

- Chinzo Dandar
- Khanh Tang
- Julia Khurelbataar
- Ben Tingle
- John Gutierrez

Roth Lab @ UNC

Bryan Roth
Sheng Wang
Tao Che

NextMove Software

Roger Sayle
John Mayfield

- Jiankun Lyu
- Stefan Gahbauer
- Brian Bender
- Trent Balias

Thanks!

OpenEye Scientific
Molinspiration
Molecular Networks
ChemAxon
Schrodinger

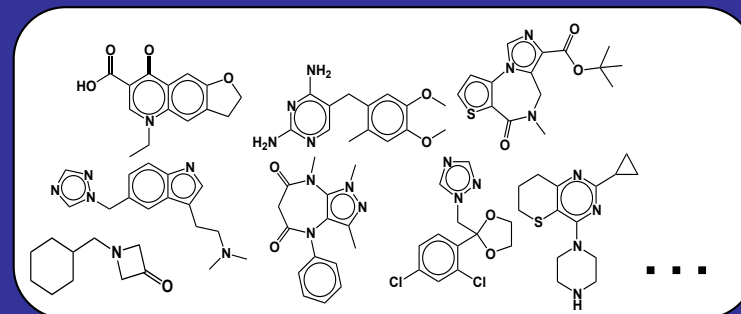
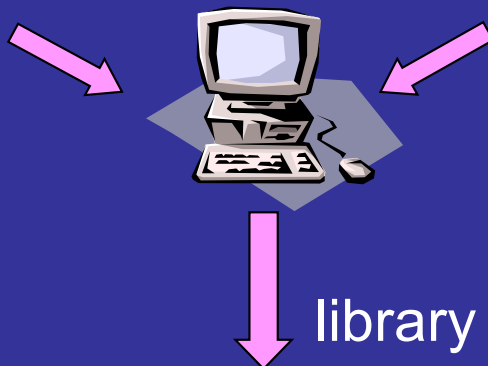
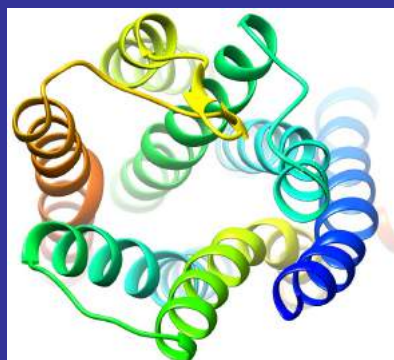
- Isha Singh
- Anat Levit
- Brian Shoichet
- Ying Yang
- Chase Webb
- Shuo Gu
- Shiming Peng

Enamine:
Yurii Moroz
A. Tolmachev

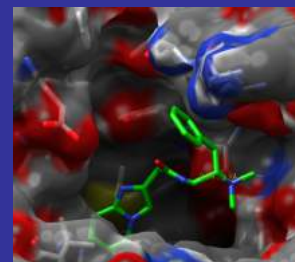
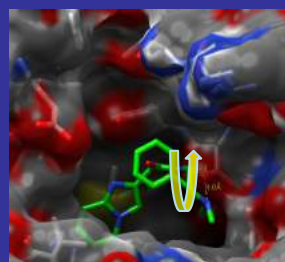
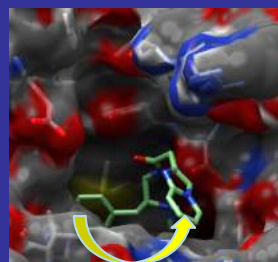
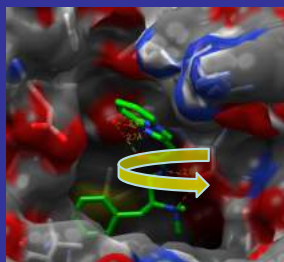
NIGMS
GM71896
GM133836

DARPA

docking large libraries for new chemotypes



library of *available* molecules



...

each in $\sim 10^6$ orientations & conformations



Score for fit

Test high-ranking molecules

Outline

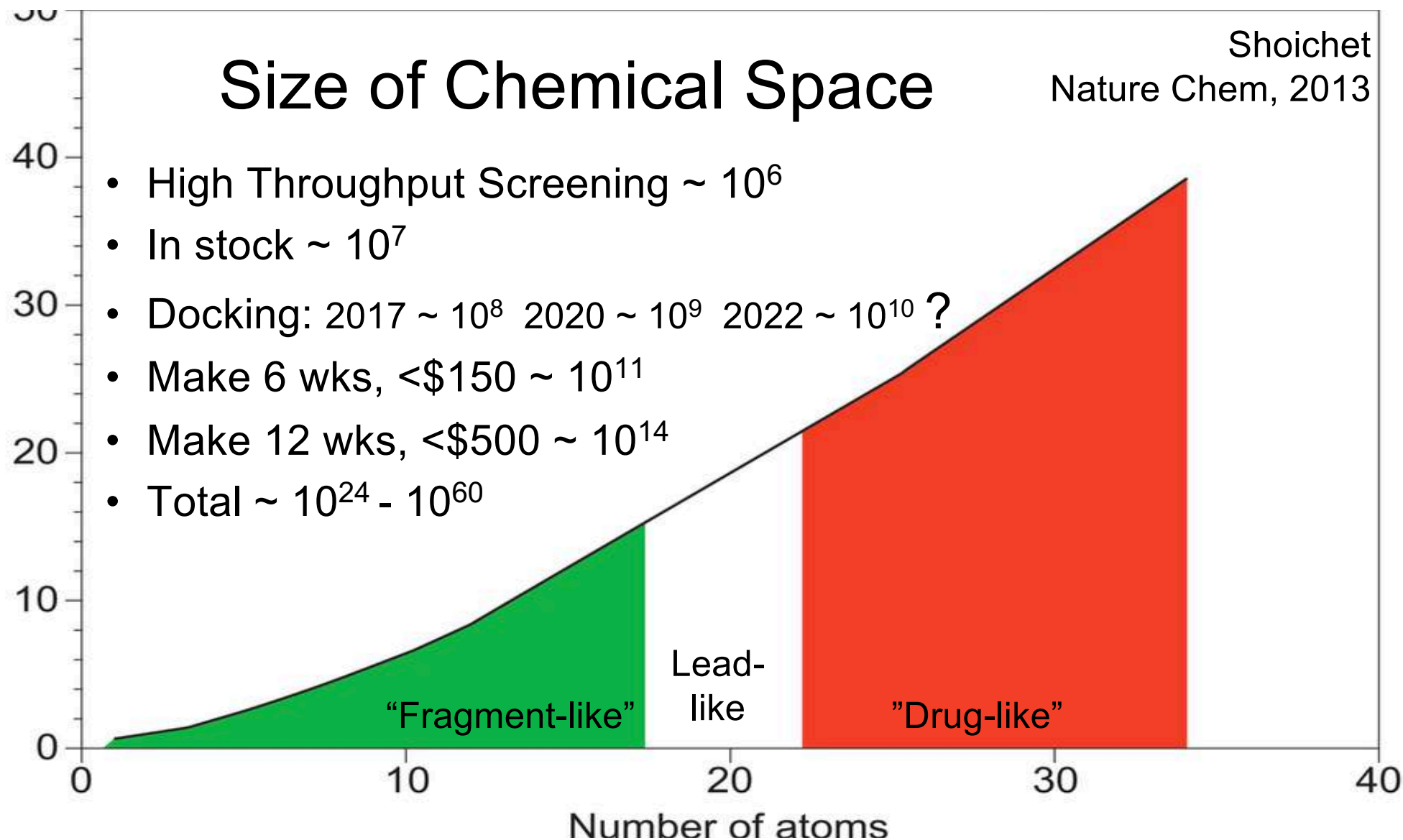
- Chemical space is big
 - ...but it is where we find new drugs
 - and can now be accessed quickly at low cost
- Docking screens in lead-like space with docking
 - How does it work
 - What can I expect?
- Free public resources you can use
 - Smallworld, Arthor, DataWarrior
 - ZINC, SEA, and much more

Size of Chemical Space

Shoichet
Nature Chem, 2013

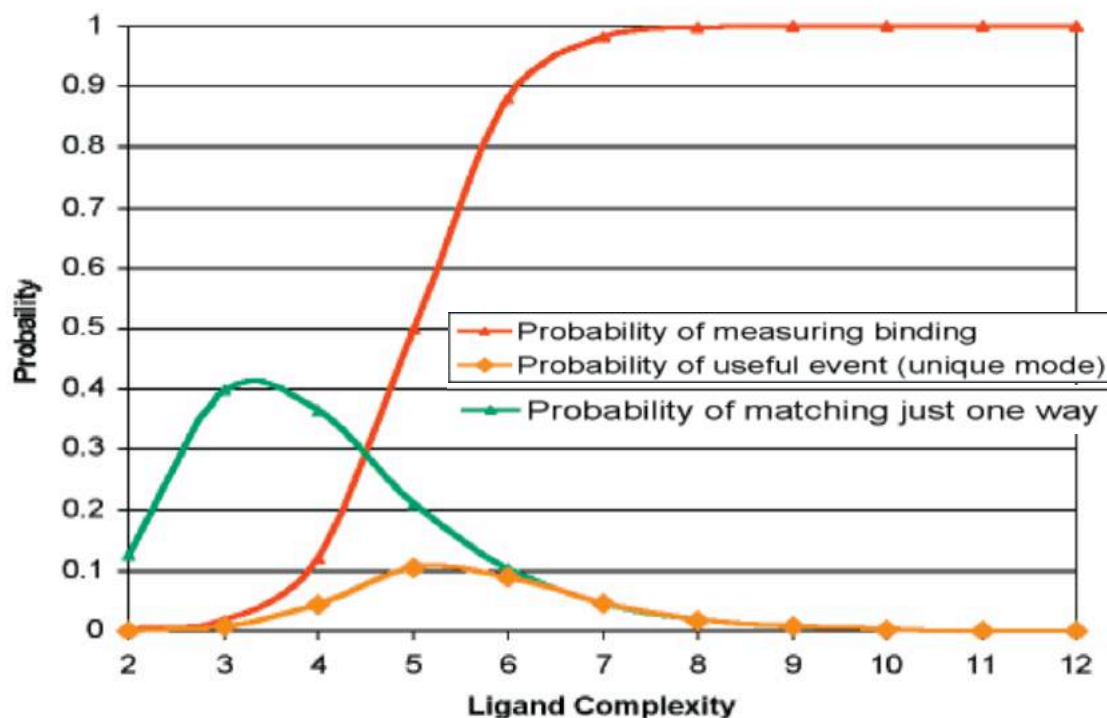
- High Throughput Screening $\sim 10^6$
- In stock $\sim 10^7$
- Docking: 2017 $\sim 10^8$ 2020 $\sim 10^9$ 2022 $\sim 10^{10}$?
- Make 6 wks, $<\$150 \sim 10^{11}$
- Make 12 wks, $<\$500 \sim 10^{14}$
- Total $\sim 10^{24} - 10^{60}$

Log (number of molecules)



Why fragments?

The Hann complexity argument



Feature Position	1	2	3	4	5	6	7	8	9
Receptor features	-	-	+	-	+	-	-	+	-
Ligand mode 1	+	+	-						
Ligand mode 2						+	+	-	
(reverse mode 3)						-	+	+	
(end wrap mode 4)	+								-
									+

Hann, Leach, Harper JCICS, 2001

Molecules you can buy

24M
(55M)
((99M))

625M
(676M)
((5B))

628M
(645M)
((100B))

LogP (up to)	Molecular Weight											LogP
	200	250	300	325	350	375	400	425	450	500	>500	
-1	35K	280K	1.3M	1.9M	3.7M	1M	304K	68K	44K	25K	5.4K	8.7M
0	174K	1.5M	6.3M	8.8M	17M	4.9M	2M	599K	403K	225K	4K	42M
1	468K	4.6M	20M	27M	53M	17M	9.2M	3.4M	2.4M	1.4M	8.5K	138M
2	624K	7.7M	37M	51M	102M	38M	26M	12M	8.8M	5.3M	23K	288M
2.5	240K	3.8M	21M	30M	61M	27M	21M	12M	8.8M	5.5M	24K	191M
3	140K	2.9M	19M	28M	56M	30M	25M	16M	12M	7.9M	39K	196M
3.5	63K	1.8M	14M	22M	45M	29M	26M	18M	15M	10M	64K	182M
4	19K	830K	8.3M	12M	18M	21M	24M	19M	17M	12M	95K	132M
4.5	2.5K	234K	4M	6.8M	12M	16M	19M	17M	16M	12M	132K	102M
5	93	35K	1.3M	2.9M	6.1M	9.4M	13M	13M	13M	10M	160K	69M
>5	28	891	46K	179K	557K	1.2M	2.1M	2.7M	3M	2.5M	818K	13M
Totals, by Weight	1.8M	24M	132M	190M	375M	195M	166M	114M	97M	67M	1.4M	1363M Substances 1.7K Tranches

Cheap
(all)
((ucsf))

		200	250	300	325	350	375	400	425	450	500	>500	LogP
LogP (up to)	-1	33K	77K	1.1M	1.4M	1.8M	372K	275K	65K	40K	19K	2.1K	5.2M
	0	134K	745K	5.2M	7.7M	10M	2M	529K	296K	296K	156K	2.4K	27M
	1	414K	3M	16M	10M	19M	5.6M	894K	298K	240K	301K	6.2K	57M
	2	586K	7.1M	20M	37M	15M	24M	3.2M	341K	60K	311K	19K	107M
	2.5	228K	3.5M	15M	16M	16M	11M	2.4M	393K	73K	65K	21K	65M
	3	131K	2.7M	14M	9.6M	20M	28M	3M	439K	109K	317K	37K	79M
	3.5	55K	1.2M	13M	20M	11M	13M	2.5M	183K	147K	458K	61K	62M
	4	14K	390K	6.1M	7.2M	9.3M	3.2M	19M	5.3M	177K	466K	91K	51M
	4.5	1.8K	50K	542K	6M	5.1M	4.7M	1.5M	4.4M	175K	519K	100K	23M
5	93	3.8K	93K	297K	67K	136K	111K	136K	145K	513K	156K	1.7M	
>5	27	767	13K	49K	42K	107K	113K	167K	205K	440K	778K	1.9M	
Totals, by Weight		1.6M	19M	92M	115M	108M	93M	34M	12M	1.7M	3.6M	1.3M	481M Protomers 6.5K Tranches

East Outskirts of Kiev – looking E



BB – 4 C right – RT left.

