HTCondor Week, May 27, 2021

Scaling Virtual Screening to Ultra-Large Virtual Chemical Libraries

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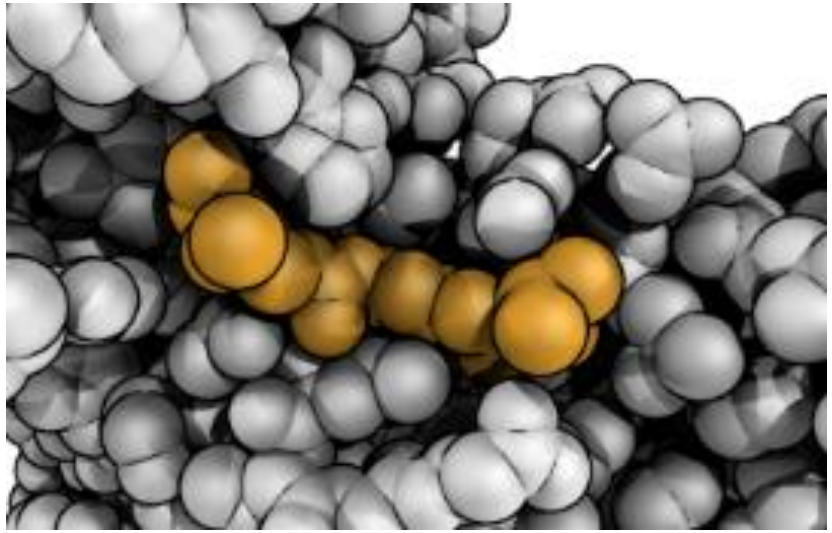
Small Molecule Screening Facility



Carbone Cancer Center
UNIVERSITY OF WISCONSIN
SCHOOL OF MEDICINE AND PUBLIC HEALTH

Open Science Grid

CENTER FOR HIGH THROUGHPUT COMPUTING

HTCondor
High Throughput Computing

Why am I here?

- To promote early-stage drug discovery efforts on campus!
- Find active molecules that modulate therapeutically relevant mechanism. Develop as probes or leads.
- Early-stage drug discovery is a needle-in-the-haystack problem—could be 10^{33} drug-like organic molecules.*
- Conventional HTS approach too expensive.

*Polishchuk PG, et al., JCAMD 2013 27(8):675-9

What is VS?

- Virtual Screen: use a computer model to evaluate a chemical library. Prioritize some subset for testing.
- VS models predict potential for compound-target interaction or assay read-out.
- Goal is in enrichment for actives. Highly enriched subset reduces costs—enables focused screening.

