

Supplementary material

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Table S1. Review of the literature related to the detection of various compounds (iridoids, phenolics, and terpenes) in *Nepeta nuda* extracts.

Compound	Type of extract	References
<i>Iridoids</i>		
<i>cis,trans</i> -Nepetalactone	EO	De Pooter et al., 1987 [61]; Kobaisy et al., 2005 104; Mancini et al., 2009 [99]; Narimani et al., 2017 [13]; Akbaba et al., 2021 [100]
	HE and AE	Kökdil et al., 1999 [40]
<i>trans,cis</i> -Nepetalactone	EO	Regnier et al., 1967 [41]; De Pooter et al., 1987 [61]; Mancini et al., 2009 [99]; Gkinis et al., 2010 [14]; Bozok et al., 2017 [4]; Narimani et al., 2017 [13]; Akbaba et al., 2021 [100]; Aćimović et al., 2022 [62]
<i>cis,cis</i> -Nepetalactone	EO	De Pooter et al., 1987 [61]; Kobaisy et al., 2005 [8]; Mancini et al., 2009 [99]; Bozari et al., 2013 [101]; Gormez et al., 2013 [6]
	HE and AE	Kökdil et al., 1999 [40]
	EA	Zaharieva et al., 2023 [11]
<i>trans,trans</i> -Nepetalactone	EO	De Pooter et al., 1987 [61]; Handjieva et al., 1996 [57]
Iridomyrmecin	EO	Handjieva et al., 1996 [57]
Isoiridomyrmecin	EO	Handjieva et al., 1996 [57]
Nepetalic acid	HE	Kökdil et al., 1999 [40]
	EO	Handjieva et al., 1996 [57]
Dehydronepetalactone	EO	Handjieva et al., 1996 [57]
	HE and AE	Kökdil et al., 1999 [40]
1,5,9- <i>epi</i> -Deoxyloganic acid	HE and AE	Kökdil et al., 1999 [40]
	MeOH	Dienaitė et al., 2018 [27]; Petrova et al., 2022 [10]
Epideoxyloganic acid hexoside	MeOH	Petrova et al., 2022 [10]
Epideoxyloganic acid pentoside	MeOH	Petrova et al., 2022 [10]
Geniposidic acid	MeOH	Petrova et al., 2022 [10]
Dihydrocornic acid	MeOH	Petrova et al., 2022 [10]
Secologanin	MeOH	Petrova et al., 2022 [10]
Verminoside	MeOH	Smiljković et al., 2018 [15]
Velpetin	MeOH	Takeda et al., 1995 [33]
Nepetanudoside A	MeOH	Takeda et al., 1995 [33]
Nepetanudoside B	MeOH	Takeda et al., 1995 [33]
Nepetanudoside C	MeOH	Takeda et al., 1995 [33]
Nepetanudoside D	MeOH	Takeda et al., 1995 [33]
Nepetanudone	HE and AE	Kökdil et al., 1998b [102]
<i>Phenolics</i>		
Genkwanin	MeOH	Jamzad et al., 2003 [43]
Isothymusin	MeOH	Jamzad et al., 2003 [43]

8-Hydroxysalvigenin	MeOH	Jamzad et al., 2003 [43]
4-Hydroxybenzoic acid	WE and EtOH	Teber and Bursal, 2020 [63]
	MeOH	Petrova et al., 2022 [10]
Acacetin	MeOH	Mišić et al., 2015 [20]
Aesculetin	MeOH	Petrova et al., 2022 [10]
Aesculin	MeOH	Mišić et al., 2015 [20]; Petrova et al., 2022 [10]
Apigenin	WE and MeOH	Dienaitė et al., 2018 [27]
	WE and EtOH	Teber and Bursal, 2020 [63]
	MeOH	Mišić et al., 2015 [20]; Aras et al., 2016 [14]; Sarikurkcu et al., 2019 [5]; Petrova et al., 2022 [10]
Apigenin 7-O-(acetyl) hexuronide	MeOH	Petrova et al., 2022 [10]
Apigenin 7-O-(acetyl-caffeoyl) hexuronide	MeOH	Petrova et al., 2022 [10]
Apigenin 7-O-(caffeoyl) hexuronide	MeOH	Petrova et al., 2022 [10]
Apigenin 7-O-(feruloyl) hexuronide	MeOH	Petrova et al., 2022 [10]
Apigenin 7-O-(sinapoyl) hexuronide	MeOH	Petrova et al., 2022 [10]
Apigenin 7-O-hexoside	MeOH	Petrova et al., 2022 [10]
Apigenin 7-O-hexuronide	MeOH	Petrova et al., 2022
Apigenin 7-O-hexuronide methyl ester	MeOH	Petrova et al., 2022 [10]
Astragalin	MeOH	Mišić et al., 2015 [20]; Petrova et al., 2022 [10]
Benzoic acid methyl ester	WE and MeOH	Dienaitė et al., 2018 [27]
Benzoyl tartaric acid	MeOH	Petrova et al., 2022 [10]
Caffeic acid	WE	Hinkov et al., 2020 [103]
	WE and EtOH	Teber and Bursal, 2020 [63]
	WE and MeOH	Dienaitė et al., 2018 [27]
	MeOH	Mišić et al., 2015 [20]; Aras et al., 2016 [14]; Sarikurkcu et al., 2019 [5]; Petrova et al., 2022 [10]
Caffeic acid hexoside	MeOH	Petrova et al., 2022 [10]
Caffeic acid hexuronide	MeOH	Petrova et al., 2022 [10]
Caffeolymalic acid	WE and MeOH	Dienaitė et al., 2018 [27]
Caffeoyltartaric acid	MeOH	Petrova et al., 2022 [10]
Calcelarioside A/B	MeOH	Smiljković et al., 2018 [15]
Chlorogenic acid	WE	Hinkov et al., 2020 [103]
	WE and MeOH	Dienaitė et al., 2018 [27]
	MeOH	Mišić et al., 2015 [20]; Aras et al., 2016 [14]; Sarikurkcu et al., 2019 [5]; Petrova et al., 2022

