## Supplementary data for article:

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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 $\left(r^{2}\right)$, limit of detection (LOD) and limit of quantification (LOQ), as revealed by UHPLC/ $\pm \mathrm{MS} / \mathrm{MS}$ analyses in SRM experiment. LOD and LOQ were separately determined in six replicate determinations at a signal-tonoise ratio $(\mathrm{S} / \mathrm{N})$ of 3 and 10 , respectively.

| Code | Compound | Ionisation mode | $\left(r^{2}\right)$ | LOD ( $\mu \mathrm{g} \mathrm{mL}{ }^{-1}$ ) | LOQ ( $\mu \mathrm{g} \mathrm{mL}{ }^{-1}$ ) |
| :---: | :---: | :---: | :---: | :---: | :---: |
| No. |  |  |  |  |  |
| 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 |

