

SUPPORTING INFORMATION

Development of Tandem Mass Spectral Library for the Detection of Triterpenoids in Plant Metabolome based on Reference Standards

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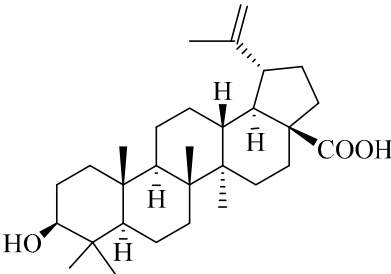
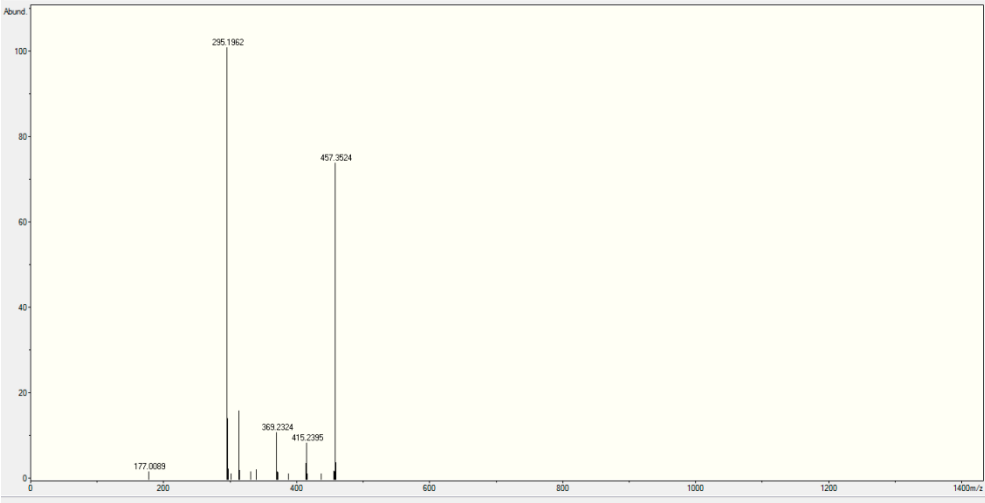
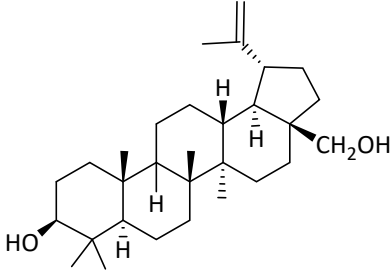
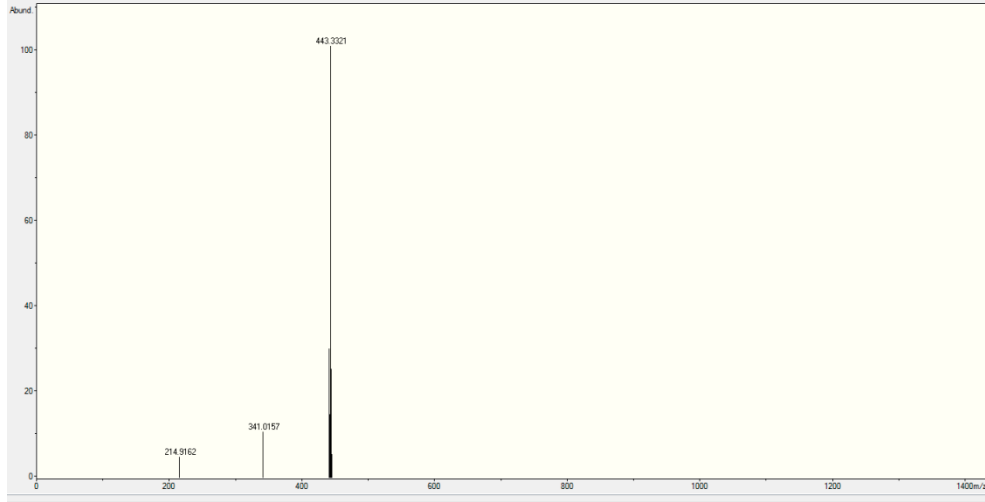
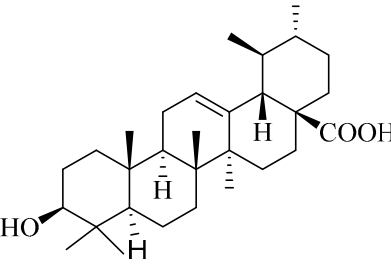
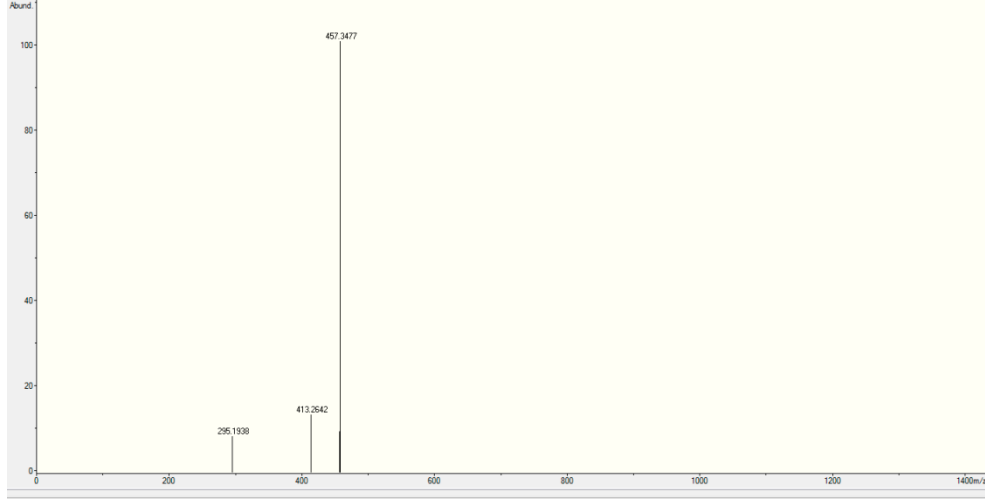
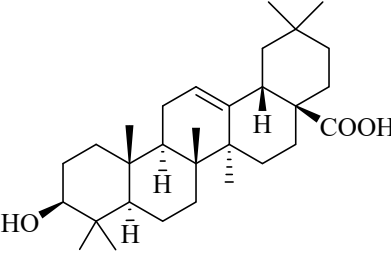
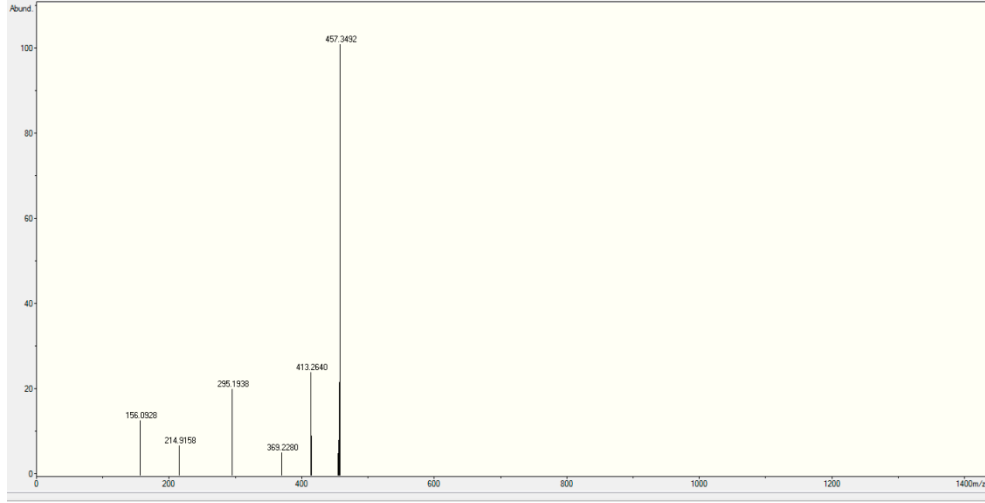
⁶ Department of Medicinal Chemistry, Uppsala Biomedical Center, Uppsala University, Sweden. hesham.el-seedi@fkog.uu.se

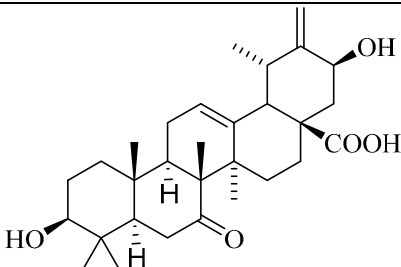
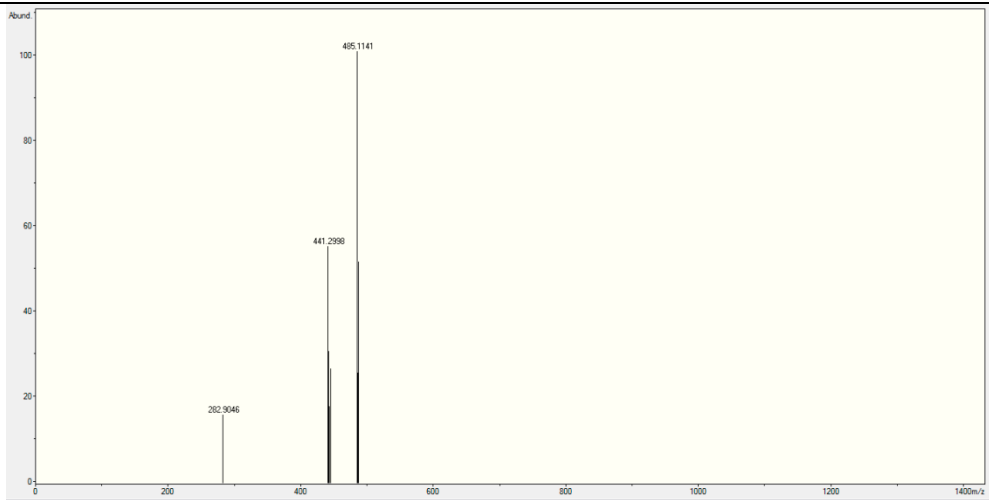
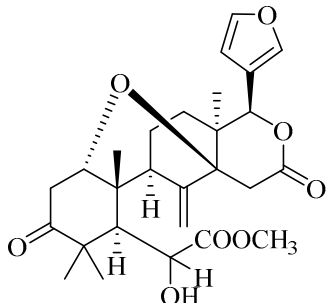
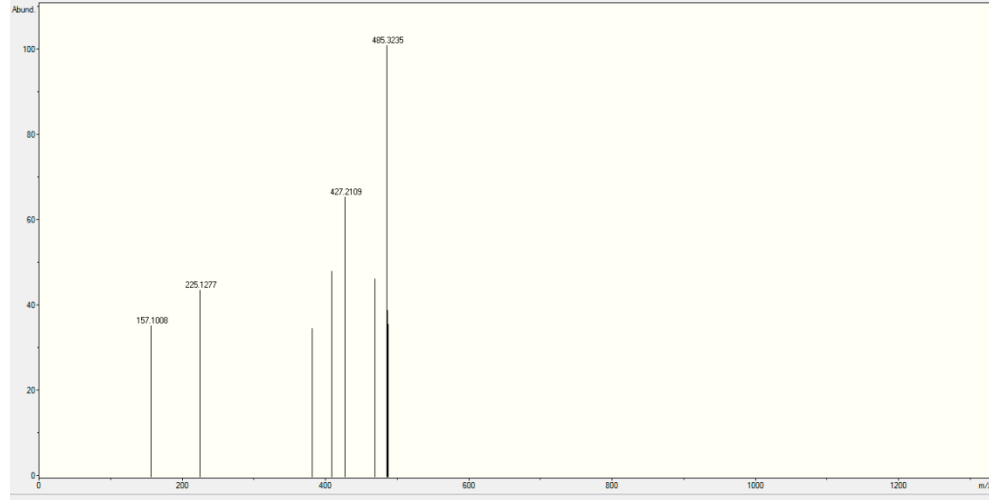
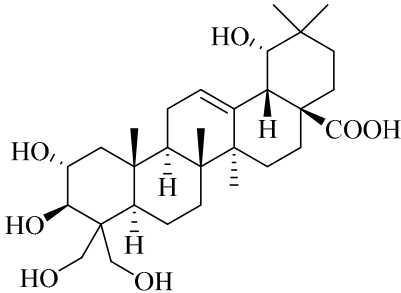
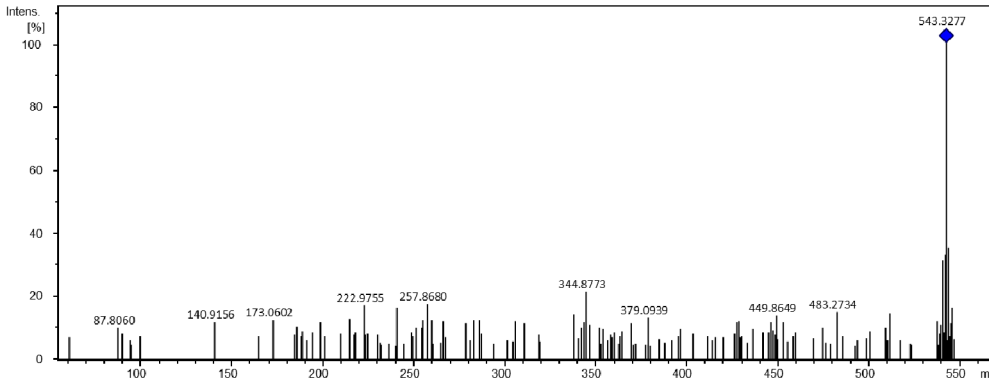
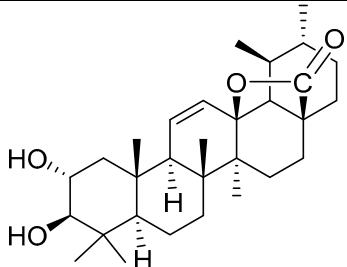
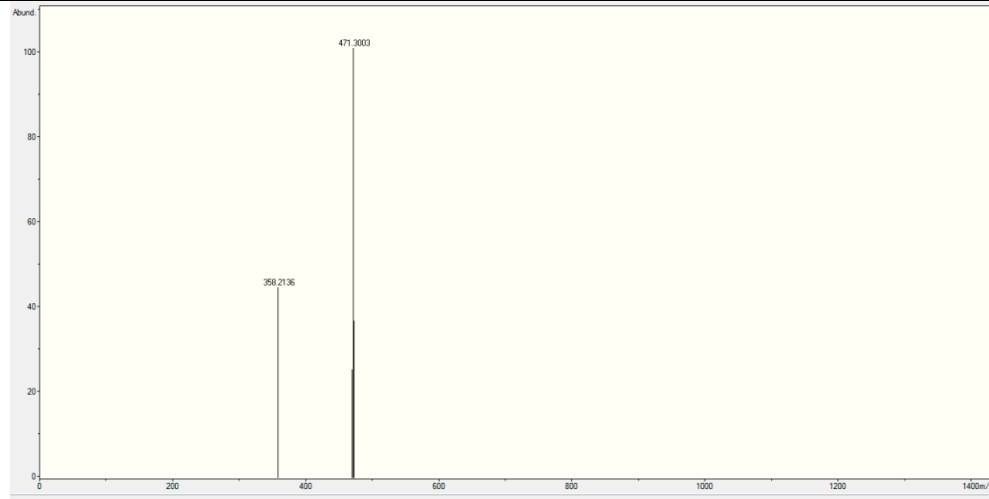
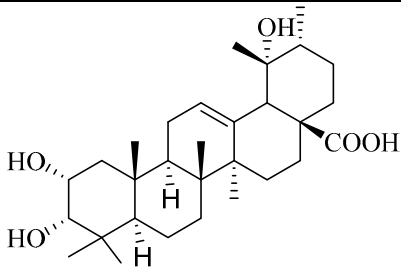
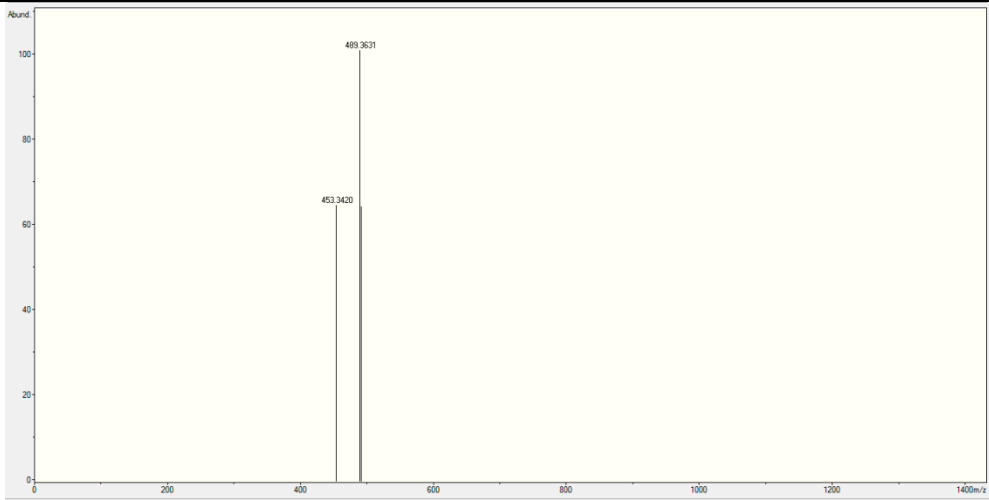
* Correspondence: musharraf1977@yahoo.com; Tel.: (+92 21 34824924-5; 4819010)

