

**Table S6:** In each of R1 to R8, given drugs and targets of drug-target pairs, the ratio of drug-target pairs which were in the corresponding cluster to all drug-target pairs between them, and the average over those of  $10^5$  clusters, each having drug-target pairs randomly selected out of the original 11,219 drug-target interactions and keeping the cluster size the same as that of the corresponding cluster.

Cluster	R1	R2	R3	R4	R5	R6	R7	R8
Ratio	1.00 (283/283)	0.9349 (287/307)	0.9946 (1848/1858)	0.9730 (180/185)	0.9652 (555/575)	0.9810 (465/474)	1.00 (222/222)	0.9933 (741/746)
Average ratio by $10^5$ random clusters (RC)	0.5663	0.5650	0.5327	0.6102	0.5234	0.5318	0.5882	0.5143
Standard deviation of RC	0.0227	0.0225	0.0658	0.0298	0.0150	0.0167	0.0262	0.0124
Max of RC	0.6612	0.6568	0.5627	0.7407	0.5873	0.6008	0.7231	0.5731