Searching chemical space for hits

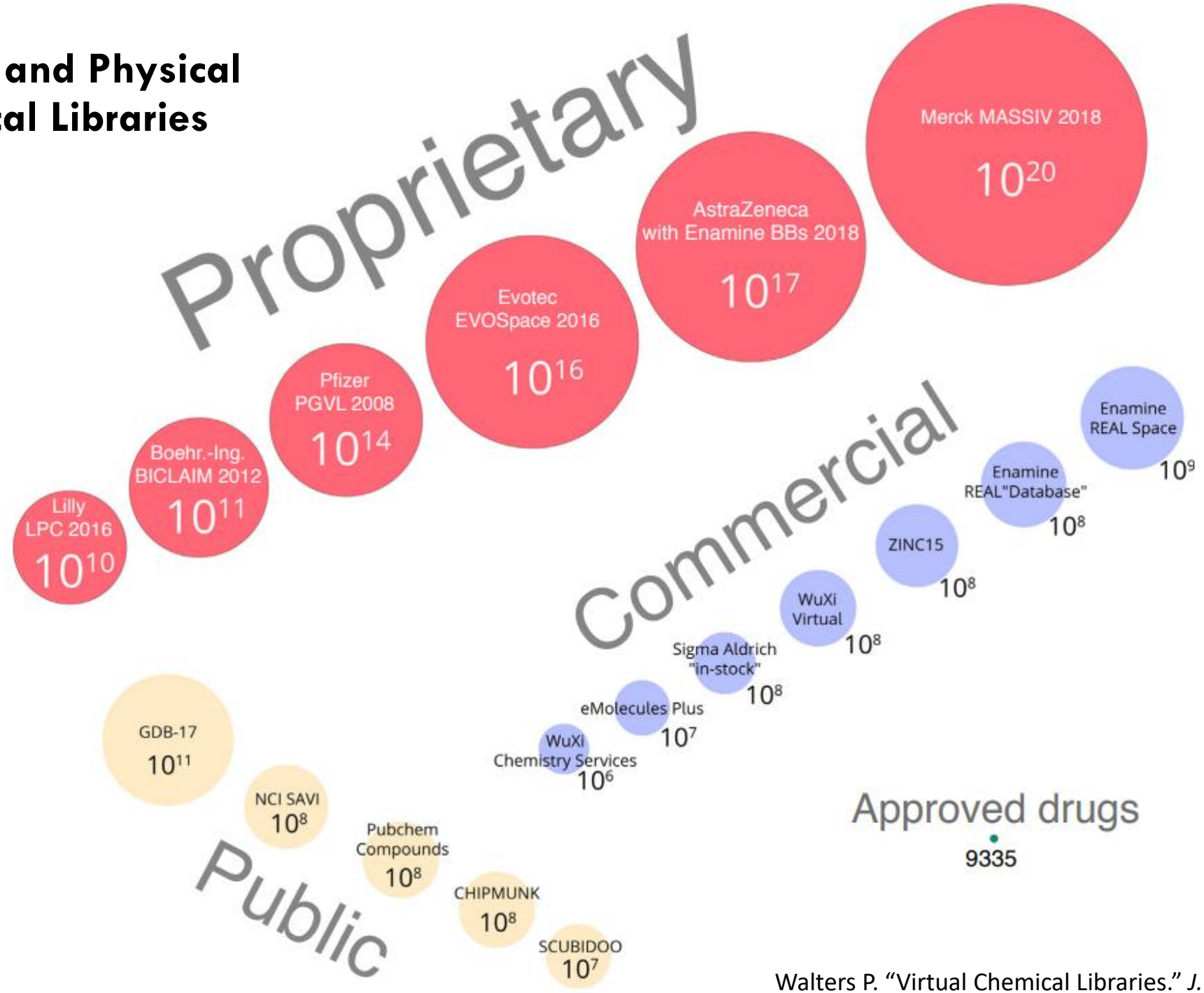
High Throughput Screening

- test 10^4-10^6 cpds
- generates valuable real data
- expensive
- noisy
- can't scale to ultra-large libraries
- Assay must be developed!

Virtual Screening + focused testing

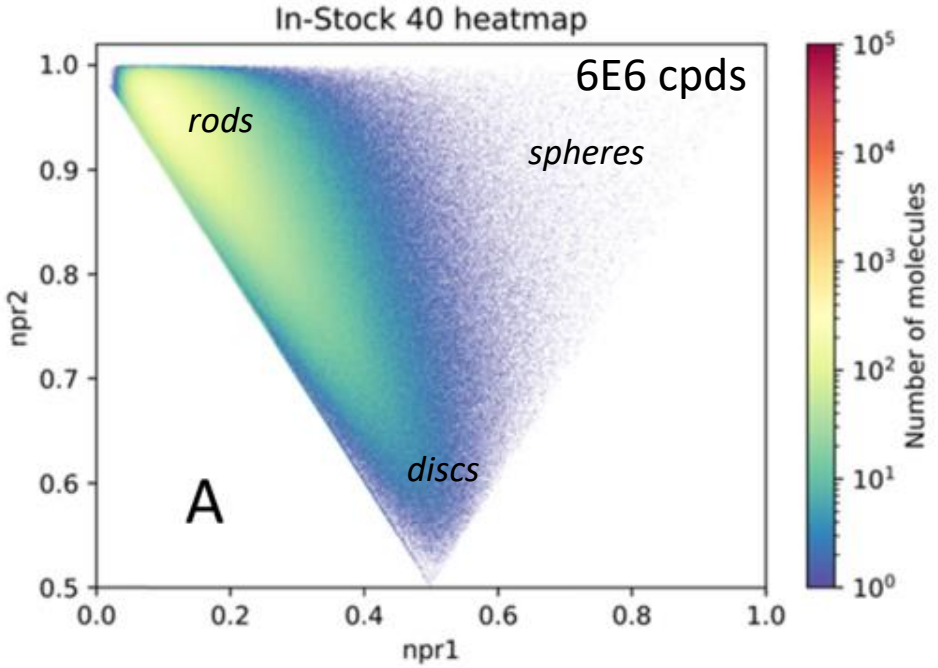
- VS 10^8-10^{12} → test 10^2-10^4 cpds
- limited real data generation
- cheap
- **VERY** noisy
- scales to ultra-large libraries (10^9-10^{12})
- VS models have data requirements

