Supporting Information For

ZINC – A free tool to discover chemistry for biology

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Keywords: ligand discovery, chemical biology, virtual screening, computational drug discovery, chemical informatics.

Running title: The ZINC database and tool

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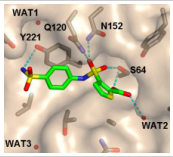
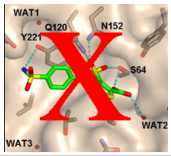
All Catalogs (212 in total)

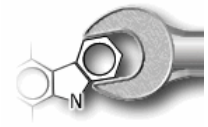
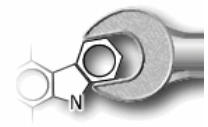
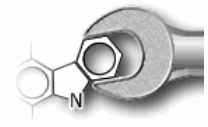
All ZINC source catalogs - commercial vendors and annotated databases - as a sortable list. Use the tabs to the right to break down this list into distinct classes.

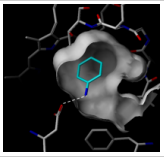
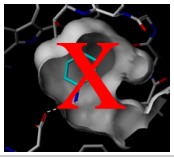
These databases have been provided to us under collaborative agreements with each respective catalog owner. Catalogs have been filtered for drug discovery relevance, and thus compounds in the original catalog may not be in ZINC. Some documentation on ZINC subsets is available.

ZINC may be used free of charge for research by individuals and institutions. Whereas you are free to share the results of a ZINC search or a screen of molecules from ZINC, you may not redistribute major portions of ZINC without the express written permission of John Irwin.

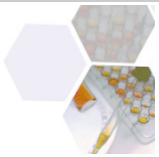
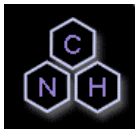
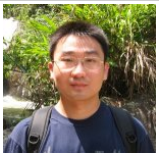
Vendor	Name	Last Updated	Purchasability	Vendor Catalog Size	ZINC Entries	Filtered	Unique	Browse	Download Usual Subset
ACB BLOCKS	ACB Blocks	2011-12-06	Items In Stock	6273	5519	122	512	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
Accela ChemBio Inc.	Accela ChemBio Inc	2010.5	Items In Stock	3124	3300	169	294	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
ACROS ORGANICS	Acros Organics	2012-02-02	Items In Stock	20953	15514	3023	215	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
adesis inc	Adesis	2011-08-22	Items In Stock	1482	1297	272	329	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
AF ChemPharm	AF ChemPharm	2012-02-01	Items In Stock	1051	1352	35	943	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
AldrichCPR	Aldrich CPR	2012-01-20	Items In Stock	169308	181332	6871	71634	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
Alfa Pyridines	Alfa Pyridines	2010.11	Items In Stock	61654	59648	10410	54929	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
Alfa Aesar A Johnson Matthey Company	Alfa-Aesar	2012-01-27	Items In Stock	25102	16440	10440	945	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
Amadis Chemical	Amadis Chemical	2011-12-13	Items In Stock	39265	41381	4795	9198	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
AMBINTER	Ambinter	2012-01-30	Boutique	5053511	5119481	154919	1089911	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase

	Ambinter Natural Products	2011-12-07	Boutique	32998	36057	4317	2943	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Amidohydrolase AH-EFI	2011-11-01	Collaborations Only	470	848	2	20	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Amino acid derivatives (EFI)	2011-12-20	Collaborations Only	246	243	0	20	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	AmpC ligands	2008.7	Not for Sale (Annotated)	21	21	0	0	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	AmpC non-binders	2008.7	Not for Sale (Annotated)	84	119	0	17	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	AnalytiCon Discovery Natural Derivatives	2012-02-16	Items In Stock	23278	24488	41	1690	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	AnalytiCon Discovery NP	2012-02-15	Items In Stock	4719	10119	933	3501	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	AnalytiCon Discovery NP BB	2012-02-15	Items In Stock	148	149	0	64	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Angene	2012-02-15	Items In Stock	2687	2684	75	520	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	APAC Sourcing Solutions	2008.12	Agent	30312	31587	3155	12251	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Apeiron Synthesis	2012-01-02	Items In Stock	12	12	0	3	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	APIChem	2010.2	Items In Stock	13844	14773	1326	376	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Apollo Scientific	2012-02-03	Items In Stock	44578	43850	5409	8327	Overview Basic Targets	SMILES SDF MOL2

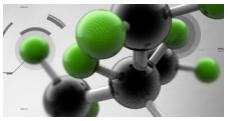
Limited								Focus	Flexibase
	Aronis	2011-08-22	Items In Stock	24118	27859	812	112	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Aronis (Make on Request)	2011-11-16	Made On Demand	302612	254331	21326	94970	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Aronis BuildingBlocks	2011-08-22	Items In Stock	1374	1709	27	8	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	ARVI	2011-09-06	Items In Stock	90044	82878	10751	535	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Asinex	2011-10-05	Items In Stock	360240	508494	17456	41910	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Asinex Building Blocks	2012-03-01	Items In Stock	37429	45680	169	534	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	AsisChem	2011-12-06	Items In Stock	212949	235555	12814	897	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	AsisChem Building Blocks	2011-12-06	Items In Stock	18514	21401	610	1461	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	AstaTech	2011-08-23	Items In Stock	8467	9067	267	1060	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Asymchem	2007-05	Items In Stock	1029	711	286	187	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Bachem	2012-01-08	Items In Stock	4776	4355	351	1770	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Beijing Advanced Technology	2012-02-01	Items In Stock	32	32	0	4	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase

	Bepharm Ltd	2012-01-05	Items In Stock	5456	5620	216	201	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	BindingDB.org	2012-01-03	Not for Sale (Annotated)	345529	400626	26865	39162	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	BioBlocks	2011-12-06	Items In Stock	2989	3024	6	157	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	BioSynth	2012-02-02	Items In Stock	6121	5968	1067	1507	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Bosche Scientific	2011-08-22	Items In Stock	17512	18893	1138	1555	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Calbiochem	2008.1	Items In Stock	665	761	101	369	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Cayman Chemical	2012-02-01	Items In Stock	2525	4715	108	3096	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	CCP W191G binders	2011-10-05	Not For Sale (Model System)	43	56	0	3	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	CCP W191G non-binders	2011-10-05	Not For Sale (Model System)	17	24	0	1	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	ChEBI	2012-01-26	Not for Sale (Annotated)	16563	11596	2072	888	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	ChEMBL DrugStore	2011-09-14	Not for Sale (Annotated)	1437	1508	96	69	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	ChEMBL11	2011-09-08	Not for Sale (Annotated)	1059560	1211557		75602	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase

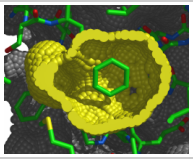
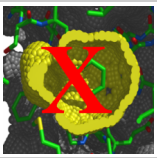
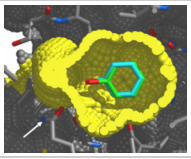
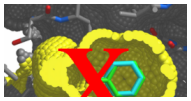
ChEMBL	ChEMBL12	2011-12-19	Not for Sale (Annotated)	1076486	1223663	62410	92843	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
ChEMBL	ChEMBL12 10uM	2011-12-29	Not for Sale (Annotated)	238073	274827	15604	27266	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
ChEMBL	ChEMBL13	2011-08-30	Not for Sale (Annotated)	1000000		0	0	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
ChemBridge	ChemBridge	2012-01-02	Items In Stock	801103	1111884	8991	68213	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
ChemBridge BB	ChemBridge BuildingBlocks	2012-03-02	Items In Stock	13741	16523	237	128	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
ChemDiv The chemistry of cures	ChemDiv	2011-09-02	Items In Stock	673640	843113	40974	1206	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
ChemDiv The chemistry of cures	ChemDiv BuildingBlocks	2011-11-16	Items In Stock	50104	59264	739	9453	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
江苏弘和药物研发有限公司 ChemFuture PharmaTech (Jiangsu), Ltd.	ChemFuture PharmTech	2011-10-27	Items In Stock	1324	1349	80	91	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
CHEMICAL BLOCK	Chemical Block	2011-08-25	Items In Stock	125754	181020	9867	8654	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
CHEMICAL BLOCK	Chemical Block BB	2011-08-22	Items In Stock	5564	6763	115	9	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
ChemiK A Custom Synthesis Specialist	Chemik	2011-08-23	Items In Stock	3962	3675	290	47	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
Chemivate .com	Chemivate	2011-08-23	Items In Stock	1108	1456	3	0	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
ChemMol	ChemMol	2011-12-04	Agent	82462	57568	5586	9867	Overview Basic	SMILES SDF

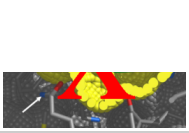
								Targets Focus	MOL2 Flexibase
chemonaut	Chemonaut	2012-02-23	Agent	4202600	4684344	153160	338869	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	CiVentiChem	2011-12-13	Items In Stock	2462	2646	99	1108	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	CNH Technologies	2009.10	Items In Stock	244	217	18	32	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
CDD COLLABORATIVE DRUG DISCOVERY	Collaborative Drug Discovery	2011-11-17	Not for Sale (Annotated)	1261617	1536878	31915	43687	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
COMBI-BLOCKS Inc.	Combi-Blocks	2011-12-06	Items In Stock	3320	1586	1564	7	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
UsefulChem combiugi	CombiUgi	2009.11	Boutique	117450	106087		106074	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	DiPeptides (Hao)	2011-12-20	Collaborations Only	5922	2911	0	239	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
DrugBank Drugs	DrugBank-approved	2012-01-26	Not for Sale (Annotated)	1408	1761	85	92	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
DrugBank Experimental	DrugBank-experimental	2012-01-26	Not for Sale (Annotated)	5046	10253	897	738	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
DrugBank Nutriceuticals	DrugBank-nutriceuticals	2012-01-26	Not for Sale (Annotated)	75	115	3	4	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	DrugBank-Street Drugs	2012-01-26	Not for Sale (Annotated)	172	279	0	43	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
								Overview	SMILES

DrugBank Drugs	DrugBank-withdrawn	2012-01-26	Not for Sale (Annotated)	66	88	3	4	Basic Targets Focus	SDF MOL2 Flexibase
eMolecules	eMolecules	2012-01-25	Agent	4632369	5639322	144517	55968	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
Enamine	Enamine	2012-02-23	Items In Stock	1485558	2016185	2192	90230	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
Enamine	Enamine BB Make on Demand	2011-12-05	Boutique	467397	630398	836	470429	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
Enamine	Enamine Building Blocks	2012-02-06	Items In Stock	55640	65718	1403	3730	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
Enamine	Enamine-REAL	2012-01-18	Made On Demand	15188791	7438306	11376	6456152	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
ENDOTHERM LIFE SCIENCE MOLECULES	EndoTherm	2012-01-20	Items In Stock	2230	2274	248	774	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
EFI EN	Enolase EN-EFI	2011-10-25	Collaborations Only	4358	87	0	6	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
EFI EN	Enolase via KEGG (EFI)	2011-12-21	Collaborations Only	8973	6351	34	409	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
Enzo Life Sciences	Enzo Life Sciences	2010.2	Items In Stock	1172	1295	253	376	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
EUROASIA'S	Euroasia	2009.10	Items In Stock	85	73	14	25	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
EvoBlocks Your Unique Chemical Partner	EvoBlocks	2012-02-23	Items In Stock	8367	10455	198	788	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
FDA	FDA-approved drugs (via DSSTOX)	2005-03-01	Not for Sale (Annotated)	1217	3180	28	507	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase

	FineTech	2011-07-27	Items In Stock	4909	4735	510	132	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Florida Heterocyclic Compounds	2011-09-15	Items In Stock	32056	41192	3467	2696	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Fluorochem	2012-02-08	Items In Stock	58004	58993	3391	1292	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Focus Synthesis	2011-08-23	Items In Stock	2339	2284	289	624	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Fragmenta	2012-03-02	Items In Stock	1699	2011	79	821	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Frinton	2011-12-06	Items In Stock	1187	1313	124	32	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Frontier	2012-01-18	Items In Stock	65119	75889	2173	4839	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Frontier Scientific BB	2012-01-18	Items In Stock	18025	17112	2166	675	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Glutathione Transferrase GST-EFI	2011-11-22	Collaborations Only	39	52	3	5	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Haloacid dehalogenase HAD-EFI	2011-10-25	Collaborations Only	108	111	7	12	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Human Metabolome Database	2011-08-23	Not for Sale (Annotated)	7886	4467	4280	333	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	IBScreen	2011-12-05	Items In Stock	439481	598713	16543	595	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase

	IBScreen Bioactives	2012-01-27	Items In Stock	754	945	31	69	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	IBScreen BuildingBlocks	2011-11-29	Items In Stock	10723	12559	363	96	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	IBScreen NP	2011-11-29	Items In Stock	46940	69363	741	596	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Indofine	2012-02-02	Items In Stock	1593	1826	168	259	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Indofine Natural Products	2012-02-02	Items In Stock	56	113	3	28	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Infarmatik	2010.5	Items In Stock	212	299	0	249	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Infarmatik (make-on-demand)	2011-11-16	Boutique	8422	21016	50	20773	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Infospectrum	2011-08-23	Items In Stock	2032	2003	254	207	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Innovapharm	2011-11-28	Boutique	316315	392259	51737	1674	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Innovapharm BB Make on Demand	2011-11-16	Boutique	64423	82616	1313	18575	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Innovapharm Building Blocks	2011-11-16	Boutique	17519	22597	391	226	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Innovapharm Make-on-Demand	2011-11-16	Boutique	230897	766734	180951	512873	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase

IS Chemical Technology INNOVATIVE SERVICE	IS Chem Tech (Make on Demand)	2011-11-16	Made On Demand	304	351	21	0	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
IS Chemical Technology INNOVATIVE SERVICE	IS Chem. Tech Building Blocks	2011-09-14	Items In Stock	3646	3776	487	0	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
IS Chemical Technology INNOVATIVE SERVICE	IS Chemical Technology	2011-09-14	Items In Stock	44063	40572	4038	3851	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
EFI IS	Isoprenoid synthase IS-EFI	2011-11-30	Collaborations Only	13	14	1	11	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
IUPHAR DATABASE International Union of Basic and Clinical Pharmacology	IUPHAR Database	2011-07-27	Not for Sale (Annotated)	1967	2276	203	256	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
KEGG VIA PubChem	KEGG via PubChem	2011-11-28	Not for Sale (Annotated)	19960	19851	2242	1666	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Key Organics Building Blocks	2012-03-05	Items In Stock	7574	8873	44	105	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	KeyOrganics	2012-03-05	Items In Stock	53955	67384	1191	1316	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	KeyOrganics Bioactives	2012-03-05	Items In Stock	640	679	90	51	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	L99A binders	2011-10-05	Not For Sale (Model System)	74	71	43	2	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	L99A non-binders	2011-10-05	Not For Sale (Model System)	68	64	0	2	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	L99A/M102Q binders	2011-10-05	Not For Sale (Model System)	94	101	0	3	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	L99A/M102Q non-binders	2011-10-05	Not For Sale (Model System)	24	26	0	0	Overview Basic Targets	SMILES SDF MOL2

								Focus	Flexibase
	Labotest	2011-09-06	Items In Stock	106756	124842	9332	4308	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Labotest Building Blocks	2011-08-25	Items In Stock	3165	3412	297	3	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Letopharm	2011-01-14	Items In Stock	26534	26509	2462	895	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Life Chemicals	2011-12-04	Items In Stock	344693	414730	5751	9055	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Life Chemicals (Virtual)	2011-11-16	Made On Demand	408701	459378	30338	112538	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Life Chemicals Building Blocks	2011-11-22	Items In Stock	26270	31091	31	392	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Matrix Scientific	2011-09-06	Items In Stock	55377	64855	2223	946	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Maybridge	2011-12-19	Items In Stock	55810	70821	1560	2288	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Maybridge Building Blocks	2011-12-16	Items In Stock	6048	6216	473	37	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Maybridge Hit Finder	2011-03-10	Items In Stock	14400	19584	217	1206	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	MicroCombiChem	2011-11-22	Items In Stock	770	906	29	797	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	MicroCombiChem BB	2011-11-22	Items In Stock	841	1014	35	715	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase

	MicroCombiChem BB Make-on-demand	2011-11-22	Made On Demand	607	716	0	524	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	MicroCombiChem Make-on-demand	2011-11-22	Made On Demand	47	14	33	14	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	MicroSource	2004-10	Items In Stock	2117	3879	102	648	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	mlsmr2	2011-04-13	Not for Sale (Annotated)	237280	292273	6758	47761	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	mlsmr3 AMPC Oliv	2011-04-13	Not for Sale (Annotated)	517196	537314	17713	92235	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	MLSMR4 May2011	2011-04-27	Not for Sale (Annotated)	366867	473598		14599	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Molcan	2011-09-12	Items In Stock	1240	1332	62	486	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Molecular Diversity Preservation International	2011-12-05	Items In Stock	22181	26918	743	11024	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Molport	2012-02-08	Agent	4421283	5554673	148649	675996	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	MP Biomedicals	2009.10	Items In Stock	19769	18066	5412	3007	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Nagase	2011-11-02	Items In Stock	78	79	2	26	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	NCI Diversity II	2009.4	Not for Sale (Annotated)	1364	1880	5	342	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	NCI Plated 2007	2011-09-21	Items In Stock	139735	87374	21235	59580	Overview Basic Targets	SMILES SDF MOL2

								Focus	Flexibase
	Oakwood Chemical	2011-09-20	Items In Stock	43273	46166	2317	2356	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Otava	2011-12-13	Items In Stock	157744	197185	8853	1236	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Otava (Virtual)	2011-11-16	Boutique	339583	443391	11396	372762	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Otava BB Make-to-order	2012-01-05	Boutique	1681032	1765749	9082	994967	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
PBMR Labs Ukraine	PBMR Labs	2010.4	Items In Stock	379034	482755	20572	63554	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
peakdale	Peakdale	2011-12-06	Items In Stock	15339	17066	330	15117	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
PepTech	PepTech	2011-12-16	Items In Stock	2380	1692	771	552	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
PHARMEKS	Pharmeks	2011-12-29	Items In Stock	259523	379166	24183	28810	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
EFI EN	Phosphate sugars (EFI)	2011-12-20	Collaborations Only	199	86	0	9	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
PRESTWICK CHEMICAL INC.	Prestwick Chemical	2011-07-26	Items In Stock	1200	1968	124	177	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Princeton BioMolecular BuildingBlocks	2011-05-17	Boutique	70252	82853	1221	22071	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Princeton BioMolecular Research	2011-05-26	Items In Stock	910414	1084177	54683	54403	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase

	Princeton NP	2011-12-06	Items In Stock	45785	49381	43	2543	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
PubChem	PubChem	2011-05-17	Not for Sale (Annotated)	31453252	15467019	3193633	5367313	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
RSci	Ryan Scientific	2006.5	Agent	185372	120266	6527	200	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
RSci	Ryan Scientific BB	2012-02-15	Items In Stock	145634	119719	6300	1080	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
Scientific Exchange, Inc. Supplier of HTS compounds	Scientific Exchange	2011-03-09	Agent	47455	58907	15043	7389	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
Scientific Exchange, Inc. Supplier of HTS compounds	Scientific Exchange (make on demand)	2011-11-16	Agent	1161526	1293626	24497	438426	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
Scientific Exchange, Inc. Supplier of HTS compounds	Scientific Exchange Building Blocks	2011-02-16	Agent	25504	33568	190	8930	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
SelleckBio.com	Selleck BioChemicals	2011-11-28	Items In Stock	563	614	35	0	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
SelleckBio.com	Selleck BioChemicals NP	2011-11-29	Items In Stock	130	136	17	0	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
Selleck Chemicals	Selleck Chemicals	2011-11-18	Items In Stock	1089	1134	74	263	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
Sequoia Research Products	Sequoia Research Products	2011-10-05	Items In Stock	2266	2407	384	100	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
SINOF	Shanghai Sinofluoro Scientific	2012-02-24	Items In Stock	1535	1353	137	53	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase

