horticulturae

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Supplementary Materials

Phenolic Profiles of Six Unexplored Asteraceae Species from Asia: Comparison of Wild and Cultivated Plants

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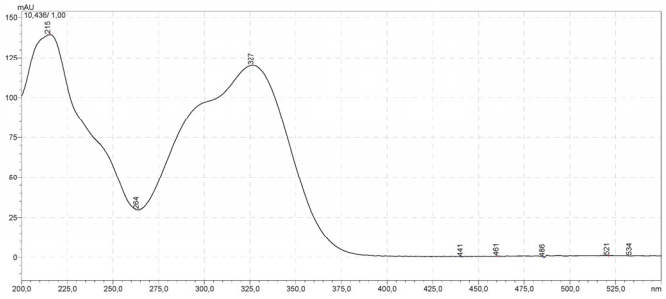
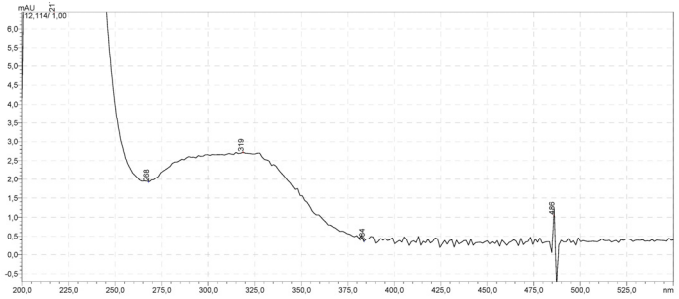
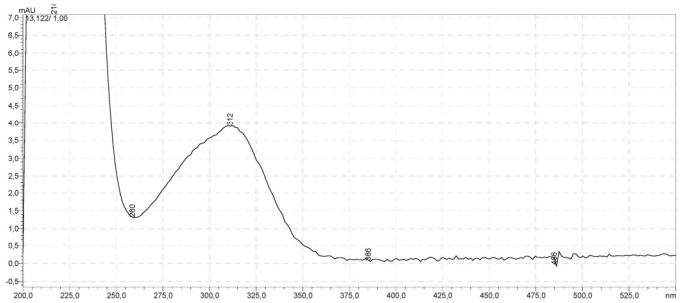
Supplementary content



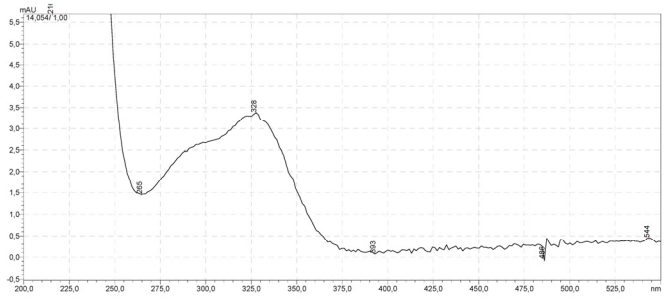
Caffeoyl-quinic acids, *trans*-; dicaffeoyl-quinic acids



Caffeoyl-quinic acids, *cis*-



p-Coumaroyl-quinic acids



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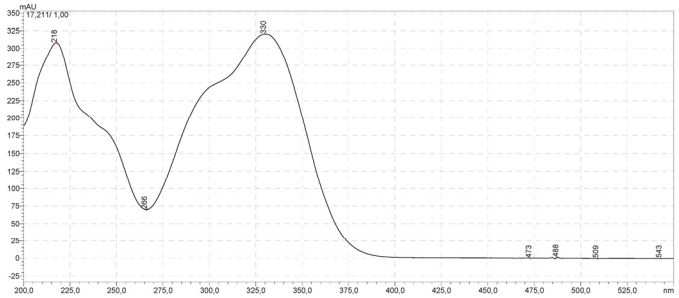
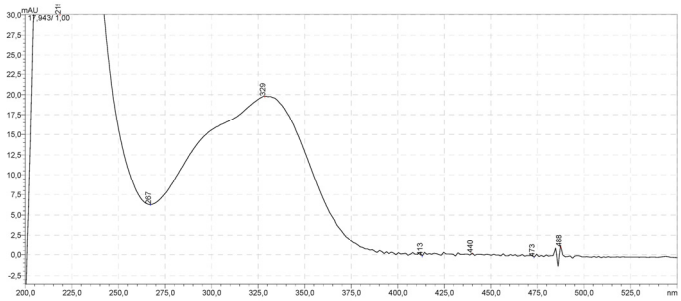
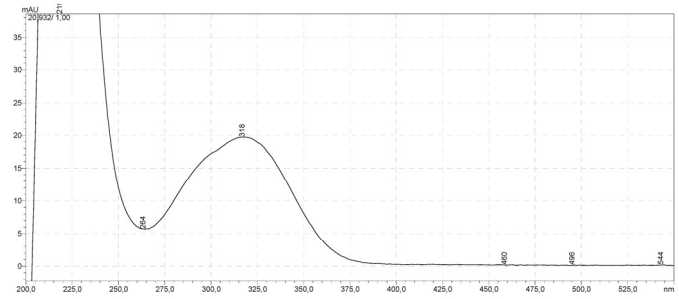


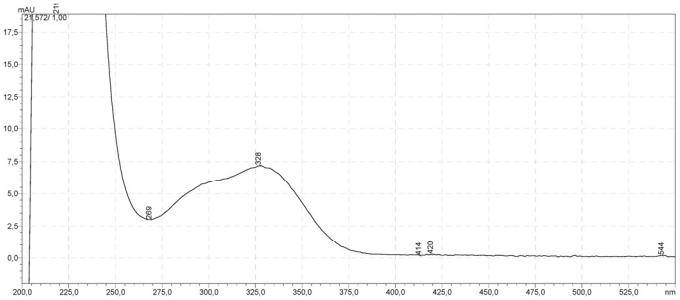
Cichoric acid, *trans*,*trans*-; caftaric acid



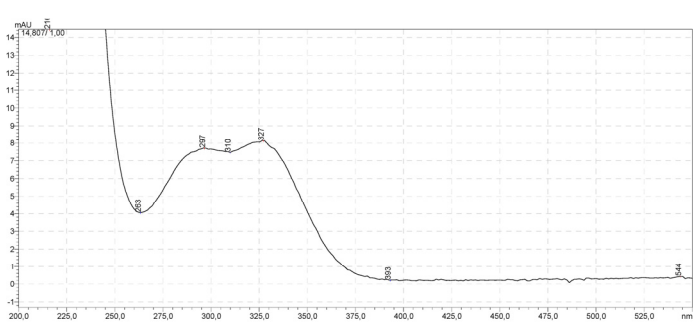
Cichoric acid, *cis*,*trans*-



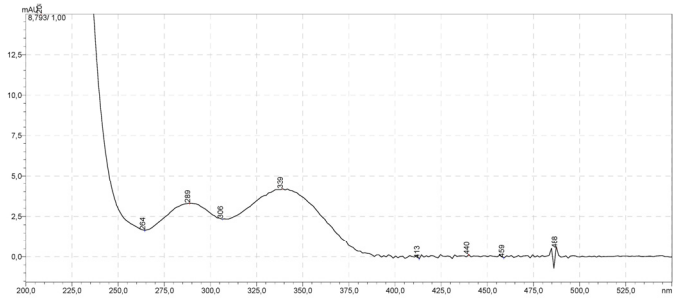
p-Coumaroyl-caffeoyl-tartaric acid



Feruloyl-caffeoyl-tartaric acid

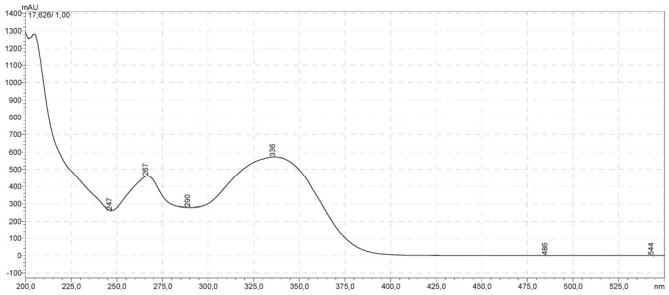


Vanilloyl quinic acids, divanilloyl quinic acids

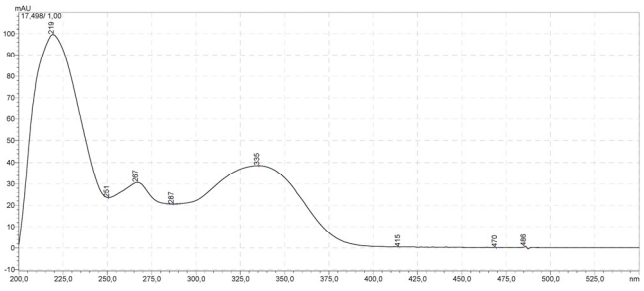


Cichoriin

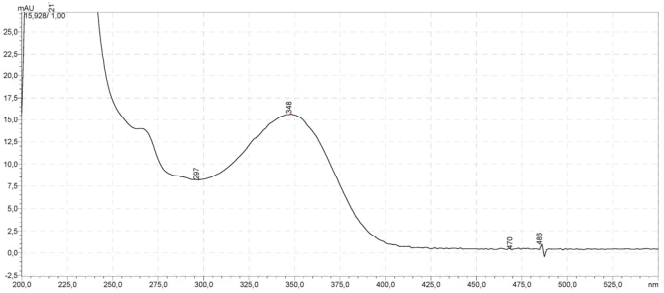
Figure S1. Typical UV spectra of the basic phenolic compounds found in six Asteraceae species.



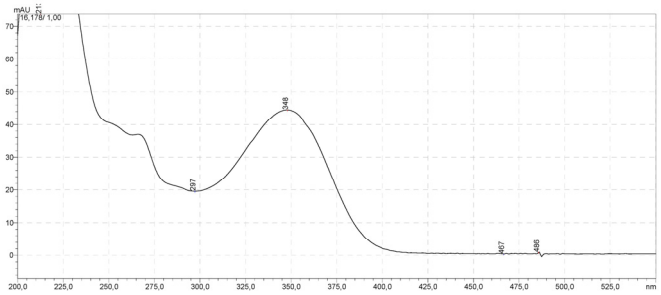
Apigenin 7-*O*-glycosides



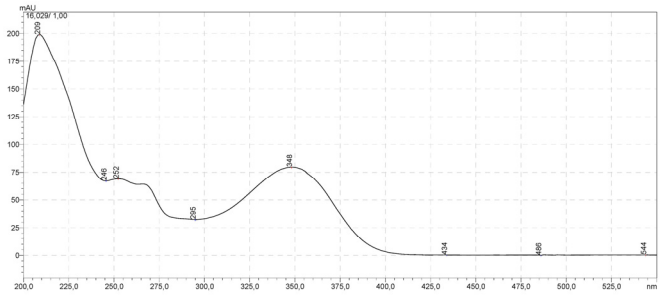
Acacetin/pectolinarigenin 7-*O*-glycosides



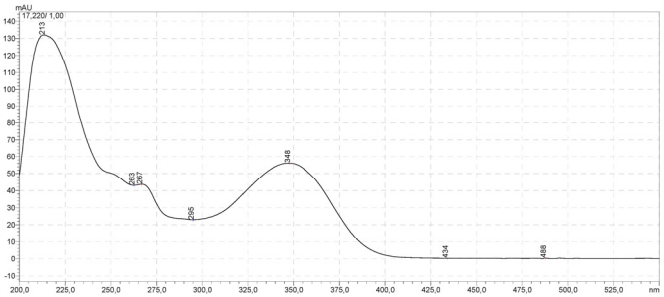
Luteolin 7-*O*-glycosides



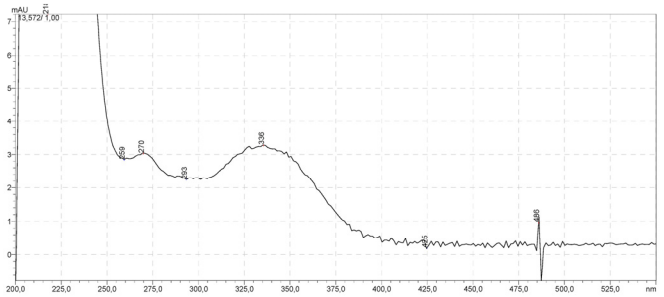
Chrysoeriol 7-*O*-glycosides



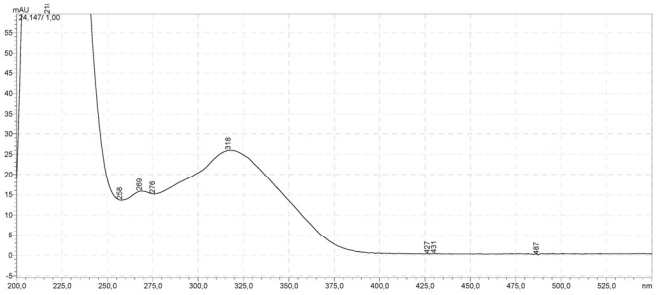
Luteolin 7-O-(2″-*O*-(6‴-*O*-acetyl)-glucosyl)-glucoside



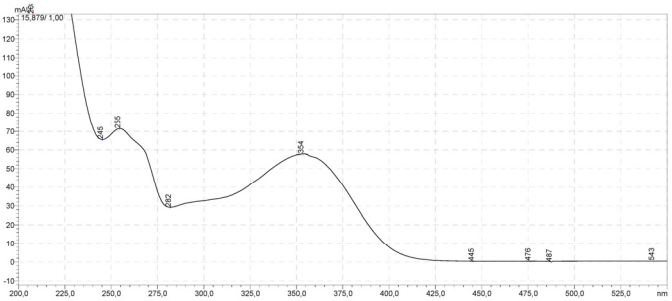
Chrysoeriol 7-O-(2″-*O*-(6‴-*O*-acetyl)-glucosyl)-glucoside



Schaftoside

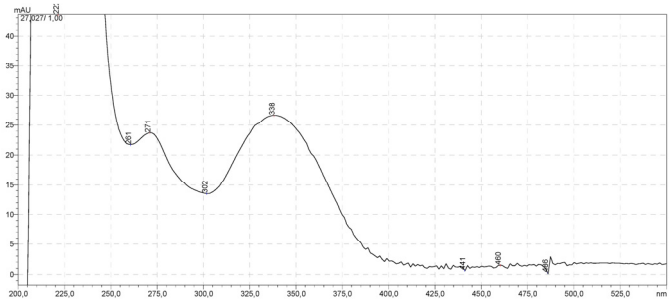


Echitin, echinacin

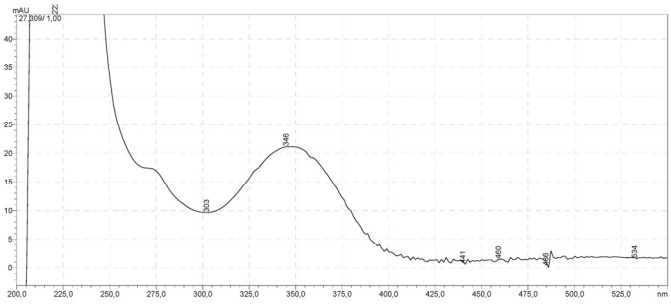


Quercetin/isorhamnetin 3-*O*-glycosides

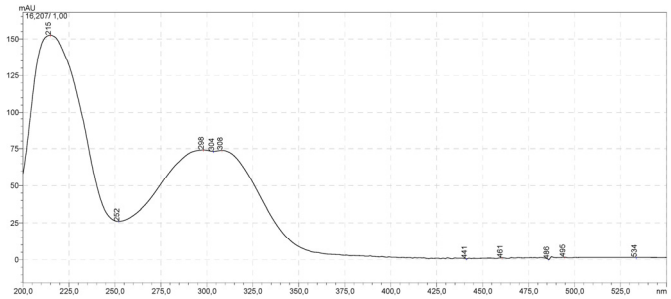
Figure S1. *Continuation*.