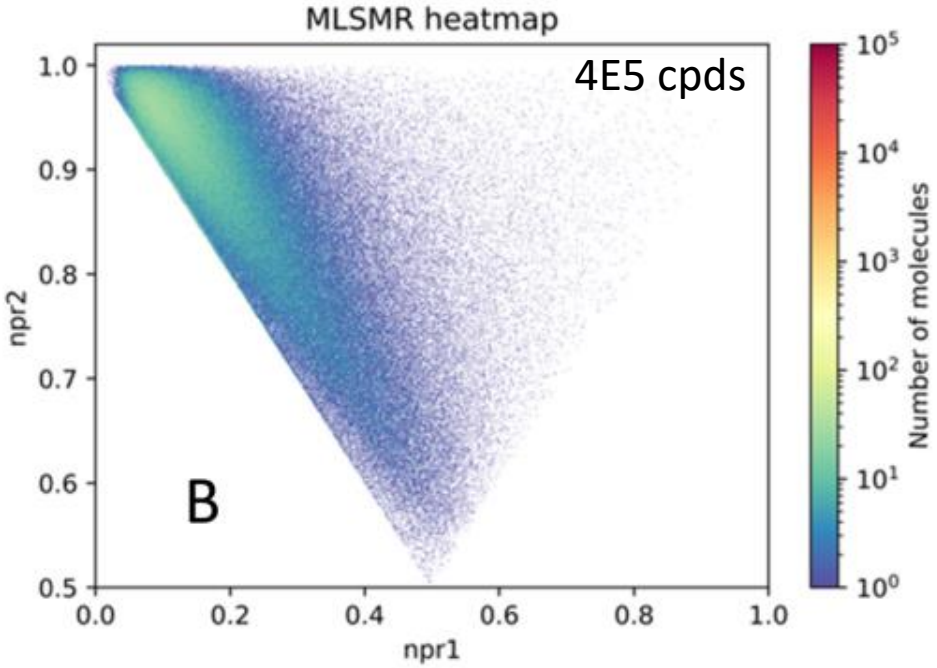
Virtual and Physical Chemical Libraries

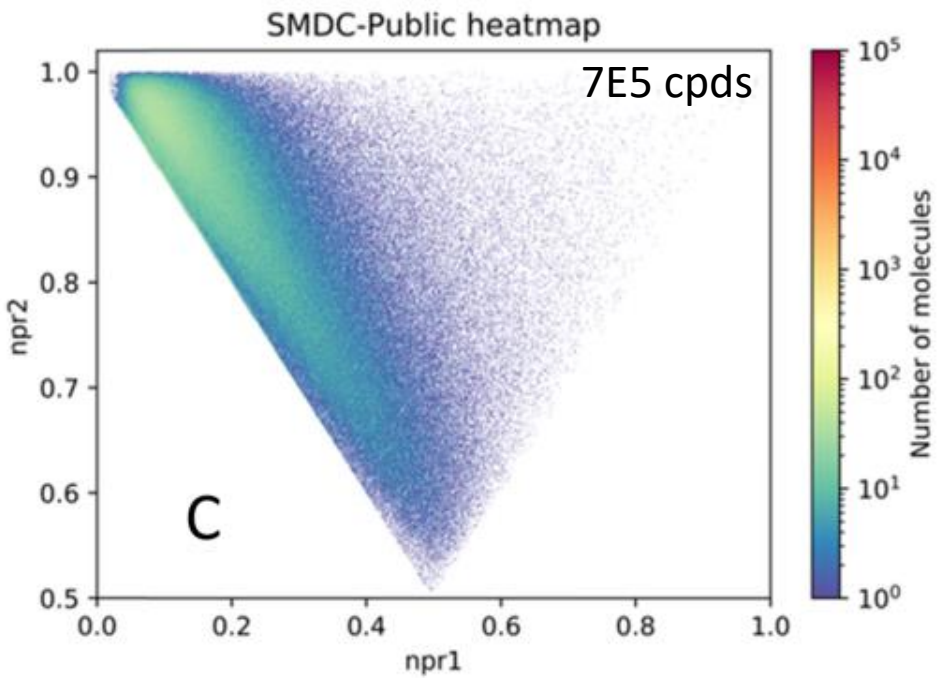


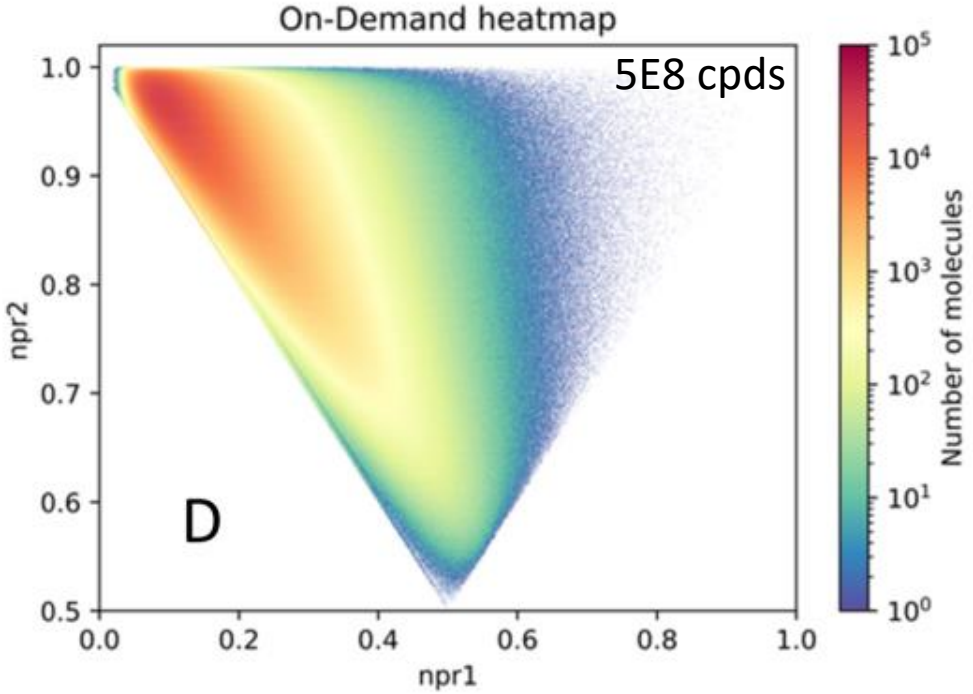
Hoffmann & Gastreich "The next level in chemical space navigation: going far beyond enumerable compound libraries." *Drug Discovery Today*, 2019, 24, 5, 1148-1156.

Walters P. "Virtual Chemical Libraries." *J. Med. Chem*. 2019, 62, 3, 1116-1124