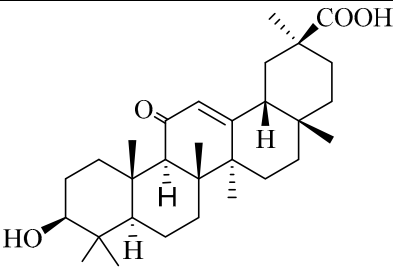
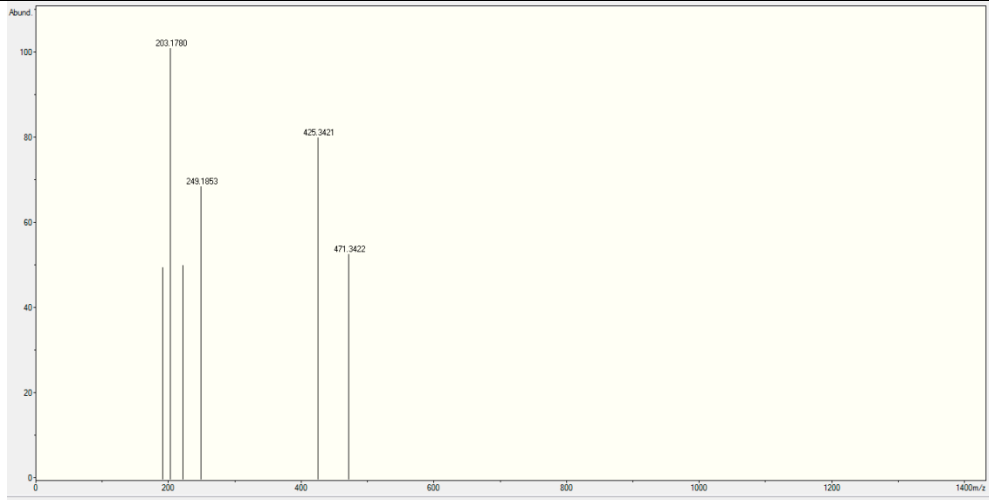
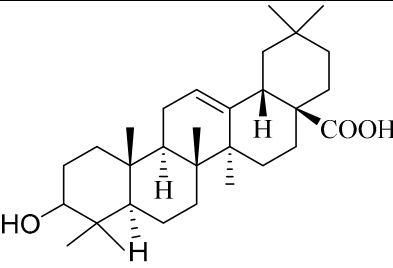
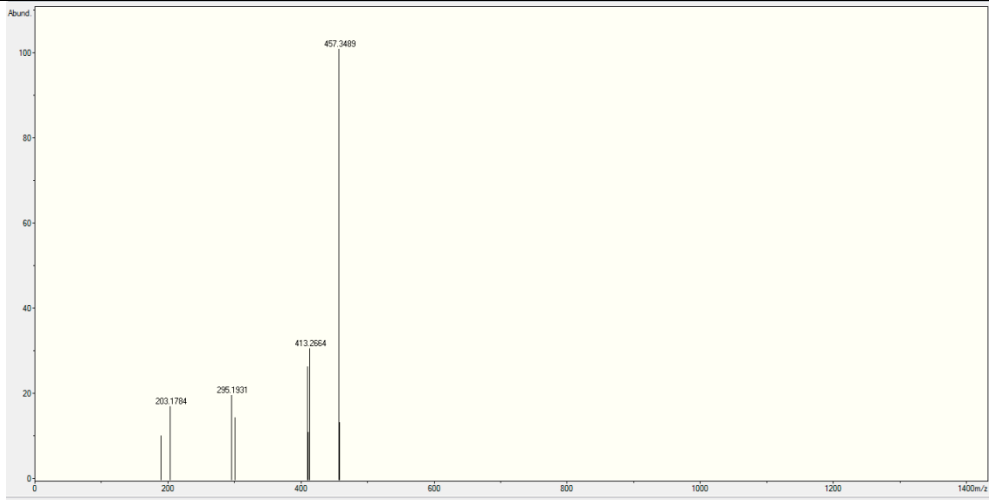
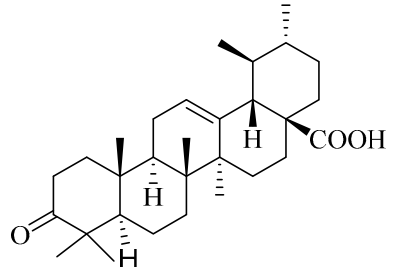
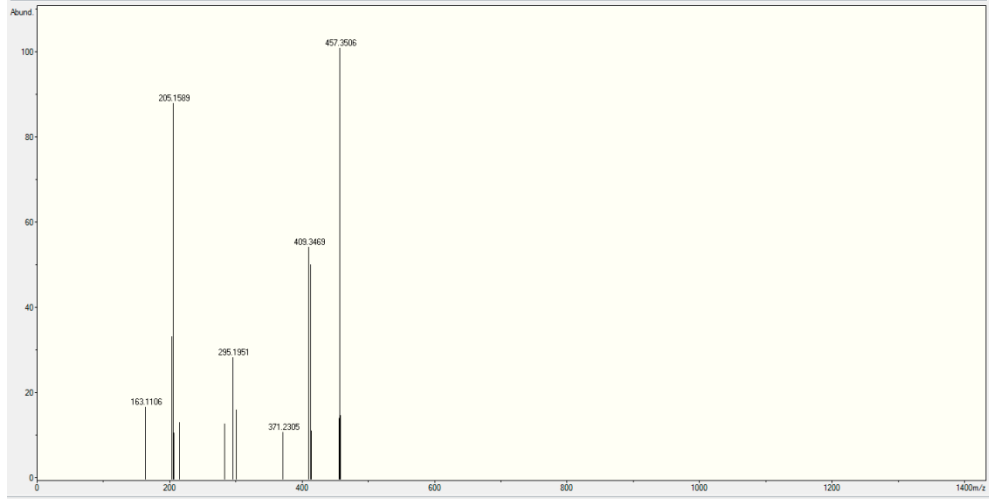
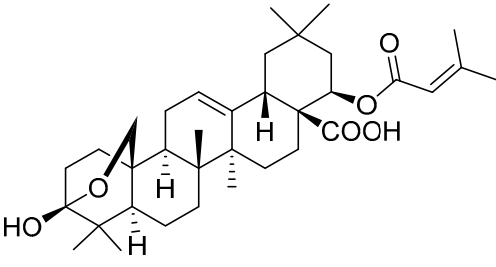
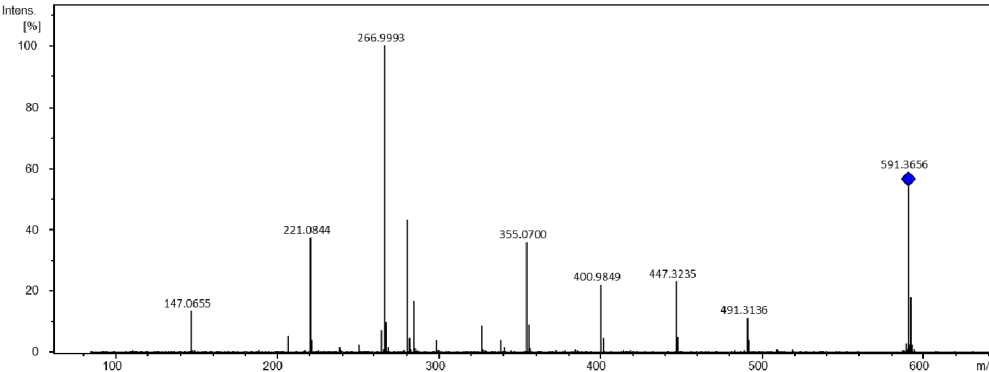
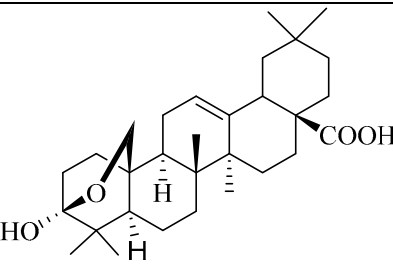
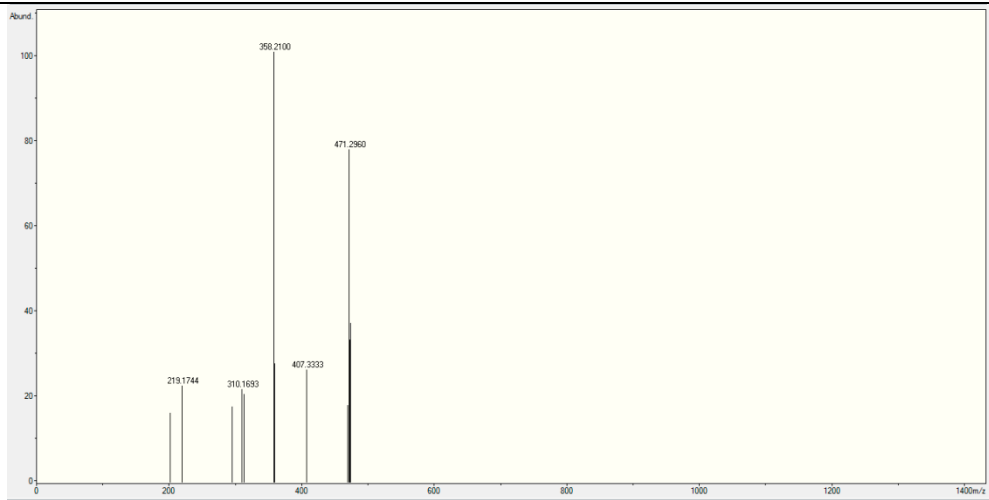
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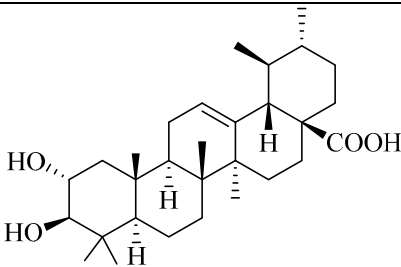
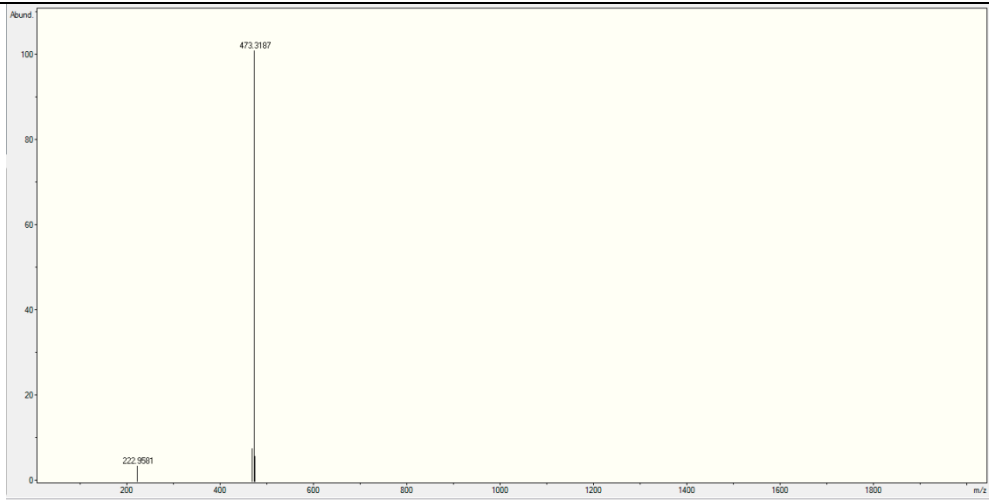
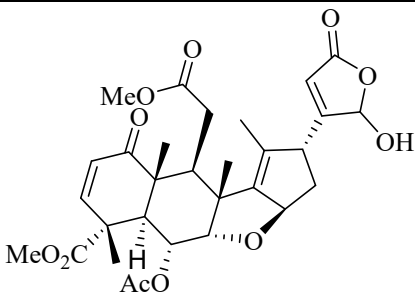
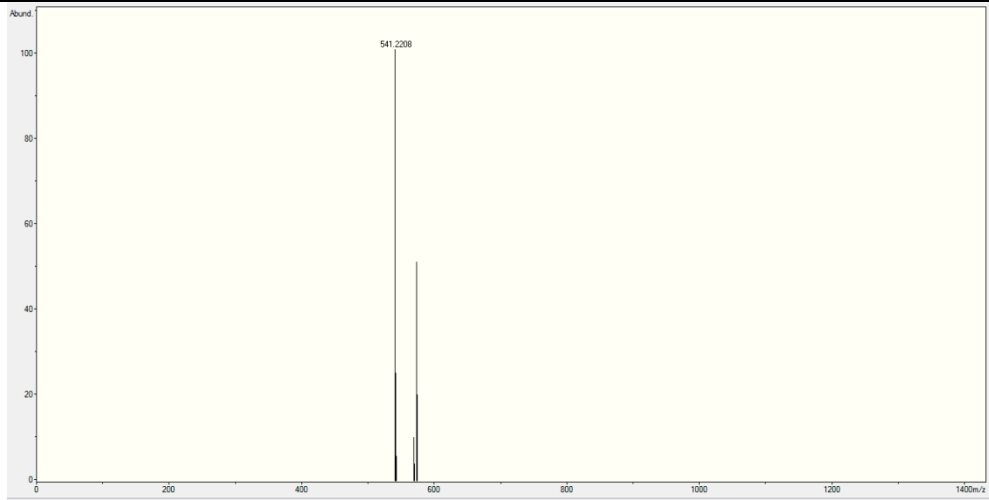
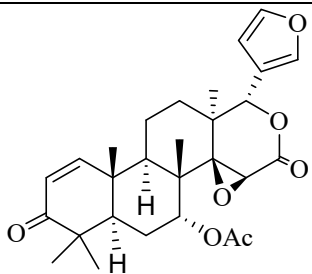
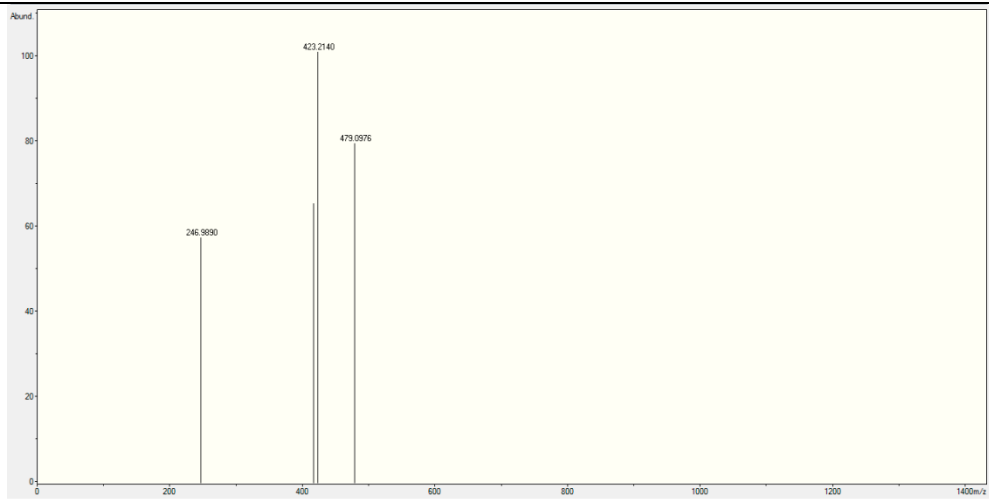
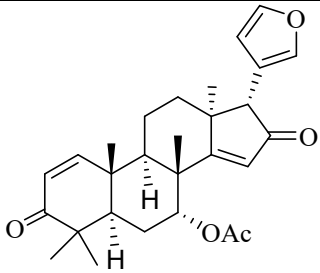
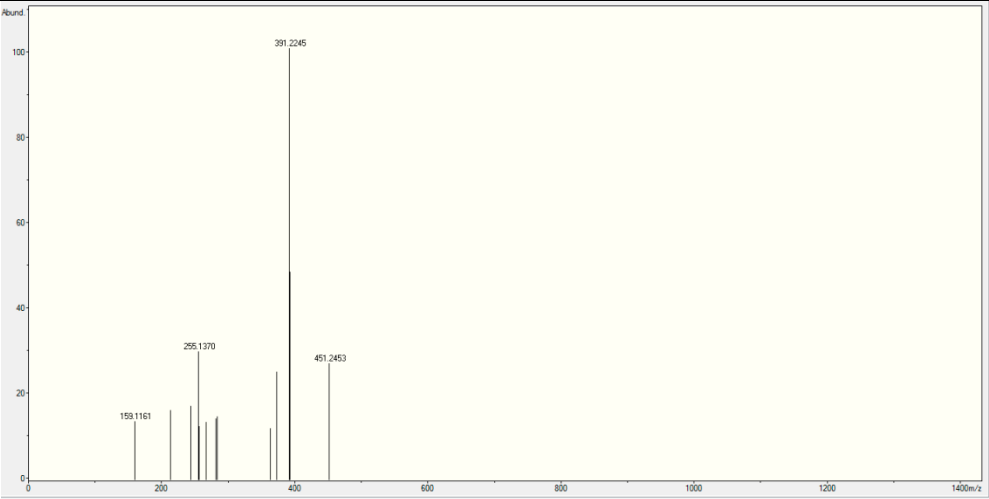
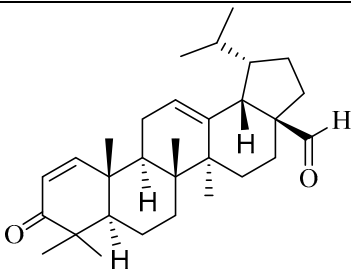
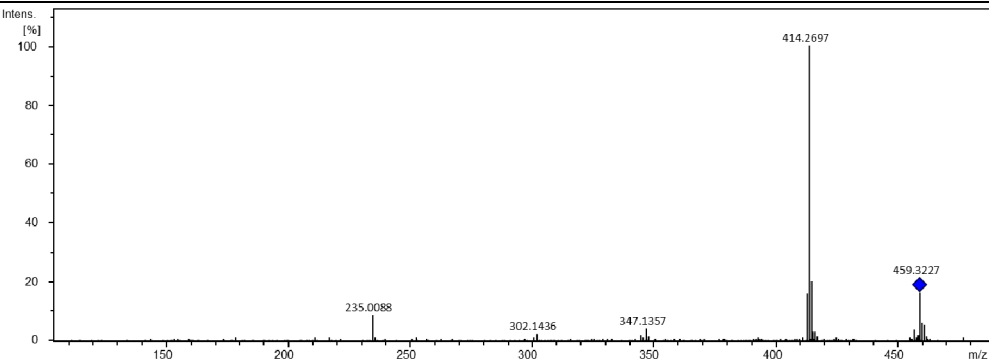
Table S1: All Standard triterpenoids sstructures, classes and MS/MS spectra in the constructed Library

