Supporting Information

***Rec. Nat. Prod*. 20:1 (2026):e25093633**

Delving into the phytochemical constituents and biological activities of *Scorzonera coriacea* extracts: new perspectives from *in vitro* and *in silico* studies

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S1. UHPLC–MS/MS analysis of polyphenolic compounds

The phytochemical analysis of the tested extracts was assessed according to the previously reported method using high-performance liquid chromatographic (HPLC) analysis joined with an ESI-MS/MS spectrometer detector. This technique allowed tentative identification of phytoconstituents based on the molecular weights. The plant extract (100 µg/ml) was dissolved in methanol (HPLC-grade) and then filtered via a membrane disc (0.20 µm). Then, the filtrate (10 µL) was injected into HPLC-ESI-MS/MS. The used HPLC instrument has the following specifications: Waters® stocked with a reversed-phase C-18 column (ACQUITY UPLC-BEH C-18, particle size ~ 1.7 µm, dimensions = 2.1 × 50 mm). Before injection, the mobile phase was filtered through a membrane disc filter (0.2 µm) and sonicated. The elution period took 35 min using gradient elution (water and methanol acidified with 0.1% formic acid) with a flow rate of 0.2 mL/min. On an XEVO TQD triple quadrupole instrument, positive and negative ions were acquired using ESI-MS. Waters® Corporation, Milford, MA 01757, U.S.A. supplied the HPLC unit and mass spectrometer. Edwards®, U.S.A., provided the vacuum pump at desolvation temperatures of 150 and 440 °C. The mass spectra were obtained using the software Masslynx 4.1 at an ESI range m/z of 100–1000. To tentatively identify the obtained mass spectra, the peak retention time (tR) and their fragmentation pattern were compared with the reported data in the literature.

Assays for Total Phenolic and Flavonoid Contents

The total phenolic content was determined by employing the methods given in the literature with some modification. Sample solution (0.25 mL) was mixed with diluted Folin–Ciocalteu reagent (1 mL, 1:9, v/v) and shaken vigorously. After 3 min, Na_2CO_3 solution (0.75 mL, 1%) was added and the sample absorbance was read at 760 nm after a 2 h incubation at room temperature. The total phenolic content was expressed as milligrams of gallic acid equivalents (mg GAE/g extract)(Uysal et al., 2017).

The total flavonoid content was determined using the $AlCl_3$ method. Briefly, sample solution (1 mL) was mixed with the same volume of aluminum trichloride (2%) in methanol. Similarly, a blank was prepared by adding sample solution (1 mL) to methanol (1 mL) without $AlCl_3$. The sample and blank absorbances were read at 415 nm after a 10 min incubation at room temperature. The absorbance of the blank was subtracted from that of the sample. Rutin was used as a reference standard and the total flavonoid content was expressed as milligrams of rutin equivalents (mg RE/g extract) (Uysal et al., 2017).

Determination of Antioxidant and Enzyme Inhibitory Effects

Antioxidant (DPPH and ABTS radical scavenging, reducing power (CUPRAC and FRAP), phosphomolybdenum and metal chelating (ferrozine method)) and enzyme inhibitory activities (cholinesterase (Elmann's method), tyrosinase (dopachrome method), α-amylase (iodine/potassium iodide method), α -glucosidase (chromogenic PNPG method) and pancreatic lipase (*p*-nitrophenyl butyrate (p-NPB) method) were determined using the methods previously described by Uysal et al. (Uysal et al., 2017) and Grochowski et al. (Grochowski et al., 2017)

For the DPPH (1,1-diphenyl-2-picrylhydrazyl) radical scavenging assay: Sample solution was added to 4 mL of a 0.004% methanol solution of DPPH. The sample absorbance was read at 517 nm after a 30 min incubation at room temperature in the dark. DPPH radical scavenging activity was expressed as milligrams of trolox equivalents (mg TE/g extract).

For ABTS (2,2′-azino-bis(3-ethylbenzothiazoline) 6-sulfonic acid) radical scavenging assay: Briefly, ABTS+ was produced directly by reacting 7 mM ABTS solution with 2.45 mM potassium persulfate and allowing the mixture to stand for 12–16 in the dark at room temperature. Prior to beginning the assay, ABTS solution was diluted with methanol to an absorbance of 0.700 ± 0.02 at 734 nm. Sample solution was added to ABTS solution (2 mL) and mixed. The sample absorbance was read at 734 nm after a 30 min incubation at room temperature. The ABTS radical scavenging activity was expressed as milligrams of trolox equivalents (mg TE/g extract).

For CUPRAC (cupric ion reducing activity) activity assay: Sample solution was added to premixed reaction mixture containing $CuCl_2$ (1 mL, 10 mM), neocuproine (1 mL, 7.5 mM) and NH_4Ac buffer (1 mL, 1 M, pH 7.0). Similarly, a blank was prepared by adding sample solution (0.5 mL) to premixed reaction mixture (3 mL) without $CuCl_2$. Then, the sample and blank absorbances were read at 450 nm after a 30 min incubation at room temperature. The absorbance of the blank was subtracted from that of the sample. CUPRAC activity was expressed as milligrams of trolox equivalents (mg TE/g extract).

For FRAP (ferric reducing antioxidant power) activity assay: Sample solution was added to premixed FRAP reagent (2 mL) containing acetate buffer (0.3 M, pH 3.6), 2,4,6-tris(2-pyridyl)-S-triazine (TPTZ) (10 mM) in 40 mM HCl and ferric chloride (20 mM) in a ratio of 10:1:1 (v/v/v). Then, the sample absorbance was read at 593 nm after a 30 min incubation at room temperature. FRAP activity was expressed as milligrams of trolox equivalents (mg TE/g extract).

For phosphomolybdenum method: Sample solution was combined with 3 mL of reagent solution (0.6 M sulfuric acid, 28 mM sodium phosphate and 4 mM ammonium molybdate). The sample absorbance was read at 695 nm after a 90 min incubation at 95 °C. The total antioxidant capacity was expressed as millimoles of trolox equivalents (mmol TE/g extract).

For metal chelating activity assay: Briefly, sample solution was added to $FeCl_2$ solution (0.05 mL, 2 mM). The reaction was initiated by the addition of 5 mM ferrozine (0.2 mL). Similarly, a blank was prepared by adding sample solution (2 mL) to $FeCl_2$ solution (0.05 mL, 2 mM) and water (0.2 mL) without ferrozine. Then, the sample and blank absorbances were read at 562 nm after 10 min incubation at room temperature. The absorbance of the blank was sub-tracted from that of the sample. The metal chelating activity was expressed as milligrams of EDTA (disodium edetate) equivalents (mg EDTAE/g extract).

For Cholinesterase (ChE) inhibitory activity assay: Sample solution (was mixed with DTNB (5,5-dithio-bis(2-nitrobenzoic) acid, Sigma, St. Louis, MO, USA) (125 µL) and AChE (acetylcholines-terase (Electric ell acetylcholinesterase, Type-VI-S, EC 3.1.1.7,Sigma)), or BChE (butyrylcholinesterase (horse serum butyrylcholinesterase, EC 3.1.1.8, Sigma)) solution (25 µL) in Tris–HCl buffer (pH 8.0) in a 96-well microplate and incubated for 15 min at 25 °C. The reaction was then initiated with the addition of acetylthiocholine iodide (ATCI, Sigma) or butyrylthiocholine chloride (BTCl, Sigma) (25 µL). Similarly, a blank was prepared by adding sample solution to all reaction reagents without enzyme (AChE or BChE) solution. The sample and blank absorbances were read at 405 nm after 10 min incubation at 25 °C. The absorbance of the blank was subtracted from that of the sample and the cholinesterase inhibitory activity was expressed as galanthamine equivalents (mgGALAE/g extract).

For Tyrosinase inhibitory activity assay: Sample solution was mixed with tyrosinase solution (40 µL, Sigma) and phosphate buffer (100 µL, pH 6.8) in a 96-well microplate and incubated for 15 min at 25 °C. The reaction was then initiated with the addition of L-DOPA (40 µL, Sigma). Similarly, a blank was prepared by adding sample solution to all reaction reagents without enzyme (tyrosinase) solution. The sample and blank absorbances were read at 492 nm after a 10 min incubation at 25 °C. The absorbance of the blank was subtracted from that of the sample and the tyrosinase inhibitory activity was expressed as kojic acid equivalents (mgKAE/g extract).

For α-amylase inhibitory activity assay: Sample solution was mixed with α-amylase solution (ex-porcine pancreas, EC 3.2.1.1, Sigma) (50 µL) in phosphate buffer (pH 6.9 with 6 mM sodium chloride) in a 96-well microplate and incubated for 10 min at 37 °C. After pre-incubation, the reaction was initiated with the addition of starch solution (50 µL, 0.05%). Similarly, a blank was prepared by adding sample solution to all reaction reagents without enzyme (α-amylase) solution. The reaction mixture was incubated 10 min at 37 °C. The reaction was then stopped with the addition of HCl (25 µL, 1 M). This was followed by addition of the iodine-potassium iodide solution (100 µL). The sample and blank absorbances were read at 630 nm. The absorbance of the blank was subtracted from that of the sample and the α-amylase inhibitory activity was expressed as acarbose equivalents (mmol ACE/g extract).

For α-glucosidase inhibitory activity assay: Sample solution was mixed with glutathione (50 µL), α-glucosidase solution (from Saccharomyces cerevisiae, EC 3.2.1.20, Sigma) (50 µL) in phosphate buffer (pH 6.8) and PNPG (4-N-trophenyl-α-D-glucopyranoside, Sigma) (50 µL) in a 96-well microplate and incubated for 15 min at 37 °C. Similarly, a blank was prepared by adding sample solution to all reaction reagents without enzyme (α-glucosidase) solution. The reaction was then stopped with the addition of sodium carbonate (50 µL, 0.2 M). The sample and blank absorbances were read at 400 nm. The absorbance of the blank was subtracted from that of the sample and the α-glucosidase inhibitory activity was expressed as acarbose equivalents (mmol ACE/g extract).

Table S1. Parameters of LC/MS/MS method

Compound name	Expected RT (min)	Polarity	Precursor (m/z)	Product 1 (m/z)	Collision Energy 1 (V)	Product 2 (m/z)	Collision Energy 2 (V)
Apigenin-7-glucoside	6.60	Negative	431.250	238.967	50.04	268.050	34.12
Apigenin	7.70	Positive	271.300	118.883	30.63	152.883	29.47
Caffeic acid	5.62	Negative	179.033	106.967	21.83	134.967	15.26
Luteolin 7-rutinoside	5.60	Negative	593.317	150.883	62.57	285.050	37.65
Luteolin	7.80	Negative	285.033	132.883	34.67	150.883	26.18
Orientin	6.20	Negative	447.200	327.050	21.48	357.050	19.61
Quercetin	7.80	Negative	301.050	150.883	21.23	178.967	17.49

Table S2. Validation data for the quantified phenolic compounds.

Compound name	Ionization mode	Parent m/z	Linear regression equation	R^2	Linearity range, mg/L	Linearity range, mg/ kg	LOD/ LOQ µg/L	Re-covery, %
Apigenin 7-glucoside	Negative	431.250	Y = 0.228047*X +0.000584383	0.997	0.01 – 2.50	0.5 - 125	2/6	103.2
Apigenin	Positive	271.300	Y = 0.230611*X +0.020491	99.91	0.01 - 5.00	0.5 - 250	2 / 6	99.26
Caffeic acid	Negative	179.033	Y = 0.247735*X +0.061756	0.979	0.25 – 2.50	12.5 - 125	10/30	102.4
Luteolin	Negative	285.033	Y = 0.0787429*X +0.0000165593	0.999	0.01 – 1.00	0.5 - 50	2/6	98.0
Luteolin 7-rutinoside	Negative	593.317	Y = 0.372884*X +0.0000635256	0.999	0.01 – 0.50	0.5 - 25	2/6	98.0
Orientin	Negative	447.200	Y = 0.141617*X - 0.000309574	0.999	0.01 – 2.00	0.5 - 100	2/6	102.0
Quercetin	Negative	301.050	Y = 0.250951*X - 0.012511	0.999	0.01 – 5.00	0.5 - 250	3/9	98.84

Table S3: Docking grid center coordinates and box dimensions for the selected protein targets.

Target Protein	**PDB ID**	**Center X, Y, Z**	**Grid Size X, Y, Z**
AChE	7E3H	-54.44, 32.90, -28.65	25, 25, 25
BChE	6EQP	32.16, -16.33, 40.73	25, 25, 25
Tyrosinase	6QXD	21.81, 12.22, 91.40	25, 25, 25
Amylase	2QV4	14.188, 48.964, 22.886	28, 28, 24
Glucosidase	7KBJ	-18.79, 2.18, 15.75	25, 25, 25
AKT	4GV1	-17.903, 0.789, 15.945	20,38,34
BRPF1	5MWZ	-9.411, 9.221, 6.159	40,40,40
CDK2	6GUE	-6.463, -24.101, 25.309	40,40,40
CDK4	2W96	5.126, -5.071, 74.401	42,64,74
CyclinD1	2W99	15.991, 26.615, 49.003	26,30,26
MYC	1NKP	71.779, 68.731, 41.5	60,72,40
PD-1	5N2F	32.621, 17.007, 130.416	30,30,30
TERT	5CQG	3.629, -3.75, -45.599	126,98,126
PPARγ	1I7I	13.814,18.569,16.359	66,46,106

Table S4: The docking score (kcal/mol) and interacting residues of the protein.

Compound	Target	PDB ID	Binding energy	RMSD	Interaction
					Type and Binding site
Kaempferol-3-O-glucoside	Amylase	2QV4	-8.7	**0.8**	Hbond- GLN:63;GLN:63;ARG:195;ASP:300;ASP:300;HIS:305 Hydrophobic- TRP:58;TRP:59;TYR:62 Pi-Stacking- TRP:59 Salt Bridge- HIS:305
Catechin	Amylase	2QV4	-8.8	**0.9**	Hbond- GLN:63;GLN:63;ARG:195;ARG:195;GLU:233;ASP:300;ASP:300;ASP:300;HIS:305 Hydrophobic- TRP:58;TRP:59;TRP:59 Pi-Stacking- TYR:62
Eupatorin	Amylase	2QV4	-8.0	**0.4**	Hbond- GLN:63 Hydrophobic- TRP:59;TYR:62;LEU:165 Pi-Stacking- TRP:59
Dihydroxy-Trimethoxyflavone	Amylase	2QV4	-8.2	**0.2**	Hbond- ARG:195;ASP:197;HIS:201;HIS:299;ASP:300 Hydrophobic- LYS:200;LYS:200;ILE:235;ILE:235 Pi-Stacking- HIS:201
Quercetin	Amylase	2QV4	-9.1	**0.1**	Hbond- TYR:62;GLN:63;ARG:195;ARG:195;GLU:233;HIS:299 Hydrophobic- TRP:58;TRP:59;TYR:62 Pi-Stacking- TRP:59;TYR:62
Kaempferol	Amylase	2QV4	-8.7	**0.2**	Hbond- GLN:63;HIS:101;ARG:195;ASP:197 Hydrophobic- TRP:58;TRP:59;TYR:62 Pi-Stacking- TRP:59
Eriodictyol-7-O-neohesperidoside	Amylase	2QV4	-10.1	**0.6**	Hbond- GLN:63;ARG:195;ASP:197;LYS:200;LYS:200;HIS:201;ILE:235;ILE:235;HIS:299 Hydrophobic- TRP:58;TRP:59;TRP:59;TYR:62;LEU:162 Salt Bridge- HIS:201

5-Caffeoylquinic acid	Amylase	2QV4	-8.3	**0.2**	Hbond- GLN:63;ALA:198;HIS:201;GLU:233;GLU:233;GLU:233 Hydrophobic- TRP:59;TYR:62;ILE:235 Pi-Stacking- TRP:59 Salt Bridge- HIS:299
Taxifolin	Amylase	2QV4	-9.2	**0.5**	Hbond- GLN:63;ARG:195;ARG:195;ASP:197;GLU:233;HIS:299 Hydrophobic- TRP:58;TRP:59;TYR:62 Pi-Stacking- TRP:59;TYR:62
Isoquercitrin	Amylase	2QV4	-8.9	**1.1**	Hbond- GLN:63;GLN:63;ASP:197;HIS:299;ASP:300;ASP:300;HIS:305 Hydrophobic- TRP:58;TRP:59 Pi-Stacking- TRP:59 Salt Bridge- HIS:305
Afzelin	Amylase	2QV4	-9.3	**0.1**	Hbond- ARG:195;ARG:195;ASP:197;LYS:200;HIS:201;HIS:299;HIS:305 Hydrophobic- TRP:58
Quercetin-3-O-rutinoside	Amylase	2QV4	-9.2	**0.8**	Hbond- GLN:63;GLN:63;ARG:195;ALA:198;SER:199;LYS:200;LYS:200;ILE:235;ILE:235;HIS:299;HIS:305 Hydrophobic- TRP:58;TRP:58;TYR:62;TYR:151 Pi-Stacking- TRP:59;TRP:59;TRP:59;HIS:201 Salt Bridge- HIS:201;HIS:305
Myricetin	Amylase	2QV4	-9.3	**1.1**	Hbond- TYR:62;GLN:63;ARG:195;GLU:233;HIS:299;ASP:300 Hydrophobic- TRP:58;TYR:62;TYR:62 Pi-Stacking- TRP:59;TRP:59
Diosmetin	Amylase	2QV4	-8.2	**0.3**	Hbond- GLN:63;HIS:101 Hydrophobic- TRP:58;TRP:58;TRP:59;TYR:62;TYR:62 Pi-Stacking- TRP:59;TRP:59
Malvidin 3-O-beta-D-glucoside	Amylase	2QV4	-7.9	**1.9**	Hbond- GLN:63;ARG:195;GLU:233;GLU:233;HIS:299;ASP:300;HIS:305;HIS:305 Hydrophobic- TRP:59;THR:163;LEU:165
3-5-Dicaffeoylquinic acid	Amylase	2QV4	-8.7	**0.2**	Hbond- TRP:59;GLN:63;ARG:195;ARG:195;ASP:197;GLU:233;GLU:233;HIS:299;ASP:300 Hydrophobic- TRP:58;TRP:59;TRP:59;TYR:62;TYR:62;LEU:162 Salt Bridge- HIS:305;HIS:305
Diosmetin-7-O-glucoside	Amylase	2QV4	-9.4	**0.5**	Hbond- HIS:101;THR:163;ASP:197;ALA:198;ASP:300 Hydrophobic- TRP:58;TRP:59;TRP:59;LEU:165