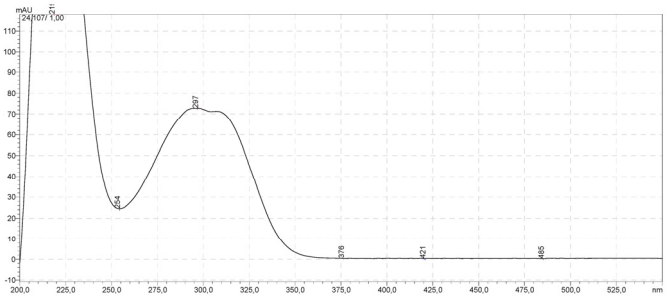
Cirsiliol



Chrysosplenetin



Tri-*p*-coumaroyl spermines / spermidines



Tetra-*p*-coumaroyl spermines

Figure S1. *Continuation*.

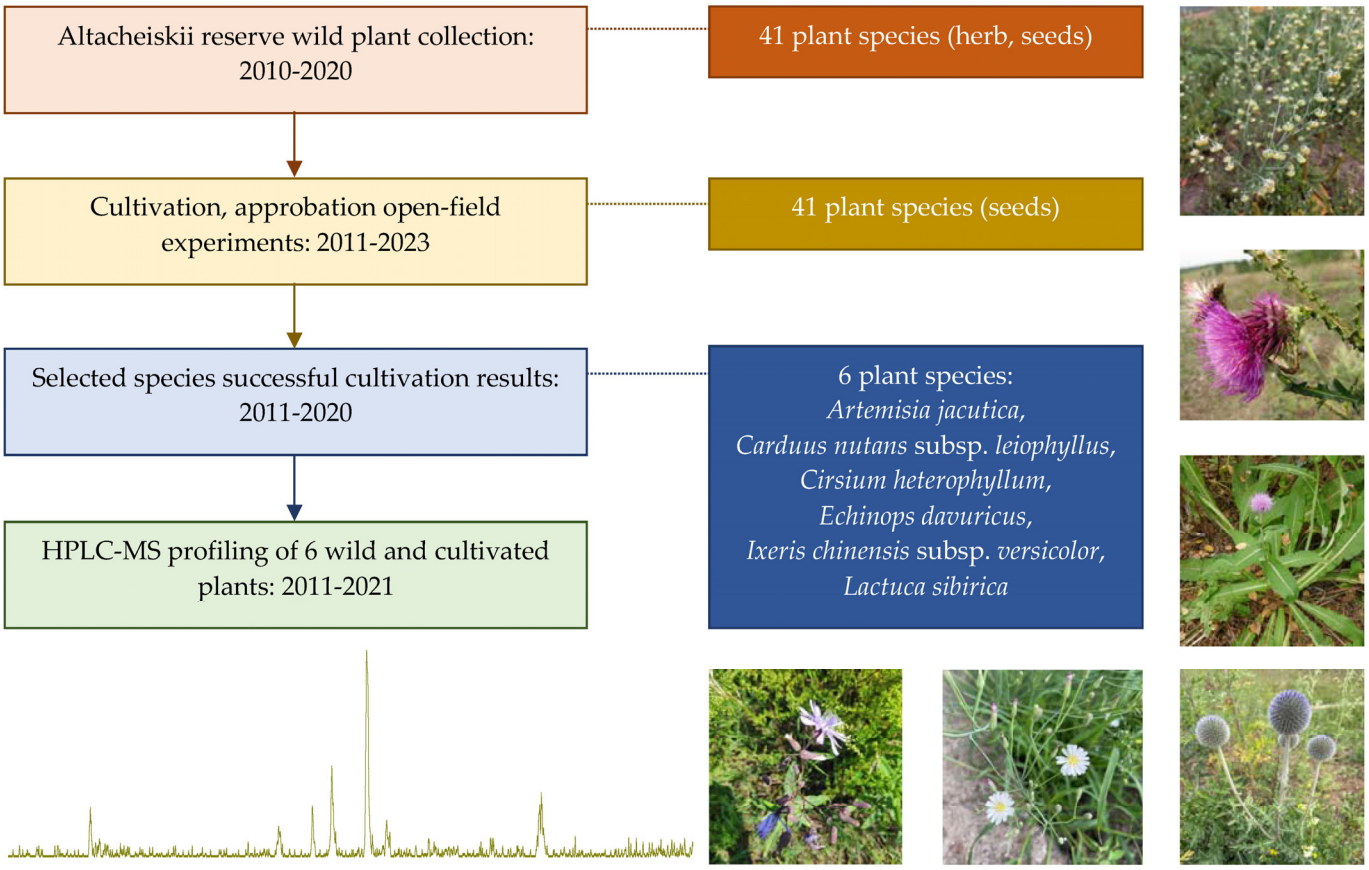


Figure S2. Flow chart for the experimental design.

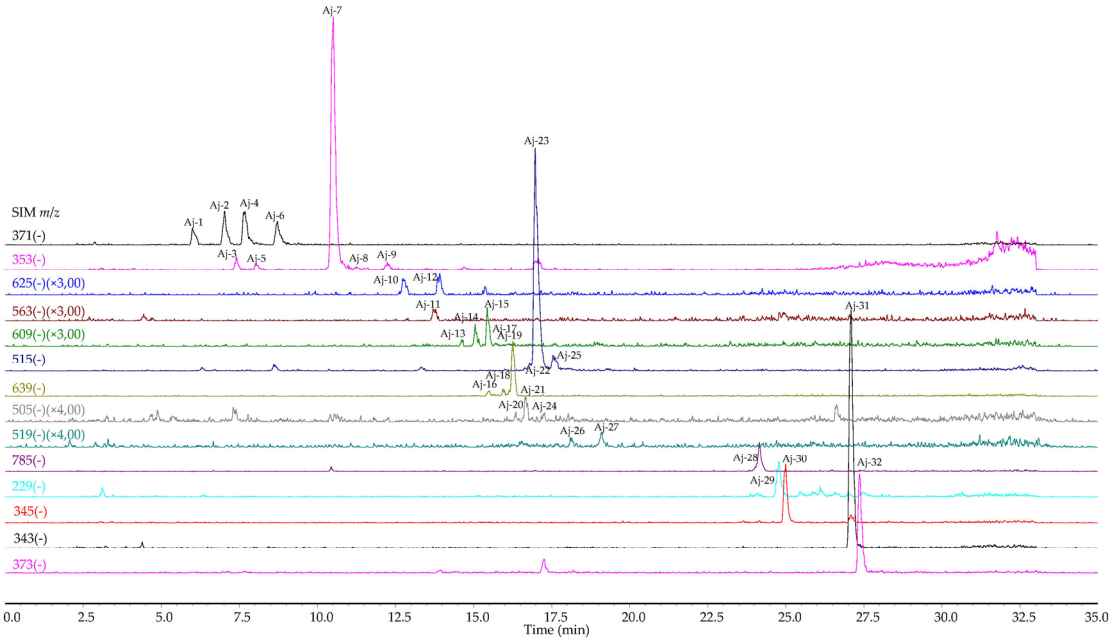


Figure S3. HPLC-MS chromatograms of *Artemisia jacutica* herb (wild sample AJW-1) in SIM mode (negative ionization; SIM *m/z* values in left panel). Compounds Aj-1–Aj-32 description see in Table S1.

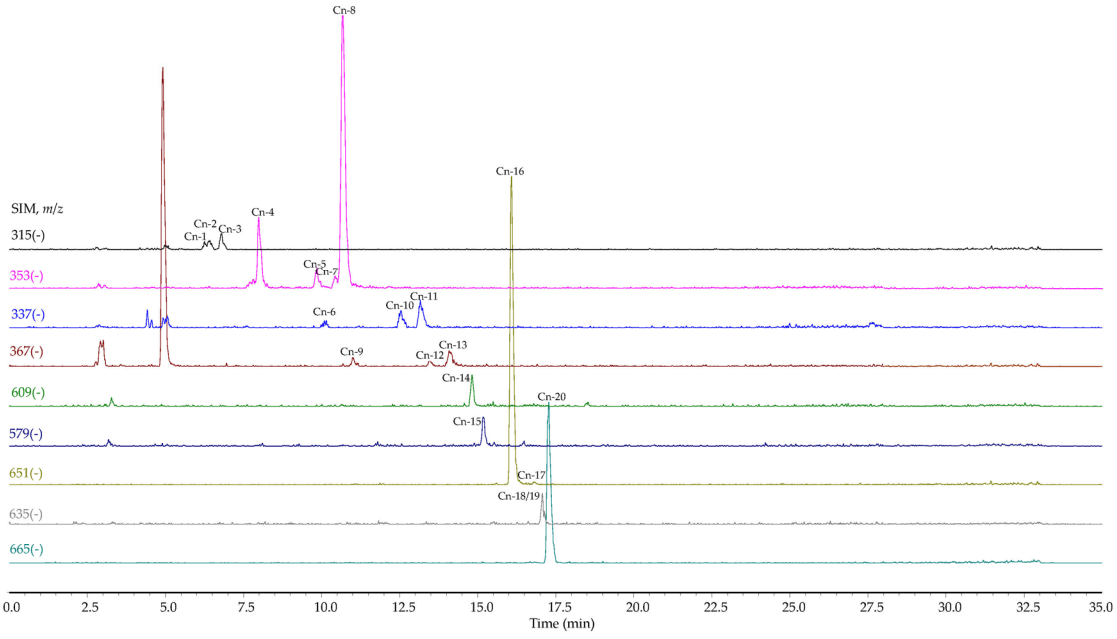


Figure S4. HPLC-MS chromatograms of *Carduus nutans* subsp. *leiophyllus* herb (wild sample CNW-1) in SIM mode (negative ionization; SIM *m/z* values in left panel). Compounds Cn-1–Cn-20 description see in Table S2.

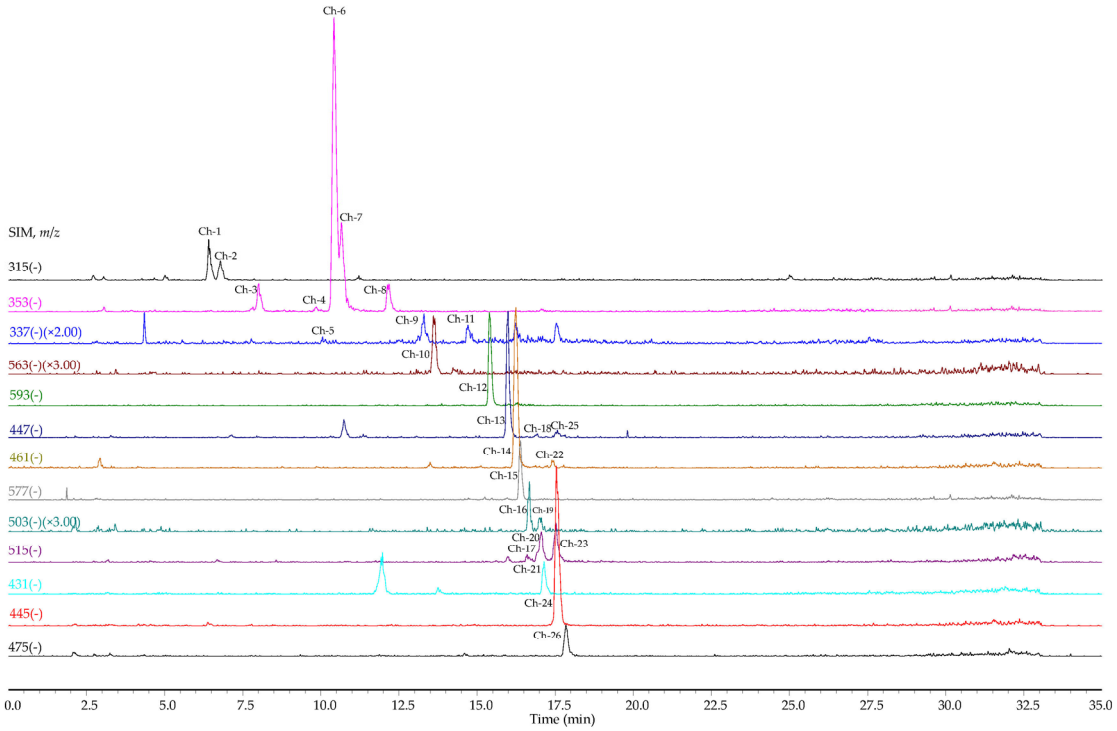


Figure S5. HPLC-MS chromatograms of *Cirsium heterophyllum* herb (wild sample CHW-1) in SIM mode (negative ionization; SIM *m*/*z* values in left panel). Compounds Ch-1–Ch-24 description see in Table S4.

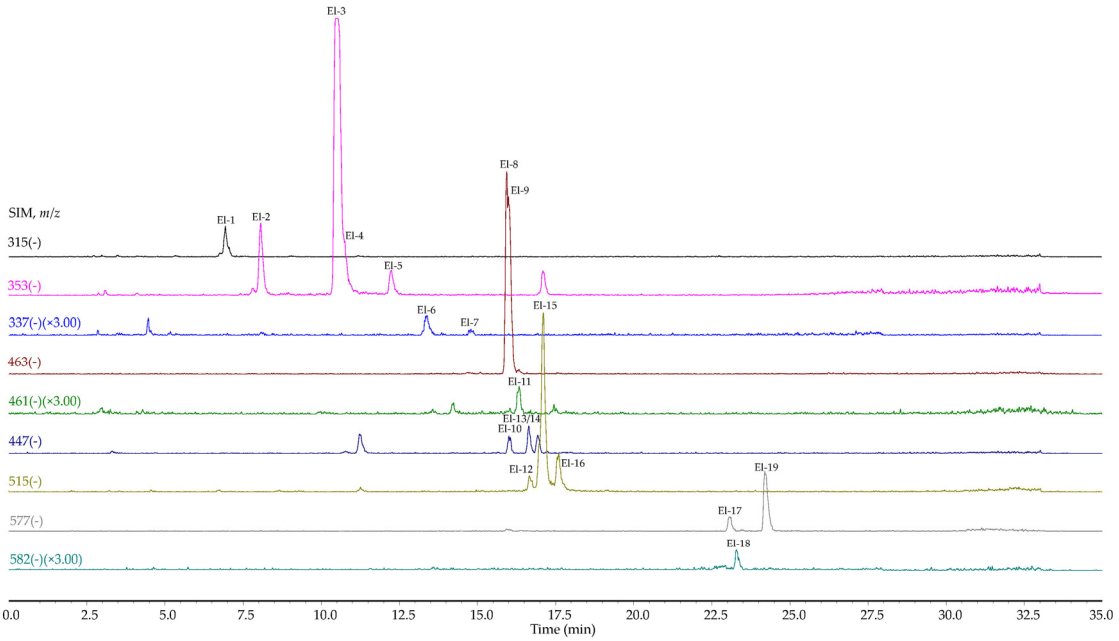


Figure S6. HPLC-MS chromatograms of *Echinops davuricus* herb (wild sample ELW-1) in SIM mode (negative ionization; SIM *m*/*z* values in left panel). Compounds El-1–El-19 description see in Table S5.

