https://zinc20.docking.org

ZINC Substances Catalogs Tranches Biological More About

ZINC20

Welcome to ZINC, a free database of commercially-available compounds for virtual screening. ZINC contains over 230 million purchasable compounds in ready-to-dock, 3D formats. ZINC also contains over 750 million purchasable compounds you can search for analogs in under a minute.

ZINC is provided by the Irwin and Shoichet Laboratories in the Department of Pharmaceutical Chemistry at the University of California, San Francisco (UCSF). We thank NIGMS for financial support (GM71896).

To cite ZINC, please reference: Irwin, Tang, Young, Dandarchuluun, Wong, Khurelbaatar, Moroz, Mayfield, Sayle, *J. Chem. Inf. Model 2020*, in press. https://pubs.acs.org/doi/10.1021/acs.jcim.0c00675. You may also wish to cite our previous papers: Sterling and Irwin, *J. Chem. Inf. Model, 2015* *http://pubs.acs.org/doi/abs/10.1021/acs.jcim.5b00559*. Irwin, Sterling, Mysinger, Bolstad and Coleman, *J. Chem. Inf. Model, 2012* DOI: 10.1021/ci3001277 or Irwin and Shoichet, *J. Chem. Inf. Model. 2005;45(1):177-82* PDF, DOI.

Getting Started

- Getting Started
- What's New
- About ZINC 20 Resources
- Current Status / In Progress
- Why are ZINC results "estimates"?

Explore Resources

Chemistry
Tranches, Substances, 3D Representations, Rings, Patterns
And More
Catalogs, Genes, ATC Codes

Ask Questions

You can use ZINC for **general** questions such as

- How many substances in current clinical trials have PAINS patterns? (150)
- How many natural products have names in ZINC and are not for sale? (9296) get them as SMILES, names and calculated logP
- How many endogenous human metabolites are there? (47319) and how many of these can I buy? (8271) How many are FDA approved drugs? (94)
- How many compounds known to aggregate are in current clinical trials? (60)
- How many epigenetic targets have compounds known? (53) and Which of these substances can I buy? (278)
- How many ligands are there for the NMDA 1 ion channel GRIN1? (662) and How many of these are for sale? (60)
- More...

ZINC20 News

- ZINC20 has been released

Caveat Emptor: We do not guarantee the quality of any molecule for any purpose and take no responsibility for errors arising from the use of this database. ZINC is provided in the hope that it will be useful, but you must use it at your own risk.

Rep. 2D 3D React. Standard Purch. Wait OK pH N/A Charge N/A

Highest Reactivity
Anodyne
Bother
Clean
Standard ✓
Reactive
Hot
Exclusive

Molecular Weight (up to, Daltons)

LogP (up to)	200	250	300	325	350	375	400	425	450	500	>500	Totals, by LogP
-1	27,791	172,563	710,795	[illegible]	[illegible]	786,738	276,834	116,066	92,417	77,790	7,310	5,582,780
0	139,434	934,776	3,655,384	[illegible]	[illegible]	3,498,214	1,663,579	708,919	570,546	507,344	4,734	27,417,112
1	362,437	2,884,636	12,030,074	[illegible]	[illegible]	11,885,957	6,807,876	3,178,487	2,648,581	2,412,998	9,940	92,025,779
2	467,220	4,584,223	22,941,206	[illegible]	[illegible]	26,752,849	17,839,254	9,349,272	8,099,970	7,686,687	24,554	193,701,135
2.5	167,513	2,136,113	12,849,121	17,977,157	38,682,058	18,584,223	13,812,274	8,111,104	7,197,414	6,979,014	24,126	126,520,117
3	90,548	1,570,772	11,037,383	16,282,627	34,831,558	19,940,391	16,037,132	10,339,743	9,362,233	9,118,717	37,422	128,648,526
3.5	36,748	929,872	7,920,574	12,490,662	27,380,104	18,703,024	16,485,194	11,784,160	10,774,472	10,693,411	58,791	117,257,012
4	9,017	369,565	4,332,131	6,472,808	10,487,856	13,034,155	14,329,253	11,683,208	10,891,465	11,003,975	86,262	82,699,695
4.5	993	86,613	1,814,492	3,457,942	6,367,225	8,853,064	10,320,054	9,945,353	9,486,869	9,825,079	117,980	60,275,664
5	150	13,393	536,018	1,405,708	3,168,584	4,995,850	6,471,525	7,025,034	6,976,742	7,325,833	144,297	38,063,134
>5	39	1,097	22,854	103,521	376,905	927,395	1,670,856	2,195,160	2,588,702	3,052,048	767,762	11,706,339
Totals, by Weight	1,301,890	13,683,623	77,850,034	111,452,617	232,841,447	127,961,860	105,713,831	74,436,506	68,689,411	68,682,896	1,283,178	**883,897,293** Substances **1.9K** Tranches

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Rep. 2D 3D React. Standard Purch. In-Stock pH N/A Charge N/A