	[10]	
Chrysin	MeOH	Mišić et al., 2015 [20]
Chrysoeriol	WE	Hinkov et al., 2020 [103]
Cinnamic acid	MeOH	Mišić et al., 2015 [20]
	WE	Hinkov et al., 2020 [103]
Cirsimaritin	WE	Hinkov et al., 2020 [103]
	MeOH	Jamzad et al., 2003 [43]; Petrova et al., 2022 [10]
Clinopodic acid A	MeOH	Petrova et al., 2022 [10]
Coumaric acid	WE and EtOH	Teber and Bursal, 2020 [63]
	MeOH	Aras et al., 2016 [14]
Dicaffeoylquinic acid	MeOH	Mišić et al., 2015 [20]
Dimetoxycinnamic acid	MeOH	Mišić et al., 2015 [20]
Ethyl caffeate	MeOH	Petrova et al., 2022 [10]
Eryodictyol	MeOH	Petrova et al., 2022 [10]
Eukovoside	MeOH	Smiljković et al., 2018 [15]
Ferulic acid	WE	Hinkov et al., 2020 [103]
	WE and MeOH	Dienaitė et al., 2018 [27]
	MeOH	Mišić et al., 2015 [20]; Sarikurkcu et al., 2019 [5]; Petrova et al., 2022 [10]
Feruloyltartaric acid	MeOH	Petrova et al., 2022 [10]
Galangin	MeOH	Mišić et al., 2015 [20]
Gallic acid	WE	Hinkov et al., 2020 [103]
	MeOH	Petrova et al., 2022 [10]
Gallic acid hexoside	MeOH	Petrova et al., 2022 [10]
Gentisic acid	MeOH	Petrova et al., 2022 [10]
Hispidulin	MeOH	Petrova et al., 2022 [10]
Hydroxybenzoic acid hexoside	MeOH	Mišić et al., 2015 [20]; Petrova et al., 2022 [10]
Isorhamnetin	MeOH	Petrova et al., 2022 [10]
Kaempferol	WE and EtOH	Teber and Bursal, 2020 [63]
	MeOH	Aras et al., 2016 [14]
Kaempferol dimethyl ether	MeOH	Mišić et al., 2015 [20]
Kaempferol monomethyl ether	MeOH	Mišić et al., 2015 [20]
Ligstroside hexoside	MeOH	Smiljković et al., 2018 [15]
Lithospermic acid A	MeOH	Smiljković et al., 2018 [15]
Luteolin	WE and MeOH	Dienaitė et al., 2018
	MeOH	Mišić et al., 2015 [20]; Aras et al., 2016 [14]
Luteolin 7-O-diglucuronide	WE and MeOH	Dienaitė et al., 2018 [27]
Luteolin 7-O-(feruloyl) hexuronide	MeOH	Petrova et al., 2022 [10]
Luteolin 7-O-hexuronide	MeOH	Petrova et al., 2022 [10]
Luteolin 7-O-(caffeoyl) hexuronide	MeOH	Petrova et al., 2022 [10]

Luteolin 7-O-(acetyl) hexuronide	MeOH	Petrova et al., 2022 [10]
Methyl rosmanirate	MeOH	Petrova et al., 2022 [10]
Methyl salvianolate	MeOH	Petrova et al., 2022 [10]
Myricetin	WE and EtOH	Teber and Bursal, 2020 [63]
Nepetoidin B	MeOH	Petrova et al., 2022 [10]
Naringenin	MeOH	Mišić et al., 2015 [20]; Petrova et al., 2022 [10]
Plantamajoside	MeOH	Smiljković et al., 2018 [15]
Plantamajoside hexoside	MeOH	Smiljković et al., 2018 [15]
Protocatechuic acid	WE and EtOH	Teber and Bursal, 2020 [63]
	WE	Hinkov et al., 2020 [103]
	MeOH	Mišić et al., 2015 [20]; Smiljković et al., 2018 [15]; Sarikurkcu et al., 2019 [5]; Petrova et al., 2022 [10]
Quercetin	WE and EtOH	Teber and Bursal, 2020 [63]
	WE	Hinkov et al., 2020 [103]
	MeOH	Mišić et al., 2015 [20]
Quercetin dimethyl ether	MeOH	Mišić et al., 2015 [20]
Quercetin trimethyl ether	MeOH	Mišić et al., 2015 [20]
Quercetin tetramethyl ether	MeOH	Mišić et al., 2015 [20]
Rhamnetin	MeOH	Aras et al., 2016 [14]
Rosmarinic acid	WE and MeOH	Dienaitė et al., 2018 [27]
	WE	Hinkov et al., 2020 [103]
	MeOH	Mišić et al., 2015 [20]; Aras et al., 2016 [14]; Smiljković et al., 2018 [15]; Petrova et al., 2022 [10]
Rutin	WE	Hinkov et al., 2020 [103]
	MeOH	Petrova et al., 2022 [10]
Salvianolic acid A	MeOH	Smiljković et al., 2018 [15]
Salvianolic acid B	MeOH	Smiljković et al., 2018 [15]
Salvianolic acid C	MeOH	Petrova et al., 2022 [10]
Syringic acid	WE and MeOH	Dienaitė et al., 2018 [27]
	MeOH	Mišić et al., 2015 [20]; Petrova et al., 2022 [10]
Syringic acid hexoside	MeOH	Mišić et al., 2015 [20]
Thymusin	MeOH	Petrova et al., 2022 [10]
Umbelliferone	WE and MeOH	Dienaitė et al., 2018 [27]
Vanillic acid	WEs	Hinkov et al., 2020 [103]
	MeOH	Mišić et al., 2015 [20]; Petrova et al., 2022 [10]
Vanillin	MeOH	Petrova et al., 2022 [10]
Xanthomicrol	MeOH	Petrova et al., 2022 [10]
Other monoterpenes		

1,8-Cineole (eucalyptol)	EO	De Pooter et al., 1987 [61]; Sarer and Konuklugil, 1996 [104]; Chalchat et al., 1998 [60]; Kökdil et al., 1998a [54]; Kobaisy et al., 2005 [8]; Malenčić et al., 2008 [105]; Alim et al., 2009 [56]; Mancini et al., 2009 [99]; Gkinis et al., 2010 [14]; Kilic et al., 2011 [55]; Bozari et al., 2013 [101]; Bozok et al., 2017 [4]; Narimani et al., 2017 [13]; Akbaba et al., 2021 [100]; Aćimović et al., 2022 [62]; Semiz et al., 2022 [106]
	MeOH	Sarikurkcü et al., 2019 [5]
Dehydro-1,8-cineole	EA	Zaharieva et al., 2023 [11]
	EO	Kobaisy et al., 2005 [8]
α-Pinene	EO	De Pooter et al., 1987 [61]; Kökdil et al., 1998a [54]; Chalchat et al., 1998 [60]; Kobaisy et al., 2005 [8]; Gkinis et al., 2010 [14]; Kilic et al., 2011 [55]; Semiz et al., 2022 [106]
Sabinene	EO	De Pooter et al., 1987 [61]; Chalchat et al., 1998 [60]; Kökdil et al., 1998a [54]; Kobaisy et al., 2005 [8]; Gkinis et al., 2010 [14]; Kilic et al., 2011 [55]; Aćimović et al., 2022 [62]
	EA	Zaharieva et al., 2023 [11]
β-Pinene	EO	De Pooter et al., 1987 [61]; Chalchat et al., 1998 [60]; Kökdil et al., 1998a [54]; Alim et al., 2009 [56]; Kilic et al., 2011 [55]; Aćimović et al., 2022 [62]; Semiz et al., 2022 [106]
	EA	Zaharieva et al., 2023 [11]
Myrcene	EO	De Pooter et al., 1987 [61]; Chalchat et al., 1998 [60]; Kökdil et al., 1998a [54]; Alim et al., 2009 [56]; Gkinis et al., 2010 [14]; Aćimović et al., 2022 [62]; Semiz et al., 2022 [106]
	EA	Zaharieva et al., 2023 [11]
Limonene	EO	De Pooter et al., 1987 [61]; Kökdil et al., 1998a [54]
	EA	Zaharieva et al., 2023 [11]
Terpineol	EO	De Pooter et al., 1987 [61]; Akbaba et al., 2021 [100]; Semiz et al., 2022 [106]
β-Ocimene	EO	Kökdil et al., 1998a [54]; Kobaisy et al., 2005 [8]; Gkinis et al., 2010 [14]; Semiz et al., 2022 [106]
	EA	Zaharieva et al., 2023 [11]
γ-Terpinene	EO	Kökdil et al., 1998a [54]; Kobaisy et al., 2005 [8]; Gkinis et al., 2010 [14]; Aćimović et al., 2022 [62]; Semiz et al., 2022 [106]
<i>p</i>-Mentha-2,4(8)-diene	EO	Kobaisy et al., 2005 [8]
Pinocarvone	EO	Kobaisy et al., 2005 [8]
Terpinen-4-ol	EO	Kökdil et al., 1998a [54]; Kobaisy et al., 2005 [8]; Semiz et al., 2022 [106]