Apigenin 6-C-glucoside 8-C-arabinoside	Amylase	2QV4	-9.3	**1.0**	Hbond- GLN:63;THR:163;GLY:164;ARG:195;ARG:195;ASP:197;HIS:299;HIS:305;HIS:305 Hydrophobic- TYR:62
1-3-Dicaffeoylquinic acid	Amylase	2QV4	-7.5	**0.5**	Hbond- ASP:197;ALA:307 Hydrophobic- THR:163 Salt Bridge- LYS:200;LYS:200;HIS:201
Orientin	Amylase	2QV4	-8.3	**0.6**	Hbond- GLN:63;THR:163;ARG:195;ARG:195;HIS:299;HIS:305;HIS:305;HIS:305 Hydrophobic- TRP:58 Pi-Stacking- TYR:62
Isoorientin	Amylase	2QV4	-8.8	**0.3**	Hbond- GLN:63;ASN:105;ALA:106;GLY:164;ARG:195;ARG:195;ALA:198;GLU:233;HIS:299;ASP:300 Hydrophobic- TRP:58;TYR:62;LEU:165 Pi-Stacking- TYR:62
Kaempferol-3-O-glucoside	AChE	7E3H	-8.5	**0.3**	Hbond- GLY:120;GLY:120;TYR:124;TYR:124;TYR:124;SER:125;GLY:126;PHE:295;HIS:447 Hydrophobic- TRP:86;TYR:337;PHE:338;TYR:341
Catechin	AChE	7E3H	-9.6	**1.0**	Hbond- TYR:72;ASP:74;GLY:120;TYR:133;GLU:202;TYR:337;TYR:337 Hydrophobic- ASP:74;TRP:86;TYR:124 Pi-Stacking- TRP:86;TRP:86
Dihydroxy-Trimethoxyflavone	AChE	7E3H	-8.3	**0.5**	Hbond- TRP:86;TYR:124 Hydrophobic- TYR:124;PHE:297;PHE:338;PHE:338 Pi-Stacking- TYR:341
Quercetin	AChE	7E3H	-9.8	**0.0**	Hbond- GLN:71;TYR:72;ASP:74;ASP:74;GLY:120;TYR:133;GLU:202;TYR:337 Hydrophobic- ASP:74;TRP:86 Pi-Stacking- TRP:86;TRP:86;TYR:124
Kaempferol	AChE	7E3H	-9.8	**0.4**	Hbond- TRP:86;GLY:120;GLY:120;TYR:124;TYR:124 Hydrophobic- TRP:86;TYR:337;PHE:338;TYR:341
5-Caffeoylquinic acid	AChE	7E3H	-8.8	**0.7**	Hbond- GLY:120;GLY:120;TYR:124;GLU:202;TYR:337;TYR:341 Hydrophobic- TRP:86;TRP:86;TRP:86;TYR:124;PHE:297 Salt Bridge- HIS:447
Taxifolin	AChE	7E3H	-9.6	**0.6**	Hbond- GLN:71;ASP:74;GLY:120;GLY:126;TYR:133;TYR:133;TYR:337;TYR:337;HIS:447 Hydrophobic- ASP:74;TRP:86;TRP:86

					Pi-Stacking- TRP:86;TYR:124
Isoquercitrin	AChE	7E3H	-8.7	**0.8**	Hbond- TRP:86;GLY:120;GLY:121;TYR:124;SER:125;GLY:126;GLU:202;GLU:202;PHE:295 Hydrophobic- TRP:86;TYR:337;PHE:338;TYR:341
Afzelin	AChE	7E3H	-8.3	**1.1**	Hbond- TRP:86;TYR:124;TYR:124;SER:125;GLY:126;GLU:202;PHE:295 Hydrophobic- TRP:86;TRP:86;TYR:337;PHE:338;TYR:341
4-Hydroxycoumarin	AChE	7E3H	-7.6	**0.3**	Hbond- TYR:124;TYR:124;TYR:337 Hydrophobic- TYR:337 Pi-Stacking- TRP:86;TRP:86;TRP:86
Myricetin	AChE	7E3H	-9.9	**0.5**	Hbond- GLN:71;ASP:74;ASP:74;ASN:87;GLY:120;GLY:120;TYR:133;TYR:337;TYR:337 Hydrophobic- TRP:86 Pi-Stacking- TRP:86;TRP:86
Diosmetin	AChE	7E3H	-8.8	**0.4**	Hbond- GLY:120;GLU:202;TYR:337 Hydrophobic- TRP:86;TRP:86;PHE:297
3-5-Dicaffeoylquinic acid	AChE	7E3H	-7.5	**1.0**	Hbond- TRP:86;GLY:120;SER:125;GLY:126;TYR:337;TYR:337 Hydrophobic- TYR:72;ASP:74;TRP:86;TYR:124;PHE:338;TYR:341 Salt Bridge- HIS:447
1-3-Dicaffeoylquinic acid	AChE	7E3H	-8.1	**0.5**	Hbond- GLN:71;ASP:74;GLY:121;SER:125;SER:125;GLY:126;ALA:127;TYR:337 Hydrophobic- TYR:72;ASP:74;TRP:86;TRP:86;TRP:86;TYR:124;PHE:297 Salt Bridge- HIS:447
Hydroxycoumarin	AChE	7E3H	-7.6	**0.3**	Hbond- TYR:124;TYR:337 Hydrophobic- TRP:86;TYR:337 Pi-Stacking- TRP:86;TRP:86;TRP:86
Caffeic Acid	AChE	7E3H	-7.4	**0.1**	Hbond- GLY:120;TYR:124;TYR:133;TYR:133;TYR:337 Hydrophobic- TRP:86;TRP:86 Pi-Stacking- TRP:86
Orientin	AChE	7E3H	-9.5	**0.6**	Hbond- TYR:72;TYR:72;ASP:74;GLY:120;TYR:133;GLU:202;TYR:337;TYR:341;TYR:341 Hydrophobic- ASP:74;TRP:86;TRP:86;TRP:86;TYR:124

Umbelliferone	AChE	7E3H	-7.5	**0.5**	Hbond- TYR:124 Hydrophobic- TRP:86;TRP:86;TYR:337 Pi-Stacking- TRP:86;TRP:86
Kaempferol-3-O-glucoside	glucosidase	7KBJ	-8.2	**0.8**	Hbond- GLU:248;LEU:252;GLY:253;GLY:254;GLU:287;TYR:291;ARG:334;ARG:334;ARG:352 Hydrophobic- TRP:331 Pi-Stacking- TYR:291 Salt Bridge- ARG:352
Catechin	glucosidase	7KBJ	-8.4	**1.0**	Hbond- GLU:248;TYR:291;ARG:334;ARG:352 Hydrophobic- LEU:252;ILE:257;TYR:291
Eupatorin	glucosidase	7KBJ	-7.9	**0.1**	Hbond- GLY:253;ARG:334;LEU:344 Hydrophobic- PHE:350 Pi-Cation- ARG:352;ARG:352
Dihydroxy-Trimethoxyflavone	glucosidase	7KBJ	-7.3	**0.5**	Hbond- GLY:264;TYR:291 Hydrophobic- LEU:344
Quercetin	glucosidase	7KBJ	-8.4	**0.3**	Hbond- GLU:248;GLY:264;ASN:265;MET:289;TYR:291;TYR:291;ARG:334;ARG:352 Hydrophobic- LEU:252;ILE:257;TYR:291
Kaempferol	glucosidase	7KBJ	-8.2	**0.8**	Hbond- ASN:265;TYR:291;ARG:334;ARG:352 Hydrophobic- ILE:257;TYR:291
Eriodictyol-7-O-neohesperidoside	glucosidase	7KBJ	-8.6	**nd**	Hbond- GLN:247;GLY:253;GLY:254;LYS:283;MET:289;TYR:291;LEU:344;ALA:345;ARG:352;ARG:352;ARG:352 Hydrophobic- VAL:249;LEU:252;LEU:344;PHE:350 Salt Bridge- ARG:352
5-Caffeoylquinic acid	glucosidase	7KBJ	-8.8	**4.5**	Hbond- GLN:247;GLU:248;ASP:251;LEU:252;GLY:253;GLY:254;LYS:283;ARG:334;ARG:334;ALA:345;ARG:352 Hydrophobic- LEU:252;TYR:291;LEU:344 Salt Bridge- LYS:283;ARG:352
Taxifolin	glucosidase	7KBJ	-8.3	**0.6**	Hbond- GLU:248;GLY:253;ASN:265;ARG:334;ARG:352;ARG:352 Hydrophobic- LEU:252;ILE:257;TYR:291

Isoquercitrin	glucosidase	7KBJ	-8.1	**1.1**	Hbond- GLU:248;ASP:251;LEU:252;GLY:253;GLY:254;TYR:291;ARG:334;ARG:334;ARG:352;ARG:352 Hydrophobic- TRP:331 Pi-Stacking- TYR:291 Salt Bridge- ARG:352
Afzelin	glucosidase	7KBJ	-8.5	**0.5**	Hbond- GLU:248;GLU:248;LEU:252;GLY:253;GLY:254;TYR:291;ARG:334;ARG:334 Hydrophobic- TRP:331 Pi-Stacking- TYR:291 Salt Bridge- ARG:352
Quercetin-3-O-rutinoside	glucosidase	7KBJ	-8.8	**6.5**	Hbond- TYR:246;TYR:246;ASP:251;LEU:252;GLY:253;SER:290;ARG:352;ARG:352;ARG:352 Hydrophobic- TYR:291;TRP:331 Salt Bridge- ARG:352
Myricetin	glucosidase	7KBJ	-7.7	**0.8**	Hbond- GLN:247;MET:289;TYR:291;TYR:291;TYR:291 Pi-Cation- ARG:352
Diosmetin	glucosidase	7KBJ	-8.3	**0.5**	Hbond- GLN:247;ARG:334 Hydrophobic- LEU:252;TYR:291;TYR:291
3-5-Dicaffeoylquinic acid	glucosidase	7KBJ	-9.1	**4.5**	Hbond- GLN:247;ASP:251;LEU:252;GLY:253;GLY:254;LYS:283;MET:289;ALA:345;TYR:348;ARG:352 Hydrophobic- LEU:252;LEU:252;LEU:344 Salt Bridge- ARG:352
Diosmetin-7-O-glucoside	glucosidase	7KBJ	-9.8	**0.5**	Hbond- GLU:248;GLU:248;LEU:252;GLY:253;LYS:283;SER:290;SER:290;ARG:334;ARG:352;ARG:352;ARG:352 Hydrophobic- PHE:350;PHE:350 Salt Bridge- ARG:352 Pi-Cation- ARG:352;ARG:352
1-3-Dicaffeoylquinic acid	glucosidase	7KBJ	-8.4	**1.0**	Hbond- PHE:237;PHE:237;PRO:238;GLY:240;ASP:251;ASP:251;GLY:253;ARG:267;PHE:271;MET:289;ARG:334;ALA:345 Hydrophobic- PHE:237;LEU:252;GLU:270;TYR:291;TRP:331;LEU:344 Salt Bridge- LYS:283;LYS:283;ARG:352
Orientin	glucosidase	7KBJ	-7.1	**0.2**	Hbond- GLY:264;SER:290;TYR:291;TYR:291;ARG:334;ARG:352;ARG:352;ARG:352 Hydrophobic- LEU:344;PHE:350 Pi-Cation- ARG:352;ARG:352

Isoorientin	glucosidase	7KBJ	-9.3	**0.2**	Hbond- GLU:248;LYS:283;LEU:344;ALA:345;TYR:348;TYR:348;ARG:352;ARG:352 Hydrophobic- TYR:291;LEU:344;PHE:350 Pi-Cation- ARG:334
Kaempferol-3-O-glucoside	BChE	6EQP	-10.4	**0.7**	Hbond- ASP:70;GLY:78;GLY:115;GLY:115;TYR:128;SER:198 Pi-Stacking- PHE:329;PHE:329;TYR:332
Catechin	BChE	6EQP	-8.8	**0.2**	Hbond- TRP:82;GLY:115;TYR:128;ALA:328;ALA:328 Hydrophobic- TRP:82;TRP:430 Pi-Stacking- TRP:82;TRP:82
Dihydroxy-Trimethoxyflavone	BChE	6EQP	-7.9	**0.4**	Hbond- ASP:70;THR:120 Hydrophobic- LEU:286 Pi-Stacking- TRP:231;TRP:231;PHE:329
Quercetin	BChE	6EQP	-8.9	**0.6**	Hbond- GLY:116;GLY:117;ALA:199 Hydrophobic- LEU:286;PHE:398 Pi-Stacking- TRP:82;TRP:231;TRP:231;PHE:329;HIS:438
Kaempferol	BChE	6EQP	-9.0	**0.8**	Hbond- GLY:115;GLY:115;THR:120;ALA:328 Hydrophobic- TRP:82;TYR:332;TRP:430 Pi-Stacking- TRP:82;TRP:82
Eriodictyol-7-O-neohesperidoside	BChE	6EQP	-8.7	**5.3**	Hbond- TRP:82;GLY:115;GLY:115;GLY:115;THR:120;THR:120;TYR:128;HIS:438 Hydrophobic- VAL:288;PHE:329;TYR:332;TRP:430
5-Caffeoylquinic acid	BChE	6EQP	-8.9	**0.9**	Hbond- GLY:115;GLY:115;TYR:128;GLU:197 Hydrophobic- TRP:82 Pi-Stacking- PHE:329
Taxifolin	BChE	6EQP	-8.8	**0.6**	Hbond- TRP:82;GLY:115;GLU:197;HIS:438 Hydrophobic- TRP:82;TRP:82;TRP:430
Isoquercitrin	BChE	6EQP	-10.6	**1.0**	Hbond- ASP:70;ASP:70;TRP:82;GLY:115;GLY:115;TYR:128;TYR:128;SER:198;PRO:285;TYR:332;HIS:438 Pi-Stacking- PHE:329;PHE:329;TYR:332
Afzelin	BChE	6EQP	-10.4	**0.7**	Hbond- ASP:70;GLY:115;TYR:128;TYR:128;SER:198;SER:198;LEU:286;TYR:332 Hydrophobic- TRP:82;TYR:332 Pi-Stacking- PHE:329;PHE:329

Quercetin-3-O-rutinoside	BChE	6EQP	-9.4	**0.3**	Hbond- ASP:70;GLY:78;SER:79;TRP:82;TRP:82;GLY:115;GLY:116;THR:120;GLU:197;TRP:430 Hydrophobic- ALA:328;PHE:329;PHE:329
Myricetin	BChE	6EQP	-8.8	**0.2**	Hbond- GLY:115;GLY:115;TYR:128;TYR:128;PRO:285 Hydrophobic- TRP:82;PHE:329 Pi-Stacking- TRP:82;TRP:82
Diosmetin	BChE	6EQP	-8.2	**0.5**	Hbond- GLY:117;SER:287 Hydrophobic- VAL:288;PHE:329 Pi-Stacking- TRP:82;PHE:329
Malvidin 3-O-beta-D-glucoside	BChE	6EQP	-10.0	**2.0**	Hbond- GLY:115;GLY:115;TYR:128;TYR:128;GLU:197;SER:198;ALA:328;TYR:440 Hydrophobic- PHE:329;TYR:332;TRP:430
3-5-Dicaffeoylquinic acid	BChE	6EQP	-9.4	**5.3**	Hbond- TRP:82;TRP:82;SER:198;LEU:286;TRP:430;TYR:440 Hydrophobic- TRP:82;TRP:82;ALA:328;PHE:329 Salt Bridge- HIS:438
Diosmetin-7-O-glucoside	BChE	6EQP	-8.6	**0.5**	Hbond- GLY:115;GLY:117;GLY:117;TYR:128;GLU:197;SER:198;ALA:328 Hydrophobic- TRP:82;TRP:82;PHE:329 Pi-Stacking- TRP:82
1-3-Dicaffeoylquinic acid	BChE	6EQP	-9.0	**0.6**	Hbond- ASP:70;TRP:82;TRP:82;TRP:82;TRP:82;GLY:115;GLY:116;GLY:117;TYR:128;SER:198;HIS:438 Hydrophobic- ASP:70;TRP:82;TRP:82;TRP:82;THR:120
Orientin	BChE	6EQP	-9.4	**0.6**	Hbond- THR:120;THR:120 Hydrophobic- ASP:70 Pi-Stacking- PHE:329
Umbelliferone	BChE	6EQP	-7.0	**0.4**	Hbond- GLY:115;HIS:438 Hydrophobic- TRP:82 Pi-Stacking- TRP:82;TRP:82;TRP:82
Kaempferol-3-O-glucoside	AKT	4GV1	-8.0	**0.7**	Hbond- PHE:161;GLY:162;LYS:179;THR:195;ASP:274;LYS:276;ASP:292 Hydrophobic- PHE:161;LEU:295
Catechin	AKT	4GV1	-7.9	**0.5**	Hbond- LYS:158;ALA:230 Hydrophobic- LEU:156;VAL:164;VAL:164;ALA:177;PHE:438

