

## Supplementary Information

**Table S1.** The estimated values of logP and *in silico* permeability across model interfaces.

Name	logP	Human Jejunal Effective Permeability (cm/s × 10 <sup>4</sup> )	Permeability (MDCK) (cm/s × 10 <sup>7</sup> )	Permeability (Rabbit Cornea) (cm/s × 10 <sup>7</sup> )	Permeability (Skin) (cm/s × 10 <sup>7</sup> )
4	3.46	3.34	71.79	71.94	0.17
5	4.01	3.57	59.96	87.65	0.05
6	4.13	3.75	52	84.62	0.05
7	3.82	4.47	88.73	204.61	42.42
8	4.42	5.07	89.45	238.88	37.93
9	4.52	5.37	74.74	233.1	45.62
10	4.71	5.04	236.57	208	1.69
11	5.27	5.64	249.17	280.16	15.74
12	5.4	5.94	230.41	249.71	15.02
13	4.95	5.19	290.51	208.37	7.16
14	5.5	5.78	306.07	262.44	64.34
15	5.63	6.08	287.23	243.42	67.2

**Table S2.** The estimated solubility in water and biorelevant gastro-intestinal fluids.

Name	Solubility Water (mg/mL)	Intrinsic Solubility (mg/mL)	Solubility at pH = 7.4 (mg/mL)	Solubility in FaSSGF (mg/mL)	Solubility in FaSSIF (mg/mL)	Solubility in FeSSIF (mg/mL)
4	0.00128	0.00116	0.00154	0.01030	0.03820	0.09760
5	0.00066	0.00058	0.00075	0.00546	0.02320	0.06990
6	0.00079	0.00071	0.00087	0.00475	0.02100	0.06440
7	0.00138	0.00115	0.00239	0.01400	0.30900	0.09010
8	0.00070	0.00051	0.00138	0.00579	0.17400	0.06340
9	0.00080	0.00060	0.00144	0.00495	0.15600	0.05630
10	0.00037	0.00037	0.00037	0.00721	0.01800	0.01730
11	0.00019	0.00019	0.00019	0.00360	0.01120	0.01230
12	0.00026	0.00026	0.00026	0.00308	0.01020	0.01140
13	0.00039	0.00039	0.00039	0.00535	0.01350	0.01410
14	0.00021	0.00021	0.00021	0.00275	0.00874	0.01020
15	0.00028	0.00028	0.00028	0.00234	0.00797	0.00942

FaSSGF—Fast State Simulated Gastric Fluid; FaSSIF—Fast State Simulated Intestinal Fluid; FeSSIF—Fed State Simulated Intestinal Fluid.

Portions of these results were generated by ADMET Predictor™ software provided by Simulations Plus, Inc., Lancaster, CA, USA.

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