiles of vegetables and fruits from the Chenopodi-aceae and Cactaceae. <i>Z. Fur. Naturforschung Sect. C J. Biosci.</i> 2007, 62, 311–318.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Esteves, L.C.; Machado, C.O.; Gonçalves, L.C.P.; Cavalcante, V.F.; Obeid, G.; Correra, T.C.; Bastos, E.L. Structural Effects on the Antioxidant Properties of Amino Acid Betaxanthins. <i>Antioxidants</i> 2022, 11, 2259.</p>									

Lysine-bx

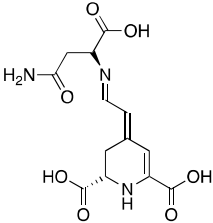
Chemical structure										
Name:	Lysine-bx									
Chemical Formula	C ₁₅ H ₂₁ N ₃ O ₆									
Molecular weight	339.35									
Monoisotopic mass	339.1430									
m/z [M+H]	340.1503									
Theoretical fragments (m/z)	340.15	339.14	338.13	337.13	336.12	325.14	324.16	323.12	322.14	321.11
		320.12	319.09	318.11	312.16	311.15	310.14	309.11	308.16	307.13
		306.14	305.11	304.13	303.1	302.11	301.08	300.16	298.14	297.11
		296.16	295.09	294.14	293.14	292.13	291.13	290.15	289.12	288.13
		287.1	286.12	285.09	284.16	283.09	282.14	281.08	280.17	279.13
		278.15	277.12	276.13	275.1	274.12	273.12	271.11	270.08	269.08
		268.13	267.06	266.15	265.12	264.17	263.07	262.16	261.12	260.14
		259.11	257.09	255.1	254.09	253.08	252.13	251.07	250.12	249.05
		248.08	247.11	246.06	245.06	243.11	241.08	239.07	238.16	237.05
		236.09	235.07	234.12	233.09	232.05	231.08	225.09	224.08	223.07
		222.06	221.06	219.08	217.06	213.09	212.08	211.07	210.06	209.06
		208.05	207.08	206.07	205.06	204.05	198.08	197.13	196.06	195.08
		194.04	193.06	192.05	191.05	190.04	185.13	184.06	183.05	182.1
		181.1	180.07	179.08	178.05	177.07	176.03	175.05	171.11	170.1
		168.03	167.08	166.07	165.07	164.07	163.09	159.11	158.1	157.1
		156.09	155.08	154.09	153.08	152.07	151.09	150.02	149.07	148.08
		147.11	146.1	145.1	144.09	143.08	142.11	141.1	140.07	139.09
		138.05	137.03	136.08	134.06	132.1	131.12	130.09	129.08	128.07
		127.09	126.05	125.11	124.08	123.07	122.06	121.05	120.04	119.12
		117.1	116.03	115.03	114.09	113.06	112.08	111.04	110.06	109.08
		108.08	105.03							
	<p>Svenson, J.; Smallfield, B.M.; Joyce, N.I.; Sanson, C.E.; Perry, N.B. Betalains in red and yellow varieties of the Andean tuber crop ulluco (<i>Ullucus tuberosus</i>). <i>J. Agric. Food Chem.</i> 2008, 56, 7730–7737.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Esteves, L.C.; Machado, C.O.; Gonçalves, L.C.P.; Cavalcante, V.F.; Obeid, G.; Correra, T.C.; Bastos, E.L. Structural Effects on the Antioxidant Properties of Amino Acid Betaxanthins. <i>Antioxidants</i> 2022, 11, 2259.</p>									

Polar uncharged-type

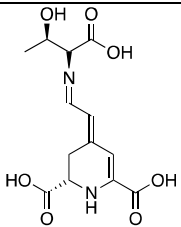
Glutamine-bx

Chemical structure										
Name:	Glutamine-bx (Vulgaxanthin I)									
Chemical Formula	C ₁₄ H ₁₇ N ₃ O ₇									
Molecular weight	339.30									
Monoisotopic mass	339.1066									
m/z [M+H]	340.1139									
Theoretical fragments (m/z)	340.11	339.11	338.1	337.09	336.08	325.1	324.12	323.09	322.1	321.07
		320.09	319.08	318.07	313.1	312.12	311.11	310.1	309.07	308.12
		307.09	306.11	305.08	304.09	303.06	302.08	300.12	299.09	298.1
		297.07	296.12	295.09	294.11	293.1	292.09	291.06	290.11	289.08
		288.1	287.07	286.08	285.07	284.12	283.12	282.11	281.08	280.13
		279.1	278.11	277.08	276.1	275.09	274.08	273.09	272.1	271.07
		270.11	269.08	268.09	267.06	266.11	265.07	264.13	263.07	262.12
		261.09	260.1	259.07	258.09	255.1	254.11	253.08	252.1	251.07
		250.08	249.05	248.08	247.07	246.12	245.06	244.11	243.08	241.08
		239.07	238.08	237.05	236.1	235.07	234.09	233.06	232.05	231.08
		225.09	224.08	223.07	222.06	221.06	220.07	219.08	218.07	217.06
		213.09	212.08	211.07	210.06	209.06	208.05	207.08	206.07	205.06
		204.05	198.08	197.09	196.06	195.08	194.04	193.06	192.05	191.05
		190.04	185.09	184.06	183.05	182.07	181.06	180.07	179.08	178.05
		177.07	176.03	175.05	171.08	170.07	168.03	167.08	166.07	165.07
		164.03	163.05	159.08	158.07	157.06	156.05	155.05	154.07	153.04
		152.07	151.06	150.02	149.07	148.04	147.08	146.07	145.06	144.05
		143.05	142.07	141.07	140.03	139.05	138.05	137.07	136.08	134.06
		132.07	131.08	130.05	129.04	128.03	127.05	126.02	125.07	124.04
		123.06	122.02	121.05	120.04	119.08	117.07	116.03	115.03	114.05
		113.02	112.04	111.01	110.02	109.08	108.04	105.03	103.09	102.05
		101.07	100.04							
	<p>Piattelli, M.; Minale, L.; Nicolaus, R.A. Pigments of centrospermae—V. <i>Phytochemistry</i> 1965, 4, 817–823.</p> <p>Stintzing, F.C.; Schieber, A.; Carle, R. Identification of betalains from yellow beet (<i>Beta vulgaris</i> L.) and cactus pear [<i>Opuntia ficus-indica</i> (L.) Mill.] by high-performance liquid chromatography–electrospray ionization mass spectroscopy. <i>J. Agric. Food Chem.</i> 2002, 50, 2302–2307.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Esteves, L.C.; Machado, C.O.; Gonçalves, L.C.P.; Cavalcante, V.F.; Obeid, G.; Correra, T.C.; Bastos, E.L. Structural Effects on the Antioxidant Properties of Amino Acid Betaxanthins. <i>Antioxidants</i> 2022, 11, 2259.</p>									

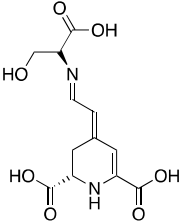
Asparagine-bx

Chemical structure										
Name:	Asparagine-bx (Vulgaxanthin III)									
Chemical Formula	C ₁₃ H ₁₅ N ₃ O ₇									
Molecular weight	325.28									
Monoisotopic mass	325.0910									
m/z [M+H]	326.0983									
Theoretical fragments (m/z)	326.1	325.09	324.08	323.07	311.09	310.1	309.07	308.09	307.06	306.07
		305.06	299.09	298.1	297.1	296.09	295.06	294.11	293.08	292.09
		291.06	290.08	289.05	288.06	286.1	285.07	284.09	283.06	282.11
		281.08	280.09	279.08	278.08	277.08	276.1	275.07	274.08	273.05
		272.07	270.11	269.1	268.09	267.06	266.11	265.08	264.1	263.07
		262.08	261.09	260.07	259.07	258.09	257.06	256.09	255.04	254.08
		253.08	252.1	251.07	250.12	249.05	248.1	247.07	246.09	245.06
		244.07	243.04	241.08	240.1	239.07	238.08	237.05	236.07	235.07
		234.12	233.06	232.11	231.04	230.09	229.06	225.09	224.1	223.07
		222.09	221.06	220.07	219.04	218.04	217.06	213.09	212.08	211.07
		210.06	209.06	208.05	207.08	206.07	205.06	204.05	197.09	196.06
		195.08	194.04	193.06	192.05	191.05	190.04	184.06	183.05	182.04
		181.06	180.07	179.08	178.05	177.07	176.03	175.05	171.08	170.04
		169.06	168.05	167.05	166.07	165.07	164.03	163.05	158.04	157.06
		156.05	154.05	153.07	152.07	151.09	150.02	149.07	145.06	144.05
		143.05	142.05	141.03	140.06	139.03	138.05	137.03	136.08	135.06
		134.02	133.06	132.05	131.05	130.04	129.07	128.06	127.05	126.02
		125.03	124.04	123.07	122.02	121.05	120.04	118.05	117.07	116.03
		115.03	114.02	113.03	112.06	111.06	110.02	109.04	108.01	105.07
Reference	<p>Kugler, F.; Stintzing, F.C.; Carle, R. Identification of betalains from petioles of differently colored Swiss chard (<i>Beta vulgaris</i> L. ssp. cicla Alef. Cv. Bright Lights) by high-performance liquid chromatography-electrospray ionization mass spectrometry. <i>J. Agric. Food Chem.</i> 2004, 52, 2975–2981.</p> <p>Hempel, J.; Bohm, H. Betaxanthin pattern of hairy roots from <i>Beta vulgaris</i> var lutea and its alteration by feeding of amino acids. <i>Phytochemistry</i> 1997, 44, 847–852.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Esteves, L.C.; Machado, C.O.; Gonçalves, L.C.P.; Cavalcante, V.F.; Obeid, G.; Correra, T.C.; Bastos, E.L. Structural Effects on the Antioxidant Properties of Amino Acid Betaxanthins. <i>Antioxidants</i> 2022, 11, 2259.</p>									

Threonine-bx

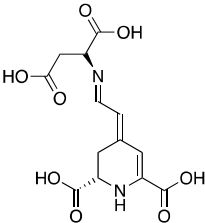
Chemical structure										
Name:	Threonine-bx									
Chemical Formula	C ₁₃ H ₁₆ N ₂ O ₇									
Molecular weight	312.28									
Monoisotopic mass	312.0958									
m/z [M+H]	313.1030									
Theoretical fragments (m/z)	313.1	312.1	311.09	310.08	298.08	297.07	296.1	295.09	294.08	293.08
		292.07	287.09	285.11	284.1	283.09	282.08	281.11	280.11	279.1
		278.09	277.08	276.07	275.07	273.11	271.09	270.08	269.08	268.07
		267.06	266.09	265.08	264.07	263.1	262.07	261.09	260.08	259.07
		258.06	257.11	256.11	255.1	254.09	253.08	252.11	251.07	250.09
		249.09	248.08	247.07	245.06	243.1	242.09	241.08	240.09	239.07
		238.09	237.05	236.08	235.07	234.1	233.06	232.08	231.08	230.07
		229.06	228.09	227.1	226.07	225.09	224.08	223.07	222.06	221.06
		219.08	217.06	215.08	213.09	212.08	211.07	210.06	209.06	208.05
		207.08	206.07	205.06	204.05	198.08	197.09	196.06	195.08	194.04
		193.06	192.05	191.05	190.04	184.06	183.05	182.04	181.06	180.07
		179.08	178.05	177.07	176.03	175.05	170.04	169.07	168.03	167.08
		166.07	165.07	164.03	163.05	158.04	157.04	156.07	155.06	154.05
		153.07	152.07	151.06	150.02	149.07	147.06	144.07	143.06	142.05
		141.07	140.03	139.05	138.05	137.05	136.04	134.06	132.07	131.06
		130.05	129.04	128.03	126.05	125.05	124.04	123.04	121.05	120.07
		119.06	118.05	117.04	116.03	115.06	114.05	113.05	112.04	111.03
		110.06	108.04	105.05	104.07	103.04	102.03	101.02	100.04	
	<p>Kugler, F.; Graneis, S.; Stintzing, F.C.; Carle, R. Studies on betaxanthin profiles of vegetables and fruits from the Chenopodi-aceae and Cactaceae. <i>Z. Fur. Naturforschung Sect. C J. Biosci.</i> 2007, 62, 311–318.</p> <p>Slimen, I.B.; Najjar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Esteves, L.C.; Machado, C.O.; Gonçalves, L.C.P.; Cavalcante, V.F.; Obeid, G.; Correra, T.C.; Bastos, E.L. Structural Effects on the Antioxidant Properties of Amino Acid Betaxanthins. <i>Antioxidants</i> 2022, 11, 2259.</p>									