Eupatorin	AKT	4GV1	-7.8	**0.3**	Hbond- LYS:158;LYS:158 Hydrophobic- LEU:156;VAL:164;VAL:164
Dihydroxy-Trimethoxyflavone	AKT	4GV1	-7.8	**0.4**	Hbond- LYS:158;LYS:179;ASP:292 Hydrophobic- LEU:156;VAL:164;VAL:164;ALA:177;PHE:438
Quercetin	AKT	4GV1	-8.1	**0.5**	Hbond- LYS:158;GLU:228;ALA:230 Hydrophobic- VAL:164;ALA:177;PHE:438
Kaempferol	AKT	4GV1	-7.9	**7.0**	Hbond- LYS:158;LYS:158;GLU:228;ALA:230;ALA:230 Hydrophobic- VAL:164;ALA:177;PHE:438
Eriodictyol-7-O-neohesperidoside	AKT	4GV1	-9.4	**0.6**	Hbond- LEU:156;LYS:179;GLU:228;GLU:228;ALA:230;LYS:276
5-Caffeoylquinic acid	AKT	4GV1	-8.3	**0.4**	Hbond- THR:160;PHE:161;GLY:162;LYS:179;ALA:230;ASP:292 Hydrophobic- LEU:156;LEU:156;VAL:164;VAL:164;PHE:438
Taxifolin	AKT	4GV1	-7.6	**0.5**	Hbond- LYS:158;ALA:230;GLU:278;THR:291 Hydrophobic- LEU:156;VAL:164;PHE:438
Isoquercitrin	AKT	4GV1	-8.2	**1.0**	Hbond- GLY:159;PHE:161;GLY:162;LYS:179;LYS:276;GLY:294 Hydrophobic- PHE:161;LEU:295
Afzelin	AKT	4GV1	-8.2	**1.0**	Hbond- LYS:179;LYS:276;ASN:279 Hydrophobic- LEU:295
Quercetin-3-O-rutinoside	AKT	4GV1	-9.3	**0.1**	Hbond- LYS:158;LYS:179;HIS:194;LYS:276;ASN:279 Hydrophobic- VAL:164;PHE:438 Salt Bridge- LYS:276
Myricetin	AKT	4GV1	-8.3	**0.3**	Hbond- LYS:158;LYS:158;GLU:228;ALA:230;ALA:230;GLU:234 Hydrophobic- VAL:164;ALA:177;PHE:438
Diosmetin	AKT	4GV1	-7.8	**0.4**	Hbond- GLU:228;ALA:230;ALA:230 Hydrophobic- VAL:164;ALA:177;ALA:230;THR:291
Malvidin 3-O-beta-D-glucoside	AKT	4GV1	-8.3	**2.0**	Hbond- GLY:157;GLY:157;GLY:159;THR:160;PHE:161;GLY:162;LYS:179;ASP:292;PHE:293;GLY:294;LEU:295 Pi-Stacking- PHE:161

3-5-Dicaffeoylquinic acid	AKT	4GV1	-10.4	**1.0**	Hbond- PHE:161;GLY:162;GLU:198;ALA:230;ALA:230;ASN:279;ASP:292;GLY:294 Hydrophobic- PHE:161;VAL:164;ALA:177;LYS:179;LEU:181;LEU:181;PHE:438 Salt Bridge- LYS:276 Pi-Cation- LYS:179
Diosmetin-7-O-glucoside	AKT	4GV1	-9.4	**0.4**	Hbond- LYS:158;LYS:158;ASP:274;ASN:279;ASN:279 Hydrophobic- VAL:164;VAL:164 Salt Bridge- LYS:179
Apigenin 6-C-glucoside 8-C-arabinoside	AKT	4GV1	-8.6	**1.1**	Hbond- LYS:179;GLU:191;ASP:274;LYS:276;ASN:279;ASN:279;THR:291;ASP:292;ASP:292;ASP:292;ASP:292;GLY:294;ASP:439 Hydrophobic- PHE:236;GLU:278;PHE:442
1-3-Dicaffeoylquinic acid	AKT	4GV1	-9.5	**0.5**	Hbond- LYS:158;GLY:162;LYS:179;GLU:198;GLU:198;ALA:230;ALA:230;ASN:279;GLY:294 Hydrophobic- LEU:156;LEU:156;PHE:161;VAL:164;VAL:164;LEU:181;PHE:438 Pi-Cation- LYS:179
Orientin	AKT	4GV1	-8.7	**0.5**	Hbond- GLY:157;LYS:158;GLY:162;VAL:164 Hydrophobic- VAL:164;ALA:177;PHE:438;PHE:442
Umbelliferone	AKT	4GV1	-7.0	**0.5**	Hbond- ALA:230 Hydrophobic- LEU:156;LEU:156;VAL:164;VAL:164;ALA:177;TYR:229;PHE:438
Isoorientin	AKT	4GV1	-8.5	**1.0**	Hbond- THR:160;THR:160;PHE:161;GLY:162;GLY:162;LYS:179;ALA:230;LYS:276 Hydrophobic- LEU:156;LEU:156;VAL:164;VAL:164;PHE:438
Kaempferol-3-O-glucoside	PD-1	5N2F	-7.9	**1.0**	Hbond- THR:20;ASN:63;GLN:66;ALA:121;LYS:124;ARG:125;ARG:125 Hydrophobic- TYR:123 Pi-Stacking- TYR:56;TYR:123 Salt Bridge- LYS:124
Catechin	PD-1	5N2F	-9.4	**0.8**	Hbond- ILE:54;MET:115;ILE:116;ILE:116;ASP:122 Hydrophobic- ILE:54;TYR:56;MET:115;MET:115;ALA:121;ALA:121;TYR:123 Pi-Stacking- TYR:56
Eupatorin	PD-1	5N2F	-9.9	**0.3**	Hbond- ASN:63;GLN:66 Hydrophobic- TYR:56;TYR:56;MET:115;ALA:121;TYR:123;TYR:123 Pi-Stacking- TYR:56

Dihydroxy-Trimethoxyflavone	PD-1	5N2F	-7.7	**0.3**	Hbond- ASN:63;GLN:66 Pi-Stacking- TYR:123
Quercetin	PD-1	5N2F	-9.5	**0.7**	Hbond- TYR:56;ASN:63;GLN:66;ASP:122 Hydrophobic- ILE:54;TYR:56;TYR:56;MET:115;ALA:121;TYR:123;TYR:123 Pi-Stacking- TYR:56
Kaempferol	PD-1	5N2F	-9.2	**0.2**	Hbond- SER:117;ALA:121;TYR:123 Hydrophobic- TYR:56;MET:115;MET:115;ALA:121;ALA:121;TYR:123;TYR:123
Eriodictyol-7-O-neohesperidoside	PD-1	5N2F	-10.7	**0.6**	Hbond- PHE:19;ASN:63;GLN:66;ILE:116;TYR:123;ARG:125;ARG:125 Hydrophobic- ILE:54;TYR:56;MET:115;MET:115;ALA:121;TYR:123;TYR:123;LYS:124 Pi-Stacking- TYR:56 Salt Bridge- LYS:124;LYS:124
5-Caffeoylquinic acid	PD-1	5N2F	-9.2	**0.7**	Hbond- TYR:56;ASP:61;ASN:63;GLN:66;MET:115;SER:117;TYR:123;LYS:124;ARG:125;ARG:125 Hydrophobic- TYR:56;TYR:56;TYR:56;TYR:123;TYR:123
Taxifolin	PD-1	5N2F	-9.5	**0.6**	Hbond- ILE:54;TYR:56;ASN:63;GLN:66;SER:117;ALA:121 Hydrophobic- ILE:54;TYR:56;TYR:123
Isoquercitrin	PD-1	5N2F	-8.0	**1.0**	Hbond- ASN:63;GLN:66;GLN:66;LYS:124;ARG:125;ARG:125 Hydrophobic- TYR:123;TYR:123;LYS:124 Pi-Stacking- TYR:56 Salt Bridge- LYS:124
Afzelin	PD-1	5N2F	-8.5	**0.9**	Hbond- PHE:19;ASP:61;ASP:61;ASN:63;ASN:63;GLN:66;GLN:66;LYS:75;ARG:125 Hydrophobic- LYS:124;LYS:124 Pi-Stacking- TYR:123 Pi-Cation- LYS:124
4-Hydroxycoumarin	PD-1	5N2F	-7.7	**0.4**	Hbond- MET:115;SER:117 Hydrophobic- ILE:54;TYR:56;ALA:121;TYR:123
Quercetin-3-O-rutinoside	PD-1	5N2F	-9.6	**0.2**	Hbond- ASP:61;ASN:63;GLN:66;GLN:66;GLN:66 Hydrophobic- ILE:54;TYR:56;VAL:76;LYS:124
Myricetin	PD-1	5N2F	-9.6	**1.0**	Hbond- TYR:56;TYR:56;ASN:63;GLN:66;MET:115 Hydrophobic- ILE:54;TYR:56;TYR:56;TYR:123;TYR:123

					Pi-Stacking- TYR:56
Diosmetin	PD-1	5N2F	-10.0	**0.3**	Hbond- TYR:56;ASN:63;GLN:66;GLN:66;SER:117 Hydrophobic- ILE:54;TYR:56;TYR:56;ALA:121;TYR:123 Pi-Stacking- TYR:56
Malvidin 3-O-beta-D-glucoside	PD-1	5N2F	-7.6	**20.4**	Hbond- THR:20;GLN:66;ASP:73;LYS:75;ALA:121;ASP:122;LYS:124;ARG:125;ARG:125 Hydrophobic- TYR:56;TYR:56;ALA:121;TYR:123;TYR:123 Pi-Stacking- TYR:56;TYR:56 Salt Bridge- LYS:75
3-5-Dicaffeoylquinic acid	PD-1	5N2F	-9.9	**1.0**	Hbond- PHE:19;TYR:56;ASN:63;GLN:66;ALA:121;ASP:122 Hydrophobic- ILE:54;TYR:56;TYR:56;VAL:68;MET:115;MET:115;ALA:121
Diosmetin-7-O-glucoside	PD-1	5N2F	-10.4	**0.5**	Hbond- PHE:19;ILE:54;GLN:66;SER:117;ALA:121;ALA:121;ASP:122 Hydrophobic- ILE:54;TYR:56;VAL:68;MET:115;ALA:121;TYR:123 Pi-Stacking- TYR:56
Apigenin 6-C-glucoside 8-C-arabinoside	PD-1	5N2F	-8.3	**0.9**	Hbond- PHE:19;PHE:19;THR:20;GLN:66;ALA:121;ALA:121;ASP:122;LYS:124;ARG:125;ARG:125 Hydrophobic- TYR:56;TYR:123;LYS:124
1-3-Dicaffeoylquinic acid	PD-1	5N2F	-10.1	**8.8**	Hbond- TYR:56;ASP:61;ASP:61;ASN:63;GLN:66;MET:115;SER:117;ASP:122;ASP:122;TYR:123;ARG:125;ARG:125 Hydrophobic- ILE:54;TYR:56;TYR:56;ALA:121;ASP:122;LYS:124 Salt Bridge- LYS:124
Hydroxycoumarin	PD-1	5N2F	-7.7	**0.5**	Hbond- ILE:116;ILE:116;ASP:122 Hydrophobic- ILE:54;TYR:56;MET:115;ALA:121;TYR:123
Caffeic Acid	PD-1	5N2F	-7.5	**1.1**	Hbond- GLN:66;ILE:116;SER:117 Hydrophobic- ILE:54;TYR:56;TYR:56;TYR:56;MET:115;ALA:121;TYR:123
Orientin	PD-1	5N2F	-9.1	**0.7**	Hbond- PHE:19;TYR:56;ASN:63;ASN:63;GLN:66;ASP:73;ALA:121;ASP:122 Hydrophobic- ILE:54;TYR:56;TYR:56;TYR:56;VAL:76;ALA:121;TYR:123;TYR:123
Umbelliferone	PD-1	5N2F	-7.5	**0.2**	Hbond- GLN:66;ILE:116;ASP:122 Hydrophobic- TYR:123

Isoorientin	PD-1	5N2F	-9.4	**1.1**	Hbond- TYR:56;ASN:63;GLN:66;GLN:66;SER:117;ALA:121;ALA:121;TYR:123 Hydrophobic- MET:115;ALA:121;ALA:121;TYR:123;TYR:123;TYR:123
Kaempferol-3-O-glucoside	CDK4	2W96	-9.6	**0.3**	Hbond- THR:20;ASN:63;GLN:66;ALA:121;LYS:124;ARG:125;ARG:125 Hydrophobic- TYR:123 Pi-Stacking- TYR:56;TYR:123 Salt Bridge- LYS:124 Pi-Cation- LYS:124
Catechin	CDK4	2W96	-9.0	**0.7**	Hbond- ALA:16;LYS:35;VAL:96;ASP:99;ASP:99;LYS:142;ASN:145;ASP:158 Hydrophobic- ASP:99;GLU:144
Eupatorin	CDK4	2W96	-8.1	**0.3**	Hbond- ALA:16;HIS:95;ARG:101;ARG:101;LYS:142 Hydrophobic- GLU:144;LEU:147;ALA:157
Dihydroxy-Trimethoxyflavone	CDK4	2W96	-8.3	**0.4**	Hbond- ALA:16;LYS:35;ARG:101;ARG:101;LYS:142 Hydrophobic- VAL:20;ALA:33;GLU:144;LEU:147;ALA:157 Pi-Cation- LYS:35
Quercetin	CDK4	2W96	-9.2	**0.1**	Hbond- ALA:16;LYS:35;ASP:99;ASP:99;THR:102;LYS:142;ASN:145;ASN:145;ASP:158;ASP:158 Hydrophobic- ASP:99;GLU:144
Kaempferol	CDK4	2W96	-8.9	**0.3**	Hbond- ALA:16;LYS:35;ASP:99;ASP:99;ASP:99;LYS:142 Hydrophobic- ASP:99;GLU:144;LEU:147
Eriodictyol-7-O-neohesperidoside	CDK4	2W96	-9.6	**0.5**	Hbond- VAL:14;GLY:15;ALA:16;LYS:35;ARG:101;LYS:142;ASN:145;ASP:158;ASP:158 Hydrophobic- VAL:20;ALA:33;LEU:147 Salt Bridge- LYS:142
5-Caffeoylquinic acid	CDK4	2W96	-8.5	**1.0**	Hbond- GLY:15;GLY:15;TYR:17;LYS:35;HIS:95;VAL:96;VAL:96;ARG:101 Hydrophobic- VAL:20 Salt Bridge- LYS:35;ARG:101
Taxifolin	CDK4	2W96	-9.3	**0.8**	Hbond- ALA:16;LYS:35;VAL:96;ASP:99;ASP:99;LYS:142;ASN:145;ASN:145;ASP:158 Hydrophobic- ASP:99;GLU:144;LEU:147
Isoquercitrin	CDK4	2W96	-9.2	**4.9**	Hbond- ASN:63;GLN:66;GLN:66;LYS:124;ARG:125;ARG:125 Hydrophobic- TYR:123;TYR:123;LYS:124 Pi-Stacking- TYR:56 Salt Bridge- LYS:124