α-Terpineol	EO	Kökdil et al., 1998a [54]; Kobaisy et al., 2005 [8]
Myrtenal	EO	Kobaisy et al., 2005 [8]; Gkinis et al., 2010 [14]; Aćimović et al., 2022 [62]
Carvone	EO	Kobaisy et al., 2005 [8]; Kökdil et al., 1998a [54]
Geraniol	EO	Kobaisy et al., 2005 [8]
α-Thujene	EO	Gkinis et al., 2010 [14]
<i>p</i>-Cymene	EO	Gkinis et al., 2010 [14]; Semiz et al., 2022 [106]
<i>cis</i>-Sabinene hydrate	EO	Gkinis et al., 2010 [14]
Terpinolene	EO	Gkinis et al., 2010 [14]
Linalool	EO	Kökdil et al., 1998a [54]; Gkinis et al., 2010 [14]; Akbaba et al., 2021 [100]; Semiz et al., 2022 [106]
Pinocarveol	EO	Kökdil et al., 1998a [54]
Pulegone	EO	Handjieva et al., 1996 [57]; Mancini et al., 2009 [99]; Narimani et al., 2017 [13]
Camphene	EO	Kilic et al., 2011 [55]; Alim et al., 2009 [56]
Camphor	EO	Kilic et al., 2011 [55]; Semiz et al., 2022 [106]
Borneol	EO	Kilic et al., 2011 [55]; Semiz et al., 2022 [106]
Tricyclene	EO	Semiz et al., 2022 [106]
3-Carene	EO	Semiz et al., 2022 [106]
<i>Sesquiterpenes</i>		
β-Caryophyllene	EO	De Pooter et al., 1987 [61]; Handjieva et al., 1996 [57]; Kökdil et al., 1998a [54]; Kobaisy et al., 2005 [8]; Malenčić et al., 2008 [105]; Gkinis et al., 2010 [14]; Bozari et al., 2013 [101]; Akbaba et al., 2021 [100]
14-Hydroxy-9-<i>epi</i>-(E)- caryophyllene	EO	Gkinis et al., 2010 [14]
14-Hydroxy-δ-cadinene	EO	Kobaisy et al., 2005 [8]
14-Oxy-α-muurolene	EO	Kobaisy et al., 2005 [8]
Allo-aromadendrene	EO	Kökdil et al., 1998a [54]; Kobaisy et al., 2005 [8]
Aromadendrene	EO	Kökdil et al., 1998a [54]; Gkinis et al., 2010 [14]; Bozari et al., 2013 [101]
Bicyclogermacrene	EO	Kobaisy et al., 2005 [8]; Bozari et al., 2013 [101]
	EA	Zaharieva et al., 2023 [11]
Cadinene	EO	De Pooter et al., 1987 [61]; Kökdil et al., 1998a [54]; Gkinis et al., 2010 [14]; Bozari et al., 2013 [101]; Aćimović et al., 2022 [62]
Caryophyllene	EO	Bozari et al., 2013 [101]
	EA	Zaharieva et al., 2023 [11]
Caryophyllene oxide	EO	De Pooter et al., 1987 [61]; Sarer and Konuklugil, 1996 [104]; Chalchat et al., 1998 [60]; Gkinis et al., 2010 [14]; Bozok et al., 2017 [4]; Narimani et al., 2017 [13]; Akbaba et al., 2021 [100]; Aćimović et al., 2022 [62]; Semiz et al., 2022 [106]
Cedr-8-(15)-en-9-α-ol	EO	Kobaisy et al., 2005 [8]
Cedrol	EO	Kobaisy et al., 2005 [8]

<i>cis</i> -Calamenen-10-ol	EO	Gkinis et al., 2010 [14]
<i>cis</i> -murola-4(14),5-diene	EO	Kobaisy et al., 2005 [8]
Copaene	EO	De Pooter et al., 1987 [61]; Kökdil et al., 1998a [54]; Bozari et al., 2013 [101]
Cubenol	EO	Bozari et al., 2013 [101]
Elemol	EO	Kökdil et al., 1998a [54]; Gkinis et al., 2010 [14]; Bozari et al., 2013 [101]; Gormez et al., 2013 [6]; Narimani et al., 2017 [13]; Akbaba et al., 2021 [100]
Epi- α -muurolol	EO	Kobaisy et al., 2005 [8]
Farnesol	EO	Kökdil et al., 1998a [54]; Semiz et al., 2022 [106]
Geijerene	MeOH	Sarikurkcü et al., 2019 [5]
Germacrene	EO	Bozari et al., 2013 [101]
Germacrene-D	EO	De Pooter et al., 1987 [61]; Chalchat et al., 1998 [60]; Kökdil et al., 1998a [54]; Kobaisy et al., 2005 [8]; Malenčić et al., 2008 [105]; Alim et al., 2009 [56]; Gkinis et al., 2010 [14]; Kilic et al., 2011 [55]; Bozok et al., 2017 [4]; Narimani et al., 2017 [13]; Akbaba et al., 2021 [100]; Aćimović et al., 2022 [62]; Semiz et al., 2022 [106]
	EA	Zaharieva et al., 2023 [11]
Globulol	EO	Kökdil et al., 1998a [54]
Hinesol acetate	EO	Kobaisy et al., 2005 [8]
Humulene	EA	Zaharieva et al., 2023 [11]
Humulene epoxide II	EO	Kobaisy et al., 2005 [8]; Gkinis et al., 2010 [14]
Humulene oxide	EO	Kökdil et al., 1998a [54]
Iso-longifolol	EO	Kobaisy et al., 2005 [8]
Khusinol	EO	Kobaisy et al., 2005 [8]
Ledol	EO	Kökdil et al., 1998a [54]
Longifolene	EO	Kobaisy et al., 2005 [8]
Nerolidol	EO	Sarer and Konuklugil, 1996 [104]
Oplopanone	EO	Kobaisy et al., 2005 [8]
Palustrol	EO	Akbaba et al., 2021 [100]
Sesquiphellandrene	EO	Handjieva et al., 1996; Gkinis et al., 2010
Spathulenol	EO	Sarer and Konuklugil, 1996 [104]; Chalchat et al., 1998 [60]; Kökdil et al., 1998a [54]; Kobaisy et al., 2005 [8]; Malenčić et al., 2008 [105]; Mancini et al., 2009 [99]; Bozari et al., 2013 [101]; Gormez et al., 2013 [6]; Narimani et al., 2017 [13]; Akbaba et al., 2021 [100]
T-Cadinol	EO	Kökdil et al., 1998a [54]
<i>trans</i> -Caryophyllene	EO	Sarer and Konuklugil, 1996 [104]; Chalchat et al., 1998 [60]; Alim et al., 2009 [56]; Kilic et al., 2011 [55]; Gormez et al., 2013 [6]; Bozok et al., 2017 [4]; Narimani et al., 2017 [13]; Aćimović et al.,

