

Table S4. ADME data of all compounds

ID	Molecule Name	cLogP	Polar surface area (Å ²)	Aqueous Solubility (μM)	Human PPB (%)	Human Liver Microsome CLint (μL/min/mg)	Rat Hepatocyte CLint (μL/min/10 ⁶ cells)	LogD _{7.4}
1	NEU-961	6.4	75	0.3	> 99	140	20	-
2	NEU-1021	2.7	100	7.3	88	-	-	3.1
3	NEU-1022	2.7	100	3.2	97	-	-	4.2
4	NEU-1027	2.3	91	4.2	94	-	-	3.2
5	NEU-1026	4.1	78	< 1	> 99	-	-	-
6	NEU-1029	4.6	75	100	99	270	44	< 1
7	NEU-1030	4.7	66	-	> 99	150	15	-
8	NEU-1031	5.2	66	-	-	290	-	-
9	NEU-1926	4	75	9	-	350	58	4.2
10	NEU-1927	5.6	75	-	> 99	280	79	4.5
11	NEU-1929	3	78	-	92	400	49	3.7
12	NEU-1930	4.2	78	-	98	390	260	4.4
13	NEU-1931	6.4	75	< 1	> 99	110	24	4.8
14	NEU-1060	6.2	66	< 1	> 99	54	24	3.4
15	NEU-1899	6.9	66	< 0.1	100	35	35	4.1
16	NEU-1900	5.8	63	12	> 99	< 3	17	4.6
17	NEU-2076	7.3	53	-	-	-	-	-
18	NEU-2152	6.0	78	-	-	-	-	-
19	NEU-2086	6.6	78	1	-	21	4.6	4.7
20	NEU-2077	6.6	78	-	-	-	-	-
21	NEU-1898	6.8	73	0.2	100	29	48	4.3
22	NEU-1953	2.1	83	44	87	180	130	3.3
23	NEU-1956	4.4	66	< 1	98	170	45	4.3
	NEU-1018	3.5	110	< 1	98	-	-	3.4
	NEU-1019	2.9	78	175	85	-	-	2
	NEU-1020	1.9	91	> 1000	57	-	-	-0.5
	NEU-1023	3.4	78	< 1	99	-	-	4.2
	NEU-1024	2.5	120	< 1	97	-	-	3.7
	NEU-1025	3.5	91	4.8	99	-	-	4.1
	NEU-1028	2.2	100	1.5	93	-	-	3.4
	NEU-1957	3.2	99	< 1	91	120	51	3.3
	NEU-2087	4	63	2	97	8	5	3.5
	NEU-2088	1.7	79	1	-	130	5	2.6

	NEU-2090	4.8	78	570	99	-	7.2	3.3
	NEU-2091	2.5	95	26	-	-	9.3	2.8
	NEU-2093	4.8	78	-	-	45	2.3	-
	NEU-2094	2.5	95	2	-	-	-	2.9
	NEU-2096	3.1	69	810	88	-	10	2.2
	NEU-2129	1.8	69	4	-	25	290	2.9
	NEU-2130	4	52	-	-	-	-	
	NEU-2131	2.4	64	6	98	160	-	3.8
	NEU-2133	2.6	64	4	99	190	290	4
	NEU-2134	4.9	47	0.1	> 99	> 300	193	4.8
	NEU-2141	2.5	76	4	91	68	270	3.3
	NEU-2142	1.9	81	570	59	13	32	2
	NEU-2143	1.6	81	-	63	10	66	1.9
	NEU-2144	1.7	81	100	69	10	16	2.4
	NEU-2145	1	100	3	75	42	> 300	2.1
	NEU-2146	1.8	91	-	68	8	120	1.8
	NEU-2147	2	81	160	57	12	37	1.7
	NEU-2148	2.4	76	2	-	28	9	3.5
	NEU-2149	3.2	76	1	96	54	> 300	3.7
	NEU-2150	1.8	89	-	-	-	-	-
	NEU-2151	1.2	101	-	-	-	-	-