					Pi-Cation- LYS:124
Afzelin	CDK4	2W96	-10.0	**1.0**	Hbond- LYS:35;ASP:97;ASP:99;ASP:99;ARG:101;LYS:142;ASN:145;ASP:158;ASP:158 Hydrophobic- VAL:20;ASP:99;GLU:144;LEU:147;LEU:147;ALA:157 Pi-Cation- LYS:35
Quercetin-3-O-rutinoside	CDK4	2W96	-9.4	**0.0**	Hbond- VAL:14;VAL:14;GLY:15;GLY:15;ALA:16;TYR:17;HIS:95;VAL:96;VAL:96;ASP:97;ASP:99;ASP:99;ARG:101 Hydrophobic- VAL:20;LEU:147 Salt Bridge- ARG:101 Pi-Cation- LYS:35
Myricetin	CDK4	2W96	-9.1	**0.8**	Hbond- ALA:16;LYS:35;VAL:96;ASP:97;ASP:99;ASP:99;LYS:142;ASN:145;ASN:145;ASP:158 Hydrophobic- ASP:99;GLU:144;LEU:147
Diosmetin	CDK4	2W96	-8.9	**0.3**	Hbond- ALA:16;ASP:99;ASP:99;LYS:142;ASN:145;ASN:145;ASP:158 Hydrophobic- ASP:99;GLU:144
Malvidin 3-O-beta-D-glucoside	CDK4	2W96	-8.7	**0.6**	Hbond- GLY:15;ALA:16;TYR:17;LYS:35;HIS:95;VAL:96;ASP:97;ASP:99;ARG:101;THR:102 Hydrophobic- VAL:20;ALA:33;ALA:157
3-5-Dicaffeoylquinic acid	CDK4	2W96	-9.1	**0.2**	Hbond- ALA:16;TYR:17;HIS:95;VAL:96;ARG:101;ASP:158;ASP:158;TRP:179 Hydrophobic- GLU:144;ALA:157 Salt Bridge- LYS:35;ARG:101;LYS:142;LYS:142
Diosmetin-7-O-glucoside	CDK4	2W96	-9.5	**0.5**	Hbond- ALA:16;ASP:99;ASP:99;ASP:99;THR:102;THR:102;LYS:142;ASN:145;ASP:158 Hydrophobic- ASP:99;GLU:144;LEU:147 Salt Bridge- ARG:101
Apigenin 6-C-glucoside 8-C-arabinoside	CDK4	2W96	-8.3	**5.7**	Hbond- GLY:15;ALA:16;TYR:17;LYS:35;HIS:95;VAL:96;ARG:101;ARG:101;LYS:142;GLU:144;ASN:145;ASP:158 Hydrophobic- ILE:12
1-3-Dicaffeoylquinic acid	CDK4	2W96	-8.9	**5.5**	Hbond- VAL:14;GLY:15;ALA:16;HIS:95;VAL:96;ASP:97;ASP:99;ASP:99;LYS:142;ASP:158 Hydrophobic- ILE:12;ILE:12;VAL:20;VAL:20 Salt Bridge- LYS:35;LYS:35

Orientin	CDK4	2W96	-9.1	**0.7**	Hbond- ALA:16;TYR:17;LYS:35;HIS:95;ASP:97;ARG:101;GLU:144;ASP:158 Hydrophobic- VAL:20
Isoorientin	CDK4	2W96	-8.8	**0.3**	Hbond- LYS:35;ASP:99;ASP:99;ARG:101;ASP:158 Hydrophobic- ALA:33;LEU:147
Kaempferol-3-O-glucoside	BRPF1	5MWZ	-7.6	**0.5**	Hbond- SER:654;SER:654;SER:654;GLU:655;ASN:708 Hydrophobic- PRO:658;GLU:661
Eupatorin	BRPF1	5MWZ	-7.1	**0.3**	Hbond- TYR:665;ASN:708 Hydrophobic- VAL:657;PRO:658;VAL:662;TYR:665;TYR:707
Dihydroxy-Trimethoxyflavone	BRPF1	5MWZ	-7.1	**0.3**	Hbond- SER:654;SER:654;GLU:655 Hydrophobic- VAL:657;VAL:657;VAL:662;TYR:665;TYR:707;TYR:707;PHE:714
Quercetin	BRPF1	5MWZ	-7.0	**1.0**	Hbond- ASN:651;ILE:652;GLU:655;GLU:655;ASN:708;ASN:708 Hydrophobic- TYR:707
Eriodictyol-7-O-neohesperidoside	BRPF1	5MWZ	-7.5	**0.6**	Hbond- SER:654;GLU:655;GLU:655;GLU:661;ASN:708 Hydrophobic- ILE:652;VAL:657;VAL:657;TYR:665;TYR:707;PHE:714
5-Caffeoylquinic acid	BRPF1	5MWZ	-7.5	**0.4**	Hbond- SER:654;SER:654;GLU:655;GLU:655;GLU:655;ASN:708 Hydrophobic- VAL:657;VAL:657;PHE:714
Taxifolin	BRPF1	5MWZ	-7.0	**0.4**	Hbond- ILE:652;GLU:655;PRO:656;ASN:708 Hydrophobic- TYR:707
Afzelin	BRPF1	5MWZ	-7.1	**0.7**	Hbond- SER:654;SER:654;GLU:655;GLU:655;GLU:661 Hydrophobic- GLU:655;VAL:657;PRO:658;GLU:661
Quercetin-3-O-rutinoside	BRPF1	5MWZ	-7.9	**0.7**	Hbond- SER:654;SER:654;GLU:655;GLU:655;GLU:655;GLU:661;ASN:708 Hydrophobic- GLU:655;VAL:657;PRO:658;VAL:662
Myricetin	BRPF1	5MWZ	-7.1	**1.0**	Hbond- GLU:655;GLU:655;ASN:708;ASN:708 Hydrophobic- TYR:707
Diosmetin	BRPF1	5MWZ	-7.4	**0.4**	Hbond- ASN:703;ASN:708 Hydrophobic- VAL:657;PRO:658;GLU:661;VAL:662;TYR:665;TYR:707

Malvidin 3-O-beta-D-glucoside	BRPF1	5MWZ	-7.9	**2.1**	Hbond- GLY:650;ILE:652;SER:654;SER:654;GLU:655;GLU:655;ASN:708 Hydrophobic- PRO:658;PHE:714;PHE:714
3-5-Dicaffeoylquinic acid	BRPF1	5MWZ	-8.5	**0.9**	Hbond- SER:654;SER:654;GLU:655;GLU:655;LEU:659;TYR:665;ILE:700;ASN:708 Hydrophobic- PHE:653;PRO:656;VAL:657;TYR:665;PHE:714;PHE:714
Diosmetin-7-O-glucoside	BRPF1	5MWZ	-7.7	**0.6**	Hbond- TYR:665;TYR:707;ASN:708;ALA:709 Hydrophobic- VAL:657;VAL:657;TYR:665;TYR:707;PHE:714 Pi-Stacking- PHE:714
1-3-Dicaffeoylquinic acid	BRPF1	5MWZ	-7.3	**0.5**	Hbond- SER:654;SER:654;GLU:655;GLU:655;ASN:708;ASN:708 Hydrophobic- VAL:657;VAL:657;PRO:658;GLU:661
Orientin	BRPF1	5MWZ	-7.7	**0.5**	Hbond- SER:654;SER:654;GLU:655;GLU:661;TYR:665;ASN:708 Hydrophobic- VAL:657;VAL:657;TYR:665;TYR:707;PHE:714
Isoorientin	BRPF1	5MWZ	-7.1	**0.8**	Hbond- SER:654;SER:654;GLU:655;ASN:708 Hydrophobic- ILE:652;VAL:657;VAL:657;PHE:714
Eupatorin	PPAR	1i7i	-7.0	**0.4**	Hbond- SER:342 Hydrophobic- ARG:288;ARG:288;ILE:341;ILE:341
Afzelin	PPAR	1i7i	-7.2	**0.4**	Hbond- LEU:340 Hydrophobic- PHE:287;PHE:287;ARG:288;ILE:341;ILE:341
Diosmetin	PPAR	1i7i	-7.2	**0.4**	Hbond- LEU:340;SER:342 Hydrophobic- ARG:288;ARG:288;ILE:341;ILE:341
3-5-Dicaffeoylquinic acid	PPAR	1i7i	-7.1	**nd**	Hbond- LYS:263 Hydrophobic- GLN:283;PHE:287;PHE:287;ARG:288;ARG:288;ILE:341;ILE:341
Kaempferol-3-O-glucoside	CDK2	6GUE	-8.4	**0.8**	Hbond- TYR:180;GLU:12;LYS:33;HIS:84;ASP:86;LYS:129;ASP:145 Hydrophobic- VAL:163;TYR:15;GLN:131;GLN:131;ALA:144 Salt Bridge- ARG:50;ARG:126;ARG:150
Catechin	CDK2	6GUE	-8.8	**0.5**	Hbond- TYR:180;LYS:33;GLU:51;ASP:86;ASP:145 Hydrophobic- VAL:163;ILE:10;PHE:80;LEU:134;LEU:134;ALA:144 Salt Bridge- ARG:50;ARG:126;ARG:150

Eupatorin	CDK2	6GUE	-8.9	**0.4**	Hbond- TYR:180;LYS:33;LEU:83;ASP:86;ASP:86;LYS:89 Hydrophobic- VAL:163;ILE:10;ILE:10;VAL:18 Salt Bridge- ARG:50;ARG:126;ARG:150
Dihydroxy-Trimethoxyflavone	CDK2	6GUE	-8.5	**0.4**	Hbond- TYR:180;GLU:12;TYR:15;ASP:86 Hydrophobic- VAL:163;VAL:18;ALA:31;LEU:134;ALA:144 Pi-Stacking- PHE:80 Salt Bridge- ARG:50;ARG:126;ARG:150
Quercetin	CDK2	6GUE	-8.9	**0.0**	Hbond- TYR:180;LYS:33;GLU:51;ASP:86;ASP:86;GLN:131;ASP:145 Hydrophobic- VAL:163;ILE:10;LEU:134;LEU:134;ALA:144;ASP:145 Salt Bridge- ARG:50;ARG:126;ARG:150
Kaempferol	CDK2	6GUE	-8.8	**0.8**	Hbond- TYR:180;LYS:33;GLU:51;ASP:86;ASP:86;GLN:131;ASP:145 Hydrophobic- VAL:163;ILE:10;LEU:134;LEU:134;ALA:144;ASP:145 Salt Bridge- ARG:50;ARG:126;ARG:150
Eriodictyol-7-O-neohesperidoside	CDK2	6GUE	-9.3	**0.4**	Hbond- TYR:180;LYS:33;LEU:83;HIS:84;ASP:86;ASP:127;LYS:129;ASN:132;ASP:145;ASP:145 Hydrophobic- VAL:163;VAL:18;ALA:31 Pi-Stacking- TYR:15 Salt Bridge- ARG:50;ARG:126;ARG:150 Pi-Cation- LYS:129
5-Caffeoylquinic acid	CDK2	6GUE	-8.3	**1.0**	Hbond- TYR:180;LYS:33;LEU:83;HIS:84;LYS:89;ASP:145 Hydrophobic- VAL:163;ILE:10;ILE:10;LEU:134;ASP:145 Salt Bridge- ARG:50;ARG:126;ARG:150
Taxifolin	CDK2	6GUE	-8.7	**0.4**	Hbond- TYR:180;GLU:81;LEU:83;LYS:89 Hydrophobic- VAL:163;ILE:10;VAL:18;ALA:31;GLN:85;LYS:89 Salt Bridge- ARG:50;ARG:126;ARG:150
Isoquercitrin	CDK2	6GUE	-9.1	**0.7**	Hbond- TYR:180;TYR:15;GLU:81;LEU:83;ASP:86;ASP:86;LYS:89;ASP:145 Hydrophobic- VAL:163;ILE:10;VAL:18;ALA:31;LEU:83 Salt Bridge- ARG:50;ARG:126;ARG:150
Afzelin	CDK2	6GUE	-8.7	**0.8**	Hbond- TYR:180;LYS:33;HIS:84;LYS:129;ASP:145 Hydrophobic- VAL:163;TYR:15;ASP:86;GLN:131;ALA:144 Salt Bridge- ARG:50;ARG:126;ARG:150

4-Hydroxycoumarin	CDK2	6GUE	-7.2	**0.5**	Hbond- TYR:180;ASP:145 Hydrophobic- VAL:163;ILE:10;VAL:18;VAL:18;PHE:80;LEU:134 Salt Bridge- ARG:50;ARG:126;ARG:150;LYS:33
Quercetin-3-O-rutinoside	CDK2	6GUE	-8.9	**0.5**	Hbond- TYR:180;ILE:10;ILE:10;THR:14;TYR:15;LYS:33;LYS:129;ASN:132;ASP:145;ASP:145 Hydrophobic- VAL:163;ILE:10;TYR:15;TYR:15;VAL:18;ALA:31;GLN:131 Salt Bridge- ARG:50;ARG:126;ARG:150;LYS:33;LYS:129 Pi-Cation- LYS:129
Myricetin	CDK2	6GUE	-8.9	**0.4**	Hbond- TYR:180;TYR:15;LYS:33;ASP:86;ASP:145 Hydrophobic- VAL:163;ILE:10;ASP:145 Salt Bridge- ARG:50;ARG:126;ARG:150
Diosmetin	CDK2	6GUE	-8.7	**0.6**	Hbond- TYR:180;ILE:10;LYS:33;GLU:81;LEU:83 Hydrophobic- VAL:163;ILE:10;VAL:18;ALA:31;PHE:80 Salt Bridge- ARG:50;ARG:126;ARG:150
Malvidin 3-O-beta-D-glucoside	CDK2	6GUE	-9.2	**0.6**	Hbond- TYR:180;GLU:12;GLU:12;LYS:33;ASP:86;LYS:129;GLN:131 Hydrophobic- VAL:163;ILE:10;VAL:18;VAL:18;LEU:134 Salt Bridge- ARG:50;ARG:126;ARG:150
3-5-Dicaffeoylquinic acid	CDK2	6GUE	-9.4	**0.7**	Hbond- TYR:180;GLU:12;GLU:12;TYR:15;TYR:15;LEU:83;LEU:83;HIS:84 Hydrophobic- VAL:163;ILE:10;TYR:15;VAL:18;VAL:18;ALA:31;VAL:64;PHE:80;GLN:131;LEU:134;LEU:134 Salt Bridge- ARG:50;ARG:126;ARG:150;LYS:33;LYS:129
Diosmetin-7-O-glucoside	CDK2	6GUE	-9.3	**0.3**	Hbond- TYR:180;GLU:12;TYR:15;TYR:15;LYS:89;LYS:129;ASN:132;ASP:145;ASP:145 Hydrophobic- VAL:163;ILE:10;ILE:10;VAL:18;LYS:89;LEU:134 Salt Bridge- ARG:50;ARG:126;ARG:150
Apigenin 6-C-glucoside 8-C-arabinoside	CDK2	6GUE	-8.5	**0.5**	Hbond- TYR:180;TYR:15;LEU:83;ASP:86;LYS:89 Hydrophobic- VAL:163;LEU:134;ALA:144;ASP:145 Salt Bridge- ARG:50;ARG:126;ARG:150
1-3-Dicaffeoylquinic acid	CDK2	6GUE	-9.2	**8.3**	Hbond- TYR:180;LEU:83;ASP:86;ASP:86;LYS:129;ASP:145;ASP:145;ASP:145 Hydrophobic- VAL:163;ILE:10;TYR:15;VAL:18;GLN:131;LEU:134 Salt Bridge- ARG:50;ARG:126;ARG:150;LYS:33
Hydroxycoumarin	CDK2	6GUE	-7.5	**0.5**	Hbond- TYR:180;LYS:33;ASP:145 Hydrophobic- VAL:163;VAL:18;ALA:31;VAL:64;PHE:80;PHE:80;LEU:134;ALA:144

					Salt Bridge- ARG:50;ARG:126;ARG:150;LYS:33
Orientin	CDK2	6GUE	-10.3	**0.5**	Hbond- TYR:180;GLU:12;TYR:15;TYR:15;LYS:33;LEU:83;ASP:86;ASP:145;ASP:145;ASP:145 Hydrophobic- VAL:163;ILE:10;ALA:31;PHE:80;LEU:134;LEU:134;ALA:144 Salt Bridge- ARG:50;ARG:126;ARG:150
Umbelliferone	CDK2	6GUE	-7.5	**0.1**	Hbond- TYR:180;LEU:83 Hydrophobic- VAL:163;ALA:31;VAL:64;PHE:80;PHE:80;PHE:80;LEU:134 Salt Bridge- ARG:50;ARG:126;ARG:150;LYS:33
Isoorientin	CDK2	6GUE	-8.4	**1.0**	Hbond- TYR:180;GLU:12;THR:14;TYR:15;LEU:83;LEU:83;LYS:129;ASN:132;ASP:145 Hydrophobic- VAL:163;ILE:10;TYR:15;VAL:18;ALA:31;LEU:134;LEU:134 Salt Bridge- ARG:50;ARG:126;ARG:150 Pi-Cation- LYS:129
Kaempferol-3-O-glucoside	Tert	5CQG	-8.9	**3.0**	Hbond- ALA:195;ALA:195;ILE:252;ILE:252;ASP:254;ALA:255;TYR:256;GLN:308;ASN:369;ASN:369 Hydrophobic- ASN:192;PHE:193;PHE:193;ARG:253
Catechin	Tert	5CQG	-8.8	**0.1**	Hbond- MET:482;ARG:486;PHE:494;TRP:498 Hydrophobic- PHE:494;ILE:497;LEU:554 Pi-Stacking- PHE:494;PHE:494;TYR:551
Eupatorin	Tert	5CQG	-8.4	**0.6**	Hbond- ARG:486;ARG:486 Hydrophobic- PHE:494;PHE:494;ILE:497;ILE:550;TYR:551;LEU:554 Pi-Stacking- PHE:494
Dihydroxy-Trimethoxyflavone	Tert	5CQG	-8.3	**1.0**	Hbond- GLY:553 Hydrophobic- MET:482;ILE:550;TYR:551 Pi-Stacking- PHE:494
Quercetin	Tert	5CQG	-8.4	**17.2**	Hbond- GLY:495;TRP:498 Hydrophobic- PHE:494;ILE:550;TYR:551;LEU:554 Pi-Stacking- PHE:494
Kaempferol	Tert	5CQG	-8.5	**0.2**	Hbond- ILE:550;GLY:553 Hydrophobic- PHE:494;ILE:550;LEU:554 Pi-Stacking- PHE:494;TYR:551

