

Supporting Information for:

Systems Chemistry: Using Thermodynamically Controlled Networks to Assess Molecular Similarity

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Effector	Receptor					
	(1)(3) ₂	(3) ₄	(3) ₃	(1)(2)(3)	(1) ₂ (3)	(1) ₂ (2) ₂
4	0.715	8.62	0.163	0.0673	0.0832	0.408
5	1.08	10.5	0.193	0.120	0.189	1.19
6	0.832	5.63	0.662	0.588	0.729	1.14
7	0.740	6.57	0.257	0.295	0.378	1.38
8	0.589	8.44	0.244	0.328	0.346	1.32
9	1.49	4.38	0.496	0.433	0.389	1.32
10	0.844	5.53	0.433	0.413	0.431	1.31
11	0.767	4.33	0.519	0.599	0.826	1.067
12	1.16	0.773	1.02	0.932	0.930	1.08
13	0.775	0.683	0.889	0.909	0.757	1.06
14	0.550	1.22	0.849	0.920	1.26	0.994
15	1.18	0.654	1.06	1.06	0.868	1.11
16	1.08	1.10	1.00	0.905	1.10	1.07
17	1.20	0.746	1.01	0.944	0.876	1.07
18	0.880	1.25	0.945	0.941	0.982	1.08
19	1.01	0.919	1.02	0.974	0.931	1.09
20	0.917	0.787	1.10	1.03	0.944	0.836
21	1.02	1.01	0.746	0.922	0.611	1.15
22	1.45	1.26	0.913	0.919	0.746	1.17
23	0.502	1.01	0.997	0.917	1.19	1.05
24	1.22	0.744	0.995	0.936	0.873	1.13
25	1.10	0.735	0.942	0.924	0.840	1.11
26	1.00	0.511	0.570	0.755	0.589	1.17
27	0.867	1.28	1.94	0.967	0.709	1.14
28	0.801	1.10	1.05	0.933	1.04	1.06

Table 1. Amplification factors of receptors upon addition of different effectors.