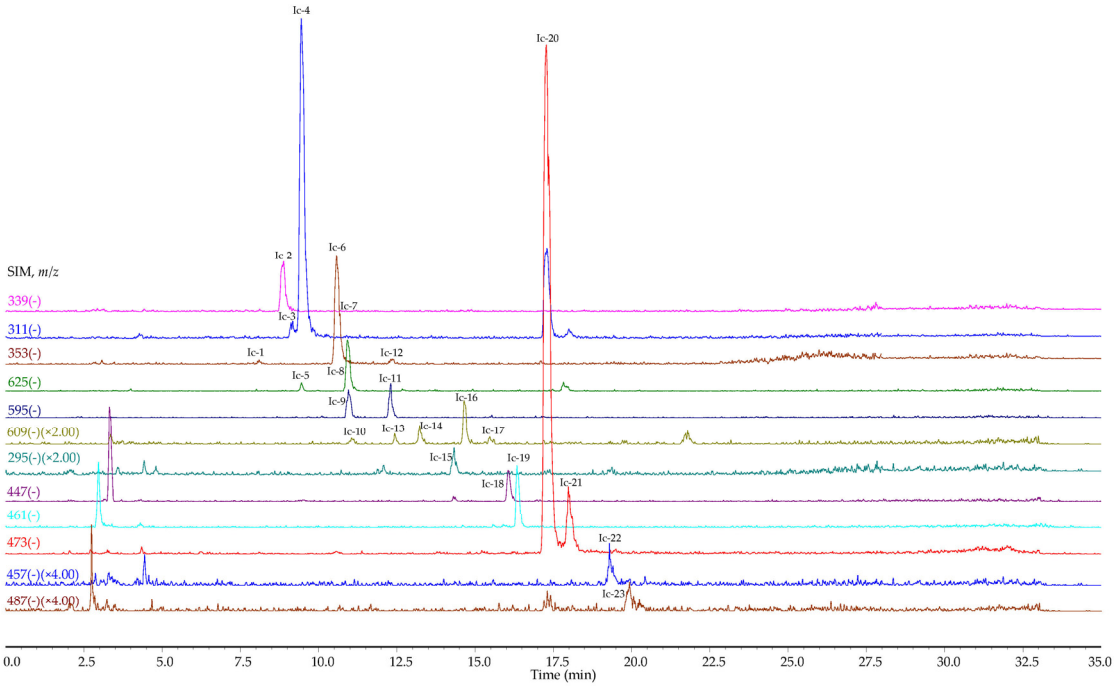


Figure S7. HPLC-MS chromatograms of *Ixeris chinensis* subsp. *versicolor* herb (wild sample ICW-1) in SIM mode (negative ionization; SIM *m*/*z* values in left panel). Compounds Ic-1–Ic-23 description see in Table S6.

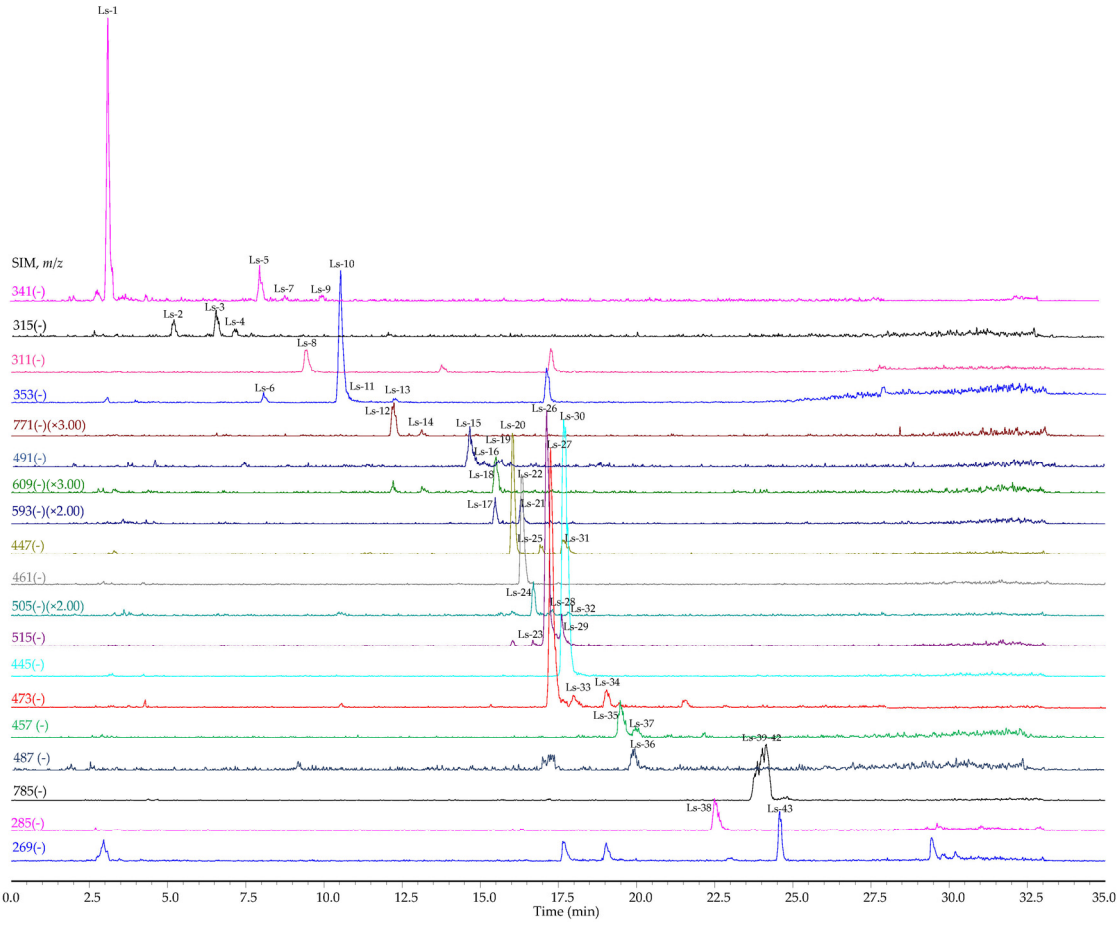


Figure S8. HPLC-MS chromatograms of *Lactuca sibirica* herb (wild sample LSW-1) in SIM mode (negative ionization; SIM *m*/*z* values in left panel). Compounds Ls-1–Ls-41 description see in Table S7.

Table S1. Description of wild samples of Asteraceae species collected in Altacheiskii reserve (https://baikalzapovednik.ru/altacheisky#rec54745054; accessed on 10 April 2024) for a period 2010–2020 and information on cultivation success.

No	Species	Seed and Herb Collection Year	Approbations Years	Cultivation Results*
AAW-1	*Achillea asiatica* Serg.	2010	2011, 2012, 2013	Ambiguously
ADW-1	*Antennaria dioica* (L.) Gaertn.	2014	2015, 2016	Failed
AGW-1	*Arctogeron gramineum* (L.) DC	2012	2013, 2014, 2015	Ambiguously
ANW-1	*Artemisia anethifolia* Web. ex Stechm.	2015	2016, 2017, 2018	Ambiguously
AEW-1	*Artemisia desertorum* Spreng.	2010	2011, 2012, 2013	Ambiguously
AFW-1	*Artemisia frigida* Willd.	2011	2012, 2014	Ambiguously
AIW-1	*Artemisia integrifolia* L.	2017	2018, 2019	Ambiguously
AJW-1	*Artemisia jacutica* Drobow	2016	2017, 2019, 2021	2-year cultivation success
APW-1	*Artemisia palustris* L.	2019	2020, 2021, 2022	Ambiguously
AUW-1	*Artemisia pubescens* var. *pubescens*	2020	2021, 2022	Ambiguously
ASW-1	*Artemisia sericea* Weber ex Stechm.	2020	2021, 2022	Ambiguously
ATW-1	*Artemisia tanacetifolia* L.	2010	2011, 2012, 2013	Ambiguously
ALW-1	*Aster alpinus* L.	2020	2021, 2022	Ambiguously
ABW-1	*Aster biennis* Ledeb.	2011	2012, 2013	Ambiguously
ARW-1	*Aster tataricus* L.	2010	2011, 2012, 2013	Ambiguously
CHW-1	*Cacalia hastata* L.	2018	2019, 2020	Ambiguously
CNW-1	*Carduus nutans* subsp. *leiophyllus* (Petrovič) Arènes	2015	2016, 2018, 2020	2-year cultivation success
CEW-1	*Cirsium esculentum* (Siev.) C.A. Mey.	2012	2013, 2014, 2015	Ambiguously
CHW-1	*Cirsium heterophyllum* (L.) Hill	2014	2015	6-year cultivation success
CSW-1	*Cirsium serratuloides* (L.) Hill	2019	2020, 2022	Ambiguously
CBW-1	*Crepis bungei* Ledeb.	2012	2013, 2014, 2015	Ambiguously
CTW-1	*Crepis tectorum* L.	2015	2016, 2017	Ambiguously
EDW-1	*Echinops davuricus* Fisch. ex Hornem.	2010	2011	9-year cultivation success
EAW-1	*Erigeron acris* L.	2017	2018, 2019	Ambiguously
FSW-1	*Filifolium sibiricum* (L.) Kitam.	2011	2012, 2013	Failed
GDW-1	*Galatella davurica* DC.	2014	2015, 2016, 2017	Failed
ICW-1	*Ixeris chinensis* subsp. *versicolor* (Fisch. ex Link) Kitam.	2014	2015	4-year cultivation success
LSW-1	*Lactuca sibirica* (L.) Benth. ex Maxim.	2014	2015	5-year cultivation success
LAW-1	*Leibnitzia anandria* (L.) Nakai	2018	2019, 2020	Failed
NPW-1	*Neopallasia pectinata* Poljak.	2020	2021, 2022, 2023	Ambiguously
PBW-1	*Pentanema britannica* (L.) D.Gut.Larr., Santos-Vicente, Anderb., E.Rico & M.M.Mart.Ort.	2014	2015, 2016, 2017	Ambiguously
PDW-1	*Picris davurica* Fisch.	2017	2018, 2019, 2020	Ambiguously
SAW-1	*Saussurea amara* (L.) DC.	2020	2021, 2022	Ambiguously
SSW-1	*Saussurea salicifolia* (L.) DC.	2010	2011, 2012	Ambiguously
SUW-1	*Scorzonera austriaca* Willd.	2018	2019, 2020	Ambiguously
SEW-1	*Senecio erucifolius* L.	2017	2018, 2019	Ambiguously
SDW-1	*Solidago dahurica* (Kitag.) Kitag. ex Juz.	2015	2016, 2017, 2019	Ambiguously
TLW-1	*Taraxacum leucanthum* (Ledeb.) Ledeb.	2014	2015, 2016, 2017	Failed
TIW-1	*Tephroseris integrifolia* (L.) Holub	2019	2020, 2021, 2022	Ambiguously
TSW-1	*Tephroseris subdentata* (Bunge) Holub	2011	2012, 2013, 2014	Ambiguously
YTW-1	*Youngia tenuifolia* (Willd.) Babc. et Stebb.	2015	2016, 2017, 2018	Ambiguously

* Ambiguously—mixed results, more research needed. Failed—failed to achieve successful cultivation.

Table S2. Plant cultivation conditions of six Asteraceae species.

Species	Experimental Field Size, m×m	Experimental Fields, n (No.)	Distance Between Plants, m	Soil Description	Climatic Data
Artemisia jacutica	50 × 60	3 (24-1b-1, 24-1b-2, 24-1b-3)	0.6	Soil type: Dark humus. Fertile Layer: 70–90 cm. Soil P_2O_5 content: 22–24 mg/100 g. Soil K_2O content: 60–64 mg/100 g. pH: 7.4. Humus content: 8–9%. Total N: 0.5–0.6%. C : N Ratio: 10–11. No organic/inorganic fertilizers used.	Average annual precipitation: 230-250 mm. Frost-free period: 110-116 days. Sum of temperatures above 10°C: 1900–2000.
Carduus nutans subsp. *leiophyllus*	70 × 70	4 (24-1b-7, 24-1b-8, 24-1b-9, 24-1b-10)	1.2		
Cirsium heterophyllum	50 × 40	3 (24-1b-15, 24-1b-16, 24-1b-17)	0.6		
Echinops davuricus	70 × 90	3 (24-1b-27, 24-1b-28, 24-1b-29)	0.5		
Ixeris chinensis subsp. *versicolor*	40 × 40	4 (24-1b-35, 24-1b-36, 24-1b-37, 24-1b-38)	0.3		
Lactuca sibirica	40 × 50	5 (24-1b-52, 24-1b-53, 24-1b-54, 24-1b-55, 24-1b-56)	0.4		

Table S3. Plant sample description for HPLC assay.

Species	Experimental Field No	Year of Collection (plant age, years; sample numbers = repetition, one dry sample weight, kg)
Artemisia jacutica	24-1b-1	2021 (1; 5/0.1), 2022 (2; 5/0.5)
	24-1b-2	2021 (1; 5/0.1), 2022 (2; 5/0.7)
	24-1b-3	2021 (1; 5/0.1), 2022 (2; 5/0.6)
Carduus nutans subsp. *leiophyllus*	24-1b-7	2020 (1; 5/0.8), 2021 (2; 5/2.5)
	24-1b-8	2020 (1; 5/0.7), 2021 (2; 5/2.0)
	24-1b-9	2020 (1; 5/0.7), 2021 (2; 5/3.5)
	24-1b-10	2020 (1; 5/0.9), 2021 (2; 5/1.5)
Cirsium heterophyllum	24-1b-15	2015 (1; 5/0.2), 2016 (2; 5/0.7), 2018 (4; 5/1.4), 2020 (6; 5/2.9)
	24-1b-16	2015 (1; 5/0.1), 2016 (2; 5/0.6), 2018 (4; 5/1.2), 2020 (6; 5/2.4)
	24-1b-17	2015 (1; 5/0.2), 2016 (2; 5/0.5), 2018 (4; 5/1.2), 2020 (6; 5/2.5)
Echinops davuricus	24-1b-27	2011 (1; 4/0.3), 2013 (3; 4/0.9), 2015 (5; 4/1.6), 2017 (7; 4/1.7), 2019 (9; 4/1.5)
	24-1b-28	2011 (1; 4/0.2), 2013 (3; 4/0.8), 2015 (5; 4/1.2), 2017 (7; 4/1.4), 2019 (9; 4/1.5)
	24-1b-29	2011 (1; 4/0.4), 2013 (3; 4/0.8), 2015 (5; 4/1.4), 2017 (7; 4/1.4), 2019 (9; 4/1.5)
Ixeris chinensis subsp. *versicolor*	24-1b-35	2015 (1; 6/0.1), 2016 (2; 6/0.2), 2017 (3; 6/0.3), 2018 (4; 6/0.3)
	24-1b-36	2015 (1; 6/0.08), 2016 (2; 6/0.2), 2017 (3; 6/0.3), 2018 (4; 6/0.3)
	24-1b-37	2015 (1; 6/0.1), 2016 (2; 6/0.2), 2017 (3; 6/0.3), 2018 (4; 6/0.3)
	24-1b-38	2015 (1; 6/0.1), 2016 (2; 6/0.2), 2017 (3; 6/0.3), 2018 (4; 6/0.3)
Lactuca sibirica	24-1b-52	2015 (1; 5/0.1), 2016 (2; 5/0.2), 2017 (3; 5/0.4), 2019 (5; 5/0.3)
	24-1b-53	2015 (1; 5/0.1), 2016 (2; 5/0.15), 2017 (3; 5/0.3), 2019 (5; 5/0.3)
	24-1b-54	2015 (1; 5/0.1), 2016 (2; 5/0.2), 2017 (3; 5/0.3), 2019 (5; 5/0.3)
	24-1b-55	2015 (1; 5/0.1), 2016 (2; 5/0.17), 2017 (3; 5/0.4), 2019 (5; 5/0.3)
	24-1b-56	2015 (1; 5/0.1), 2016 (2; 5/0.2), 2017 (3; 5/0.4), 2019 (5; 5/0.3)

Table S4. Reference standards used for HPLC profiling and quantification.