2022 [62]		
Valerianol	EO	Kobaisy et al., 2005 [8]
Viridiflorol	EO	Kökdil et al., 1998a [54]
α-Cadinol	EO	Kökdil et al., 1998a [54]; Akbaba et al., 2021 [100]
α-Calacorene	EO	Gkinis et al., 2010 [14]
α-Copaene-11-ol	EO	Kökdil et al., 1998a [54]
α-Copaene-8-ol	EO	Kökdil et al., 1998a [54]
α-Gurjunene	EA	Zaharieva et al., 2023 [11]
α-Humulene	EO	Chalchat et al., 1998 [60]; Kökdil et al., 1998a [54]; Alim et al., 2009 [56]; Mancini et al., 2009 [99]; Gkinis et al., 2010 [14]; Bozari et al., 2013 [101]; Narimani et al., 2017 [13]; Semiz et al., 2022 [106]
α-Muurolene	EO	Kobaisy et al., 2005 [8]
α-neo-Clovene	EO	Kobaisy et al., 2005 [8]
β-Acoradienol	EO	Kobaisy et al., 2005 [8]
β-Bisabolene	EO	Handjieva et al., 1996 [57]; Chalchat et al., 1998 [60]; Kobaisy et al., 2005 [8]; Mancini et al., 2009 [99]; Gkinis et al., 2010 [14]; Bozok et al., 2017 [4]; Akbaba et al., 2021 [100]
β-Bourbonene	EO	De Pooter et al., 1987 [61]; Gkinis et al., 2010 [14]; Bozari et al., 2013 [101]; Aćimović et al., 2022 [62]; Semiz et al., 2022 [106]
	EA	Zaharieva et al., 2023 [11]
β-Caryophyllene oxide	EO	Kökdil et al., 1998a [54]; Kobaisy et al., 2005 [8]; Handjieva et al., 1996 [57]
β-Copaene	EA	Zaharieva et al., 2023 [11]
β-Elemene	EO	De Pooter et al., 1987 [61]; Kökdil et al., 1998a [54]; Bozari et al., 2013 [101]; Aćimović et al., 2022 [62]; Semiz et al., 2022 [106]
	EA	Zaharieva et al., 2023 [11]
β-Eudesmol	EO	Kökdil et al., 1998a [54]
β-Farnesene	EO	De Pooter et al., 1987 [61]; Handjieva et al., 1996 [57]; Kökdil et al., 1998a [54]; Gkinis et al., 2010 [14]; Semiz et al., 2022 [106]
β-Gurjunene	EO	Kobaisy et al., 2005 [8]; Gkinis et al., 2010 [14]; Bozari et al., 2013 [101]
β-Sesquiphellandrene	EO	Kökdil et al., 1998a [54]
γ-Muurolene	EO	Kobaisy et al., 2005 [8]

EA – ethyl acetate; EO - essential oil; HE – hexane extract; AE acetone extract; MeOH – methanolic extract, EtOH – ethanol extract; WE – water extract.

Table S2. Peak areas of compounds identified using QToF MS in eleven different *Nepeta nuda* leaf extracts.

No	Compound name	Selište	Brodica	Debeli Lug	Rtanj	Straža	Vinatovača	Vlasina	Donji Krivodol	Janjska reka	Židilje	Gornje Selo
<i>Hydroxybenzoic acid derivatives</i>												
1	Galloyl hexoside	68827419	49816429	79828266	73984855	78642392	67790250	1025496	96043299	151584704	9944625	116560317
2	Gallic acid	NF	NF	NF	666419	641442	NF	NF	861967	NF	NF	347965
3	Dihydroxybenzoic acid	NF	NF	NF	NF	NF	NF	NF	2981235	1582865	NF	NF
4	Dihydroxybenzoic acid hexoside	63411934	49721319	25869910	66379401	49791202	38673114	35114408	73940725	95890976	83266823	50583519
5	Vanillic acid hexoside	5096132	9828399	3759343	4750432	8596501	2703691	6793888	15344418	14002208	16205044	9491045
6	Hydroxybenzoic acid	24508576	79935361	7886827	14440272	19071606	8408490	56529193	37886718	14715451	102528578	7924664
7	Dihydroxybenzoic acid hexoside isomer	12954831	NF	NF	12132645	6527028	6661118	NF	4129682	4820412	25901016	NF
8	Dihydroxybenzoic acid isomer	19658394	4064622	12551063	13480677	17322582	7576350	841385	10869299	6196600	14342630	4484404
9	Vanillic acid	NF	NF	NF	NF	NF	NF	NF	NF	NF	27164940	NF
10	Hydroxybenzoic acid hexoside	33194428	14106799	21334299	33791934	17046752	29033835	14280943	10419373	9936991	45087692	16336170
<i>Hydroxycinnamic acid derivatives</i>												
11	Syringic acid hexoside	29706413	33543218	8696094	5630572	12505794	11710762	NF	40657590	13074155	11966385	8047841
12	Caffeoyltartaric acid	40785804	NF	NF	16568466	3612252	14081695	3554261	15876633	10361020	10008515	8970271
13	Caffeoyltartronic acid	53416241	209866014	39981858	43287883	44433410	70356425	35580171	19515495	152252095	37020720	80246154
14	Caffeic acid hexoside	NF	NF	NF	NF	NF	NF	5539026	16505840	8484834	6743288	7775625
15	Caffeoylglycolic acid	58168302	141123128	31016355	85825889	91553739	87743135	28306582	33705890	114860323	44433768	121946874
16	Umbelliferone	59483038	80804701	59597102	55754706	59831867	86395479	48349032	39080170	141986798	53406341	110779397
17	Caffeoyltartronic acid isomer	161398227	184313820	126013508	166047694	160487978	191467841	119735953	117874185	245135613	151786278	182440956
18	Sinapic acid	5140121	1035830	6546941	11896636	2309679	10746993	NF	NF	3996981	NF	1338253
19	Caffeic acid hexoside isomer	NF	9274609	6363094	7692410	9580335	7946026	1878689	11355444	10668173	4505813	11061228
20	Dihydrocaffeic acid hexoside	3754961	5503630	4004414	4348926	6040352	3410555	1821104	5120358	3581450	3146137	2646418
21	Caffeic acid	22634446	24737043	16377622	16146058	20981301	17556206	NF	34342711	20628972	NF	6202734
22	Feruloyltartaric acid	33093009	NF	NF	24356075	NF	NF	3583088	47545873	5842950	3431502	NF
23	Ethyl caffeate	114910260	64749527	60921967	100382768	61146940	63604577	77670595	88896805	98859092	54107105	110553041

