

Supplemental data

Table S1: Log*P*-values of various flavonoids

| | Tsopelas et al. | | | Rothwell | Dai | Toxnet | ChemSpider | | PubChem | Ø |
|------------------------|-----------------|-------|-------|--------------------|------|--------|------------|------|---------|-------------|
| | cal. | exp.1 | exp.2 | | | | cal. | exp. | | |
| Acacetin | 3.20 | 2.56 | 2.71 | | | 3.41 | 3.14 | 1.46 | 2.1 | 2.65 |
| Apigenin | 1.74 | 2.05 | 2.28 | 2.92 | | 3.02 | 2.10 | 1.14 | 1.7 | 2.12 |
| Baicalein | 3.04 | 1.94 | 2.65 | | 3.19 | | 3.31 | 2.63 | 1.7 | 2.64 |
| Biochanin A (Olmelin) | 3.07 | 2.75 | 3.48 | | | | 3.14 | 1.36 | 3.0 | 2.80 |
| Catechin | | | | 0.41 ¹⁾ | | | 0.49 | 0.85 | 0.4 | 0.54 |
| Chrysin | 3.52 | 2.53 | 3.01 | | | 3.52 | 2.88 | 1.85 | 2.1 | 2.77 |
| 3',4'-Dihydroxyflavone | 2.64 | 2.60 | 2.72 | | | | 3.08 | 1.86 | 2.8 | 2.62 |
| 2',3'-Dihydroxyflavone | 2.87 | 2.59 | 3.20 | | | | 3.40 | | 2.8 | 2.97 |
| Daidzein | 2.91 | 2.56 | 3.10 | 2.51 | | 2.55 | 2.78 | 1.12 | 2.5 | 2.50 |
| (-)-Epicatechin | 0.51 | 1.63 | 2.05 | | | | 0.49 | 0.85 | 0.4 | 0.99 |
| Eriodictyol | 2.02 | 2.20 | 3.02 | | | 2.02 | 2.59 | 1.14 | 2.0 | 2.14 |
| Formononetin | 2.58 | 2.04 | 2.39 | | | 3.11 | 2.96 | 1.44 | 2.8 | 2.47 |
| Galangin | 2.85 | 2.55 | 2.77 | | | 2.44 | 2.83 | 2.20 | 2.3 | 2.56 |
| Glycetein | | | | 1.97 | | | 2.57 | 1.36 | 2.4 | 2.08 |
| Genistein | 2.57 | 2.18 | 2.87 | 3.04 | | 2.8 | 2.57 | 1.36 | 2.4 | 2.47 |
| Hesperetin | 2.60 | 2.92 | 3.17 | | | 2.60 | 2.90 | 1.03 | 2.4 | 2.52 |
| Hispidulin | 2.49 | 2.68 | 2.74 | | | | 1.60 | 1.38 | 1.7 | 1.98 |
| Isoliquiritigenin | 2.96 | 2.29 | 2.95 | | 3.04 | | 3.11 | 1.67 | 3.2 | 2.75 |
| Isorhamnetin | 2.16 | 1.81 | 2.49 | | | | 1.76 | 1.73 | 1.9 | 1.98 |
| Kaempferide | 2.82 | 2.53 | 2.81 | | | | 2.74 | 1.81 | 2.2 | 2.49 |
| Kaempferol | 2.45 | 2.37 | 2.44 | | | 1.96 | 2.05 | 1.49 | 1.9 | 2.09 |
| Luteolin | 2.53 | 2.22 | 3.09 | 3.22 | | 2.53 | 2.40 | 1.49 | 1.4 | 2.36 |
| Liquiritigenin | | | | | 2.79 | | 2.76 | 0.87 | 2.2 | 2.16 |
| Morin | 1.54 | 1.75 | 1.96 | | | 1.54 | 1.61 | 1.40 | 1.5 | 1.61 |
| Myricetin | 1.63 | 1.98 | 1.84 | | | 1.42 | 2.11 | 2.18 | 1.2 | 1.89 |
| Naringenin | 2.52 | 2.97 | 2.98 | 2.60 | | 2.52 | 3.19 | 0.79 | 2.4 | 2.50 |
| Quercetin | 2.06 | 2.21 | 2.45 | 1.82 | | 1.48 | | 1.37 | 1.5 | 1.84 |
| Silibinin (Silybin) | 2.06 | 2.31 | 2.87 | | | | 2.59 | 0.86 | 2.59 | 2.21 |
| Tamarixetin | 2.18 | 2.03 | 2.52 | | | | 2.42 | 1.73 | 1.9 | 2.13 |
| Tangeretin | 2.87 | 2.87 | 3.01 | | | | 2.66 | 2.58 | 3.00 | 2.83 |
| Wogonin | 2.80 | 2.62 | 2.83 | | 3.43 | | 2.14 | 2.09 | 3.00 | 2.70 |

