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 | Compound | Ionisation mode | (r ²) | LOD (µg mL-1) | LOQ (µg mL ⁻¹) |
|------|-------------------------|-----------------|-------------------|---------------|----------------------------|
| No. | | | | | |
| 71 | Quinic acid | -HESI | 0.9970 | 0.010 | 0.025 |
| 3 | Caffeic acid | -HESI | 0.9987 | 0.010 | 0025 |
| 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 | 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 |