

Building
Blocks



Screening
Compounds



Expanded
Space



Compound
Sets



Lead-like compounds

980 000

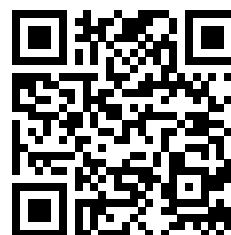
high-quality set, comply with Ro4
diversity sets available



ChEMBL analogs

2 600 000

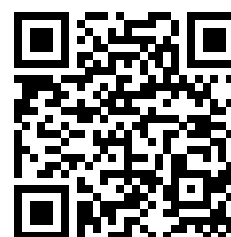
ChEMBL actives
and their analogs



CNS-Focused library

94 100

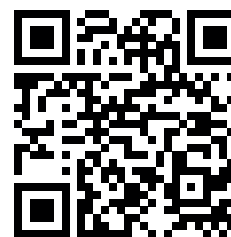
neutral or basic compounds
comply with criteria for
CNS-permeable compounds



Covalent Modifiers

71 400

common covalent warheads
single warhead



CHEM SPACE

Delivering Discovery

Drug Impurities

370

impurities of drugs from
EU and US Pharmacopoeias



Drug Repurposing

870

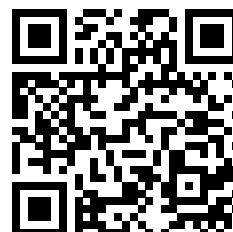
compounds with proven activity
information on targets



High QED compounds

284 100

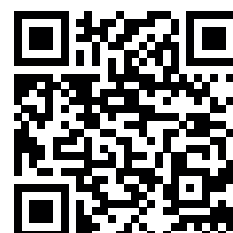
Drug-like compounds
QED score 0.9-0.95



PPI Modulators

6 400

large, not greasy molecules
"hot spot" paradigm



Pre-Plated sets

total 144 600

5 sets: Diversity, Fragments,
LeadLike, Representative, Unique