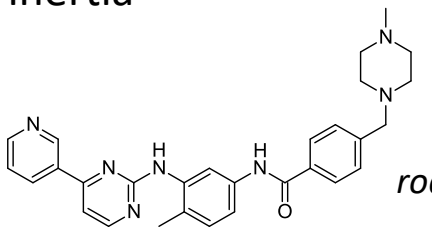




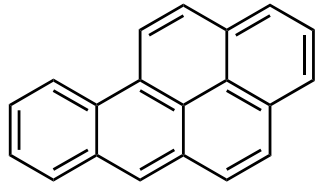




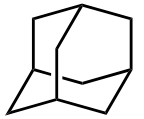
NPMI = normalized ratios of principle moments of inertia



rods



discs



spherical

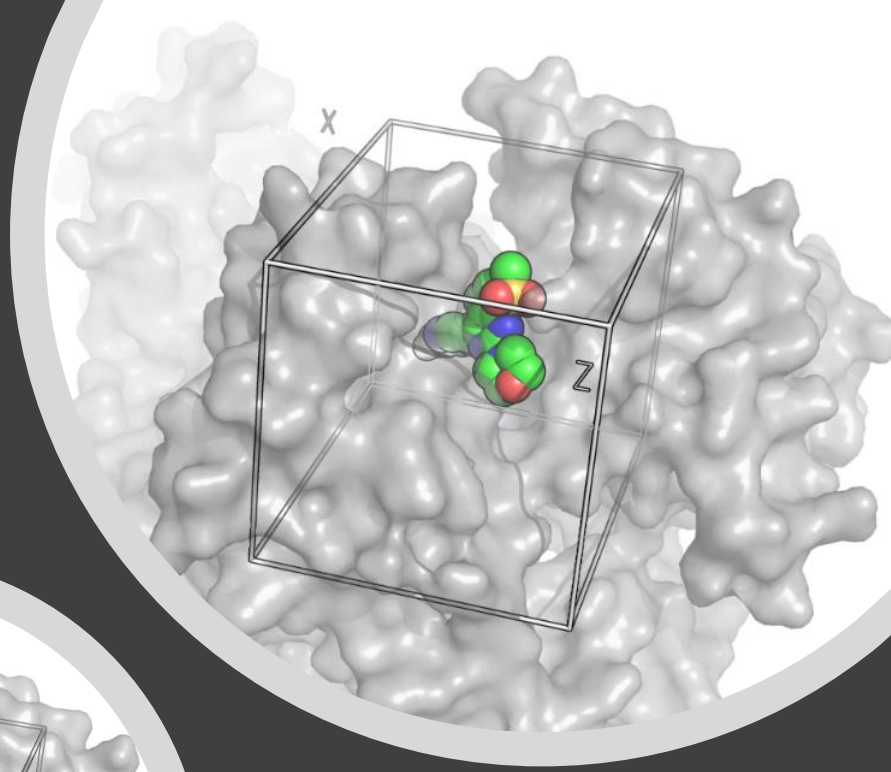
Irwin JJ et al., "ZINC20—A Free Ultralarge-Scale Chemical Database for Ligand Discovery." *J. Chem. Inf. Model*. 2020, **60**, 6065-6075.