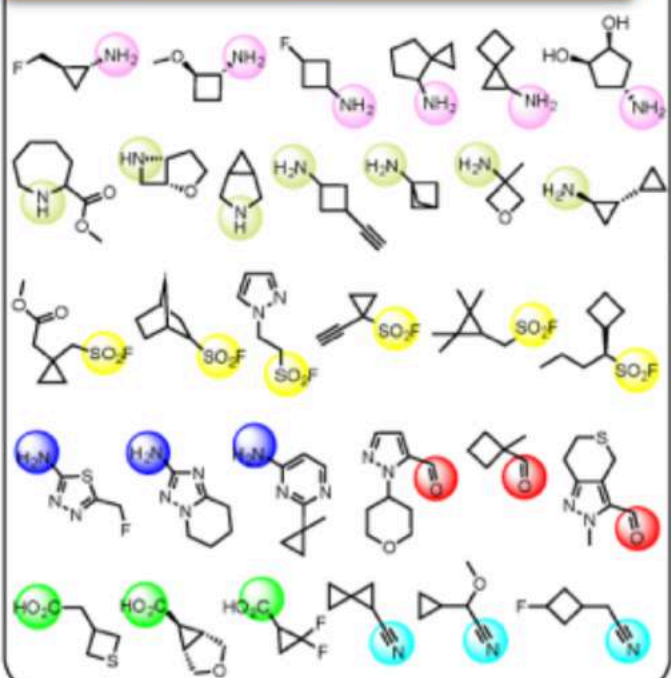
#BB>200,000



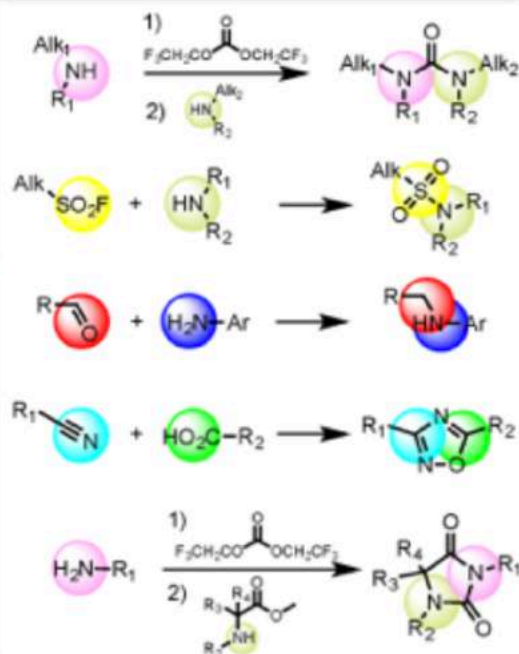
make-on-demand library: 109 2-component reactions 200,000 building blocks



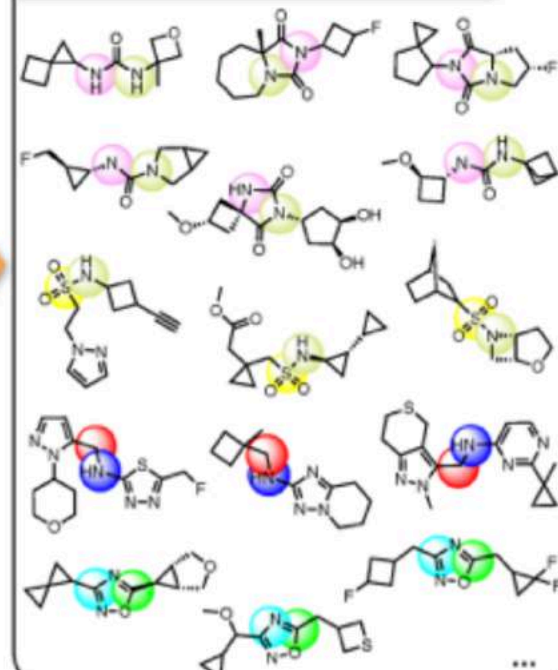
Example building blocks



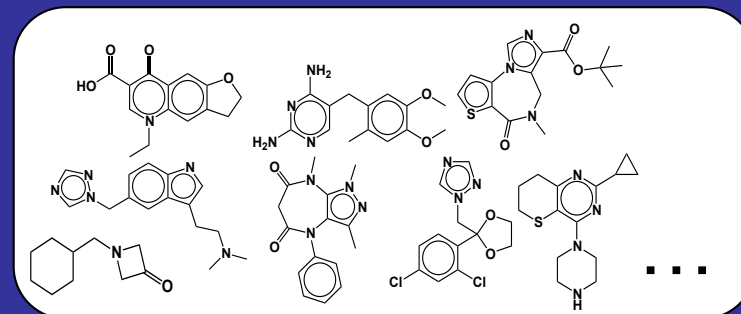
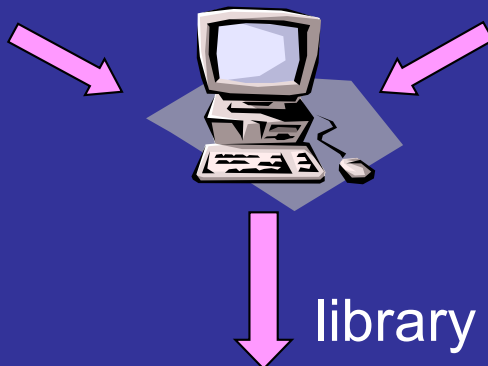
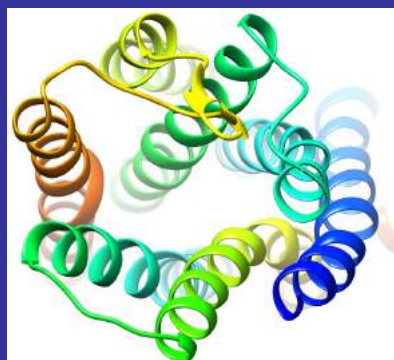
Example reactions



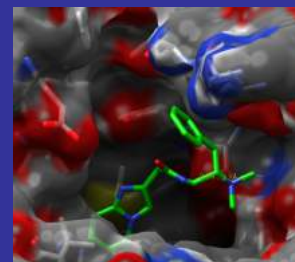
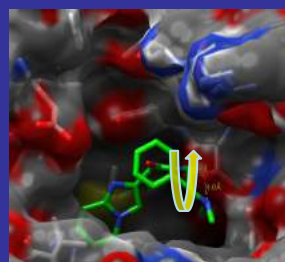
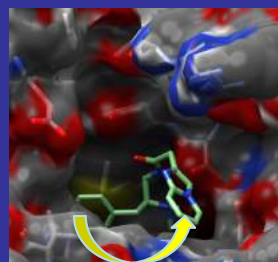
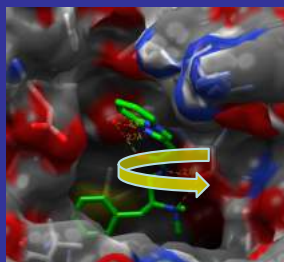
Example products



docking large libraries for new chemotypes



library of *available* molecules



...

each in $\sim 10^6$ orientations & conformations



Score for fit

Test high-ranking molecules

fast, grid-based DOCK3.7 scoring function (a miracle it ever works)

Mysinger, *JCIM* 2010
Fischer, *Nature Chem.* 2014
Balius, *PNAS*, 2017

$$\Delta G_{\text{interact}} - \Delta G_{\text{solv, L}} - \Delta G_{\text{solv, R}}$$

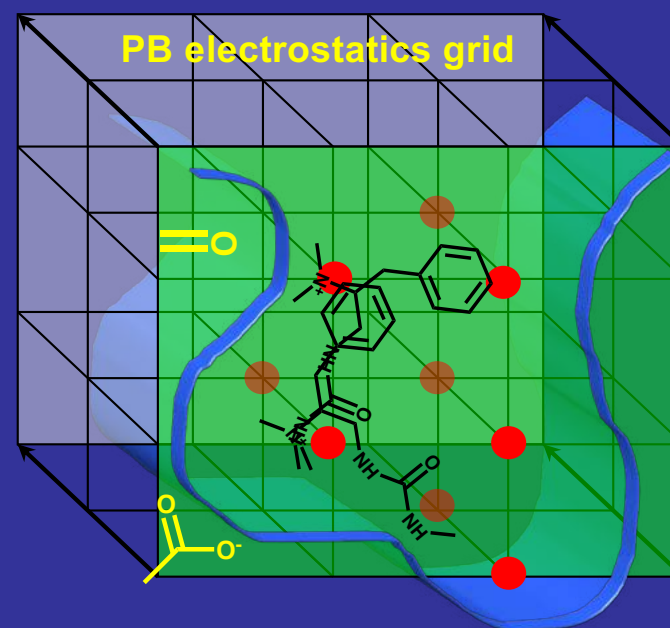
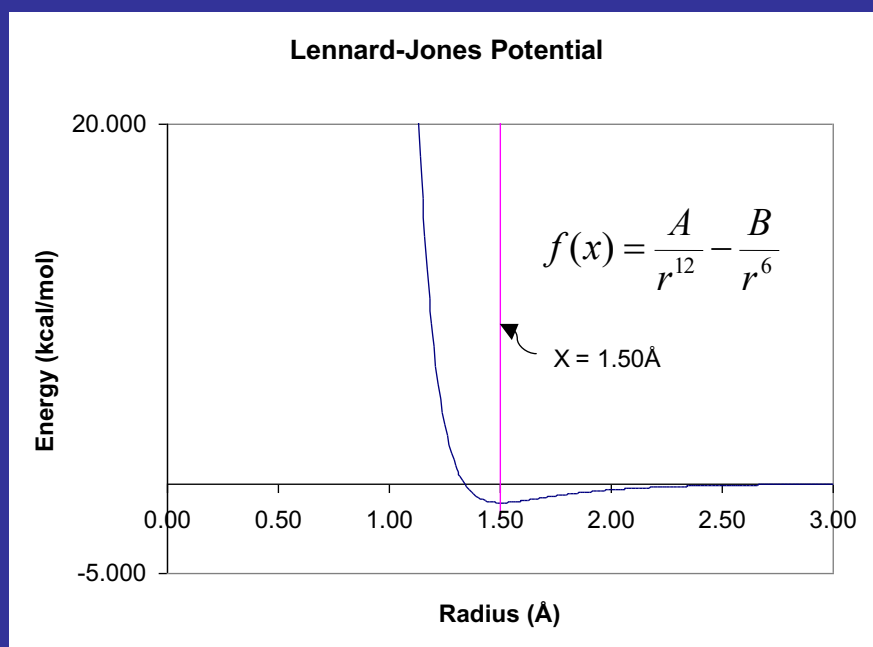
$$\sum (q_i * PB_i + v_i * P_{v,i})$$

$$GB_{\text{ligand}} + IST_{\text{receptor}}$$

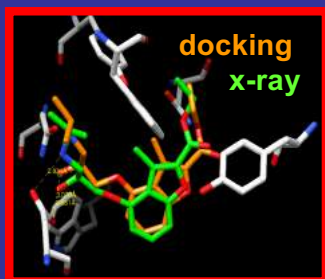
$$= \Delta G_{\text{bind}}$$

$$= \Delta G_{\text{inter}}$$

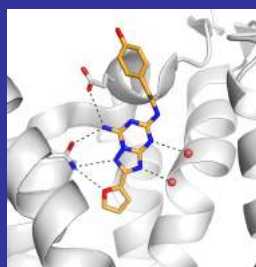
$$= \Delta G_{\text{solv}}$$



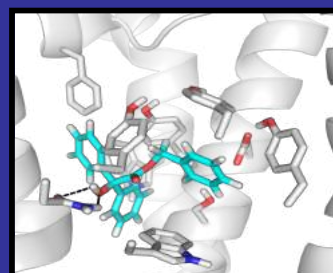
GPCR docking: 17 to 58% hit rates, nM activities, novel ligands, new biology, xray confirmation



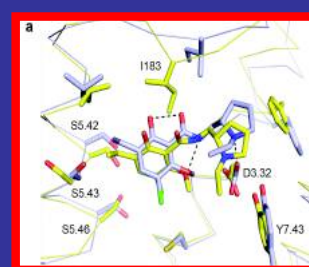
β 2AR: 25%
0.01 to 3 μ M
Kolb, *PNAS* 2009



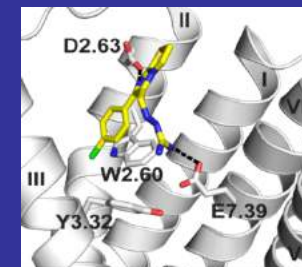
A2a: 35%
0.2 to 3 μ M
Carlsson, *JMC* 2010



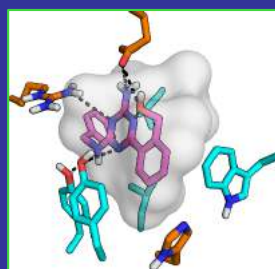
CHRM3: 58%
0.4 to 40 μ M
Kruze, *Mol Pharm* 2013



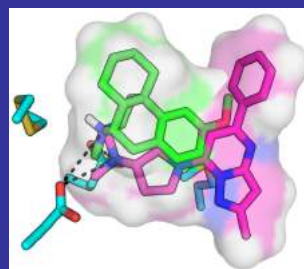
D3 23%
0.2 to 3 μ M
Carlsson, *NCB* 2011



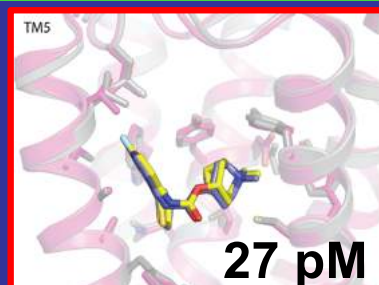
CXCR4: 17%
0.3 to 30 μ M
Mysinger, *PNAS* 2012



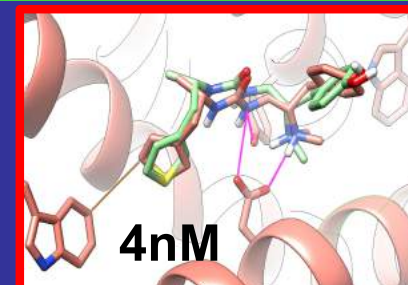
GPR68: 1 μ M PAM
Huang, *Nature* 2015



MRGPRX2: 6%
0.7 μ M
Lansu *NCB* 2017



CHRM3
Liu, *PNAS* 2018



MOR: 30% 2 to 14 μ M
Manglik *Nature* 2016
Kobilka, Skinniotis, unpub

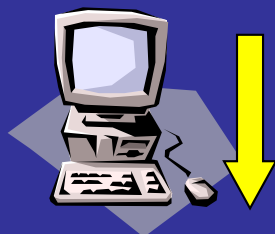
an explosion in readily-accessible molecules



