

Supplementary data for article:

Banjanac, T.; Dragićević, M.; Šiler, B.; Gašić, U.; Bohanec, B.; Nestorović Živković, J.; Trifunović, S.; Mišić, D. Chemodiversity of Two Closely Related Tetraploid *Centaurium* Species and Their Hexaploid Hybrid: Metabolomic Search for High-Resolution Taxonomic Classifiers. *Phytochemistry* **2017**, *140*, 27–44.

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Table S1. Calibration data of 20 targeted compounds, including correlation coefficient (r^2), limit of detection (LOD) and limit of quantification (LOQ), as revealed by UHPLC/ \pm MS/MS analyses in SRM experiment. LOD and LOQ were separately determined in six replicate determinations at a signal-to-noise ratio (S/N) of 3 and 10, respectively.

Code No.	Compound	Ionisation mode	(r^2)	LOD ($\mu\text{g mL}^{-1}$)	LOQ ($\mu\text{g mL}^{-1}$)
71	Quinic acid	-HESI	0.9970	0.010	0.025
3	Caffeic acid	-HESI	0.9987	0.010	0.025
10	<i>p</i> -Coumaric acid	-HESI	0.9936	0.025	0.050
13	Ferulic acid	-HESI	0.9950	0.100	0.200
12	Sinapic acid	-HESI	0.9939	0.010	0.025
17	Luteolin	-HESI	0.9903	0.010	0.025
19	Apigenin	-HESI	0.9948	0.005	0.010
26	Rutin	-HESI	0.9956	0.005	0.010
25	Isoquercitrin	-HESI	0.9987	0.010	0.025
29	Astragalin	-HESI	0.9909	0.005	0.010
21	Quercetin	-HESI	0.9939	0.005	0.010
20	Kaempferol	-HESI	0.9911	0.010	0.025
18	Naringenin	-HESI	0.9981	0.010	0.025
47	Decussatin	+HESI	0.9944	0.010	0.025
53	Eustomin	+HESI	0.9920	0.005	0.010
48	Methylbellidifolin	+HESI	0.9983	0.100	0.250
55	Demethyleustomin	+HESI	0.9987	0.005	0.010
68	Swertiaarin	-HESI	0.9970	0.025	0.100
70	Gentiopicrin	-HESI	0.9990	0.010	0.025
69	Sweroside	-HESI	0.9973	0.050	0.100