

Phytochemical Analysis and Antiproliferative Activity of *Ulex gallii* Planch. (Fabaceae), a Medicinal Plant from Galicia (Spain)

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Table S1. Database of flavonoids present in *Ulex* species.

Metabolite	Formula	Type	Mode	Ion	Collision Energy	<i>m/z</i>	Relative intensity	Database	Reference
Isowighteone	C ₂₀ H ₁₈ O ₅	LC-ESI-QTOF	[M-H] ⁻	C ₂₀ H ₁₇ O ₅ ⁻	10 eV 20 eV	177.0188, 319.0970, 337.1076/ 177.0188, 295.0970, 307.0970, 319.0970, 337.1076	2.7847, 3.68867, 86.9560/ 44.8500, 2.2009, 4.2065, 3.2897, 48.8165	HMDB (Predicted)	https://hmdb.ca/spectra/ms_ms/158859 https://hmdb.ca/spectra/ms_ms/158860
Limonianin	C ₂₀ H ₁₆ O ₅	LC-ESI-QTOF	[M-H] ⁻	C ₂₀ H ₁₅ O ₅ ⁻	10 eV 20 eV	217.0501, 309.0763, 317.0814, 335.0919/ 191.0708, 251.0344, 319.0606, 335.0919	0.6327, 0.8304, 0.5542, 94.8013/ 2.0200, 5.5959, 2.2507, 74.3874	HMDB (Predicted)	https://hmdb.ca/spectra/ms_ms/155106 https://hmdb.ca/spectra/ms_ms/155107
Isopruneitin	C ₁₆ H ₁₂ O ₅	LC-ESI-QTOF	[M-H] ⁻	C ₁₆ H ₁₁ O ₅ ⁻	20V	196.0486, 240.0427, 268.0371, 283.0608	7.2022, 92.7647, 95.2782, 100.0000	MoNA (Experimental)	https://mona.fiehnlab.ucdavis.edu/spectra/display/VF-NPL-QTOF004611
Dihydromyricetin	C ₁₅ H ₁₂ O ₈	LC-ESI-QTOF	[M-H] ⁻	C ₁₅ H ₁₁ O ₈ ⁻	10 eV 20 eV	151.0032, 153.0188, 301.0348, 319.0454/ 125.0239, 151.0031, 301.0348, 319.0454	7.2372, 3.1921, 3.0270, 67.0856/ 7.6694, 15.6284, 4.6647, 25.8881	HMDB (Predicted)	https://hmdb.ca/spectra/ms_ms/22583 https://hmdb.ca/spectra/ms_ms/22584
Genistein	C ₁₅ H ₁₀ O ₅	LC-ESI-QTOF LC-ESI-ITTOF	[M-H] ⁻	C ₁₅ H ₉ O ₅ ⁻	10 eV 20 eV	133.0274, 181.0631, 201.0554, 269.04355 269.0400, 269.3396, 270.0498, 271.0455, 540.1046	5.6, 2.7, 1.5, 100/ 1.906, 5.2535, 3.7033, 4.5508, 19.4843	MoNA (Experimental) HMDB (Experimental)	https://mona.fiehnlab.ucdavis.edu/spectra/display/RIKENPlasma005451 https://hmdb.ca/spectra/ms_ms/6394
Quercetin 3,7-diglucoside	C ₂₇ H ₃₀ O ₁₇	LC-ESI-QTOF	[M-H] ⁻	C ₂₇ H ₂₉ O ₁₇ ⁻	30 eV	301.0000, 463.000, 505.0000	20.00, 100.00, 10.00	MoNA (Experimental)	https://mona.fiehnlab.ucdavis.edu/spectra/display/PM016302
Isopruneitin-7-O-glucoside	C ₂₂ H ₂₂ O ₁₀	LC-ESI-QTOF	[M-H] ⁻	C ₂₂ H ₂₁ O ₁₀ ⁻	-	282.0514, 283.0586, 445.1175	100.0000, 82.9099, 4.0310	MoNA (Experimental)	https://mona.fiehnlab.ucdavis.edu/spectra/display/VF-NPL-QTOF005060
Neoisoliquiritin	C ₂₁ H ₂₂ O ₉	LC-ESI-QTOF	[M-H] ⁻	C ₂₁ H ₂₁ O ₉ ⁻	10 eV 20 eV	119.0497, 237.0552, 255.0657, 417.1186 119.0497, 237.0552, 255.0657, 417.1186	3.8957, 4.1872, 21.2357, 31.6361 5.8093, 6.4842, 37.4759, 4.5595	HMDB (Predicted)	https://hmdb.ca/spectra/ms_ms/137952 https://hmdb.ca/spectra/ms_ms/137953
Daidzein	C ₁₅ H ₁₀ O ₄	UHPLC-ESI-QTOF	[M-H] ⁻	C ₁₅ H ₉ O ₄ ⁻	30 eV	223.0453, 224.0506, 253.0501, 253.3113	12.21, 11.81, 100.00, 8.71	HMDB (Experimental)	https://hmdb.ca/spectra/ms_ms/5886
Inermin	C ₁₆ H ₁₂ O ₅	LC-ESI-QTOF	[M-H] ⁻	C ₁₆ H ₁₁ O ₅ ⁻	10 eV 20 eV	237.0552, 253.0501, 265.0501, 283.0606 237.0551, 253.0500, 265.0500, 283.0606	2.3492, 2.7754, 1.2463, 88.7910 7.7075, 13.6947, 6.7467, 54.4447	HMDB (Predicted)	https://hmdb.ca/spectra/ms_ms/22295 https://hmdb.ca/spectra/ms_ms/22296