Serine-bx

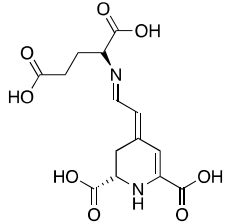
Chemical structure										
Name:	Serine-bx									
Chemical Formula	C ₁₂ H ₁₄ N ₂ O ₇									
Molecular weight	298.25									
Monoisotopic mass	298.0801									
m/z [M+H]	299.0874									
Theoretical fragments (m/z)	299.09	298.08	297.07	296.06	295.06	284.08	283.09	282.08	281.08	280.07
		279.06	277.05	271.09	270.08	269.08	268.07	267.06	266.09	265.08
		264.07	263.07	262.06	261.05	259.09	257.08	256.08	255.1	254.09
		253.08	252.07	251.07	250.06	249.05	248.06	247.07	246.06	245.06
		243.1	242.09	241.08	240.07	239.07	238.09	237.09	236.08	235.07
		234.06	233.06	232.05	231.04	229.08	228.07	227.07	226.07	225.09
		224.08	223.07	222.06	221.09	219.08	217.06	214.07	213.09	212.08
		211.07	210.06	209.06	208.05	207.08	206.07	205.06	204.05	198.08
		197.09	196.06	195.08	194.04	193.06	192.05	191.05	190.04	184.06
		183.05	182.04	181.06	180.07	179.08	178.05	177.07	176.03	175.05
		174.04	170.04	169.05	168.03	167.08	166.07	165.07	164.03	163.05
		158.04	157.04	156.07	155.06	154.05	153.07	152.07	151.06	150.02
		149.07	147.06	144.07	142.05	141.04	140.03	139.05	138.05	137.03
		136.08	134.06	132.03	130.05	129.04	128.03	126.05	125.05	124.04
		123.04	122.02	121.05	120.04	118.05	117.04	116.03	115.03	114.02
		113.05	112.04	111.03	110.06	108.04	107.07	106.05	105.04	104.03
		103.03	102.02	101.05	100.04					
Reference	<p>Stintzing, F.C.; Schieber, A.; Carle, R. Identification of betalains from yellow beet (<i>Beta vulgaris</i> L.) and cactus pear [<i>Opuntia ficus-indica</i> (L.) Mill.] by high-performance liquid chromatography–electrospray ionization mass spectroscopy. <i>J. Agric. Food Chem.</i> 2002, 50, 2302–2307.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Esteves, L.C.; Machado, C.O.; Gonçalves, L.C.P.; Cavalcante, V.F.; Obeid, G.; Correra, T.C.; Bastos, E.L. Structural Effects on the Antioxidant Properties of Amino Acid Betaxanthins. <i>Antioxidants</i> 2022, 11, 2259.</p>									

Negatively charged-type

Aspartic acid-bx

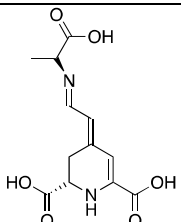
Chemical structure										
Name:	Aspartic acid-bx (Miraxanthin II)									
Chemical Formula	C ₁₃ H ₁₄ N ₂ O ₈									
Molecular weight	326.26									
Monoisotopic mass	326.0750									
m/z [M+H]	327.0823									
Theoretical fragments (m/z)	327.08	326.07	325.07	324.06	312.07	311.09	310.08	309.07	308.06	307.06
		306.05	299.09	298.08	297.07	296.06	295.09	294.08	293.08	292.07
		291.06	290.05	289.05	287.09	285.07	284.08	283.09	282.08	281.08
		280.07	279.06	278.05	277.08	276.07	275.07	274.06	273.05	272.04
		271.09	270.08	269.08	268.07	267.06	266.09	265.08	264.07	263.07
		262.06	261.05	259.07	257.08	256.07	255.06	254.07	253.08	252.07
		251.07	250.06	249.05	248.08	247.07	246.06	245.06	244.05	243.04
		242.07	241.08	240.05	239.07	238.07	237.05	236.06	235.07	234.06
		233.06	232.05	231.04	229.06	226.07	225.09	224.08	223.07	222.06
		221.06	220.06	219.04	218.04	217.06	213.09	212.08	211.07	210.06
		209.06	208.05	207.08	206.07	205.06	204.05	197.09	196.06	195.08
		194.04	193.06	192.05	191.05	190.04	184.06	183.05	182.04	181.06
		180.07	179.08	178.05	177.07	176.03	175.05	172.06	170.04	169.04
		168.03	167.08	166.07	165.07	164.03	163.05	158.04	157.04	156.03
		154.05	153.07	152.03	151.09	150.02	149.07	146.04	145.04	144.03
		143.02	142.01	141.04	140.03	139.03	138.05	137.03	136.04	134.04
		133.04	132.03	131.02	130.05	129.04	128.03	127.03	126.02	125.05
		124.04	123.07	122.02	121.05	120.04	119.03	118.05	117.02	116.01
		115	114.02	113.05	112.04	111.03	110.02	109.02	108.01	106.05
		105.03								
Reference	<p>Piattelli, M.; Minale, L.; Nicolaus, R.A. Pigments of centrospermae—V. <i>Phytochemistry</i> 1965, 4, 817–823.</p> <p>Gandía-Herrero, F.; García-Carmona, F.; Escribano, J. Development of a protocol for the semisynthesis and purification of betaxanthins. <i>Phytochem. Anal.</i> 2006, 17, 262–269.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Esteves, L.C.; Machado, C.O.; Gonçalves, L.C.P.; Cavalcante, V.F.; Obeid, G.; Correra, T.C.; Bastos, E.L. Structural Effects on the Antioxidant Properties of Amino Acid Betaxanthins. <i>Antioxidants</i> 2022, 11, 2259.</p>									

Glutamic acid-bx

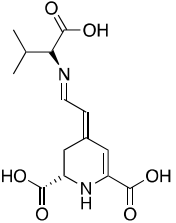
Chemical structure										
Name:	Glutamic acid-bx (Vulgaxanthin II)									
Chemical Formula	C ₁₄ H ₁₆ N ₂ O ₈									
Molecular weight	340.29									
Monoisotopic mass	340.0907									
m/z [M+H]	341.0979									
Theoretical fragments (m/z)	341.1	340.09	339.08	338.07	326.09	325.1	324.1	323.09	322.08	321.07
		320.06	319.06	313.1	312.1	311.09	310.08	309.11	308.06	307.09
		306.08	305.08	304.07	303.06	301.1	299.09	298.09	297.11	296.1
		295.09	294.08	293.08	292.07	291.06	290.09	289.08	288.07	287.07
		286.06	285.11	284.1	283.09	282.08	281.08	280.07	279.1	278.09
		277.08	276.07	275.07	273.09	271.09	270.08	269.08	268.07	267.06
		266.09	265.08	264.07	263.07	262.06	261.09	260.08	259.07	256.08
		255.1	254.07	253.08	252.05	251.07	250.06	249.05	248.08	247.07
		246.06	245.06	243.08	241.08	239.07	238.07	237.05	236.08	235.07
		234.06	233.06	232.05	231.08	225.09	224.08	223.07	222.06	221.06
		220.08	219.08	218.07	217.06	213.09	212.08	211.07	210.06	209.06
		208.05	207.08	206.07	205.06	204.05	198.08	197.09	196.06	195.08
		194.04	193.06	192.05	191.05	190.04	186.08	184.06	183.05	182.04
		181.06	180.07	179.08	178.05	177.07	176.03	175.05	172.06	171.05
		170.04	168.03	167.08	166.05	165.07	164.03	163.05	160.06	159.05
		158.04	157.04	156.03	155.06	154.05	153.04	152.07	151.09	150.05
		149.07	148.06	147.05	146.04	145.04	144.03	143.06	142.05	141.04
		140.03	139.05	138.05	137.03	136.08	134.06	133.05	132.07	131.03
		130.03	129.02	128.03	127	126.05	125.05	124.04	123.03	122.02
		121.05	120.07	118.05	117.05	116.03	115.04	114.05	113.02	112.02
		111.01	110.06	108.04	104.07					
Reference	<p>Piattelli, M.; Minale, L.; Nicolaus, R.A. Pigments of centrospermae—V. <i>Phytochemistry</i> 1965, 4, 817–823.</p> <p>Kugler, F.; Stintzing, F.C.; Carle, R. Identification of betalains from petioles of differently colored Swiss chard (<i>Beta vulgaris</i> L. ssp. <i>cicla</i> Alef. Cv. Bright Lights) by high-performance liquid chromatography-electrospray ionization mass spectrometry. <i>J. Agric. Food Chem.</i> 2004, 52, 2975–2981.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Esteves, L.C.; Machado, C.O.; Gonçalves, L.C.P.; Cavalcante, V.F.; Obeid, G.; Correra, T.C.; Bastos, E.L. Structural Effects on the Antioxidant Properties of Amino Acid Betaxanthins. <i>Antioxidants</i> 2022, 11, 2259.</p>									