SIGMA-ALDRICH	Sigma Aldrich (Building Blocks)	2012-01-20	Items In Stock	77614	37659	19217	5306	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
SINOVA	Sinova	2008.6	Items In Stock	3335	3074	122	1828	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
SMDC	SMDC CDiv Carboxamide	2012-02-20	Not for Sale (Annotated)	4417	5516	205	132	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
SMDC	SMDC CDiv Diverse	2012-02-21	Not for Sale (Annotated)	50000	69194	33	1334	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
SMDC	SMDC CDiv Kinase	2012-02-20	Not for Sale (Annotated)	10000	11581	2	531	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
SMDC	SMDC ChBr Diverse	2012-02-20	Not for Sale (Annotated)	23865	32099	124	2541	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
SMDC	SMDC ChBr Premium	2012-02-20	Not for Sale (Annotated)	30000	44774	3	3647	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
SMDC	SMDC Iconix	2012-02-20	Not for Sale (Annotated)	909	1065	45	25	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
SMDC	SMDC Life and Maybridge	2012-02-20	Not for Sale (Annotated)	2451	2756	5	9	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
SMDC	SMDC MicroSource	2012-02-20	Not for Sale (Annotated)	2160	3404		277	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
specs chemistry solutions for drug discovery	Specs	2011-12-13	Items In Stock	203434	273915	15181	26461	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
specs chemistry solutions for drug discovery	Specs Building Blocks	2011-12-06	Items In Stock	8523	9239	254	269	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	Specs Natural							Overview Basic	SMILES SDF

specs chemistry solutions for drug discovery	Products	2011-12-06	Items In Stock	456	651	107	31	Targets Focus	MOL2 Flexibase
SPECTRUM CHEMICALS & LABORATORY PRODUCTS	spectrum	2011-08-23	Items In Stock	2320	4885	324	477	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
SynChem SYNCHEM	SynChem	2007	Items In Stock	937	1011	14	0	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
SYNCHEM	SYNCHEM OHG	2008.6	Items In Stock	2127	2003	214	744	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
Synergy Scientific Ltd	Synergy Scientific BB	2012-01-09	Items In Stock	4295	4323	142	0	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
SynQuest Laboratories, Inc.	SynQuest Laboratories	2007	Items In Stock	3516	2218	1509	94	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
SYNTHON LAB	Synthon-Lab	2011-10-07	Items In Stock	54436	81096	2645	2209	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
SYNTHONIX ELEMENTS OF PROGRESS	Synthonix	2007	Items In Stock	1817	1505	341	425	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
	TCI	2012-03-01	Items In Stock	20310	17320	2570	1110	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
TCM DATABASE @TAIWAN http://tcm.cmu.edu.tw YC Lab	TCM Database @ Taiwan	2011-11-16	Collaborations Only	15747	6595	2876	280	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
TimTec Your Full Service Partner for Drug Discovery Since 1995	TimTec	2011-12-19	Items In Stock	205589	258020	13373	1410	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
TimTec Your Full Service Partner for Drug Discovery Since 1995	TimTec BB Make on Demand	2011-12-14	Made On Demand	32334	39213	1271	55	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
TimTec Your Full Service Partner for Drug Discovery	TimTec Building Blocks	2011-12-16	Items In Stock	35307	40779	1373	188	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase

TimTec	TimTec Make-on-Demand	2012-01-09	Made On Demand	678040	811436	22665	2821	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
TimTec	TimTec Natural Derivatives	2011-12-07	Items In Stock	3040	4961	67	314	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
TOCRIS bioscience	Tocris	2005.10	Items In Stock	974	1177	162	284	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
TRC	Toronto Research Chemicals	2012-03-05	Items In Stock	20083	25239	1713	8149	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
TOSLAB	Toslab	2011-12-07	Items In Stock	22065	29502	4935	6315	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
TOSLAB	Toslab Building Blocks	2011-12-06	Items In Stock	1222	1647	94	533	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
Tractus	Tractus	2012-02-07	Items In Stock	75547	78161	2421	3480	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
Trylead chemical	Trylead Chemical	2008.12	Items In Stock	8242	7745	1168	12	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
TYGER	Tyger	2005.10	Items In Stock	2670	3345	150	1381	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
ubichem PHARMA SERVICES	Ubichem	2008.11	Items In Stock	1220	1230	87	380	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
UEFS.br UNIVERSIDADE ESTADUAL DE FEIRA DE SANTANA	UEFS Natural Products	2011-11-29	Collaborations Only	503	473	7	382	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
UM-BBD	UMBBD	2011-12-05	Not for Sale (Annotated)	1319	1517	172	79	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
								Overview	SMILES

UkrOrgSynthesis	UORSY	2012-03-05	Items In Stock	1300403	1494307	16560	594215	Basic Targets Focus	SDF MOL2 Flexibase
UkrOrgSynthesis	UORSY BB Make-on-demand	2012-03-02	Boutique	5996815	7803833	42983	6678245	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
VIT LABORATORY	Vitas-M	2012-01-02	Items In Stock	1101501	1352753	62523	11487	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
VIT LABORATORY	Vitasm-M Building Blocks	2011-12-13	Items In Stock	17968	19871	401	4	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase
ZANNAN 上海赞南药业有限公司 ZANNAN PHARMA LTD.	Zannan	2009.5	Items In Stock	1514	2893	73	2158	Overview Basic Targets Focus	SMILES SDF MOL2 Flexibase

Filtering rules in effect at docking.org

For each set of filtering rules, we provide them in raw text and also in an graphic form. Thanks to Mattias Rarey and his group for SMARTSviewer.

Basic filters: applied to all vendor catalogs

- text: rules_default.txt
- graphic: graphic version

Annotated catalog filters

Catalogs of biologically active molecules are filtered using more permissive rules (because they are active).

- text: rules_annotated.txt
- graphic: graphic version

Secondary filters

Molecules are annotated as potentially problematic if they match any of these filters.

yuck rules

The "clean" subsets in ZINC have any molecule matching any of these two yuck rule sets filtered out. Editorial comment: We do not endorse either set of yuck rules. They are provided merely as a convenience to users. Many perfectly good actives and over 1/2 of purchasable chemistry are filtered out by these rules. caveat emptor

- text: rules_yuck.txt
- graphic: graphic version

yuck1 rules

A second set of rules.

- text: rules_yuck1.txt
- graphic: graphic version

Blaster rules

During upload and DOCK Blaster, we are more tolerant of ligands since they bind (i.e. in the PDB). These are like the rules for

- text: rules_blaster.txt
- graphic: graphic version

Many thanks to David M. Lorber for the filtering script and our colleagues at drug companies for advice. As always at docking.org, the sole responsibility for any errors is John Irwin's.

Finally, a wide range of SMARTS definitions.