Formononetin	C ₁₆ H ₁₂ O ₄	LC-ESI-QTOF	[M-H] ⁻	C ₁₆ H ₁₁ O ₄ ⁻	10 eV	223.409, 251.0328, 252.0426, 267.0662	1.4404, 30.8938, 100.0000	MoNA (Experimental)	https://mona.fiehnlab.ucdavis.edu/spectra/display/VF-NPL-QTOF007716
Genistin	C ₂₁ H ₂₀ O ₁₀	LC-ESI-QTOF	[M-H] ⁻	C ₂₁ H ₁₉ O ₁₀ ⁻	10 eV 20 eV	103.0395, 269.0450, 413.0872, 431.0978 73.0290, 269.0450, 413.0873, 431.0978	3.1718, 28.8188, 3.7217, 38.9856 3.1659, 7.4359, 3.5405, 5.7824	HMDB (Predicted)	https://hmdb.ca/spectra/ms_ms/19073 https://hmdb.ca/spectra/ms_ms/19074
Soyasapogenol B	C ₃₀ H ₅₀ O ₃	LC-ESI-QTOF	[M-H] ⁻	C ₃₀ H ₄₉ O ₃ ⁻	10 eV 20 eV	421.3470, 427.3576, 439.3576, 457.3682 427.3576, 439.3576, 441.3368, 457.3681	4.2356, 5.0888, 23.4589, 51.2316 4.0092, 27.7025, 1.1133, 21.81467	HMDB (Predicted)	https://hmdb.ca/spectra/ms_ms/164916 https://hmdb.ca/spectra/ms_ms/164917
Resokaempferol	C ₁₅ H ₁₀ O ₅	LC-ESI-QTOF	[M-H] ⁻	C ₁₅ H ₁₅ O ₅ ⁻	10 eV 20 eV	269.0449, 270.0476, 271.0469 224.0447, 239.0320, 269.0408, 270.436	100.00, 12.61, 1.70 1.70, 2.30, 100.00, 10.41	HMDB (Experimental)	https://hmdb.ca/spectra/ms_ms/373875 https://hmdb.ca/spectra/ms_ms/373876
Luteolin-4-O-glucoside	C ₂₁ H ₂₀ O ₁₁	LC-ESI-QTOF	[M-H] ⁻	C ₂₁ H ₁₉ O ₁₁ ⁻	10 eV	285.0388, 286.0418, 287.0416, 441.0925	100.00, 17.80, 2.60, 68.20	MoNA (Predicted)	https://mona.fiehnlab.ucdavis.edu/spectra/display/RIKENPlasma005697
Luteolin-7-O-glucoside	C ₂₁ H ₂₀ O ₁₁	LC-ESI-QTOF	[M+FA-H] ⁻	C ₂₁ H ₁₉ O ₁₁ ⁻	10 eV	284.0297, 284.0559, 285.0418, 447.0932	15.0847, 12.4764, 23.7698, 100.0000	MoNA (Experimental)	https://mona.fiehnlab.ucdavis.edu/spectra/display/CCMSLIB00000846983