Hydrophobic-type

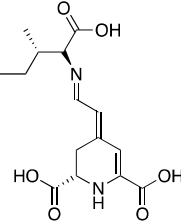
Alanine-bx

Chemical structure										
Name:	Alanine-bx									
Chemical Formula	C ₁₂ H ₁₄ N ₂ O ₆									
Molecular weight	282.25									
Monoisotopic mass	282.0852									
m/z [M+H]	283.0925									
Theoretical fragments (m/z)	283.09	282.08	281.08	280.07	279.06	268.08	267.06	266.09	265.08	264.07
		263.07	255.1	254.09	253.08	252.07	251.1	250.06	249.09	248.08
		247.07	246.06	245.06	243.1	241.08	240.09	239.1	238.09	237.09
		236.08	235.07	234.08	233.09	232.06	231.08	229.06	227.1	226.09
		225.09	224.08	223.11	222.1	221.09	220.08	219.08	218.07	217.06
		213.09	212.08	211.07	210.06	209.06	208.05	207.11	206.07	205.1
		204.05	203.08	201.07	198.08	197.09	196.06	195.08	194.04	193.06
		192.05	191.05	190.04	184.06	183.05	182.04	181.06	180.07	179.08
		178.05	177.07	176.03	175.05	174.05	170.04	169.05	168.03	167.08
		166.07	165.07	164.03	163.05	161.07	158.04	157.04	156.03	154.05
		153.07	152.07	151.06	150.02	149.07	148.08	147.06	144.03	142.05
		141.07	140.07	139.05	138.05	137.03	136.08	134.06	132.03	130.05
		129.04	128.03	126.05	125.05	124.04	123.04	122.06	121.05	120.04
		116.03	115.03	114.05	113.05	112.04	111.03	110.06	109.05	108.04
		107.04	106.03	105.03	102.02	101.05	100.04			
References	<p>Kugler, F.; Stintzing, F.C.; Carle, R. Identification of betalains from petioles of differently colored Swiss chard (<i>Beta vulgaris</i> L. ssp. <i>cicla</i> Alef. Cv. Bright Lights) by high-performance liquid chromatography-electrospray ionization mass spectrometry. <i>J. Agric. Food Chem.</i> 2004, 52, 2975–2981.</p> <p>Piattelli, M.; Minale, L.; Nicolaus, R.A. Pigments of centrospermae—V. <i>Phytochemistry</i> 1965, 4, 817–823.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Esteves, L.C.; Machado, C.O.; Gonçalves, L.C.P.; Cavalcante, V.F.; Obeid, G.; Correra, T.C.; Bastos, E.L. Structural Effects on the Antioxidant Properties of Amino Acid Betaxanthins. <i>Antioxidants</i> 2022, 11, 2259.</p>									

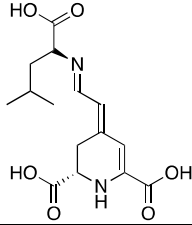
Valine-bx

Chemical structure										
Name:	Valine-bx									
Chemical Formula	C ₁₄ H ₁₈ N ₂ O ₆									
Molecular weight	310.31									
Monoisotopic mass	310.1165									
m/z [M+H]	311.1238									
Theoretical fragments (m/z)	311.12	310.12	309.11	308.1	297.11	296.1	295.13	294.12	293.11	292.11
		291.1	290.09	289.08	283.13	282.12	281.11	280.11	279.13	278.09
		277.12	276.11	275.1	274.09	273.09	271.13	270.08	269.08	268.07
		267.06	266.13	265.12	264.11	263.1	262.11	261.12	260.09	259.11
		257.09	255.13	254.13	253.12	252.11	251.07	250.13	249.12	248.12
		247.11	246.1	245.09	241.12	240.11	239.1	238.11	237.09	236.12
		235.14	234.1	233.13	232.05	231.11	230.07	229.1	226.11	225.09
		224.08	223.11	222.06	221.09	220.1	219.08	217.06	213.09	212.08
		211.07	210.06	209.06	208.05	207.08	206.07	205.06	204.05	203.12
		202.09	198.08	197.09	196.06	195.08	194.04	193.06	192.05	191.05
		190.04	184.06	183.05	182.04	181.06	180.07	179.08	178.05	177.07
		176.03	175.05	174.04	170.04	169.05	168.1	167.08	166.07	165.07
		164.03	163.05	158.04	157.04	156.1	154.05	153.08	152.07	151.06
		150.09	149.07	148.08	147.06	144.03	142.09	141.08	140.03	139.05
		138.05	137.08	136.08	135.07	134.06	132.03	130.05	129.08	128.07
		127.06	126.05	125.05	124.08	123.04	122.08	121.05	120.04	118.09
		117.08	116.07	115.06	114.05	113.08	112.08	111.07	110.06	108.04
		107.07	106.07	105.03	103.08	102.02	101.06	100.05		
References	<p>Stintzing, F.C.; Schieber, A.; Carle, R. Identification of betalains from yellow beet (<i>Beta vulgaris</i> L.) and cactus pear [<i>Opuntia ficus-indica</i> (L.) Mill.] by high-performance liquid chromatography–electrospray ionization mass spectroscopy. <i>J. Agric. Food Chem.</i> 2002, 50, 2302–2307.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Esteves, L.C.; Machado, C.O.; Gonçalves, L.C.P.; Cavalcante, V.F.; Obeid, G.; Correra, T.C.; Bastos, E.L. Structural Effects on the Antioxidant Properties of Amino Acid Betaxanthins. <i>Antioxidants</i> 2022, 11, 2259.</p>									

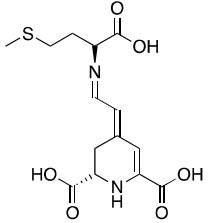
Isoleucine-bx

Chemical structure										
Name:	Isoleucine-betaxanthin (Isovulgaxanthin IV)									
Chemical Formula	C ₁₅ H ₂₀ N ₂ O ₆									
Molecular weight	324.33									
Monoisotopic mass	324.1321									
m/z [M+H]	325.1394									
Theoretical fragments (m/z)	325.14	324.13	323.12	322.12	311.12	310.12	309.14	308.14	307.13	306.12
		305.11	304.11	303.1	297.14	296.14	295.13	294.12	293.15	292.11
		291.13	290.13	289.12	288.11	287.1	285.14	283.13	282.08	281.15
		280.14	279.13	278.13	277.12	276.11	275.14	274.09	273.12	271.11
		270.08	269.08	268.07	267.06	266.13	265.15	264.15	263.14	262.13
		261.12	260.12	259.11	257.09	255.13	254.13	253.12	252.12	251.07
		250.06	249.05	248.08	247.14	246.06	245.13	244.08	243.11	241.08
		240.12	239.07	238.11	237.12	236.13	235.11	234.11	233.06	232.05
		231.04	225.09	224.08	223.07	222.06	221.09	220.1	219.08	218.12
		217.06	216.1	213.09	212.08	211.07	210.06	209.06	208.05	207.08
		206.07	205.06	204.05	198.08	197.09	196.06	195.08	194.04	193.06
		192.05	191.05	190.04	184.06	183.05	182.12	181.06	180.07	179.08
		178.05	177.07	176.03	175.05	170.04	168.03	167.08	166.09	165.07
		164.11	163.05	162.09	158.04	157.04	156.1	155.09	154.05	153.07
		152.07	151.09	150.09	149.07	148.08	147.06	144.1	143.09	142.09
		141.08	140.07	139.05	138.09	137.03	136.08	134.06	132.1	131.09
		130.09	129.08	128.03	127.1	126.09	125.08	124.08	123.07	121.05
		120.04	117.08	116.03	115.08	114.07	113.06	112.08	111.07	110.1
		108.04	105.03	104.11	102.05	101.05	100.04			
References	<p>Stintzing, F.C.; Schieber, A.; Carle, R. Identification of betalains from yellow beet (<i>Beta vulgaris</i> L.) and cactus pear [<i>Opuntia ficus-indica</i> (L.) Mill.] by high-performance liquid chromatography–electrospray ionization mass spectroscopy. <i>J. Agric. Food Chem.</i> 2002, 50, 2302–2307.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Esteves, L.C.; Machado, C.O.; Gonçalves, L.C.P.; Cavalcante, V.F.; Obeid, G.; Correra, T.C.; Bastos, E.L. Structural Effects on the Antioxidant Properties of Amino Acid Betaxanthins. <i>Antioxidants</i> 2022, 11, 2259.</p>									

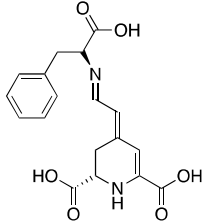
Leucine-bx

Chemical structure										
Name:	Leucine-bx (Vulgaxanthin IV)									
Chemical Formula	C ₁₅ H ₂₀ N ₂ O ₆									
Molecular weight	324.33									
Monoisotopic mass	324.1321									
m/z [M+H]	325.1394									
Theoretical fragments (m/z)	325.14	324.13	323.12	322.12	310.13	309.14	308.14	307.13	306.12	305.11
		304.11	303.1	297.14	296.14	295.13	294.12	293.15	292.11	291.13
		290.13	289.12	288.11	287.1	285.14	283.09	282.08	281.15	280.14
		279.13	278.13	277.12	276.11	275.14	274.09	273.12	271.11	270.08
		269.08	268.07	267.06	266.13	265.15	264.15	263.14	262.13	261.12
		260.12	259.11	257.09	255.13	254.13	253.12	252.12	251.07	250.06
		249.05	248.12	247.14	246.06	245.13	243.11	241.08	240.12	239.07
		238.11	237.12	236.13	235.11	234.11	233.06	232.05	231.04	225.09
		224.08	223.07	222.06	221.06	220.1	219.11	218.12	217.06	216.1
		213.09	212.08	211.07	210.06	209.06	208.05	207.08	206.07	205.06
		204.05	198.08	197.09	196.06	195.08	194.04	193.06	192.05	191.05
		190.04	184.06	183.05	182.12	181.06	180.07	179.08	178.05	177.07
		176.03	175.05	174.04	170.04	169.05	168.03	167.08	166.09	165.07
		164.11	163.05	162.09	158.04	157.04	156.1	155.09	154.05	153.07
		152.07	151.09	150.09	149.07	148.08	147.06	144.1	143.09	142.09
		141.08	140.07	139.05	138.09	137.03	136.08	134.06	132.1	131.09
		130.09	129.08	128.03	127.1	126.09	125.08	124.08	123.07	122.08
		121.05	120.04	117.08	116.03	115.08	114.07	113.06	112.08	111.07
		110.1	108.04	107.07	106.07	105.03	104.11	102.02	101.06	100
References	<p>Kugler, F.; Stintzing, F.C.; Carle, R. Identification of betalains from petioles of differently colored Swiss chard (<i>Beta vulgaris</i> L. ssp. cicla Alef. Cv. Bright Lights) by high-performance liquid chromatography-electrospray ionization mass spectrometry. <i>J. Agric. Food Chem.</i> 2004, 52, 2975–2981.</p> <p>Hempel, J.; Bohm, H. Betaxanthin pattern of hairy roots from <i>Beta vulgaris</i> var lutea and its alteration by feeding of amino acids. <i>Phytochemistry</i> 1997, 44, 847–852.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Esteves, L.C.; Machado, C.O.; Gonçalves, L.C.P.; Cavalcante, V.F.; Obeid, G.; Correra, T.C.; Bastos, E.L. Structural Effects on the Antioxidant Properties of Amino Acid Betaxanthins. <i>Antioxidants</i> 2022, 11, 2259.</p>									