- text: smarts_use.txt
- graphic: graphic version

Last updated: October 2011.

```
#special flags
50.0 500.0 MOLWT
STRIPSALTS yes
0 10 CHIRALITY enumerate
ALLOWED_ATOMS C N O S P Cl F Br I H

# normal format is (min, max, name, SMARTS)

#rules
5 40 Non-Hydrogen_atoms [a,A]
2 40 carbons [#6]
0 20 N,O,S [#7,#8,#16]
0 1 Sulfonyl_halides S(=O)(=O)[Cl,Br]
0 1 Acid_halides [S,C](=[O,S])[F,Br,Cl,I]
0 1 Alkyl_halides [Br,Cl,I][CX4;CH,CH2]
0 0 Phosphenes cPc
0 0 Heptanes [CD1][CD2][CD2][CD2][CD2][CD2][CD2]
0 0 Perchlorates OCl(O)(O)(O)
0 7 Fluorines F
0 6 Cl,Br,I [Cl,Br,I]
0 0 Carbazides O=CN=[N+]=[N-]
0 0 Acid_anhydrides C(=O)OC(=O)
0 0 Peroxides OO
0 1 Iso(thio)cyanates N=C=[S,O]
0 1 Thiocyanates SC#N
0 0 Phosphoranes C=P
0 0 P/S_halides [P,S][Cl,Br,F,I]
#0 0 Carbodiimides N=C=N
0 0 Cyanohydrines N#CC[OH]
0 0 Carbazides O=CN=[N+]=[N-]
0 1 Sulfate_esters COS(=O)O[C,c]
0 1 Sulfonates COS(=O)(=O)[C,c]
0 0 Pentafluorophenyl_esters C(=O)Oc1c(F)c(F)c(F)c(F)c1(F)
0 0 Paranitrophenyl_esters C(=O)Oc1ccc(N(=O)=O)cc1
0 0 HOBt_esters C(=O)Onnn
0 0 Triflates OS(=O)(=O)C(F)(F)F
0 0 Lawesson's_reagents P(=S)(S)S
0 0 Phosphoramides NP(=O)(N)N
0 0 Aromatic_azides cN=[N+]=[N-]
0 2 Quaternary_C,Cl,I,P,S [C+,Cl+,I+,P+,S+]
0 2 Beta_carbonyl_quaternary_N C(=O)C[N+,n+]
0 2 Acylhydrazides [N;R0][N;R0]C(=O)
0 0 Chloramidines [Cl]C([C&R0])=N
0 0 Isonitriles [N+]#[C-]
0 0 Triacyloximes C(=O)N(C(=O))OC(=O)
0 0 Acyl_cyanides N#CC(=O)
0 0 Sulfonyl_cyanides S(=O)(=O)C#N
0 0 Cyanophosphonates P(OCC)(OCC)(=O)C#N
0 0 Azocyanamides [N;R0]=[N;R0]C#N
0 0 Azoalkanals [N;R0]=[N;R0]CC=O
0 2 (Thio)epoxides,aziridines C1[O,S,N]C1
0 2 Benzylic_quaternary_N cC[N+]
0 2 Thioesters C[O,S;R0][C;R0](=S)
0 3 Diand_Triphosphates P(=O)([OH])OP(=O)[OH]
0 2 Aminooxy(oxo) [#7]O[#6,#16]=O
0 2 nitros N(~[OD1])~[OD1]
0 2 Imines C=[N;R0]*
0 2 Acrylonitriles N#CC=C
0 2 Propenals C=CC(=O)[!#7;!#8]
0 1 Quaternary_N [nD1+,ND4+]
```

```
#special flags
50.0 600.0 MOLWT
STRIPSALTS yes
0 20 CHIRALITY enumerate
ALLOWED_ATOMS C N O S P Cl F Br I H

# normal format is (min, max, name, SMARTS)

#rules
4 50 Non-Hydrogen_atoms [a,A]
1 49 carbons [#6]
```

```
#special flags
80.0 999.0 MOLWT
STRIPSALTS yes
0 10 CHIRALITY
ALLOWED_ATOMS C N O S P Cl F Br I H

# normal format is (min, max, name, SMARTS)

#rules
0 0 Sulfonyl_halides S(=O)(=O)[Cl,Br]
0 0 Acid_halides [S,C](=[O,S])[F,Br,Cl,I]
0 0 Alkyl_halides [Br,Cl,I][CX4;CH,CH2]
0 0 Phosphenes cPc
0 0 Heptanes [CD1][CD2][CD2][CD2][CD2][CD2][CD2]
0 0 Perchlorates OCl(O)(O)(O)
0 7 Fluorines F
0 6 Cl,Br,I [Cl,Br,I]
0 0 Carbazides O=CN=[N+]=[N-]
0 0 Acid_anhydrides C(=O)OC(=O)
0 0 Peroxides OO
0 0 Iso(thio)cyanates N=C=[S,O]
0 0 Thiocyanates SC#N
0 0 Phosphoranes C=P
0 0 P/S_halides [P,S][Cl,Br,F,I]
0 0 Carbodiimides N=C=N
0 0 Cyanohydrines N#CC[OH]
0 0 Carbazides O=CN=[N+]=[N-]
0 0 Sulfate_esters COS(=O)O[C,c]
0 0 Sulfonates COS(=O)(=O)[C,c]
0 0 Pentafluorophenyl_esters C(=O)Oc1c(F)c(F)c(F)c(F)c1(F)
0 0 Paranitrophenyl_esters C(=O)Oc1ccc(N(=O)=O)cc1
0 0 HOBt_esters C(=O)Onnn
0 0 Triflates OS(=O)(=O)C(F)(F)F
0 0 Lawesson's_reagents P(=S)(S)S
0 0 Phosphoramides NP(=O)(N)N
0 0 Aromatic_azides cN=[N+]=[N-]
0 0 Quaternary_C,Cl,I,P,S [C+,Cl+,I+,P+,S+]
0 0 Beta_carbonyl_quaternary_N C(=O)C[N+,n+]
0 0 Acylhydrazides [N;R0][N;R0]C(=O)
0 0 Chloramidines [Cl]C([C&R0])=N
0 0 Isonitriles [N+]#[C-]
0 0 Triacyloximes C(=O)N(C(=O))OC(=O)
0 0 Acyl_cyanides N#CC(=O)
0 0 Sulfonyl_cyanides S(=O)(=O)C#N
0 0 Cyanophosphonates P(OCC)(OCC)(=O)C#N
0 0 Azocyanamides [N;R0]=[N;R0]C#N
0 0 Azoalkanals [N;R0]=[N;R0]CC=O
0 0 (Thio)epoxides,aziridines C1[O,S,N]C1
0 0 Benzylic_quaternary_N cC[N+]
0 0 Thioesters C[O,S;R0][C;R0](=S)
0 0 Diand_Triphosphates P(=O)([OH])OP(=O)[OH]
0 0 Aminooxy(oxo) [#7]O[#6,#16]=O
0 0 nitros N(~[OD1])~[OD1]
0 0 Imines C=[N;R0]*
0 0 Acrylonitriles N#CC=C
0 0 Propenals C=CC(=O)[!#7;!#8]
0 0 Quaternary_N [nD4+,ND4+]
0 0 azo [N;D2;$(N=[N;D2]);!$(N(=N)~[#7,#8,#15,#16]);!$(N=N~[#7,#8,#15,#16])]
0 0 Azide N=[N+]=[N-]
0 0 epoxide C1CO1
```

```
0 0 chloroformate C(=O)Cl
0 0 benzylic_halide c[CD2X4][F,Cl,Br,I]
0 0 thioether CSC
0 0 thiol [SD1]
0 0 disulfide S-S