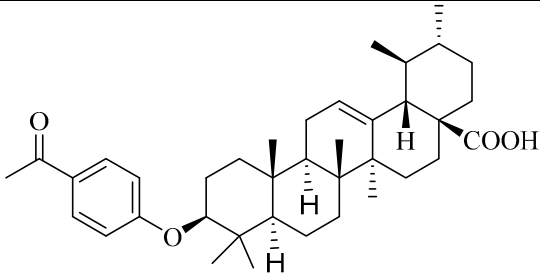
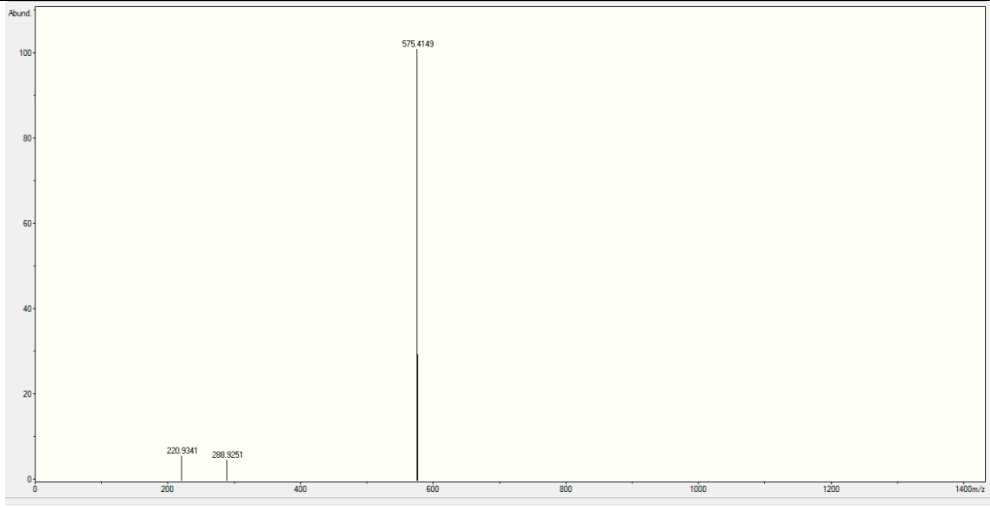
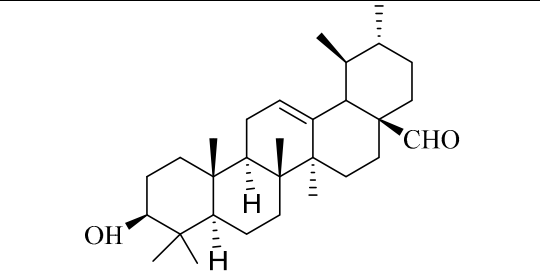
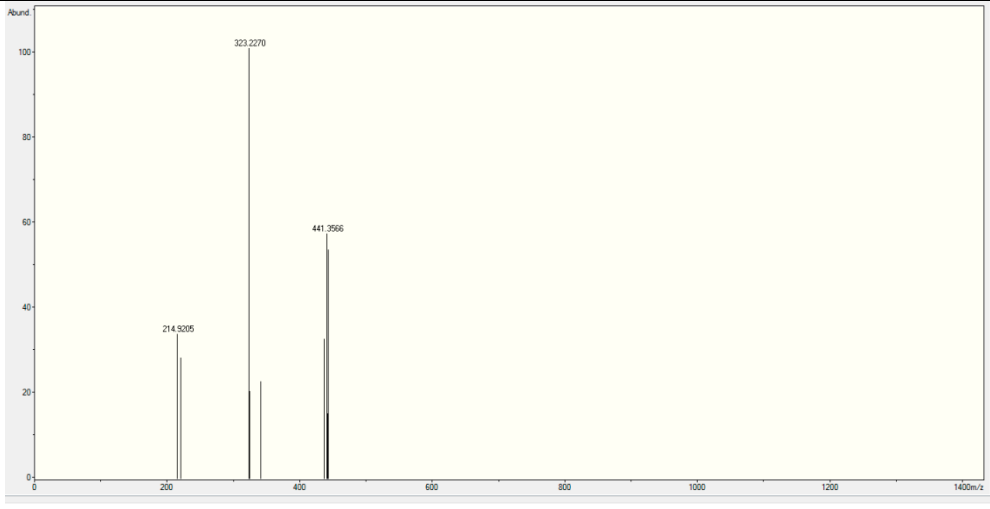
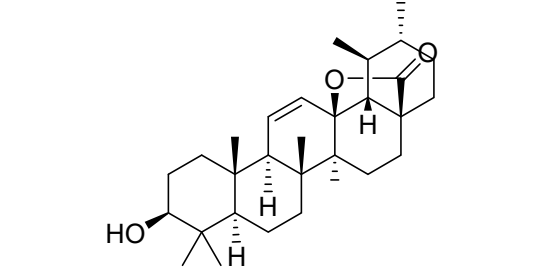
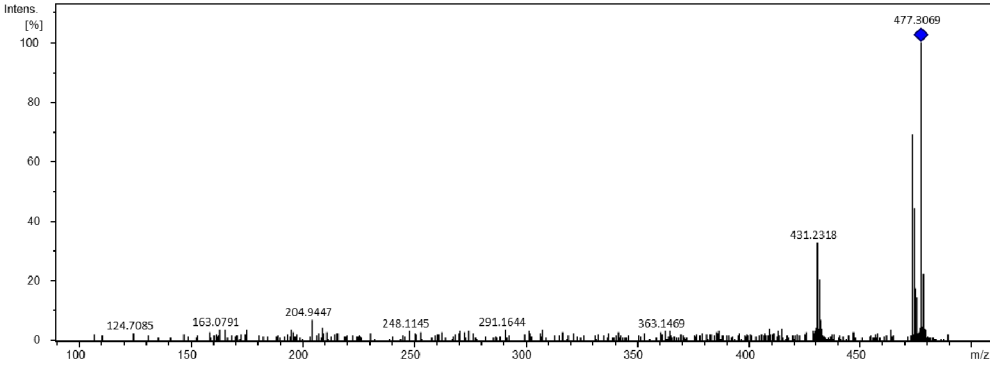
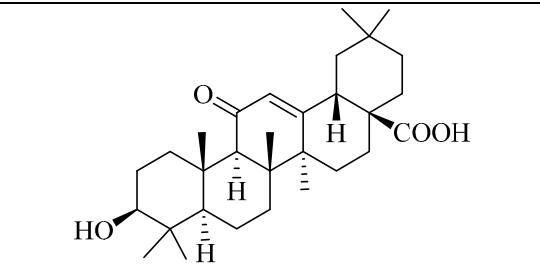
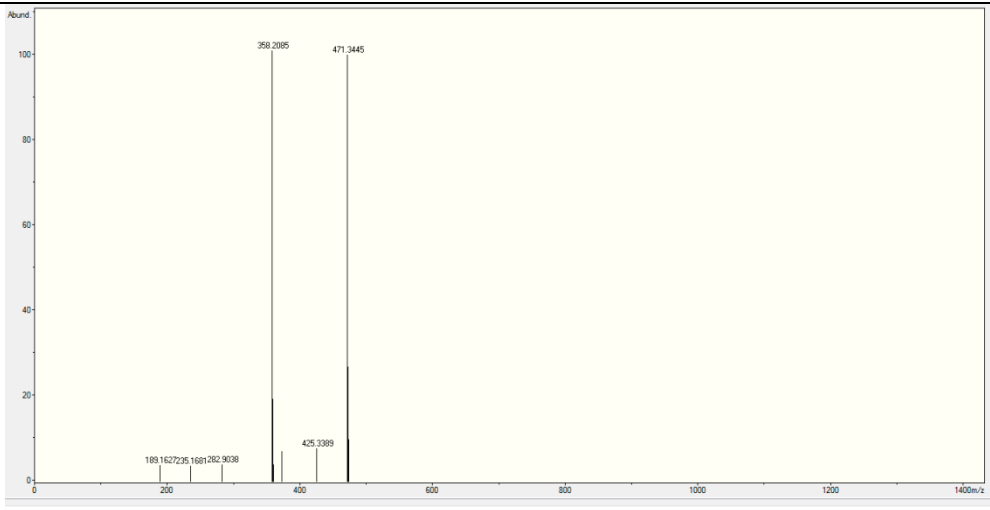
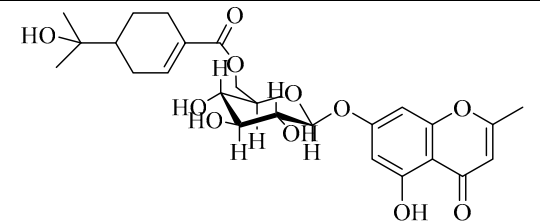
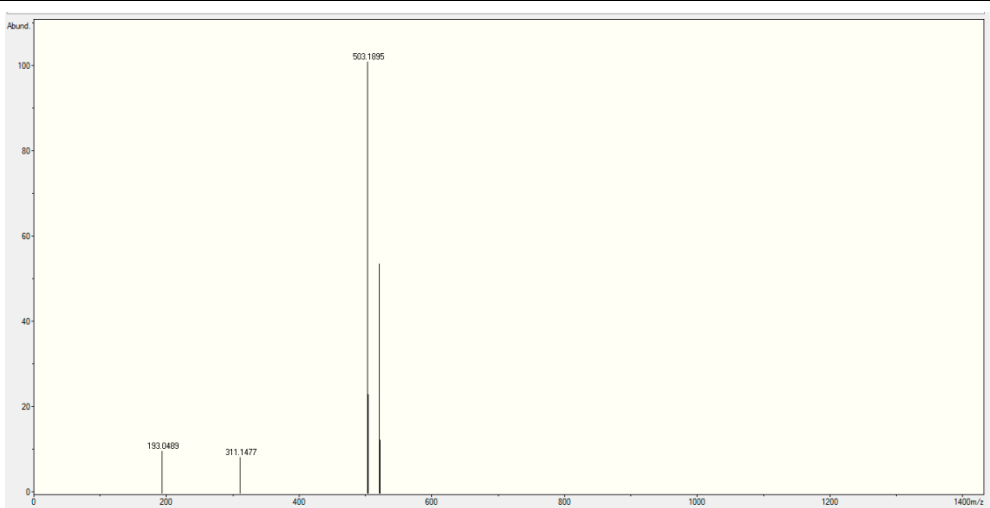
Table S1: All Standard triterpenoids structures, classes, and MS/MS spectra in the constructed Library