Analyzed Compound	Reference Compound. HPLC-Profiling	Reference Compound. Quantification
Benzoates		
Protocatechuic acid *O*-hexosides	Protocatechuic acid 4-*O*-β-glucoside. ChemFaces. Cat. No.: CFN95557. Purity ≥98%	Protocatechuic acid 4-*O*-β-glucoside. ChemFaces. Cat. No.: CFN95557. Purity ≥98%
Protocatechuic acid 4-*O*-glucoside		
Vanilloyl quinic acid (probably 1-*O*-isomer) Vanilloyl quinic acid (probably 4-*O*-isomer) Vanilloyl quinic acid (probably 5-*O*-isomer)	Putative identification. Ref. [40–42]	Vanillic acid 4-β-D-glucoside. MedChemExpress. Cat. No.: HY-114760. Purity ≥98%. Conversion factor (difference in MW): 0.97.
Divanilloyl quinic acid (probably 3,4-*O*-isomer) Divanilloyl quinic acid (probably 3,5-*O*-isomer) Divanilloyl quinic acid (probably 4,5-*O*-isomer)		Vanillic acid 4-β-D-glucoside. MedChemExpress. Cat. No.: HY-114760. Purity ≥98%. Conversion factor (difference in MW): 0.67.
Coumarins		
Esculetin 7-*O*-glucoside	Cichoriin. ChemFaces. Cat. No.: CFN95196. Purity ≥98%	Cichoriin. ChemFaces. Cat. No.: CFN95196. Purity ≥98%
Hydroxycinnamates		
3-*O*-Caffeoyl glucaric acid 4-*O*-Caffeoyl glucaric acid 2-*O*-Caffeoyl glucaric acid 5-*O*-Caffeoyl glucaric acid	Laboratory collection. Ref. [43]	*trans*-Caffeoyl-6-*O*-D-gluconic acid. MedChemExpress. Cat. No.: HY-N11466. Purity ≥98%. Conversion factor (difference in MW): 0.96.
Caftaric acid isomer Caftaric acid	Caftaric acid. ChemFaces. Cat. No.: CFN00384. Purity ≥98%	Caftaric acid. ChemFaces. Cat. No.: CFN00384. Purity ≥98%
Cichoric acid (*di-trans* isomer) Cichoric acid (*cis-trans* isomer) Cichoric acid (*cis-cis* isomer)	Cichoric acid. ChemFaces. Cat. No.: CFN99725. Purity ≥98%	Cichoric acid. ChemFaces. Cat. No.: CFN99725. Purity ≥98%
Coutaric acid	Coutaric acid. SLS Scientific Laboratory Supplies. Cat. No.: SIGPHL83843. Purity ≥96%	Coutaric acid. SLS Scientific Laboratory Supplies. Cat. No.: SIGPHL83843. Purity ≥96%
p-Coumaroyl-caffeoyl-tartaric acids	Putative identification. Ref. [44,45]	Cichoric acid. ChemFaces. Cat. No.: CFN99725. Purity ≥98%. Conversion factor (difference in MW): 1.04.
Feruloyl-caffeoyl-tartaric acid		Cichoric acid. ChemFaces. Cat. No.: CFN99725. Purity ≥98%. Conversion factor (difference in MW): 0.81.
3-*O*-*p*-Coumaroyl quinic acid	3-*O*-*p*-Coumaroylquinic acid. Sigma-Aldrich. Cat. No.: 935557. Purity ≥95%	3-*O*-*p*-Coumaroylquinic acid. Sigma-Aldrich. Cat. No.: 935557. Purity ≥95%
4-*O*-*p*-Coumaroyl quinic acid	4-*O*-Coumaroylquinic acid. ChemFaces. Cat. No.: CFN95508. Purity ≥98%	4-*O*-Coumaroylquinic acid. ChemFaces. Cat. No.: CFN95508. Purity ≥98%
5-*O*-*p*-Coumaroyl quinic acid	5-*O*-Coumaroylquinic acid. ChemFaces. Cat. No.: CFN95507. Purity ≥98%	5-*O*-Coumaroylquinic acid. ChemFaces. Cat. No.: CFN95507. Purity ≥98%
3-*O*-Caffeoyl quinic acid (*trans*-)	Chlorogenic acid. MedChemExpress. Cat. No.: HY-N0055. Purity ≥99.35%.	Chlorogenic acid. MedChemExpress. Cat. No.: HY-N0055. Purity ≥99.35%.
4-*O*-Caffeoyl quinic acid (*trans*-) 4-*O*-Caffeoyl quinic acid (*cis*-)	Cryptochlorogenic acid. MedChemExpress. Cat. No.: HY-N0787. Purity ≥99.88%.	Cryptochlorogenic acid. MedChemExpress. Cat. No.: HY-N0787. Purity ≥99.88%.
5-*O*-Caffeoyl quinic acid (*trans*-)	Neochlorogenic acid. MedChemExpress. Cat. No.: HY-N0722. Purity ≥99.07%.	Neochlorogenic acid. MedChemExpress. Cat. No.: HY- N0722. Purity ≥99.07%.
5-*O*-Caffeoyl quinic acid (*cis*-)	*Cis*-5-Caffeoylquinic acid. BenchChem. Cat. No.: B1222021. Purity ≥98%.	*Cis*-5-Caffeoylquinic acid. BenchChem. Cat. No.: B1222021. Purity ≥98%.
3,4-Di-*O*-caffeoyl quinic acid	3,4-Dicaffeoylquinic acid. MedChemExpress. Cat. No.: HY-N0057. Purity ≥98.64%.	3,4-Dicaffeoylquinic acid. MedChemExpress. Cat. No.: HY-N0057. Purity ≥98.64%.
3,5-Di-*O*-caffeoyl quinic acid	3,5-Di-*O*-caffeoylquinic acid. ChemFaces. Cat. No.: CFN93712. Purity ≥98%	3,5-Di-*O*-caffeoylquinic acid. ChemFaces. Cat. No.: CFN93712. Purity ≥98%

4,5-Di-*O*-caffeoyl quinic acid	4,5-Di-*O*-caffeoyl quinic acid. MedChemExpress. Cat. No.: HY-N11077. Purity ≥98%.	4,5-Di-*O*-caffeoyl quinic acid. MedChemExpress. Cat. No.: HY-N11077. Purity ≥98%.
3-*O*-Feruloyl quinic acid	3-*O*-Feruloyl quinic acid. ChemFaces. Cat. No.: CFN92393. Purity ≥98%.	3-*O*-Feruloyl quinic acid. ChemFaces. Cat. No.: CFN92393. Purity ≥98%.
4-*O*-Feruloyl quinic acid	4-*O*-Feruloyl quinic acid. ChemFaces. Cat. No.: CFN92392. Purity ≥98%.	4-*O*-Feruloyl quinic acid. ChemFaces. Cat. No.: CFN92392. Purity ≥98%.
5-*O*-Feruloyl quinic acid	5-*O*-Feruloyl quinic acid. ChemFaces. Cat. No.: CFN92889. Purity ≥98%.	5-*O*-Feruloyl quinic acid. ChemFaces. Cat. No.: CFN92889. Purity ≥98%.
	Flavonoids	
Apigenin 7-*O*-glucoside	Apigenin 7-*O*-glucoside. Extrasynthese. Cat. No.: 1004 S. Purity ≥99%.	Apigenin 7-*O*-glucoside. Extrasynthese. Cat. No.: 1004 S. Purity ≥99%.
Apigenin 7-*O*-glucuronide	Apigenin 7-*O*-glucuronide. MedChemExpress. Cat. No.: HY-N1454. Purity ≥98.83%.	Apigenin 7-*O*-glucuronide. MedChemExpress. Cat. No.: HY-N1454. Purity ≥98.83%.
Apigenin 7-*O*-rutinoside	Isorhoifolin. Cayman Chemical. Cat. No.: 34036. Purity ≥95%	Isorhoifolin. Cayman Chemical. Cat. No.: 34036. Purity ≥95%
Apigenin 7-*O*-(2″-*O*-*p*-coumaroyl)-glucoside Apigenin 7-*O*-(6″-*O*-*p*-coumaroyl)-glucoside	Laboratory collection. Ref. [46]	Apigenin 4'-*O*-(2'',6''-di-*O*-*E*-*p*-coumaroyl)glucoside. ChemFaces. Cat. No.: CFN95276. Purity ≥98%. Conversion factor (difference in MW): 1.25.
Apigenin di-*O*-hexoside-*O*-acetates	Putative identification. Ref. [47]	Apigenin 7-*O*-glucoside. Extrasynthese. Cat. No.: 1004 S. Purity ≥99%. Conversion factor (difference in MW): 0.68.
Apigenin 6-*C*-glucoside-8-*C*-arabinoside	Schaftoside. ChemFaces. Cat. No.: CFN90197. Purity ≥98%.	Schaftoside. ChemFaces. Cat. No.: CFN90197. Purity ≥98%.
Acacetin 7-*O*-glucoside	Tilianin. ChemFaces. Cat. No.: CFN92764. Purity ≥98%.	Tilianin. ChemFaces. Cat. No.: CFN92764. Purity ≥98%.
Luteolin 5-*O*-glucoside	Luteolin 5-*O*-glucoside. MedChemExpress. Cat. No.: HY-N2008. Purity ≥97.18%.	Luteolin 5-*O*-glucoside. MedChemExpress. Cat. No.: HY-N2008. Purity ≥97.18%.
Luteolin 7-*O*-glucoside	Luteolin 7-glucoside. Sigma-Aldrich. Cat. No.: 49968. Purity ≥98%.	Luteolin 7-glucoside. Sigma-Aldrich. Cat. No.: 49968. Purity ≥98%
Luteolin 3′-*O*-glucoside	Luteolin 3′-glucoside. Phytolab GmbH & Co. KG. Cat. No.: 85840. Purity ≥98%.	Luteolin 3′-glucoside. Phytolab GmbH & Co. KG. Cat. No.: 85840. Purity ≥98%.
Luteolin 4′-*O*-glucoside	Luteolin 4′-*O*-glucoside. Extrasynthese. Cat. No.: 1412 S. Purity ≥98%.	Luteolin 4′-*O*-glucoside. Extrasynthese. Cat. No.: 1412 S. Purity ≥98%.
Luteolin 7-*O*-rutinoside	Luteolin 7-rutinoside. MedChemExpress. Cat. No.: HY-N6647. Purity ≥98.47%.	Luteolin 7-rutinoside. MedChemExpress. Cat. No.: HY-N6647. Purity ≥98.47%.
Luteolin 7-*O*-(2″-*O*-glucosyl)-glucoside	Laboratory collection. Ref. [48]	Luteolin 7-glucoside. Sigma-Aldrich. Cat. No.: 49968. Purity ≥98%. Conversion factor (difference in MW): 0.73.
Luteolin 7-*O*-(2″-*O*-(6‴-*O*-acetyl)-glucosyl)-glucoside	Isolated in present work.	Luteolin 7-glucoside. Sigma-Aldrich. Cat. No.: 49968. Purity ≥98%. Conversion factor (difference in MW): 0.69.
Luteolin *O*-hexoside-*O*-pentoside	Putative identification. Ref. [49]	Luteolin 7-glucoside. Sigma-Aldrich. Cat. No.: 49968. Purity ≥98%. Conversion factor (difference in MW): 0.77.
Luteolin di-*O*-hexoside-*O*-acetate	Putative identification. Ref. [49]	Luteolin 7-glucoside. Sigma-Aldrich. Cat. No.: 49968. Purity ≥98%. Conversion factor (difference in MW): 0.67.
Luteolin tri-*O*-hexosides	Putative identification. Ref. [49]	Luteolin 7-glucoside. Sigma-Aldrich. Cat. No.: 49968. Purity ≥98%. Conversion factor (difference in MW): 0.58.
Chrysoeriol 7-*O*-glucoside	Chrysoeriol 7-*O*-glucoside. ChemFaces. Cat. No.: CFN93021. Purity ≥98%.	Chrysoeriol 7-*O*-glucoside. ChemFaces. Cat. No.: CFN93021. Purity ≥98%.
Chrysoeriol 4′-*O*-glucoside	Laboratory collection. Ref. [50]	Chrysoeriol 7-*O*-glucoside. ChemFaces. Cat. No.: CFN93021. Purity ≥98%.

