

Supplementary Material

# Characterization of Flavonoids and Polyphenolic Compounds and Solubility Determination of Luteolin in Water, Nonpolar, Polar Aprotic and Protic Solvents using FTIR-ATR spectroscopy

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**Table S1.** Real amount of dissolved luteolin (mg.mL<sup>-1</sup>) in different solvents mixed in proportions of 0.3, 0.03 and 0.003 mg.mL<sup>-1</sup> at 27 °C.

Solvent	0.3 mg.mL <sup>-1</sup>	0.03 mg.mL <sup>-1</sup>	0.003 mg.mL <sup>-1</sup>
DMSO	0.31 ± 0.08	0.023 ± 0.002	0.0021 ± 0.0004
THF	0.30 ± 0.03	0.022 ± 0.008	0.0020 ± 0.0008
Butanol	0.29 ± 0.08	0.014 ± 0.005	0.0019 ± 0.0002
1,4-dioxane	0.28 ± 0.03	0.015 ± 0.012	0.0014 ± 0.0011
Methanol	0.28 ± 0.04	0.023 ± 0.009	0.0023 ± 0.0013
Diethyl ether	0.27 ± 0.06	0.026 ± 0.012	0.002 ± 0.001
Ethanol	0.25 ± 0.05	0.018 ± 0.001	0.0019 ± 0.0001
Ethyl acetate	0.25 ± 0.04	0.013 ± 0.007	0.0014 ± 0.0008
Acetone	0.21 ± 0.04	0.020 ± 0.004	0.0018 ± 0.0005
Propanol	0.21 ± 0.03	0.014 ± 0.010	0.0019 ± 0.0004
Acetonitrile	0.20 ± 0.02	0.017 ± 0.001	0.0016 ± 0.0005
Dichloromethane	0.004 ± 0.001	0.0009 ± 0.0007	0.0003 ± 0.0001
Water	0.002 ± 0.001	0.0013 ± 0.0004	0.0008 ± 0.0001
Toluene	0	0	0
Benzene	0	0	0

**Table S2.** Experimental solubilities of luteolin in several solvents calculated in mole fractions at 27 °C.

Solvent	Solubility of Luteolin in Mole Fraction	Density of Solvents Used to Calculate Mole Fractions (g mL <sup>-1</sup> ) [1]
Diethyl ether	9.87·10 <sup>-5</sup> ± 2.35·10 <sup>-5</sup>	0.713
Butanol	9.17·10 <sup>-5</sup> ± 2.51·10 <sup>-5</sup>	0.810
THF	8.63·10 <sup>-5</sup> ± 1.15·10 <sup>-5</sup>	0.883
1,4 – dioxane	8.48·10 <sup>-5</sup> ± 9.69·10 <sup>-6</sup>	1.033
Ethyl acetate	8.44·10 <sup>-5</sup> ± 1.43·10 <sup>-5</sup>	0.895
DMSO	7.86·10 <sup>-5</sup> ± 2.30·10 <sup>-5</sup>	1.092
Propanol	5.45·10 <sup>-5</sup> ± 7.55·10 <sup>-6</sup>	0.803
Acetone	5.43·10 <sup>-5</sup> ± 1.12·10 <sup>-5</sup>	0.785

<b>Ethanol</b>	$5.04 \cdot 10^{-5} \pm 1.04 \cdot 10^{-5}$	0.789
<b>Methanol</b>	$3.90 \cdot 10^{-5} \pm 4.99 \cdot 10^{-6}$	0.791
<b>Acetonitrile</b>	$3.63 \cdot 10^{-5} \pm 3.39 \cdot 10^{-6}$	0.786
<b>Dichloromethane</b>	$8.86 \cdot 10^{-7} \pm 1.44 \cdot 10^{-7}$	1.326
<b>Water</b>	$1.48 \cdot 10^{-7} \pm 4.53 \cdot 10^{-8}$	0.998
<b>Toluene</b>	0	0.867
<b>Benzene</b>	0	0.877

[1] Common Solvents Used in Organic Chemistry: Table of Properties Available online: <https://organicchemistrydata.org/solvents/> (Accessed on 20 October 2021).