24	Caffeoylmalic acid	210267762	164098824	111186310	380481585	151365388	144450892	152314740	211795201	199124003	148005607	161803742
25	Feruloylmalic acid	27143201	15653101	21628843	21992137	9499374	12330849	9446397	49854724	30176239	10983446	10567449
26	Rosmarinic acid	97839486	107208254	82019387	79263330	107171359	97070097	NF	89021322	110638581	62039338	104245548
27	Ferulic acid	13367694	10490861	8399330	11715530	14443554	18751777	7515372	9589311	18913418	13435876	10183613
28	Clinopodic acid A	NF	NF	NF	NF	NF	NF	NF	NF	NF	NF	16306924
29	Nepetoidin A or B	NF	NF	NF	NF	10052962	NF	NF	8961568	33059163	34868387	NF
<i>Iridoid glycosides</i>												
30	Aucubin	3019416	2689171	5338978	3019459	3255214	4637743	3064093	4435849	6832249	3845968	3279941
31	6 α -Hydroxyadoxoside	19484203	13488419	6568908	14283131	36467093	6616257	31729833	13479475	11468254	5977208	40606265
32	Nepetanudoside C + HCOOH	5537833	11181290	29067501	15046558	19400049	8908500	8230991	7942952	15183005	18881823	5862898
33	5-Deoxylamiol	19593137	24494721	24957926	9936655	50436747	40817816	20464364	NF	20122951	23185789	15044820
34	1,5,9- <i>epi</i> -Deoxyloganic acid hexoside + HCOOH	9912956	7771022	6748864	2582677	24392436	10354180	6756417	10481429	18632018	14873179	5864643
35	Nepetanudoside A + HCOOH	219831446	204795379	173077488	115271002	NF	146761959	209497923	205541731	205357373	188145894	275430921
36	1,5,9- <i>epi</i> -Deoxyloganic acid	111955667	76169497	73617210	79031859	97131270	154857663	90398682	20053831	62831952	90858335	49198745
37	Nepetaside	3395628	16623346	3363498	4191534	2848206	3619512	14428017	NF	3689419	7953326	6265567
38	6-Deoxylamioside	5048880	5256522	3966211	2575392	3486690	4906205	6195053	6237366	7057259	5113908	5518474
<i>Iridoid aglycones</i>												
39	Genipin	8865495	NF	NF	NF	NF	NF	NF	6460335	NF	NF	12899143
40	5,9-Dehydronepetalactone	8058755	NF	7486301	3472251	21689929	17255035	7265040	4539049	7807331	11149421	4756406
41	Nepetaside aglycone acetate	54099027	70435147	52541529	62745360	63223568	63927228	59681311	NF	46338721	73924859	75690546
42	Loganetin	88517703	91295588	81247238	98334527	NF	65664042	107839654	100917123	100705964	84788881	102136704
43	Deoxygeniposide aglycone	77828214	86499150	67312571	52223239	NF	60143136	78194774	114290918	126285108	13720293	85576134
44	Nepetalactol	23303592	16502440	NF	13825490	18481582	NF	18522741	17091497	22562544	17815600	NF
45	7-Deoxyloganetic acid	121019548	75925978	96813941	72097502	118181110	127088860	102196575	10291008	53206251	93304101	38923416
46	Nepetaracemoside B aglycone	64747741	50298886	67645008	43946505	64888731	82791929	59128004	NF	27033511	47448657	14968975
47	Nepetalactone	5081237	NF	NF	4366095	NF	2247981	6294609	NF	NF	NF	NF
48	De-4-methylnepetalactol	3092473	1868459	1448789	2858439	NF	NF	3749565	2492500	2404847	NF	2805553

49	7-Deoxyloganetin	NF	864478	NF	NF	NF	NF	NF	NF	NF	NF	NF
50	Nepetalic acid	2105121	963989	583051	990798	922668	2013698	1930162	631680	1514519	1196966	736319
51	Dihydronepetalactone	NF	5142957	NF	NF	NF	NF	NF	NF	2283601	NF	NF
52	Nepetalactone	NF	NF	NF	1456878	NF	NF	1899632	NF	1877026	NF	940246
53	Nepetalactol acetate	5085035	9415261	4807244	NF	5041691	NF	NF	8031114	NF	NF	5300142
54	Nepetalactone	5706798	NF	NF	NF	NF	26674714	NF	NF	NF	NF	2164527
<i>Flavonoid glycosides</i>												
55	Luteolin 7-O-(6"-hexosyl)-hexuronide	NF	5728957	NF	2777467	5683670	3079868	4487511	12142195	10280978	5619287	10176381
56	Luteolin 7-O-(2"-hexuronyl)-hexuronide	8378788	NF	8584864	15804190	NF	12241555	NF	12683796	NF	NF	NF
<i>Flavonoid aglycones</i>												
57	Thymusin	NF	NF	7723680	15217674	NF	7261445	NF	12273791	NF	12590588	3187246
58	Chrysoeriol	NF	NF	NF	NF	NF	11940081	NF	6419231	NF	NF	NF
59	Cirsimaritin	32215074	NF	41417833	28527724	36441038	58175168	16470535	74323702	10551524	59829445	11404089
60	Xanthomicrol	27315930	11283766	6945961	45626248	22559361	19578337	3689246	9379672	6387221	17857379	10261790
61	Acacetin	NF	NF	NF	NF	NF	21219670	NF	13980521	NF	13393970	NF
62	Salvigenin	259848289	113593466	140176896	149531432	180503029	239060447	140641534	133228890	122340436	199990146	137798708
<i>Other metabolites</i>												
63	Quinic acid	12638782	4345002	13867590	NF	2850656	10717683	80343463	6945857	5026079	31408322	1630708
64	3-(3,4-Dihydroxyphenyl)-lactic acid	18023840	11383440	14114567	6543041	11255499	13742909	NF	33485089	39092982	3953959	24653454
65	Hexenyl-pentosyl-hexoside	2796589	NF	NF	10831451	51545148	16230725	3855288	NF	NF	11880396	NF
66	Schizonepetin	8357111	7781772	6585958	NF	18590582	13967535	NF	3827262	6279403	9249708	NF
67	12-O-Hexosyl-jasmonate	78592256	79622350	68539143	81204375	91302772	92381522	88577591	49740313	62038918	75626213	80306694
68	Schizonepetin isomer	3875462	11557505	NF	4558663	3929896	4118665	4519467	NF	NF	NF	NF
69	2,5-Dimethyl-hexanedioic acid	18571094	10480083	17055171	18451911	16860753	11191572	16007140	15367235	15494307	11849984	21912657
70	2-Carboxy-3-methyl-cyclopentaneacetic acid	NF	1173303	NF	890418	1392178	2307865	NF	978045	1084270	828665	1011595
71	Argolic acid A rhamnoside	19652507	9266785	14805373	16841551	13887886	16895772	19891487	8523679	9101520	11879339	14577691
72	2-Carboxy- α ,3-dimethyl-cyclopentaneacetic acid	4100956	1446551	3165395	3718776	2754972	2575205	3048148	1869599	1989732	1722892	2199813

73	9-Oxononanoic acid	NF	48791557	61090022	60535187	36035201	77607432	67750156	71017852	62100259	44586670	77357382
74	2-Carboxy-3-methyl- cyclopentaneacetic acid isomer	NF	NF	8705348	9371719	12861977	9242889	9384400	6824961	10857976	10881622	9528147
75	Argolic acid A	14895035	11225966	12679788	14442303	15948198	14134338	10740518	8651484	9957215	NF	14439798
76	Argolic acid A methyl ether rhamnoside	49438884	23945371	10207828	15343403	13304173	14361581	10788595	5777299	10869489	14588601	12447571
77	Nepetonic acid	47887031	46455500	49155212	45408988	29125191	58594330	51375418	53182891	47908818	34023140	59445119
78	2-Carboxy- α ,3-dimethyl- cyclopentaneacetic acid dimethyl ester	328977	6316302	NF	NF	NF	NF	NF	NF	NF	NF	4917518

NF – not found.