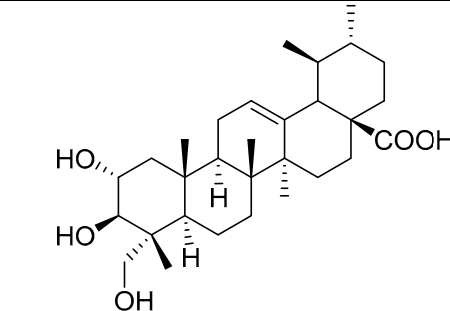
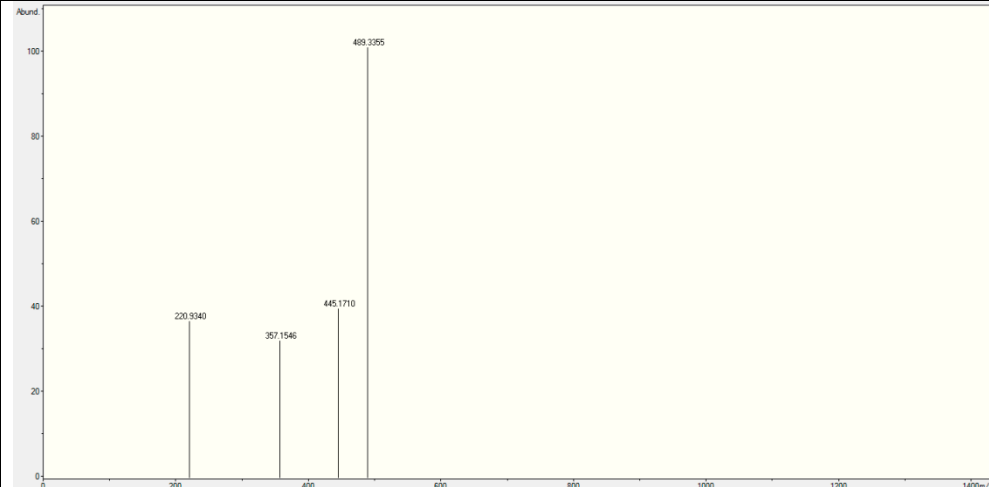
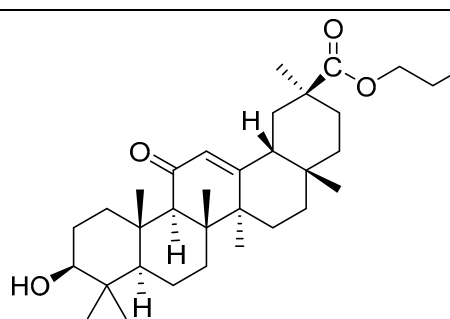
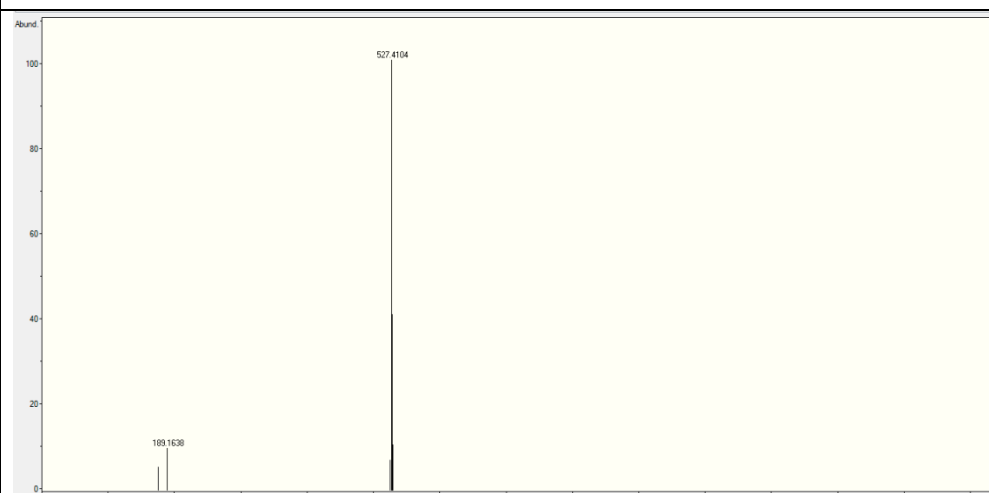
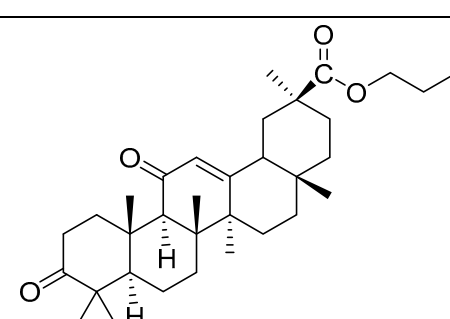
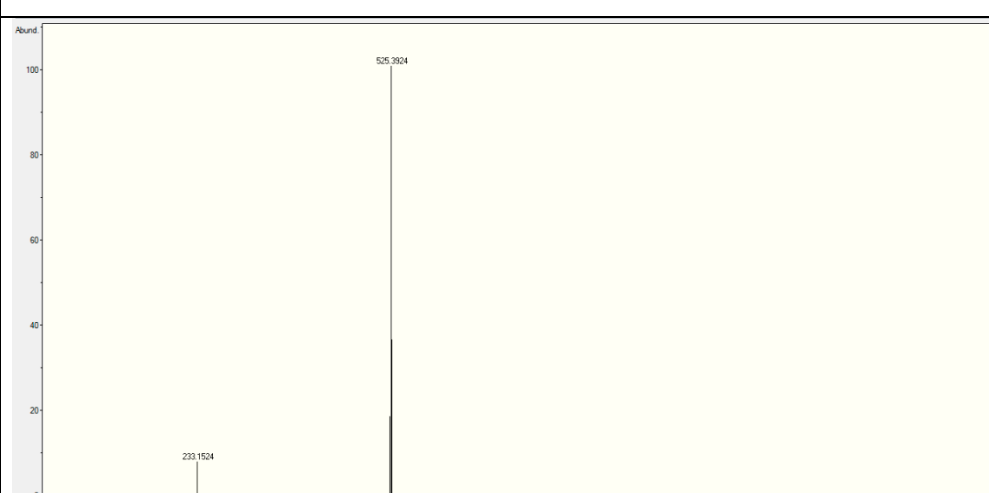
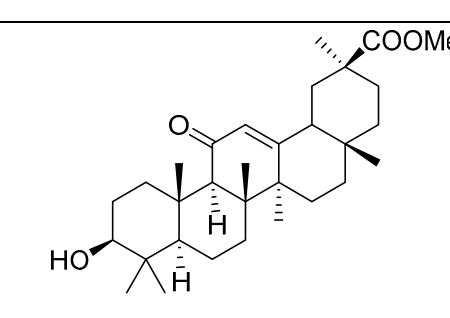
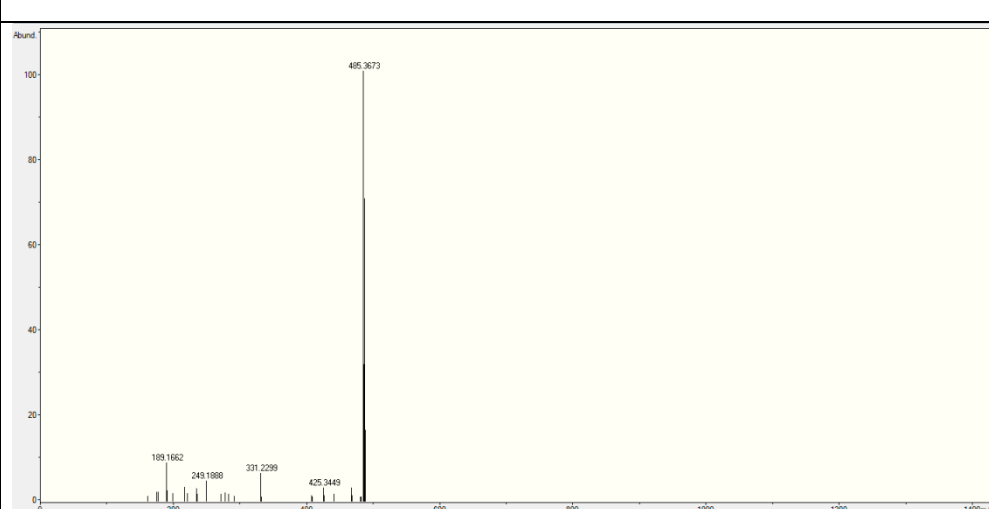
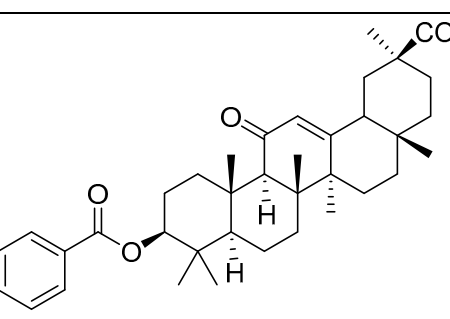
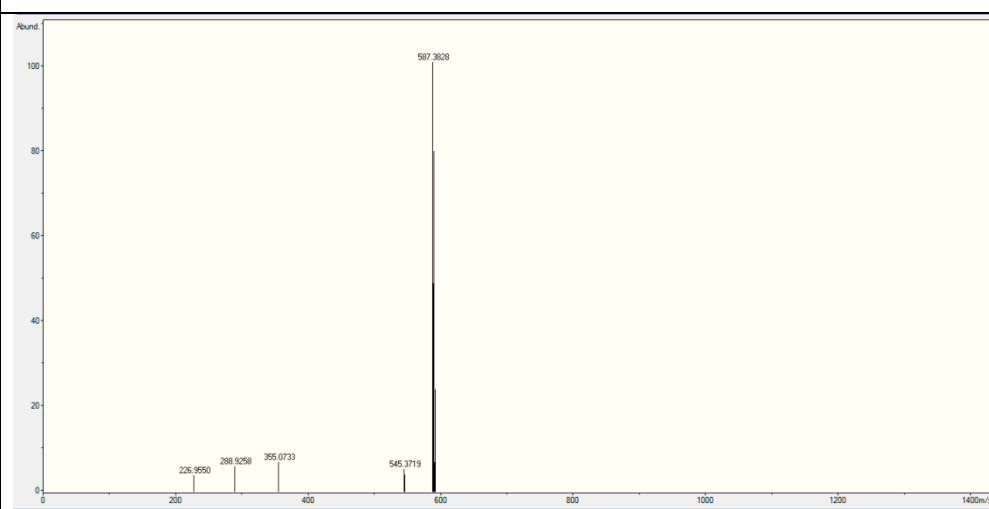
S.No.	Name (Barcode)	Subclass of Compounds	Structure/Exact Mass/Chemical Formula	Spectra in constructed library
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2.	Betulin (STD004)	lupane	<div></div> <div>Chemical Formula: C₃₀H₅₀O₂ Exact Mass: 442.3811</div>	
3.	Ursolic acid (STD007)	Ursane	<div></div> <div>Chemical Formula: C₃₀H₄₈O₃ Exact Mass: 456.3603</div>	
4.	Oleanolic Acid (STD011)	Oleanane	<div></div> <div>Chemical Formula: C₃₀H₄₈O₃ Exact Mass: 456.3603</div>	