Compilation of log*P*-values from Tsopelas et al. (2017), Rothwell et al. (2005), and Dai et al. (2008) as well as from the databases Toxnet, PubChem (National Library of Medicine) and ChemSpider (Royal Society of Chemistry). Tsopelas et al. (2017) presented data calculated (cal.) using ADME Boxes v. 3.0 software (Pharma Algorithms), as well as experimental data obtained by applying the compounds to two different immobilized artificial membranes (exp.1 and exp.2). In the same manner, at ChemSpider calculated (cal.) as well as experimental log*P*-values are listed. ¹⁾ This log*P* is taken from Poaty et al., 2009. Ø: arithmetic average of all log*P*-values listed for a certain substance.

Table S2: Log*P*-values of various flavonoid-glycosides

| | Tsopelas et al. | | | Rothwell | Dai | Toxnet | ChemSpider | | PubChem | Ø |
|--|-----------------|-------|-------|----------|------|--------|------------|-------|---------|--------------|
| | cal. | exp.1 | exp.2 | | | | cal. | exp. | | |
| Vitexin 2-O-rhamnoside (Apigenin-8-C-glucoside) | -0.09 | 1.17 | 1.45 | | | | (1.86) | -1.54 | -0.9 | 0.02 |
| Baicalein-7-glucuronide (Baicalin) | 0.62 | 1.34 | 1.57 | | 1.28 | | 0.31 | 1.05 | 1.1 | 1.03 |
| Daidzein-7-glucoside (Daidzin) | 0.44 | 1.37 | 1.94 | | 0,32 | | 0.45 | -0.18 | 0.7 | 0.72 |
| Daidzein-8-C-glucoside (Puerarin) | 1.34 | 1.74 | 1.91 | | | | 1.95 | -0.72 | 0.0 | 1.04 |
| Genistein-7-glucoside (Genistin) | 0.45 | 1.88 | 2.07 | 0.97 | | | 0.79 | -0.26 | 0.9 | 0.97 |
| Myricetin-3-rhamnoside (Myricitrin) | 0.12 | 1.54 | 2.21 | | | | 1.98 | 1.15 | 0.5 | 1.25 |
| Naringenin-7-rhamnosyl- glucoside (Naringin) | -0.44 | 1.56 | 1.80 | | | -0.44 | (2.73) | -1.35 | -0.5 | 0.10 |
| Quercetin-3-glucoside (Isoquercitrin) | -0.46 | 1.59 | 1.94 | | | -0.10 | 1.75 | 0.10 | 0.4 | 0.75 |
| Quercetin-3-glucoside (xylo-hexofuranoside) | | | | 0,76 | | | | 0.82 | 0.4 | 0.66 |
| Quercetin-3-rhamnoside (Quercitrin) | 0.43 | 1.53 | 2.33 | | | | 0.21 | 0.80 | 0.9 | 1.03 |
| Quercetin-4'-glucoside (Spiraeoside) | -0.39 | 1.07 | 1.42 | | | | -0.38 | 0.10 | 0.40 | 0.37 |
| Rutin (Quercetin- 3-rhamnoglucoside) | -0.86 | 1.10 | 1.61 | -0.64 | | -2.02 | (1.76) | -074 | -1.3 | -0.41 |
| Wogonin-7-glucoside | | | | | 1.16 | | | | 1.2 | 1.18 |

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