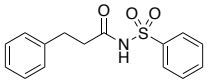
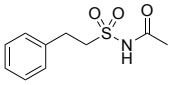
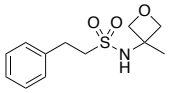
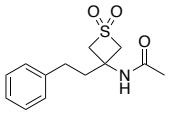
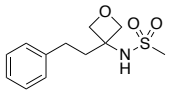
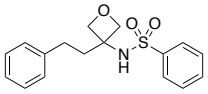
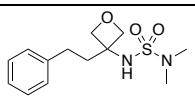
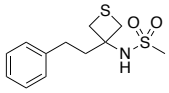
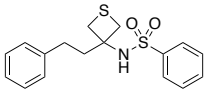
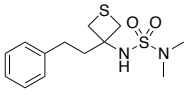
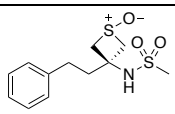
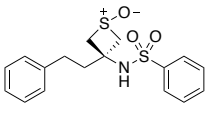
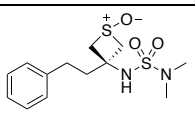
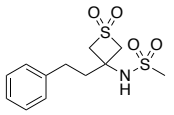
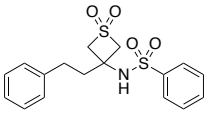
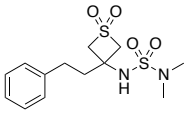
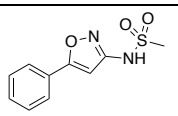
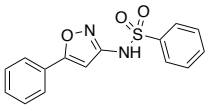
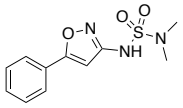
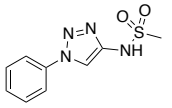
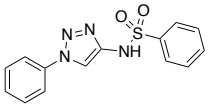
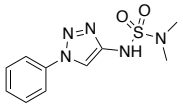
Experimental Properties of Test Compounds

Molecule ID	*Structure*	*mp (°C)*[a]	*% Stability aq. buffer pH 7.4*[b]	*Intrinsic solubility (mol/L)*[c]	*logP*[d]	*logD$_{7.4}$*[e]	*PAMPA*			*pK$_d$*[j]
							Pe (cm/s)[g]	*% retention*[h]	*log$_{Papp}$*[i]	
SM25		107.8–108.5	100.0	9.97E–4	2.67 ±0.01	–0.09	1.64E–6	–3.05E-2	–5.79	4.49 ±0.04
SM26		76.2–78.4	91.4	8.65E–2	1.04 ±0.01	–0.87	1.00E–06	–5.00E–2	–6.00	4.91 ±0.01
SM27		ND§	100.0	8.71E–2	‡	1.56†	6.79E–6	–3.20E–2	–5.17	10.45 ±0.01
SM28		135.3–136.8	94.5	1.62E–3	‡	1.18†	2.11E–6	-1.20E-2	–5.68	>12
SM29		71.4–71.9	100.0	2.65E–2	1.61 ±0.03	1.61	8.44E–6	0.157	–5.1	10.05 ±0.01
SM30		105.8–107.2	94.1	6.38E–4	‡	2.76†	7.06E–6	0.260	–5.2	10.29 ±0.12
SM31		ND	93.7	3.47E–2	‡	1.96†	1.02E–5	5.89E–2	–4.99	11.02 ±0.01
SM32		115.2–116.0	91.5	1.43E–3	‡	2.44†	1.46E–05	0.439	–4.8	10.45 ±0.02
SM33		74.2–75.8	92.8	1.10E–3	‡	2.96†	ND	ND	ND	>12
SM34		56.6–58.9	93.5	2.20E–3	‡	2.83†	1.14E–5	0.373	–4.9	11.93 ±0.05
SM35		151.2–154.2	100.0	2.20E–2	0.88 ±0.02	0.87	ND	ND	ND	9.87 ±0.01
SM36		135.3–136.8	90.3	4.268E–2	‡	0.76†	2.91E–6	5.07E–2	–5.54	9.80 ±0.06
SM37		127.1–127.8	93.4	1.06E–2	‡	1.45†	3.41E–6	7.13E–2	–5.47	10.33 ±0.02

SM38		108.3–108.7	100.0	4.32E–2	‡	1.03[†]	3.66E–06	–3.00E-3	–5.4	9.44 ±0.02
SM39		182.5–184.2	98.3	1.06E-3	‡	1.89[†]	ND	ND	ND	10.22 ±0.15
SM40		100.2–101.5	100.0	8.16E–3	1.83 ±0.05	1.82	4.43E–6	0.105	–5.35	9.58 ±0.01
SM41		158.0–158.8	97.7	3.85E–2	0.58 ±0.02	–0.42	1.16E–6	3.42E–2	–5.94	5.22 ±0.01
SM42		164.8–166.0	95.5	2.17E–3	1.76 ±0.03	0.99	5.79E–6	–4.81E–2	–5.24	6.62 ±0.02
SM43		152.5–152.9	97.3	2.36E–2	0.85 ±0.01	0.42	2.87E–6	0.131	–5.54	5.62 ±0.02
SM44		156.0–157.5	93.5	1.05E–2	1.16 ±0.03	0.06	2.42E–6	–4.07E–2	–5.62	6.34 ±0.01
SM45		163.7–164.5	93.3	3.62E–4	2.55 ±0.04	1.06	4.09E–6	2.76E–4	–5.39	5.93 ±0.05
SM46		158.5–159.7	93.9	2.75E–3	1.72 ±0.01	0.69	3.77E–6	–4.43E–2	–5.42	6.42 ±0.01

[a] Melting point of crystalline material; [b] Test compound (%) remaining after 5 h of incubation at rt in aqueous buffer (pH 7.4) as determined by LC/MS analyses; [c] Intrinsic solubility determined from the general solubility equation (GSE) by using experimentally determined logP and mp values; [d] Log of the partition coefficient between *n*-octanol and water (unless otherwise noted, logP determinations were conducted via potentiometric titrations using a Sirius T3, Pion); [e] Log of the distribution coefficient between *n*-octanol and aqueous buffer at pH 7.4 (unless otherwise noted, $\log D_{7.4}$ determinations were conducted via potentiometric titrations using a Sirius T3, Pion); [f] Calculated values using ChemAxon[37]; [g] Effective permeability (PAMPA assay run by Analiza); [h] Membrane retention; [i] Log of the apparent permeability coefficient (P_{app}); [j] pK_a values determined by potentiometric titrations using a Sirius T3, Pion (values in brackets are from [30]); [§] Test compound was an oil; [†] $\log D_{7.4}$ value determined via shake-flask assay (experiment run by Analiza); [‡] logP value is considered equal to the $\log D_{7.4}$ as these compounds exhibit pK_a values >9.4; ND = not determined.