Eriodictyol-7-O-neohesperidoside	Tert	5CQG	-8.9	**1.4**	Hbond- TYR:170;TYR:170;ASN:192;ALA:195;ILE:252;ARG:253;GLN:308;ASP:343;ASN:369 Hydrophobic- TYR:170;PHE:193;ARG:194;LYS:372
5-Caffeoylquinic acid	Tert	5CQG	-8.3	**0.9**	Hbond- MET:482;ARG:486;ARG:486;PHE:494;GLY:495;TRP:498 Hydrophobic- MET:482;PHE:494;ILE:550;TYR:551;LEU:554 Pi-Stacking- PHE:494 Salt Bridge- ARG:557
Taxifolin	Tert	5CQG	-8.2	**0.7**	Hbond- TRP:498 Hydrophobic- PHE:494;ILE:550;TYR:551;LEU:554 Pi-Stacking- PHE:494
Isoquercitrin	Tert	5CQG	-8.8	**1.1**	Hbond- GLN:190;ILE:252;ASP:254;ASP:254;ALA:255;TYR:256;GLN:308;ASN:369;ASN:369 Hydrophobic- LYS:189;ASN:192;PHE:193
Afzelin	Tert	5CQG	-8.6	**0.7**	Hbond- ALA:195;ILE:252;ARG:253;ARG:253;ASP:254;ALA:255;GLN:308;GLN:308 Hydrophobic- ASN:192;PHE:193;PHE:193;ARG:253;TYR:256
Quercetin-3-O-rutinoside	Tert	5CQG	-8.7	**6.7**	Hbond- ASN:192;ALA:195;ALA:195;ASP:254;ASP:254;ASP:254;ALA:255;TYR:256;HIS:304;ASP:343;ASN:369;ASN:369;LYS:372 Hydrophobic- ASP:343
Myricetin	Tert	5CQG	-8.3	**0.9**	Hbond- PHE:494;TRP:498 Hydrophobic- ILE:550;TYR:551;LEU:554 Pi-Stacking- PHE:494
Diosmetin	Tert	5CQG	-8.5	**8.3**	Hbond- GLY:553 Hydrophobic- PHE:494;ILE:497;TYR:551;LEU:554;LEU:554 Pi-Stacking- PHE:494
Malvidin 3-O-beta-D-glucoside	Tert	5CQG	-7.8	**6.7**	Hbond- ASN:192;ARG:194;ILE:252;ASP:254;ALA:255;GLN:308 Hydrophobic- ASN:192;ARG:253
3-5-Dicaffeoylquinic acid	Tert	5CQG	-8.7	**3.1**	Hbond- ARG:486;ARG:486;ASN:492;PHE:494;TRP:498;ILE:550;GLY:553;LEU:554 Hydrophobic- ARG:486;PHE:494;PHE:494;PHE:494;PHE:494;ILE:550;TYR:551;LEU:554 Salt Bridge- ARG:557

Diosmetin-7-O-glucoside	Tert	5CQG	-8.5	**48.5**	Hbond- TYR:170;TYR:170;GLN:190;PHE:193;ALA:195;ASP:254;GLN:308;ASN:369 Hydrophobic- ARG:194 Pi-Stacking- TYR:170
Apigenin 6-C-glucoside 8-C-arabinoside	Tert	5CQG	-8.3	**0.9**	Hbond- ASN:192;ASP:254;ASP:254;ASP:254;GLN:308;ASP:343;ASN:369 Hydrophobic- TYR:170;PHE:193
1-3-Dicaffeoylquinic acid	Tert	5CQG	-7.5	**44.2**	Hbond- ASN:192;ASN:192;ASP:254;ASP:254;ALA:255;GLN:308 Hydrophobic- LYS:189;ASN:192;ARG:253;ASP:254;TYR:256 Salt Bridge- ARG:194;ARG:194
Orientin	Tert	5CQG	-8.6	**0.7**	Hbond- ARG:486;ARG:486;GLU:549;GLY:553 Hydrophobic- PHE:494;PHE:494;PHE:494;PHE:494;ILE:550;TYR:551;LEU:554
Isoorientin	Tert	5CQG	-8.4	**0.8**	Hbond- ASN:192;ASN:192;ALA:195;ASP:254;ALA:255;GLN:308;VAL:342;ASP:343 Hydrophobic- TYR:170;PHE:193;PHE:193 Pi-Stacking- PHE:193
Kaempferol-3-O-glucoside	CyclinD1	2W99	-7.3	**1.1**	Hbond- CYS:68;GLU:75;LYS:180;LYS:180;GLN:183;GLN:183 Hydrophobic- LYS:180 Pi-Cation- LYS:180
Catechin	CyclinD1	2W99	-7.0	**0.3**	Hbond- CYS:68;HIS:158;GLN:183;GLN:183 Hydrophobic- LEU:65;GLU:69;GLU:75;PHE:78
Quercetin	CyclinD1	2W99	-7.1	**1.1**	Hbond- CYS:68;GLU:69 Hydrophobic- GLU:69;ALA:187
Kaempferol	CyclinD1	2W99	-7.1	**1.0**	Hbond- GLU:75 Hydrophobic- GLU:69;ALA:187
Eriodictyol-7-O-neohesperidoside	CyclinD1	2W99	-7.6	**8.7**	Hbond- GLU:69;GLN:176;ARG:179;LYS:180;GLN:183;THR:184 Hydrophobic- GLU:75
Isoquercitrin	CyclinD1	2W99	-7.3	**0.5**	Hbond- CYS:68;GLU:69;LYS:72;LYS:180;LYS:180;GLN:183;GLN:183 Hydrophobic- LYS:180 Pi-Cation- LYS:180
Afzelin	CyclinD1	2W99	-7.7	**0.6**	Hbond- GLU:69;HIS:158;LYS:180;GLN:183

					Hydrophobic- GLU:75;PHE:78;LYS:180;GLN:183
Quercetin-3-O-rutinoside	CyclinD1	2W99	-8.2	**0.6**	Hbond- GLU:75;HIS:158;GLN:176;LYS:180;GLN:183;GLN:183;THR:184 Hydrophobic- LEU:65;GLU:69;GLU:75
Myricetin	CyclinD1	2W99	-7.0	**1.1**	Hbond- CYS:68;GLU:75;GLN:183 Hydrophobic- GLU:69;ALA:187
Malvidin 3-O-beta-D-glucoside	CyclinD1	2W99	-7.1	**2.1**	Hbond- GLU:69;HIS:158;LYS:180;GLN:183 Hydrophobic- GLU:75;PHE:78;GLN:183;ALA:187
3-5-Dicaffeoylquinic acid	CyclinD1	2W99	-7.3	**1.0**	Hbond- CYS:73;GLU:75;GLU:75;GLU:75;GLU:75;PHE:78;GLN:183 Hydrophobic- GLU:69;GLN:183
Diosmetin-7-O-glucoside	CyclinD1	2W99	-7.9	**0.4**	Hbond- CYS:73;PHE:78;THR:184;THR:191;GLN:261 Hydrophobic- LEU:65;THR:184;ALA:187;LEU:188
Apigenin 6-C-glucoside 8-C-arabinoside	CyclinD1	2W99	-7.2	**0.7**	Hbond- GLN:183 Hydrophobic- LEU:65;THR:184;ALA:187;LEU:188
Orientin	CyclinD1	2W99	-7.7	**0.6**	Hbond- CYS:68;GLU:69;GLU:75;PHE:78;HIS:158
Isoorientin	CyclinD1	2W99	-7.0	**0.9**	Hbond- CYS:68;GLU:70;LYS:72;HIS:158;GLN:183 Hydrophobic- LYS:72;LYS:72 Pi-Cation- LYS:72

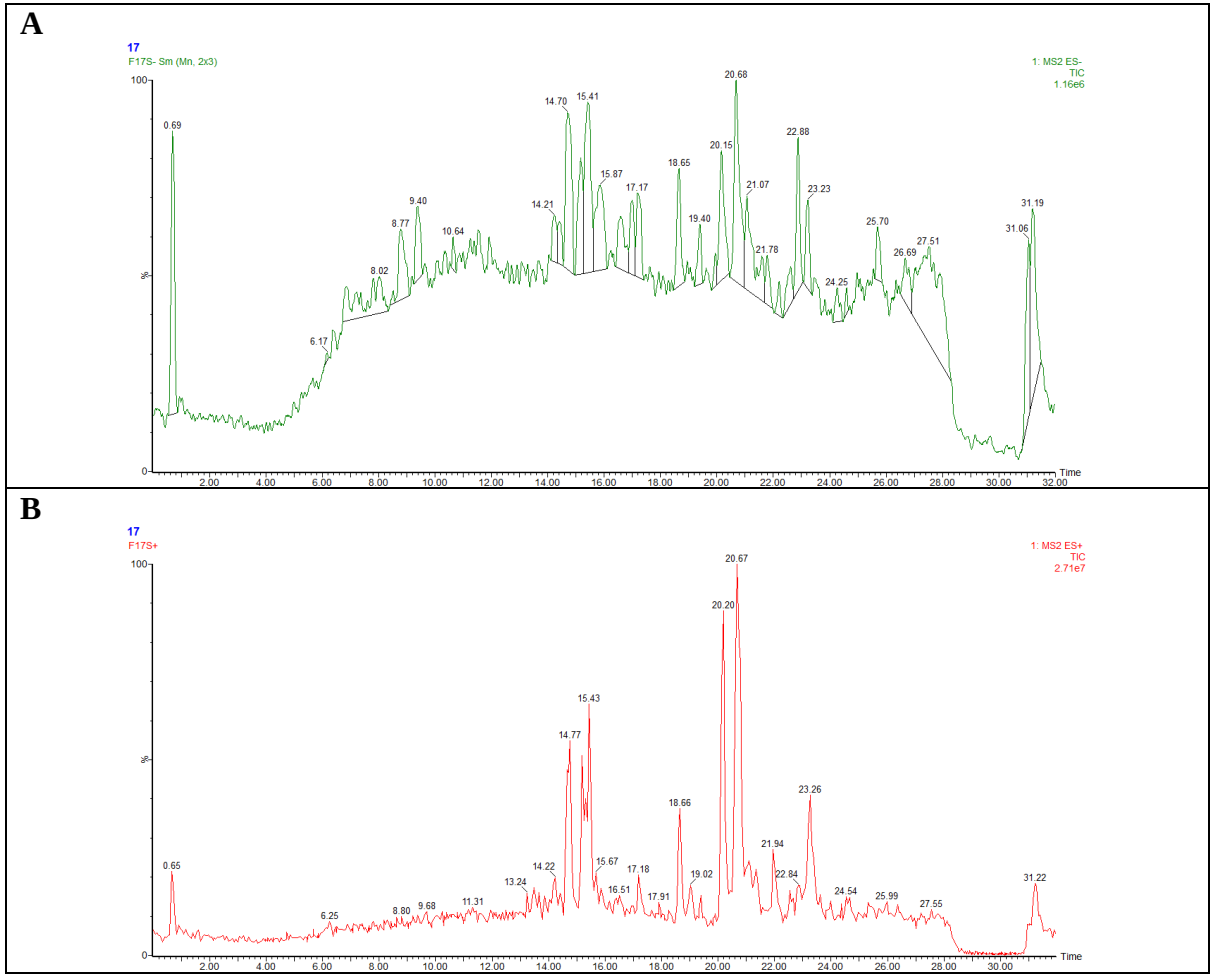

Figure S1. Total ion chromatogram (TIC) of the aerial parts ethyl acetate extract of *S. coriacea* in negative ion mode (A) and positive ion mode (B)

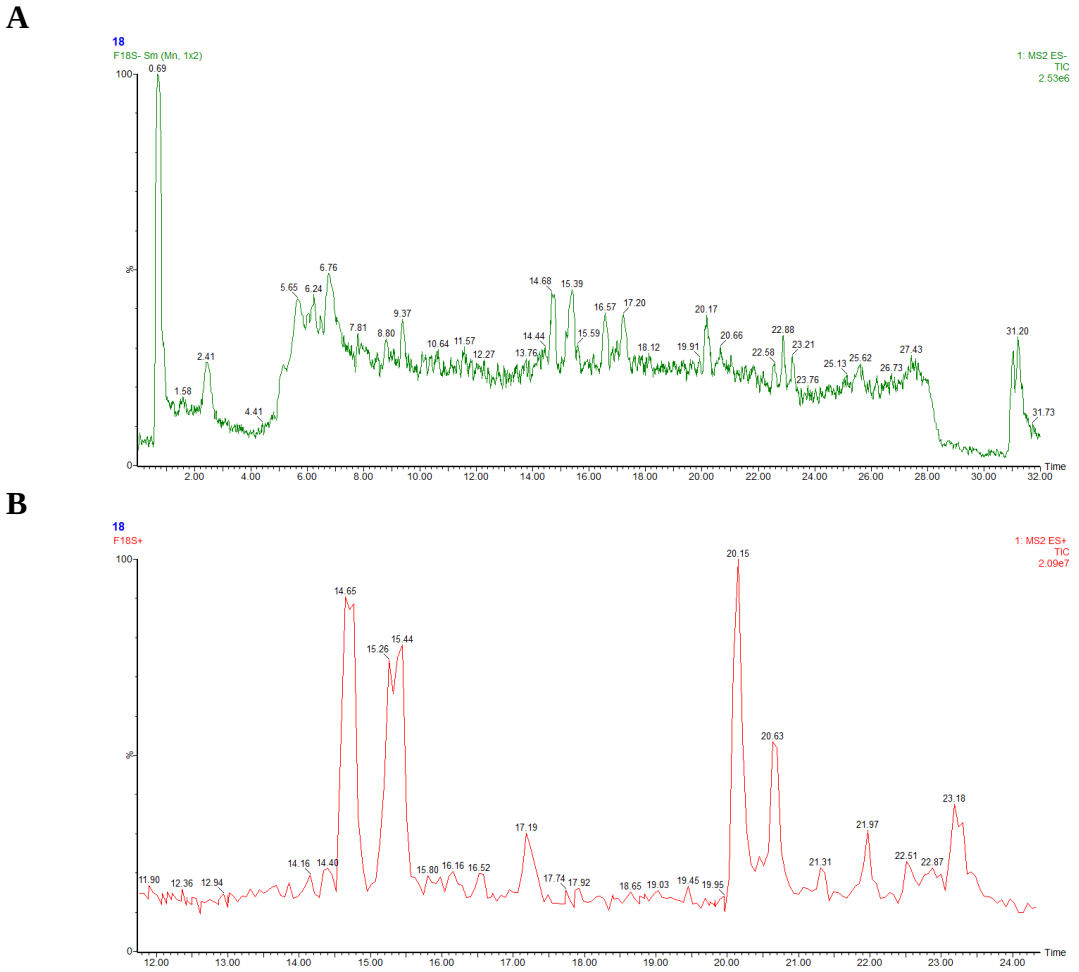

Figure S2. Total ion chromatogram (TIC) of the aerial parts ethanol extract of *S. coriacea* in negative ion mode (A) and positive ion mode (B)

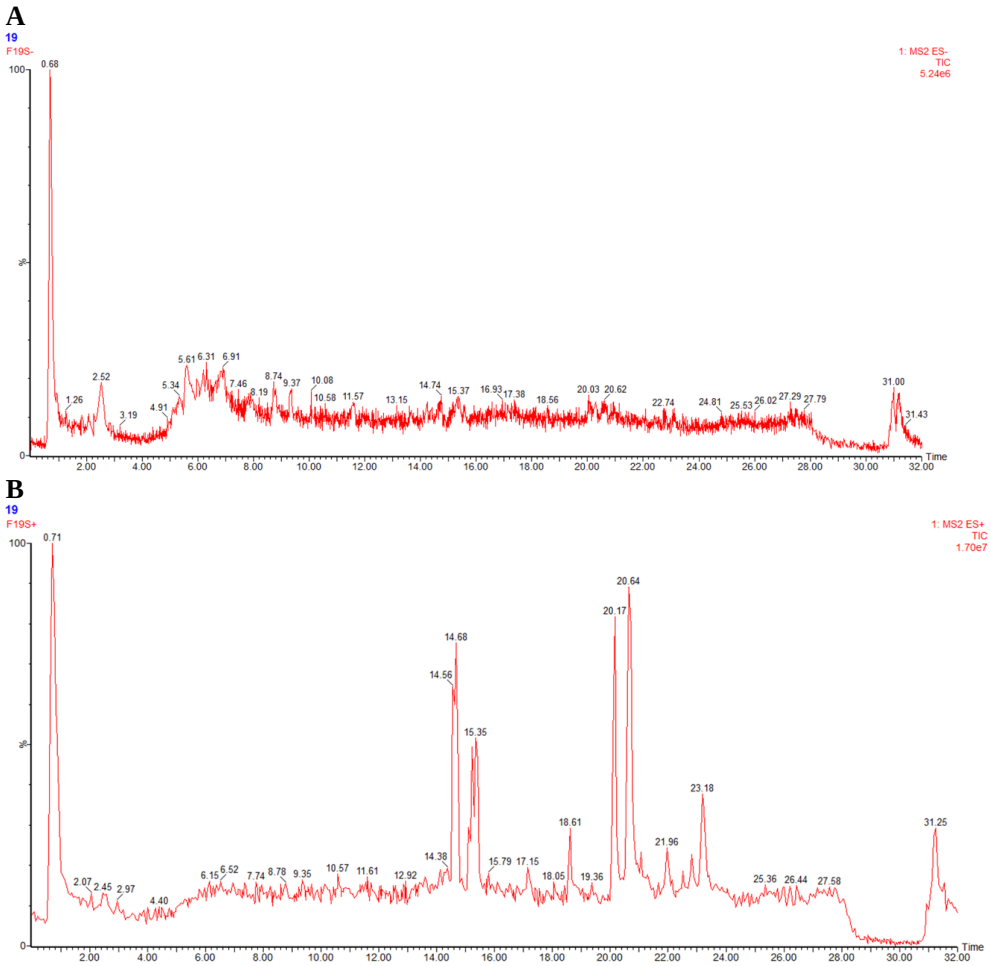

Figure S3. Total ion chromatogram (TIC) of the aerial parts ethanol/water extract of *S. coriacea* in negative ion mode (A) and positive ion mode (B)

