Appendix S1. Retention time (tR) and optimised mass spectrometric parameters for the detection of the compounds under study. The quantification of the compounds was based on appropriate Multiple Reaction Monitoring (MRM) of ion pairs. Hy: L-hyoscyamine; HBA: Hydroxybenzoic acid; HCA: Hydroxycinnamic acid; Ps: Psoralen; 8M: Dihydronepetalactone; Bg: Bergapten.

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| --- | --- | --- | --- | --- | --- |
| **Compound** | **tR (min)** | **Ionization Mode** | **Cone (V)** | **Collision Energy (eV)** | **MRM** |
| Hy | 1.2 | ES+ | 40 | 25 | 290.30 → 124.23 |
| HBA | 1.8 | ES- | 30 | 15 | 137.00 → 93.05 |
| HCA | 2.2 | ES- | 25 | 15 | 163.10 → 118.96 |
| Ps | 6.8 | ES+ | 40 | 25 | 187.00 → 131.16 |
| 8M | 7.4 | ES+ | 40 | 20 | 217.17 → 161.10 |
| Bg | 9.0 | ES+ | 40 | 20 | 217.17 → 202.03 |