0 0 aldehyde  [CD2](=O)
0 0 N_O_bonds N-O
0 0 N_N_bonds N-N
0 0 michael [$([CH1,CH2]=CC=O)]
```

```
#special flags
50.0 700.0 MOLWT
STRIPSALTS yes
#0 10 CHIRALITY enumerate
ALLOWED_ATOMS C N O S P Cl F Br I H

# normal format is (min, max, name, SMARTS)

#rules
0 0 rule2 *C(=S)[N,S]
0 0 rule3 *O[N+](=O)[O-]
0 0 rule4 *OCS(=O)(=O)O
0 0 rule5 *OS(=O)(=O)O
0 0 rule6 [#6;R3;!r7][#6;R3;!r7][#6;R3;!r7]1[#6;R3;!r7][#6;R3;!r7][#6;R3;!r7]**1
0 0 rule7 [#7,#8;r9,r10,r11,r12,r13,r14,r15,r16,r17,r18][#6;R][#6;R]
[#7,#8;r9,r10,r11,r12,r13,r14,r15,r16,r17,r18][#6;R][#6;R]
[#7,#8;r9,r10,r11,r12,r13,r14,r15,r16,r17,r18]
0 0 rule8 [$([2H]),$([3H])]
0 0 rule9 [$([CH](C#N)([F,Cl,Br,I])),$([CH](C=O)([F,Cl,Br,I])),$([CH](N(=O)=O)
([F,Cl,Br,I]))]
0 0 rule10
[$([Np]),$([Ru]),$([Sr]),$([Rh]),$([Se]),$([Pd]),$([Sc]),$([Bi]),$([Ag]),$([Ti]),$([A
l]),$([Cd]),$([V]),$([In]),$([Cr]),$([Sn]),$([Mn]),$([La]),$([Fe]),$([Er]),$([Tm]),$(
[Yb]),$([Lu]),$([Hf]),$([Ta]),$([W]),$([Re]),$([Co]),$([Os]),$([Ni]),$([Ir]),$([Cu]),
$([Zn]),$([Ga]),$([Pu]),$([Ge]),$([Am]),$([As]),$([Cm]),$([Y]),$([Bk]),$([Zr]),$([Cf]
),$([Nb]),$([Es]),$([Fm]),$([Ce]),$([No]),$([Pr]),$([Nd]),$([Pm]),$([Sm]),$([Eu]),$([
Gd]),$([Tb]),$([Dy]),$([Ho]),$([Pt]),$([Au]),$([Hg]),$([Tl]),$([Pb]),$([Ac]),$([Th]),
$([Pa]),$([Mo]),$([U]),$([Tc]),$([Te])]
0 0 rule11 [$(C(=O));H1][C;X4]
0 0 rule12 [$(C(=O)c);H1]
0 0 rule13 [$(C(=O)N);H1]
0 0 rule14 [*;H1]OC(=[O,S])[N,O,S]
0 0 rule15 [*][C;!R](=O)[C;!R](=O)[*]
0 0 rule16 [*][C;!R](=O)C[C;!R](=O)[*]
0 0 rule17 [*]1=[!N]-C(=O)-C(=O)-[!N]=[*]1
0 0 rule18 [B]
0 0 rule19 [C,c]C(=O)[F,Cl,Br,I,$(S(=O)(=O))]
0 0 rule20 [C,c]C(=O)C(=O)[C,c]
0 0 rule21 [C,c]C(=O)C[F,Cl,Br,I,$(S(=O)(=O))]
0 0 rule22 [C,c]OP(=O)(=O)C[C,c]
0 0 rule23 [C,c]OS(=O)(=O)C[C,c]
0 0 rule24 [C,c]OS(=O)O[C,c]
0 0 rule25 [C,S,P](=O)[OH].[C,S,P](=O)[OH].[C,S,P](=O)[OH].[C,S,P](=O)[OH]
0 0 rule26 [C;H2]=[C][N,O]
0 0 rule27 [C;X4;H2][C;R0](=O)[C;H3]
0 0 rule28 [C;X4;R0][C;X4;R0][C;R0](=[N;R0][C;X4;R0])[C;X4;R0]
0 0 rule29 [C;X4][O,N,S;D2;R0][O,N,S;D2;R0][CX4,H]
0 0 rule30 [C]=[C][Cl,Br,I,F]
0 0 rule31 [C+,Cl+,I+,P+,S+]
0 0 rule32 [CH2]=C-C=O
0 0 rule33 [Cl,Br,I,F]CC(=O)[O,N]
0 0 rule34 [Cl,Br,I].[Cl,Br,I].[Cl,Br,I].[Cl,Br,I].[Cl,Br,I].[Cl,Br,I]
0 0 rule35 [Cl,Br,I][CX4;CH,CH2]
0 0 rule36 [Cl,I]([*])[*]
0 0 rule37 [Cl][$(C=O);!$(C(=O)N)]
0 0 rule38 [Cl]C([C&R0])=N
0 0 rule39 [F,Cl,Br,I,$(S(=O)(=O))]C([F,Cl,Br,I,$(S(=O)(=O))])([F,Cl,Br,I,$(S(=O)
(=O))])C(=O)[C;X4;H2]
0 0 rule40 [F,Cl,Br,I,$(S(=O)(=O))]c1ncccn1
0 0 rule41 [F,Cl,Br,I][$([C,S]=[O,S]);!$([C,S](=[O,S])N)]
```

```
0 0 rule42 [N&D2](=O)
0 0 rule43 [N,O,S]C#N
0 0 rule44 [N;D4]
0 0 rule45 [N;R0][N;R0]C(=O)
0 0 rule46 [N;R0]=[N;R0]C#N
0 0 rule47 [N;R0]=[N;R0]CC=O
0 0 rule48 [N+,n+][N-,n-]
0 0 rule49 [N+]#[C-]
0 0 rule50 [O;H1]c1ccccc1[O;H1]
0 0 rule51 [O]=[N][C,N]
0 0 rule52 [P,S][Cl,Br,F,I]
0 0 rule53 [P]
0 0 rule54 [S;!R]C(=[S,O;!R])([!O;!S;!N])
0 0 rule55 [SH]
0 0 rule56 [Si]
0 0 rule57 C#N.C#N.C#N.C#N
0 0 rule58 c([OH])c([OH])c([OH])
0 0 rule59 c([OH])c([OH])cc([OH])
0 0 rule60 C(=O)[C;!H0][N+,n+]
0 0 rule61 C(=O)[N,O]C(=O)
0 0 rule62 C(=O)C[N,O]CC(=O)
0 0 rule63 C(=O)N(C(=O))OC(=O)
0 0 rule64 C(=O)OC(=O)
0 0 rule65 C(=O)Oc1c(F)c(F)c(F)c(F)c1(F)
0 0 rule66 C(=O)Oc1ccc(N(=O)=O)cc1
0 0 rule67 C(=O)Onnn
0 0 rule68 C=N[N;H1]
0 0 rule69 C=P
0 0 rule70 C1(=O)OCC1
0 0 rule71 C1(O)C(O)C(O)C(O)OC1
0 0 rule72 C1[N;H1]CCC(=O)C1
0 0 rule73 C1[O,S,N]C1
0 0 rule74 c1c(=O)nc(=O)c1
0 0 rule75 CC[C;H1;!R]=[C;H1;!R]C(=O)[C;X4;!R]
0 0 rule76 CCC([C;H2]C(=O)[C;X4])[F,Cl,Br,I,$(S(=O)(=O))]
0 0 rule77 N#CC(=O)
0 0 rule78 N#CC[OH]
0 0 rule79 N[CH2]C#N
0 0 rule80 N[Cl,Br,I,F]
0 0 rule81 N=C=[S,O]
0 0 rule82 N=C=N
0 0 rule83 N=NC(=S)N
0 0 rule84 N1CN1
0 0 rule85 NOS(=O)(=O)
0 0 rule86 NP(=O)(N)N
0 0 rule87 O=C1[#6]~[#6]C(=O)[#6]~[#6]1
0 0 rule88 O=CN=[N+]=[N-]
0 0 rule89 O=CO[n,$(N(C=O)(C=O))]
0 0 rule90 OO
0 0 rule91 OS(=O)(=O)C(F)(F)F
0 0 rule92 P(=O)([OH])OP(=O)[OH]
0 0 rule93 P(=S)(S)S
0 0 rule94 P(OCC)(OCC)(=O)C#N
0 0 rule95 S(=O)(=O)[F,Cl,Br,I,$(S(=O)(=O))]
0 0 rule96 S(=O)(=O)C#N
0 0 rule97 S~S
0 0 rule98 s1****1[N;H2]
0 0 rule99 s1nccn1
0 0 rule100 SC#N
```