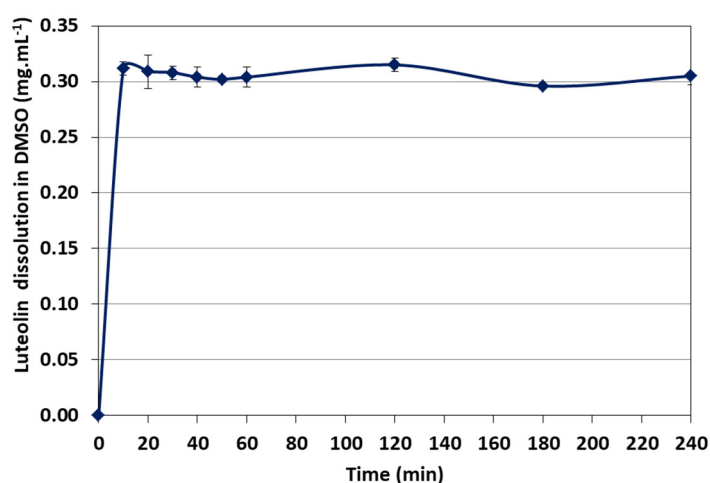


Figure S1. Luteolin dissolution with time.

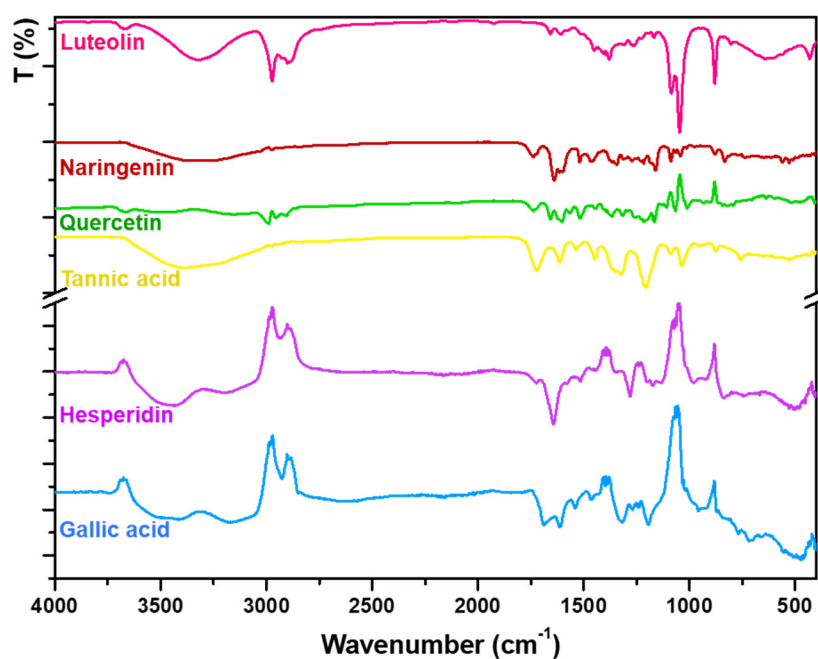


Figure S2. FTIR-ATR spectra of luteolin, naringenin, quercetin, tannic acid, hesperidin and gallic acid in ethanol after the solvent spectrum has been subtracted.

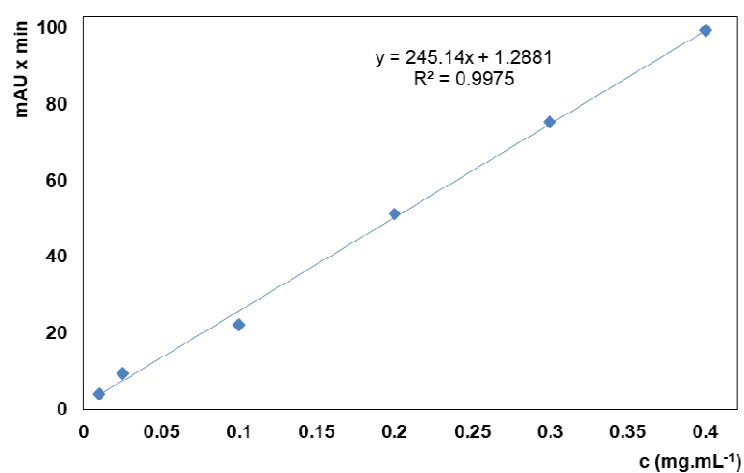


Figure S3. Calibration curve of luteolin in DMSO for HPLC analysis.