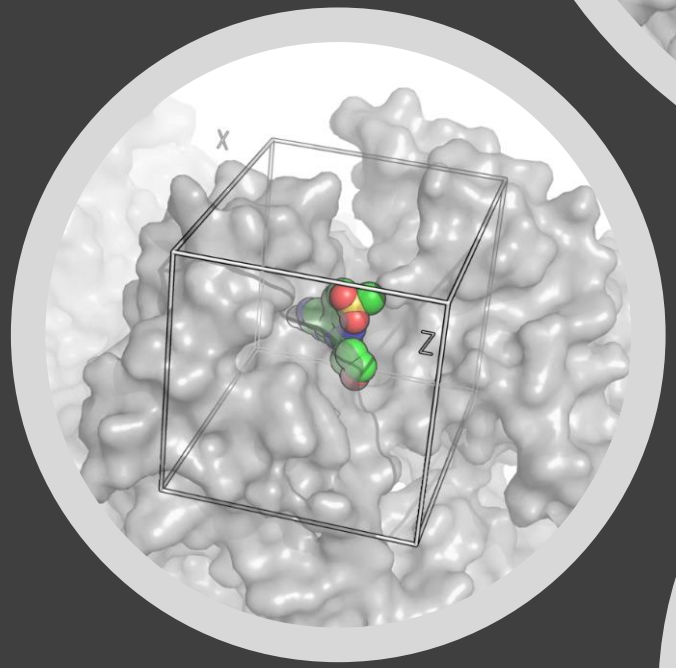
Structure-based virtual screening

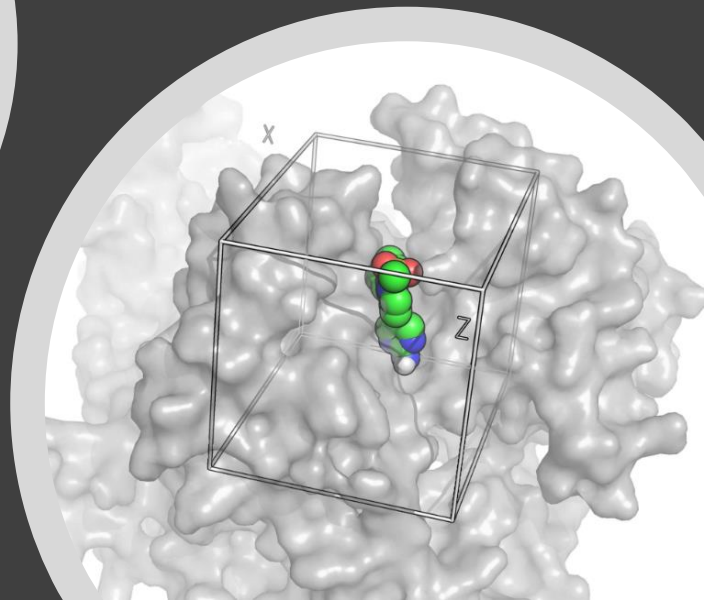
SBVS

What is docking?

- Docking uses 3D molecular models to determine the optimal compound binding orientation on a given target.
- Search is guided by a scoring function that evaluates favorability of each sampled configuration.
- Many docking programs exist with different search strategies and scoring functions.
- Docking score is crude estimate of binding favorability for a given compound.

