

Leadlikeness analysis NovaCore and PharmaCore libraries

NovaCore: 65882 structures
PharmaCore: 51126 structures

Hits on structural filters:

	NovaCore	PharmaCore
Aldehydes	79	74
Aliph. (thio)esters	779	419
Michael acceptors	280	842
HN-NH and N-NH2	1	0
N-oxides	102	53
Vinyllic halogens	26	182
Carbamates	399	410
Acyclic diketyls	87	76
Aliph. Ketones	25	11
Thiadizoles	280	202
= 4 x CH2		

Hits on property filters:

MW > 450	451	20052
cLogP > 4.50	1600	1042
cLogSW < -6.00	175	92
Rot. Bonds > 10	1598	131
Leadlike structures	59288 (90.0%)	27077 (53.0%)

Note that all the filters are run sequentially, meaning that some structures may in fact hit more than one filter (which is suggested by this list)!

Uniqueness:

Both libraries have been compared to a 4.8M structure database, consisting of all commercially offered compounds (June 2006).

Duplicates found:

NovaCore: 28
PharmaCore: 224