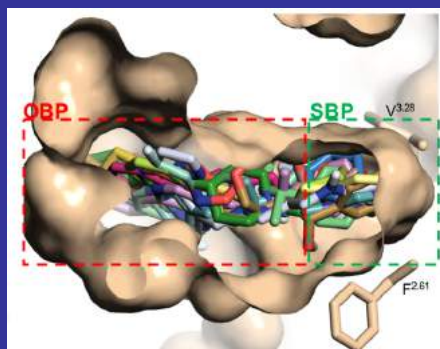
Yurii Moroz



3.5→350
million
compounds



225 trillion
complexes



docking libraries, 1991 to 2019
270,000,000

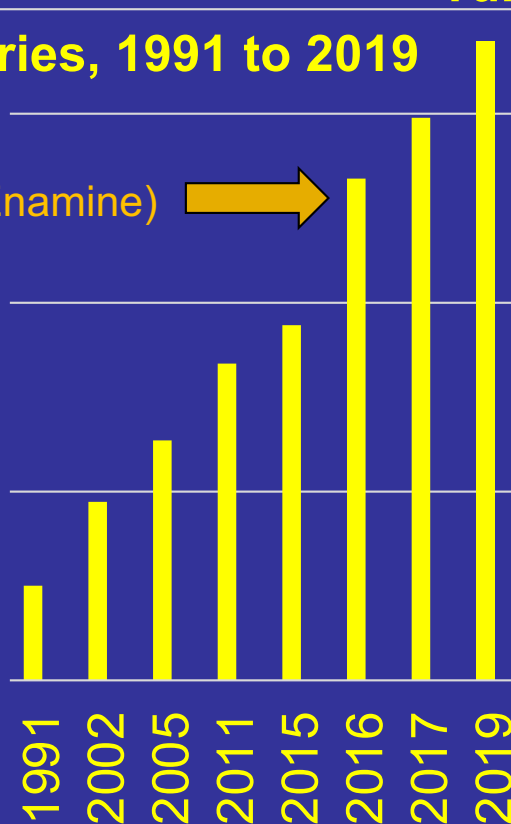
make-on-demand (Enamine)



9,000,000

300,000

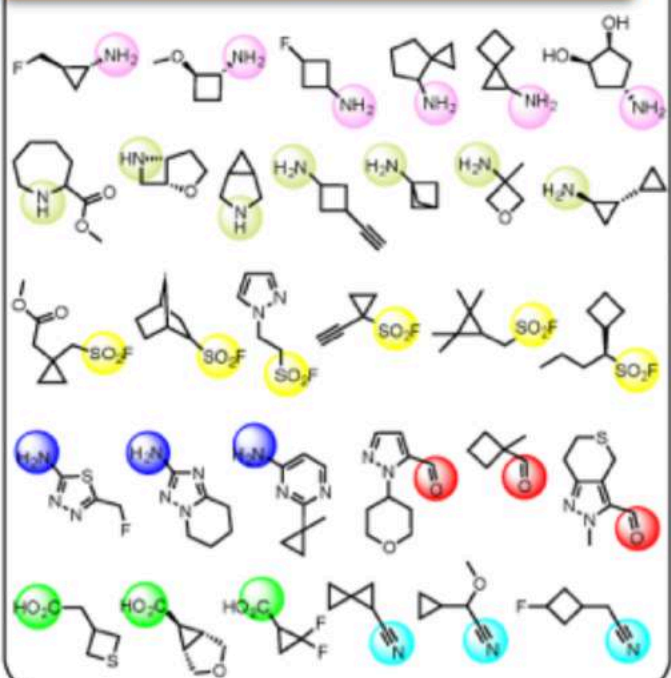
10,000



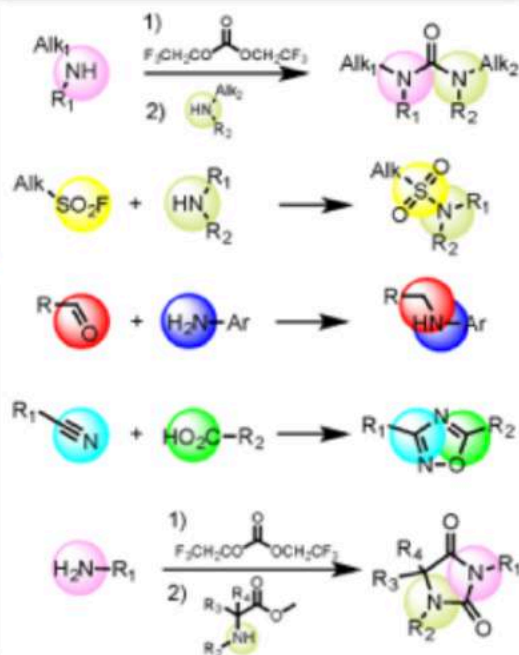
make-on-demand library: 109 2-component reactions > 200,000 building blocks



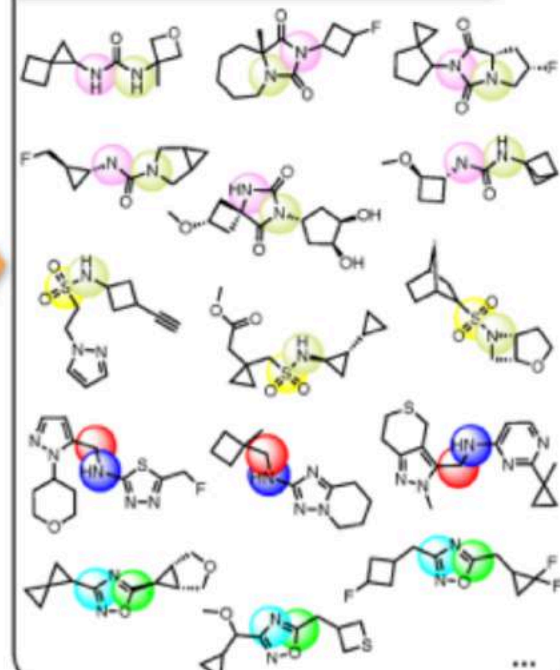
Example building blocks



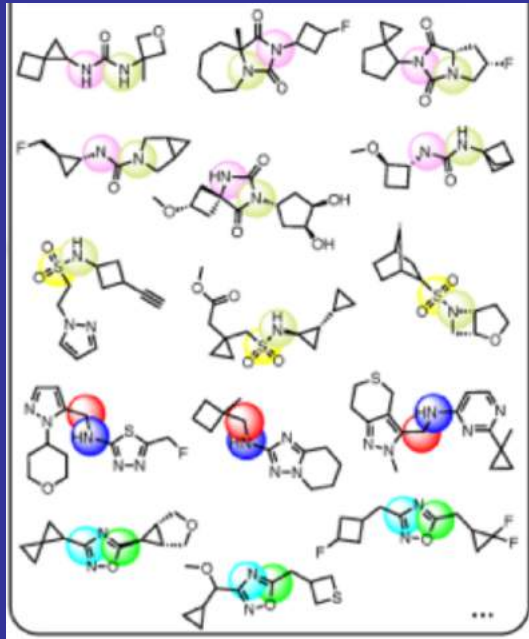
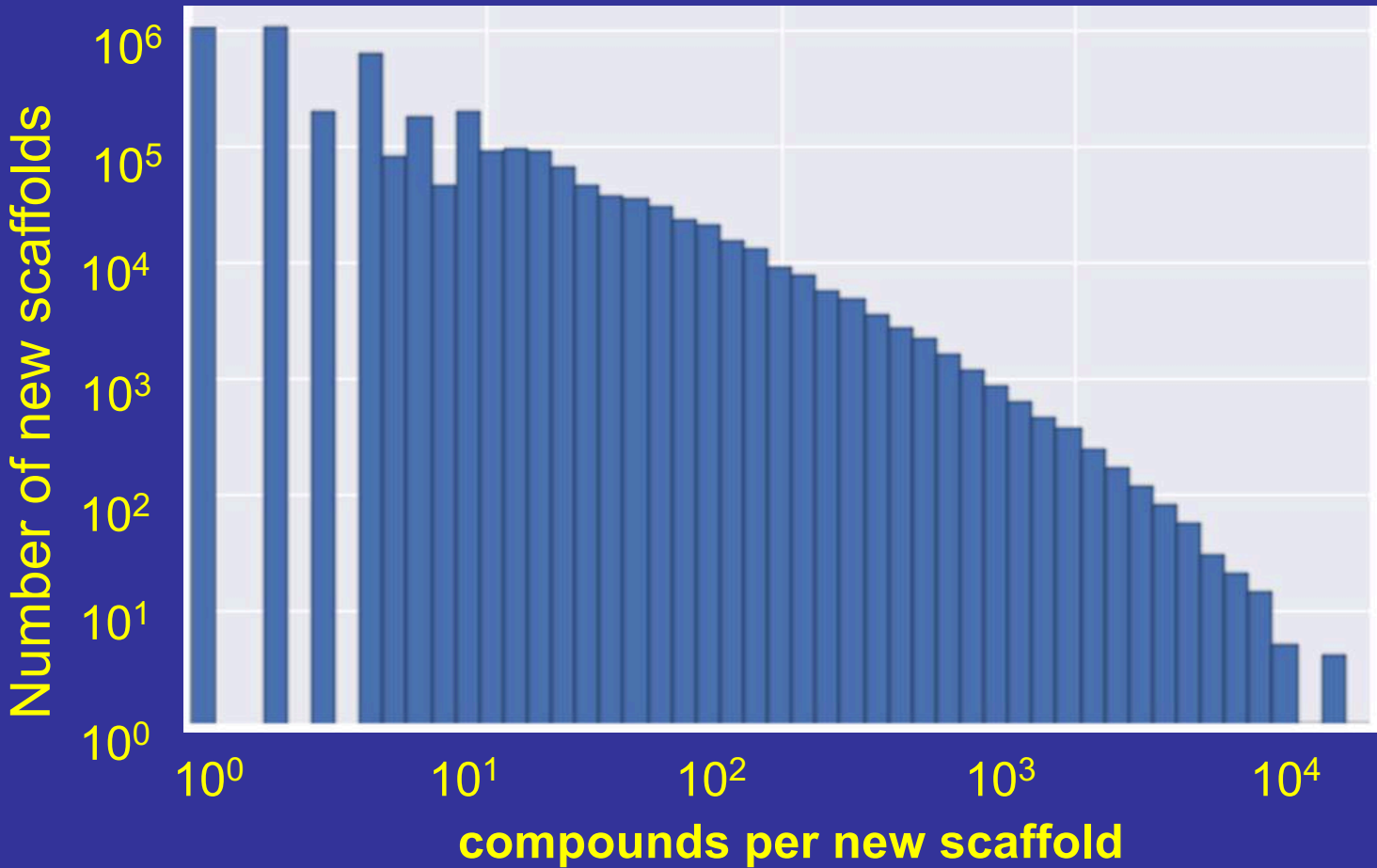
Example reactions