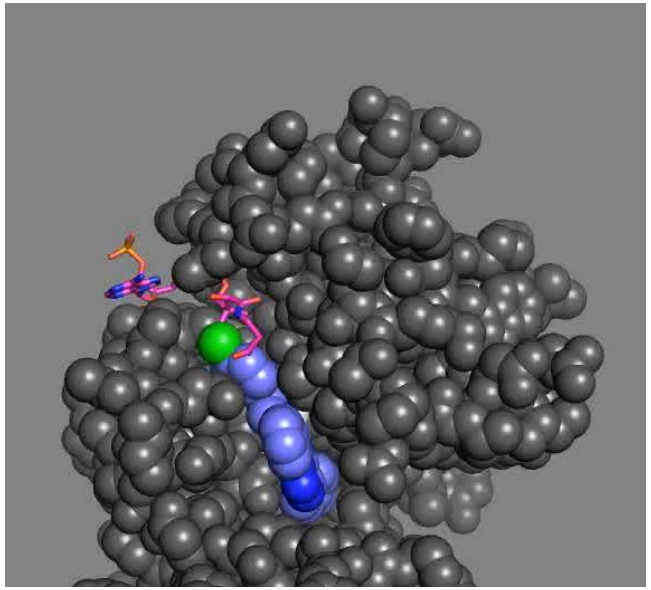






Structure-based virtual screening

Dock Compound Library



MOLID	SCORE
ZINC36206438	58.63
ZINC59310217	58.72
ZINC61596674	56.35
ZINC67458535	47.40
CHEMBL1221861	60.66
ZINC10123401	52.39
ZINC64526095	66.13
ZINC24002103	56.72
ZINC09612655	58.84
ZINC24002105	38.95
CHEMBL38532	74.19
ZINC40824467	50.10
ZINC59829723	58.29
ZINC37520295	44.78
ZINC49812309	38.01
ZINC14558020	53.31
CHEMBL472090	58.71
ZINC36207525	69.07
ZINC14010625	68.48
CHEMBL274782	63.97
ZINC63949457	55.35
ZINC39657146	48.74
ZINC23197109	58.72
ZINC25520953	63.14
ZINC09282496	43.71
ZINC60343267	62.18
ZINC58790750	62.53
CHEMBL400392	65.96
ZINC52096905	49.96
ZINC48922871	49.59
ZINC33058380	45.11
ZINC64684798	56.64
ZINC21076300	68.36
ZINC29461868	50.65
CHEMBL26183	58.56
ZINC61908006	66.40
ZINC15429053	54.10
CHEMBL323258	74.94
ZINC05091951	58.47
ZINC02759924	48.25
ZINC54596097	42.68
ZINC19899314	65.54
ZINC53113244	38.99
ZINC40947055	61.87
ZINC36611787	60.04
CHEMBL419085	65.96
ZINC35844701	58.57
ZINC01296699	39.07
ZINC39914438	49.68
ZINC00706129	48.34
ZINC34747432	52.55
ZINC43220997	47.45
ZINC37619890	54.49
ZINC15666896	55.50

