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/±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 (μg $mL^{-1}$) | LOQ (μg $mL^{-1}$) |
|---|---|---|---|---|---|
| **71** | Quinic acid | -HESI | 0.9970 | 0.010 | 0.025 |
| **3** | Caffeic acid | -HESI | 0.9987 | 0.010 | 0..025 |
| **10** | *p*-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** | Swertiamarin | -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 |