Example products



**library is diverse: 7 million new scaffolds
in 138 million compounds**



How most screening compounds get made

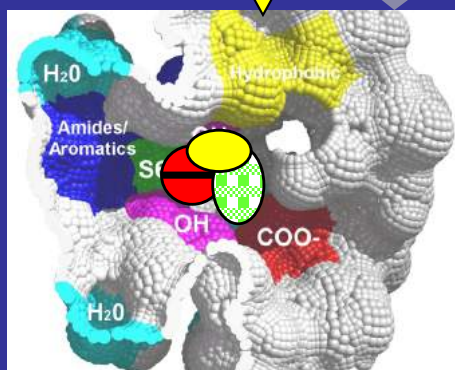




docking 99 million compounds vs β -lactamase predicts new chemotypes



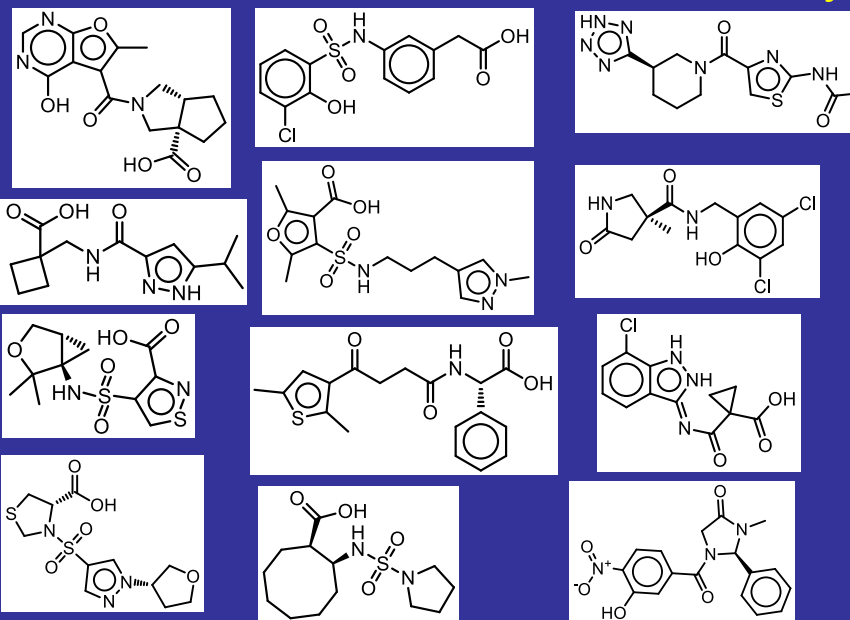
99 million
cmpds



28,310 core hours



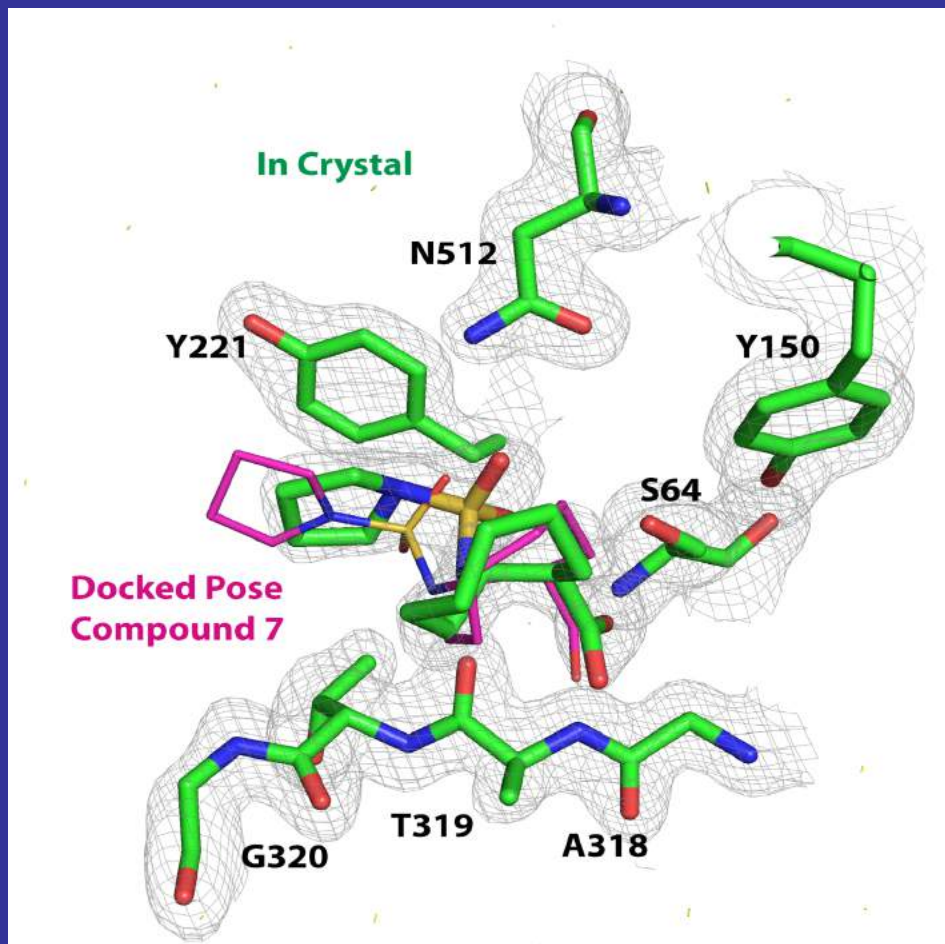
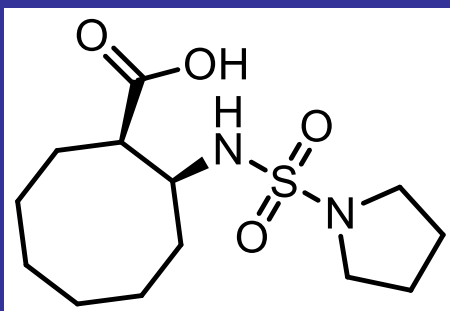
cannot resemble knowns nor 3.5 million library



44 WACs picked from top 3000 clusters

JK Lyu, Trent Balius, Isha Singh, *Nature* 2019

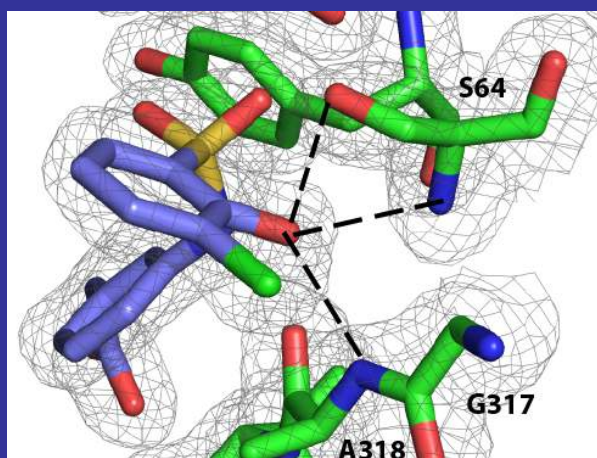
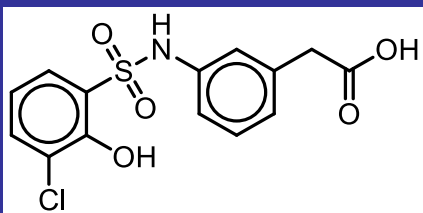
99 million vs β -lactamase: 11% hit rate,
x-ray structure confirms a docking prediction



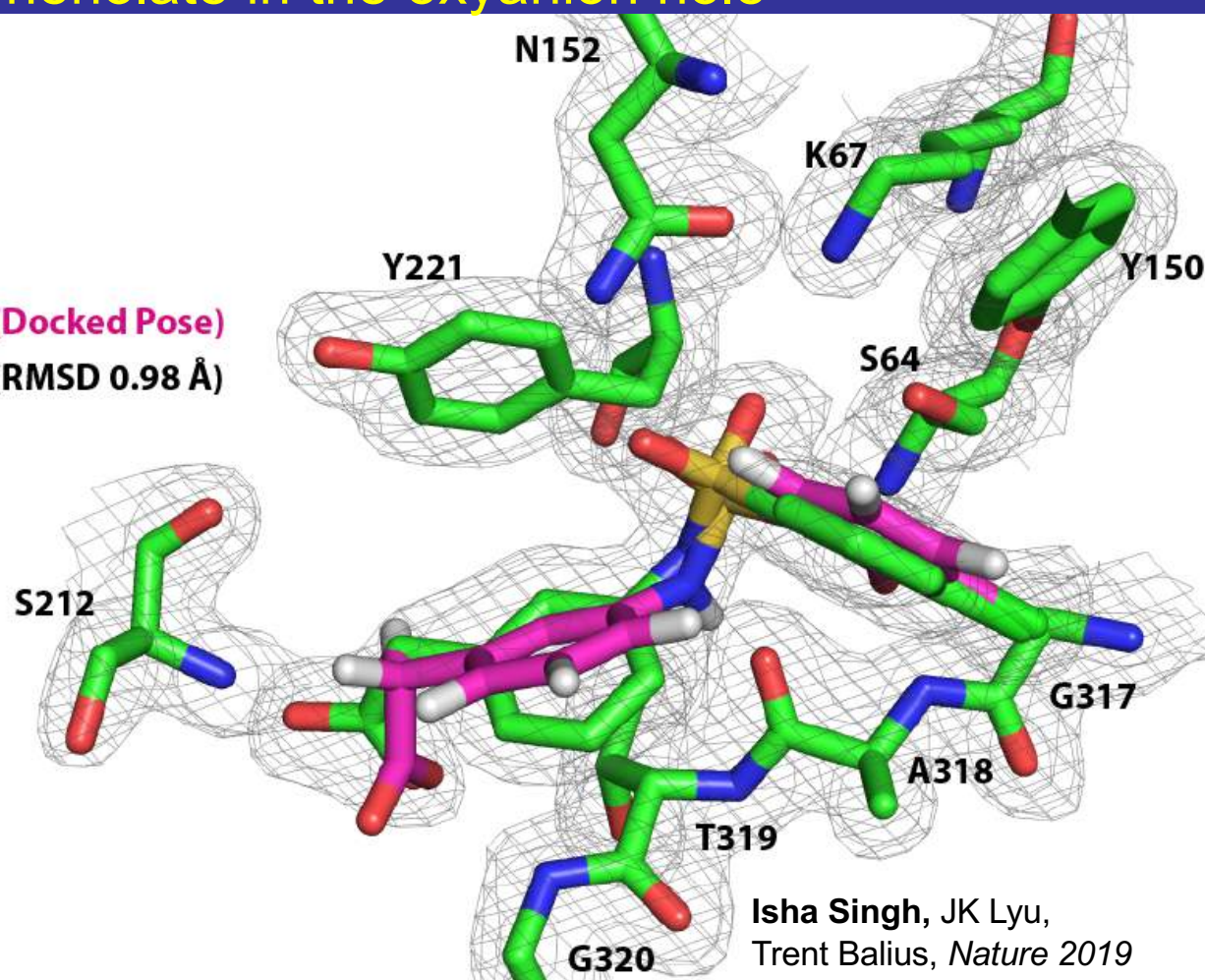
Isha Singh, JK Lyu,
Trent Balias, *Nature* 2019



99 million vs β -lactamase: 11% hit rate, unprecedented
1.3 μ M phenolate in the oxyanion hole



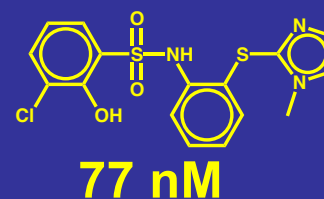
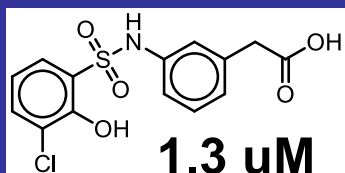
(Docked Pose)
(RMSD 0.98 Å)



Isha Singh, JK Lyu,
Trent Balias, *Nature* 2019

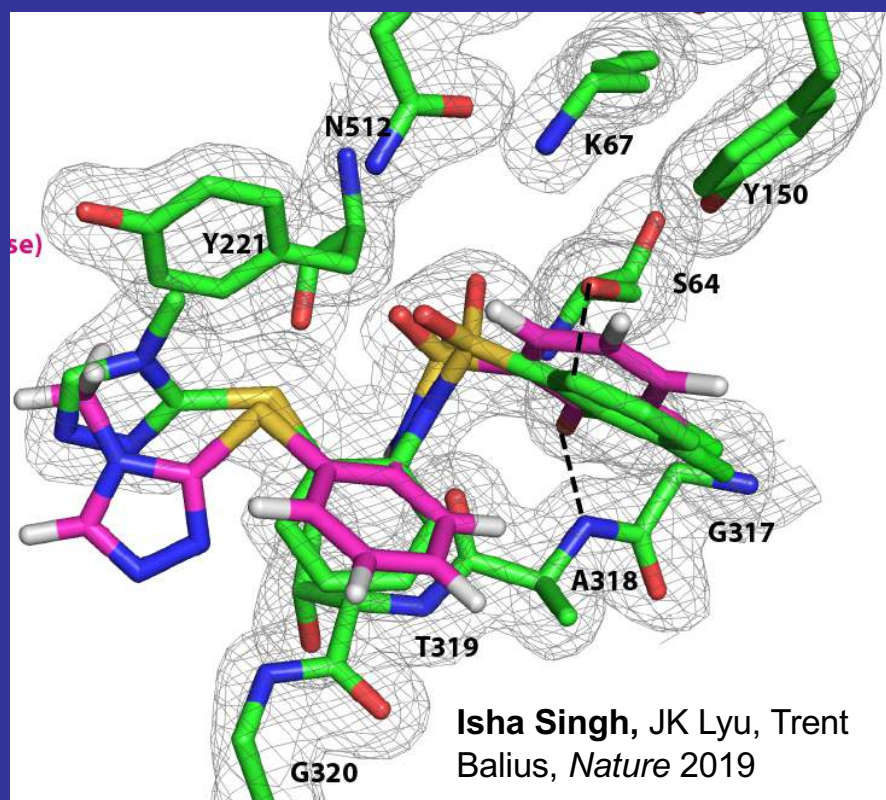
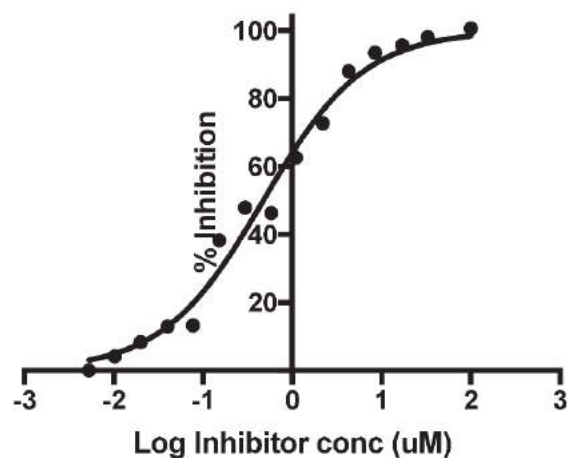


analog-by-catalog to 77 nM



**>400 analogs
docked, test 11**

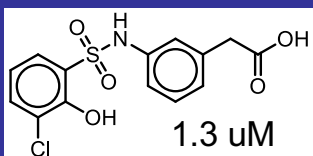
Compound 67 (C10 analog)



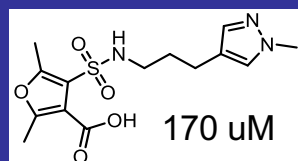
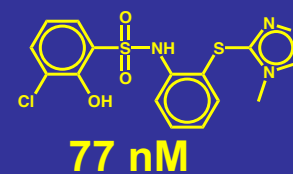
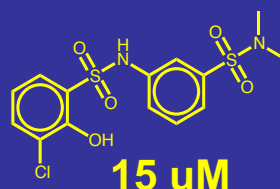
Isha Singh, JK Lyu, Trent
Balius, *Nature* 2019

**analog-by-catalog optimization:
>2000 possible analogs, which are best?**

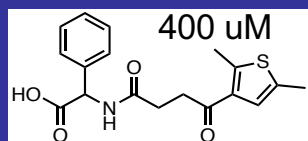
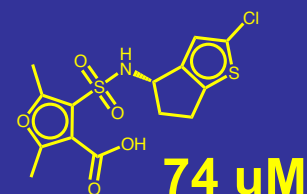
Isha Singh



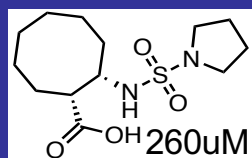
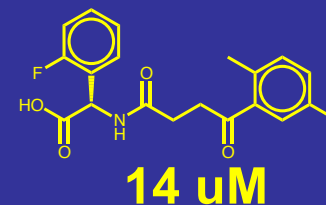
test 11



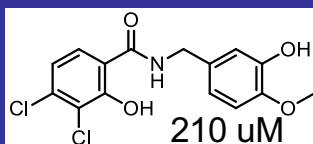
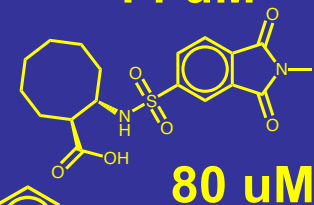
test 15



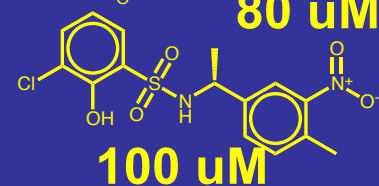
test 31



test 19



test 14

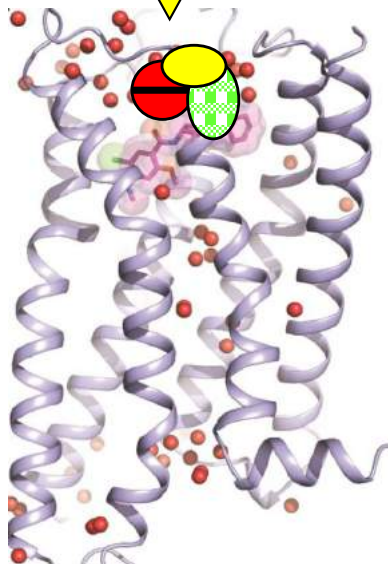
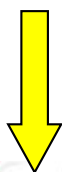


How many ligands *findable* in the library?