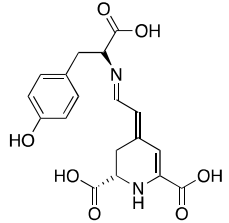
Methionine-bx

Chemical structure										
Name:	Methionine-bx (Miraxanthin I)									
Chemical Formula	C ₁₄ H ₁₈ N ₂ O ₆ S									
Molecular weight	342.37									
Monoisotopic mass	342.0886									
m/z [M+H]	343.0958									
Theoretical fragments (m/z)	343.1	342.09	341.08	340.07	328.08	327.1	326.09	325.09	324.08	323.07
		322.06	321.05	315.1	314.09	313.09	312.08	311.11	310.07	309.09
		308.08	307.07	306.07	305.06	303.1	301.09	300.09	299.11	298.1
		297.09	296.08	295.09	294.08	293.08	292.06	291.08	289.06	287.11
		286.1	285.09	284.08	283.11	282.08	281.1	280.09	279.1	278.09
		277.08	276.07	275.07	273.09	272.08	271.07	270.08	269.08	268.07
		267.06	266.05	265.1	264.07	263.07	262.06	261.09	260.08	259.07
		258.08	257.1	256.06	255.08	254.08	253.06	252.05	251.07	250.09
		249.09	248.04	247.07	246.06	245.06	243.08	242.08	241.1	240.07
		239.07	238.05	237.05	236.08	235.07	234.1	233.09	232.08	231.08
		229.06	227.08	225.09	224.08	223.07	222.06	221.06	219.11	217.1
		215.08	213.09	212.08	211.07	210.06	209.06	208.05	207.08	206.07
		205.06	204.05	200.07	199.07	198.08	197.09	196.06	195.08	194.04
		193.06	192.05	191.05	190.04	188.07	186.06	185.05	184.04	183.05
		182.04	181.06	180.07	179.08	178.05	177.07	176.03	175.05	174.06
		173.05	170.04	169.06	168.05	167.08	166.07	165.07	164.03	163.05
		162.06	161.05	160.04	159.03	158.04	157.04	156.05	154.05	153.07
		152.07	151.06	150.06	149.07	148.04	147.03	146.03	145.06	144.05
		143.04	142.03	141.07	140.03	139.05	138.05	137.05	136.04	135.05
		134.06	133.03	132.02	131.02	130.03	129	128.05	126.05	125.05
		124.04	123.04	122.06	121.05	120.05	119.02	118.01	117.04	116.03
		115.02	114.05	113.05	112.04	111.03	110.06	108.04	106.07	105.04
		104.05	103.02	102.04	101.01	100				
References	<p>Piattelli, M.; Minale, L.; Nicolaus, R.A. Pigments of centrospermae—V. <i>Phytochemistry</i> 1965, 4, 817–823.</p> <p>Gandía-Herrero, F.; García-Carmona, F.; Escribano, J. Development of a protocol for the semisynthesis and purification of betaxanthins. <i>Phytochem. Anal.</i> 2006, 17, 262–269.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Esteves, L.C.; Machado, C.O.; Gonçalves, L.C.P.; Cavalcante, V.F.; Obeid, G.; Correra, T.C.; Bastos, E.L. Structural Effects on the Antioxidant Properties of Amino Acid Betaxanthins. <i>Antioxidants</i> 2022, 11, 2259.</p>									

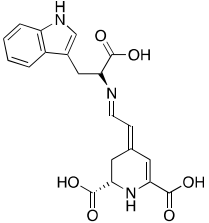
Phenylalanine-bx

Chemical structure										
Name:	Phenylalanine-bx									
Chemical Formula	C ₁₈ H ₁₈ N ₂ O ₆									
Molecular weight	358.3358.35005									
Monoisotopic mass	358.1165									
m/z [M+H]	359.1238									
Theoretical fragments (m/z)	359.12	358.12	357.11	356.1	344.11	343.13	342.12	341.11	340.11	339.1
		338.09	337.08	331.13	330.12	329.11	328.12	327.13	326.1	325.12
		324.11	323.1	322.09	321.09	320.08	319.13	317.11	316.12	315.13
		314.13	313.12	312.11	311.1	310.09	309.12	308.09	307.11	305.09
		303.13	302.13	301.12	300.11	299.14	298.13	297.12	296.12	295.11
		294.1	293.09	289.12	288.11	287.1	286.11	285.12	284.12	283.14
		282.08	281.08	280.07	279.11	277.1	274.11	273.12	272.09	271.11
		270.11	269.09	268.1	267.06	266.09	265.08	264.07	263.07	262.06
		261.05	258.11	257.13	256.1	255.15	254.08	253.08	252.07	251.07
		250.06	249.05	248.08	247.07	246.06	245.06	243.11	242.12	241.1
		240.1	239.07	238.09	237.09	236.08	235.07	234.06	233.06	232.05
		231.04	228.1	227.12	225.1	224.08	223.07	222.06	221.09	219.08
		217.06	216.1	215.09	214.09	213.09	212.08	211.07	210.06	209.06
		208.05	207.08	206.07	205.06	204.1	202.09	201.08	200.07	199.1
		198.09	197.09	196.06	195.08	194.04	193.06	192.05	191.05	190.09
		189.08	185.08	184.08	183.05	182.04	181.06	180.07	179.08	178.05
		177.08	176.07	175.05	174.05	172.08	170.04	169.05	168.03	167.08
		166.09	165.07	164.07	163.06	162.05	161.08	160.08	159.07	158.04
		157.04	156.03	154.05	153.07	152.07	151.09	150.09	149.06	148.05
		147.04	146.06	144.08	142.05	141.07	140.03	139.05	138.09	137.03
		136.08	135.07	134.06	133.06	132.06	131.05	130.05	129.03	128.03
		126.02	125.05	124.04	123.07	122.1	121.06	120.08	119.05	118.07
		117.06	116.03	115.03	114.05	113.05	112.04	111.03	110.02	109.06
		108.04	107.05	106.07	105.03	103.05	102.02	101.04	100	
References	<p>Stintzing, F.C.; Schieber, A.; Carle, R. Identification of betalains from yellow beet (<i>Beta vulgaris</i> L.) and cactus pear [<i>Opuntia ficus-indica</i> (L.) Mill.] by high-performance liquid chromatography–electrospray ionization mass spectroscopy. <i>J. Agric. Food Chem.</i> 2002, 50, 2302–2307.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Esteves, L.C.; Machado, C.O.; Gonçalves, L.C.P.; Cavalcante, V.F.; Obeid, G.; Correra, T.C.; Bastos, E.L. Structural Effects on the Antioxidant Properties of Amino Acid Betaxanthins. <i>Antioxidants</i> 2022, 11, 2259.</p>									

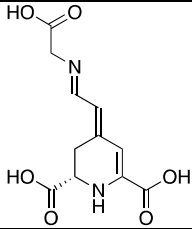
Tyrosine-bx

Chemical structure										
Name:	Tyrosine-bx (Portulacaxanthin II)									
Chemical Formula	C ₁₈ H ₁₈ N ₂ O ₇									
Molecular weight	374.35									
Monoisotopic mass	374.1114									
m/z [M+H]	375.1187									
Theoretical fragments (m/z)	375.12	374.11	373.1	372.1	360.11	359.12	358.12	357.11	356.1	355.09
		354.08	353.08	347.12	346.12	345.11	344.11	343.13	342.1	341.11
		340.11	339.1	338.09	337.08	336.07	335.12	333.11	332.11	331.13
		330.12	329.11	328.11	327.1	326.09	325.12	324.09	323.1	322.09
		321.09	320.08	319.13	318.12	317.11	316.11	315.13	314.13	313.12
		312.11	311.1	310.09	309.09	305.11	304.11	303.1	302.1	301.12
		300.11	299.14	298.09	297.12	295.11	293.09	290.1	289.12	288.09
		287.1	286.11	285.09	284.09	283.07	282.08	281.08	280.07	279.06
		274.11	273.12	272.09	271.14	270.08	269.09	268.07	267.06	266.09
		265.08	264.07	263.07	262.06	261.05	259.11	258.11	257.09	256.1
		253.08	252.07	251.07	250.06	249.05	248.08	247.07	246.06	245.06
		244.1	243.11	241.1	239.07	238.09	237.09	236.08	235.07	234.06
		233.06	232.1	231.04	230.08	225.09	224.08	223.07	222.06	221.09
		220.1	219.08	218.08	217.07	216.07	215.05	214.09	213.09	212.08
		211.07	210.06	209.06	208.05	207.08	206.08	205.07	204.05	201.08
		200.07	199.06	198.05	197.09	196.06	195.08	194.04	193.07	192.07
		191.05	190.05	188.07	184.06	183.05	182.08	181.06	180.07	179.06
		178.05	177.08	176.07	175.06	174.05	170.04	169.05	168.03	167.08
		166.07	165.05	164.05	163.04	162.05	161.05	160.08	158.04	157.04
		156.03	154.09	153.07	152.07	151.09	150.02	149.06	148.05	147.04
		146.04	145.03	144.04	142.05	141.07	140.03	139.05	138.09	137.06
		136.08	135.04	134.06	133.05	132.03	131.05	130.05	129.04	128.03
		126.02	125.06	124.04	123.04	122.08	121.03	120.04	119.05	118.04
		117.03	116.03	115.03	114.05	113.05	112.04	111.04	110.02	108.04
		107.05	106.04	105.03						
References	<p>Trezzini, G.F.; Zrýd, J.-P. Two betalains from <i>Portulaca grandiflora</i>. <i>Phytochemistry</i> 1991, 30, 1897–1899.</p> <p>Kugler, F.; Stintzing, F.C.; Carle, R. Identification of betalains from petioles of differently colored Swiss chard (<i>Beta vulgaris</i> L. ssp. <i>cicla</i> Alef. Cv. Bright Lights) by high-performance liquid chromatography-electrospray ionization mass spectrometry. <i>J. Agric. Food Chem.</i> 2004, 52, 2975–2981.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Esteves, L.C.; Machado, C.O.; Gonçalves, L.C.P.; Cavalcante, V.F.; Obeid, G.; Correra, T.C.; Bastos, E.L. Structural Effects on the Antioxidant Properties of Amino Acid Betaxanthins. <i>Antioxidants</i> 2022, 11, 2259.</p>									

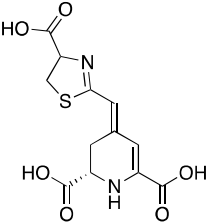
Tryptophan-bx

Chemical structure										
Name:	Tryptophan-bx									
Chemical Formula	C ₂₀ H ₁₉ N ₃ O ₆									
Molecular weight	397.39									
Monoisotopic mass	397.1274									
m/z [M+H]	398.1347									
Theoretical fragments (m/z)	398.13	397.13	396.12	395.11	383.12	382.14	381.13	380.12	379.12	378.11
		377.1	371.12	370.14	369.13	368.12	367.13	366.14	365.11	364.13
			363.12	362.11	361.11	360.1	358.14	356.12	355.13	354.14
				352.13	351.12	350.11	349.12	348.13	347.1	346.12
					342.14	341.14	340.13	339.12	338.15	337.14
						333.09	332.1	328.13	327.12	326.11
							321.1	320.14	319.08	318.12
								316.11	313.12	312.13
									311.1	310.12
										309.12
										308.1
										307.11
										306.09
										305.1
										304.09
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										102.02
										100
References	<p>Cai, Y.-Z.; Sun, M.; Corke, H. Characterization and application of betalain pigments from plants of the Amaranthaceae. <i>Trends Food Sci. Technol.</i> 2005, 16, 370–376.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Esteves, L.C.; Machado, C.O.; Gonçalves, L.C.P.; Cavalcante, V.F.; Obeid, G.; Correra, T.C.; Bastos, E.L. Structural Effects on the Antioxidant Properties of Amino Acid Betaxanthins. <i>Antioxidants</i> 2022, 11, 2259.</p>									

