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Set	Unique by Complex	Unique UniProt	Unique SCOP families
Synthetic small	1,525	518	165
molecules	(1,206)	(385)	(143)
Approved drugs	201 (95)	155 (76)	67 (46)
Oral drugs	134 (68)	93 (49)	24 (19)
Protein-protein			
interaction	30 (25)	9 (9)	7 (7)
inhibitors			
Natural	1505 (283)	1159 (216)	346 (134)
molecules	1303 (203)	1133 (210)	310 (131)
Small peptides	557 (467)	288 (238)	98 (83)
Obligate	161	161	293
dimers			
Transient dimers	154	154	183
Homo			
quaternary	12,034	7,177	2,711
interfaces			
Hetero			
quaternary	2,271	1,709	897
interfaces			
Protein-protein			
complexes SM	15	15	13
inhibited			

Supplementary Table S2. Number of entries in each set of molecules. The non-redundant sets are considering non-redundant set of interactions for the complexes (protein-ligand or protein-protein interaction). From these sets protein redundancy is removed by selecting unique UniProt identifiers and removed structural domains redundancy by selecting unique SCOP families. Numbers in parenthesis are the number of unique small molecules in each set. Numbers for unique UniProt and SCOP families for protein complexes refer to distinct pairs of UniProt identifiers or SCOP family respectively.