138 million vs. dopamine D4

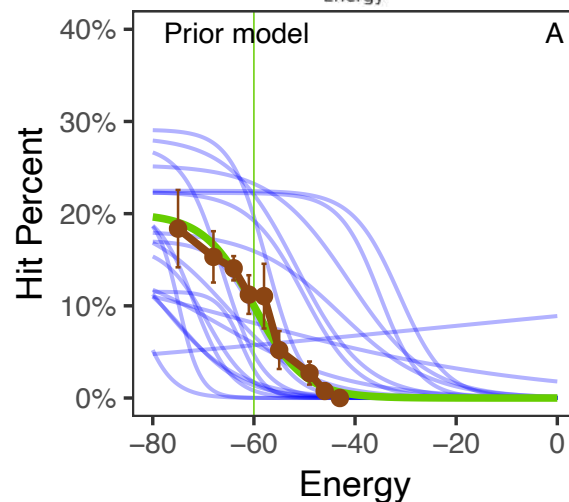
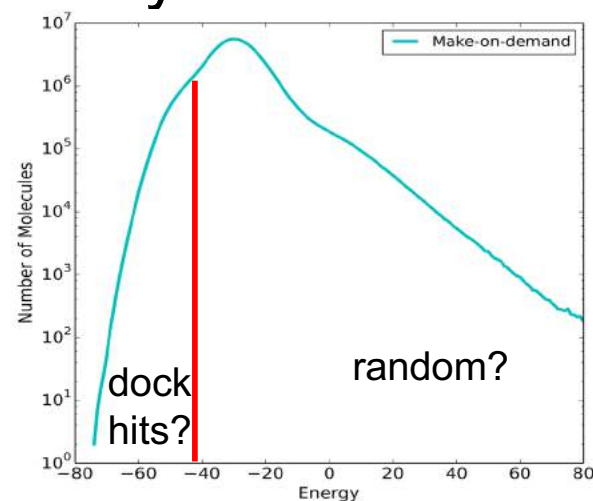


138 million molecules
 10^{14} complexes
1 mol/sec; 10^3 cores
1.8 cluster days



~~Test 30~~

Test 549



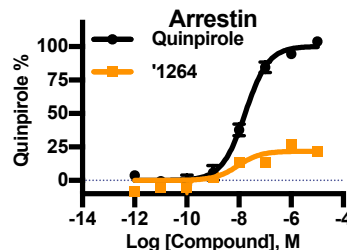
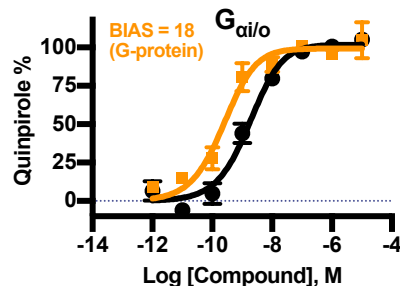
JK Liu, A Levit, T Balias, M. O'Meara, *Nature* 2019

from top ranked: novel, selective, potent D4 ligands

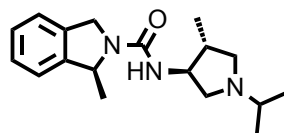
Sheng Wang
Bryan Roth

ZINC361131264, 18x bias

Rank: 1067

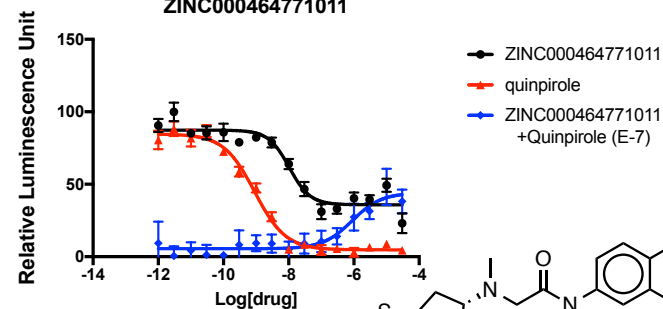


D4 = 0.18 nM
D2 > 10,000 nM
D3 > 10,000 nM

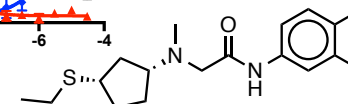


Rank: 936

ZINC000464771011

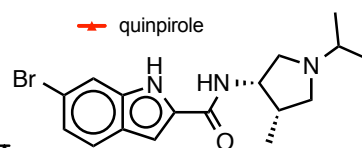
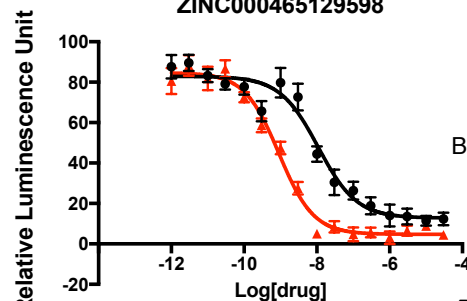


D4 = 10 nM
D2 > 10,000 nM
D3 > 10,000 nM



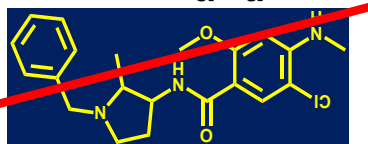
ZINC000465129598

Rank: 1565



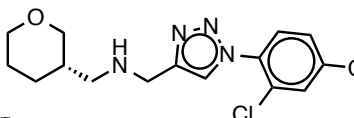
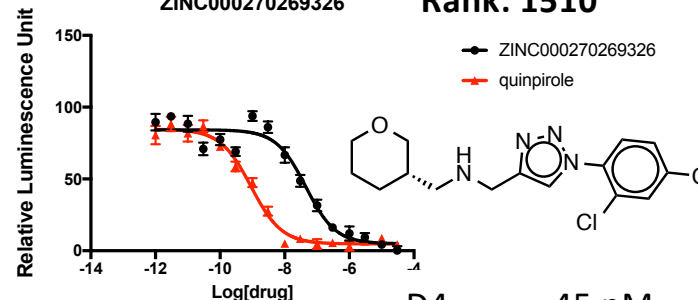
D4 = 11 nM
D2 > 10,000 nM
D3 > 10,000 nM