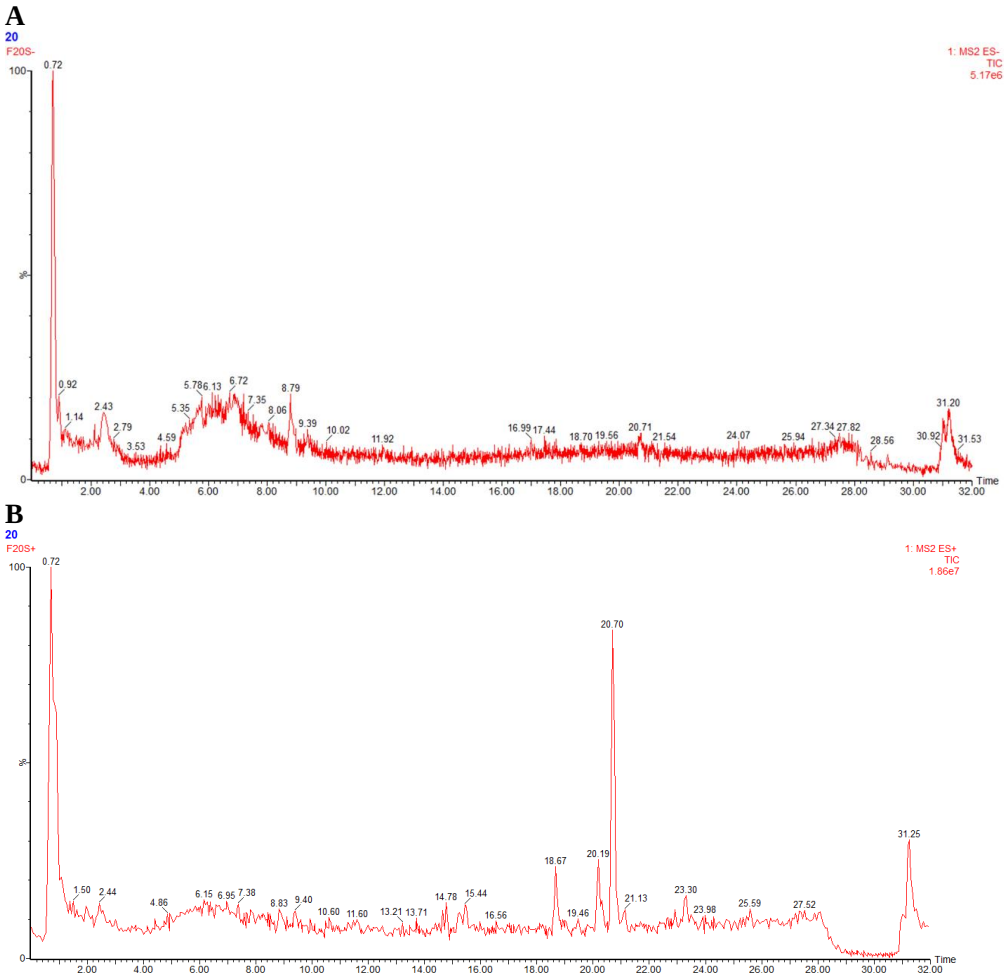

Figure S4. Total ion chromatogram (TIC) of the aerial parts water extract of *S. coriacea* in negative ion mode (A) and positive ion mode (B)

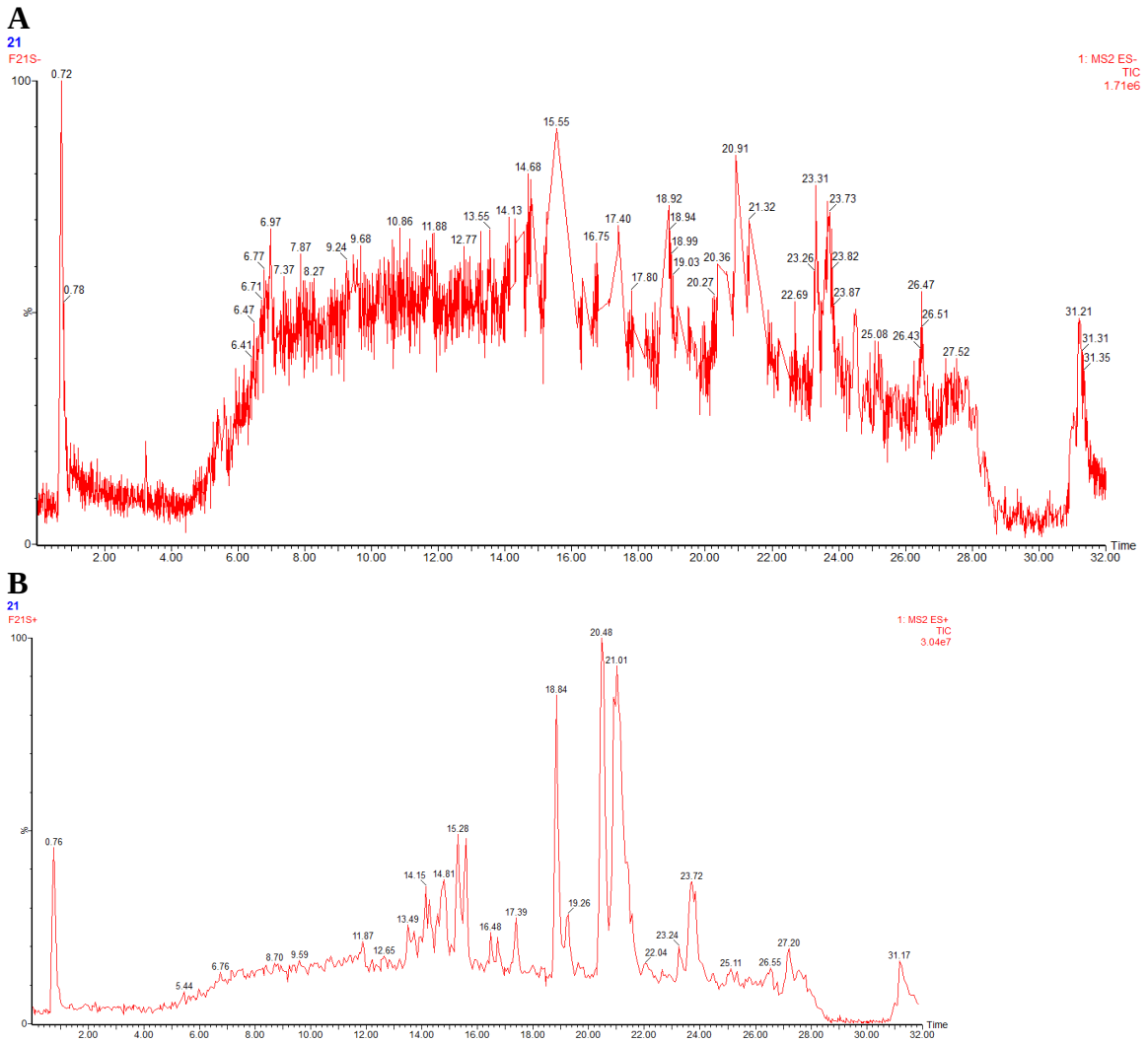

Figure S5. Total ion chromatogram (TIC) of the roots ethyl acetate extract of *S. coriacea* in negative ion mode (A) and positive ion mode (B)

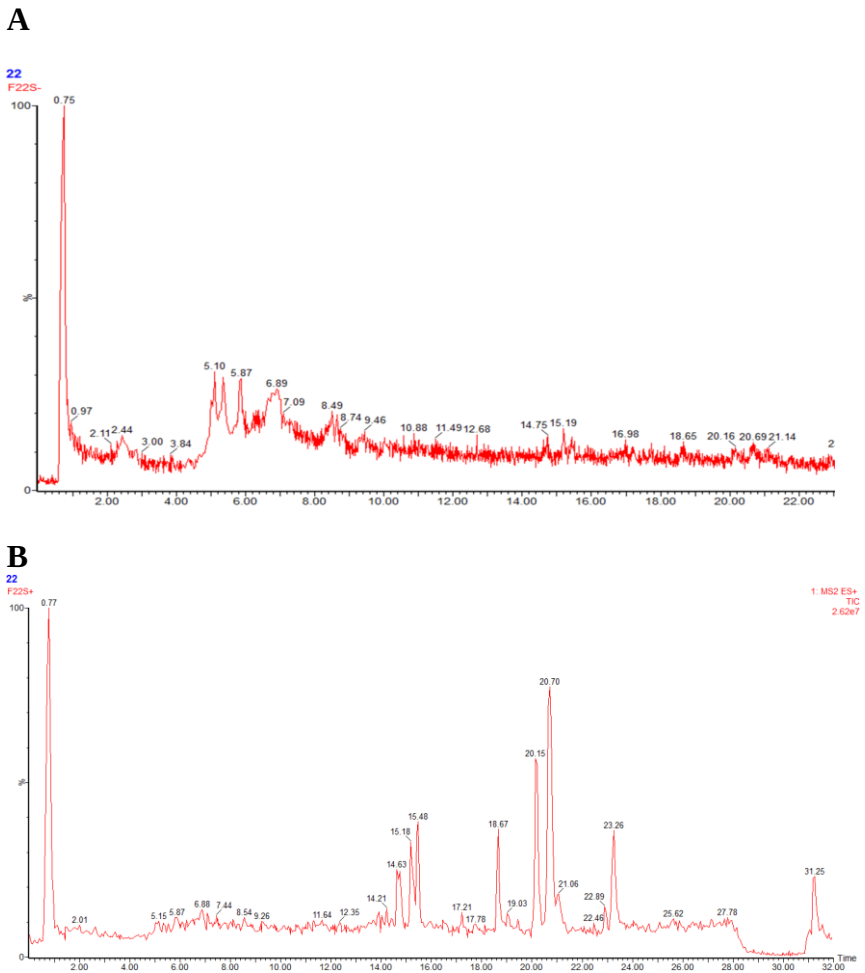

Figure S6. Total ion chromatogram (TIC) of the roots ethanol extract of *S. coriacea* in negative ion mode (A) and positive ion mode (B)

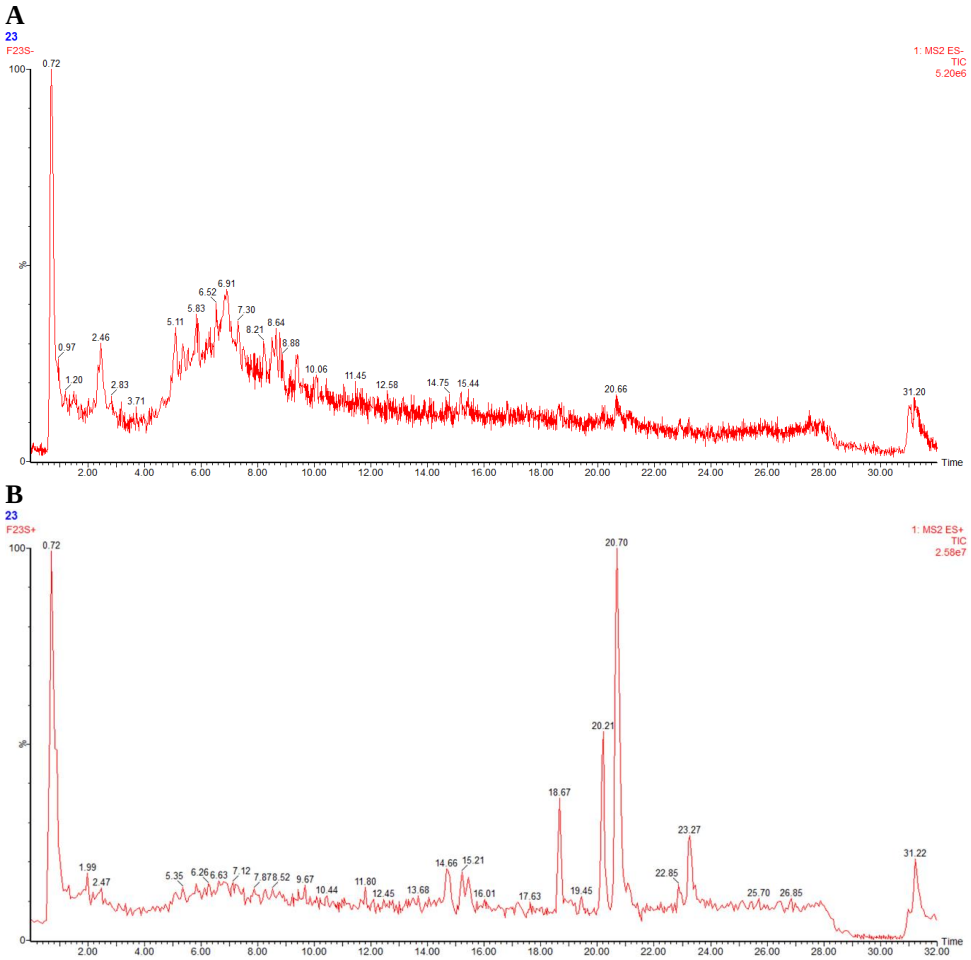

Figure S7. Total ion chromatogram (TIC) of the roots ethanol/water extract of *S. coriacea* in negative ion mode (A) and positive ion mode (B)

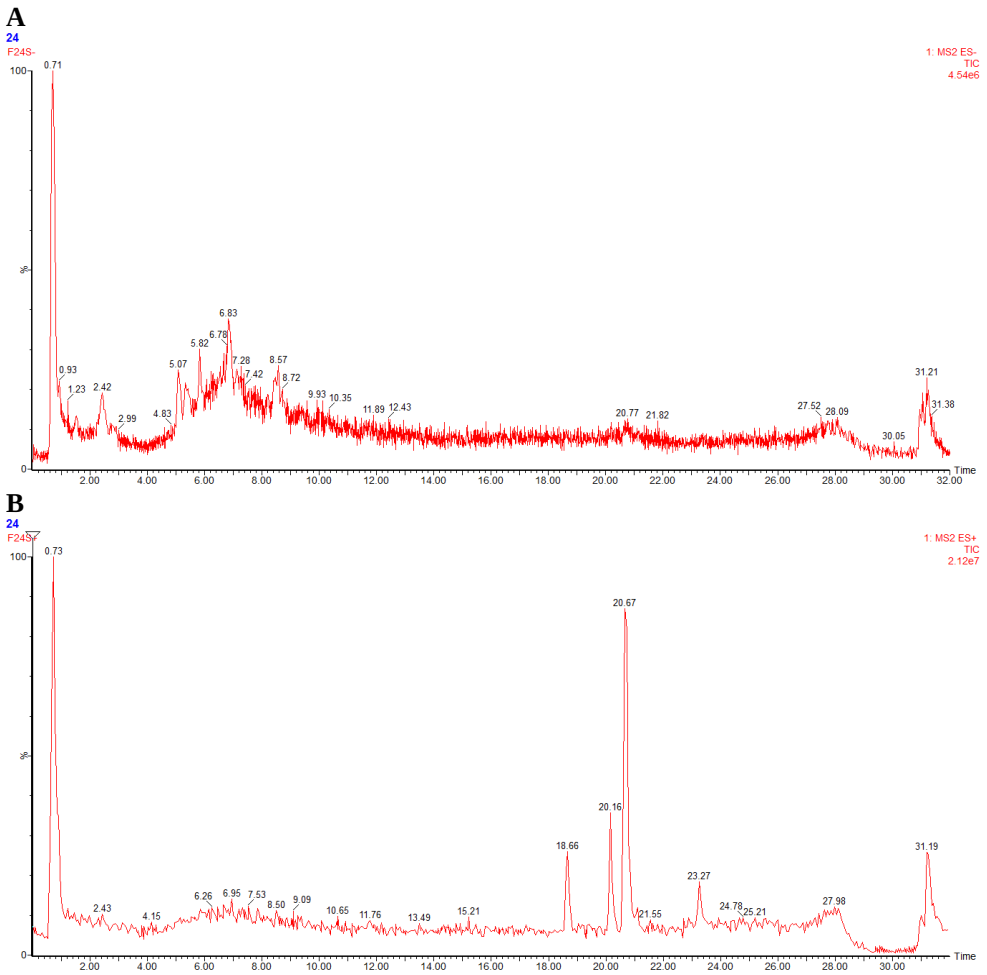

Figure S8. Total ion chromatogram (TIC) of the roots water extract of *S. coriacea* in negative ion mode (A) and positive ion mode (B)

