Molecular BioSystems

Supplementary material

The topology of drug-target interaction networks: implicit dependence on drug properties and target families

Jordi Mestres,[a] Elisabet Gregori-Puigjané,[a] Sergi Valverde[bc] and Ricard V. Solé[bd]

[a] *Chemogenomics Laboratory, Research Unit on Biomedical Informatics, Institut Municipal d'Investigació Mèdica, Parc de Recerca Biomèdica, Doctor Aiguader 88, 08003 Barcelona, Catalonia, Spain. Email: jmestres@imim.es; Tel: +34-93-3160540; Fax: +34-93-3160550*
[b] *Complex Systems Laboratory, Universitat Pompeu Fabra, Barcelona, Catalonia, Spain*
[c] *CNRS-UMR, Université Paul Sabatier, Toulouse, France*
[d] *Santa Fe Institute, New Mexico, USA*

Table S1 Distribution of the number of drugs (in bold), mean number of interactions and degree of the drug-target network (in italics) from known experimental data and *in silico* projections (in parenthesis).

		MW		
		<300	**[300,400]**	**>400**
clogP	**>4**	**49** 9.2 (30.9) *2.6 (6.3)*	**81** 9.3 (20.2) *3.2 (4.8)*	**89** 7.4 (11.2) *2.6 (3.3)*
	(3,4]	**49** 7.6 (18.0) *2.0 (3.5)*	**49** 6.3 (14.7) *1.7 (2.5)*	**31** 4.0 (5.3) *1.1 (1.3)*
	(2,3]	**66** 4.4 (15.1) *1.6 (3.3)*	**57** 8.8 (14.8) *2.6 (3.0)*	**29** 4.0 (5.5) *1.2 (1.4)*
	(1,2]	**61** 4.1 (10.7) *1.5 (2.4)*	**41** 4.1 (7.7) *1.3 (2.1)*	**10** 2.6 (5.9) *0.8 (0.9)*
	<1	**121** 4.5 (8.3) *1.7 (2.3)*	**42** 3.3 (5.2) *1.1 (1.4)*	**27** 2.4 (6.7) *0.9 (1.2)*

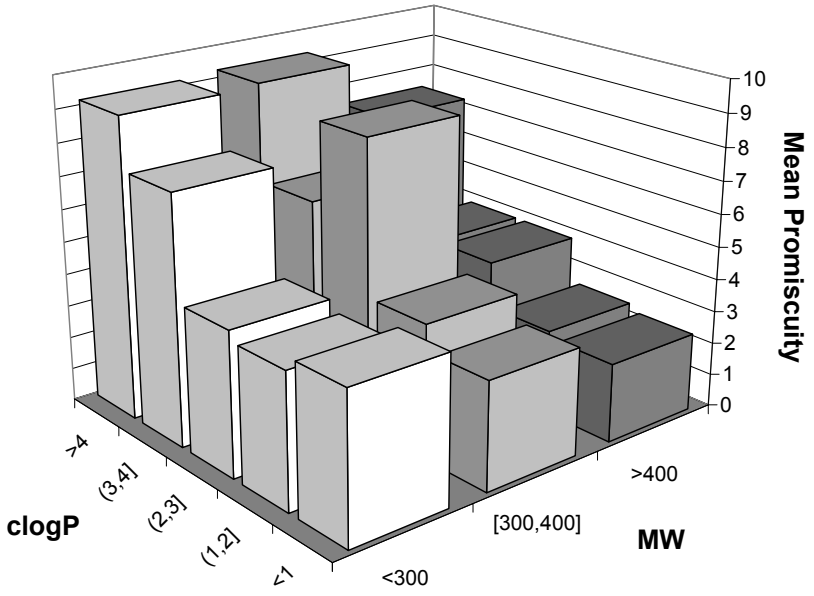

Fig. S1 Variation of the mean promiscuity of drugs contained within value ranges of molecular weight (MW) and hydrophobicity (clogP) as extracted from currently available experimental data