Different from
Nemonapride



ZINC000270269326

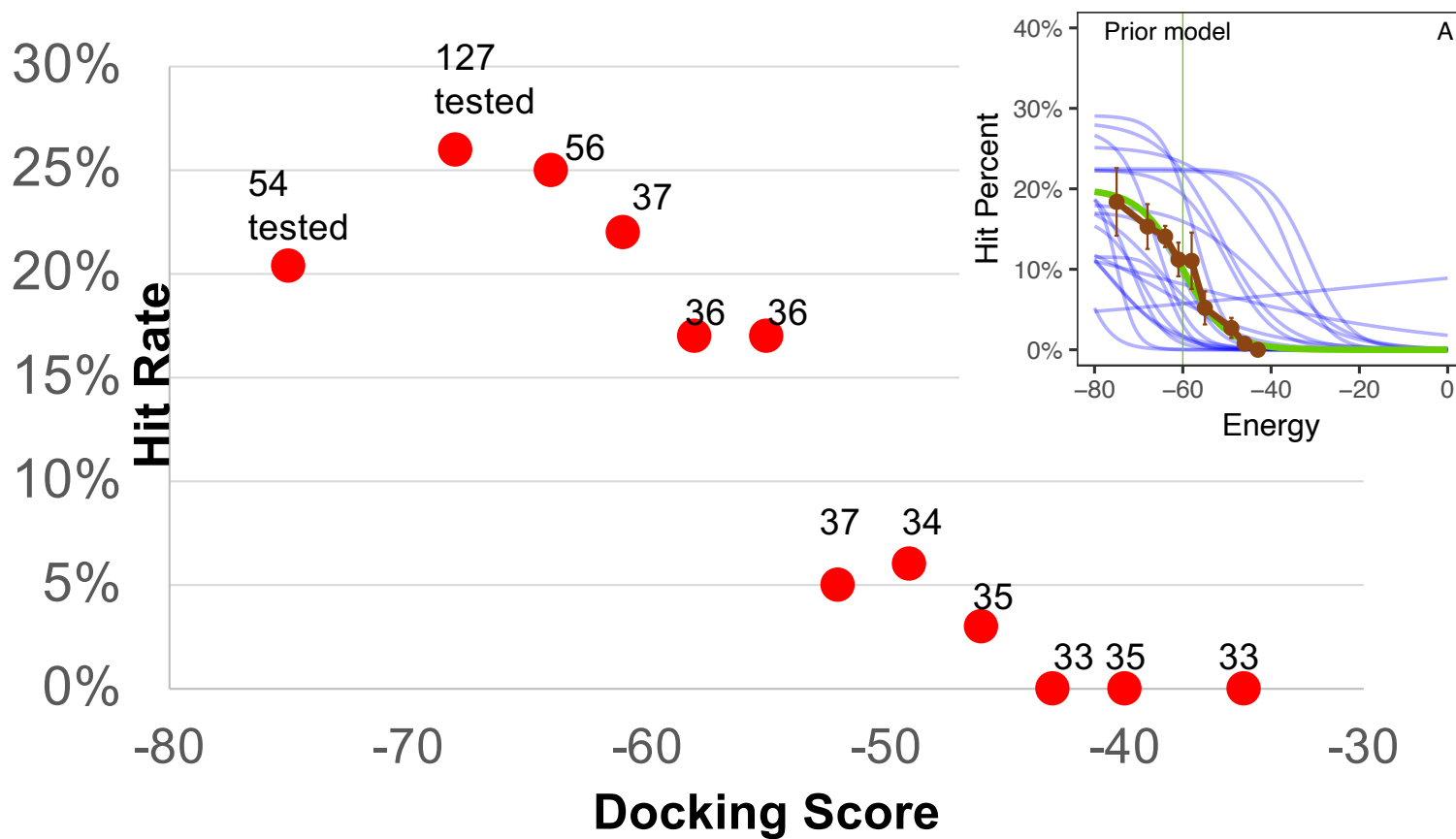
Rank: 1510



D4 = 45 nM
D2 > 10,000 nM
D3 > 10,000 nM

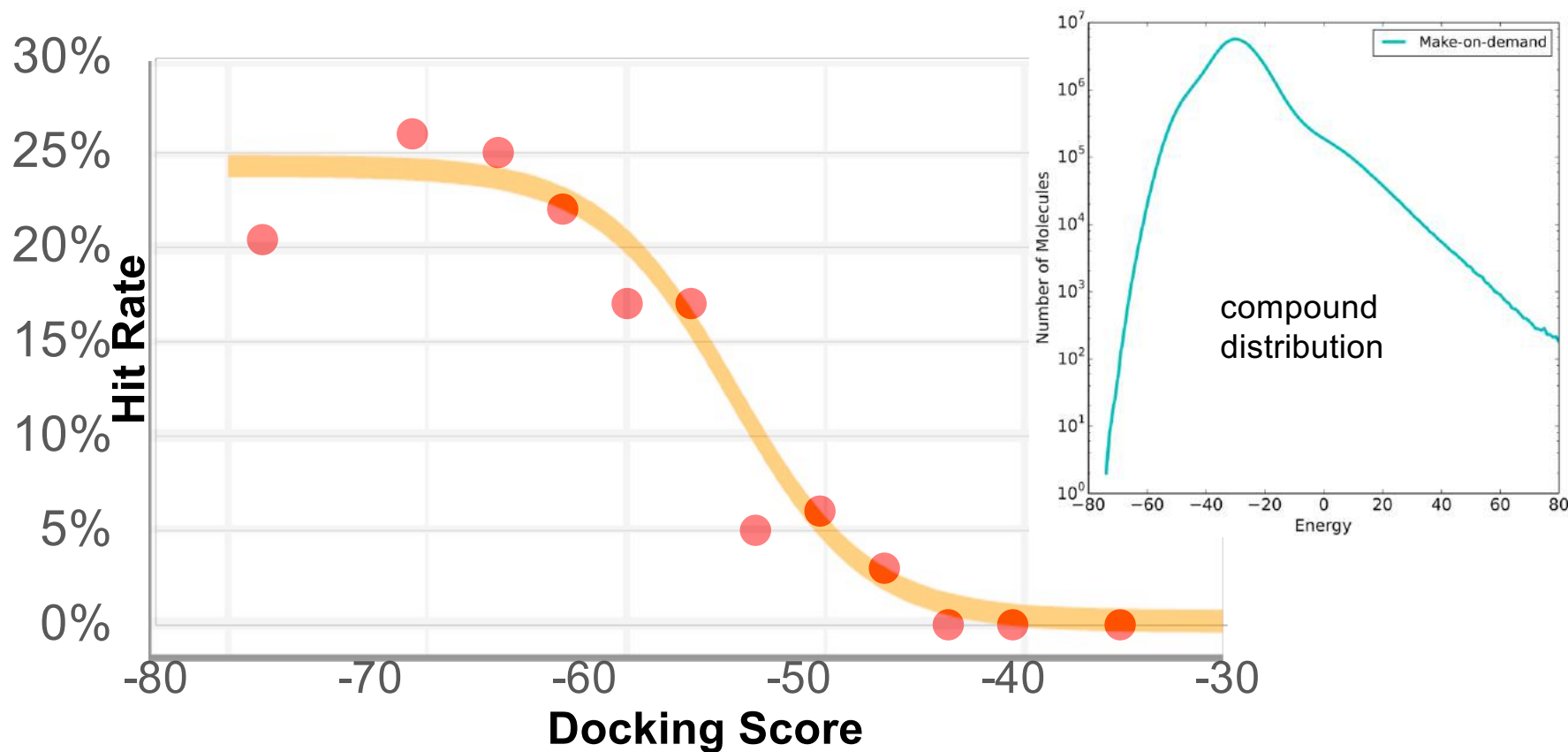
	ZINC000270269326
IC50	4.496e-008

hit rates correlate with docking rank



Sheng Wang, Bryan Roth, *Nature* 2019

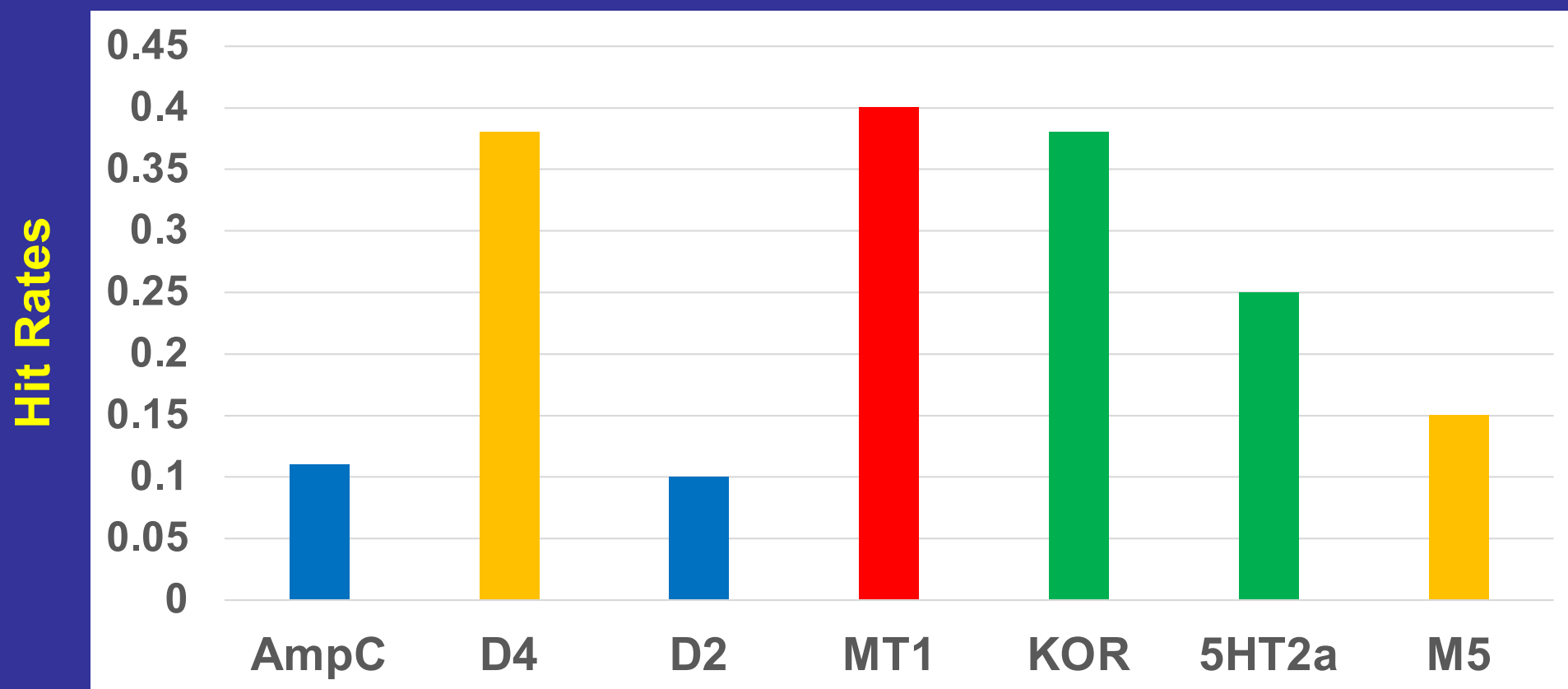
AUC predicts 479,000 ($\pm 40\%$) DRD4 actives (10 μM)
in 72,000 ($\pm 30\%$) scaffold families



Matt O'Meara, *Nature* 2019

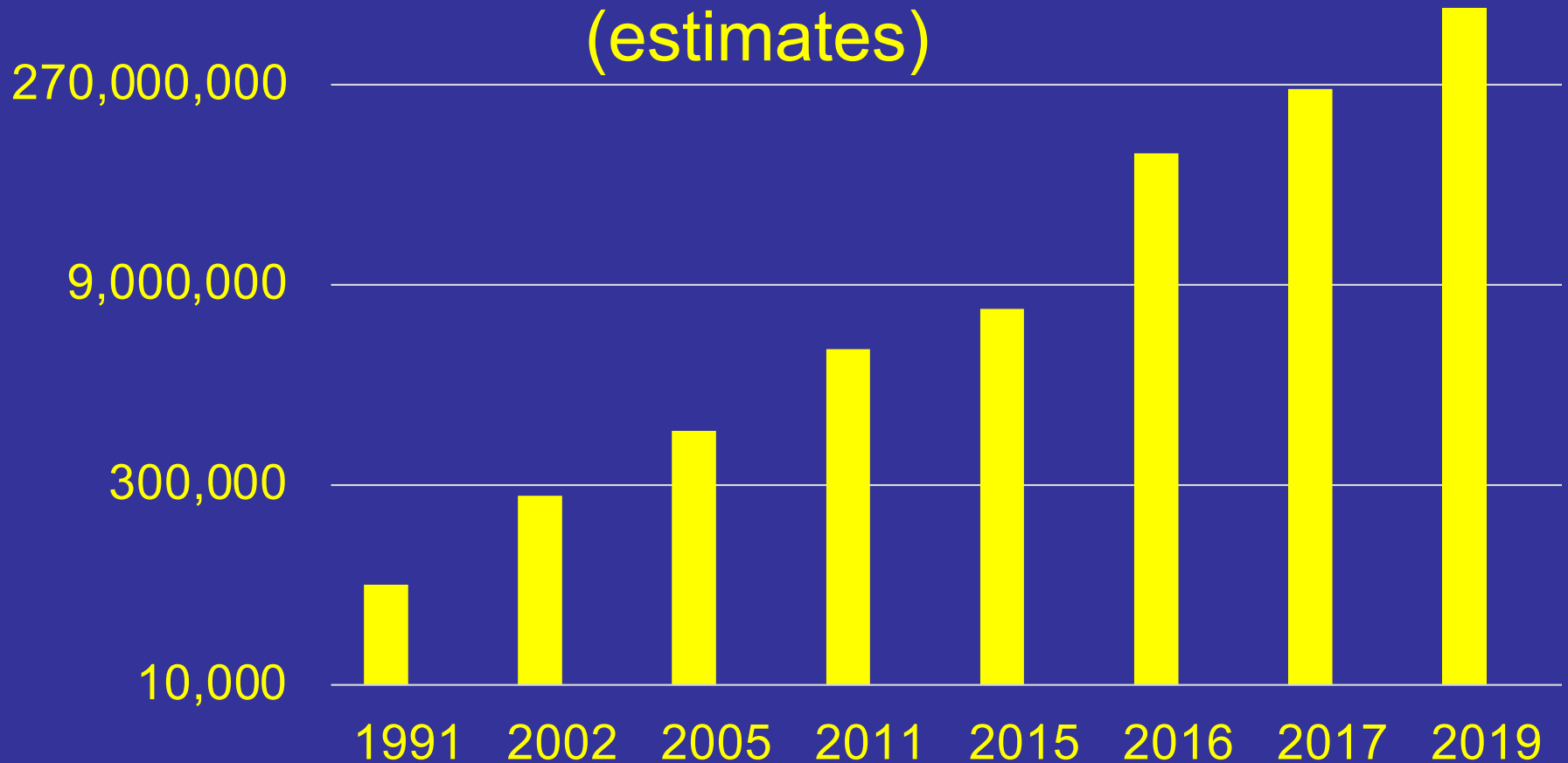
high hit rates in LSD campaigns vs over a dozen targets

■ 10pm to 1 nM ■ 0.1 to 10nM ■ 0.5 to 5uM ■ 0.1 to 1uM ■ 3 to 10 uM



Dockable libraries keep growing

End 2020: 1 billion, 2021: 4 billion, 2022 10 billion
(estimates)



Free Public Resources and how to use them

Smallworld

for

similarity

sw.docking.org

NextMove Software

Roger A. Sayle

sw.docking.org/search.html

SmallWorld Search Manage Datasets

Version 4.0.1

Query

Chemical structure: NCCc1ccc(O)c(O)c1

Identifier: NCCc1ccc(O)c(O)c1

DataSet: BB-All-2020Q2-26.7M

Search Type: SmallWorld ☒ Advanced

Advanced Options

Distance: 0 4

Anon Distance: 0 4

Terminal: 0 4 Up 0 4 Down

Ring: 0 4 Up 0 4 Down

Linker: 0 4 Up 0 4 Down

Mutation: 0 4 Major 0 4 Minor

Substitution: 0 4

Hybridisation: 0 4

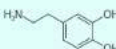
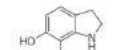
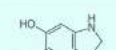
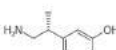
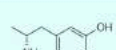
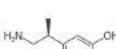
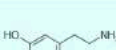
Scoring Methods

Atom Alignment ☒ Aligns and scores each hit relative to the query atom types, differences are categorised as MAJ, MIN, HYB, SUB

SMARTS Alignment ☐ Treat input as SMARTS and align and score each hit relative to the query atom expressions in the input (Important: Turn off Atom Alignment!)

ECFP4 ☒ Extended Connectivity Circular Fingerprint

Results

Compound	Distance	ECFP4	Daylight	Anon Distance	Unlabelled MCES	TDN	TUP	RDN	RUP	LDN	LUP
 ZINC000000033882 SWIDX: B11R1.248 MW: 153.18 MF: C ₉ H ₁₁ NO ₂	0	1.00	1.00	0	11	0	0	0	0	0	0
 ZINC000116886618 SWIDX: B12R2.1042 MW: 151.16 MF: C ₉ H ₉ NO ₂	1	0.30	0.51	1	11	0	0	0	1	0	0
 ZINC000005161652 SWIDX: B12R2.203 MW: 151.16 MF: C ₉ H ₉ NO ₂	1	0.29	0.52	1	11	0	0	0	1	0	0
 ZINC000029561199 SWIDX: B12R1.131 MW: 167.21 MF: C ₉ H ₁₃ NO ₂	1	0.39	1.00	1	11	0	1	0	0	0	0
 ZINC000002038644 SWIDX: B12R1.23 MW: 167.21 MF: C ₉ H ₁₃ NO ₂	1	0.47	0.87	1	11	0	1	0	0	0	0
 ZINC000029561203 SWIDX: B12R1.131 MW: 167.21 MF: C ₉ H ₁₃ NO ₂	1	0.39	1.00	1	11	0	1	0	0	0	0
 ZINC000000406211 SWIDX: B12R1.227 MW: 137.18 MF: C ₈ H ₁₁ NO	1	0.59	0.90	1	10	1	0	0	0	0	0
 ZINC000037629258 SWIDX: B12R1.131											

Showing 1 to 8 of 9,650 entries

Arthor for substructure

arthor.docking.org

NextMove Software

Roger A. Sayle

Not Secure | arthor.docking.org

evennewer newer new Daily weekly students Monthly projects DOCK Utils ID idioms dbs

Arthor Search Databases API

NEW X R Z ↺ ↻ X I

C N O S F Cl Br I X

Enter SMILES, Name, Identifier...

Automatically search on draw or type

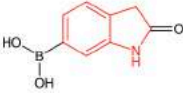
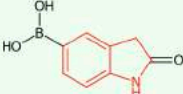
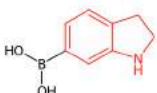
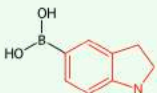
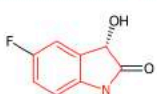
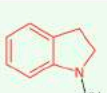
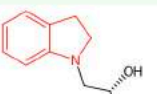
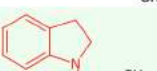
Search Type: Substructure SMARTS Formula

Ring systems Chains Properties

Databases:

- ZINC-All-19Q4-1.4B
- BB-All-For-Sale-19Q4-26M
- BB-Stock-19Q4-1.6M
- ZINC-All-For-Sale-19Q4-1.4B**
- HMDBMetabolites-20Q1-585
- In-Stock-19Q4-13.8M
- ZINC-Interesting-2019Q4-307K
- M-Enamine-20Q1-408M
- Mcule_ultimate_200407_c8bx14
- ZINC-On-Demand-19Q4-311M
- S-Enamine-20Q1-803M
- TCNMP-20Q1-37438
- Wait-OK-19Q4-1 1R

Matched **20,000** results in **1059** ms

1		ZINC000169905266 C ₈ H ₈ BNO ₃ 176.965
2		ZINC000169961300 C ₈ H ₈ BNO ₃ 176.965
3		ZINC000169983550 C ₈ H ₁₀ BNO ₂ 162.981
4		ZINC000169810253 C ₈ H ₁₀ BNO ₂ 162.981
5		ZINC000000111128 C ₈ H ₆ FNO ₂ 167.137
6		ZINC000000153910 C ₈ H ₁₀ N ₂ 134.178
7		ZINC000000254639 C ₁₁ H ₁₅ NO ₂ 193.242
8		ZINC000000254643 C ₁₁ H ₁₅ NO ₂

Author for patterns

author.docking.org

NextMove Software

Roger A. Sayle

Author Search Databases API Version 3.3.2

N-S(=O)(=O).c1nn[nH]1.C-C(=O)-O-[CD1]

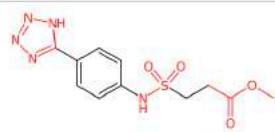
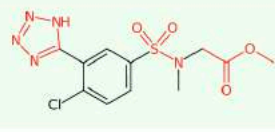
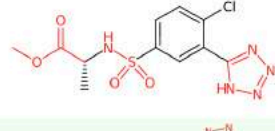
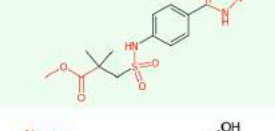
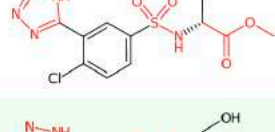
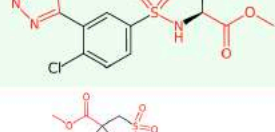
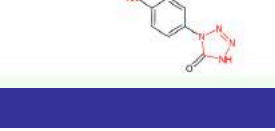
Automatically search on draw or type

Search Type: Substructure **SMARTS** Formula

Databases:

- ZINC-All-19Q4-1.4B
- BB-All-For-Sale-19Q4-26M
- BB-Stock-19Q4-1.6M
- ZINC-All-For-Sale-19Q4-1.4B**
- HMDBMetabolites-20Q1-585
- In-Stock-19Q4-13.8M
- ZINC-Interesting-2019Q4-307K
- M-Enamine-20Q1-408M
- Mcule_ultimate_200407_c8bx14
- ZINC-On-Demand-19Q4-311M
- S-Enamine-20Q1-803M
- TCNMP-20Q1-37438
- Wait-OK-19Q4-1.1B
- World-Drugs-20Q1-3004
- WuXi-2019Q4-339M

Matched **116** results in **7388** ms

- **ZINC000290466704**
C₁₁H₁₃N₅O₄S
311.318
- **ZINC000281645045**
C₁₁H₁₂ClN₅O₄S
345.763
- **ZINC000281936077**
C₁₁H₁₂ClN₅O₄S
345.763
- **ZINC000288659304**
C₁₃H₁₇N₅O₄S
339.371
- **ZINC000281919548**
C₁₁H₁₂ClN₅O₅S
361.762
- **ZINC000281919554**
C₁₁H₁₂ClN₅O₅S
361.762
- **ZINC000288215968**
C₁₃H₁₇N₅O₅S
355.370