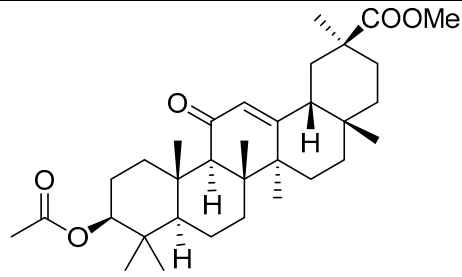
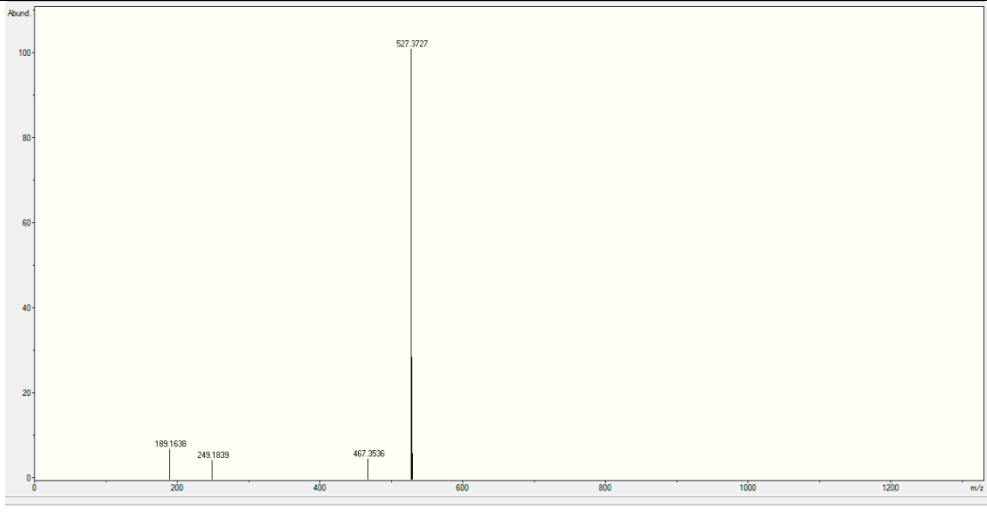
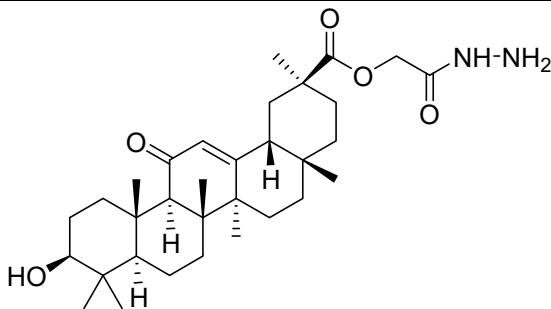
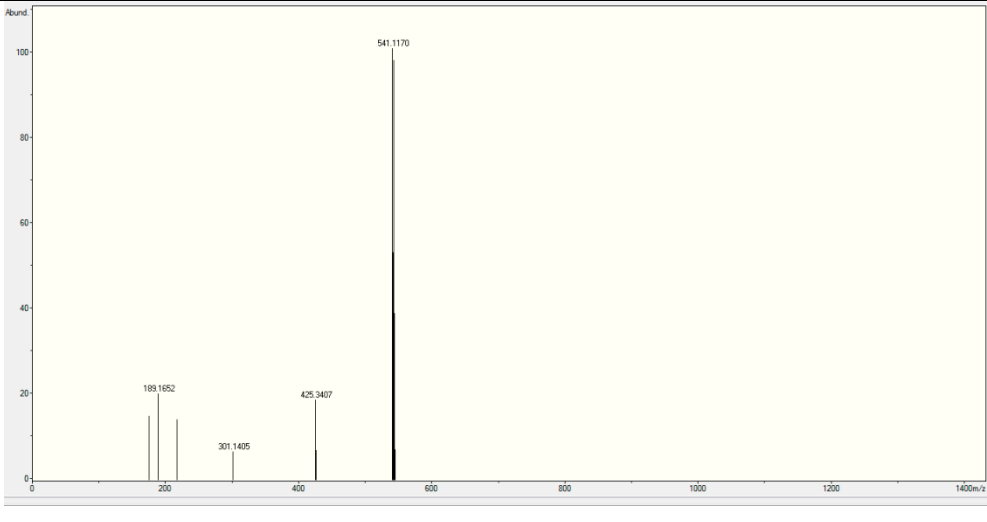
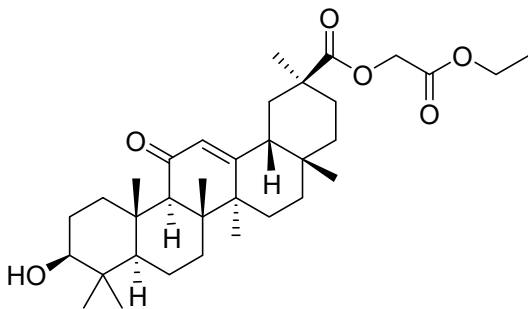
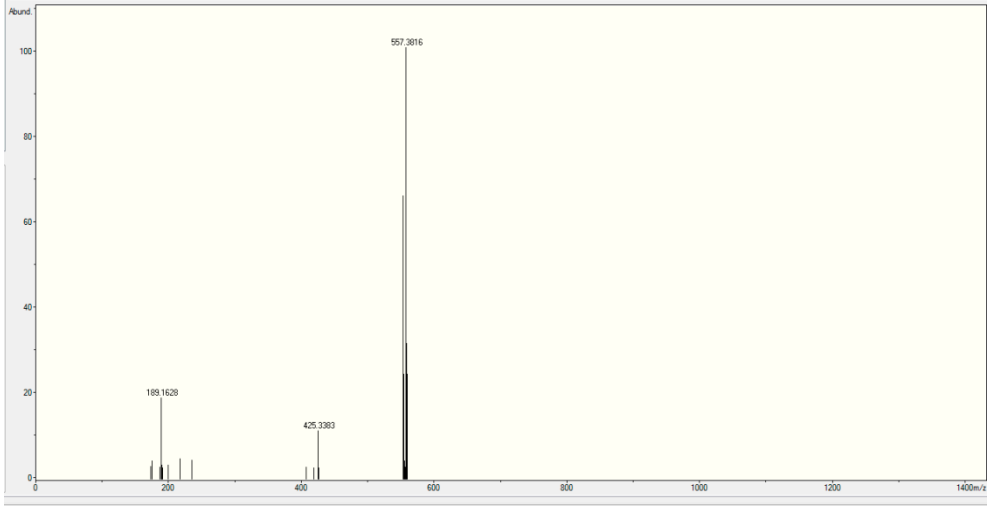
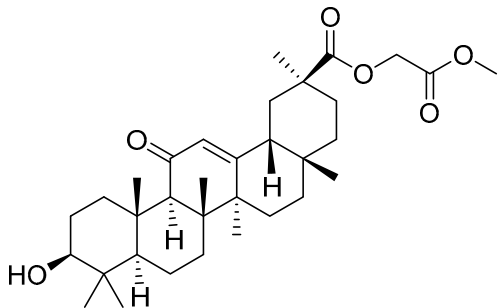
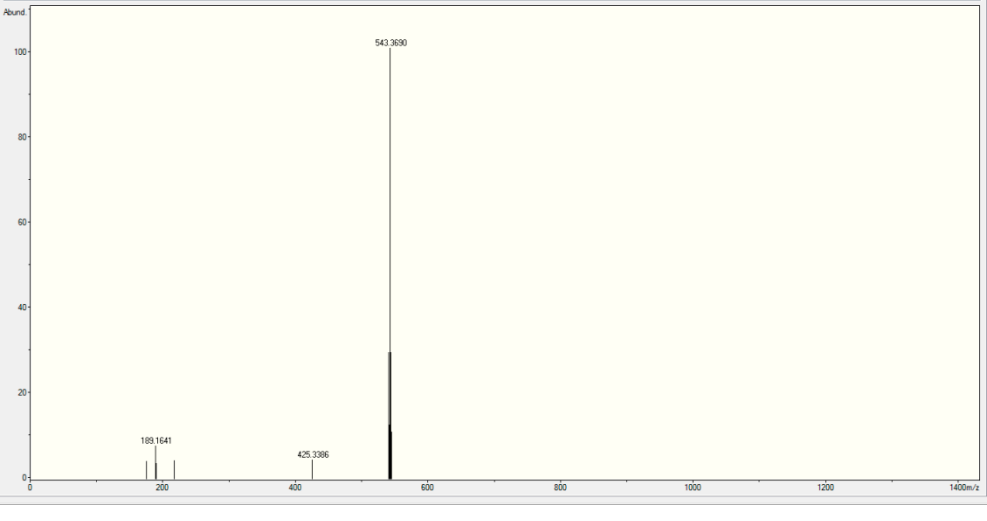
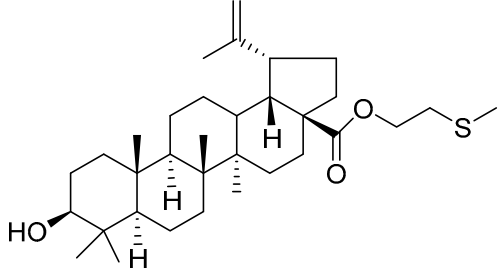
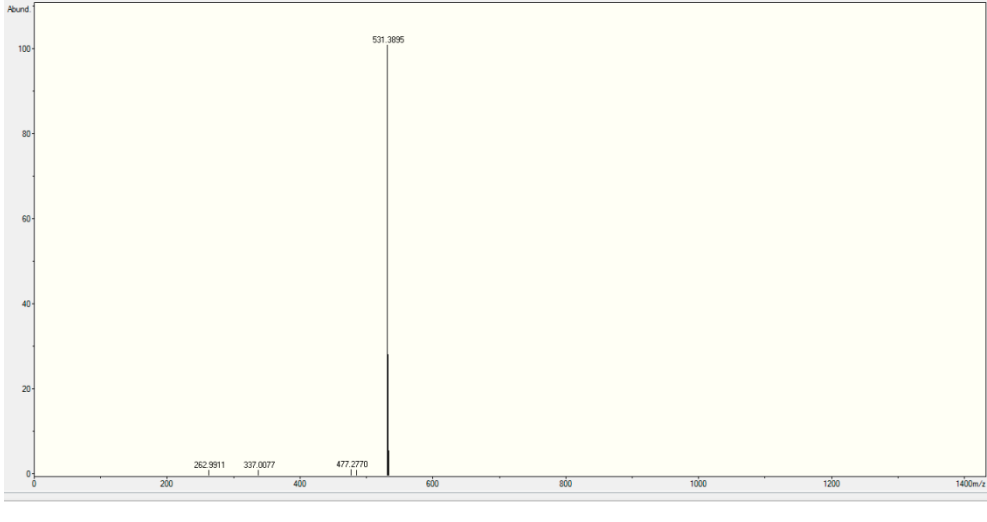
5.	Silymin A (AAC139)	Ursane	<div></div> <div>Chemical Formula: C₃₀H₄₄O₅ Exact Mass: 484.3189</div>	<div></div> <table><tr><th>m/z</th><th>Abund.</th></tr><tr><td>282.9046</td><td>15</td></tr><tr><td>441.2998</td><td>55</td></tr><tr><td>485.1141</td><td>100</td></tr></table>	m/z	Abund.	282.9046	15	441.2998	55	485.1141	100														
m/z	Abund.																									
282.9046	15																									
441.2998	55																									
485.1141	100																									
6.	Intybusoloid (AAC169)	Limonoid	<div></div> <div>Chemical Formula: C₂₇H₃₄O₈ Exact Mass: 486.2254</div>	<div></div> <table><tr><th>m/z</th><th>Abund.</th></tr><tr><td>157.1008</td><td>35</td></tr><tr><td>225.1277</td><td>45</td></tr><tr><td>427.2109</td><td>65</td></tr><tr><td>485.3225</td><td>100</td></tr></table>	m/z	Abund.	157.1008	35	225.1277	45	427.2109	65	485.3225	100												
m/z	Abund.																									
157.1008	35																									
225.1277	45																									
427.2109	65																									
485.3225	100																									
7.	Bellerigenin B (AAC192)	Oleanane	<div></div> <div>Chemical Formula: C₃₀H₄₈O₇ Exact Mass: 520.3400</div>	<div></div> <table><tr><th>m/z</th><th>Intens. [%]</th></tr><tr><td>87.8060</td><td>5</td></tr><tr><td>140.9156</td><td>10</td></tr><tr><td>173.0602</td><td>10</td></tr><tr><td>222.9755</td><td>15</td></tr><tr><td>257.8680</td><td>15</td></tr><tr><td>344.8773</td><td>25</td></tr><tr><td>379.0939</td><td>10</td></tr><tr><td>449.8649</td><td>10</td></tr><tr><td>483.2734</td><td>10</td></tr><tr><td>543.3277</td><td>100</td></tr></table>	m/z	Intens. [%]	87.8060	5	140.9156	10	173.0602	10	222.9755	15	257.8680	15	344.8773	25	379.0939	10	449.8649	10	483.2734	10	543.3277	100
m/z	Intens. [%]																									
87.8060	5																									
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379.0939	10																									
449.8649	10																									
483.2734	10																									
543.3277	100																									
8.	ilelatifol D (AAC196)	Ursane	<div></div> <div>Chemical Formula: C₃₀H₄₆O₄ Exact Mass: 470.3396</div>	<div></div> <table><tr><th>m/z</th><th>Abund.</th></tr><tr><td>356.2136</td><td>45</td></tr><tr><td>471.3003</td><td>100</td></tr></table>	m/z	Abund.	356.2136	45	471.3003	100																
m/z	Abund.																									
356.2136	45																									
471.3003	100																									
9.	Euscaphic acid (AAC198)	Ursane	<div></div> <div>Chemical Formula: C₃₀H₄₈O₅ Exact Mass: 488.3502</div>	<div></div> <table><tr><th>m/z</th><th>Abund.</th></tr><tr><td>453.3420</td><td>65</td></tr><tr><td>489.3631</td><td>100</td></tr></table>	m/z	Abund.	453.3420	65	489.3631	100																
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453.3420	65																									
489.3631	100																									

