

ZINC15 Tranches

Rep.2D3DReact. Standard ▼Purch. Wait OK ▼pH N/A ▼Charge N/A ▼														
Molecular Weight (up to, Daltons)														
LogP (up to)		200	250	300	325	350	375	400	425	500	>500	Totals, by LogP		
	-1	31,520	210,198	784,279	1,124,026	2,310,970	854,208	300,607	56,7	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,	7,879,918	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?