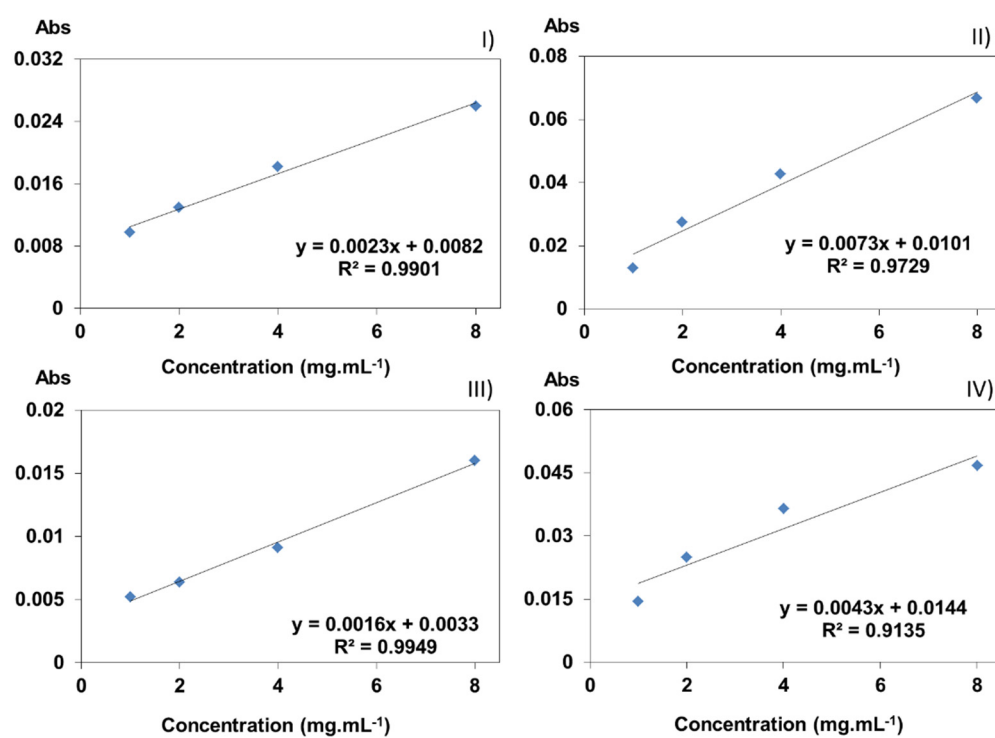
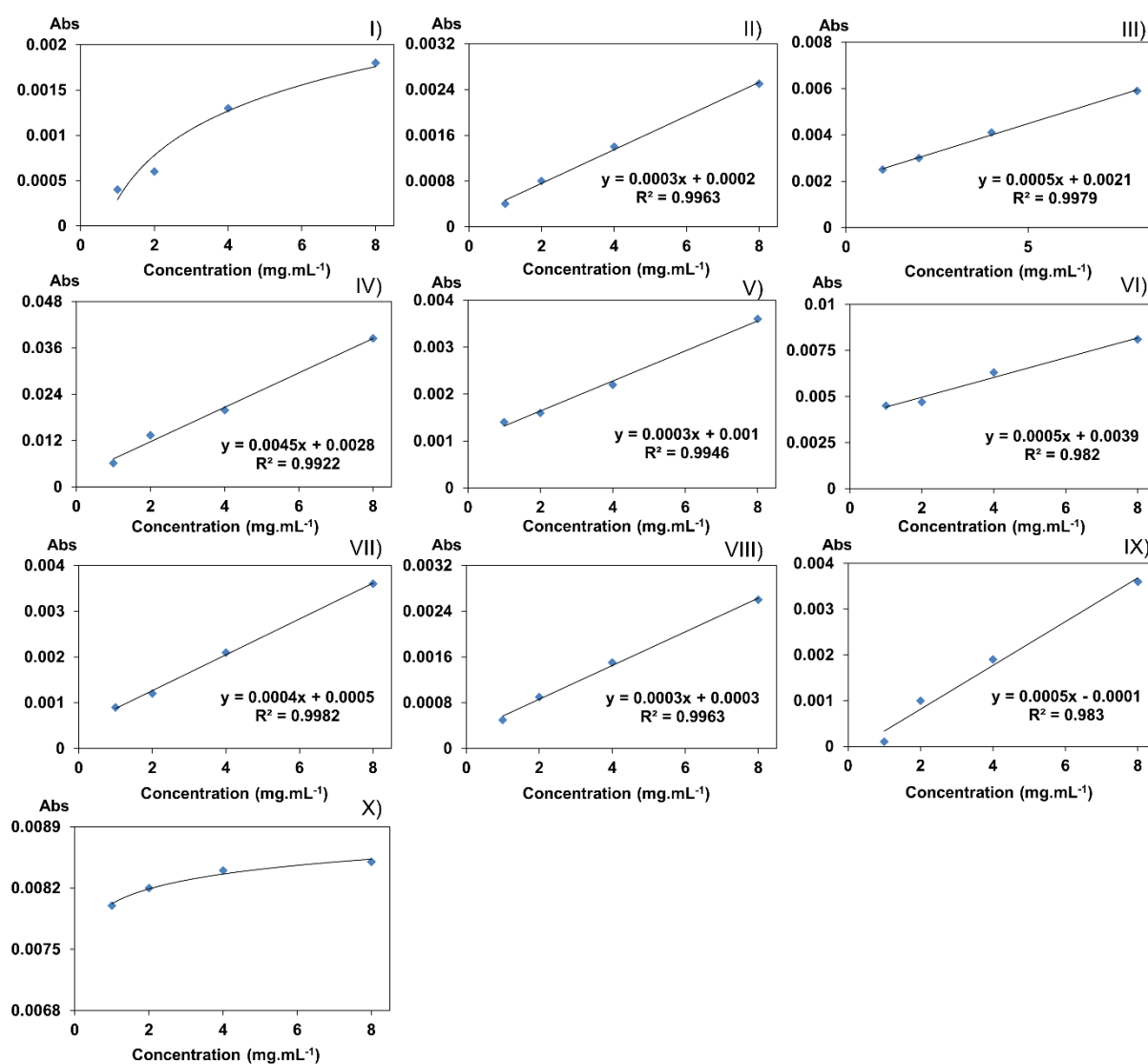