ZINC:Command language

From DISI

You can control ZINC-12 remotely by hand writing URLs. This document is a guide to how to use them.

URLs are generally of the form: http://zinc.docking.org/results?category.field=argument&category2.field2=argument2

Multiple queries and format instructions may be supplied in a single transaction.

Contents

- 1 Quick Search Bar
- 2 Structure
- 3 Catalog
- 4 ZINC ID
- 5 Annotation
- 6 Prediction
- 7 Clustered Targets
- 8 Reports, Formats, Filters

Quick Search Bar

You can access all the functionality of the Quick Search Bar using the /find/ command.

```
e.g.  http://zinc.docking.org/find/12346+3432+3343
e.g.  http://zinc.docking.org/find/drug:ibuprofen
```

Structure

The SMILES and SMARTS must be URL encoded.

```
structure.similarity=n where 0<=n<=1
structure.smiles=<SMILES>
structure.substructure=<SMARTS>
```

```
e.g. http://zinc.docking.org/results.?structure.smiles=C1CCCCC1&structure.similarity=1.
```

Catalog

```
catalog.purchasability={not-for-sale, in-stock, on-demand, boutique, agent, collabocule
catalog.name=<name>
```

```
e.g. http://zinc.docking.org/results?catalog.purchasablity=in-stock
e.g. http://zinc.docking.org/results?catalog.name=:ChemBridge,Molport
```

ZINC ID

```
zinc.id =
```

```
e.g.http://zinc.docking.org/results?zinc.id=29323
```

Annotation

```
annotation.swiss_prot=Q9R297
annotation.uniprot=HRH1_HUMAN
annotation.term=:Q9R297,HRH1_HUMAN
```

```
e.g.http://zinc.docking.org/results?annotation.uniprot=HRH1_HUMAN
```

Prediction

```
prediction.swiss_prot=Q9R297
prediction.uniprot=HRH1_HUMAN
```

```
 e.g.http://zinc.docking.org/results?prediction.swissprot=Q112345
```

Clustered Targets

```
target.code=drd2-1-e
```

```
e.g.http://zinc.docking.org/results?target.code=drd2-1-e
```

Reports, Formats, Filters

```
page.format=X where X = sdf, mol2, smi, Flexibase
filter.representation=X where X= usual, single, metal, all, ref, mid, hi, lo
filter.purchasability=X where X= in-stock, on-demand, purchasable, not-for-sale, all, .
```

```
e.g. http://zinc.docking.org/results?annotation.name=DRD2_HUMAN&filter.purchasability=p
```

Retrieved from "http://wiki.bkslab.org/index.php/ZINC:Command_language"

Category: ZINC

Quick Search Bar

From DISI

(Redirected from QSB)

The Quick Search Bar may be used to enter free-form text to query ZINC. The goal is to offer fast google-like simplicity. The input is interpreted as follows. Wildcards are supported

Number(s)

If it is a number, interpret as a ZINC ID. To force this behavior, prefix with zinc:

```
e.g. (All are supported)
     zinc:32768
     32768
     32768 55535 7
```

Number-Number-Number

If it is of the form number-number-number, interpret as a CAS number. For force this behavior, prefix with cas:

```
e.g. (All are supported)
      cas:5-6-10
      6-54-2
      3-5-6 3-4-2
```

Contents

- 1 Number(s)
- 2 Number-Number-Number
- 3 SMILES and SMARTS
- 4 Name
- 5 Target
- 6 Catalog

SMILES and SMARTS

If it is a valid SMILES, interpret as "90% similar to". To force this behavior, prefix with smiles:

Optionally after SMILES (SMARTS) add identical, exact, substructure, 80% or 0.8 (or any value) for corresponding searches.

```
e.g. (All are supported)
     smiles:O=C1CCN1 substructure
```

```
    smiles:O=C1CCN1 77%
    C1CCNCC1 exact
```

Name

Attempt to interpret as name of molecule. To force this behavior, prefix with name: or drug:

```
e.g.  (All are supported)
      drug:cetirizine
      drug:*pram
      ibuprofen
```

Target

Attempt to interpret as target name. Uniprot and SwissProt codes as well as target names are supported. To force this behavior, prefix with target:

```
e.g. (All are supported)
     target:5ht1a*
     target:hdac*
     target:DRD2_HUMAN
     DRD2_HUMAN
     target:Q2LFS1
```

Catalog

Attempt to interpret as catalog name. To force this behavior, prefix with catalog:

```
e.g. (All are supported)
     ChemBridge
     catalog:Enamine
     catalog:asin
```

Attempt to interpret as a catalog code, optionally prefixed with catalog name. Thus

```
e.g. (All are supported)
     ChemBridge T12345
     vendor:ChemBridge T12345
     Enamine 194394*
     vendor:12345 (any compound called 12345 by any vendor)
```

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How to link to ZINC

From DISI

How to link to ZINC.