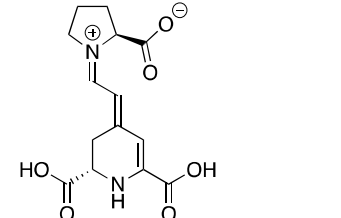
Glycine-bx

Chemical structure										
Name:	Glycine-bx (Portulacaxanthin III)									
Chemical Formula	C ₁₁ H ₁₂ N ₂ O ₆									
Molecular weight	268.22									
Monoisotopic mass	268.0695									
m/z [M+H]	269.0768									
Theoretical fragments (m/z)	269.08	268.07	267.06	266.05	265.05	254.07	253.08	252.07	251.07	250.06
		249.05	241.08	240.07	239.07	238.07	237.09	236.06	235.07	234.06
		233.06	232.05	231.04	229.08	227.07	226.07	225.09	224.08	223.07
		222.06	221.09	220.06	219.08	218.04	217.06	215.05	213.09	212.08
		211.07	210.06	209.09	208.08	207.08	206.07	205.06	204.05	203.05
		199.07	198.06	197.06	196.06	195.08	194.04	193.1	192.05	191.08
		190.04	189.07	187.05	184.06	183.05	182.04	181.06	180.07	179.05
		178.05	177.03	176.03	175.09	174.04	173.07	170.04	169.04	168.07
		167.06	166.05	165.04	164.03	163.05	162.05	161.07	160.04	158.04
		157.04	156.03	154.05	153.07	152.07	151.06	150.05	149.07	148.06
		147.06	146.05	144.03	142.05	140.03	139.06	138.05	137.07	136.08
		135.06	134.06	132.03	130.05	129.04	128.03	126.05	125.05	124.04
		123.04	121.05	116.03	115.03	114.05	113.05	112.04	111.03	110.02
		109.05	108.04	107.07	106.03	105.03	102.02	100.04		
References	<p>Trezzini, G.F.; Zrýd, J.-P. Two betalains from <i>Portulaca grandiflora</i>. <i>Phytochemistry</i> 1991, 30, 1897–1899.</p> <p>Kugler, F.; Stintzing, F.C.; Carle, R. Identification of betalains from petioles of differently colored Swiss chard (<i>Beta vulgaris</i> L. ssp. <i>cicla</i> Alef. Cv. Bright Lights) by high-performance liquid chromatography-electrospray ionization mass spectrometry. <i>J. Agric. Food Chem.</i> 2004, 52, 2975–2981.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Esteves, L.C.; Machado, C.O.; Gonçalves, L.C.P.; Cavalcante, V.F.; Obeid, G.; Correra, T.C.; Bastos, E.L. Structural Effects on the Antioxidant Properties of Amino Acid Betaxanthins. <i>Antioxidants</i> 2022, 11, 2259.</p>									

Cysteine-bx

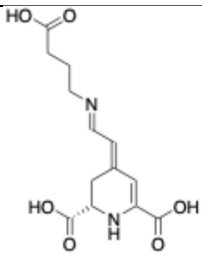
Chemical structure										
Name:	Cysteine-bx									
Chemical Formula	C ₁₂ H ₁₂ N ₂ O ₆ S									
Molecular weight	312.30									
Monoisotopic mass	312.0416									
m/z [M+H]	313.0489									
Theoretical fragments (m/z)	313.05	312.04	311.03	310.03	309.02	299.03	298.04	297.05	296.05	295.04
		294.03	293.02	285.05	284.05	283.04	282.04	281.06	280.03	279.04
		278.04	277.03	276.02	275.01	273.05	271.04	270.04	269.06	268.05
		267.04	266.04	265.06	264.03	263.05	262.02	261.03	259.02	257.06
		256.05	255.04	254.04	253.06	252.06	251.05	250.04	249.03	248.04
		247.02	243.04	242.04	241.03	240.03	239.05	238.04	237.07	236.03
		235.05	234.06	233.04	231.04	228.03	227.05	226.02	225.03	224.04
		223.02	222.02	221	219.08	217.06	215.05	213.03	212.04	211.05
		210.02	209.06	208.01	207.02	206.03	205.04	204.01	199.05	197.04
		196.04	195.02	194.04	193.06	191.05	189.07	184.06	183.05	182.04
		181.04	180.05	179.03	178.03	170.03	169.02	168.01	167.06	166.05
		165.04	164.03	163.05	158.04	157.04	156.01	154.03	153.02	152.02
		151.01	149.07	147.06	144.01	142.05	140.03	139.06	138.05	137.03
		136.04	132.01	131	130	128.99	127.98	126	124.04	123.07
		121.05	116.03	115.03	114	113.05	111.99	111.03	109.97	105
References	Esteves, L.C.; Machado, C.O.; Gonçalves, L.C.P.; Cavalcante, V.F.; Obeid, G.; Corra, T.C.; Bastos, E.L. Structural Effects on the Antioxidant Properties of Amino Acid Betaxanthins. <i>Antioxidants</i> 2022 , <i>11</i> , 2259.									

Proline-bx

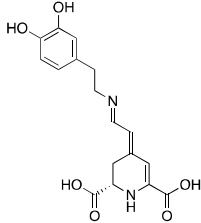
Chemical structure	
Name:	Proline-bx (Indicaxanthin)
Chemical Formula	C ₁₄ H ₁₆ N ₂ O ₆
Molecular weight	308.29
Monoisotopic mass	308.1008
m/z [M+H]	309.1081
Theoretical fragments (m/z)	<div style="display: flex; justify-content: space-between;"> 309.11 308.1 307.09 306.08 305.08 297.11 295.09 294.08 293.11 292.11 </div> <div style="display: flex; justify-content: space-between;"> 291.1 290.09 289.08 287.07 283.09 282.08 281.08 280.07 279.1 </div> <div style="display: flex; justify-content: space-between;"> 278.09 277.12 276.11 275.1 274.09 273.09 272.08 271.07 269.08 </div> <div style="display: flex; justify-content: space-between;"> 268.07 267.06 266.05 265.08 264.07 263.07 262.06 261.09 259.11 </div> <div style="display: flex; justify-content: space-between;"> 257.09 255.1 254.09 253.08 252.07 251.07 250.06 249.09 248.12 </div> <div style="display: flex; justify-content: space-between;"> 247.07 246.1 245.06 244.08 243.08 241.08 239.07 238.09 237.09 </div> <div style="display: flex; justify-content: space-between;"> 236.08 235.07 234.1 233.06 232.08 231.04 229.06 225.09 224.08 </div> <div style="display: flex; justify-content: space-between;"> 223.07 222.06 221.09 220.08 219.08 218.07 217.06 213.09 211.07 </div> <div style="display: flex; justify-content: space-between;"> 210.06 209.06 208.05 207.08 206.07 205.06 204.13 203.12 202.11 </div> <div style="display: flex; justify-content: space-between;"> 201.1 200.07 197.07 196.06 195.08 194.04 193.06 192.05 191.05 </div> <div style="display: flex; justify-content: space-between;"> 190.04 182.04 180.07 179.08 178.05 177.1 176.03 175.09 170.04 </div> <div style="display: flex; justify-content: space-between;"> 168.03 167.08 166.07 165.07 164.06 163.05 162.04 161.07 154.09 </div> <div style="display: flex; justify-content: space-between;"> 152.07 151.09 150.05 149.07 140.07 138.09 136.08 127.06 126.05 </div> <div style="display: flex; justify-content: space-between;"> 125.05 124.08 122.06 116.07 115.06 114.05 113.05 112.04 111.07 </div> <div style="display: flex; justify-content: space-between;"> 110.06 109.05 108.04 101.06 100.05 </div>
References	<p>Impellizzeri, G.; Piattelli, M. Biosynthesis of indicaxanthin in <i>Opuntia ficus-indica</i> fruits. <i>Phytochemistry</i> 1972, 11, 2499–2502.</p> <p>Stintzing, F.C.; Schieber, A.; Carle, R. Identification of betalains from yellow beet (<i>Beta vulgaris</i> L.) and cactus pear [<i>Opuntia ficus-indica</i> (L.) Mill.] by high-performance liquid chromatography-electrospray ionization mass spectroscopy. <i>J. Agric. Food Chem.</i> 2002, 50, 2302–2307.Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Esteves, L.C.; Machado, C.O.; Gonçalves, L.C.P.; Cavalcante, V.F.; Obeid, G.; Correra, T.C.; Bastos, E.L. Structural Effects on the Antioxidant Properties of Amino Acid Betaxanthins. <i>Antioxidants</i> 2022. 11, 2259.</p>

Special cases

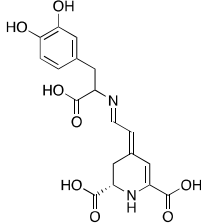
γ -aminobutyric acid-bx

Chemical structure										
Name:	γ -aminobutyric acid-bx									
Chemical Formula	$C_{13}H_{16}N_2O_6$									
Molecular weight	296.28									
Monoisotopic mass	296.1008									
m/z [M+H]	297.1081									
Theoretical fragments (m/z)	297.11	296.1	295.09	294.08	283.09	282.08	281.11	280.11	279.1	278.09
		277.08	276.07	275.07	270.08	269.11	268.07	267.06	266.09	265.12
		264.07	263.1	262.09	261.09	260.08	259.07	257.11	255.1	254.1
		253.12	252.11	251.1	250.09	249.05	248.08	247.11	246.06	245.09
		243.08	241.12	240.11	239.07	238.09	237.12	236.12	235.11	234.1
		233.09	232.08	231.08	227.1	226.09	225.09	224.08	223.07	222.06
		221.13	220.08	219.11	217.1	215.08	213.09	212.08	211.07	210.06
		209.06	208.05	207.08	206.07	205.06	204.05	198.08	197.09	196.06
		195.08	194.04	193.06	192.05	191.05	190.04	189.1	188.07	184.06
		183.05	182.04	181.06	180.07	179.08	178.05	177.07	176.03	175.05
		174.04	170.04	169.05	168.03	167.08	166.07	165.07	164.03	163.05
		158.04	157.04	156.03	154.05	153.07	152.07	151.06	150.02	149.07
		147.06	144.03	142.05	141.07	140.03	139.05	138.05	137.03	136.08
		135.07	134.06	132.03	130.05	129.04	128.07	127.06	126.05	125.05
		124.04	123.04	122.06	121.05	120.04	116.03	115.06	114.05	113.05
		112.04	111.03	110.06	108.04	107.07	106.07	105.03	104.07	103.06
		102.05	101.05	100						
References	<p>Spórna-Kucab, A.; Tekieli, A.; Grzegorzczak, A.; Świątek, Ł.; Rajtar, B.; Skalicka-Woźniak, K.; Starzak, K.; Nemzer, B.; Pietrzkowski, Z.; Wybraniec, S. Metabolite profiling analysis and the correlation with biological activity of betalain-rich <i>Portulaca grandiflora</i> Hook. extracts. <i>Antioxidants</i> 2022, 11, 1654.</p> <p>Wybraniec, S.; Nowak-Wydra, B.; Mitka, K.; Kowalski, P.; Mizrahi, Y. Minor betalains in fruits of <i>Hylocereus</i> species. <i>Phytochemistry</i> 2007, 68, 251–259.</p> <p>Kugler, F.; Stintzing, F.C.; Carle, R. Identification of betalains from petioles of differently colored Swiss chard (<i>Beta vulgaris</i> L. ssp. <i>cicla</i> Alef. Cv. Bright Lights) by high-performance liquid chromatography-electrospray ionization mass spectrometry. <i>J. Agric. Food Chem.</i> 2004, 52, 2975–2981.</p>									