Figure S4. Calibration curves from the IR spectra of I) quercetin at  $1654 \text{ cm}^{-1}$ , II) naringenin at  $1637 \text{ cm}^{-1}$ , III) luteolin at  $1612 \text{ cm}^{-1}$  and IV) tannic acid at  $1716 \text{ cm}^{-1}$  dissolved in ethanol.



**Figure S5.** Luteolin calibration curves from the IR spectra in: **I)** methanol at 1658 cm<sup>-1</sup>, **II)** ethanol at 1656 cm<sup>-1</sup>, **III)** acetone at 1164 cm<sup>-1</sup>, **IV)** ethyl acetate at 1655 cm<sup>-1</sup>, **V)** 1,4-dioxane at 1656 cm<sup>-1</sup>, **VI)** DMSO at 1655 cm<sup>-1</sup>, **VII)** propanol at 1656 cm<sup>-1</sup>, **VIII)** THF at 1658 cm<sup>-1</sup>, **IX)** butanol at 1656 cm<sup>-1</sup>.



**Figure S6.** Dissolution of luteolin at concentrations 1, 2, 4, 6, 8, 10 mg.mL<sup>-1</sup> before (left) and after centrifugation (right) in I) methanol, II) ethanol, III) acetone, IV) ethyl acetate, V) 1,4-dioxane, VI) DMSO, VII) propanol, VIII) THF, IX) butanol, X) diethyl ether, XI) acetonitrile, XII) dichloromethane and XIII) water. Samples I, IV, V, X, XI, XII) and XIII) present sedimentation.



**Figure S7.** Luteolin dissolved in distinct solvents.