Supplementary Information

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

Name	logP	Human Jejunal Effective Permeability (cm/s × 10⁴)	Permeability (MDCK) (cm/s × 10⁷)	Permeability (Rabbit Cornea) (cm/s × 10⁷)	Permeability (Skin) (cm/s × 10⁷)
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.