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Systems chemistry

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Published in:
Journal of Systems Chemistry

DOI:
[10.1186/1759-2208-4-2](https://doi.org/10.1186/1759-2208-4-2)

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Document Version
Publisher's PDF, also known as Version of record

Publication date:
2013

[Link to publication in University of Groningen/UMCG research database](#)

Citation for published version (APA):

Saggiomo, V., Hristova, Y. R., Ludlow, R. F., & Otto, S. (2013). Systems chemistry: using thermodynamically controlled networks to assess molecular similarity. *Journal of Systems Chemistry*, 4(2). <https://doi.org/10.1186/1759-2208-4-2>

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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.