Quercetin-O-glucoside	C ₂₁ H ₂₀ O ₁₂	LC-ESI-QTOF	[M-H] ⁻	C ₂₁ H ₁₉ O ₁₁ ⁻	-	255.0274, 271.0261, 300.0258, 301.0351, 463.0889	10.39, 23.35, 100.00, 87.02, 98.06	HMDB (Experimental)	https://hmdb.ca/spectra/ms_ms/440558
Eriodictyol 7-O-glucoside	C ₂₁ H ₂₂ O ₁₁	LC-ESI-QTOF	[M-H] ⁻	C ₂₁ H ₂₁ O ₁₁ ⁻	10 eV	287.0533, 288.0582, 289.0566, 449.1077	100.00, 15.40, 2.40, 23.30	MoNA (Experimental)	https://mona.fiehnlab.ucdavis.edu/spectra/display/RIKENPlasma006155
Rutin	C ₂₇ H ₃₀ O ₁₆	LC-ESI-QTOF	[M-H] ⁻	C ₂₇ H ₂₉ O ₁₆ ⁻	10 eV 20 eV	163.0606, 301.0348, 591.1349, 609.1455 272.0281, 301.0344, 609.1456	6.3662, 18.8843, 6.0445, 20.6713 16.00, 91.00, 99.00	HMDB (Predicted) MassBank EU (Experimental)	https://hmdb.ca/spectra/ms_ms/273297 https://massbank.eu/MassBank/RecordDisplay?id=MSBNK-Washington_State_Univ-BML00141&dsn=Washington_State_Univ
Liquiritin	C ₂₁ H ₂₂ O ₉	LC-ESI-QTOF	[M-H] ⁻	C ₂₁ H ₂₁ O ₈ ⁻	10 eV 20 eV	237.0551, 255.0657, 399.1079, 417.1185 161.0449, 237.0551, 255.0865, 417.1186	4.5417, 24.9801, 3.3249, 34.4403 3.5209, 5.8702, 43.2606, 4.9646	HMDB (Experimental)	https://hmdb.ca/spectra/ms_ms/168057 https://hmdb.ca/spectra/ms_ms/168058
Apigenin 4-O-glucoside	C ₂₁ H ₂₀ O ₁₀	LC-ESI-QTOF	[M+FA-H] ⁻	C ₂₁ H ₁₉ O ₁₀ ⁻	20 eV	268.0384, 269.0450, 431.0997	17.6810, 91.3639, 100.0000	MoNA (Experimental)	https://mona.fiehnlab.ucdavis.edu/spectra/display/CCMSLIB00000847310
Apigenin 7-O-glucoside	C ₂₁ H ₂₀ O ₁₀	LC-ESI-QTOF	[M-H] ⁻	C ₂₁ H ₁₉ O ₁₁ ⁻	10 eV 20 eV	103.0395, 269.0449, 413.0872, 431.0978	3.0945, 27.6401, 9.3458, 37.5765	HMDB (Predicted)	https://hmdb.ca/spectra/ms_ms/148638

