



Figure S1: An enlargement of the matrix of Fig.3, including all major clusters of both significant substructure pairs and drug-target pairs. From left to right on the three columns on the right-hand side of the matrix, in the first column, an element is colored red if the corresponding drug-target pair has an approved drug; otherwise blue. In the middle column, an element is colored red if the corresponding drug-target pair has GPCR; otherwise blue. In the right column, an element colored red if the target of the corresponding drug-target pair is a membrane protein; otherwise blue.