

**Table S3. Lipophilic ligand efficiency (LLE) values for all compounds**

ID	Molecule Name	Log P	<i>L. major</i> amastigote EC <sub>50</sub> (μM)	<i>L. major</i> LLE <sup>a</sup>	<i>T.b.</i> <i>brucei</i> EC <sub>50</sub> (μM)	<i>T.b.</i> <i>brucei</i> LLE <sup>a</sup>	<i>T. cruzi</i> amastigote EC <sub>50</sub> (μM)	<i>T. cruzi</i> LLE <sup>a</sup>
1	NEU-961	6.4	1.6	-0.63	0.079	0.67	0.73	-0.29
2	NEU-1021	2.7	3.1	2.8	2.5	2.9	> 50	< 1.6
3	NEU-1022	2.7	19	2.0	0.62	3.5	9.7	2.3
4	NEU-1027	2.3	20	2.4	0.91	3.8	16	2.5
5	NEU-1026	4.1	2.1	1.6	0.27	2.5	2.8	1.5
6	NEU-1029	4.6	1.4	1.3	0.22	2.1	3.8	0.86
7	NEU-1030	4.7	3.4	0.75	> 50	-0.42	> 50	< -0.42
8	NEU-1031	5.2	2.4	0.38	0.65	0.95	> 50	< -0.94
9	NEU-1926	4.0	4.4	1.4	0.52	2.3	1.9	1.80
10	NEU-1927	5.6	0.78	0.56	0.27	1.0	1.4	0.30
11	NEU-1929	3.0	3.9	2.4	0.69	3.1	9.9	2.0
12	NEU-1930	4.2	6.2	1.0	0.7	2.0	5.4	1.1
13	NEU-1931	6.4	0.2	0.27	0.48	-0.11	> 50	< -2.1
14	NEU-1060	6.2	1.5	-0.42	0.006	2.0	0.09	0.81
15	NEU-1899	6.9	0.96	-0.83	0.14	0.0039	4.7	-1.5
16	NEU-1900	5.8	0.83	0.24	0.11	1.1	0.92	0.20
17	NEU-2076	7.3	1.2	-1.4	0.12	-0.36	2.1	-1.6
18	NEU-2152	6.0	0.87	0.030	0.16	0.77	2.7	-0.46
19	NEU-2086	6.6	2.5	-1.0	0.12	0.29	2.7	-1.1
20	NEU-2077	6.6	1.2	-0.71	0.098	0.38	4.3	-1.3
21	NEU-1898	6.8	1.1	-0.84	0.15	0.024	0.6	-0.58
22	NEU-1953	2.1	2.5	3.5	0.43	4.3	6	3.1
23	NEU-1956	4.4	2	1.3	0.91	1.7	0.62	1.8
	NEU-1018	3.4	17	1.4	> 50	0.89	> 50	< 0.89
	NEU-1019	2.9	22	1.8	5.4	2.4	> 50	< 1.4
	NEU-1020	1.9	22	2.7	> 50	2.4	> 50	< 2.4
	NEU-1023	3.4	8.4	1.7	0.6	2.8	25	1.2
	NEU-1024	2.5	19	2.2	3	3.0	> 50	< 1.8
	NEU-1025	3.5	8.7	1.6	1.5	2.3	8.8	1.6
	NEU-1028	2.2	4	3.2	> 50	2.1	> 50	< 2.1
	NEU-1957	3.2	21	1.5	21	1.5	> 50	< 1.1
	NEU-2087	4.0	29	0.57	0.91	2.1	> 50	< 0.33
	NEU-2088	1.7	3	3.8	0.29	4.9	> 50	< 2.6
	NEU-2090	4.8	2.3	0.88	0.35	1.7	> 20	< -0.061
	NEU-2091	2.5	5.3	2.8	0.38	4.0	> 20	< 2.2
	NEU-2093	4.8	4.6	0.58	0.34	1.7	8.1	0.33

	<b>NEU-2094</b>	2.5	3.2	3.0	0.81	3.6	> 50	< 1.8
	<b>NEU-2096</b>	3.1	7.9	2.0	0.91	2.9	17	1.6
	<b>NEU-2129</b>	1.8	33	2.7	3.3	3.7	2.4	3.8
	<b>NEU-2130</b>	4.0	29	0.54	2.6	1.6	1.9	1.7
	<b>NEU-2131</b>	2.4	35	2.0	4.8	2.9	4.7	2.9
	<b>NEU-2133</b>	2.6	33	1.8	5.3	2.6	0.79	3.5
	<b>NEU-2134</b>	4.9	27	-0.35	> 20	< -0.22	1.2	1.0
	<b>NEU-2141</b>	2.5	24	2.1	4.4	2.8	22	2.1
	<b>NEU-2142</b>	1.9	26	2.7	23	2.7	> 50	< 2.4
	<b>NEU-2143</b>	1.6	28	3.0	14	3.3	> 50	< 2.7
	<b>NEU-2144</b>	1.7	28	2.9	14	3.2	> 50	< 2.6
	<b>NEU-2145</b>	1.0	28	3.6	4.7	4.4	> 50	< 3.4
	<b>NEU-2146</b>	1.8	27	2.8	17	3.0	> 50	< 2.5
	<b>NEU-2147</b>	2.0	5.5	3.3	49	2.3	> 50	< 2.3
	<b>NEU-2148</b>	2.4	4.7	2.9	7.6	2.7	> 50	< 1.9
	<b>NEU-2149</b>	3.2	5.3	2.1	2.3	2.5	> 50	< 1.1
	<b>NEU-2150</b>	1.8	31	2.7	29	2.8	21	2.9
	<b>NEU-2151</b>	1.2	26	3.4	2.3	4.4	> 50	< 3.1

<sup>a</sup>Lipophilic ligand efficiency (LLE):  $pEC_{50} - \text{LogP}$