SEA: Similarity Ensemble Approach

for drug targets of small molecules

sea.bkslab.org

SEA Search Server Home Library Search **Datasets** Recent Jobs

Similarity ensemble approach (SEA)

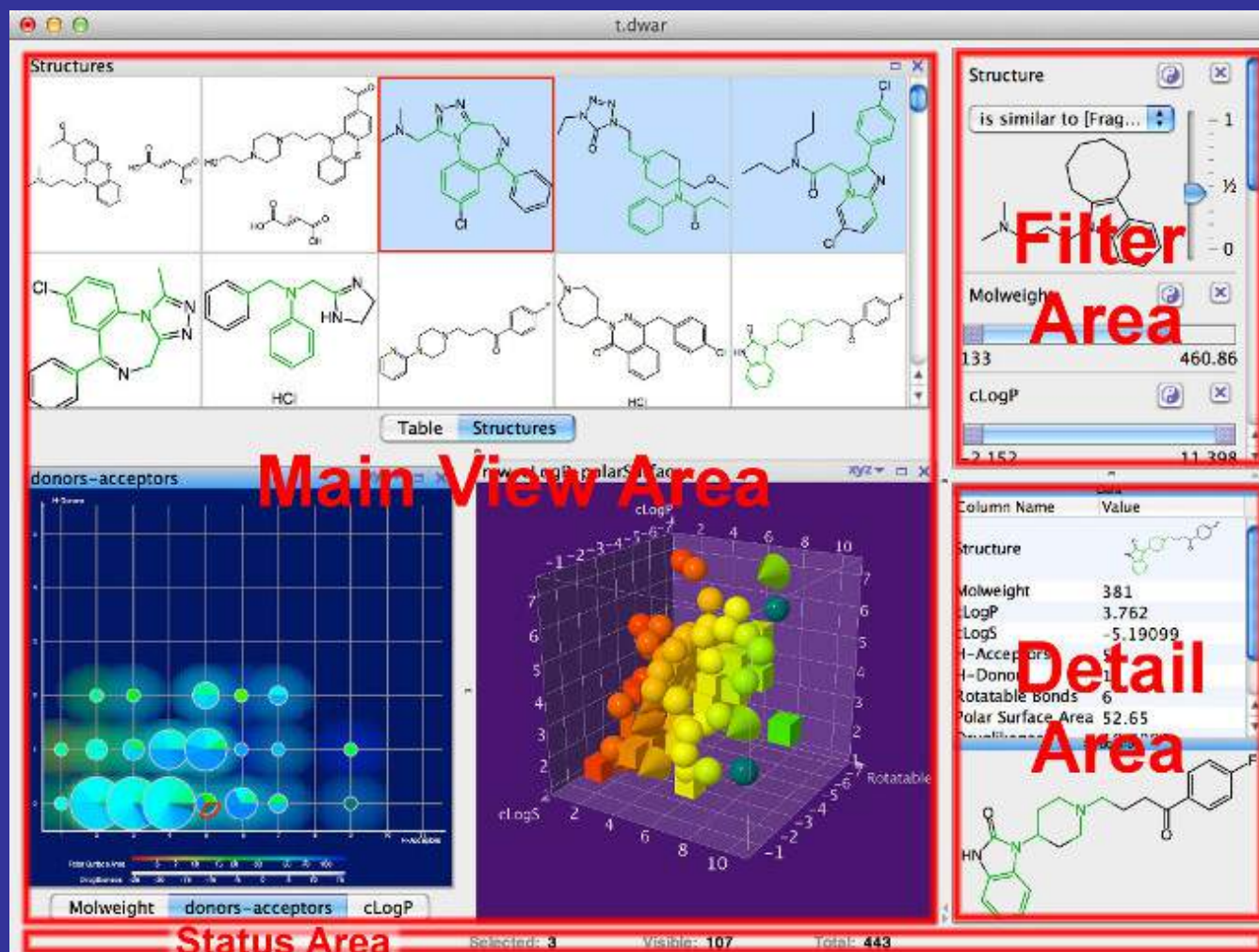
Results of Job: [search_2999be86-6bc4-4c9a-9829-9471d4e026ee](#) 

Query	Target Key	Target Name	Description	P-Value	MaxTC
 my_compound	KCNC1_RAT	Kcnc1	Potassium voltage-gated channel subfamily C member 1	3.02e-70	0.67
	MTP_HUMAN	MTTP	Microsomal triglyceride transfer protein large subunit	4.816e-32	0.32
	SYFA_STAAU	pheS	Phenylalanine--tRNA ligase alpha subunit	6.234e-24	0.34
	CA2D2_RAT	Cacna2d2	Voltage-dependent calcium channel subunit alpha-2/delta-2	3.145e-22	0.34
	CAC1A_HUMAN	CACNA1A	Voltage-dependent P/Q-type calcium channel subunit alpha-1A	3.145e-22	0.34
	CACB1_HUMAN	CACNB1	Voltage-dependent L-type calcium channel subunit beta-1	3.145e-22	0.34
	TYTR_TRYCR	TPR	Trypanothione reductase	1.11e-16	0.34
	KCNK2_HUMAN	KCNK2	Potassium channel subfamily K member 2	6.328e-15	0.67
	5HT2C_RAT	Htr2c	5-hydroxytryptamine receptor 2C	1.965e-14	0.72

Datawarrior

free from
openmolecules.org

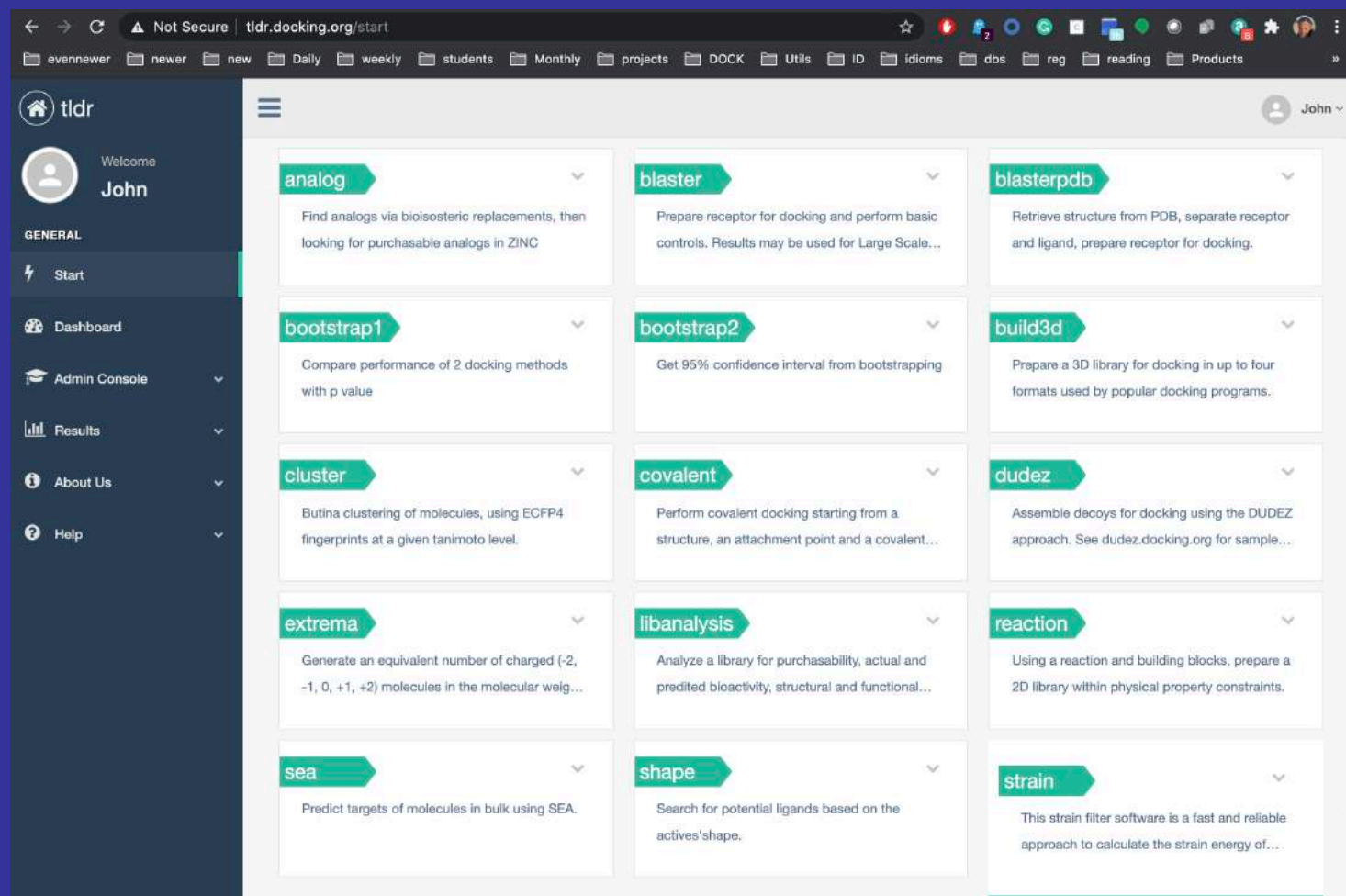
Thomas Sander
of idorsia.com



TLDR's a Ligand Discovery Resource

for free web-
based tools

tldr.docking.org



DUD DUD-E DUD-EZ

for
docking
benchmarks

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even newer | newer | new | Daily | weekly | students | Monthly | projects | DOCK | Utils | ID | idioms | dbs »

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D U D • E

A Database of Useful Decoys: Enhanced

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Welcome to DUD•E, an enhanced and rebuilt version of DUD, a directory of useful decoys. DUD-E is designed to help benchmark molecular docking programs by providing challenging decoys. It contains:

- 22,886 active compounds and their affinities against 102 targets, an average of 224 ligands per target
- 50 decoys for each active having similar physico-chemical properties but dissimilar 2-D topology.

mol2 and SDF format now available in all packages for actives and decoys. [July 14]

DUD-E is provided by the [Shoichet Laboratory](#) in the [Department of Pharmaceutical Chemistry](#) at the [University of California, San Francisco \(UCSF\)](#). To cite DUD-E, please reference **Mysinger MM, Carchia M, Irwin JJ, Shoichet BK J. Med. Chem., 2012, Jul 5. doi 10.1021/jm300687e**.

We thank [NIGMS](#) for financial support (GM71896 to BKS and JJI). For correspondence about DUD-E, please write John Irwin jji at cgl dot ucsf dot edu.

DUD-E may be downloaded [target-by-target](#), organized by [subset](#) such as GPCR and kinase, or [all at once](#). You may also [generate your own](#) decoys.

DUD-E is a research tool which we have tried to make as useful and as correct as we know how. Anticipating that problems will undoubtedly be found, we have set up a [DUDE wiki page](#) and a [DUDE Facebook page](#) to allow the community to share problems or observations. We will endeavor to put right any problems promptly, as best we can.

Browse
the DUD•E targets

Download
the default DUD•E package

Make Decoys
for your own ligands

UCSF DOCK

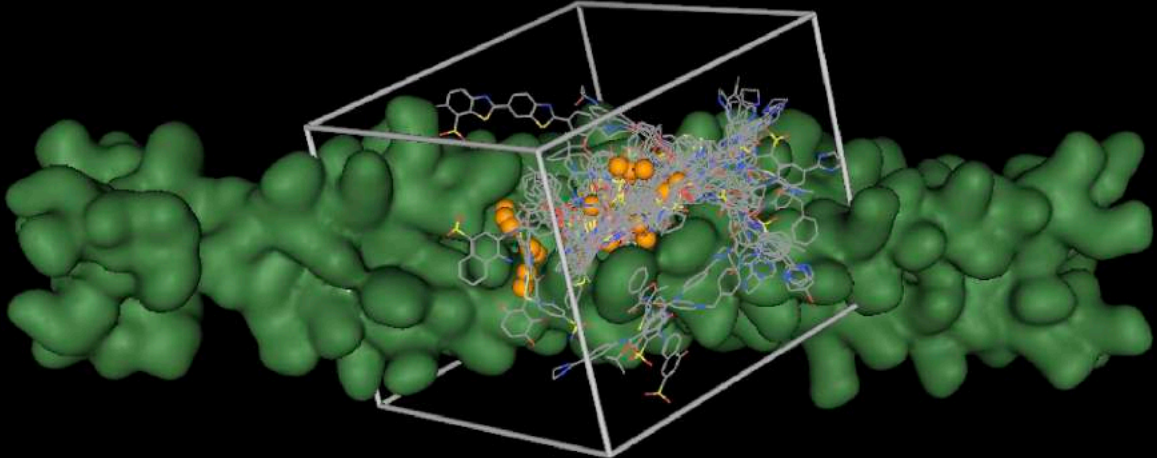
molecular
docking
software

← → ↻ Not Secure | dock.compbio.ucsf.edu

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UCSF 

The Official UCSF DOCK Web-site



NEW and IMPROVED:
Release of DOCK 3.7!
Release of DOCK 6.9!