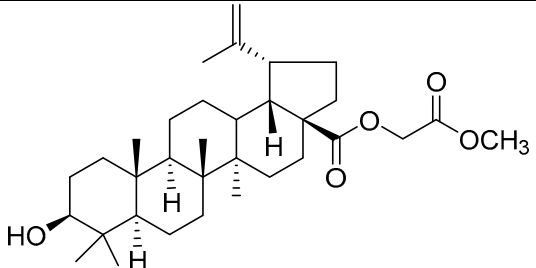
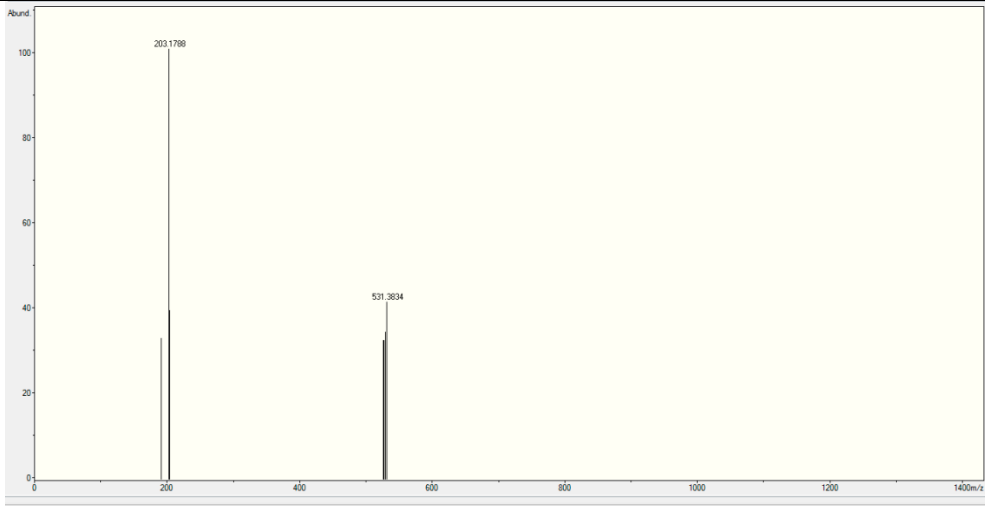
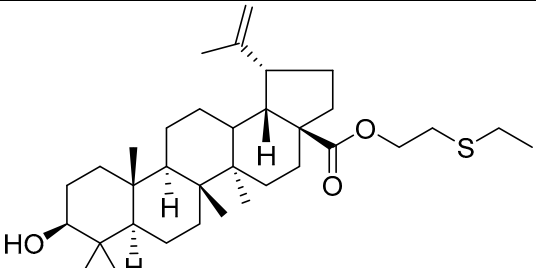
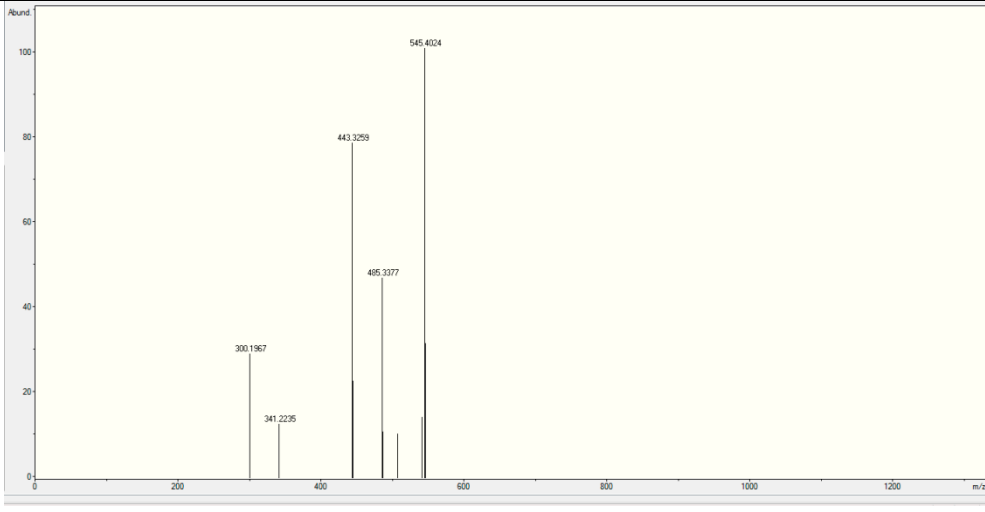
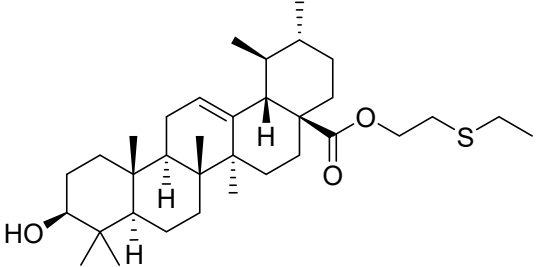
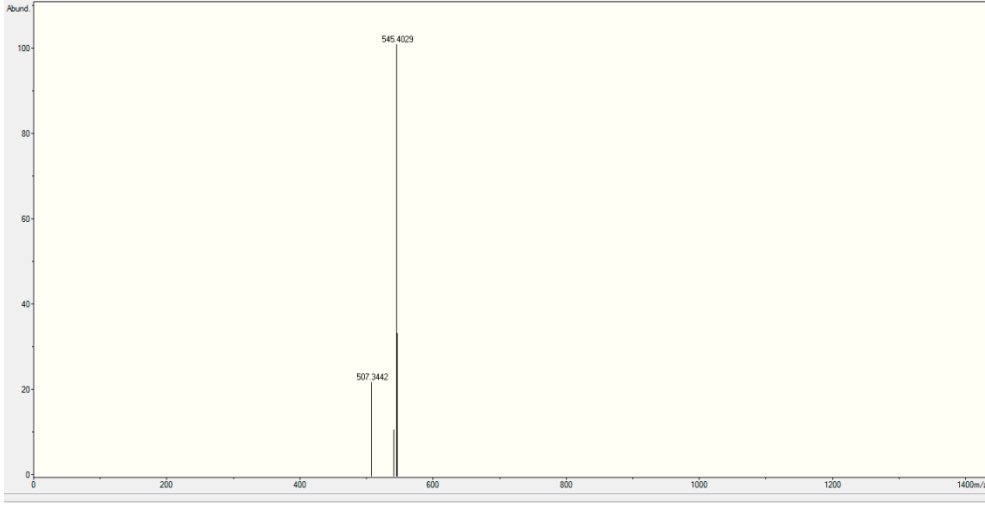
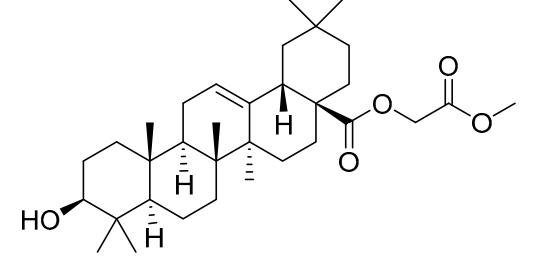
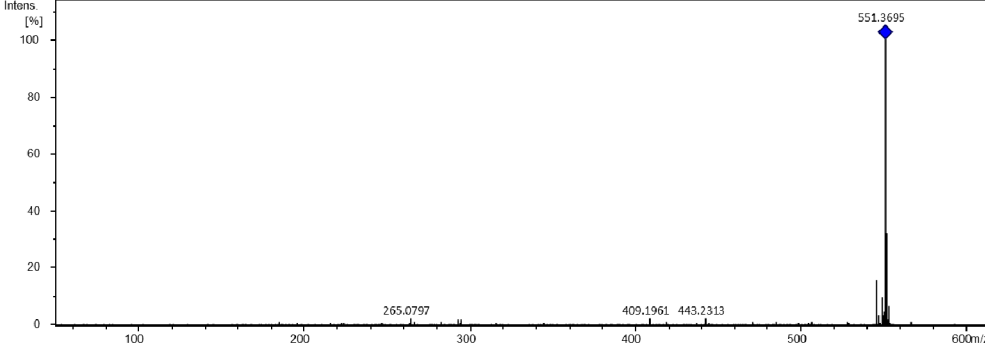
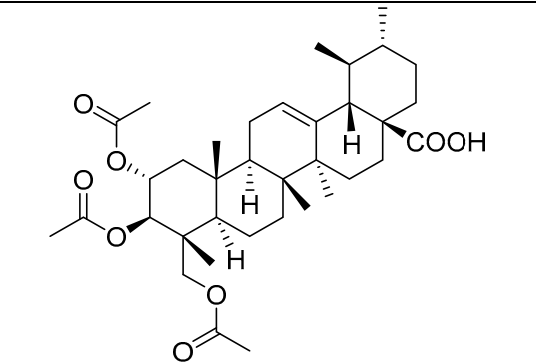
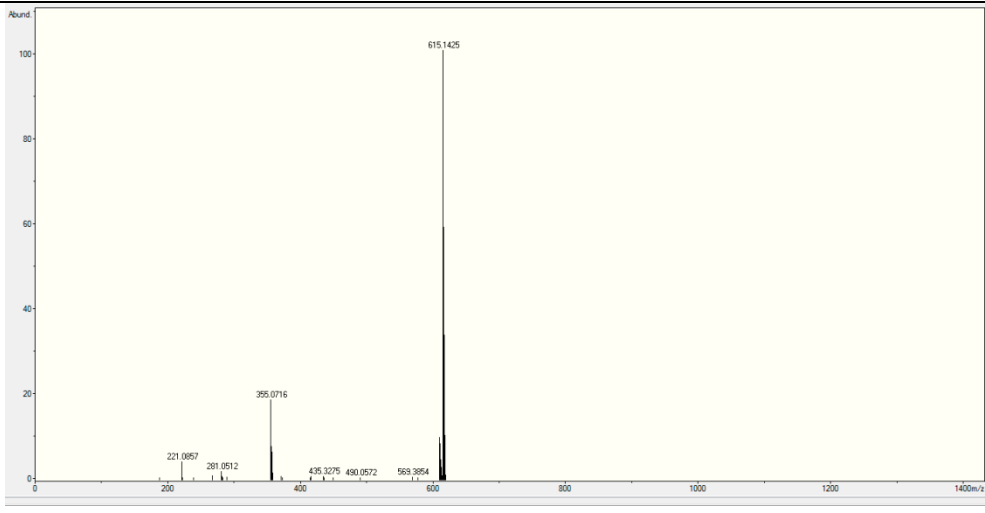
10.	Glycyrrhetic acid (AAC411)	oleanane	<div></div> <div>Chemical Formula: C₃₀H₄₆O₄ Exact Mass: 470.3396</div>	<div></div>
11.	Oleanoic acid (AAC451)	Oleanane	<div></div> <div>Chemical Formula: C₃₀H₄₈O₃ Exact Mass: 456.3603</div>	<div></div>
12.	Ursonic acid (AAC452)	Ursane	<div></div> <div>Chemical Formula: C₃₀H₄₆O₃ Exact Mass: 454.3447</div>	<div></div>
13.	Lantanilic acid (AAC456)	Oleanane	<div></div> <div>Chemical Formula: C₃₅H₅₂O₆ Exact Mass: 568.3764</div>	<div></div>
14.	3,25-epoxy-3a,hydroxy-olean-12-en-28-oic acid (AAC457)	Oleanane	<div></div> <div>Chemical Formula: C₃₀H₄₆O₄ Exact Mass: 470.3396</div>	<div></div>

