

Building
Blocks



Screening
Compounds



Expanded
Space



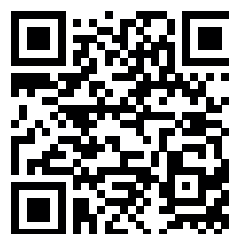
Compound
Sets



General Fragments

93 800

comply with Ro3
no undesirable moieties



3D-Shaped Fragments

770

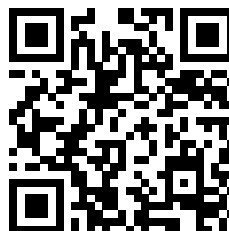
disc- and sphere-like molecules
plane-of-best fit ≥ 0.6



Selected Fragments - Acids

10 800

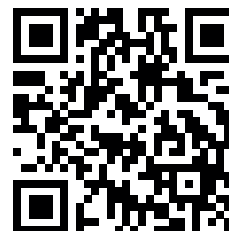
comply with Ro3
contain carboxylic acid



Selected Fragments - Amines

10 800

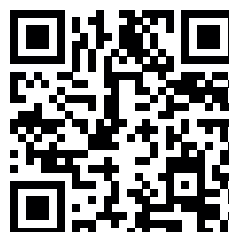
comply with Ro3
contain free amino group



Covalent Fragments

11 000

common covalent warheads
single warhead



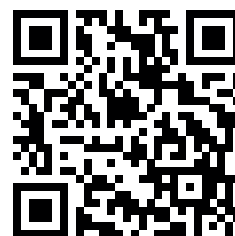
CHEM SPACE

Delivering Discovery

Fluorinated Fragments

17 600

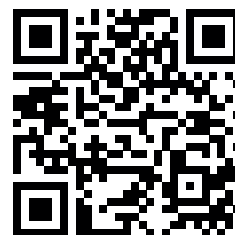
mono F-, CHF₂-, and CF₃-groups
one F-containing group



«Heavy» Fragments

3 800

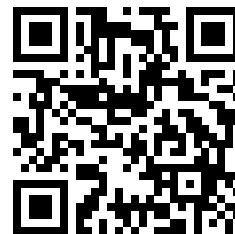
Br- and I-containing compounds
no active halogens



Saturated Fragments

9 100

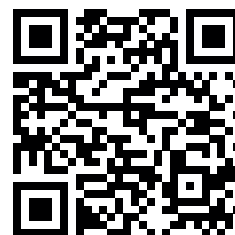
high Fsp³
Rotating bonds ≤ 1



Singleton Fragments

2 100

no close analogs in purchasable space
high diversity within the set



Spiro Fragments

2 900

comply with Ro3
contain spiro moiety