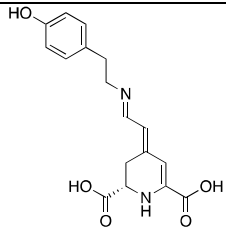
Dopamine-bx

Chemical structure										
Name:	Dopamine-bx (Miraxanthin V)									
Chemical Formula	C ₁₇ H ₁₈ N ₂ O ₆									
Molecular weight	346.34									
Monoisotopic mass	346.1165									
m/z [M+H]	347.1238									
Theoretical fragments (m/z)	347.12	346.12	345.11	344.1	343.09	332.11	331.13	330.12	329.11	328.11
		327.1	326.09	325.08	319.13	318.12	317.11	316.12	315.13	314.1
		313.12	312.09	311.1	310.09	309.09	307.13	305.11	304.12	303.13
		302.13	301.12	300.11	299.1	293.11	291.13	290.13	289.12	288.11
		287.14	286.11	285.12	284.12	283.11	281.09	277.12	276.11	275.1
		274.11	273.09	272.09	271.11	270.11	262.11	261.1	260.09	259.14
		258.14	257.13	256.1	246.11	245.13	244.1	243.11	242.08	241.1
		240.09	237.09	236.08	235.07	231.11	230.12	229.1	228.1	224.08
		223.07	222.06	221.09	219.08	218.12	216.1	213.09	212.08	211.07
		210.06	209.06	208.08	207.08	206.07	205.06	204.1	203.09	202.09
		197.09	196.06	195.08	194.04	193.06	192.1	191.05	190.04	189.08
		188.07	184.06	183.05	182.04	181.06	180.07	179.08	178.05	177.08
		176.03	175.05	174.04	170.04	169.05	168.03	167.08	166.07	165.08
		164.07	163.06	162.05	161.07	158.04	157.04	156.03	154.09	153.07
		152.07	151.06	150.05	149.05	148.04	147.07	146.05	145.04	144.03
		143.02	142.05	141.07	140.03	139.05	138.05	137.06	136.08	135.04
		134.06	133.05	132.03	130.05	129.04	128.03	126.05	125.05	124.04
		123.04	122.04	121.05	120.04	119.05	118.04	116.03	115.03	114.05
		113.05	112.04	111.04	110.06	109.03	108.02	107.05	106.04	105.03
		102.02	100							
References	<p>Piattelli, M.; Minale, L.; Nicolaus, R.A. Pigments of centrospermae—V. <i>Phytochemistry</i> 1965, 4, 817–823.</p> <p>Kobayashi, N.; Schmidt, J.; Wray, V.; Schliemann, W. Formation and occurrence of dopamine derived betacyanins. <i>Phytochemistry</i> 2001, 56, 429–436.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Esteves, L.C.; Machado, C.O.; Gonçalves, L.C.P.; Cavalcante, V.F.; Obeid, G.; Correra, T.C.; Bastos, E.L. Structural Effects on the Antioxidant Properties of Amino Acid Betaxanthins. <i>Antioxidants</i> 2022, 11, 2259.</p>									

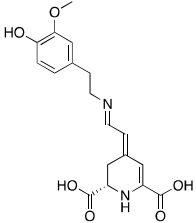
L-DOPA-bx

Chemical structure										
Name:	L-DOPA-bx (Dopaxanthin)									
Chemical Formula	C ₁₈ H ₁₈ N ₂ O ₈									
Molecular weight	390.35									
Monoisotopic mass	390.1063									
m/z [M+H]	391.1136									
Theoretical fragments (m/z)	391.11	390.11	389.1	388.09	376.1	375.12	374.11	373.1	372.1	371.09
		370.08	363.12	362.11	361.1	360.11	359.12	358.09	357.11	356.1
		355.09	354.08	353.08	352.07	351.12	349.1	348.11	347.12	346.12
		345.11	344.1	343.09	342.08	341.11	340.08	339.1	338.09	337.08
		336.07	335.12	334.12	333.11	332.1	331.13	330.12	329.11	328.11
		327.1	326.09	325.08	321.11	320.1	319.09	318.1	317.11	316.11
		315.13	314.09	313.12	311.1	309.09	306.1	305.11	304.08	303.1
		302.1	301.08	300.09	299.07	290.1	289.12	288.09	287.14	286.07
		285.09	284.09	283.11	282.08	281.08	280.07	279.06	275.1	274.11
		273.09	272.09	269.08	268.07	267.06	266.09	265.08	264.07	263.07
		262.06	261.05	260.09	259.11	257.09	253.08	252.07	251.07	250.06
		249.05	248.09	247.07	246.08	245.06	239.07	238.09	237.09	236.09
		235.07	234.08	233.07	232.06	231.04	230.08	229.07	228.07	225.09
		224.08	223.07	222.08	221.07	219.08	217.07	216.07	215.06	214.05
		213.09	212.08	211.07	210.06	209.07	208.06	207.08	206.04	205.06
		204.07	198.08	197.07	196.06	195.05	194.04	193.06	192.07	191.06
		190.05	184.06	183.05	182.04	181.05	180.07	179.03	178.05	177.07
		176.07	175.05	174.04	170.04	169.05	168.07	167.08	166.07	165.07
		164.05	163.04	162.03	161.02	160.04	158.04	157.04	156.03	154.09
		153.05	152.07	151.04	150.05	149.05	148.04	147.04	146.04	144.03
		142.05	141.05	140.03	139.05	138.05	137.02	136.08	135.04	134.04
		133.03	130.05	129.04	128.03	127.04	126.02	125.05	124.04	123.04
		122.04	121.05	120.04	119.05	118.04	116.03	115.03	114.05	113.05
		112.04	111.04	110.02	109.03	108.02	107.05	106.04	105.03	
References	<p>Gandía-Herrero, F.; Escribano, J.; García-Carmona, F. Betaxanthins as substrates for tyrosinase. An approach to the role of tyrosinase in the biosynthetic pathway of betalains. <i>Plant Physiol.</i> 2005, 138, 421–432.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Esteves, L.C.; Machado, C.O.; Gonçalves, L.C.P.; Cavalcante, V.F.; Obeid, G.; Correra, T.C.; Bastos, E.L. Structural Effects on the Antioxidant Properties of Amino Acid Betaxanthins. <i>Antioxidants</i> 2022, 11, 2259.</p>									

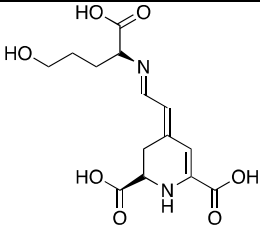
Tyramine-bx

Chemical structure										
Name:	Tyramine-bx (Miraxanthin III)									
Chemical Formula	C ₁₇ H ₁₈ N ₂ O ₅									
Molecular weight	330.34									
Monoisotopic mass	330.1216									
m/z [M+H]	331.1288									
Theoretical fragments (m/z)	331.13	330.12	329.11	328.11	327.1	316.12	315.13	314.13	313.12	312.11
		311.1	310.09	309.09	303.13	302.13	301.12	300.12	299.14	298.11
		297.12	296.09	295.11	294.1	293.09	291.13	289.12	288.12	287.14
		286.13	285.12	284.12	283.11	277.12	275.14	274.13	273.12	272.12
		271.14	270.11	269.13	268.12	267.11	265.1	261.12	260.12	259.11
		258.11	257.09	256.1	255.11	254.12	253.1	246.11	245.1	244.1
		243.15	242.14	241.13	240.1	239.12	237.09	236.08	235.07	232.13
		230.12	229.13	228.1	227.12	226.09	225.1	224.08	223.07	222.06
		221.09	219.08	215.12	214.12	213.09	212.08	211.07	210.06	209.06
		208.08	207.08	206.07	205.06	204.05	203.05	202.12	200.11	197.09
		196.06	195.08	194.04	193.06	192.05	191.05	190.04	188.11	187.1
		186.09	184.06	183.05	182.04	181.06	180.07	179.08	178.05	177.07
		176.11	175.05	174.09	173.08	172.08	170.04	169.05	168.03	167.08
		166.07	165.07	164.03	163.05	162.09	161.08	160.08	158.04	157.04
		156.03	154.05	153.07	152.07	151.09	150.09	149.08	148.08	147.07
		146.06	145.04	144.03	143.02	142.05	141.07	140.03	139.05	138.09
		137.03	136.08	135.07	134.06	133.05	132.04	131.07	130.05	129.04
		128.03	126.02	125.05	124.04	123.07	122.08	121.06	120.04	119.05
		118.04	117.06	116.03	115.03	114.05	113.05	112.04	111.03	110.02
		109.03	108.04	107.05	106.04	105.03	104.06	102.02	100	
References	<p>Piattelli, M.; Minale, L.; Nicolaus, R.A. Pigments of centrospermae—V. <i>Phytochemistry</i> 1965, 4, 817–823.</p> <p>Schliemann, W.; Cai, Y.; Degenkold, T.; Schmidt, J.; Corke, H. Betalains of <i>Celosia argentea</i>. <i>Phytochemistry</i> 2001, 58, 159–165.</p> <p>Slimen, I.B.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalains. <i>J. Agric. Food Chem.</i> 2017, 65, 675–689.</p> <p>Esteves, L.C.; Machado, C.O.; Gonçalves, L.C.P.; Cavalcante, V.F.; Obeid, G.; Correra, T.C.; Bastos, E.L. Structural Effects on the Antioxidant Properties of Amino Acid Betaxanthins. <i>Antioxidants</i> 2022, 11, 2259.</p>									

3-methoxy-tyramine-bx

Chemical structure										
Name:	3-methoxy-tyramine-bx									
Chemical Formula	C ₁₈ H ₂₀ N ₂ O ₆									
Molecular weight	360.37									
Monoisotopic mass	360.1321									
m/z [M+H]	361.1394									
Theoretical fragments (m/z)	361.14	360.13	359.12	358.12	357.11	346.13	345.14	344.14	343.13	342.12
		341.11	340.11	339.1	333.14	332.14	331.13	330.12	329.11	328.11
		327.13	326.1	325.12	324.11	323.1	321.14	319.13	318.13	317.15
		316.14	315.13	314.13	313.12	312.11	311.1	309.09	307.13	305.15
		304.14	303.13	302.13	301.15	300.12	299.14	298.13	297.12	295.11
		291.13	290.13	289.12	288.12	287.1	286.11	285.12	284.13	283.11
		276.12	275.12	274.11	273.16	272.15	271.14	270.11	260.13	259.14
		258.11	257.13	256.1	255.11	254.1	245.13	244.13	243.11	242.12
		237.09	236.08	235.07	232.13	230.12	224.08	223.07	222.06	221.09
		219.08	218.12	217.11	216.1	213.09	212.08	211.07	210.06	209.06
		208.08	207.08	206.12	205.06	204.1	203.09	202.09	197.09	196.06
		195.08	194.04	193.06	192.1	191.09	190.04	184.06	183.05	182.04
		181.06	180.07	179.09	178.09	177.07	176.07	175.05	174.04	170.04
		169.05	168.1	167.08	166.09	165.08	164.07	163.06	162.05	161.08
		158.04	157.04	156.03	154.05	153.07	152.07	151.08	150.02	149.06
		148.05	147.07	146.05	145.04	144.03	143.02	142.05	141.07	140.03
		139.05	138.05	137.06	136.05	135.09	134.06	133.06	132.06	130.05
		129.04	128.03	126.02	125.06	124.04	123.04	122.04	121.06	120.06
		119.05	116.03	115.03	114.05	113.05	112.04	111.03	110.02	109.06
		108.02	107.05	106.04	105.07	103.05	102.02	100		
References	Piattelli, M.; Minale, L.; Nicolaus, R.A. Pigments of centrospermae—V. <i>Phytochemistry</i> 1965 , 4, 817–823. Schliemann, W.; Cai, Y.; Degenkold, T.; Schmidt, J.; Corke, H. Betalains of <i>Celosia argentea</i> . <i>Phytochemistry</i> 2001 , 58, 159–165. Belhadj Slimen, I.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalain. <i>J. Agric. Food Chem.</i> 2017 , 65, 675–689, Correction in 2017 , 65, 1466.									