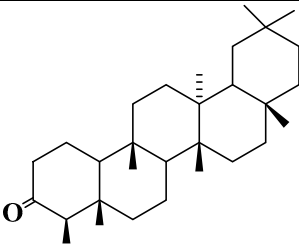
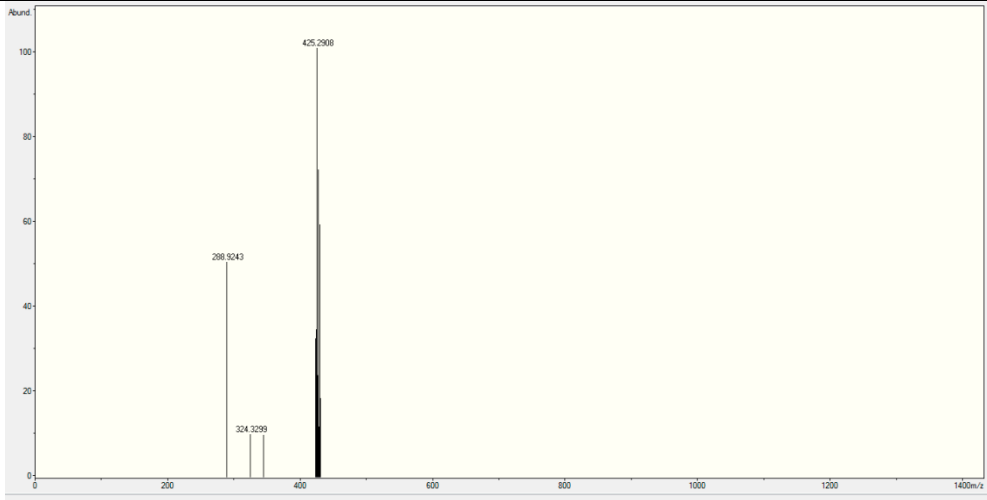
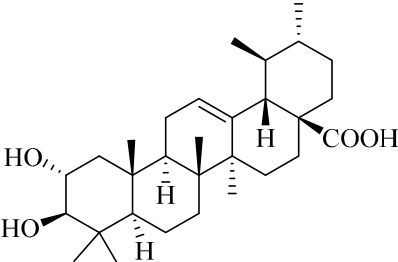
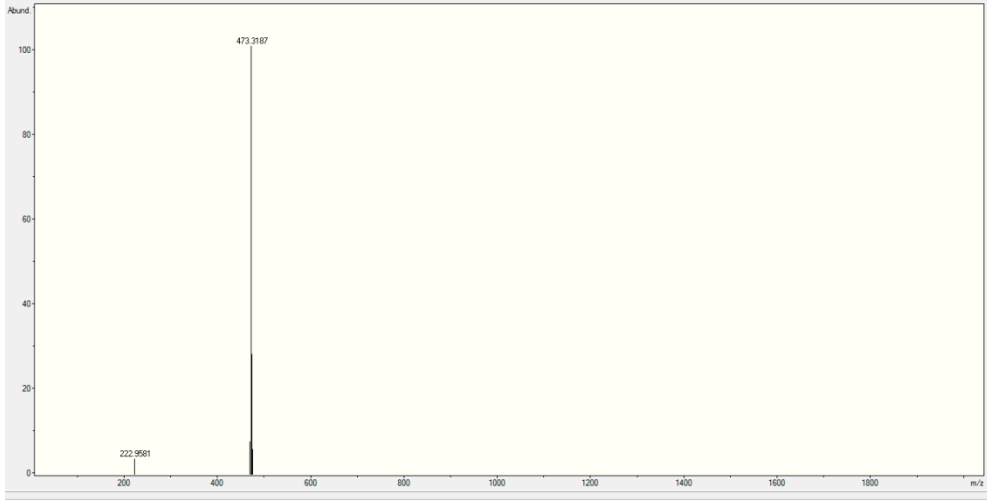
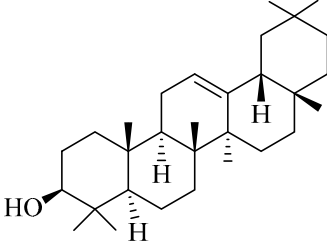
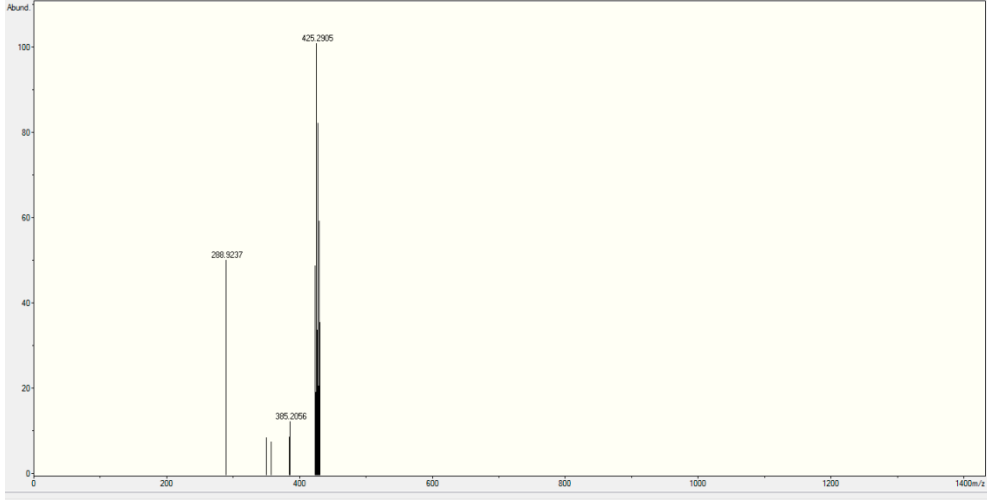
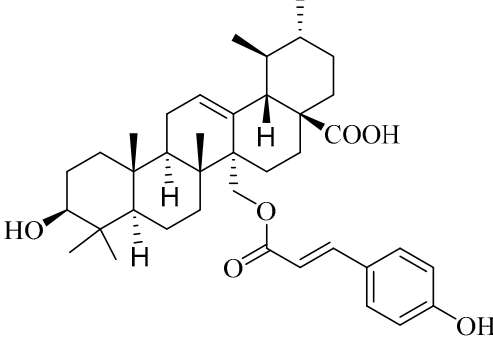
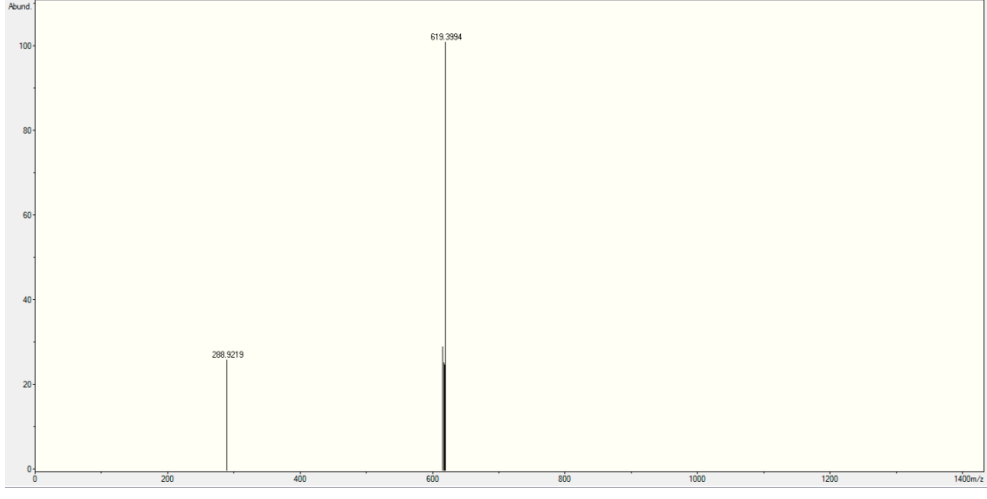
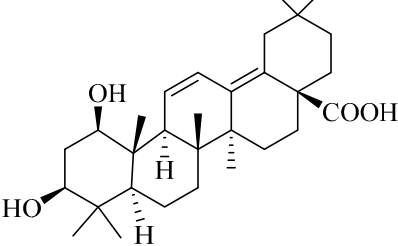
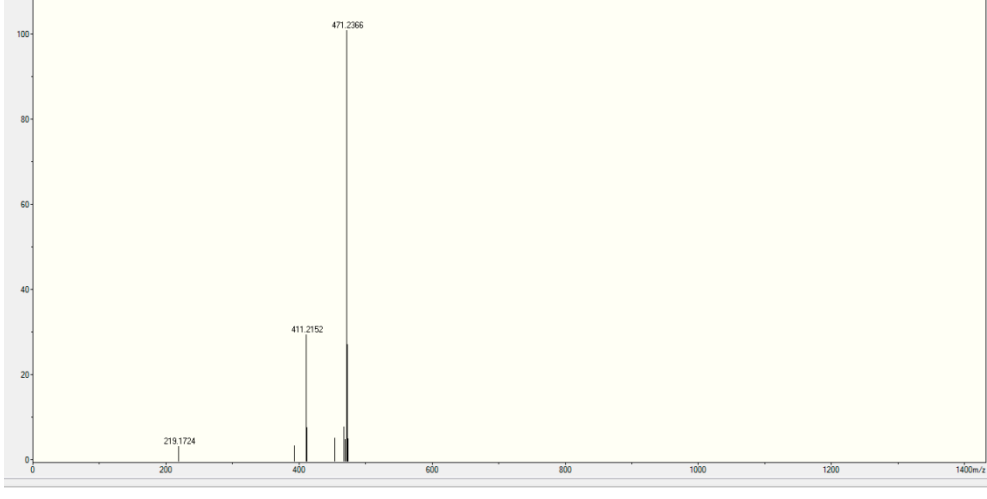
15.	2-a hydroxyurasolic acid (AAC515)	Ursane	<div></div> <div>Chemical Formula: C₃₀H₄₈O₄ Exact Mass: 472.3553</div>	<div></div> <table><tr><th>m/z</th><th>Abund.</th></tr><tr><td>222.9561</td><td>~2</td></tr><tr><td>473.3167</td><td>100</td></tr></table>	m/z	Abund.	222.9561	~2	473.3167	100						
m/z	Abund.															
222.9561	~2															
473.3167	100															
16.	Nimbinolide (AAC690)	Limonoid	<div></div> <div>Chemical Formula: C₃₀H₃₆O₁₁ Exact Mass: 572.2258</div>	<div></div> <table><tr><th>m/z</th><th>Abund.</th></tr><tr><td>541.2208</td><td>100</td></tr></table>	m/z	Abund.	541.2208	100								
m/z	Abund.															
541.2208	100															
17.	Gedunin (AAC691)	Limonoid	<div></div> <div>Chemical Formula: C₂₈H₃₄O₇ Exact Mass: 482.2305</div>	<div></div> <table><tr><th>m/z</th><th>Abund.</th></tr><tr><td>246.9890</td><td>~55</td></tr><tr><td>423.2140</td><td>100</td></tr><tr><td>473.0576</td><td>~75</td></tr></table>	m/z	Abund.	246.9890	~55	423.2140	100	473.0576	~75				
m/z	Abund.															
246.9890	~55															
423.2140	100															
473.0576	~75															
18.	Azadiradione (AAC694)	Limonoid	<div></div> <div>Chemical Formula: C₂₈H₃₄O₅ Exact Mass: 450.2406</div>	<div></div> <table><tr><th>m/z</th><th>Abund.</th></tr><tr><td>159.1161</td><td>~15</td></tr><tr><td>255.1370</td><td>~25</td></tr><tr><td>391.2245</td><td>100</td></tr><tr><td>451.2453</td><td>~25</td></tr></table>	m/z	Abund.	159.1161	~15	255.1370	~25	391.2245	100	451.2453	~25		
m/z	Abund.															
159.1161	~15															
255.1370	~25															
391.2245	100															
451.2453	~25															
19.	3-Oxolup-1:12- diene, 28-al (AAC715)	Lupane	<div></div> <div>Chemical Formula: C₃₀H₄₄O₂ Exact Mass: 436.3341</div>	<div></div> <table><tr><th>m/z</th><th>Intens. [%]</th></tr><tr><td>235.0088</td><td>~10</td></tr><tr><td>302.1436</td><td>~5</td></tr><tr><td>347.1357</td><td>~5</td></tr><tr><td>414.2697</td><td>100</td></tr><tr><td>459.3227</td><td>~15</td></tr></table>	m/z	Intens. [%]	235.0088	~10	302.1436	~5	347.1357	~5	414.2697	100	459.3227	~15
m/z	Intens. [%]															
235.0088	~10															
302.1436	~5															
347.1357	~5															
414.2697	100															
459.3227	~15															

