

**Metabolomic approach for a rapid identification of natural products with cytotoxic activity  
against human colorectal cancer cells**

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**SUPPLEMENTARY INFORMATION**

**Table S1** Main metabolites detected in the studied plant extracts. <sup>1</sup>H-NMR data are measured in ppm and coupling constants (J) in Hertz.

Plant Species	Metabolites	Chemical shift values
<i>Astragalus boeticus</i>	Cycloartanes	0.37 (H19, d, J=4.6); 0.57 (H19, d, J=4.6); 0.99 (H30, s); 1.01 (H28, s); 1.06 (H29, s); 1.24 (H18, s); 1.24 (H26, s); 1.26 (H21, s); 1.34 (H27, s)
	Kaempferol	6.32 (H6, d, J = 2.1); 6.53 (H8, d, J = 2.1); 7.00 (H2'/H6', d, J = 8.4); 8.03 (H3'/H5', d, J = 8.4)
	Quercetin	6.27 (H6, d, J = 2.1); 6.52 (H8, d, J = 2.1); 6.99 (H5', d J = 8.5); 7.60 (H6', dd, J = 8.5, 2.1); 7.65 (H2', d J = 2.1)
<i>Lathyrus cicera</i>	Kaempferol derivative 1	6.52 (H6, d, J = 2.1); 6.78 (H8, d, J = 2.1); 7.06 (H2'/H6', d, J = 8.4); 8.02 (H3'/H5', d, J = 8.4)
	L-homoarginine	1.63 (H6, m); 1.87 (H4, m); 3.20 (H7, t)
	γ-pyrone	6.69 (d, J=5.1); 8.17 (d, J=5.1)
<i>Lathyrus clymenum</i>	Kaempferol	see <i>A. boeticus</i>
	Catechin	2.52 (H4b, dd); 2.82 (H4a, dd); 5.95 (H6, d, J = 2.1 Hz); 6.03 (H8, d, J = 2.1); 6.94–6.96 (ring B, ov)
<i>Medicago minima</i>	Daidzein	6.96 (H3'/H5', d J = 9.0); 6.97 (H8, d J = 2.0); 7.04 (H6, dd J = 9.0, 2.0); 7.43 (H2'/H6', d J = 9.0); 8.06 (H5, d J = 9.0); 8.21 (H2, s)
	Daidzin	5.24 (H1'', d, J = 7.8); 6.96 (H3'/H5', d J = 9.0); 7.28 (H8, d J = 2.0); 7.25 (H6, dd J = 9.0, 2.0); 7.41 (H2'/H6', d J = 9.0); 8.17 (H5, d J = 9.0); 8.29 (H2, s)
	Genistein	6.31 (H6, d J = 2.0), 6.47 (H8, d J = 2.0), 7.05 (H3'/H5', d J = 9.0); 7.44 (H2'/H6', d J = 9.0); 8.21 (H2, s)
	Phenylpropanoid	6.42 (H8, d, J = 15.9) 7.60 (H7, d, J = 15.9)
	Quercetin-7-O glucoside	5.23 (H1'', d, J = 7.8); 6.54 (H6, d, J = 2.1); 6.90 (H8, d, J = 2.1); 7.06 (H5', d, J = 8.4); 7.66 (H6', dd, J = 8.7, 2.1); 7.83 (H2', d, J = 2.1)
	Trigonelline	9.15 (H1, s); 8.86 (H3/H5, t)
<i>Melilotus neapolitanus</i>	Coumarin	6.51 (H3, d J = 9.6); 8.08 (H4, d J = 9.6); 6.89 (H6/H8, m); 7.40 (H5/H7, m)
	cis-Melilotoside	5.03 (H10, d J = 7.8); 6.06 (H3, d J = 12.6); 6.86 (H4, d J = 12.6)
	trans-Melilotoside	5.01 (H10, d J = 7.5); 6.84(H3, d J = 16.2); 7.86 (H4, d J = 16.2);
	Trigonelline	see <i>M. minima</i>
<i>Ononis variegata</i>	Caffeic acid derivative 1	6.47 (H-8', d, J = 15.9 Hz); 6.88 (H-5', d, J = 8.2 Hz); 7.09 (H6', dd, J=8.4, 2); 7.18 (H2', d, J=2.1); 7.67 (H7, d, J=15.9)
	Quercetin derivative 1	6.32 (H6, d, J = 2.1); 6.53 (H8, d, J = 2.1); 6.95 (H5', d J = 8.5); 7.55 (H6', d J = 8.5, 2.1); 7.66 (H2', d J = 2.1)
<i>Pisum sativum</i>	Flavonoids	6.31 (ring A, d, J = 2.1); 6.52 (ring A, d, J = 2.1)
<i>Trifolium campestre</i>	C6-glycosilated apigenin derivative	6.72 (H8, S); 6.91(H8, S); 7.10 (H3'/H5',d, J = 9.0 Hz); 7.93 (H2'/H6',d, J = 9.0 Hz)
	Trigonelline	see <i>M. minima</i>
<i>Trifolium cherleri</i>	Caffeic acid derivative 2	7.61 (H7, d, J=15.9); 7.18 (H2', d, J=2.1); 7.07 (H6', dd, J=8.4, 2); 6.87 (H-5', d, J = 8.2 Hz); δ 6.39 (H-8', d, J = 15.9 Hz)
	Kaempferol derivative 2	6.32 (H6, d, J = 2.1); 6.53 (H8, d, J = 2.1); 6.95 (H2'/H6', d, J = 8.4); 8.17 (H3'/H5', d, J = 8.4)
	Quercetin derivative 2	6.27 (H6, d, J = 2.1); 6.52 (H8, d, J = 2.1); 6.95 (H5', d J = 8.5); 7.55 (H6', dd, J = 8.5, 2.1); 7.61 (H2', d J = 2.1)