						251.0344, 269.0449, 413.0872, 431.0978	3.2514, 55.1915, 6.6065, 5.8183		https://hmdb.ca/spectra/ms_ms/148639
Kaempferol-5-O-glucoside	C ₂₁ H ₂₀ O ₁₁	LC-ESI-QTOF	[M-H] ⁻	C ₂₁ H ₁₉ O ₁₁ ⁻	10 eV 20eV	267.0293, 285.0399, 429.0821, 447.0927	4.2709, 24.7430, 8.0195, 33.3460	HMDB	https://hmdb.ca/spectra/ms_ms/158397
						161.0449, 267.0293, 285.0399, 429.0821	3.5939, 6.0272, 45.6949, 5.1339	(Predicted)	https://hmdb.ca/spectra/ms_ms/158398
Formononetin-O-glucoside	C ₂₂ H ₂₂ O ₉	LC-ESI-QTOF	[M-H] ⁻	C ₂₂ H ₂₁ O ₉ ⁻	10 eV 20eV	103.0395, 267.0657, 411.1079, 429.1185	3.1818, 28.4173, 7.3022, 38.9445	HMDB	https://hmdb.ca/spectra/ms_ms/17537
						237.0551, 267.0657, 411.1079, 429.1185	5.8294, 52.7782, 5.6049, 5.6364	(Predicted)	https://hmdb.ca/spectra/ms_ms/17538
Kaempferol	C ₁₅ H ₁₀ O ₆	UHPLC -ESI-QTOF	[M-H] ⁻	C ₁₅ H ₉ O ₅ ⁻	-	119.0343, 164.9985, 285.0399	79.4299, 38.6044, 33.5242	HMDB (Experimental)	https://hmdb.ca/spectra/ms_ms/6081
Naringenin	C ₁₅ H ₁₂ O ₅	UHPLC -ESI-QTOF	[M-H] ⁻	C ₁₅ H ₁₁ O ₅ ⁻	-	93.0339, 119.0501, 151.0038, 271.0606	7.61, 60.76, 60.06, 100.00	HMDB (Experimental)	https://hmdb.ca/spectra/ms_ms/5790
Apigenin	C ₁₅ H ₁₀ O ₅	LC-ESI-QTOF	[M-H] ⁻	C ₁₅ H ₉ O ₅ ⁻	10 eV 20eV	269.0458, 270.0491, 271.0507 151.0035, 227.0350, 269.0461	29.184, 4.562, 6.100 1.222, 3.906, 6.014	MassBank. EU (Experimental)	https://massbank.eu/MassBank/RecordDisplay?id=MSBNK-Fiocruz-FIO00011&dsn=Fiocruz
Liquiritigenin	C ₁₅ H ₁₂ O ₄	LC-ESI-QTOF	[M-H] ⁻	C ₁₅ H ₁₁ O ₄ ⁻	10 eV	119.0520, 135.0123, 255.0697, 255.2351	50.5431, 69.5440, 100.0000, 21.7868	MoNA (Experimental)	https://mona.fiehnlab.ucdavis.edu/spectra/display/MoNA018159