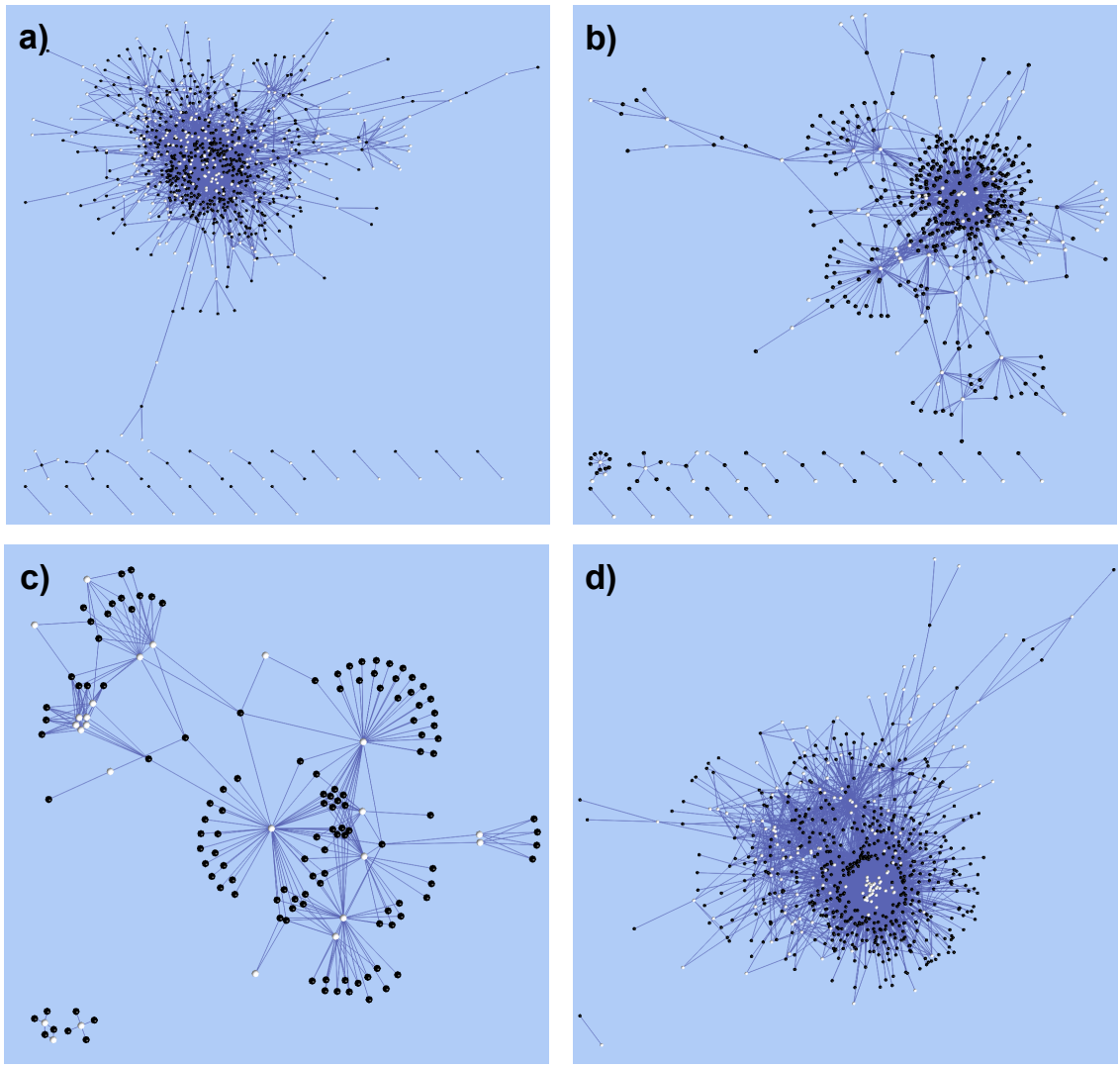

Fig. S2 Drug-target interaction networks derived for the different target families: **a)** enzymes, **b)** ion channels/transporters, **c)** nuclear receptors, and **d)** G protein-coupled receptors.