Table S3. Validation parameters of the SRM method of the UHPLC/DAD/(±)HESI-MS² for the quantification of targeted compounds.

<i>t_R</i> , min	Compounds	Ionisation mode	Molecular ion, <i>m/z</i>	MS/MS fragments, <i>m/z</i> (Collision energy, <i>eV</i>)	<i>R</i> ²	LOD, mg/L	LOQ, mg/L	Regression equation, Y = A + B*X	DAD spectra λ _{max} (nm)
1.64	Chlorogenic acid	[M - H] ⁻	353	191 (25)	0.9999	0.01	0.04	Y = 48951 + 721*X	230, 330
2.65	Caffeic acid	[M - H] ⁻	179	135 (18); 107 (18)	0.9972	0.53	1.78	Y = - 199.31 + 265.22*X	230, 330
3.43	Loganin	[M + HCOOH - H] ⁻	435	227 (20), 124 (20)	0.9999	0.13	0.45	Y = 5785 + 101*X	220
4.22	Rutin	[M - H] ⁻	609	301 (32); 271 (58)	0.9994	0.14	0.48	Y = 2700 + 167*X	270, 300, 340
4.26	Rosmarinic acid	[M - H] ⁻	359	161 (30), 133 (30)	0.9937	0.09	0.31	Y = 4778 + 1322470*X	240, 330
5.12	Astragalin	[M - H] ⁻	447	284 (29); 255 (43)	0.9976	0.30	1.00	Y = 26211 + 476*X	270, 360
5.52	1,5,9- <i>epi</i> -Deoxyloganic acid	[M + HCOOH - H] ⁻	405	359 (20), 197 (20)	0.9983	1.00	3.32	Y = 106225 + 967*X	240
5.70	Luteolin	[M - H] ⁻	285	175 (27); 134 (36)	0.9956	0.65	2.16	Y = 698354 + 4565410*X	260, 360
6.07	Apigenin	[M - H] ⁻	269	225 (23); 151 (26)	0.9911	0.65	2.16	Y = 35609 + 1488540*X	270, 360
6.20	Isorhamnetin	[M - H] ⁻	315	300 (30); 151 (25)	0.9978	0.07	0.25	Y = - 7297 + 300*X	280, 330
6.35	5,9-Dehydronepetalactone	[M + H] ⁺	165	149 (10), 77 (10)	0.9967	1.42	4.75	Y = - 1009.05 + 1.26*X	300
7.60	<i>cis,trans</i> -Nepetalactone	[M + H] ⁺	167	111 (10), 77 (10)	0.9948	0.54	1.81	Y = - 4261.36 + 17.13*X	220

LOD – limit of detection; LOQ – limit of quantification; *t_R* – retention time.

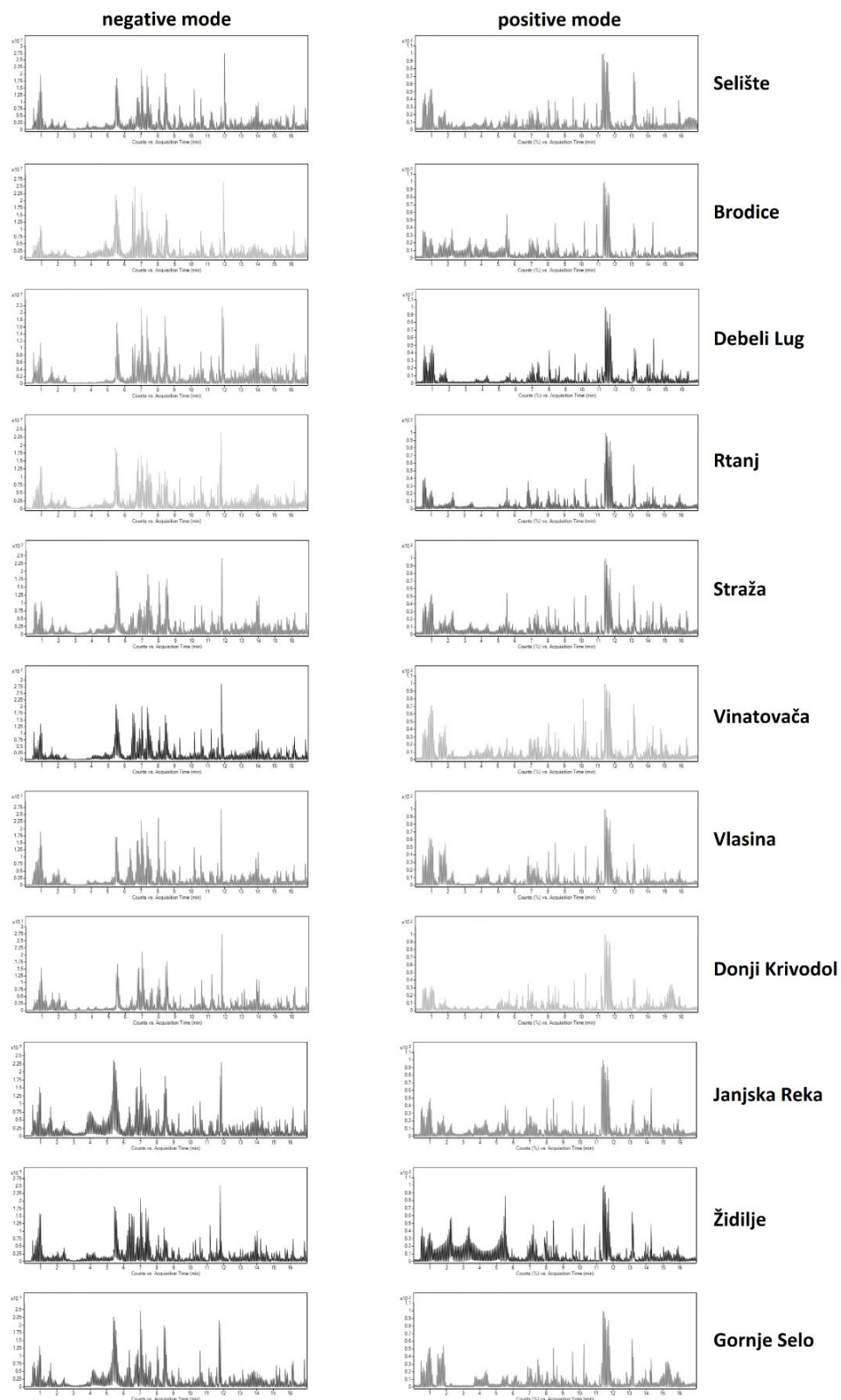


Figure S1. Base peak chromatograms, in negative and positive ionization modes, of eleven different *Nepeta nuda* leaf extracts; for peak annotation see retention times in Table 1 and peak areas from Table S2.

