

Zinc is not Commercial (ZINC15)

• freely available commercially for virtual screening

- divided into “tranches” by molecular weight and LogP, a measure of predicted hydrophobicity
- predefined subsets of ZINC15 include fragments, lead-like, and drug-like

- organized into catalogs, notably
 - by vendor
 - BindingDB.org - binding affinity database
 - DrugBank-approved - approved drugs, helpful for repurposing
 - NCI HTS libraries: plated 2007 and diversity 3.
 - Sigma Aldrich building blocks

• can search for a particular compound (SAR by catalog)

• buyer beware!



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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												