All New Chemistry – Yours to Explore

Pre-plated Diversity Sets

Life Chemicals presents a number of exclusive Pre-plated Diversity Sets composed of 50,000 novel compounds with optimal physico-chemical properties selected from Life Chemicals' collection of newly synthesized items by dissimilarity search with average Tanimoto threshold of 80%. For your convenience 5 000, 10 000, 15 000 and 20 000 non-overlapping competitively priced Diversity Sets are available. The compounds are formatted as 50uL of 10mM solutions in DMSO in 384 well plates.

- Lipinski Rule of 5 & Veber criteria compliant
- No fragment
- No reactive and unstable molecules
- Lilly MedChem Rules
- PAINS filters families A, B, C applied
- No overlap with old Life Chemicals' 50K Diversity Set

Parameters of the Diversity Sets are listed below:

Diversity	Average values							
Set	MW	HbD	HbAc	cLogP	RotB	Fsp3	PSA	Tanimoto
50K	357.29	1.38	3.77	2.51	4.91	0.35	93.67	0.79
20K	355.04	1.39	3.77	2.42	4.78	0.35	93.06	0.74
15K	357.53	1.40	3.77	2.48	4.94	0.36	91.34	0.76
10K	359.44	1.38	3.76	2.59	5.02	0.35	90.06	0.78
5K	361.31	1.34	3.78	2.76	5.11	0.33	88.52	0.80

Diversity	Number of	Number of	Number of Scaffold-	Number of
Set	compounds	Scaffolds	based compounds	Singletones
50K	50,240	2,242	42,283	7,957
20K	20,160	1,847	17,974	2,186
15K	15,040	1,947	12,904	2,136
10K	9,920	1,813	7,893	2,027
5K	5,120	1,413	3,378	1,742

To download a file with compound structures for this library, please follow this link: http://www.lifechemicals.com/downloads/14468