Chrysoeriol 7-*O*-(2″-*O*-acetyl)-glucoside Chrysoeriol 7-*O*-(6″-*O*-acetyl)-glucoside	Laboratory collection. Ref. [50]	Chrysoeriol 7-*O*-glucoside. ChemFaces. Cat. No.: CFN93021. Purity ≥98%. Conversion factor (difference in MW): 0.92.
Chrysoeriol 7-*O*-(2″-*O*-(6‴-*O*-acetyl)-glucosyl)-glucoside	Isolated in present work.	Chrysoeriol 7-*O*-glucoside. ChemFaces. Cat. No.: CFN93021. Purity ≥98%. Conversion factor (difference in MW): 0.69.
6-Hydroxyluteolin di-*O*-hexoside	Putative identification. Ref. [51]	6-Hydroxyluteolin 7-*O*-glucoside. ChemFaces. Cat. No.: CFN91094. Purity ≥98%. Conversion factor (difference in MW): 0.74.
Pectolinarigenin 7-*O*-glucoside	Pectolinarigenin 7-*O*-glucoside. Geopharma Co. Cat. No.: 35-5373-11-5. Purity ≥98%.	Pectolinarigenin 7-*O*-glucoside. Geopharma Co. Cat. No.: 35-5373-11-5. Purity ≥98%.
Kaempferol 3-*O*-neohesperidoside	Kaempferol 3-*O*-neohesperidoside. MedChemExpress. Cat. No.: HY-107207. Purity ≥99.86%.	Kaempferol 3-*O*-neohesperidoside. MedChemExpress. Cat. No.: HY-107207. Purity ≥99.86%.
Kaempferol 3-*O*-rutinoside	Nicotiflorin. Selleck Chemicals. Cat. No.: S3267. Purity ≥99.91%.	Nicotiflorin. Selleck Chemicals. Cat. No.: S3267. Purity ≥99.91%.
Kempferol 3-*O*-sophoroside	Kempferol 3-*O*-sophoroside. MedChemExpress. Cat. No.: HY-N2055. Purity ≥99.84%.	Kempferol 3-*O*-sophoroside. MedChemExpress. Cat. No.: HY-N2055. Purity ≥99.84%.
Kaempferol 3-*O*-gentiobioside	Kaempferol 3-gentiobioside. ChemFaces. Cat. No.: CFN92384. Purity ≥98%.	Kaempferol 3-gentiobioside. ChemFaces. Cat. No.: CFN92384. Purity ≥98%.
Kaempferol 7-*O*-glucoside	Kaempferol 7-*O*-glucoside. Cayman Chemical. Cat. No.: CAY34347. Purity ≥98%.	Kaempferol 7-*O*-glucoside. Cayman Chemical. Cat. No.: CAY34347. Purity ≥98%.
Kaempferol di-*O*-hexoside	Putative identification. Ref. [52]	Kempferol 3-*O*-sophoroside. MedChemExpress. Cat. No.: HY-N2055. Purity ≥99.84%.
Quercetin 3-*O*-glucoside	Isoquercitrin. Sigma-Aldrich. Cat. No.: 00140585. Purity ≥95%.	Isoquercitrin. Sigma-Aldrich. Cat. No.: 00140585. Purity ≥95%.
Quercetin 3-*O*-galactoside	Quercetin 3-D-galactoside. Cayman Chemical. Cat. No.: 18648. Purity ≥98%.	Quercetin 3-D-galactoside. Cayman Chemical. Cat. No.: 18648. Purity ≥98%.
Quercetin 3-*O*-(2″-*O*-arabinosyl)-glucoside Quercetin 3-*O*-(6″-*O*-arabinosyl)-glucoside	Putative identification. Ref. [53]	Isoquercitrin. Sigma-Aldrich. Cat. No.: 00140585. Purity ≥95%. Conversion factor (difference in MW): 0.78.
Quercetin 3-*O*-neohesperidoside	Quercetin 3-*O*-neohesperidoside. MedChemExpress. Cat. No.: HY-N7976. Purity ≥99.54%.	Quercetin 3-*O*-neohesperidoside. MedChemExpress. Cat. No.: HY-N7976. Purity ≥99.54%.
Quercetin 3-*O*-rungioside Quercetin 3-*O*-(4″-*O*-rhamnosyl)-glucoside	Laboratory collection. Ref. [54]	Rutin. Sigma-Aldrich. Cat. No.: R5143. Purity ≥94%.
Quercetin 3-*O*-rutinoside	Rutin. Sigma-Aldrich. Cat. No.: R5143. Purity ≥94%.	Rutin. Sigma-Aldrich. Cat. No.: R5143. Purity ≥94%.
Quercetin 3-*O*-sophoroside	Quercetin 3-*O*-sophoroside. ChemFaces. Cat. No.: CFN90630. Purity ≥98%.	Quercetin 3-*O*-sophoroside. ChemFaces. Cat. No.: CFN90630. Purity ≥98%.
Quercetin 3-*O*-gentiobioside	Quercetin 3-*O*-gentiobioside. MedChemExpress. Cat. No.: HY-N4089. Purity ≥99.92%.	Quercetin 3-*O*-gentiobioside. MedChemExpress. Cat. No.: HY-N4089. Purity ≥99.92%.
Quercetin 3-*O*-(2″-*O*-acetyl)-glucoside Quercetin 3-*O*-(3″-*O*-acetyl)-glucoside Quercetin 3-*O*-(4″-*O*-acetyl)-glucoside	Laboratory collection. Ref. [55]	Quercetin-3-*O*-(6-acetylglucoside). Extrasynthese. Cat. No.: 1099. Purity ≥85%.
Quercetin 3-*O*-(6″-*O*-acetyl)-glucoside	Quercetin-3-*O*-(6-acetylglucoside). Extrasynthese. Cat. No.: 1099. Purity ≥85%.	Quercetin-3-*O*-(6-acetylglucoside). Extrasynthese. Cat. No.: 1099. Purity ≥85%.
Isorhamnetin 3-*O*-(2″-*O*-acetyl)-glucoside Isorhamnetin 3-*O*-(6″-*O*-acetyl)-glucoside	Laboratory collection. Ref. [54]	Isorhamnetin 3-*O*-glucoside. MedChemExpress. Cat. No.: HY-N0777. Purity ≥99.95%. Conversion factor (difference in MW): 0.92.

Apigenin	Apigenin. ChemFaces. Cat. No.: CFN98843. Purity ≥98%.	Apigenin. ChemFaces. Cat. No.: CFN98843. Purity ≥98%.
Luteolin	Luteolin. ChemFaces. Cat. No.: CFN98784. Purity ≥98%.	Luteolin. ChemFaces. Cat. No.: CFN98784. Purity ≥98%.
Cirsiliol	Cirsiliol. MedChemExpress. Cat. No.: HY-110399. Purity ≥99.25%.	Cirsiliol. MedChemExpress. Cat. No.: HY-110399. Purity ≥99.25%.
Cirsilineol	Cirsilineol. MedChemExpress. Cat. No.: HY-119347. Purity ≥98%.	Cirsilineol. MedChemExpress. Cat. No.: HY-119347. Purity ≥98%.
Axillarin	Axillarin. ChemFaces. Cat. No.: CFN89530. Purity ≥98%.	Axillarin. ChemFaces. Cat. No.: CFN89530. Purity ≥98%.
Chrysosplenetin	Chrysosplenetin. ChemFaces. Cat. No.: CFN97026. Purity ≥98%.	Chrysosplenetin. ChemFaces. Cat. No.: CFN97026. Purity ≥98%.
	Phenylamines	
Tri-*O*-*p*-coumaroyl spermines	Putative identification. Ref. [S16]	*N*1,*N*5,*N*10-(*E*)-Tri-*p*-coumaroylspermidine. ChemFaces. Cat. No.: CFN95256. Purity ≥98%. Conversion factor (difference in MW): 0.91.
Tetra-*O*-*p*-coumaroyl spermines	Putative identification. Ref. [S16]	*N*1,*N*5,*N*10-(*E*)-Tri-*p*-coumaroylspermidine. ChemFaces. Cat. No.: CFN95256. Purity ≥98%. Conversion factor (difference in MW): 0.74.
N^1,N^5,N^{10}-Tri-*O*-(*EEE*)-*p*-coumaroyl-spermidine	*N*1,*N*5,*N*10-(*E*)-Tri-*p*-coumaroylspermidine. ChemFaces. Cat. No.: CFN95256. Purity ≥98%.	*N*1,*N*5,*N*10-(*E*)-Tri-*p*-coumaroylspermidine. ChemFaces. Cat. No.: CFN95256. Purity ≥98%.

Table S5. HPLC and mass-spectral conditions used for metabolite separation and identification.

Mode No, SPE Eluate	**Column**	**Column temp., °C**	**Eluents A/B Composition**	**Gradient Program, %B**	**Flow Rate, µL/min**
Mode 1 (for *Artemisia jacutica*, *Carduus nutans* subsp. *leiophyllus*, *Cirsium heterophyllum*, *Echinops davuricus*, *Ixeris chinensis* subsp. *versicolor*)	ReproSil-Pur 120 C18-AQ (4.6 × 250 mm, 5 µm; Dr. Maisch GmbH, Ammerbuch, Germany)	30	A: 0.1% HCOOH in water; B: 0.1% HCOOH in MeCN	0–20 min 2–80% B, 20–30 min 80–100% B, 30–35 min 100% B, 35–40 min 100–2% B	150
Mode 2 (for *Lactuca sibirica*)	ReproSil-Pur 120 C18-AQ (4.6 × 250 mm, 5 µm; Dr. Maisch GmbH, Ammerbuch, Germany)	25	A: 0.1% HCOOH in water; B: 0.1% HCOOH in MeCN	0–10 min 2–54% B, 10–20 min 54–75% B, 20–30 min 75–100% B, 30–35 min 100% B, 35–40 min 100–2% B	150
	Injection Volume, µL	**UV-Vis spectral range, nm**	**ESI Mode**	**Temperature ESI Interface / Desolvation Line / Heat Block, °C**	
Mode 1 (for *Artemisia jacutica*, *Carduus nutans* subsp. *leiophyllus*, *Cirsium heterophyllum*, *Echinops davuricus*, *Ixeris chinensis* subsp. *versicolor*)	10	200–600	Negative	300 / 200 / 400	
Mode 2 (for *Lactuca sibirica*)	10	200–600	Negative	300 / 200 / 400	
	Flow Rate Nebulizing Gas (N_2) / Heating Gas (air) / Collision-Induced Dissociation Gas (Ar), µL/min	**Source Voltage, kV**	**Collision Energy, eV**	**MS Scanning Range, *m*/*z***	
Mode 1 (for *Artemisia jacutica*, *Carduus nutans* subsp. *leiophyllus*, *Cirsium heterophyllum*, *Echinops davuricus*, *Ixeris chinensis* subsp. *versicolor*)	3 / 10 / 0.3	3	-10–-35	80–2000	
Mode 2 (for *Lactuca sibirica*)	3 / 10 / 0.3	3	-10–-35	80–2000	

Table S6. Regression equations, correlation coefficients (r^2), standard deviation (S_{YX}), limits of detection (LOD), limits of quantification (LOQ) and linear ranges for 55 reference standards.

Compound	Ionization [a]	CE [b] (eV)	Regression equation [c]		r^2	S_{YX}	LOD/LOQ (μg/mL)	Linear range (μg/mL)
			a	$b \cdot 10^6$				
Protocatechuic acid 4-*O*-β-glucoside	N	-30	0.9114	-0.6312	0.9887	$6.37 \cdot 10^{-2}$	0.23/0.70	0.7–100.0
Vanillic acid 4-β-D-glucoside	N	-15	1.0864	-0.5271	0.9983	$1.04 \cdot 10^{-2}$	0.03/0.10	0.10–500.0
Cichoriin	N	-25	1.3620	-0.0820	0.9961	$9.91 \cdot 10^{-2}$	0.21/0.72	0.8–100.0
trans-Caffeoyl-6-*O*-D-gluconic acid	N	-35	0.9562	-0.0521	0.9971	$7.79 \cdot 10^{-2}$	0.27/0.82	0.9–100.0
Caftaric acid	N	-10	2.6538	-0.1376	0.9990	$1.17 \cdot 10^{-2}$	0.01/0.04	0.10–100.0
Cichoric acid	N	-15	1.9478	-0.2369	0.9984	$1.03 \cdot 10^{-2}$	0.02/0.05	0.05–250.0
Coutaric acid	N	-10	1.5632	-0.0376	0.9983	$5.14 \cdot 10^{-2}$	0.11/0.33	0.40–100.0
3-*O*-*p*-Coumaroylquinic acid	N	-25	1.0627	-1.2531	0.9893	$0.62 \cdot 10^{-2}$	0.02/0.06	0.10–400.0
4-*O*-Coumaroylquinic acid	N	-20	1.4689	-0.3641	0.9990	$5.69 \cdot 10^{-2}$	0.12/0.38	0.40–400.0
5-*O*-Coumaroylquinic acid	N	-20	2.6340	-0.2411	0.9973	$2.74 \cdot 10^{-2}$	0.03/0.10	0.10–350.0
Chlorogenic acid	N	-15	2.4176	-1.5647	0.9994	$0.40 \cdot 10^{-2}$	0.005/0.02	0.02–300.0
Cryptochlorogenic acid	N	-15	2.7365	-1.0690	0.9996	$0.51 \cdot 10^{-2}$	0.006/0.02	0.02–300.0
Neochlorogenic acid	N	-15	2.9021	-1.4184	0.9998	$0.39 \cdot 10^{-2}$	0.004/0.01	0.02–300.0
Cis-5-Caffeoylquinic acid	N	-15	5.8022	-0.8040	0.9990	$1.14 \cdot 10^{-2}$	0.007/0.02	0.02–500.0
3,4-Dicaffeoylquinic acid	N	-10	0.1756	-0.0144	0.9967	$3.01 \cdot 10^{-2}$	0.56/1.71	2.00–850.0
3,5-Di-*O*-caffeoylquinic acid	N	-20	1.4412	-0.6211	0.9930	$11.25 \cdot 10^{-2}$	0.26/0.78	0.80–100.0
4,5-Di-*O*-caffeoyl quinic acid	N	-15	1.1123	-1.0289	0.9862	$0.41 \cdot 10^{-2}$	0.01/0.04	0.05–400.0
3-*O*-Feruloyl quinic acid	N	-20	0.9562	-0.0521	0.9971	$7.79 \cdot 10^{-2}$	0.27/0.82	0.90–100.0
4-*O*-Feruloyl quinic acid	N	-20	1.3387	-0.0284	0.9981	$9.50 \cdot 10^{-2}$	0.23/0.71	0.80–100.0
5-*O*-Feruloyl quinic acid	N	-10	0.9518	-0.0267	0.9990	$1.03 \cdot 10^{-2}$	0.03/0.10	0.10–100.0
Apigenin 7-*O*-glucoside	N	-30	1.1269	-0.9560	0.9864	$0.93 \cdot 10^{-2}$	0.02/0.08	0.10–400.0
Apigenin 7-*O*-glucuronide	N	-15	3.6748	-0.7069	0.9987	$0.90 \cdot 10^{-2}$	0.008/0.02	0.02–400.0
Isorhoifolin	N	-15	4.9634	-0.5047	0.9972	$0.63 \cdot 10^{-2}$	0.004/0.01	0.01–400.0
Apigenin 4'-*O*-(2'',6''-di-*O*-*E*-*p*-coumaroyl)glucoside	N	-30	2.3312	-0.4563	0.9803	$14.92 \cdot 10^{-2}$	0.21/0.64	0.7–100.0
Apigenin 7-*O*-glucoside	N	-25	1.1492	-0.6010	0.9980	$4.68 \cdot 10^{-2}$	0.14/0.41	0.50–400.0
Schaftoside	N	-20	1.4412	-0.6211	0.9930	$11.25 \cdot 10^{-2}$	0.26/0.78	0.8–100.0
Tilianin	N	-25	1.3620	-0.0820	0.9961	$9.91 \cdot 10^{-2}$	0.21/0.72	0.8–100.0
Luteolin 5-*O*-glucoside	N	-25	1.9634	-0.7458	0.9963	$2.59 \cdot 10^{-2}$	0.04/0.14	0.20–350.0
Luteolin 7-glucoside	N	-20	1.8233	-0.7962	0.9975	$2.02 \cdot 10^{-2}$	0.04/0.11	0.20–350.0
Luteolin 3′-glucoside	N	-15	2.0330	-0.2516	0.9992	$1.09 \cdot 10^{-2}$	0.02/0.05	0.05–300.0
Luteolin 4′-*O*-glucoside	N	-10	0.1537	-0.0189	0.9960	$3.83 \cdot 10^{-2}$	0.82/2.49	2.50–850.0
Luteolin 7-rutinoside	N	-30	1.3722	-0.0829	0.9973	$9.93 \cdot 10^{-2}$	0.24/0.72	0.80–100.0
Chrysoeriol 7-*O*-glucoside	N	-30	1.3620	-0.0820	0.9961	$9.91 \cdot 10^{-2}$	0.21/0.72	0.80–100.0
6-Hydroxyluteolin 7-*O*-glucoside	N	-20	1.0634	-0.0933	0.9902	$10.01 \cdot 10^{-2}$	0.31/0.94	1.00–100.0
Pectolinarigenin 7-*O*-glucoside	N	-10	1.9610	-0.5271	0.9993	$0.94 \cdot 10^{-2}$	0.02/0.05	0.05–250.0
Kaempferol 3-*O*-neohesperidoside	N	-15	1.1105	-0.3211	0.9937	$4.18 \cdot 10^{-2}$	0.12/0.38	0.40–400.0
Nicotiflorin	N	-30	1.9634	-0.4511	0.9952	$9.18 \cdot 10^{-2}$	0.15/0.46	0.5–100.0
Kempferol 3-*O*-sophoroside	N	-10	1.4611	-0.0731	0.9982	$4.08 \cdot 10^{-2}$	0.09/0.27	0.30–100.0
Kaempferol 3-gentiobioside	N	-10	1.5330	-0.0863	0.9985	$4.15 \cdot 10^{-2}$	0.09/0.27	0.30–100.0
Kaempferol 7-*O*-glucoside	N	-20	2.0859	-0.9171	0.9980	$6.18 \cdot 10^{-2}$	0.03/0.09	0.1–100.0
Isoquercitrin	N	-10	1.6278	-0.0428	0.9990	$7.11 \cdot 10^{-2}$	0.14/0.44	0.50–100.0
Quercetin 3-D-galactoside	N	-10	0.2569	-0.0316	0.9973	$2.52 \cdot 10^{-2}$	0.33/1.00	1.00–750.0
Quercetin 3-*O*-neohesperidoside	N	-20	1.9871	-0.6871	0.9984	$5.63 \cdot 10^{-2}$	0.09/0.28	0.40–400.0
Rutin	N	-20	1.2716	-0.7389	0.9897	$9.14 \cdot 10^{-2}$	0.23/0.72	0.80–400.0
Quercetin 3-*O*-sophoroside	N	-20	1.6705	-0.4374	0.9988	$12.79 \cdot 10^{-2}$	0.25/0.77	0.8–100.0
Quercetin 3-*O*-gentiobioside	N	-20	1.2703	-0.7911	0.9814	$15.26 \cdot 10^{-2}$	0.40/1.20	1.5–100.0
Quercetin-3-*O*-(6-acetylglucoside)	N	-20	1.1103	-0.9217	0.9901	$14.33 \cdot 10^{-2}$	0.42/1.29	1.5–100.0
Isorhamnetin 3-*O*-glucoside	N	-15	0.9375	-0.7631	0.9982	$1.42 \cdot 10^{-2}$	0.05/0.15	0.20–350.0