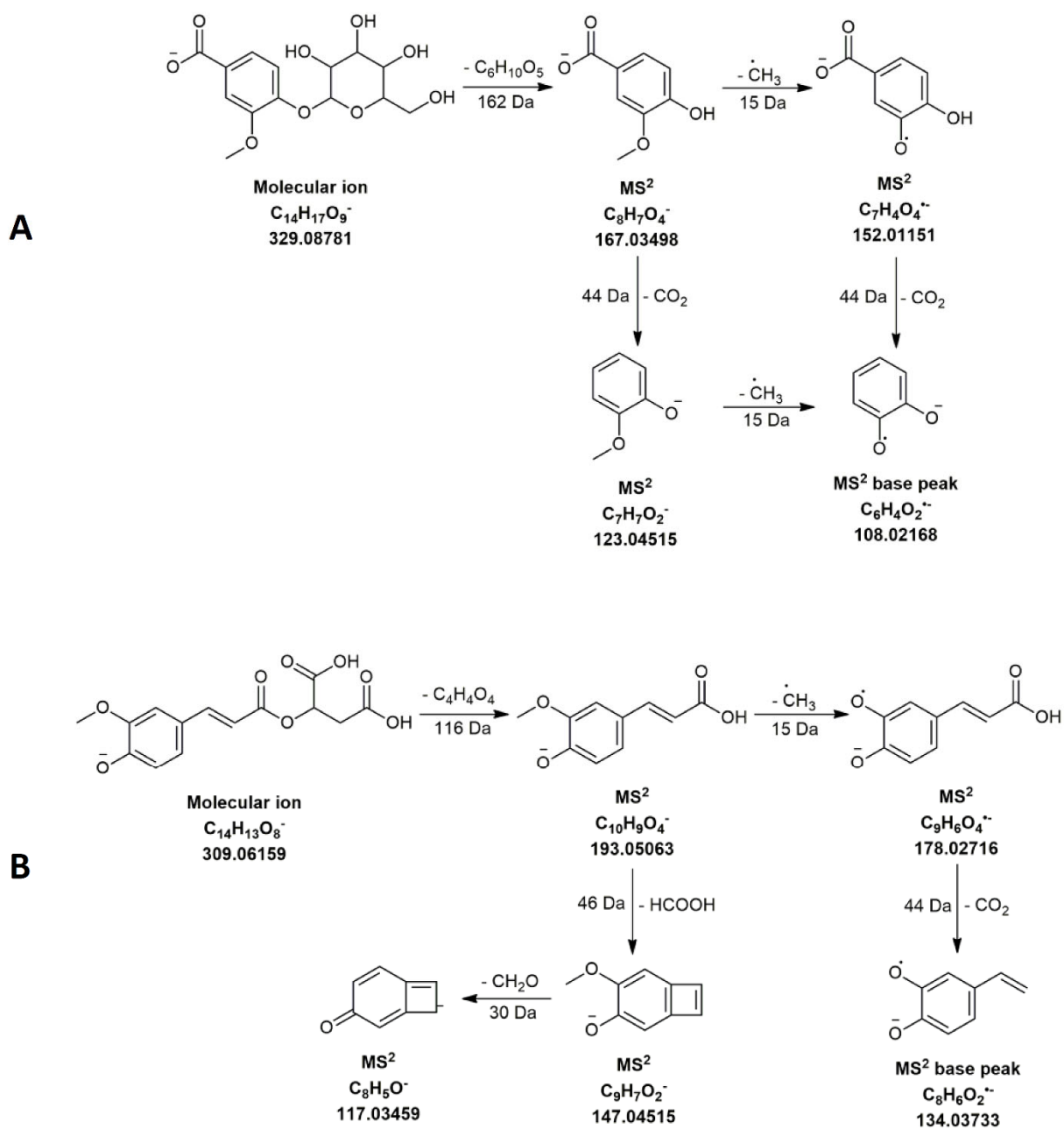


Figure S2. A proposed fragmentation pathway of (A) compound **5** (vanillic acid hexoside) and (B) compound **25** (feruloylmalic acid).

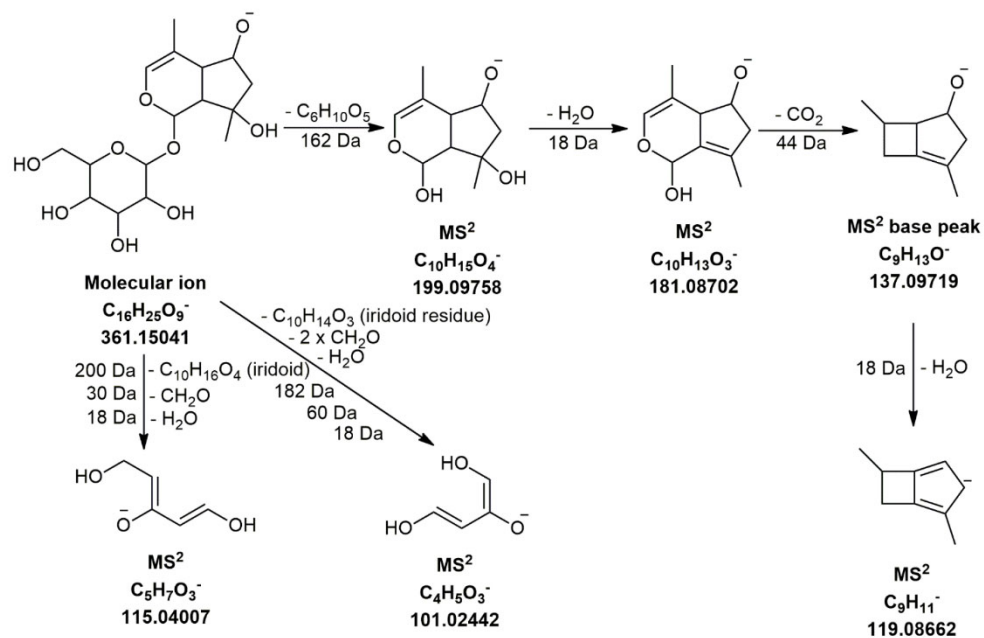


Figure S3. A proposed fragmentation pathway of compound 33 (5-deoxylamiol).