	Trigonelline	see <i>M. minima</i>
<i>Trifolium scabrum</i>	Daidzein	see <i>M. minima</i>
	Daidzin	see <i>M. minima</i>
	Genistein	see <i>M. minima</i>
	Quercetin derivative 3	6.27(H6, d, J = 2.1); 6.46 (H8, d, J = 2.1); 6.92 (H5', d J = 8.5); 7.52 (H6', d J = 8.5, 2.1); 7.58 (H2', d J = 2.1)
	Kaempferol derivative 3	6.28 (H6, d J = 2.1), 6.48 (H8, d J = 2.1), 6.93 (H3'/H5', d J = 8.5); 7.96 (H3'/H5', d, J = 8.5)
<i>Trigonella esculenta</i>	Caffeic acid derivative 3	7.59 (H7, d, J=15.9); 7.15 (H2', d, J=2.1); 7.06 (H6', dd, J=8.4, 2); 6.86 (H-5', d, J = 8.2 Hz); $\delta$ 6.38 (H-8', d, J = 15.9 Hz)
	4-hydroxyisoleucine	0.98 (H6, d, J=6.8); 1.25 (H5, d, J=6.3)
	Quercetin derivative 4	6.27 (H6, d, J = 2.1); 6.53 (H8, d, J = 2.1); 6.97 (H5', d J = 8.5); 7.67 (H6', dd, J = 8.5, 2.1); 7.75 (H2', d J = 2.1)
	Trigonelline	see <i>M. minima</i>
<i>Vicia bithynica</i>	Chlorogenic acid	6.37 (H8', d, J=15.9); 7.61 (H7', d, J=15.9); 7.14 (H5', d, J = 2.0 Hz); 7.06 (H6', d, J = 8.5; 2.2 Hz) 6.88 (d, J = 8.2); 1.84 - 2.20 (H2/H6, m); 5.45 (ring A, ov)
	Quercetin	See <i>A. boeticus</i>
	Quercetrin	0.91 (H6'', d, J = 6.0); 5.27 (H1'', d, J = 1.8); 6.31 (H6, d, J = 2.1); 6.51 (H8, d, J = 2.1); 6.98 (H5', d, J = 8.4); 7.34 (H6', dd, J = 8.7, 2.1); 7.37 (H2', d, J = 2.1)
<i>Vicia pseudocracca</i>	Quercetrin	see <i>V. bithynica</i>
	Trigonelline	see <i>M. minima</i>
<i>Vicia angustifolia</i>	Chlorogenic acid	see <i>V. bithynica</i>
	Quercetin derivative 5	6.31 (H6, d, J = 2.1); 6.56 (H8, d, J = 2.1); 7.00 (H5', d J = 8.5); 7.64 (H6', dd, J = 8.5, 2.1); 7.67 (H2', d J = 2.1)