This is how to link to ZINC from other websites.

By ZINC ID

Contents

- 1 By ZINC ID
- 2 By ChEMBL (or other catalog or vendor) ID
- 3 Dynamic link on the fly - Javascript - how to include in your page
- 4 By SMILES
- 5 By InChI
- 6 By CAS #
- 7 By Vendor / Vendor code
- 8 By Name
- 9 By Ring
- 10 By Target
  - 10.1 By SwissProt
  - 10.2 By UniProt
  - 10.3 By Target Name

- http://zinc.docking.org/substance/<zincid>

For example, to link to 16610261, use the URL

- http://zinc.docking.org/substance/16610261

By ChEMBL (or other catalog or vendor) ID

```
http://zinc.docking.org/results?page.format=zinc&filter.purchasable=purchasable&zinc.id
```

ZINC_ID can be one or more ZINC ID numbers separated by white-space. e.g.

```
wget -qO- http://zinc.docking.org/results?page.format=zinc&filter.purchasable=purchasab
```

```
http://zinc.docking.org/catalogs/chembl12/$CHEMBLID.zinc?filter.purchasability=purchasa
```

CHEMBLID can be a single chembl code. e.g: To check if the ChEMBL ID "CHEMBL25" (One of two codes for Aspirin) is purchasable you would request the following URL:

```
http://zinc.docking.org/catalogs/chembl12/CHEMBL25.zinc?filter.purchasability=purchasab
```

This will return a text file with an integer (53) corresponding to the same ZINC compound. There may be more than one compound if the ChEMBL annotation is shared between multiple ZINC Substances in which case multiple IDs will be returned, each on it's own line.

Dynamic link on the fly - Javascript - how to include in your page

The code for ChEMBL should be:

```
<script type="text/javascript" src="http://zinc.docking.org/js/embed.js"></script>
<script type="text/javascript">
window.zinc.embed(
  'zinc-link',                      // Embed in the item with id "zinc-link"
  {
    "filter.purchasability": "purchasable",
    "catalog.name": "chembl13",
    "catalog.code": "CHEMBL25"      // CHANGE THIS LINE TO APPROPRIATE CHEMBL ID
  },
  true                              // Hide on no match
                                    // Optional 4th argument will override the
                                    // default ZINC logo for one of the designer's
                                    // choice.
);
</script>
```

By SMILES

- http://zinc.docking.org/results/structure?

structure.similarity=1.0&structure.smiles=<URL-encoded-smiles>

For example, to link to benzene, c1ccccc1, use the URL

- http://zinc.docking.org/results/structure?structure.similarity=1.0&structure.smiles=c1ccccc1

Some molecules require URL encoding if they use =, (,) @, [,], +, #, \, *, ., ,

The translation is as follows: @ = %40, \ = %5c, [= %5b,] = %5d, # = %23, (= %28,) = %29, * = %2a, + = %2b, , = %2c

These are all standard hexadecimal encoding of characters that have special meaning in a URL and must be encoded to be transmitted to ZINC.

By InChI

We currently do not support InChI, but we are working on it.

By CAS

- http://zinc.docking.org/cas/<casnumber>

For example, benzene, with CAS number 71-43-2, can be looked up as follows:

- http://zinc.docking.org/cas/71-43-2

To get benzene in SMILES format, use http://zinc.docking.org/cas/71-43-2.smi

By Vendor / Vendor code

By Name

- http://zinc.docking.org/synonym/<name>

For example, to find Delta-9-THC, use: http://zinc.docking.org/synonym/delta-9-thc

To get this molecule in SDF format, use: http://zinc.docking.org/synonym/delta-9-thc.sdf

By Ring

In progress, coming soon. Format will be

http://zinc.docking.org/find/ring:indole

- in progress *

By Target

```
http://zinc.docking.org/results/combination?filter.purchasability=purchasable&annotatic
```

By SwissProt

http://zinc.docking.org/results/combination?
filter.purchasability=purchasable&annotation.name=HCN2_MOUSE

By UniProt

http://zinc.docking.org/results/combination?
filter.purchasability=purchasable&annotation.name=HCN2_MOUSE

By Target Name

ZINC processing pipeline

From DISI

(Redirected from ZPP)

Each molecule in ZINC is processed via our ZINC processing pipeline. This process is embodied in a set of scripts that we continue to refine as we discover problems.

Frankly, we hope people will simply use ZINC rather than trying to reproduce it. Still, in the interests of clarity, transparency, truth, justice and the Canadian Way (TM), here is our current protocol.

- 1. If you have 2D SDF, convert it to isomeric SMILES.
- 2. sed -e 's/N=S=N/nsn/g' 2.ism > 2-out.ism
- 3. Use molinspiration mitools/mib to eliminate broken SMILES:

```
java -jar /raid1/soft/mitools/mib.jar -singlepart -onlyOrganic -normalizeCharges -f $1
```

- 4. Use OEChem to remove molecules with problematic functional groups:

```
filter.py rules.txt 4.ism 4-out.ism  > filterlog.txt
```

see http://blaster.docking.org/filtering/rules_default.txt for current rules.

- 5. select only 4 of stereochemical expansions from previous step. We just take the first 4, but you can imagine better ways of making the selection.
- 6. get rid of bogus stereochemistry at nitrogen:

```
sed -e 's/\[N@\]/N/g' -e 's/\[N@@\]/N/g' -e 's/\[N@H+\]/\[NH+\]/g' -e 's/\[N@@H+\]/\[NH
```

- 7. If the molecule is already in ZINC, eliminate it from the list.
- 8. Generate trial 3D structure with corina.

```
corina -d neu,wh,rc,mc=1,canon -i t=smiles -o t=sdf < 1a.ism > 2.sdf
```

- 9. generate reference pH state using Schrodinger's Epik.

```
epik -ph 7.05 -ms 1 -imae A.mae -omae B.mae -WAIT
```

- 10. generate mid, hi and lo pH subsets

```
mid: setenv EPIK "-ph 7.0 -pht 1 -tp 0.20"
hi: setenv EPIK "-ph 8.5 -pht 0.75 -tp 0.20"
lo:  setenv EPIK "-ph 5.5 -pht 0.75 -tp 0.20"
epik $EPIK -imae A.mae -omae B.mae -WAIT
```

- 11. For each subset (ref, mid, hi, lo) use Corina to generate 3D model of the relevant protonated state.

```
corina -d rc,flapn,de=5,mc=2 -i t=mol2 -o t=mol2
```

That's really it. There is more to do with loading ZINC, but to generate the models, that is what we think you need to know. Good luck!

-- John Irwin. March 2009.