5-hydroxynorvaline-bx

Chemical structure										
Name:	5-hydroxynorvaline-bx									
Chemical Formula	C ₁₄ H ₁₈ N ₂ O ₇									
Molecular weight	326.30									
Monoisotopic mass	326.1114									
m/z [M+H]	327.1187									
Theoretical fragments (m/z)	327.12	326.11	325.1	324.1	312.11	311.12	310.12	309.11	308.1	307.09
		306.08	305.08	299.12	298.12	297.11	296.1	295.13	294.08	293.11
		292.11	291.1	290.09	289.08	287.12	285.11	284.11	283.13	282.12
		281.11	280.11	279.1	278.09	277.12	276.11	275.1	274.09	273.09
		272.08	271.13	270.12	269.08	268.07	267.06	266.13	265.12	264.11
		263.1	262.09	261.09	260.08	259.11	257.11	256.11	255.1	254.1
		253.08	252.05	251.07	250.06	249.05	248.12	247.11	246.1	245.09
		243.08	242.1	241.08	240.09	239.07	238.11	237.09	236.09	235.07
		234.06	233.06	232.05	231.11	229.1	226.11	225.09	224.08	223.07
		222.06	221.09	220.1	219.08	218.08	217.06	213.09	212.08	211.07
		210.06	209.06	208.05	207.08	206.07	205.06	204.05	198.08	197.09
		196.06	195.08	194.04	193.06	192.05	191.05	190.04	184.1	183.05
		182.04	181.06	180.07	179.08	178.05	177.07	176.03	175.05	172.1
		170.04	169.07	168.07	167.08	166.07	165.07	164.03	163.05	158.04
		157.07	156.03	154.05	153.07	152.07	151.09	150.05	149.07	146.08
		145.07	144.07	143.06	142.05	141.07	140.03	139.06	138.05	137.03
		136.08	134.08	133.07	132.07	131.06	130.05	129.08	128.07	127.06
		126.05	125.05	124.08	123.07	122.06	121.05	120.04	119.07	118.09
		117.05	116.05	115.04	114.05	113.05	112.08	111.07	110.06	109.05
		108.04	106.09	105.03	104.07	103.06	102.02	101.06	100	
References	Strack, D., Schmitt, D., Reznik, H., Boland, W., Grotjahn, L. and Wray, V. Humilixanthin a new betaxanthin from <i>Rivina humilis</i> . <i>Phytochemistry</i> 1987, 26, 2285-2287. Belhadj Slimen, I.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalain. <i>J. Agric. Food Chem.</i> 2017 , 65, 675–689, Correction in 2017 , 65, 1466.									

Methionine sulfoxide-bx

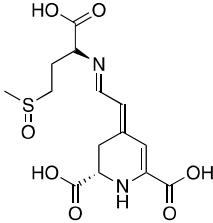
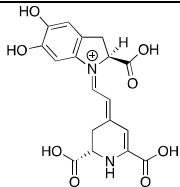
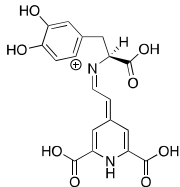
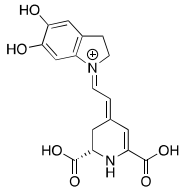
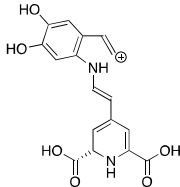
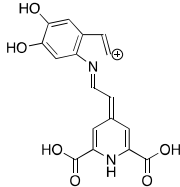
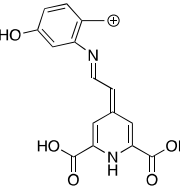
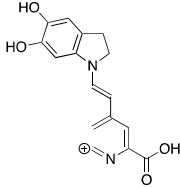
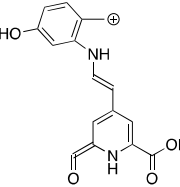
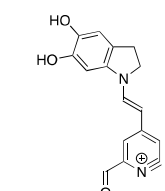
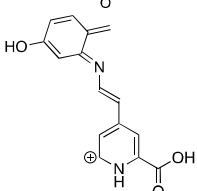
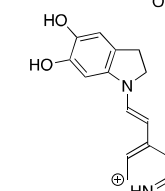
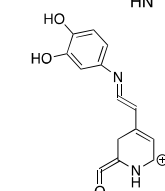
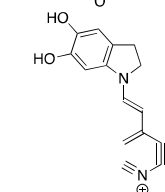
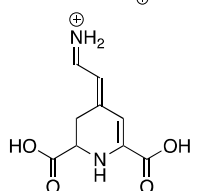
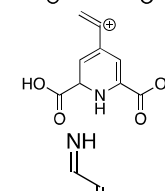
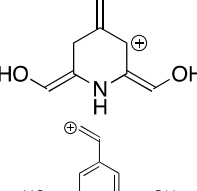
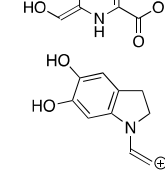

Chemical structure										
Name:	Methionine sulfoxide-bx (Miraxanthin I)									
Chemical Formula	C ₁₄ H ₁₈ N ₂ O ₇ S									
Molecular weight	358.37									
Monoisotopic mass	358.0835									
m/z [M+H]	359.0907									
Theoretical fragments (m/z)	359.09	358.08	357.08	356.07	344.08	343.1	342.09	341.08	340.07	339.06
		338.06	337.05	331.1	330.09	329.08	328.07	327.1	326.07	325.09
		324.08	323.07	322.06	321.05	319.1	317.08	316.08	315.1	314.09
		313.09	312.08	311.07	310.06	309.09	308.06	307.07	305.06	303.1
		302.09	301.09	300.08	299.11	298.1	297.09	296.08	295.09	294.08
		293.08	289.09	288.08	287.07	286.07	285.09	284.08	283.11	282.08
		281.08	280.07	279.1	278.09	277.08	276.07	275.07	274.07	273.09
		272.06	271.07	270.08	269.08	268.07	267.06	266.09	265.08	264.07
		263.07	262.06	261.09	259.07	258.08	257.1	256.06	255.1	254.05
		253.08	252.05	251.07	250.06	249.05	248.08	247.07	246.06	245.06
		243.08	242.08	241.08	240.07	239.07	238.09	237.05	236.08	235.07
		234.06	233.06	232.05	231.08	229.06	228.07	227.08	225.09	224.08
		223.07	222.06	221.06	219.08	217.06	216.07	215.06	214.05	213.09
		212.08	211.07	210.06	209.06	208.05	207.08	206.07	205.06	204.07
		202.05	201.05	200.04	199.07	198.08	197.09	196.06	195.08	194.04
		193.06	192.05	191.05	190.05	189.05	185.05	184.04	183.05	182.04
		181.06	180.07	179.08	178.05	177.05	176.04	175.05	174.02	172.04
		170.04	169.05	168.03	167.08	166.05	165.07	164.04	163.03	162.02
		161.05	160.04	159.03	158.04	157.04	156.03	154.05	153.07	152.07
		151.09	150.06	149.03	148.02	147.01	146.03	145	144.05	142.05
		141.07	140.03	139.05	138.06	137.03	136.04	135.01	134.06	133.03
		132.02	131.02	130.05	129	128.03	126.02	125.05	124.04	123.07
		122.06	121.03	120.05	119.02	118.03	117	116.03	115.03	114.05
		113.05	112.04	111.03	110.02	109.03	108.04	107.02	106.03	105.04
		104.03	103.02	102.05	101.01	100				
References	Gandía-Herrero, F.; García-Carmona, F.; Escribano, J. Development of a protocol for the semisynthesis and purification of betaxanthins. <i>Phytochem. Anal.</i> 2006 , 17, 262–269. Piattelli, M.; Minale, L.; Nicolaus, R.A. Pigments of centrospermae—V. <i>Phytochemistry</i> 1965 , 4, 817–823. Belhadj Slimen, I.; Najar, T.; Abderrabba, M. Chemical and Antioxidant Properties of Betalain. <i>J. Agric. Food Chem.</i> 2017 , 65, 675–689, Correction in 2017 , 65, 1466.									

Table S2. List of ion Fragments obtained in the Mass profile fingerprint of betalains and observed in HCD at 50 eV (Ions Relative Abundance > 5%)

Signal	<i>m/z</i>	Chemical structure of fragments
1	389.09	
2	387.07	
3	345.10	
4	343.09	
5	341.07	
6	313.08	
7	299.10	
8	297.08	

9	281.09	
10	269.09	
11	255.11	
12	255.08	
13	253.09	
14	211.07	
15	194.04	
16	179.08	
17	178.05	
18	176.07	

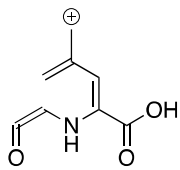
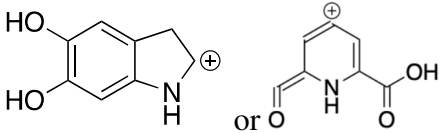
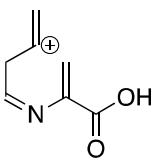
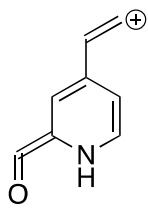
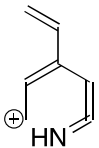
19	166.05	
20	150.05	
21	138.05	
22	132.04	
23	106.06	

Table S3. Chromatographic and HRMS data for betalains from *Beta vulgaris* extract