Apigenin	N	-20	2.4751	-0.2081	0.9976	$2.04 \cdot 10^{-2}$	0.03/0.10	0.10–350.0
Luteolin	N	-20	1.8267	-0.4160	0.9990	$11.73 \cdot 10^{-2}$	0.21/0.67	0.70–400.0
Cirsiliol	N	-15	1.1541	-0.4691	0.9987	$1.06 \cdot 10^{-2}$	0.03/0.10	0.10–350.0
Cirsilineol	N	-20	2.0384	-0.3640	0.9975	$2.02 \cdot 10^{-2}$	0.03/0.10	0.10–350.0
Axillarin	N	-10	1.2416	-0.3615	0.9901	$3.02 \cdot 10^{-2}$	0.08/0.24	0.3–100.0
Chrysosplenetin	N	-15	7.064	-1.533	0.9992	$1.92 \cdot 10^{-2}$	0.009/0.03	0.03–500.0
*N*1,*N*5,*N*10-(*E*)-Tri-*p*-coumaroylspermidine	N	-10	0.9911	-0.0379	0.9988	$2.05 \cdot 10^{-2}$	0.07/0.21	0.3–100.0

[a] Ionization mode : N—negative, P—positive. [b] CE—collision energy. [c] Regression equation: $y = a \cdot x + b$.

Table S7. Retention times (t_R), molecular formulas (MF), mass-spectral data for negative ionization (MSD), and identification level (IL) of compounds Aj-1–Aj-32 found in *Artemisia jacutica* herb.

No	t_R, min	Compound	MF	MSD, m/z	IL
Aj-1	6.00	3-*O*-Caffeoyl glucaric acid	$C_{15}H_{16}O_{11}$	371, 179	1a
Aj-2	7.01	4-*O*-Caffeoyl glucaric acid	$C_{15}H_{16}O_{11}$	371, 179	1a
Aj-3	7.41	4-*O*-Caffeoyl quinic acid (*trans*-)	$C_{16}H_{18}O_9$	353, 179	1b
Aj-4	7.66	2-*O*-Caffeoyl glucaric acid	$C_{15}H_{16}O_{11}$	371, 179	1a
Aj-5	8.06	4-*O*-Caffeoyl quinic acid (*cis*-)	$C_{16}H_{18}O_9$	353, 179	1b
Aj-6	8.71	5-*O*-Caffeoyl glucaric acid	$C_{15}H_{16}O_{11}$	371, 179	1a
Aj-7	10.51	5-*O*-Caffeoyl quinic acid (*trans*-)	$C_{16}H_{18}O_9$	353, 179	1b
Aj-8	11.28	3-*O*-Caffeoyl quinic acid (*trans*-)	$C_{16}H_{18}O_9$	353, 179	1b
Aj-9	12.25	5-*O*-Caffeoyl quinic acid (*cis*-)	$C_{16}H_{18}O_9$	353, 179	1b
Aj-10	12.77	6-Hydroxyluteolin di-*O*-hexoside	$C_{27}H_{30}O_{17}$	625, 463, 301	2
Aj-11	13.71	Schaftoside (apigenin 6-*C*-glucoside-8-*C*-arabinoside)	$C_{26}H_{28}O_{14}$	563	1b
Aj-12	13.90	Quercetin 3-*O*-gentiobioside (quercetin 3-*O*-(6″-*O*-glucosyl)-glucoside)	$C_{27}H_{30}O_{17}$	625, 463, 301	1b
Aj-13	14.61	Calendoflavobioside (quercetin 3-*O*-neohesperidoside)	$C_{27}H_{30}O_{16}$	609, 463, 301	1a
Aj-14	15.05	Rutin (quercetin 3-*O*-rutinoside)	$C_{27}H_{30}O_{16}$	609, 463, 301	1b
Aj-15	15.41	Calendoside II (quercetin 3-*O*-rungioside)	$C_{27}H_{30}O_{16}$	609, 463, 301	1a
Aj-16	15.52	Tri-*O*-*p*-coumaroyl spermine	$C_{37}H_{44}N_4O_6$	639, 493, 347, 163	2
Aj-17	15.92	Calendoside I (quercetin 3-*O*-(4″-*O*-rhamnosyl)-glucoside)	$C_{27}H_{30}O_{16}$	609, 463, 301	1a
Aj-18	15.94	Tri-*O*-*p*-coumaroyl spermine	$C_{37}H_{44}N_4O_6$	639, 493, 347, 163	2
Aj-19	16.26	Tri-*O*-*p*-coumaroyl spermine	$C_{37}H_{44}N_4O_6$	639, 493, 347, 163	2
Aj-20	16.37	Quercetin 3-*O*-(2″-*O*-acetyl)-glucoside	$C_{23}H_{22}O_{13}$	505, 463, 301	1a
Aj-21	16.67	Quercetin 3-*O*-(6″-*O*-acetyl)-glucoside	$C_{23}H_{22}O_{13}$	505, 463, 301	1a
Aj-22	16.81	3,4-Di-*O*-caffeoyl quinic acid	$C_{25}H_{24}O_{12}$	515, 353, 179	1b
Aj-23	16.97	3,5-Di-*O*-caffeoyl quinic acid	$C_{25}H_{24}O_{12}$	515, 353, 179	1b
Aj-24	17.27	Quercetin 3-*O*-(4″-*O*-acetyl)-glucoside	$C_{23}H_{22}O_{13}$	505, 463, 301	1a
Aj-25	17.57	4,5-Di-*O*-caffeoyl quinic acid	$C_{25}H_{24}O_{12}$	515, 353, 179	1b
Aj-26	18.13	Isorhamnetin 3-*O*-(2″-*O*-acetyl)-glucoside	$C_{24}H_{24}O_{13}$	519, 477, 315	1a
Aj-27	19.12	Isorhamnetin 3-*O*-(6″-*O*-acetyl)-glucoside	$C_{24}H_{24}O_{13}$	519, 477, 315	1a
Aj-28	24.17	Tetra-*O*-*p*-coumaroyl spermine	$C_{46}H_{50}N_4O_8$	785, 639, 493, 347, 163	2
Aj-29	24.80	Cirsiliol	$C_{17}H_{14}O_7$	329	1b
Aj-30	25.01	Axyllarin	$C_{17}H_{14}O_8$	345	1b
Aj-31	27.10	Cirsilineol	$C_{18}H_{16}O_7$	343	1b
Aj-32	27.37	Chrysosplenetin	$C_{19}H_{18}O_8$	373	1b

* Identification levels: (1) identified compounds after comparison of retention times, UV and mass-spectral data with previosly isolated compounds (1a) or comercial reference standard (1b); (2) putatively annotated compounds after comparison of retention times, UV and mass-spectral data with literature data.

Table S8. Retention times (t_R), molecular formulas (MF), mass-spectral data for negative ionization (MSD), and identification level (IL) of compounds Cn-1–Cn-20 found in *Carduus nutans* subsp. *leiophyllus* herb.

No	t_R, min	Compound	MF	MSD, m/z	IL
Cn-1	6.27	Protocatechuic acid *O*-hexoside (Cn-3 isomer)	$C_{13}H_{16}O_9$	315, 153	2
Cn-2	6.41	Protocatechuic acid *O*-hexoside (Cn-3 isomer)	$C_{13}H_{16}O_9$	315, 153	2
Cn-3	6.81	Protocatechuic acid 4-*O*-glucoside	$C_{13}H_{16}O_9$	315, 153	1b
Cn-4	8.01	4-*O*-Caffeoyl quinic acid (*cis*-)	$C_{16}H_{18}O_9$	353, 179	1b
Cn-5	9.84	Caffeoyl quinic acid (Cn-4/7/8 isomer)	$C_{16}H_{18}O_9$	353, 179	2
Cn-6	10.12	4-*O*-*p*-Coumaroyl quinic acid	$C_{16}H_{18}O_8$	337, 163	1a
Cn-7	10.44	5-*O*-Caffeoyl quinic acid (*trans*-)	$C_{16}H_{18}O_9$	353, 179	1b
Cn-8	10.70	3-*O*-Caffeoyl quinic acid (*trans*-)	$C_{16}H_{18}O_9$	353, 179	1b
Cn-9	11.02	4-*O*-Feruloyl quinic acid	$C_{17}H_{20}O_9$	337, 163	1a
Cn-10	12.53	5-*O*-*p*-Coumaroyl quinic acid	$C_{16}H_{18}O_8$	337, 163	1b
Cn-11	13.17	3-*O*-*p*-Coumaroyl quinic acid	$C_{16}H_{18}O_8$	337, 163	1b
Cn-12	13.50	5-*O*-Feruloyl quinic acid	$C_{17}H_{20}O_9$	337, 163	1b
Cn-13	14.08	3-*O*-Feruloyl quinic acid	$C_{17}H_{20}O_9$	337, 163	1a
Cn-14	14.83	Luteolin 7-O-(2″-*O*-glucosyl)-glucoside	$C_{27}H_{30}O_{16}$	609, 447, 285	1b
Cn-15	15.15	Luteolin *O*-hexoside-*O*-pentoside	$C_{26}H_{28}O_{15}$	579, 447, 285	2
Cn-16	16.08	Luteolin 7-O-(2″-*O*-(6‴-*O*-acetyl)-glucosyl)-glucoside (linariifolioside)	$C_{29}H_{32}O_{17}$	651, 609, 447, 285	1c
Cn-17	16.85	Luteolin di-*O*-hexoside-*O*-acetate (Cn-16 isomer)	$C_{29}H_{32}O_{17}$	651, 609, 447, 285	2
Cn-18	17.04	Apigenin di-*O*-hexoside-*O*-acetate	$C_{29}H_{32}O_{16}$	635, 593, 431, 269	2
Cn-19	17.18	Apigenin di-*O*-hexoside-*O*-acetate	$C_{29}H_{32}O_{16}$	635, 593, 431, 269	2
Cn-20	17.30	Chrysoeriol 7-O-(2″-*O*-(6‴-*O*-acetyl)-glucosyl)-glucoside	$C_{30}H_{34}O_{17}$	665, 623, 461, 299	1c

* Identification levels: (1) identified compounds after comparison of retention times, UV and mass-spectral data with previosly isolated compounds (1a) or comercial reference standard (1b) or isolated in present work (1c); (2) putatively annotated compounds after comparison of retention times, UV and mass-spectral data with literature data.

Table S9. Extraction/chromatography conditions and spectral data of luteolin 7-O-(2″-*O*-(6‴-*O*-acetyl)-glucosyl)-glucoside and chrysoeriol 7-O-(2″-*O*-(6‴-*O*-acetyl)-glucosyl)-glucoside isolated from *Carduus nutans* subsp. *leiophyllus* leaves.

