**Table S1.** Chromatographic and mass spectrometry data of the adopted UHPLC/DAD/(±)HESI–$MS^2$ analytical method for the quantification of eight targeted phenolics and iridoids in methanol extracts of *N. nuda* plants.

| | | **UHPLC/MS data** | | | | **UHPLC/DAD data** | |
|---|---|---|---|---|---|---|---|
| | Metabolite | $t_R$ [min] | $[M-H]^-$ [m/z] | Diagnostic $MS^2$ fragments [m/z] | cE [eV] | $t_R$ [min] | $\lambda_{max}$ [nm] |
| **1** | Chlorogenic acid[a] | 2.76 | 353 | 191, 127 | 30 | 2.64 | 230, 330 |
| **2** | Caffeic acid[a] | 3.02 | 179 | 135, 134 | 30 | 2.90 | 230, 330 |
| **3** | Loganin[a] | 3.43 | 435* | 227, 127 | 30 | 3.31 | 230 |
| **4** | Nepetanudoside[R] | 3.59 | 435* | 227, 101 | 30 | 3.47 | 230, 330 |
| **5** | 1,5,9-*epi*-Deoxyloganic acid[a] | 4.09 | 405* | 359, 197 | 30 | 3.97 | 240 |
| **6** | Rosmarinic acid[a] | 5.38 | 359 | 161, 133 | 30 | 5.26 | 240, 330 |
| **7** | Quercetin[a] | 6.40 | 301 | 179, 151 | 30 | 6.28 | 270, 360 |
| | Metabolite | $t_R$ [min] | $[M+H]^+$ [m/z] | Diagnostic $MS^2$ fragments [m/z] | cE [eV] | $t_R$ [min] | $\lambda_{max}$ [nm] |
| **8** | 5,9-Dehydronepetalactone[a] | 6.31 | 165 | 149, 77 | 20 | 6.19 | 300 |
| **9** | *trans*,*trans*-Nepetalactone[R] | 7.23 | 167 | 111, 77 | 20 | 7.11 | 225 |
| **10** | *cis*,*trans*-Nepetalactone[a] | 7.34 | 167 | 111, 77 | 20 | 7.22 | 225 |

Abbreviations: *- Visible as an adduct with formic acid $[M+HCOOH-H]^-$, cE- collision energy, [a]- Identified using authentic standards, [R]- Confirmed by references; $t_R$- retention time.