#	Compound	Retention time (Rt)	Relative Rt from betanin	Chemical Formula	theoretical m/z [M+H] ⁺	Observed m/z [M+H] ⁺	mass accuracy (ppm)	Fragments
1	Betalamic acid	3.23	0.94	C ₉ H ₉ NO ₅	212.0553	212.0545	-3.77	194.04, 166.05, 148.04, 138.05, 120.04, 106.03
Betanin-type								
2	Prebetanin	3.19	0.93	C ₂₄ H ₂₆ N ₂ O ₁₆ S	631.1076	631.1052	-3.8	389.09, 345.10, 343.09, 299.10, 297.08, 281.09, 269.09, 255.11, 253.09, 194.04, 166.05, 178.05, 176.07, 166.05, 150.05, 138.05, 132.04, 106.6
3	Betanin	3.43	1	C ₂₄ H ₂₆ N ₂ O ₁₃	551.1508	551.1483	-4.54	389.09, 345.10, 343.09, 299.10, 297.08, 281.09, 269.09, 255.11, 253.09, 194.04, 166.05, 178.05, 176.07, 166.05, 150.05, 138.05, 132.04, 106.6
4	Betanidin	3.44	1	C ₁₈ H ₁₆ N ₂ O ₈	389.0979	389.0964	-3.86	389.09, 345.10, 343.09, 299.10, 297.08, 281.09, 269.09, 255.11, 253.09, 194.04, 166.05, 178.05, 176.07, 166.05, 150.05, 138.05, 132.04, 106.6
5	2-decarboxy-2,3-dehydrobetanin (2-decarboxy-xanbetanin)	3.62	1.06	C ₂₃ H ₂₄ N ₂ O ₁₁	505.1453	505.1429	-4.75	343.09, 299.10, 297.08, 281.09, 269.09, 255.08, 253.09, 194.04, 178.05, 176.07, 150.05, 138.05, 132.04, 106.06
6	17-decarboxybetanin	5.83	1.7	C ₂₃ H ₂₆ N ₂ O ₁₁	507.1609	507.1591	-3.55	345.10, 299.10, 297.08, 281.09, 255.11, 253.09, 194.04, 178.05, 176.07, 150.05, 138.05, 132.04, 106.06
7	Isoprebetanin	6.01	1.75	C ₂₄ H ₂₆ N ₂ O ₁₆ S	631.1076	631.1047	-4.6	389.09, 345.10, 343.09, 299.10, 297.08, 281.09, 269.09, 255.11, 253.09, 194.04, 166.05, 178.05, 176.07, 166.05, 150.05, 138.05, 132.04, 106.6
8	Isobetanin	6.59	1.92	C ₂₄ H ₂₆ N ₂ O ₁₃	551.1508	551.1481	-4.9	389.09, 345.10, 343.09, 299.10, 297.08, 281.09, 269.09, 255.11, 253.09, 194.04, 166.05, 178.05, 176.07, 166.05, 150.05, 138.05, 132.04, 106.6
9	2-decarboxy-2,3-dehydroisobetanin (2-decarboxy-isoxanbetanin)	6.6	1.92	C ₂₃ H ₂₄ N ₂ O ₁₁	505.1453	505.1433	-3.96	343.09, 299.10, 297.08, 281.09, 269.09, 255.08, 253.09, 194.04, 178.05, 176.07, 150.05, 138.05, 132.04, 106.06
10	2,17-bidecarboxy-2,3-dehydrobetanin (2,17-bidecarboxy-xanbetanin)	7.61	2.22	C ₂₂ H ₂₄ N ₂ O ₉	461.1555	461.1534	-4.55	343.09, 299.10, 297.08, 281.09, 269.09, 255.08, 253.09, 194.04, 178.05, 176.07, 150.05, 138.05, 132.04, 106.06
11	17-decarboxyisobetanin	7.69	2.24	C ₂₃ H ₂₆ N ₂ O ₁₁	507.1609	507.1587	-4.34	345.10, 299.10, 297.08, 281.09, 255.11, 253.09, 194.04, 178.05, 176.07, 150.05, 138.05, 132.04, 106.06
12	Phyllocactin	7.71	2.25	C ₂₇ H ₂₈ N ₂ O ₁₆	637.1512	637.1497	-2.35	389.09, 345.10, 343.09, 299.10, 297.08, 281.09, 269.09, 255.11, 253.09, 194.04, 166.05, 178.05, 176.07, 166.05, 150.05, 138.05, 132.04, 106.6
13	17-decarboxyphyllocactin	8.01	2.34	C ₂₆ H ₂₈ N ₂ O ₁₄	593.1613	593.1591	-3.71	345.10, 299.10, 297.08, 281.09, 255.11, 253.09, 194.04, 178.05, 176.07, 150.05, 138.05, 132.04, 106.06
14	15-decarboxybetanin	8.29	2.42	C ₂₃ H ₂₆ N ₂ O ₁₁	507.1609	507.1591	-3.55	345.10, 299.10, 297.08, 281.09, 255.11, 253.09, 194.04, 178.05, 176.07, 150.05, 138.05, 132.04, 106.06
15	Neobetanin	8.31	2.42	C ₂₄ H ₂₄ N ₂ O ₁₃	549.1351	549.1336	-2.73	387.07, 341.07, 313.08, 299.10, 299.06, 287.08, 281.09, 269.09, 255.08, 253.09, 194.04, 178.05, 176.07, 166.05, 150.05, 132.04, 106.06
16	17-decarboxyneobetanin	8.39	2.45	C ₂₃ H ₂₄ N ₂ O ₁₁	505.1453	505.1438	-2.97	343.09, 299.10, 297.08, 281.09, 269.09, 255.08, 253.09, 194.04, 178.05, 176.07, 150.05, 138.05, 132.04, 106.06

17	Isophyllocactin	8.46	2.47	C ₂₇ H ₂₈ N ₂ O ₁₆	637.1512	637.1491	-3.3	389.09, 345.10, 343.09, 299.10, 297.08, 281.09, 269.09, 255.11, 253.09, 194.04, 166.05, 178.05, 176.07, 166.05, 150.05, 138.05, 132.04, 106.6
18	2-decarboxy-betanin	8.83	2.57	C ₂₃ H ₂₆ N ₂ O ₁₁	507.1609	507.1596	-2.56	345.10, 299.10, 297.08, 281.09, 255.11, 253.09, 194.04, 178.05, 176.07, 150.05, 138.05, 132.04, 106.06
19	17-decarboxy-isophyllocactin	9.21	2.69	C ₂₆ H ₂₈ N ₂ O ₁₄	593.1613	593.1588	-4.21	345.10, 299.10, 297.08, 281.09, 255.11, 253.09, 194.04, 178.05, 176.07, 150.05, 138.05, 132.04, 106.06
20	2-decarboxy-2,3-dehydro-neobetanin	10.06	2.93	C ₂₃ H ₂₂ N ₂ O ₁₁	503.1296	503.1277	-3.78	341.07, 327.06, 313.08, 295.07, 277.07, 267.07, 253.06, 251.08, 221.07, 195.09, 132.04, 106.06
21	2,17-bidecarboxy-2,3-dehydro-neobetanin	11.14	3.25	C ₂₂ H ₂₂ N ₂ O ₉	459.1398	459.1383	-3.27	297.08, 269.09, 251.08, 223.08, 195.09, 133.08
22	Lampranthin II	11.01	3.21	C ₃₄ H ₃₄ N ₂ O ₁₆	727.1981	727.1956	-3.44	389.09, 345.10, 343.09, 299.10, 297.08, 281.09, 269.09, 255.11, 253.09, 194.04, 166.05, 178.05, 176.07, 166.05, 150.05, 138.05, 132.04, 106.6
23	Isolampranthin II	11.34	3.31	C ₃₄ H ₃₄ N ₂ O ₁₆	727.1981	727.1948	-4.54	389.09, 345.10, 343.09, 299.10, 297.08, 281.09, 269.09, 255.11, 253.09, 194.04, 166.05, 178.05, 176.07, 166.05, 150.05, 138.05, 132.04, 106.6
Melocactin-type								
24	Melocactin	4.81	1.4	C ₃₀ H ₃₆ N ₂ O ₁₈	713.2036	713.2005	-4.35	389.09, 345.10, 343.09, 299.10, 297.08, 281.09, 269.09, 255.11, 253.09, 194.04, 166.05, 178.05, 176.07, 166.05, 150.05, 138.05, 132.04, 106.6
25	Isomelocactin	7.18	2.09	C ₃₀ H ₃₆ N ₂ O ₁₈	713.2036	713.2009	-3.79	389.09, 345.10, 343.09, 299.10, 297.08, 281.09, 269.09, 255.11, 253.09, 194.04, 166.05, 178.05, 176.07, 166.05, 150.05, 138.05, 132.04, 106.6
Apiocactin-type								
26	2'-O-apiosyl-phylllocactin	8.31	2.42	C ₃₂ H ₃₆ N ₂ O ₂₀	769.1934	769.1912	-2.86	389.09, 345.10, 343.09, 299.10, 297.08, 281.09, 269.09, 255.11, 253.09, 194.04, 166.05, 178.05, 176.07, 166.05, 150.05, 138.05, 132.04, 106.6

Continue Table S3.

#	Compound	Retention time (Rt)	Relative Rt from betanin	Chemical Formula	theoretical m/z [M+H] ⁺	Observed m/z [M+H] ⁺	mass accuracy (ppm)	Fragments
Betaxhanitins								
Positively charged-type								
27	Histamine-bx	9.04	2.64	C ₁₄ H ₁₆ N ₄ O ₄	305.1244	305.1232	-3.93	287.12, 261.13, 256.89, 211.07, 194.04, 166.05, 150.05, 138.05, 132.04, 130.05, 106.06
Polar uncharged-type								
28	Glutamine-bx	1.2	0.35	C ₁₄ H ₁₇ N ₃ O ₇	340.1139	340.1129	-2.94	323.08, 277.08, 249.08, 233.09, 231.07, 211.07, 194.04, 166.05, 150.05, 138.05, 132.04, 130.05, 106.06
29	Threonine-bx	1.52	0.44	C ₁₃ H ₁₆ N ₂ O ₇	313.103	313.1022	-2.56	269.09, 267.09, 211.07, 194.04, 166.05, 150.05, 138.05, 132.04, 130.05, 106.06
30	Serine-bx	4.77	1.39	C ₁₂ H ₁₄ N ₂ O ₇	299.0874	299.0861	-4.35	255.09, 253.09, 211.07, 194.04, 166.05, 150.05, 138.05, 132.04, 130.05, 106.06
Hydrophobic-type								
31	Alanine-bx	2.02	0.59	C ₁₂ H ₁₄ N ₂ O ₆	283.0925	283.0915	-3.53	237.08, 211.07, 194.04, 166.05, 150.05, 138.05, 132.04, 130.05, 106.06
32	Proline-bx	3.04	0.89	C ₁₄ H ₁₆ N ₂ O ₆	309.1081	309.1068	-4.21	265.11, 263.10, 235.1, 219.11, 217.09, 211.07, 194.04, 166.05, 150.05, 138.05, 132.04, 130.05, 106.06
33	Glycine-bx	6.49	1.89	C ₁₁ H ₁₂ N ₂ O ₆	269.0768	269.0758	-3.72	331.12, 239.11, 285.12, 283.10, 239.11, 211.07, 194.04, 166.05, 150.05, 138.05, 132.04, 130.05, 106.06
34	Valine-bx	7.97	2.32	C ₁₄ H ₁₈ N ₂ O ₆	311.1238	311.1229	-2.89	267.13, 265.11, 237.12, 221.12, 219.11, 211.07, 194.04, 166.05, 150.05, 138.05, 132.04, 130.05, 106.06
35	Isoleucine-bx	9.87	2.88	C ₁₅ H ₂₀ N ₂ O ₆	325.1394	325.1384	-3.08	279.13, 251.13, 235.14, 233.12, 211.07, 194.04, 166.05, 150.05, 138.05, 132.04, 130.05, 106.06
36	Leucine-bx	10.01	2.92	C ₁₅ H ₂₀ N ₂ O ₆	325.1394	325.1385	-2.77	281.14, 279.13, 251.13, 235.14, 233.12, 211.07, 194.04, 166.05, 150.05, 138.05, 132.04, 130.05, 106.06
37	Tryptophan-bx	10.12	2.95	C ₂₀ H ₁₉ N ₃ O ₆	398.1347	398.1331	-4.02	269.07, 223.07, 211.07, 194.04, 166.05, 150.05, 138.05, 132.04, 130.05, 106.06
38	Phenylalanine-bx	10.15	2.96	C ₁₈ H ₁₈ N ₂ O ₆	359.1238	359.1225	-3.62	315.13, 313.11, 269.12, 267.11, 223.12, 211.07, 194.04, 166.05, 150.05, 138.05, 132.04, 130.05, 106.06
Special case								
39	Methionine sulfoxide-bx	10.09	2.94	C ₁₄ H ₁₈ N ₂ O ₇ S	359.0907	359.0892	-4.18	267.11, 223.12, 211.07, 194.04, 166.05, 150.05, 138.05, 132.04, 130.05, 106.06