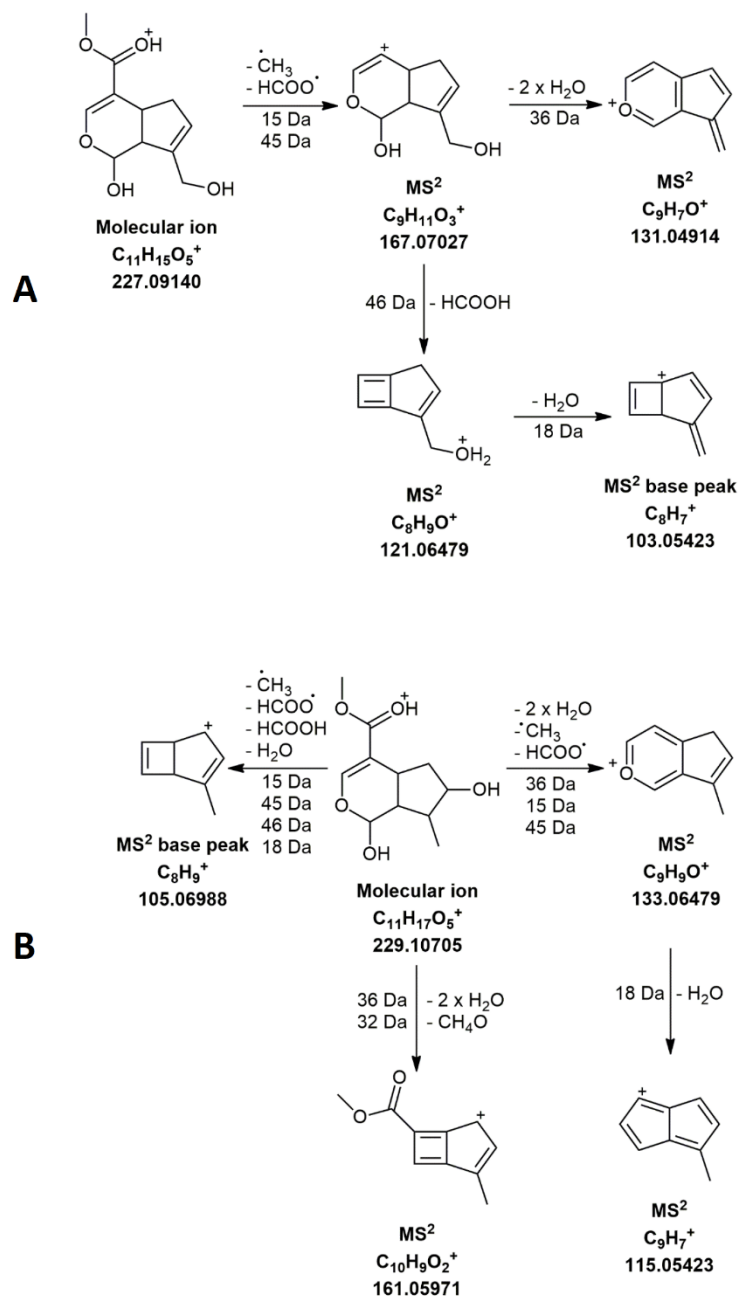


Figure S4. A proposed fragmentation pathway of **(A)** compound 39 (genipin) and **(B)** compound 42 (loganetin).

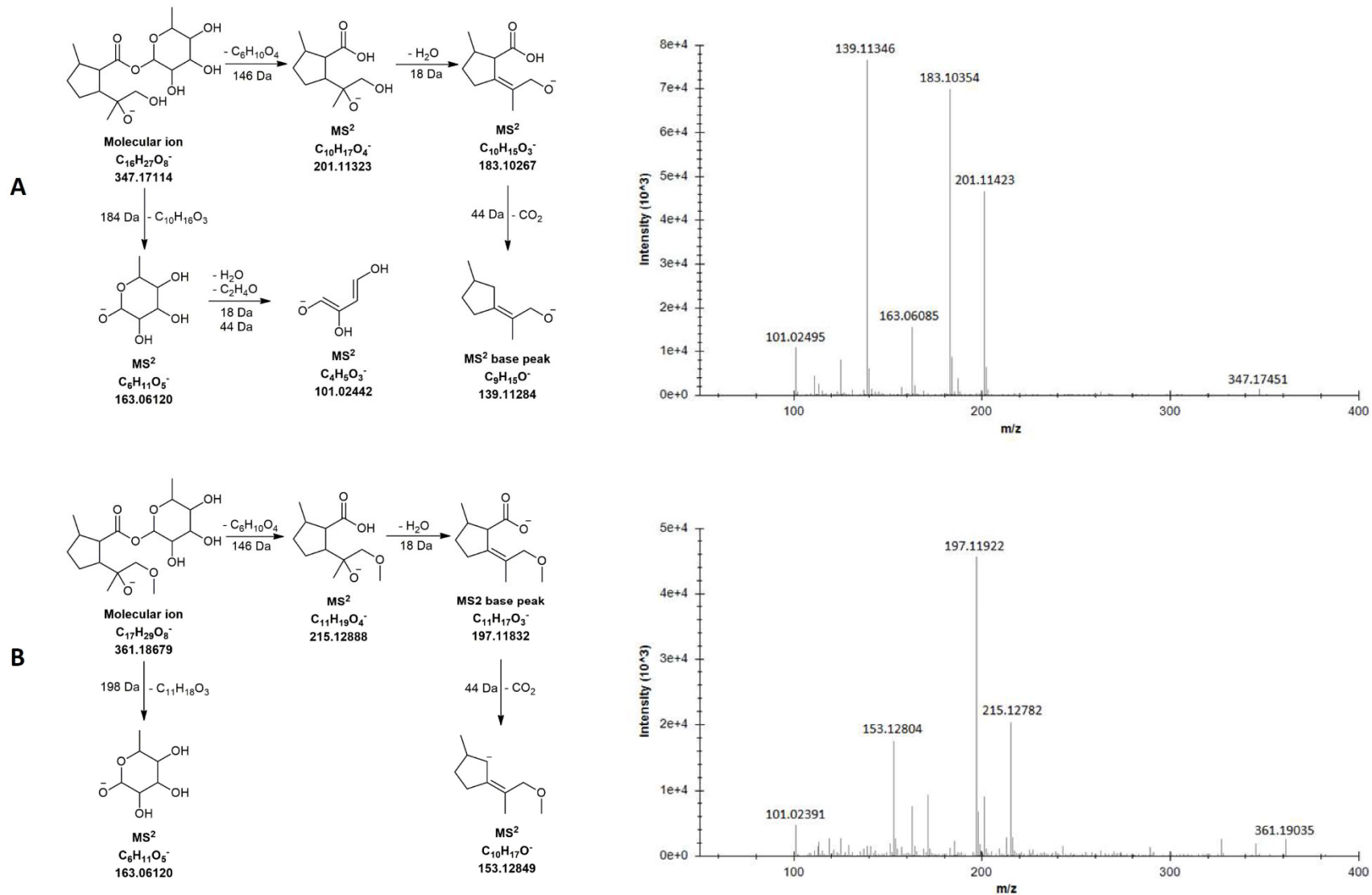


Figure S5. A proposed fragmentation pathway and MS² spectra of **(A)** compound 71 (argolic acid A rhamnoside) and **(B)** compound 76 (argolic acid A methyl ether rhamnoside).