Sort Compounds by Docking Scores

MOLID	SCORE
CHEMBL323258	74.94
CHEMBL38532	74.19
ZINC36207525	69.07
ZINC14010625	68.48
ZINC21076300	68.36
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ZINC36206438	58.63
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CHEMBL26183	58.56
ZINC05091951	58.47
ZINC59829723	58.29
ZINC24002103	56.72
ZINC64684798	56.64
ZINC61596674	56.35
ZINC15666896	55.50
ZINC63949457	55.35
ZINC37619890	54.49
ZINC15429053	54.10
ZINC14558020	53.31
ZINC34747432	52.55
ZINC10123401	52.39
ZINC29461868	50.65
ZINC40824467	50.10
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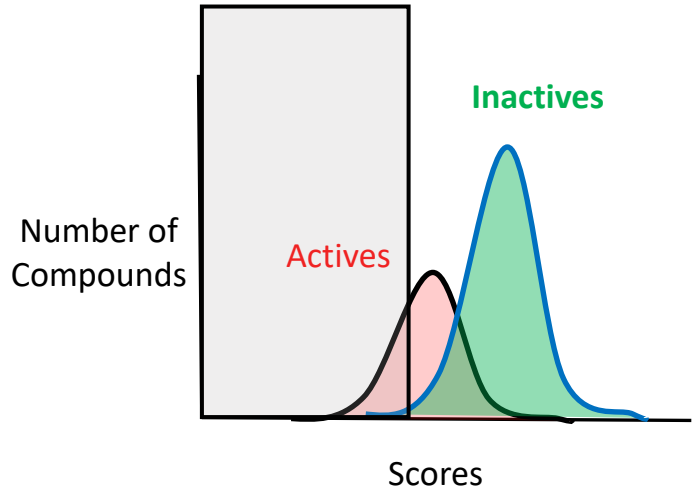
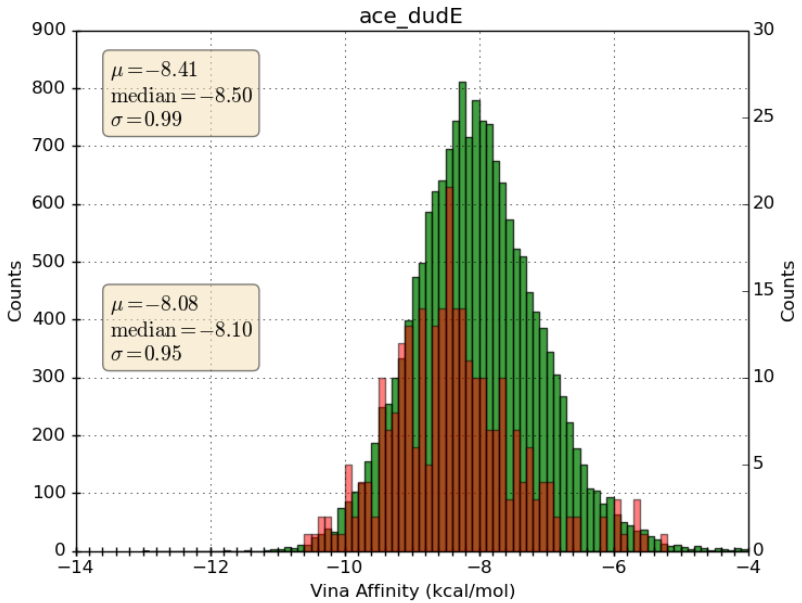
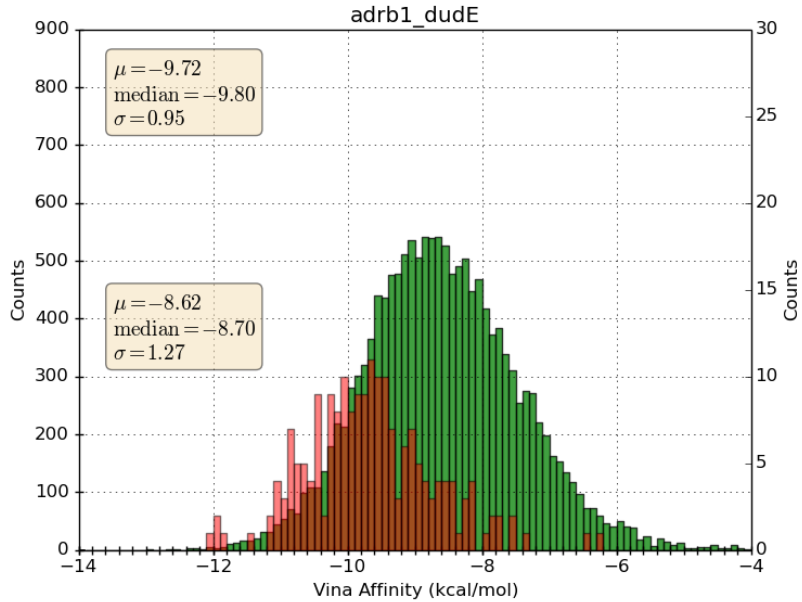
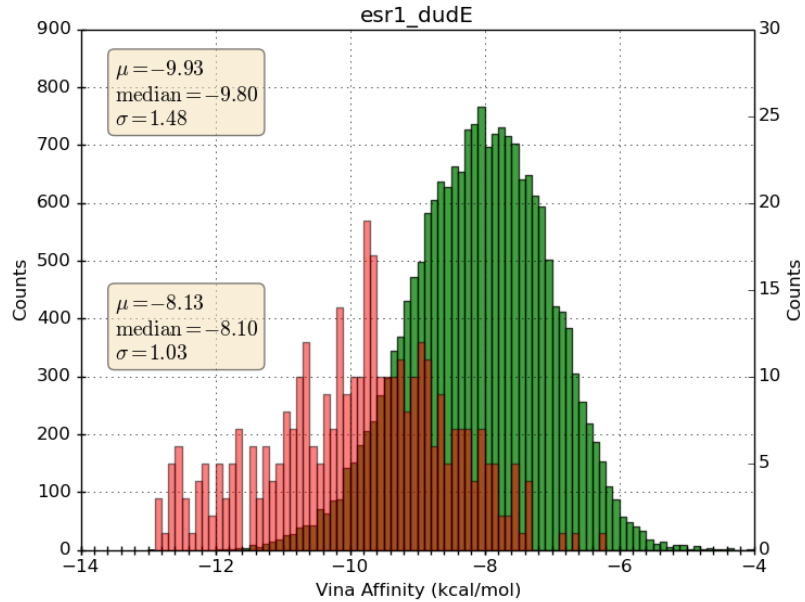
Score Distributions

