

Icagen Diversity Collection

ICAGEN, a leader in early phase drug discovery, has over two decades of experience in the evaluation, curation and assembly of diverse screening libraries for major pharmaceutical companies. This experience has been applied to the assembly of a diverse collection of drug-like molecules designed to enable client discovery programs at ICAGEN. This core collection of informative and attractive chemical starting points is continuously augmented through custom in-house design and synthesis.

As of February 2017, the screening collection comprises **170,000 highly diverse compounds with drug-like and lead-like properties** as summarized below.

Stat	mol_MW	#rotor	donorHB	acctpHB	QPlogS	QPlogPo/w	PSA	QPlogBB	Fsp3
mean	354	4	1	6	-4.2	2.8	77.2	-0.55	0.35
std	59	2	0.9	1.9	1.5	1.3	25.4	0.62	0.19
min	33	0	0	0	-19.7	-1.5	0	-15.1	0.0
25%	319	3	0.3	5	-5.2	2.0	59.5	-0.93	0.21
50%	348	4	1	6.5	-4.3	2.8	75.6	0.52	0.33
75%	391	6	1.3	7.7	-3.3	3.6	92.7	-0.13	0.47
max	620	60	19	36.6	2	7.0	180	1.55	1.0

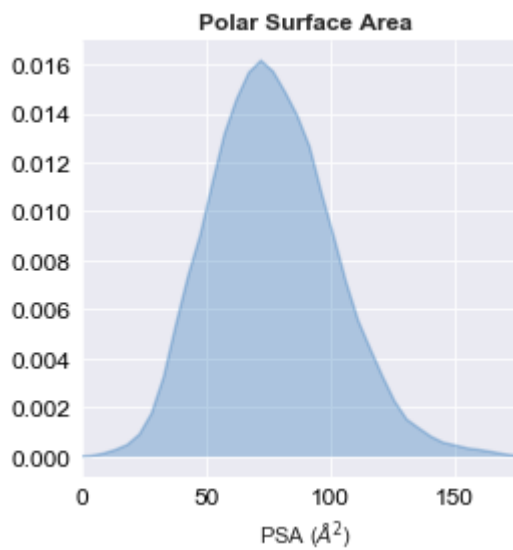
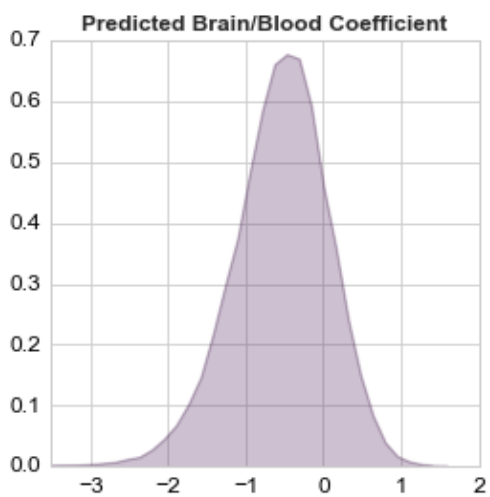
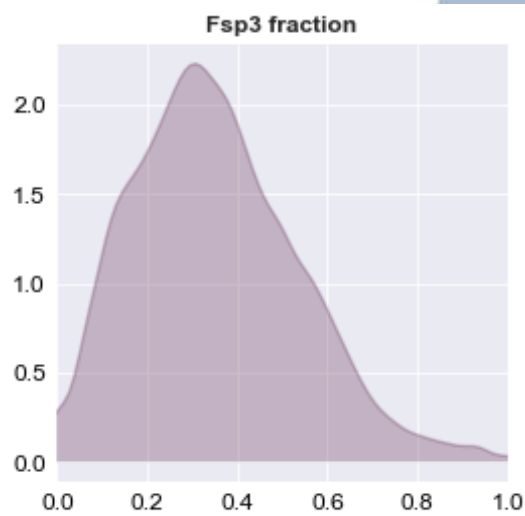
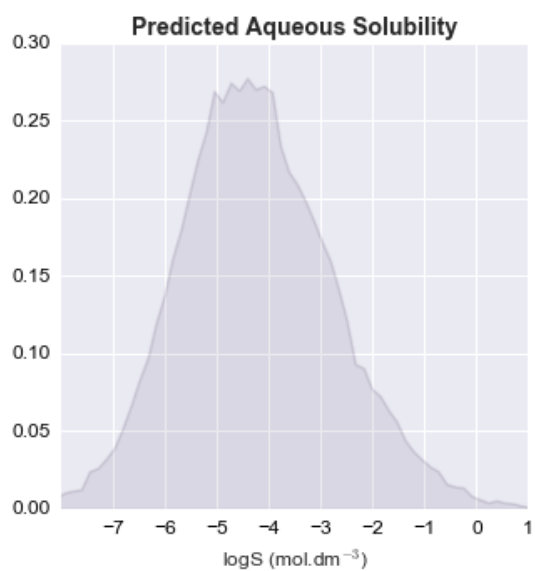
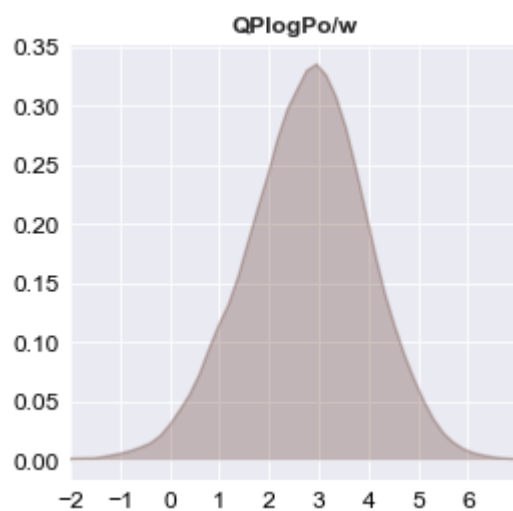
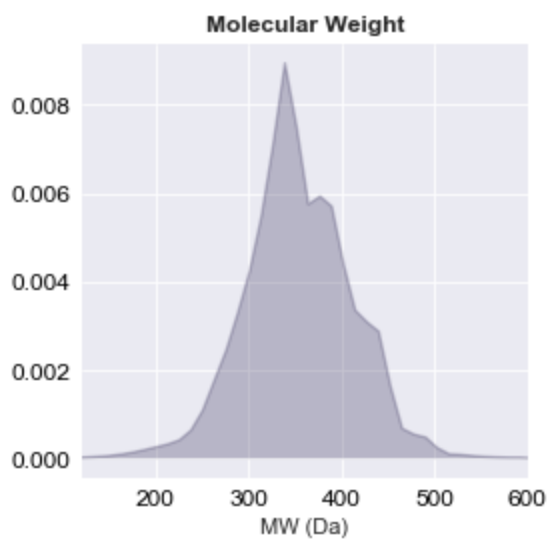
Screening Collection Assembly

