**Variable statistics for 100K diverse compounds set**

\*number of singletons - 9927

\* number of scaffolds - 4770 (1-334 compounds per scaffold)

\* diversity – 0.8617

\* number of unique heterocycles - 1635

\* number of screens - 18908

distribution data of physico-chemical parameters:

97<MW<722, av. 385

-3.6<logP< 9.1, av. 3.0

-10.0<logD<12.7, av. 2.8

-13.5<logSw<6.3, av. -3.7

0<PSA< 262, av. 82

0<Hacc< 13, av. 5

0<Hdon< 7, av. 1

0<RotB<17, av. 5

0<FSP3<100, av. 36