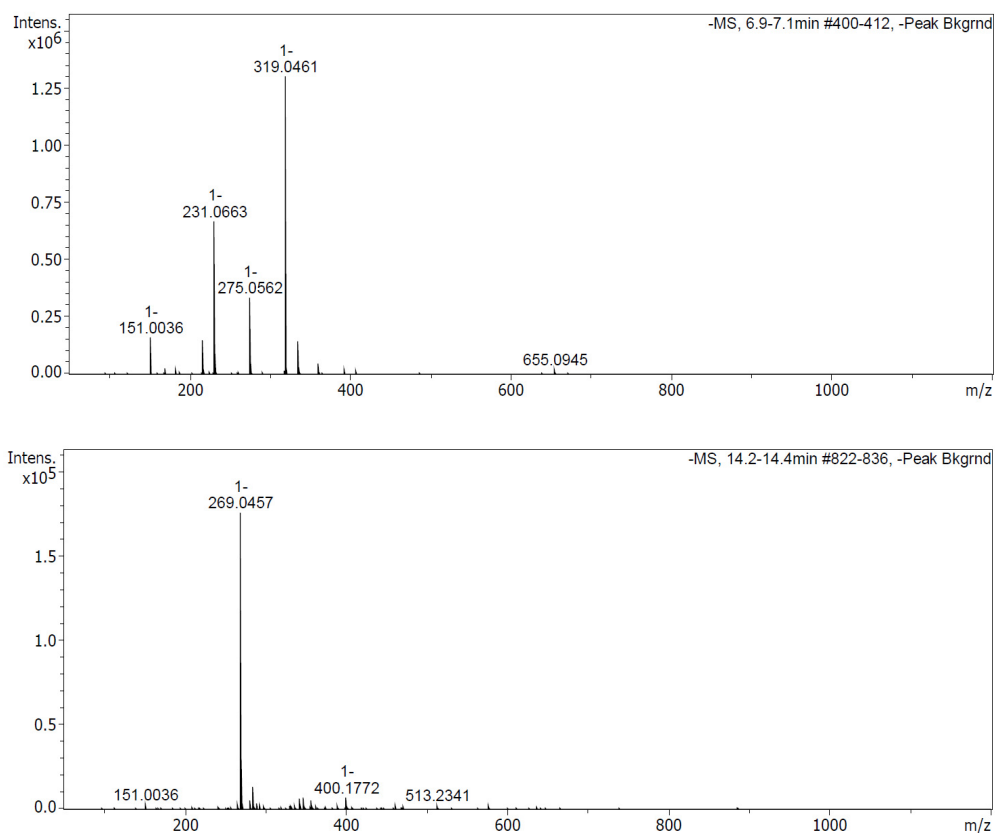


Figure S1. Mass spectrum corresponding to dihydromyricetin (top, peak 26, Rt: 7.00 min) and genistein (bottom, peak 52, Rt: 14.30) in D5 sub-fraction.

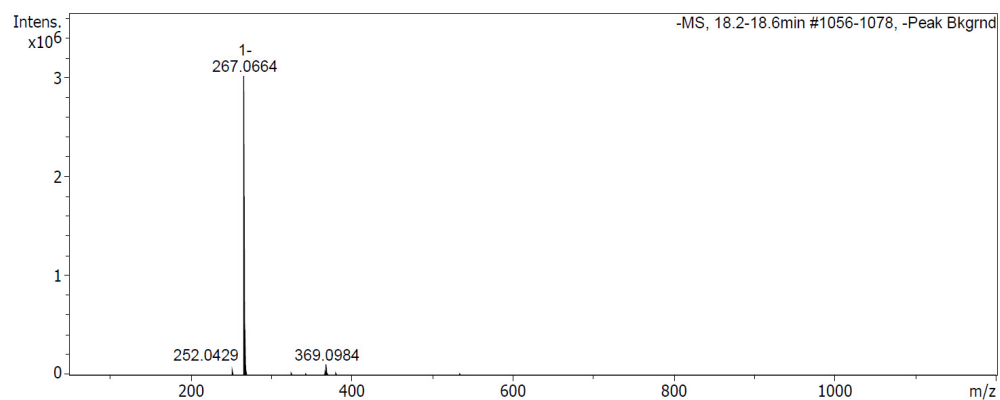


Figure S2. Mass spectrum corresponding to formononetin (peak 61, Rt: 18.40 min) in D7 sub-fraction.

