

Table S2: The experimentally measured human jejunal permeability of 29 drugs vs. the in-silico calculations of LogP with the different methods

| Drug | Value | | | | | | Classification of drug permeability with partition coefficients vs. human jejunal permeability | | | |
|---------------------|---|---------------------|---------------------|----------------------|---------------------|----------------------------|--|----------------------|---------------------|----------------------------|
| | Human permeability (x 10 ⁴ cm/s) | MLogP (BioLoom 5.0) | CLogP (BioLoom 5.0) | CLogP (ChemDraw 8.0) | ALogP (MOE 2004.03) | KLog P (Molecular Formula) | CLogP (BioLoom 5.0) | CLogP (ChemDraw 8.0) | ALogP (MOE 2004.03) | KLog P (Molecular Formula) |
| α-methyldopa | 0.1 | - | -2.26 | -2.26 | 0.44 | 0.26 | C | C | C | C |
| amoxicillin | 0.3 | -1.99 | -1.87 | -1.87 | 0.02 | 0.67 | C | C | C | C |
| antipyrine | 5.6 | 0.23 | 0.2 | 0.2 | 1.78 | 1.55 | Fn | Fn | C | Fn |
| atenolol | 0.2 | 0.16 | -0.11 | -0.11 | 0.45 | 1.33 | C | C | C | C |
| carbamazepine | 4.3 | 3.19 | 2.38 | 2.38 | 3.39 | 2.54 | C | C | C | C |
| cephalexin | 1.56 | -1.74 | -1.84 | -1.84 | 0.44 | 1.13 | Fn | Fn | Fn | Fn |
| cimetidine | 0.26 | 0.4 | 0.38 | 0.35 | 0.6 | 0.51 | C | C | C | C |
| creatinine | 0.29 | -1.76 | -1.76 | -1.77 | -1.01 | -0.46 | C | C | C | C |
| desipramine | 4.5 | 4.54 | 4.47 | 4.47 | 3.53 | 3.67 | C | C | C | C |
| enalapril | 1.57 | - | 0.67 | 0.67 | 1.6 | 1.87 | Fn | Fn | C | C |
| enalaprilat | 0.2 | - | 0.75 | 0.88 | 1.13 | 1.4 | C | C | C | C |
| fluvastatin | 2.4 | 3.8 | 4.05 | 4.05 | 4.63 | 3.53 | C | C | C | C |
| furosemide | 0.05 | 2.03 | 1.9 | 1.9 | 1.89 | 0.7 | Fp | Fp | Fp | C |
| hydrochlorothiazide | 0.04 | -0.07 | -0.36 | -0.37 | -0.35 | -0.34 | C | C | C | C |
| inogatran | 0.03 | -0.1 | -0.14 | - | 0.37 | 1.24 | C | NA | C | C |
| ketoprofen | 8.7 | 3.12 | 2.76 | 2.76 | 3.11 | 2.5 | C | C | C | C |
| levodopa | 3.4 | -2.74 | -2.82 | -2.82 | 0.05 | 0.03 | Fn | Fn | Fn | Fn |
| l-leucine | 6.2 | -1.55 | -1.67 | -1.67 | 0.44 | 0.18 | Fn | Fn | Fn | Fn |
| lisinopril | 0.33 | - | -1.82 | -1.69 | 1.24 | 1.78 | C | C | C | C |
| losartan | 1.15 | - | 3.85 | 4.11 | 4.27 | 3.59 | Fp | Fp | Fp | Fp |

| | | | | | | | | | | |
|---------------|------|-------|-------|-------|-------|-------|-----|-----|-----|-----|
| metoprolol | 1.34 | 1.88 | 1.49 | 1.49 | 1.61 | 1.87 | ref | ref | ref | ref |
| naproxen | 8.5 | 3.34 | 2.82 | 2.82 | 3.04 | 2.01 | C | C | C | C |
| phenylalanine | 6.65 | -1.52 | -1.56 | -1.56 | 0.64 | 0.93 | Fn | Fn | Fn | Fn |
| piroxicam | 6.65 | 1.98 | 1.89 | 1.89 | 1.58 | 0.91 | C | C | Fn | Fn |
| propranolol | 2.91 | 2.98 | 2.75 | 2.75 | 2.58 | 2.6 | C | C | C | C |
| ranitidine | 0.27 | 0.27 | 0.67 | 0.63 | 1.05 | 0.49 | C | C | C | C |
| terbutaline | 0.3 | 0.08 | 0.48 | 0.48 | 1.52 | 1.17 | C | C | C | C |
| valacyclovir | 1.66 | - | -1.22 | -1.22 | -0.93 | -0.62 | Fn | Fn | Fn | Fn |
| verapamil | 6.8 | 3.97 | 4.47 | 4.47 | 5.09 | 3.98 | C | C | C | C |