Minimum Purchasability
In-Stock ✓
Agent
Wait OK
Boutique
Annotated
Exclusive

Molecular Weight (up to, Daltons)

LogP (up to)	200	250	300	325	350	400	425	450	500	>500	Totals, by LogP
-1	7,447	5,685	7,652	4,072	[illegible]	2,128	1,569	1,209	2,141	6,401	45,371
0	27,933	20,326	35,387	21,903	[illegible]	9,047	4,738	3,231	3,083	4,229	166,958
1	75,706	81,653	163,888	114,245	[illegible]	44,261	20,965	12,884	11,596	8,469	729,737
2	103,414	182,568	404,153	324,853	395,876	234,773	154,906	78,406	52,184	43,906	19,454	1,994,493
2.5	37,858	102,897	268,486	240,459	326,556	208,799	149,918	85,182	59,767	50,871	19,146	1,549,939
3	21,867	83,987	250,050	244,003	364,448	257,061	200,696	123,814	91,982	85,391	30,824	1,754,123
3.5	9,604	52,471	184,966	199,778	314,985	258,411	223,888	157,406	124,425	124,006	51,525	1,701,465
4	2,996	25,449	111,741	128,633	212,911	219,598	213,677	174,283	146,493	159,913	79,541	1,475,235
4.5	626	9,399	55,607	72,796	124,642	154,106	172,335	161,544	146,636	176,682	113,058	1,187,431
5	116	2,709	21,635	34,101	62,880	90,430	112,167	120,369	123,766	172,432	141,461	882,066
>5	34	912	9,907	18,224	39,782	72,978	111,601	144,366	173,041	372,826	758,176	1,701,847
Totals, by Weight	287,601	568,056	1,513,472	1,403,067	1,991,594	1,586,860	1,394,624	1,072,642	935,618	1,202,847	1,232,284	**13,188,665** Substances **960** Tranches

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Rep. 2D 3D React. Standard Purch. In-Stock 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	[illegible]	[illegible]	7,652	4,072	4,180	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	15,904
0	[illegible]	[illegible]	35,387	21,903	22,572	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	79,862
1	[illegible]	[illegible]	163,888	114,245	122,762	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	400,895
2	[illegible]	[illegible]	404,153	324,853	395,876	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	1,124,882
2.5	[illegible]	[illegible]	268,486	240,459	326,556	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	835,501
3	[illegible]	[illegible]	250,050	244,003	364,448	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	858,501
3.5	[illegible]	[illegible]	184,966	199,778	314,985	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	699,729
4	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	0
4.5	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	0
5	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	0
>5	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	0
Totals, by Weight	0	0	1,314,582	1,149,313	1,551,379	0	0	0	0	0	0	**4,015,274** Substances **168** Tranches

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Download Tranches

168 (Non-Empty) Tranches Selected (4,015,274 Substances)

CAAA CAAB CABA CABB CACA CACB CAEA CAEB DAAA DAAB DABA DABB DACA DACB DAEA DAEB EAAA EAAB EABA EABB EACA EACB EAEA EAEB CBAA CBAB CBBA CBBB CBCA CBCB CBEA CBEB DBAA DBAB DBBA DBBB DBCA DBCB DBEA DBEB EBAA EBAB EBBA EBBB EBCA EBCB EBEA EBEB CCAA CCAB CCBA CCBB CCCA CCCB CCEA CCEB DCAA DCAB DCBA DCBB DCCA DCCB DCEA DCEB ECAA ECAB ECBA ECBB ECCA ECCB ECEA ECEB CDAA CDAB CDBA CDBB

Only If Modified Since

mm / dd / yyyy

SMILES (*.smi) Raw URLs Download

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SMILES (*.smi) ✓
2D Only
Tab-Delimited (*.txt)
3D Only
DOCK37 (*.db2.gz)
AutoDock (*.pdbqt.gz)
Mol2 (*.mol2.gz)
SDF (*.sdf.gz)

Download Tranches

168 (Non-Empty) Tranches Selected (4,015,274 Substances)

CAAA CAAB CABA CABB CACA CACB CAEA CAEB DAAA DAAB DABA DABB DACA DACB DAEA DAEB EAAA EAAB EABA EABB EACA EACB EAEA EAEB CBAA CBAB CBBA CBBB CBCA CBCB CBEA CBEB DBAA DBAB DBBA DBBB DBCA DBCB DBEA DBEB EBAA EBAB EBBA EBBB EBCA EBCB EBEA EBEB CCAA CCAB CCBA CCBB CCCA CCCB CCEA CCEB DCAA DCAB DCBA DCBB DCCA DCCB DCEA DCEB ECAA ECAB ECBA ECBB ECCA ECCB ECEA ECEB CDAA CDAB CDBA CDBB

Only If Modified Since

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DOCK Database Index
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WGET ✓
PowerShell
Flat (e.g. No AAAA/*.smi)