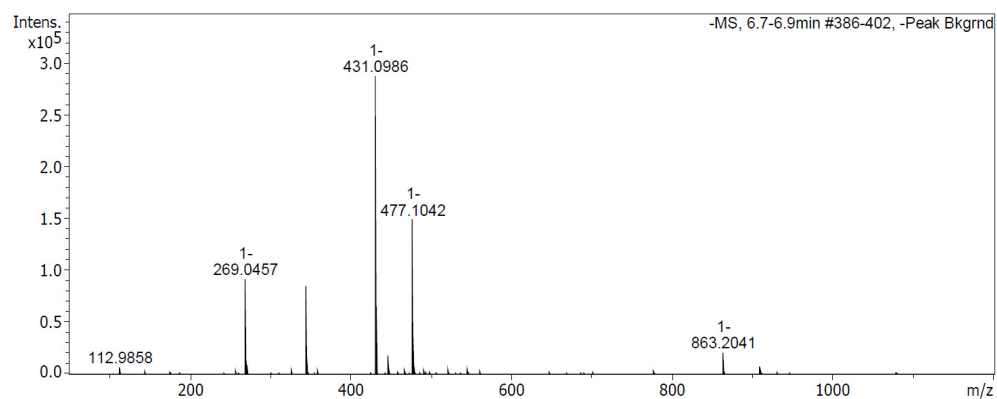
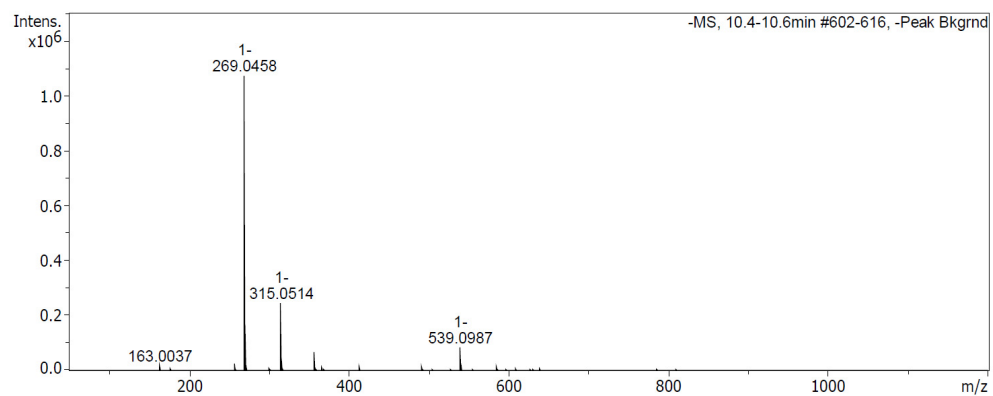


Figure S3. Mass spectrum corresponding to apigenin (top, peak 37, Rt: 10.50 min) and apigenin-4-O-glucoside (bottom, Rt: 6.87) in D8 sub-fraction.

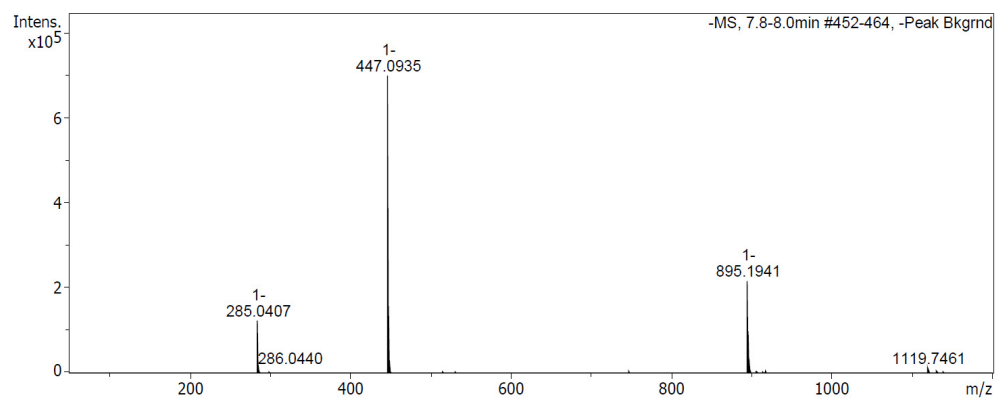


Figure S4. Mass spectrum corresponding to luteolin-4-O-glucoside (peak 10, Rt: 7.90 min) in M4 sub-fraction.