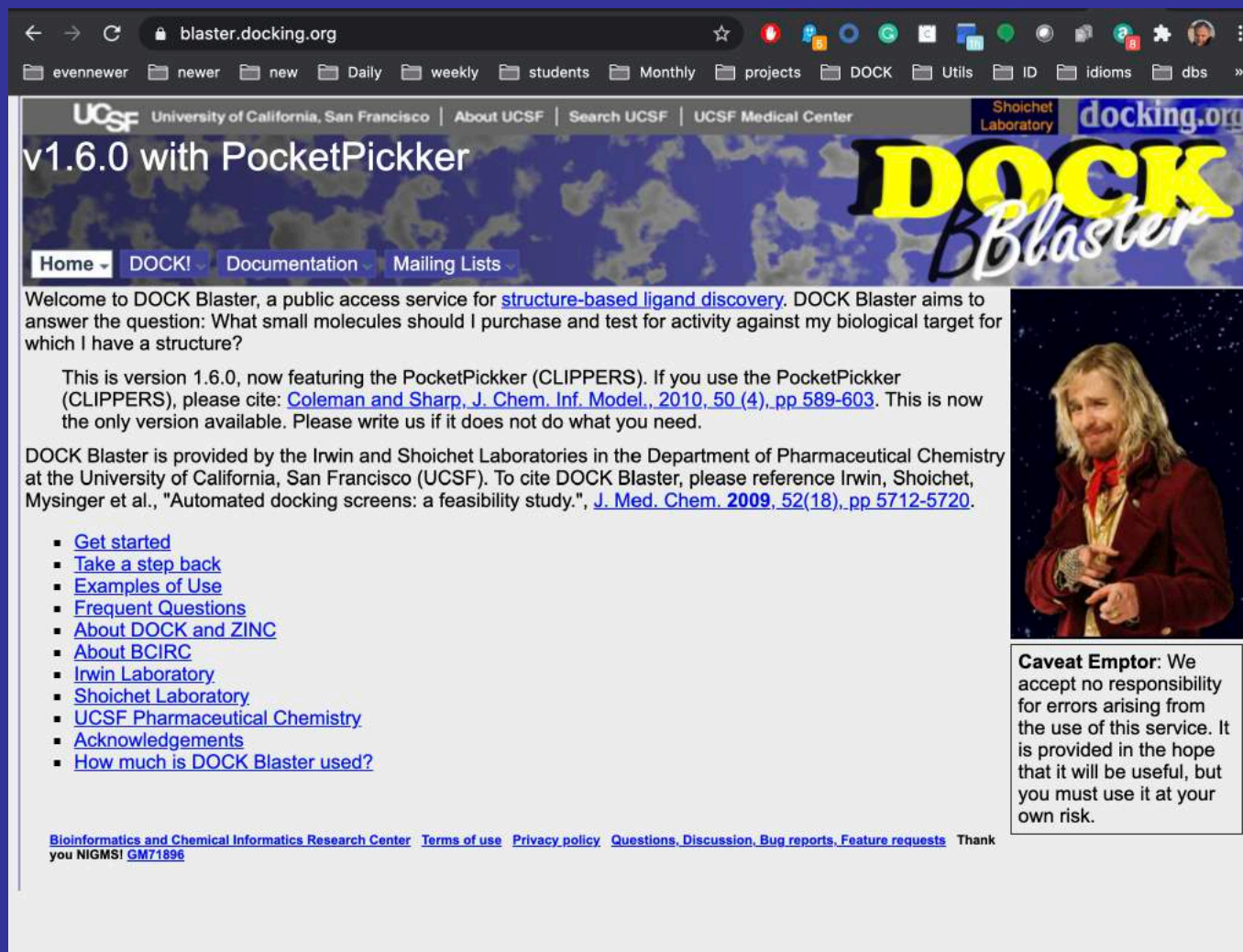
- [Kuntz Group](#)
- [Shoichet Group](#)
- [Case Group](#)
- [Rizzo Group](#)
- [Overview of DOCK](#)
- [DOCK 6](#)
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- [DOCK Related Links](#)
- [Older Versions](#)

dock.compbio.ucsf.edu

DOCK Blaster

web interface
to docking

blaster.docking.org



The screenshot shows the web interface of DOCK Blaster, version 1.6.0, which includes the PocketPicker (CLIPPERS) docking engine. The page is hosted on the University of California, San Francisco (UCSF) website. The header features the UCSF logo and navigation links for 'About UCSF', 'Search UCSF', and 'UCSF Medical Center'. The main content area welcomes users to DOCK Blaster, a public access service for structure-based ligand discovery. It provides a brief description of the service and its purpose: to answer the question of what small molecules should be purchased and tested for activity against a biological target. The page also mentions the version (1.6.0) and the docking engine (PocketPicker/CLIPPERS), along with a citation for Coleman and Sharp (2010). A list of links is provided for users to get started, take a step back, see examples of use, frequent questions, and more. A 'Caveat Emptor' disclaimer is present, stating that the service is provided as-is and users must use it at their own risk. The footer includes contact information for the Bioinformatics and Chemical Informatics Research Center and a thank you note to NIGMS.

blaster.docking.org

UCSF University of California, San Francisco | About UCSF | Search UCSF | UCSF Medical Center

v1.6.0 with PocketPicker

DOCK Blaster

Home DOCK! Documentation Mailing Lists

Welcome to DOCK Blaster, a public access service for [structure-based ligand discovery](#). DOCK Blaster aims to answer the question: What small molecules should I purchase and test for activity against my biological target for which I have a structure?

This is version 1.6.0, now featuring the PocketPicker (CLIPPERS). If you use the PocketPicker (CLIPPERS), please cite: [Coleman and Sharp, J. Chem. Inf. Model., 2010, 50 \(4\), pp 589-603](#). This is now the only version available. Please write us if it does not do what you need.

DOCK Blaster is provided by the Irwin and Shoichet Laboratories in the Department of Pharmaceutical Chemistry at the University of California, San Francisco (UCSF). To cite DOCK Blaster, please reference Irwin, Shoichet, Mysinger et al., "Automated docking screens: a feasibility study.", [J. Med. Chem. 2009, 52\(18\), pp 5712-5720](#).

- [Get started](#)
- [Take a step back](#)
- [Examples of Use](#)
- [Frequent Questions](#)
- [About DOCK and ZINC](#)
- [About BCIRC](#)
- [Irwin Laboratory](#)
- [Shoichet Laboratory](#)
- [UCSF Pharmaceutical Chemistry](#)
- [Acknowledgements](#)
- [How much is DOCK Blaster used?](#)

Caveat Emptor: We accept no responsibility for errors arising from the use of this service. It is provided in the hope that it will be useful, but you must use it at your own risk.

Bioinformatics and Chemical Informatics Research Center Terms of use Privacy policy Questions Discussion Bug reports Feature requests Thank you NIGMS! GM71896

ZINC

Database of
small
molecules for
ligand
discovery

zinc.docking.org

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even newer | newer | new | Daily | weekly | students | Monthly | projects | DOCK | Utils | ID | Idioms | dbs | reg | reading

ZINC Substances Catalogs Tranches Biological More About

Substances

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Search Using One

Isd

JSME Molecular Editor by Peter Ertl and Bruno Bierlart

Search with Nothing selected

Search Using Many

One Identifier per Line

ZINC ID, SMILES, SMARTS, InChI or Supplier Code

OR Upload a File

Choose File No file chosen

ZINC Substances Catalogs Tranches Biological More About

Added	Availability	Since	Mwt	logP	Download
2014-05-30	Premier	2015-08-08	323.44	2.905	Download

Mol Formula	Rings	Heavy Atoms	Hetero Atoms	Fraction sp ³	Tranche
C20H25N3O	4	24	4	0.45	DFAA

SMILES CCN(CC)C(=O)[C@@H]1C=C2c3cccc4[nH]cc(c34)C[C@H]2N(C)C1

InChI InChI=1S/C20H25N3O/c1-4-23(5-2)(24)14-9-16-15-7-6-8-17-19(15)13(11-21-17)10-18(16)22(3)12-14/h6-9,11,14,1i

InChI Key VAYOSLLFUXYJDT-RDXTXWAMCSA-N

Available 3D Representations

pH range	Net charge	H-bond donors	H-bond acceptors	tPSA	Rotatable bonds	Apolar desolvation	Polar desolvation	Download
Reference	1	2	1	40	3	10.12	-34.03	Download
Mid pH (7.4)	1	2	1	40	3	9.94	-42.44	Download
Mid pH (7.4)	0	1	2	39	3	7.87	-11.12	Download

Vendors (8 Total)

Sigma Aldrich (Building Blocks) L-001, L-001[CERILLIAN, L-005, L-005[CERILLIAN, L7007, L7007[SIGMA

Tetrahedron Building Blocks TS77453

Compound Cloud 5761

eMolecules 105346456, 260954711, 261082209

MuseChem R050199

Toronto Research Chemicals KIT0380, KIT1587, L488010

Annotated Catalogs (20 Total)

Ambinter Amb17616618

BindingDB.org 21342, 50241702, 86427

ChEBI CHEBI:6605

ChEMBL20 CHEMBL263881, CHEMBL269421, CHEMBL463207

ChEMBL 21 CHEMBL263881, CHEMBL269421

ChEMBL23 CHEMBL263881, CHEMBL269421

ChEMBL25 CHEMBL263881, CHEMBL269421

ChEMBL DrugStore CHEMBL263881

Substances are molecules that are loaded from catalogs. They h

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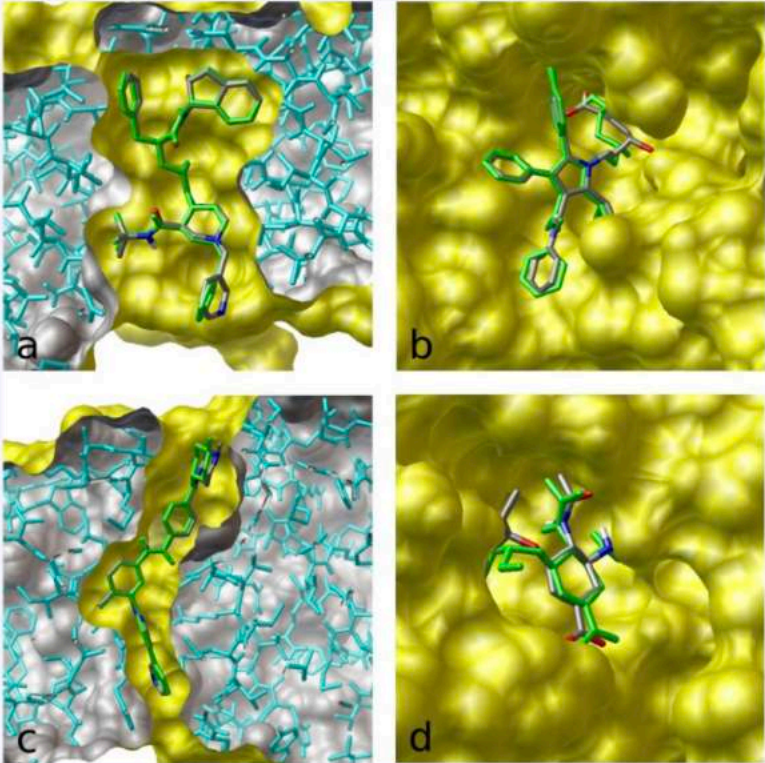
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AutoDock Vina

AutoDock Vina is an open-source program for doing [molecular docking](#). It was designed and implemented by [Dr. Oleg Trott](#) in the Molecular Graphics Lab at The Scripps Research Institute.

The image on the left illustrates the results of flexible docking (green) superimposed on the crystal structures of (a) indinavir, (b) atorvastatin, (c) imatinib, and (d) oseltamivir bound to their respective targets.



Publication

If you used AutoDock Vina in your work, please cite:

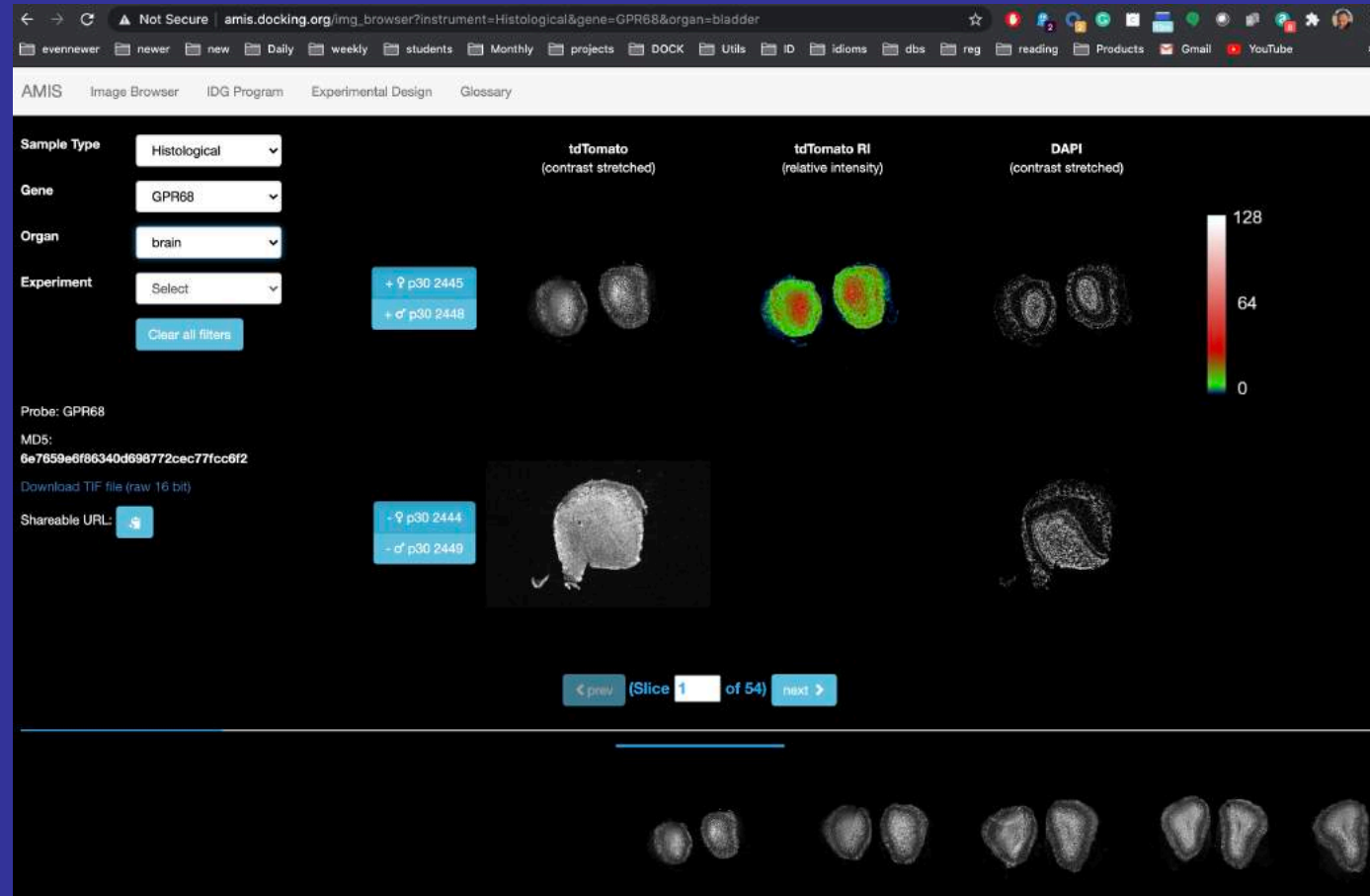
[O. Trott, A. J. Olson, AutoDock Vina: improving the speed and accuracy of docking with a new scoring function, efficient optimization and multithreading, *Journal of Computational Chemistry* 31 \(2010\) 455-461](#)

AMIS

A Mouse Image Server

Gene expression locations

amis.docking.org



Summary

- The problem of exploring chemical space
- Molecular docking as a pragmatic tool for ligand discovery using protein structure
- Inexpensive access to billions of purchasable compounds is changing how ligands are discovered
- Many free software tools you can use