ZINC15 Tranches

Rep. | **2D** | 3D   React. Standard ▾   Purch. Wait OK ▾   pH N/A ▾   Charge N/A ▾   ▦ ▾   ⬇

Predefined Subsets: All | None | Shards | Fragments | Flagments | Goldilocks | Lead-Like | Lugs | Drug-Like | Big-n-Greasy

Molecular Weight (up to, Daltons)

LogP (up to)	200	250	300	325	350	375	400	425	450	500	>500	Totals, by LogP
-1	31,520	210,198	784,279	1,124,026	2,310,970	854,208	300,607	56,?		23,759	5,598	5,801,749
0	154,788	1,095,532	3,992,760	5,390,653	10,938,346	3,784,188	1,767,726	467,?		209,867	3,862	28,410,922
1	414,273	3,374,769	13,196,175	17,182,223	34,851,540	12,860,730	7,279,946	2,568,?		1,206,882	8,249	95,133,476
2	555,197	5,533,895	25,622,912	33,383,218	88,330,050	28,983,131	19,267,814	8,741,?		8,570,868	22,307	226,760,093
2.5	214,735	2,723,802	14,831,118	19,890,876	40,686,668	20,475,678	15,126,147	8,256,?	7,??	7,879,918	23,424	137,854,889
3	125,492	2,145,037	13,281,388	18,488,586	37,136,913	22,333,418	17,838,728	11,103,726	10,986,050	6,968,806	38,186	140,446,330
3.5	57,244	1,386,997	10,135,959	14,739,692	29,791,008	21,458,732	18,737,428	13,319,769	13,704,019	9,066,863	61,984	132,459,695
4	18,215	642,659	6,131,454	8,393,140	12,628,179	15,472,307	16,892,846	13,888,572	12,864,529	10,473,721	91,903	97,497,525
4.5	2,275	180,303	2,873,064	4,781,472	7,950,935	10,959,424	12,773,295	12,430,134	11,562,431	10,654,985	127,265	74,295,583
5	94	22,897	852,691	1,984,202	4,012,544	6,416,455	8,397,678	9,229,001	8,818,548	9,234,778	155,546	49,124,434
>5	28	895	44,519	178,728	557,180	1,226,923	2,066,211	2,641,238	3,062,143	2,471,283	799,799	13,048,947
Totals, by Weight	1,573,861	17,316,984	91,746,319	125,536,816	269,194,333	144,825,194	120,448,426	82,703,885	79,387,972	66,761,730	1,338,123	**1,000,833,643** Substances / **1.7K** Tranches

How is a chemical library prepared for virtual screening?