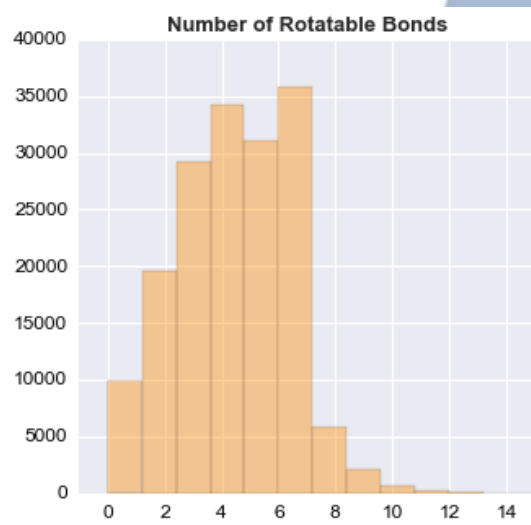
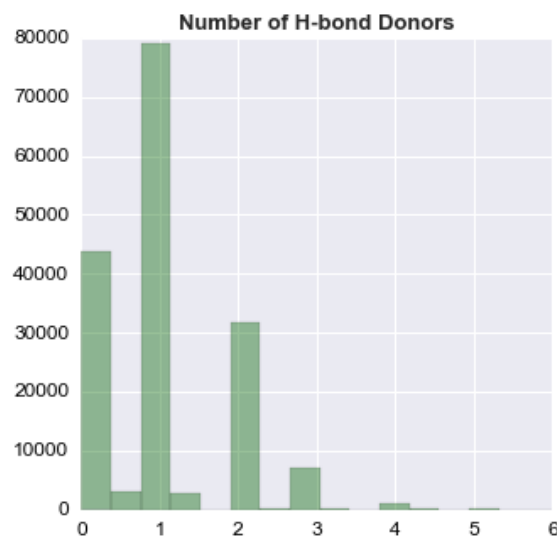
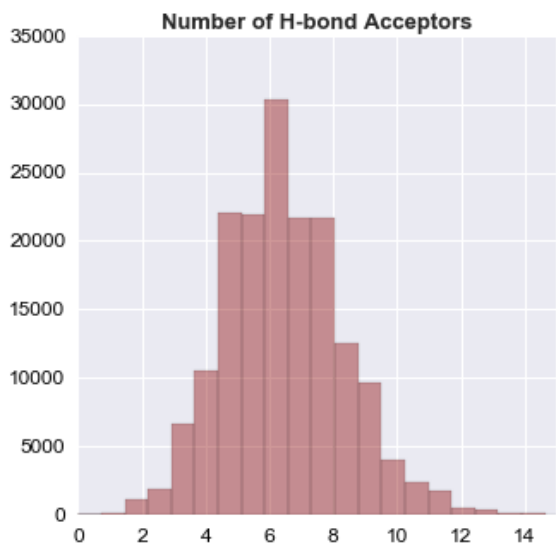
Our screening collection aims to encompass structurally diverse compounds as well as scaffolds with likely bioactivities based on published examples. The ICAGEN team employs proprietary data-mining approaches to identify newly disclosed chemotypes for traditional drug target families and novel ligands for so-called “undruggable” target classes. Through this mechanism, the collection grows in both structural novelty and biorelevance.

Testing a subset of compounds

Often complex functional assays, such as primary cell models or situations where assay components are difficult to produce, limit the practical size of a screen. The physical format of the ICAGEN collection allows for systemic and progressive diversity sampling through the use of **structurally representative subsets**.

Key library properties





[Link to QikProp Properties and Descriptors](#)

* Properties of the Icagen Screening Collection content as of February 2017; properties were calculated using QikProp (Schrodinger) and custom in-house tools.