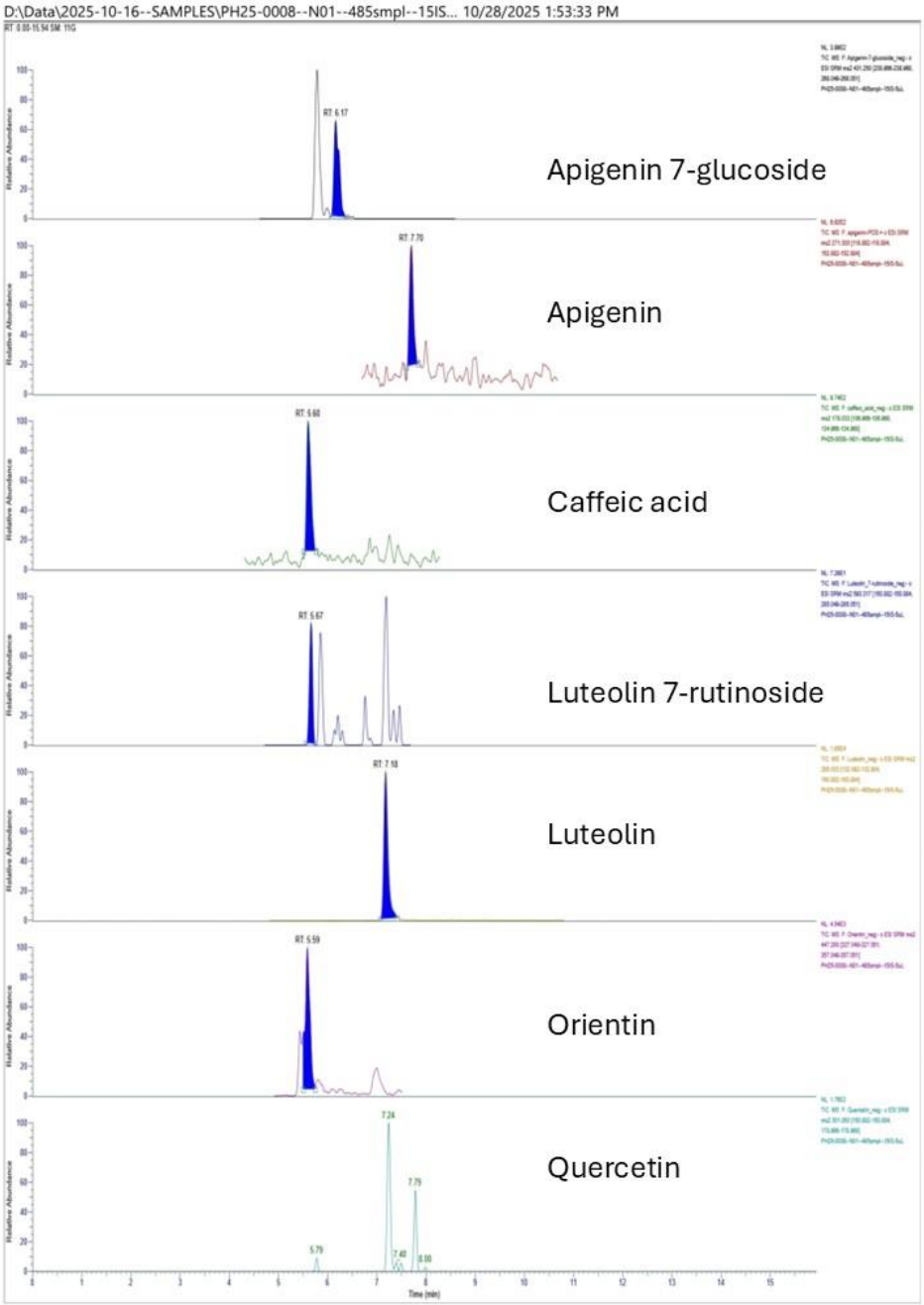

Figure S9. Chromatogram of Ethyl acetate extract from Aerial parts

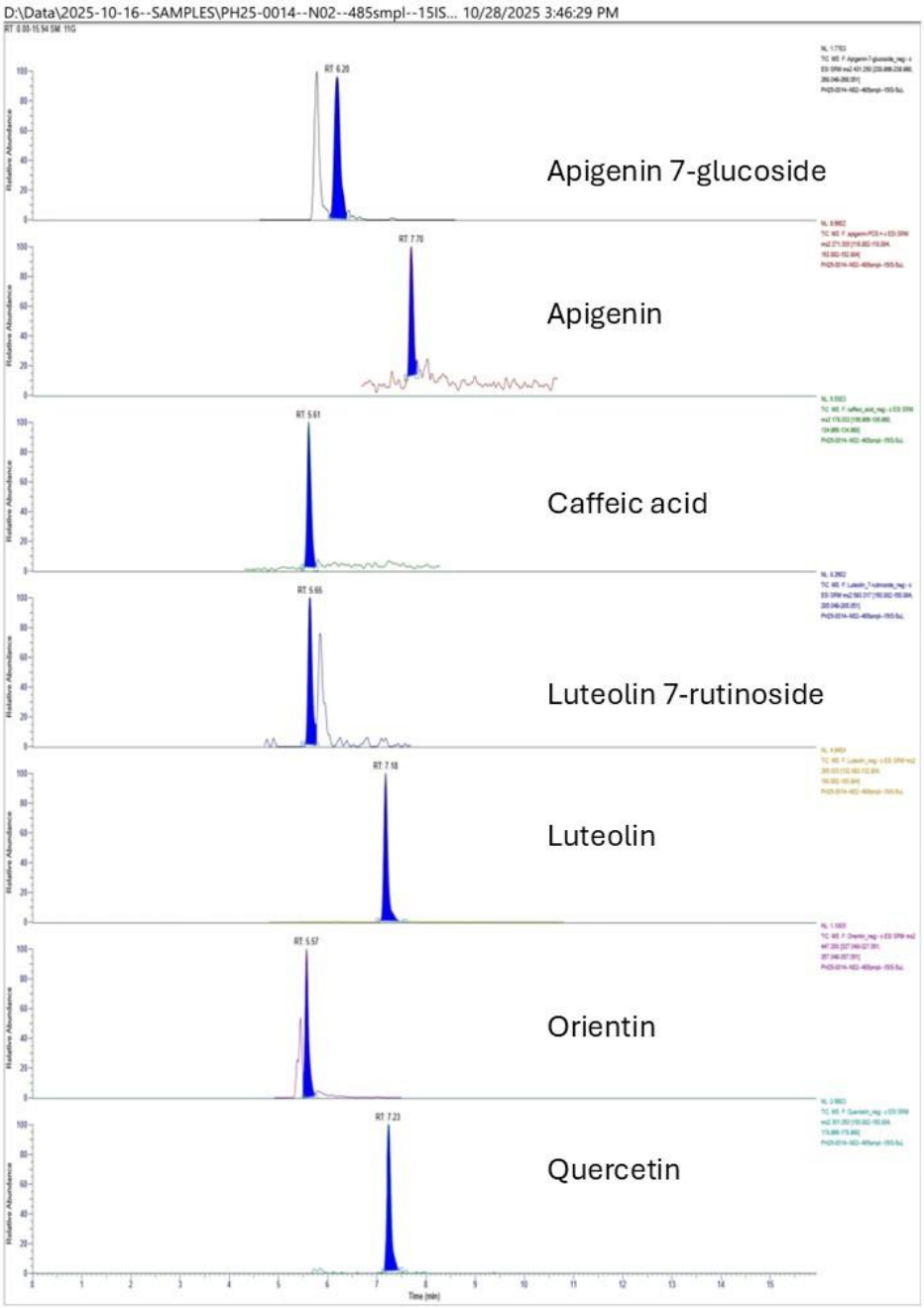

Figure S10. Chromatogram of Ethanol extract from Aerial parts

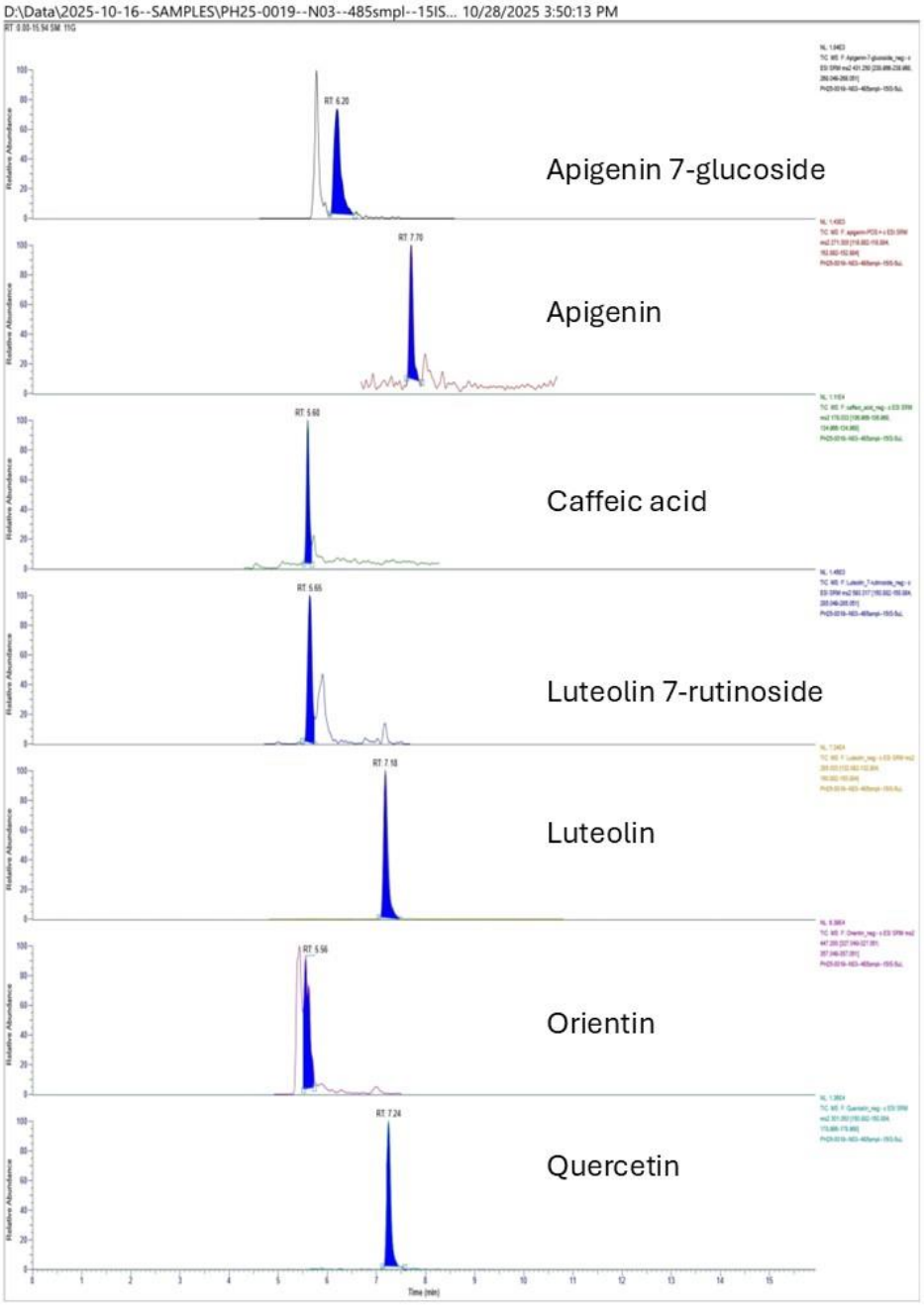

Figure S11. Chromatogram of Ethanol/Water (70%)extract from Aerial parts

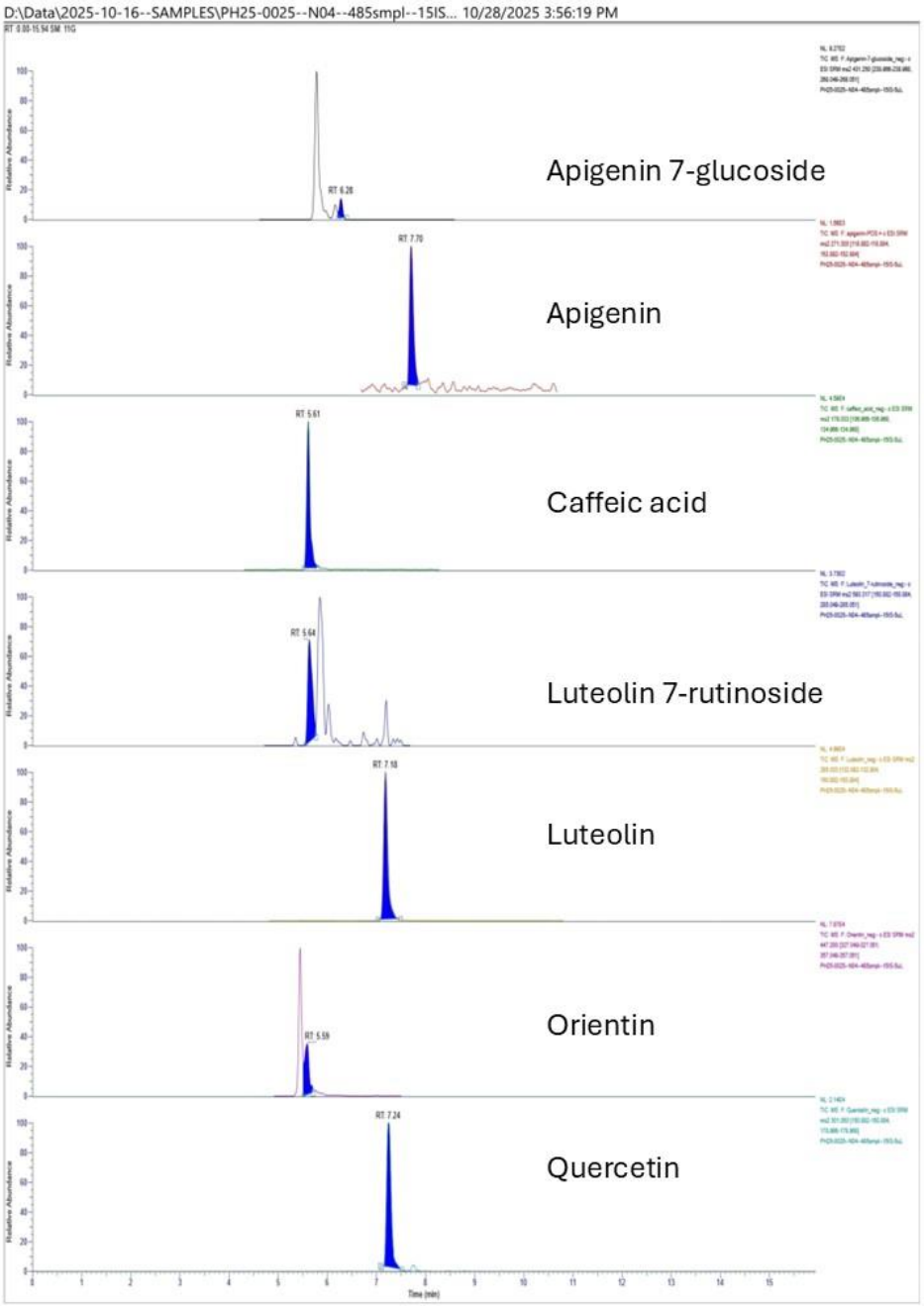

Figure S12. Chromatogram of Water extract from Aerial parts

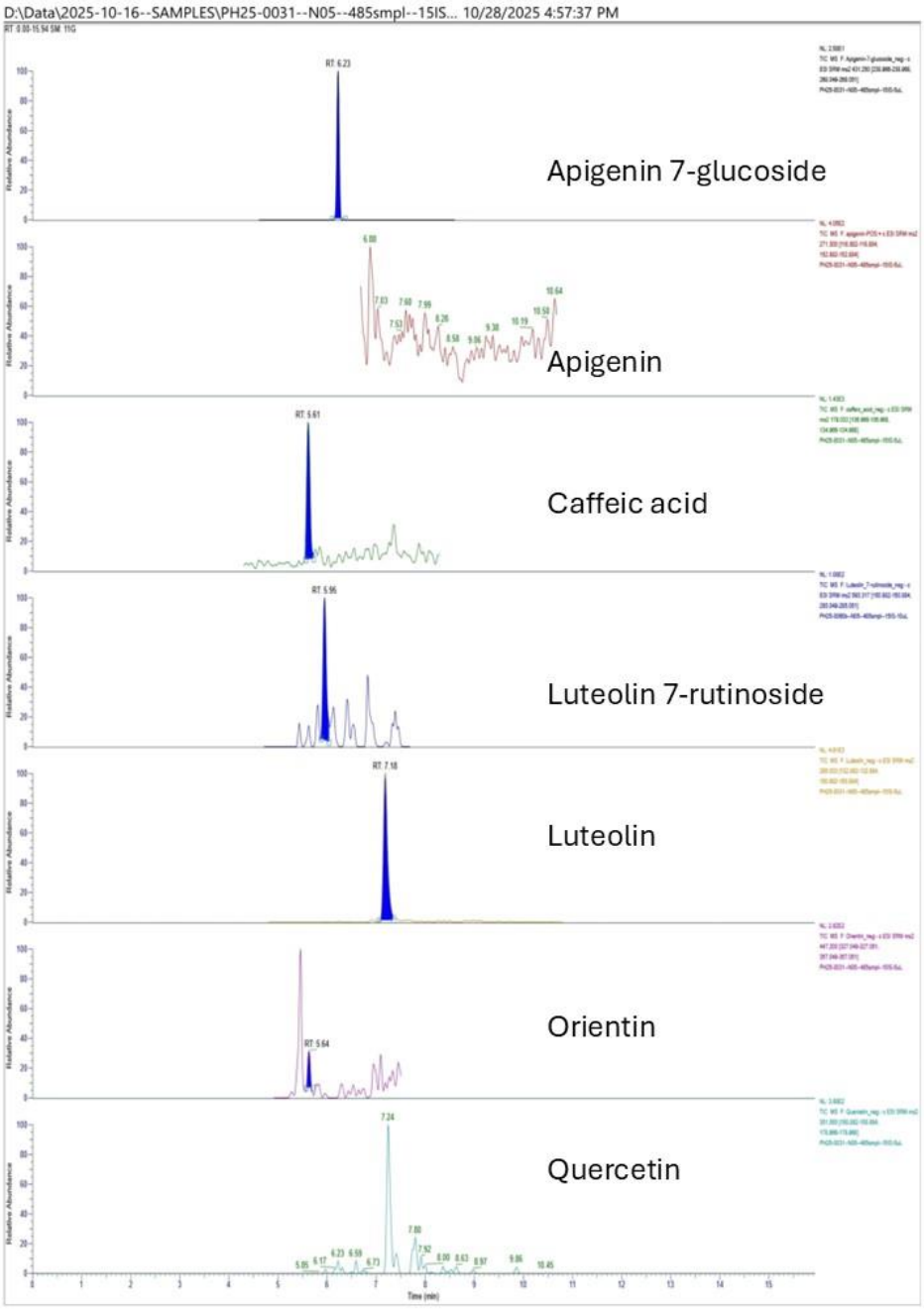

Figure S13. Chromatogram of Ethyl acetate extract from Roots

