# Supplementary Materials: Whitening Agents from *Reseda luteola* L. and Their Chemical Characterization Using Combination of CPC, UPLC-HRMS and NMR

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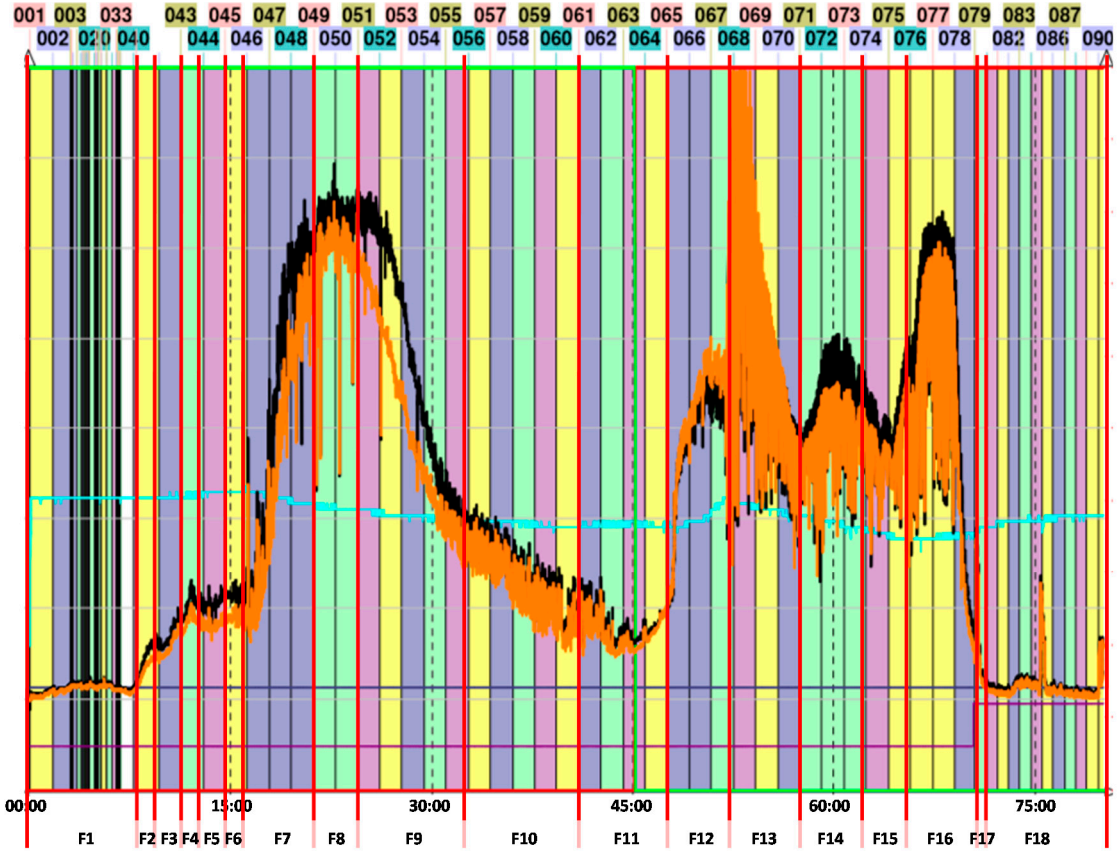
**Supplementary data 1.** The distribution coefficients *Kd* and separation factors $\alpha$ of the 4 major compounds detected in RL3-MeOH sub-extract in different solvent systems (peak identification as in Table 2).

| Solvent system | Molecule | *Kd* | $\alpha$ |
|---|---|---|---|
| ethyl acetate/water/ethanol/acetic acid (4/5/1/0.2) | 2 | 1.6 | 1.4 |
| | 3 | 8.0 | 1.1 |
| | 14 | 46.8 | 2.4 |
| | 17 | 113.6 | 1.2 |
| chloroform/methanol/water (4/3/2) | 2 | 16.6 | 3.8 |
| | 3 | 4.4 | 4.0 |
| | 14 | 1.1 | 2.5 |
| | 17 | 0.4 | 1.5 |
| chloroform/methanol/water (8/4/5) | 2 | 80.7 | 8.1 |
| | 3 | 20.4 | 1.8 |
| | 14 | 1.9 | 6.1 |
| | 17 | 0.3 | 2.8 |
| n-hexane/ethyl acetate/methanol/water/acetic acid (5/3/3.5/5/0.2) | 2 | / | / |
| | 3 | 0.0 | / |
| | 14 | 0.1 | 2.6 |
| | 17 | 0.3 | 1.2 |
| ethyl acetate/water/ethanol (4/5/1) | 2 | 1.8 | 1.4 |
| | 3 | 3.8 | 1.0 |
| | 14 | 4.6 | 1.2 |
| | 17 | 5.3 | 1.1 |
| ethyl acetate/water/ethanol/acetic acid (4/5/1/0.25) | 2 | 1.7 | 1.8 |
| | 3 | 8.5 | 1.1 |
| | 14 | 66.9 | 2.3 |
| | 17 | 153.8 | 1.1 |
| n-hexane/water/butanol (1/2/1) | 2 | 0.3 | 2.1 |
| | 3 | 0.6 | 1.4 |
| | 14 | 1.0 | 1.3 |
| | 17 | 1.3 | 1.3 |

**Supplementary data 2.** CPC chromatograms at 254 nm (in black) and 280 nm (in orange) of the RL3-MeOH sub-extract fractionation: 90 tubes collected and gathered together following the CPC chromatogram to obtain 18 fractions, named RL3-F1 to RL3-F18 respectively.




(colour online only).

**Supplementary material 3** HRESIMS and $^1$H-NMR data obtained for compounds 14 and 17, corresponding respectively to luteolin and apigenin [1].

**Compound 14 (F9)** HRESIMS *m*/*z* 287 ([M+H]$^+$, corresponding to $C_{15}H_{11}O_6$); $^1$H-NMR (200 MHz, $d_6$-DMSO): 6.25 (1H, d, J = 2 Hz), 6.43 (1H, d, J = 2 Hz), 6.67 (1H, s), 6.9 (1H, d, J = 8 Hz), 7.39 (1H, s), 7.43 (1H, d, J = 2 Hz), 12.99 (1H, s). A COSY correlation confirms the coupling of the proton at $\delta_H$ 7.39 with those at $\delta_H$ 6.9 and 7.43.

**Compound 17 (F13)** HRESIMS *m*/*z* 271 ([M + H]$^+$, corresponding to $C_{15}H_{11}O_5$); $^1$H-NMR (200 MHz, $d_6$-acetone): 6.3 (1H, d, J = 2 Hz), 6.5 (1H, d, J = 2 Hz), 6.6 (1H, s), 7 (2H, d, J = 9 Hz), 7.9 (2H, d, J = 9 Hz).

## References

1. Chaturvedula, V.S.P.; Prakash, I. Flavonoids from *Astragalus propinquus*. *J. Chem. Pharm. Res.* **2013**, *5*, 261–265.