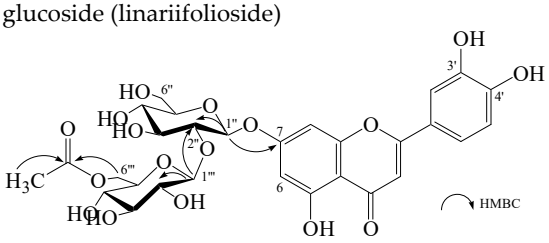
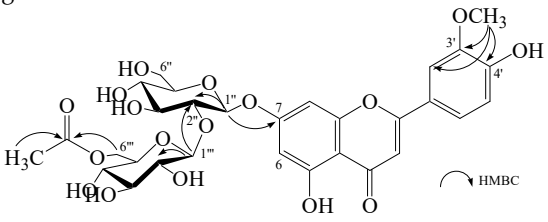
Parameter	Description
Plant extraction / chromatography	Powdered plant material (leaves, sample CNW-1; 5 kg) was extracted with MeOH in a Soxhlet apparatus. The extract was concentrated, which led to the formation of a precipitate (170 g) that was separated over Sephadex LH-20 [column chromatography, eluent EtOH (70%)] and SiO_2 (column chromatography, eluent hexane–EtOAc, 80:20→60:40) to isolate luteolin 7-O-(2″-*O*-(6‴-*O*-acetyl)-glucosyl)-glucoside (51 g) [69] and chrysoeriol 7-O-(2″-*O*-(6‴-*O*-acetyl)-glucosyl)-glucoside (35 g) [70].
Luteolin 7-O-(2″-*O*-(6‴-*O*-acetyl)-glucosyl)-glucoside (linariifolioside) 	$C_{29}H_{32}O_{17}$. UV (MeOH, λ_{max}, nm): 252, 268, 348. HR-ESI-MS, *m*/*z* 651.3281 $[M - H]^-$ (calcd. for $C_{29}H_{31}O_{17}$, 651.5500). ESI-MS, *m*/*z* (%): 651 (100) $[M - H]^-$, 609 (33) [(M – H) – acetyl]$^-$, 447 (25) [(M – H) – acetyl – glucose]$^-$, 285 (64) [(M – H) – acetyl – 2 × glucose]$^-$. ^{1}H NMR (500 MHz, DMSO-d$_6$, 298 K, δ, ppm, J/Hz): luteolin – 6.62 (1H, s; C-3), 6.35 (1H, s; C-6), 6.70 (1H, s; H-8), 7.42 (1H, d, J = 2.0; H-2′), 6.95 (1H, d, J = 8.0; H-5′), 7.45 (1H, dd, J = 2.0, 8.0; H-6′); 7-*O*-glucose – 5.35 (1H, d, J = 7.0; H-1″), 3.64 (1H, m; H-2″), 3.21–3.48 (6H, m; H-3″, H-4″, H-5″, H-3‴, H-4‴, H-5‴), 3.52 (1H, m; H-6″$_B$), 3.76 (1H, m; H-6″$_A$); 2″-*O*-glucose – 4.73 (1H, d, J = 8.0; H-1‴), 3.01 (1H, m; H-2‴), 3.21–3.48 (6H, m; H-3″, H-4″, H-5″, H-3‴, H-4‴, H-5‴), 3.80 (1H, m; H-6‴$_B$), 3.92 (1H, m; H-6‴$_A$); 6‴-*O*-acetyl – 1.85 (3H, s; COC<u>H</u>$_3$). ^{13}C NMR (125 MHz, DMSO-d$_6$, 298 K, δ, ppm): luteolin – 163.5 (C-2), 104.5 (C-3), 181.7 (C-4), 161.3 (C-5), 99.6 (C-6), 162.5 (C-7), 95.0 (C-8), 153.2 (C-9), 106.3 (C-10), 120.9 (C-1′), 113.0 (C-2′), 146.2 (C-3′), 149.1 (C-4′), 115.6 (C-5′), 119.0 (C-6′); 7-*O*-glucose – 99.5 (C-1″), 92.5 (C-2″), 75.2 (C-3″), 68.7 (C-4″), 76.9 (C-5″), 60.1 (C-6″); 2″-*O*-glucose – 104.2 (C-1‴), 74.1 (C-2‴), 75.8 (C-3‴), 69.5 (C-4‴), 73.6 (C-5‴), 62.7 (C-6‴); 6‴-*O*-acetyl – 20.1 (CO<u>C</u>H$_3$), 170.5 (<u>C</u>OCH$_3$).
Chrysoeriol 7-O-(2″-*O*-(6‴-*O*-acetyl)-glucosyl)-glucoside 	$C_{30}H_{34}O_{17}$. UV (MeOH, λ_{max}, nm): 251, 267, 348. HR-ESI-MS, *m*/*z* 665.4217 $[M - H]^-$ (calcd. for $C_{30}H_{33}O_{17}$, 665.5770). ESI-MS, *m*/*z* (%): 665 (100) $[M - H]^-$, 623 (35) [(M – H) – acetyl]$^-$, 461 (14) [(M – H) – acetyl – glucose]$^-$, 299 (54) [(M – H) – acetyl – 2 × glucose]$^-$. ^{1}H NMR (500 MHz, DMSO-d$_6$, 298 K, δ, ppm, J/Hz): chrysoeriol – 6.61 (1H, s; C-3), 6.33 (1H, s; C-6), 6.69 (1H, s; H-8), 7.56 (1H, d, J = 2.0; H-2′), 6.92 (1H, d, J = 8.0; H-5′), 7.48 (1H, dd, J = 2.0, 8.0; H-6′), 3.85 (3H, c; 3′-OC<u>H</u>$_3$); 7-*O*-glucose – 5.37 (1H, d, J = 7.0; H-1″), 3.61 (1H, m; H-2″), 3.19–3.49 (6H, m; H-3″, H-4″, H-5″, H-3‴, H-4‴, H-5‴), 3.53 (1H, m; H-6″$_B$), 3.79 (1H, m; H-6″$_A$); 2″-*O*-glucose – 4.78 (1H, d, J = 8.0; H-1‴), 3.03 (1H, m; H-2‴), 3.19–3.49 (6H, m; H-3″, H-4″, H-5″, H-3‴, H-4‴, H-5‴), 3.81 (1H, m; H-6‴$_B$), 3.96 (1H, m; H-6‴$_A$); 6‴-*O*-acetyl – 1.87 (3H, s; COC<u>H</u>$_3$). ^{13}C NMR (125 MHz, DMSO-d$_6$, 298 K, δ, ppm): chrysoeriol – 163.3 (C-2), 104.2 (C-3), 181.5 (C-4), 161.4 (C-5), 99.7 (C-6), 162.6 (C-7), 95.2 (C-8), 153.1 (C-9), 106.2 (C-10), 121.6 (C-1′), 110.9 (C-2′), 148.1 (C-3′), 150.9 (C-4′), 115.8 (C-5′), 120.1 (C-6′); 56.1 (3′-O<u>C</u>H$_3$); 7-*O*-glucose – 99.7 (C-1″), 92.2 (C-2″), 75.1 (C-3″), 68.5 (C-4″), 76.7 (C-5″), 60.2 (C-6″); 2″-*O*-glucose – 104.0 (C-1‴), 74.0 (C-2‴), 75.5 (C-3‴), 69.6 (C-4‴), 73.4 (C-5‴), 62.9 (C-6‴); 6‴-*O*-acetyl – 20.2 (CO<u>C</u>H$_3$), 170.3 (<u>C</u>OCH$_3$).

Table S10. Retention times (t_R), molecular formulas (MF), mass-spectral data for negative ionization (MSD), and identification level (IL) of compounds Ch-1–Ch-24 found in *Cirsium heterophyllum* herb.

No	t_R, min	Compound	MF	MSD, m/z	IL
Ch-1	6.41	Protocatechuic acid *O*-hexoside (Cn-3 isomer)	$C_{13}H_{16}O_9$	315, 153	2
Ch-2	6.81	Protocatechuic acid 4-*O*-glucoside	$C_{13}H_{16}O_9$	315, 153	1b
Ch-3	8.01	4-*O*-Caffeoyl quinic acid (*trans*-)	$C_{16}H_{18}O_9$	353, 179	1b
Ch-4	9.84	4-*O*-Caffeoyl quinic acid (*cis*-)	$C_{16}H_{18}O_9$	353, 179	1b
Ch-5	10.12	4-*O*-*p*-Coumaroyl quinic acid	$C_{16}H_{18}O_8$	337, 163	1a
Ch-6	10.44	5-*O*-Caffeoyl quinic acid (*trans*-)	$C_{16}H_{18}O_9$	353, 179	1b
Ch-7	10.70	3-*O*-Caffeoyl quinic acid (*trans*-)	$C_{16}H_{18}O_9$	353, 179	1b
Ch-8	12.16	5-*O*-Caffeoyl quinic acid (*cis*-)	$C_{16}H_{18}O_9$	353, 179	1b
Ch-9	12.53	5-*O*-*p*-Coumaroyl quinic acid	$C_{16}H_{18}O_8$	337, 163	1b
Ch-10	13.64	Schaftoside (apigenin 6-*C*-glucoside-8-*C*-arabinoside)	$C_{26}H_{28}O_{14}$	563	1b
Ch-11	14.73	3-*O*-*p*-Coumaroyl quinic acid	$C_{16}H_{18}O_8$	337, 163	1b
Ch-12	15.43	Scolymoside (veronicastroside, luteolin 7-*O*-rutinoside)	$C_{27}H_{30}O_{15}$	593, 447, 285	1b
Ch-13	15.98	Cynaroside (luteolin 7-*O*-glucoside)	$C_{21}H_{20}O_{11}$	447, 285	1a
Ch-14	16.24	Chrysoeriol 7-*O*-glucoside	$C_{22}H_{22}O_{11}$	461, 299	1b
Ch-15	16.39	Isorhoifolin (apigenin 7-*O*-rutinoside)	$C_{27}H_{30}O_{14}$	577, 431, 269	1b
Ch-16	16.67	Chrysoeriol 7-*O*-(2″-*O*-acetyl)-glucoside	$C_{24}H_{24}O_{12}$	503, 461, 299	2
Ch-17	16.75	3,4-Di-*O*-caffeoyl quinic acid	$C_{25}H_{24}O_{12}$	515, 353, 179	1b
Ch-18	16.93	Dracocephaloside (luteolin 3′-*O*-glucoside)	$C_{21}H_{20}O_{11}$	447, 285	1a
Ch-19	17.02	Chrysoeriol 7-*O*-(6″-*O*-acetyl)-glucoside	$C_{24}H_{24}O_{12}$	503, 461, 299	1a
Ch-20	17.04	3,5-Di-*O*-caffeoyl quinic acid	$C_{25}H_{24}O_{12}$	515, 353, 179	1b
Ch-21	17.16	Cosmosiin (apigenin 7-*O*-glucoside)	$C_{21}H_{20}O_{10}$	431, 269	1b
Ch-22	17.43	Chrysoeriol 4′-*O*-glucoside	$C_{22}H_{22}O_{11}$	461, 299	1a
Ch-23	17.55	4,5-Di-*O*-caffeoyl quinic acid	$C_{25}H_{24}O_{12}$	515, 353, 179	1b
Ch-24	17.57	Acacetin 7-*O*-glucoside	$C_{22}H_{22}O_{10}$	445, 283	1b
Ch-25	17.60	Luteolin 4′-*O*-glucoside	$C_{21}H_{20}O_{11}$	447, 285	1b
Ch-26	17.85	Pectolinarigenin 7-*O*-glucoside	$C_{22}H_{24}O_{11}$	475, 313	1b

* Identification levels: (1) identified compounds after comparison of retention times, UV and mass-spectral data with previosly isolated compounds (1a) or comercial reference standard (1b) or isolated in present work (1c); (2) putatively annotated compounds after comparison of retention times, UV and mass-spectral data with literature data.

Table S11. Retention times (t_R), molecular formulas (MF), mass-spectral data for negative ionization (MSD), and identification level (IL) of compounds El-1–El-19 found in *Echinops davuricus* herb.

No	t_R, min	Compound	MF	MSD, m/z	IL
El-1	6.81	Protocatechuic acid 4-*O*-glucoside	$C_{13}H_{16}O_9$	315, 153	1b
El-2	8.01	4-*O*-Caffeoyl quinic acid (*trans*-)	$C_{16}H_{18}O_9$	353, 179	1b
El-3	10.44	5-*O*-Caffeoyl quinic acid (*trans*-)	$C_{16}H_{18}O_9$	353, 179	1b
El-4	10.70	3-*O*-Caffeoyl quinic acid (*trans*-)	$C_{16}H_{18}O_9$	353, 179	1b
El-5	12.16	5-*O*-Caffeoyl quinic acid (*cis*-)	$C_{16}H_{18}O_9$	353, 179	1b
El-6	12.53	5-*O*-*p*-Coumaroyl quinic acid	$C_{16}H_{18}O_8$	337, 163	1b
El-7	14.73	3-*O*-*p*-Coumaroyl quinic acid	$C_{16}H_{18}O_8$	337, 163	1b
El-8	15.97	Isoquercitrin (quercetin 3-*O*-glucoside)	$C_{21}H_{20}O_{12}$	463, 301	1b
El-9	16.00	Hyperoside (quercetin 3-*O*-galactoside)	$C_{21}H_{20}O_{12}$	463, 301	1b
El-10	16.02	Cynaroside (luteolin 7-*O*-glucoside)	$C_{21}H_{20}O_{11}$	447, 285	1b
El-11	16.24	Chrysoeriol 7-*O*-glucoside	$C_{22}H_{22}O_{11}$	461, 299	1b
El-12	16.64	3,4-Di-*O*-caffeoyl quinic acid	$C_{25}H_{24}O_{12}$	515, 353, 179	1b
El-13	16.65	Luteolin 5-*O*-glucoside	$C_{21}H_{20}O_{11}$	447, 285	1b
El-14	16.93	Dracocephaloside (luteolin 3′-*O*-glucoside)	$C_{21}H_{20}O_{11}$	447, 285	1a
El-15	17.04	3,5-Di-*O*-caffeoyl quinic acid	$C_{25}H_{24}O_{12}$	515, 353, 179	1b
El-16	17.55	4,5-Di-*O*-caffeoyl quinic acid	$C_{25}H_{24}O_{12}$	515, 353, 179	1b
El-17	23.06	Echitin (apigenin 7-*O*-(2″-*O*-*p*-coumaroyl)-glucoside)	$C_{30}H_{26}O_{12}$	577, 431, 269	1a
El-18	23.29	N^1,N^5,N^{10}-Tri-*O*-(*EEE*)-*p*-coumaroyl-spermidine	$C_{34}H_{37}N_3O_6$	582, 436, 290, 163, 144	1b
El-19	24.22	Echinacin (apigenin 7-*O*-(6″-*O*-*p*-coumaroyl)-glucoside)	$C_{30}H_{26}O_{12}$	577, 431, 269	1b

* Identification levels: (1) identified compounds after comparison of retention times, UV and mass-spectral data with previosly isolated compounds (1a) or comercial reference standard (1b) or isolated in present work (1c); (2) putatively annotated compounds after comparison of retention times, UV and mass-spectral data with literature data.

Table S12. Retention times (t_R), molecular formulas (MF), mass-spectral data for negative ionization (MSD), and identification level (IL) of compounds Ic-1–Ic-25 found in *Ixeris chinensis* subsp. *versicolor* herb.

No	t_R, min	Compound	MF	MSD, m/z	IL
Ic-1	8.01	4-*O*-Caffeoyl quinic acid (*trans*-)	$C_{16}H_{18}O_9$	353, 179	1b
Ic-2	8.87	Cichoriin (esculetin 7-*O*-glucoside)	$C_{15}H_{16}O_9$	339, 177	1b
Ic-3	9.15	Caftaric acid isomer	$C_{13}H_{12}O_9$	311, 179	1b
Ic-4	9.48	Caftaric acid	$C_{13}H_{12}O_9$	311, 179	1b
Ic-5	9.52	Baimaside (quercetin 3-*O*-sophoroside)	$C_{27}H_{30}O_{17}$	625, 463, 301	1b
Ic-6	10.44	5-*O*-Caffeoyl quinic acid (*trans*-)	$C_{16}H_{18}O_9$	353, 179	1b
Ic-7	10.70	3-*O*-Caffeoyl quinic acid (*trans*-)	$C_{16}H_{18}O_9$	353, 179	1b
Ic-8	10.93	Quercetin 3-*O*-gentiobioside	$C_{27}H_{30}O_{17}$	625, 463, 301	1b
Ic-9	10.98	Quercetin 3-*O*-(2″-*O*-arabinosyl)-glucoside	$C_{26}H_{28}O_{16}$	595, 463, 301	2
Ic-10	11.08	Kaempferol di-*O*-hexoside	$C_{27}H_{30}O_{16}$	609, 447, 285	2
Ic-11	12.31	Peltatoside (quercetin 3-*O*-(6″-*O*-arabinosyl)-glucoside)	$C_{26}H_{28}O_{16}$	595, 463, 301	1b
Ic-12	12.39	5-*O*-Caffeoyl quinic acid (*cis*-)	$C_{16}H_{18}O_9$	353, 179	1b
Ic-13	12.46	Sophoraflavonoloside (kaempferol 3-*O*-sophoroside)	$C_{27}H_{30}O_{16}$	609, 447, 285	1b
Ic-14	13.22	Kaempferol 3-*O*-gentiobioside	$C_{27}H_{30}O_{16}$	609, 447, 285	1b
Ic-15	14.32	Coutaric acid	$C_{13}H_{12}O_8$	295, 163	1b
Ic-16	14.66	Calendoflavobioside (quercetin 3-*O*-neohesperidoside)	$C_{27}H_{30}O_{16}$	609, 463, 285	1a
Ic-17	15.57	Rutin (quercetin 3-*O*-rutinoside)	$C_{27}H_{30}O_{16}$	609, 463, 285	1b
Ic-18	16.07	Populnin (kaempferol 7-*O*-glucoside)	$C_{21}H_{20}O_{11}$	447, 285	1b
Ic-19	16.24	Chrysoeriol 7-*O*-glucoside	$C_{22}H_{22}O_{11}$	461, 299	1b
Ic-20	17.30	Cichoric acid (di-*trans* isomer)	$C_{22}H_{18}O_{12}$	473, 311, 179	1b
Ic-21	18.01	Cichoric acid (*cis*-*trans* isomer)	$C_{22}H_{18}O_{12}$	473, 311, 179	2
Ic-22	19.29	*p*-Coumaroyl-caffeoyl-tartaric acid	$C_{22}H_{18}O_{11}$	457, 311, 295, 179, 163	2
Ic-23	19.91	Feruloyl-caffeoyl-tartaric acid	$C_{23}H_{20}O_{12}$	587, 425, 411, 193, 179	2

* Identification levels: (1) identified compounds after comparison of retention times, UV and mass-spectral data with previosly isolated compounds (1a) or comercial reference standard (1b) or isolated in present work (1c); (2) putatively annotated compounds after comparison of retention times, UV and mass-spectral data with literature data.