20.	β -Neriursate (AAC733)	Ursane	<div><p>Chemical Formula: C₃₈H₅₄O₄ Exact Mass: 574.4022</p></div>	<div></div>
21.	Ursolaldehyde (AAC738)	Ursane	<div><p>Chemical Formula: C₃₀H₄₈O₂ Exact Mass: 440.3654</p></div>	<div></div>
22.	3b-Hydroxyurs- 11-en-13b(28)- olide (AAK089)	Ursane	<div><p>Chemical Formula: C₃₀H₄₆O₃ Exact Mass: 454.3447</p></div>	<div></div>
23.	11-Oxooleanolic acid (AAK094)	oleanane	<div><p>Chemical Formula: C₃₀H₄₆O₄ Exact Mass: 470.3396</p></div>	<div></div>
24.	5-hydroxy-7- { {6-O- {[(4R/S)-4-(1- hydroxy-1- methylethyl)cy- clohex-1-en-1- yl]-carbonyl}- D- glucopyranosyl }oxy}-2- methyl-4H-1- benzopyran-4- one (AAC039)		<div><p>Chemical Formula: C₂₆H₃₂O₁₁ Exact Mass: 520.1945</p></div>	<div></div>

25.	Asiatic acid (AAK121)	Ursane	<div><p>Chemical Formula: C₃₀H₄₈O₅ Exact Mass: 488.3502</p></div>	<div><table><caption>Mass Spectrum Data for Asiatic acid (AAK121)</caption><tr><th>m/z</th><th>Relative Abundance (%)</th></tr><tr><td>220.9340</td><td>~35</td></tr><tr><td>357.1546</td><td>~30</td></tr><tr><td>445.1710</td><td>~40</td></tr><tr><td>489.3595</td><td>100</td></tr></table></div>	m/z	Relative Abundance (%)	220.9340	~35	357.1546	~30	445.1710	~40	489.3595	100		
m/z	Relative Abundance (%)															
220.9340	~35															
357.1546	~30															
445.1710	~40															
489.3595	100															
26.	Butyl ester of glycyrrhetic acid (AAK129)	Oleanane	<div><p>Chemical Formula: C₃₄H₅₄O₄ Exact Mass: 526.4022</p></div>	<div><table><caption>Mass Spectrum Data for Butyl ester of glycyrrhetic acid (AAK129)</caption><tr><th>m/z</th><th>Relative Abundance (%)</th></tr><tr><td>189.1638</td><td>~10</td></tr><tr><td>527.4104</td><td>100</td></tr></table></div>	m/z	Relative Abundance (%)	189.1638	~10	527.4104	100						
m/z	Relative Abundance (%)															
189.1638	~10															
527.4104	100															
27.	3-oxo-30-butyl ester of glycyrrhetic acid (AAK130)	oleanane	<div><p>Chemical Formula: C₃₄H₅₂O₄ Exact Mass: 524.3866</p></div>	<div><table><caption>Mass Spectrum Data for 3-oxo-30-butyl ester of glycyrrhetic acid (AAK130)</caption><tr><th>m/z</th><th>Relative Abundance (%)</th></tr><tr><td>233.1524</td><td>~10</td></tr><tr><td>525.3824</td><td>100</td></tr></table></div>	m/z	Relative Abundance (%)	233.1524	~10	525.3824	100						
m/z	Relative Abundance (%)															
233.1524	~10															
525.3824	100															
28.	Glycyrrhetic acid methyl ester (AAK131)	oleanane	<div><p>Chemical Formula: C₃₁H₄₈O₄ Exact Mass: 484.3553</p></div>	<div><table><caption>Mass Spectrum Data for Glycyrrhetic acid methyl ester (AAK131)</caption><tr><th>m/z</th><th>Relative Abundance (%)</th></tr><tr><td>189.1662</td><td>~10</td></tr><tr><td>243.1888</td><td>~5</td></tr><tr><td>331.2299</td><td>~10</td></tr><tr><td>425.3449</td><td>~5</td></tr><tr><td>485.3673</td><td>100</td></tr></table></div>	m/z	Relative Abundance (%)	189.1662	~10	243.1888	~5	331.2299	~10	425.3449	~5	485.3673	100
m/z	Relative Abundance (%)															
189.1662	~10															
243.1888	~5															
331.2299	~10															
425.3449	~5															
485.3673	100															
29.	3-benzoyloxy-3- O-methyl ester of glycyrrhetic acid (AAK132)	oleanane	<div><p>Chemical Formula: C₃₈H₅₂O₅ Exact Mass: 588.3815</p></div>	<div><table><caption>Mass Spectrum Data for 3-benzoyloxy-3-O-methyl ester of glycyrrhetic acid (AAK132)</caption><tr><th>m/z</th><th>Relative Abundance (%)</th></tr><tr><td>226.9550</td><td>~5</td></tr><tr><td>288.9258</td><td>~10</td></tr><tr><td>355.0733</td><td>~15</td></tr><tr><td>545.3719</td><td>~5</td></tr><tr><td>587.3828</td><td>100</td></tr></table></div>	m/z	Relative Abundance (%)	226.9550	~5	288.9258	~10	355.0733	~15	545.3719	~5	587.3828	100
m/z	Relative Abundance (%)															
226.9550	~5															
288.9258	~10															
355.0733	~15															
545.3719	~5															
587.3828	100															

30.	3-acetoxy-3- methyl ester of glycyrrhetic acid (AAK133)	oleanane	<div><p>Chemical Formula: C₃₃H₅₀O₅ Exact Mass: 526.3658</p></div>	<div></div>
31.	Hydrazide of glycyrrhetic acid (AAK112)	oleanane	<div><p>Chemical Formula: C₃₂H₅₀N₂O₅ Exact Mass: 542.3720</p></div>	<div></div>
32.	Ethyl acetate ester of glycyrrhetic acid (AAK141)	oleanane	<div><p>Chemical Formula: C₃₄H₅₂O₆ Exact Mass: 556.3764</p></div>	<div></div>
33.	Methyl acetate ester of glycyrrhetic acid (AAK142)	oleanane	<div><p>Chemical Formula: C₃₃H₅₀O₆ Exact Mass: 542.3607</p></div>	<div></div>
34.	Ethyl methyl sulfide ester of betulinic acid (AAK147)	Lupane	<div><p>Chemical Formula: C₃₃H₅₄O₃S Exact Mass: 530.3794</p></div>	<div></div>

35.	Methyl acetate ester of betulinic acid (AAK152)	Lupane	<div><p>Chemical Formula: C₃₃H₅₂O₅ Exact Mass: 528.3815</p></div>	<div></div>
36.	Diethyl sulfide ester of betulinic acid (AAK155)	Lupane	<div><p>Chemical Formula: C₃₄H₅₆O₃S Exact Mass: 544.3950</p></div>	<div></div>
37.	Diethyl sulfide ester of ursolic acid (AAK172)	Ursane	<div><p>Chemical Formula: C₃₄H₅₆O₃S Exact Mass: 544.3950</p></div>	<div></div>
38.	Methyl acetate ester of oleanolic acid (AAK160)	oleanane	<div><p>Chemical Formula: C₃₃H₅₂O₅ Exact Mass: 528.3815</p></div>	<div></div>
39.	2, 3, 23-triacetoxy derivative of asiatic acid (AAK175)	Ursane	<div><p>Chemical Formula: C₃₆H₅₄O₈ Exact Mass: 614.3819</p></div>	<div></div>

40.	Friedelin (AAC150)	Friedelane	<div><p>Chemical Formula: $C_{30}H_{50}O$ Exact Mass: 426.3862</p></div>	<div></div>
41.	2 A-Hydroxyursolic acid (AAK095)	Ursane	<div><p>Chemical Formula: $C_{30}H_{48}O_4$ Exact Mass: 472.3553</p></div>	<div></div>
42.	beta-amyrin (AAD671)	Oleanane	<div><p>Chemical Formula: $C_{30}H_{50}O$ Exact Mass: 426.3862</p></div>	<div></div>
43.	3b-Hydroxy-27-p-E-coumaroyloxy-urs-12-en-28-oic acid (AAC739)	Ursane	<div><p>Chemical Formula: $C_{39}H_{54}O_6$ Exact Mass: 618.3920</p></div>	<div></div>
44.	Atriplicin (AAC401)	oleanane	<div><p>Chemical Formula: $C_{30}H_{46}O_4$ Exact Mass: 470.3396</p></div>	<div></div>