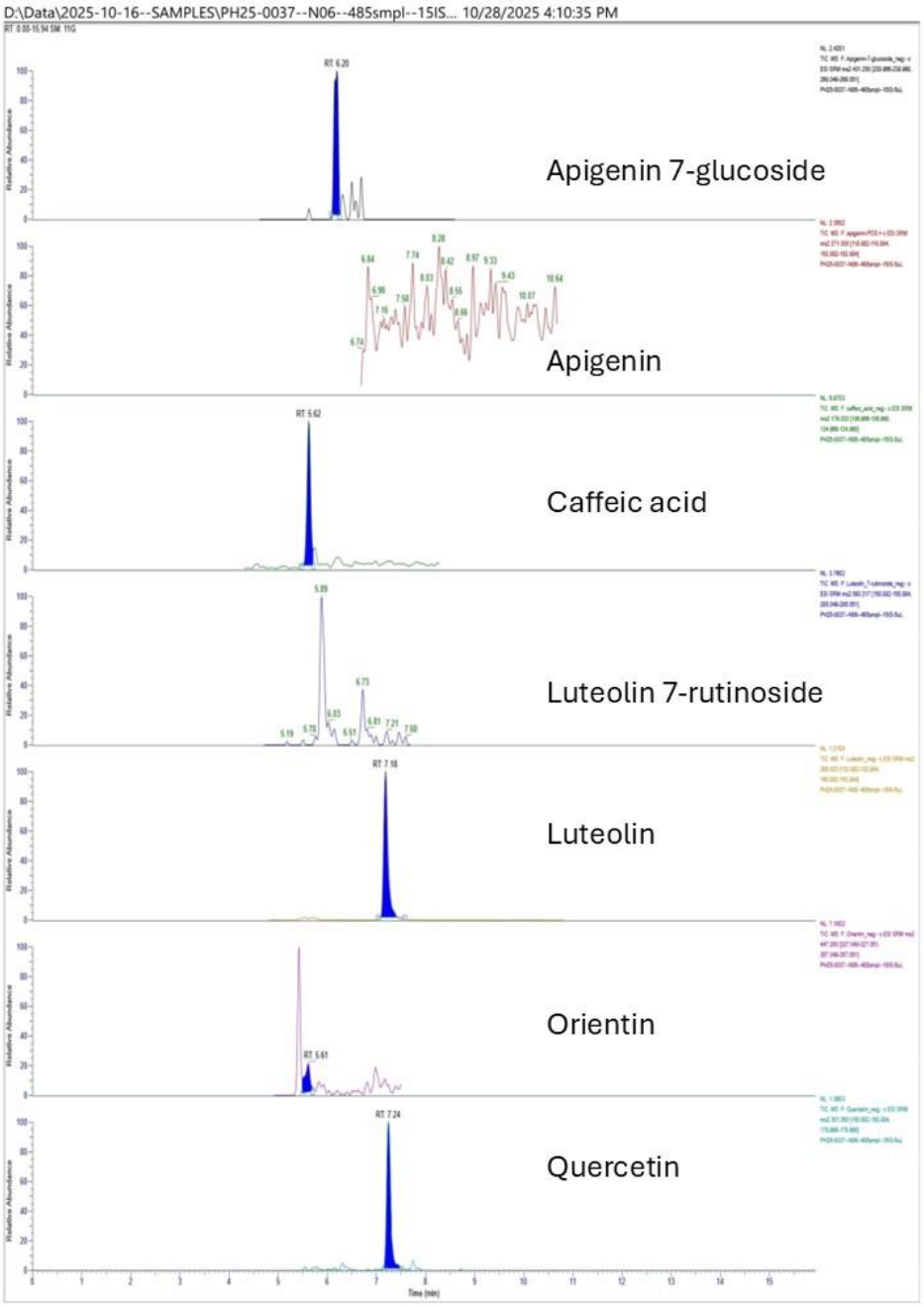

Figure S14. Chromatogram of Ethanol extract from Roots

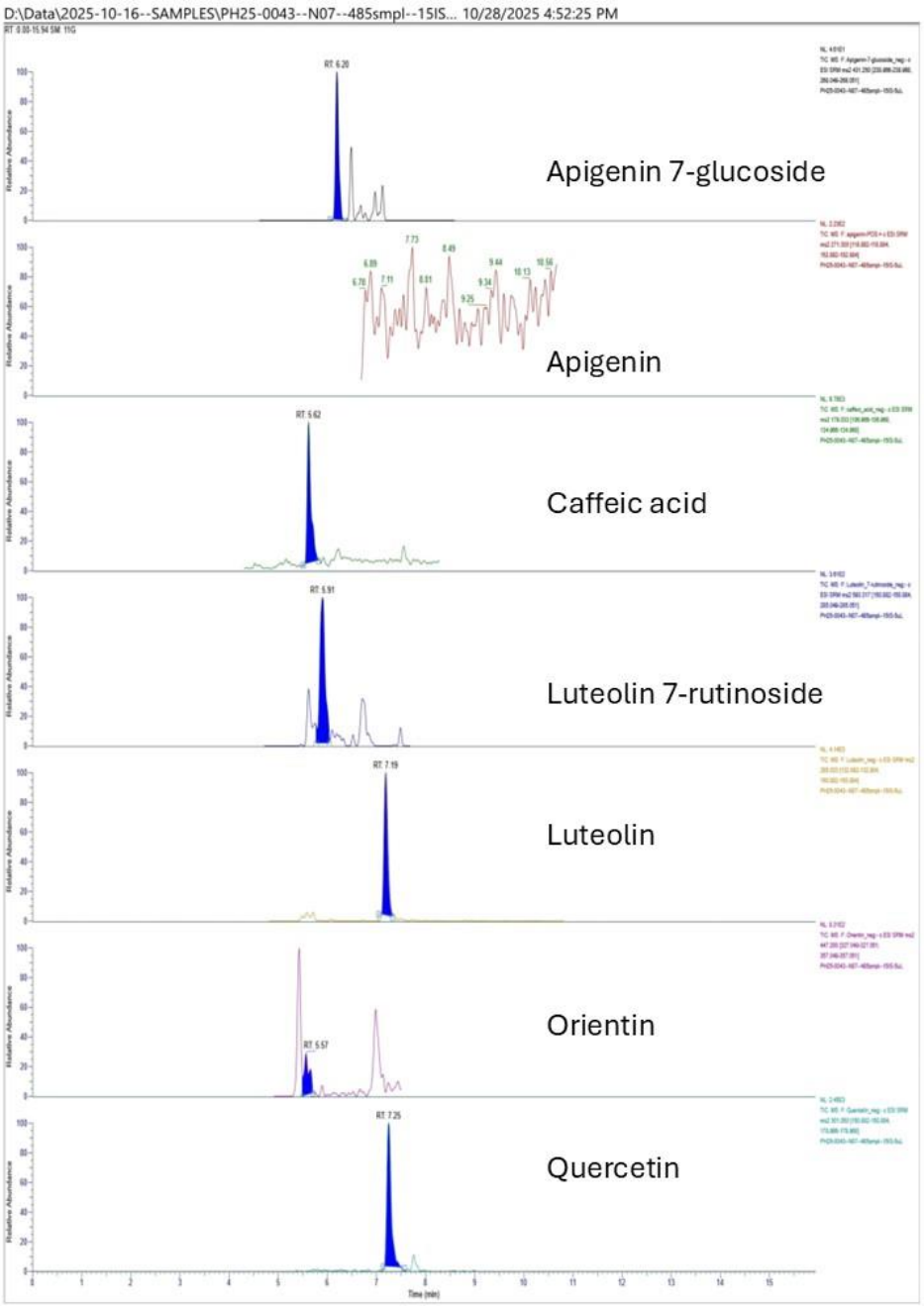

Figure S15. Chromatogram of Ethanol/Water (70%) extract from Roots

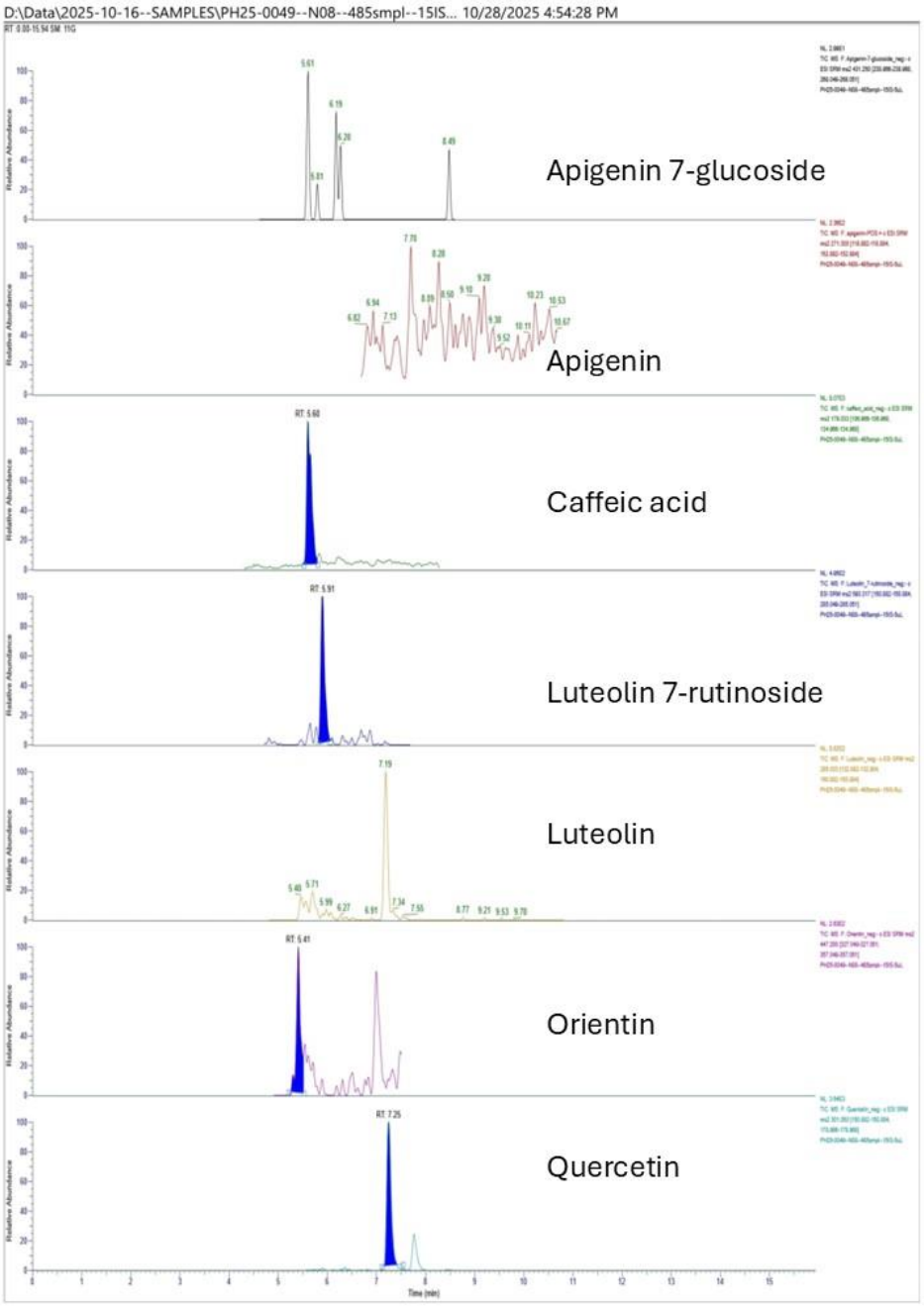

Figure S16. Chromatogram of Water extract from Roots

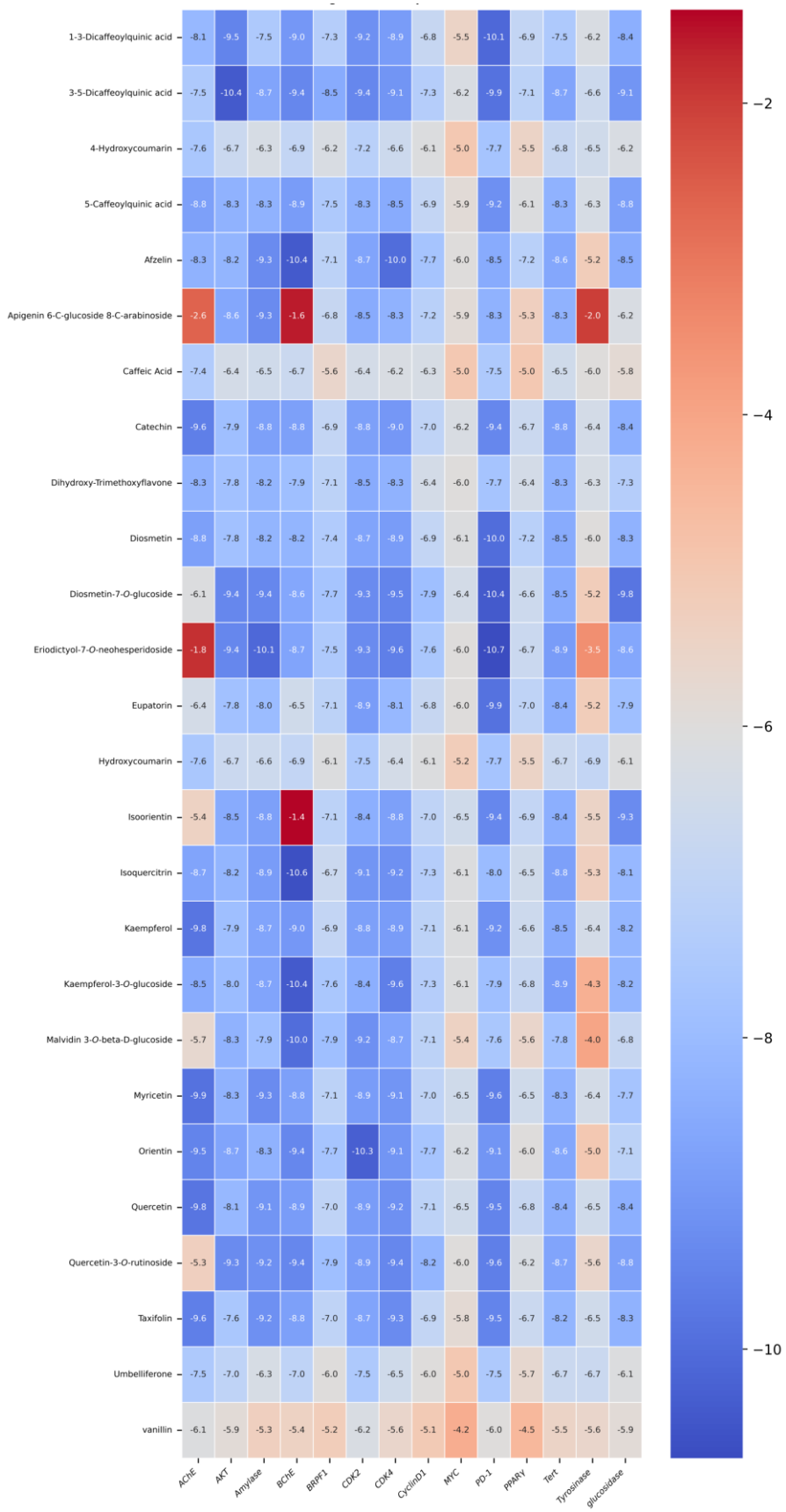

Figure S17: Binding affinity heatmap (kcal/mol) of 26 phytochemicals docked against 14 therapeutic targets. Color scale represents docking scores, with darker blue indicating stronger binding.