Table S13. Retention times (t_R), molecular formulas (MF), mass-spectral data for negative ionization (MSD), and identification level (IL) of compounds Ls-1–Ls-41 found in *Lactuca sibirica* herb.

No	t_R, min	Compound	MF	MSD, m/z	IL
Ls-1	3.09	Vanilloyl quinic acid (probably 1-*O*-isomer)	$C_{15}H_{18}O_9$	341, 167	2
Ls-2	5.32	Protocatechuic acid *O*-hexoside (Ls-4 isomer)	$C_{13}H_{16}O_9$	315, 153	2
Ls-3	6.78	Protocatechuic acid *O*-hexoside (Ls-4 isomer)	$C_{13}H_{16}O_9$	315, 153	2
Ls-4	7.41	Protocatechuic acid 4-*O*-glucoside	$C_{13}H_{16}O_9$	315, 153	1b
Ls-5	7.99	Vanilloyl quinic acid (probably 4-*O*-isomer)	$C_{15}H_{18}O_9$	341, 167	2
Ls-6	8.01	4-*O*-Caffeoyl quinic acid (*trans*-)	$C_{16}H_{18}O_9$	353, 179	1b
Ls-7	8.10	Vanilloyl quinic acid (probably 5-*O*-isomer)	$C_{15}H_{18}O_9$	341, 167	2
Ls-8	9.48	Caftaric acid	$C_{13}H_{12}O_9$	311, 179	1b
Ls-9	9.91	Vanilloyl quinic acid (probably 5-*O*-isomer)	$C_{15}H_{18}O_9$	341, 167	2
Ls-10	10.44	5-*O*-Caffeoyl quinic acid (*trans*-)	$C_{16}H_{18}O_9$	353, 179	1b
Ls-11	10.70	3-*O*-Caffeoyl quinic acid (*trans*-)	$C_{16}H_{18}O_9$	353, 179	1b
Ls-12	12.29	Luteolin tri-*O*-hexoside	$C_{33}H_{40}O_{21}$	771, 609, 447, 285	2
Ls-13	12.39	5-*O*-Caffeoyl quinic acid (*cis*-)	$C_{16}H_{18}O_9$	353, 179	1b
Ls-14	13.15	Luteolin tri-*O*-hexoside	$C_{33}H_{40}O_{21}$	771, 609, 447, 285	2
Ls-15	14.63	Divanilloyl quinic acid (probably 3,4-isomer)	$C_{23}H_{24}O_{12}$	491, 341, 167	2
Ls-16	15.05	Divanilloyl quinic acid (probably 3,5-isomer)	$C_{23}H_{24}O_{12}$	491, 341, 167	2
Ls-17	15.53	Kaempferol 3-*O*-neohesperidoside	$C_{27}H_{30}O_{15}$	593, 447, 285	1b
Ls-18	15.58	Rutin (quercetin 3-*O*-rutinoside)	$C_{27}H_{30}O_{16}$	609, 463, 301	1b
Ls-19	15.61	Divanilloyl quinic acid (probably 4,5-isomer)	$C_{23}H_{24}O_{12}$	491, 341, 167	2
Ls-20	16.08	Cynaroside (luteolin 7-*O*-glucoside)	$C_{21}H_{20}O_{11}$	447, 285	1b
Ls-21	16.31	Nicotiflorin (kaempferol 3-*O*-rutinoside)	$C_{27}H_{30}O_{15}$	593, 447, 285	1b
Ls-22	16.35	Chrysoeriol 7-*O*-glucoside	$C_{22}H_{22}O_{11}$	461, 299	1b
Ls-23	16.70	3,4-Di-*O*-caffeoyl quinic acid	$C_{25}H_{24}O_{12}$	515, 353, 179	1b
Ls-24	16.73	Quercetin 3-*O*-(6″-*O*-acetyl)-glucoside	$C_{23}H_{22}O_{13}$	505, 463, 301	1a
Ls-25	16.97	Dracocephaloside (luteolin 3′-*O*-glucoside)	$C_{21}H_{20}O_{11}$	447, 285	1a
Ls-26	17.11	3,5-Di-*O*-caffeoyl quinic acid	$C_{25}H_{24}O_{12}$	515, 353, 179	1b
Ls-27	17.30	Cichoric acid (di-*trans* isomer)	$C_{22}H_{18}O_{12}$	473, 311, 179	1b
Ls-28	17.32	Quercetin 3-*O*-(3″-*O*-acetyl)-glucoside	$C_{23}H_{22}O_{13}$	505, 463, 301	1a
Ls-29	17.60	4,5-Di-*O*-caffeoyl quinic acid	$C_{25}H_{24}O_{12}$	515, 353, 179	1b
Ls-30	17.64	Apigenin 7-*O*-glucuronide	$C_{21}H_{18}O_{11}$	445, 269	1b
Ls-31	17.69	Luteolin 4′-*O*-glucoside	$C_{21}H_{20}O_{11}$	447, 285	1b
Ls-32	17.85	Quercetin 3-*O*-(4″-*O*-acetyl)-glucoside	$C_{23}H_{22}O_{13}$	505, 463, 301	1a
Ls-33	18.01	Cichoric acid (*cis-trans* isomer)	$C_{22}H_{18}O_{12}$	473, 311, 179	2
Ls-34	19.02	Cichoric acid (*cis-cis* isomer)	$C_{22}H_{18}O_{12}$	473, 311, 179	2
Ls-35	19.29	*p*-Coumaroyl-caffeoyl-tartaric acid	$C_{22}H_{18}O_{11}$	457, 311, 295, 179, 163	2
Ls-36	19.91	Feruloyl-caffeoyl-tartaric acid	$C_{23}H_{20}O_{12}$	587, 425, 411, 193, 179	2
Ls-37	20.08	*p*-Coumaroyl-caffeoyl-tartaric acid	$C_{22}H_{18}O_{11}$	457, 311, 295, 179, 163	2
Ls-38	22.52	Luteolin	$C_{15}H_{10}O_6$	285	1b
Ls-39	23.81	Tetra-*O*-*p*-coumaroyl spermine	$C_{46}H_{50}N_4O_8$	785, 639, 493, 347, 163	2
Ls-40	23.87	Tetra-*O*-*p*-coumaroyl spermine	$C_{46}H_{50}N_4O_8$	785, 639, 493, 347, 163	2
Ls-41	24.03	Tetra-*O*-*p*-coumaroyl spermine	$C_{46}H_{50}N_4O_8$	785, 639, 493, 347, 163	2
Ls-42	24.17	Tetra-*O*-*p*-coumaroyl spermine	$C_{46}H_{50}N_4O_8$	785, 639, 493, 347, 163	2
Ls-43	24.63	Apigenin	$C_{15}H_{10}O_5$	269	1b

* Identification levels: (1) identified compounds after comparison of retention times, UV and mass-spectral data with previosly isolated compounds (1a) or comercial reference standard (1b) or isolated in present work (1c); (2) putatively annotated compounds after comparison of retention times, UV and mass-spectral data with literature data.

Table S14. Synopsis of compounds found in six Asteraceae species.

Compound	Aj	Cn	Ch	Ed	Ic	Ls
1. *Benzoates*						
1.1. Hydroxybenzoic acid glucosides						
Protocatechuic acid *O*-hexoside		√				√
Protocatechuic acid *O*-hexoside		√	√			√
Protocatechuic acid 4-*O*-glucoside		√	√	√		√
1.2. Hydroxybenzoyl quinic acids						
Vanilloyl quinic acid (probably 1-*O*-isomer)						√
Vanilloyl quinic acid (probably 4-*O*-isomer)						√
Vanilloyl quinic acid (probably 5-*O*-isomer)						√
Vanilloyl quinic acid (probably 5-*O*-isomer)						√
Divanilloyl quinic acid (probably 3,4-*O*-isomer)						√
Divanilloyl quinic acid (probably 3,5-*O*-isomer)						√
Divanilloyl quinic acid (probably 4,5-*O*-isomer)						√
2. *Coumarins*						
Esculetin 7-*O*-glucoside					√	
3. *Hydroxycinnamates*						
3.1. Caffeoyl glucaric acids						
3-*O*-Caffeoyl glucaric acid	√					
4-*O*-Caffeoyl glucaric acid	√	√				
2-*O*-Caffeoyl glucaric acid	√					
5-*O*-Caffeoyl glucaric acid	√					
3.2. Caffeoyl tartaric acids						
Caftaric acid isomer					√	
Caftaric acid					√	√
Cichoric acid (*di-trans* isomer)					√	√
Cichoric acid (*cis-trans* isomer)					√	√
Cichoric acid (*cis-cis* isomer)						√
3.3. *p*-Coumaroyl tartaric acids						
Coutaric acid					√	
3.4. Mixed tartaric acids						
p-Coumaroyl-caffeoyl-tartaric acid					√	√
Feruloyl-caffeoyl-tartaric acid					√	√
p-Coumaroyl-caffeoyl-tartaric acid						√
3.4. *p*-Coumaroyl quinic acids						
4-*O*-*p*-Coumaroyl quinic acid		√	√			
5-*O*-*p*-Coumaroyl quinic acid		√	√	√		
3-*O*-*p*-Coumaroyl quinic acid		√	√	√		
3.5. Caffeoyl quinic acids						
4-*O*-Caffeoyl quinic acid (*trans*-)	√		√	√	√	√
4-*O*-Caffeoyl quinic acid (*cis*-)	√		√	√		
5-*O*-Caffeoyl quinic acid (*trans*-)	√	√	√	√	√	√
3-*O*-Caffeoyl quinic acid (*trans*-)	√		√	√	√	√
5-*O*-Caffeoyl quinic acid (*cis*-)	√			√	√	√
3,4-Di-O-caffeoyl quinic acid	√		√	√		√
3,5-Di-O-caffeoyl quinic acid	√		√	√		√
4,5-Di-O-caffeoyl quinic acid	√		√	√		√
3.6. Feruloyl quinic acids						
4-*O*-Feruloyl quinic acid		√			√	
5-*O*-Feruloyl quinic acid		√				
3-*O*-Feruloyl quinic acid		√				

4. *Flavonoids*						
4.1. Apigenin *O*-glucosides						
Apigenin 7-*O*-glucoside			√			
Apigenin 7-*O*-glucuronide						√
Apigenin 7-*O*-rutinoside			√			
Apigenin 7-*O*-(2″-*O*-*p*-coumaroyl)-glucoside				√		
Apigenin 7-*O*-(6″-*O*-*p*-coumaroyl)-glucoside				√		
Apigenin di-*O*-hexoside-*O*-acetate		√				
Apigenin di-*O*-hexoside-*O*-acetate		√				
4.2. Apigenin *C*-glucosides						
Apigenin 6-*C*-glucoside-8-*C*-arabinoside	√		√			
4.3. Acacetin *O*-glucosides						
Acacetin 7-*O*-glucoside			√			
4.4. Luteolin *O*-glucosides						
Luteolin 5-*O*-glucoside				√		
Luteolin 7-*O*-glucoside			√	√		√
Luteolin 3′-*O*-glucoside			√	√		√
Luteolin 4′-*O*-glucoside			√			√
Luteolin 7-*O*-rutinoside			√			
Luteolin 7-*O*-(2″-*O*-glucosyl)-glucoside		√				
Luteolin 7-O-(2″-*O*-(6‴-*O*-acetyl)-glucosyl)-glucoside		√				
Luteolin *O*-hexoside-*O*-pentoside		√				
Luteolin di-*O*-hexoside-*O*-acetate		√				
Luteolin tri-*O*-hexoside						√
Luteolin tri-*O*-hexoside						√
4.5. Chrysoeriol *O*-glucosides						
Chrysoeriol 7-*O*-glucoside			√	√	√	√
Chrysoeriol 4′-*O*-glucoside			√			
Chrysoeriol 7-*O*-(2″-*O*-acetyl)-glucoside			√			
Chrysoeriol 7-*O*-(6″-*O*-acetyl)-glucoside			√			
Chrysoeriol 7-*O*-(2″-*O*-(6‴-*O*-acetyl)-glucosyl)-glucoside		√				
4.6. 6-Hydroxyluteolin *O*-glucosides						
6-Hydroxyluteolin di-*O*-hexoside	√					
4.7. Pectolinarigenin *O*-glucosides						
Pectolinarigenin 7-*O*-glucoside			√			
4.8. Kaempferol *O*-glucosides						
Kaempferol 7-*O*-glucoside					√	
Kaempferol 3-*O*-neohesperidoside						√
Kaempferol 3-*O*-rutinoside						√
Kempferol 3-*O*-sophoroside					√	
Kaempferol 3-*O*-gentiobioside					√	
Kaempferol di-*O*-hexoside					√	
4.9. Quercetin *O*-glucosides						
Quercetin 3-*O*-glucoside				√		
Quercetin 3-*O*-galactoside				√		
Quercetin 3-*O*-(2″-*O*-arabinosyl)-glucoside					√	
Quercetin 3-*O*-(6″-*O*-arabinosyl)-glucoside					√	
Quercetin 3-*O*-neohesperidoside	√				√	
Quercetin 3-*O*-rungioside	√					
Quercetin 3-*O*-(4″-*O*-rhamnosyl)-glucoside	√					
Quercetin 3-*O*-rutinoside	√				√	√
Quercetin 3-*O*-sophoroside					√	
Quercetin 3-*O*-gentiobioside	√				√	

Quercetin 3-*O*-(2″-*O*-acetyl)-glucoside	√					
Quercetin 3-*O*-(3″-*O*-acetyl)-glucoside						√
Quercetin 3-*O*-(4″-*O*-acetyl)-glucoside	√					√
Quercetin 3-O-(6″-O-acetyl)-glucoside	√					√
4.10. Isorhamnetin *O*-glucosides						
Isorhamnetin 3-*O*-(2″-*O*-acetyl)-glucoside	√					
Isorhamnetin 3-*O*-(6″-*O*-acetyl)-glucoside	√					
4.11. Flavone aglycones						
Apigenin						√
Luteolin						√
Cirsiliol	√					
Cirsilineol	√					
4.12. Flavonol aglycones						
Axillarin	√					
Chrysosplenetin	√					
5. *Phenylamines*						
5.1. Tri-*O*-*p*-coumaroyl spermines						
Tri-*O*-*p*-coumaroyl spermine	√					
Tri-*O*-*p*-coumaroyl spermine	√					
Tri-*O*-*p*-coumaroyl spermine	√					
5.2. Tetra-*O*-*p*-coumaroyl spermines						
Tetra-*O*-*p*-coumaroyl spermines						√
Tetra-*O*-*p*-coumaroyl spermine						√
Tetra-*O*-*p*-coumaroyl spermine						√
Tetra-*O*-*p*-coumaroyl spermine	√					√
5.3. Tri-*O*-*p*-coumaroyl-spermidine						
N^1,N^5,N^{10}-Tri-*O*-(*EEE*)-*p*-coumaroyl-spermidine				√		