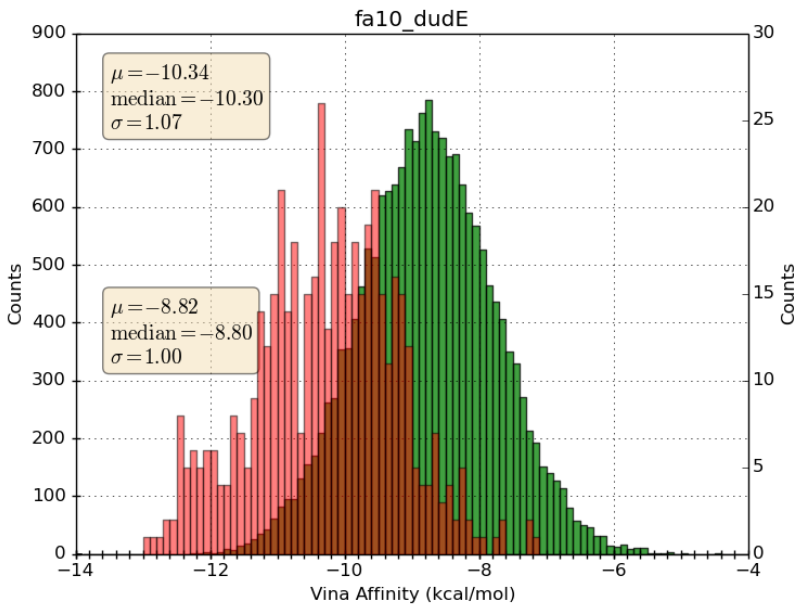


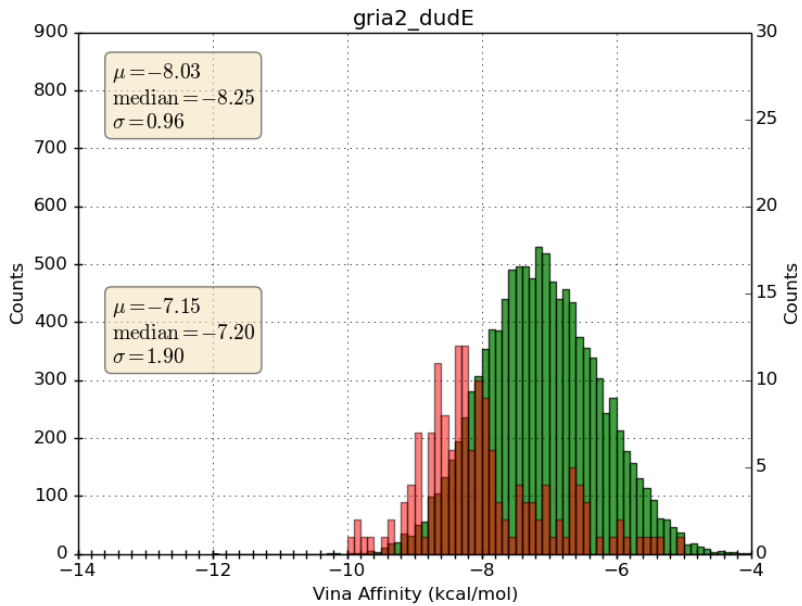
Docking-based VS performance on 6 benchmark targets from DUD-E

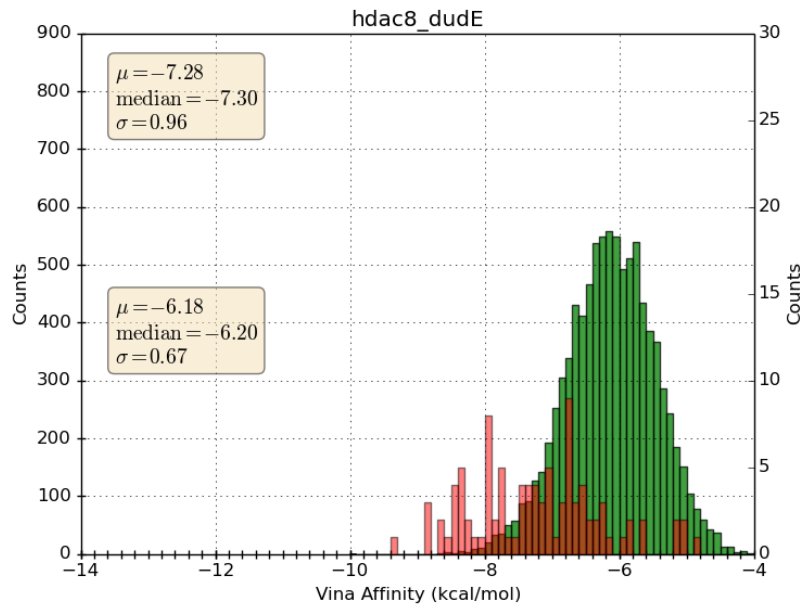






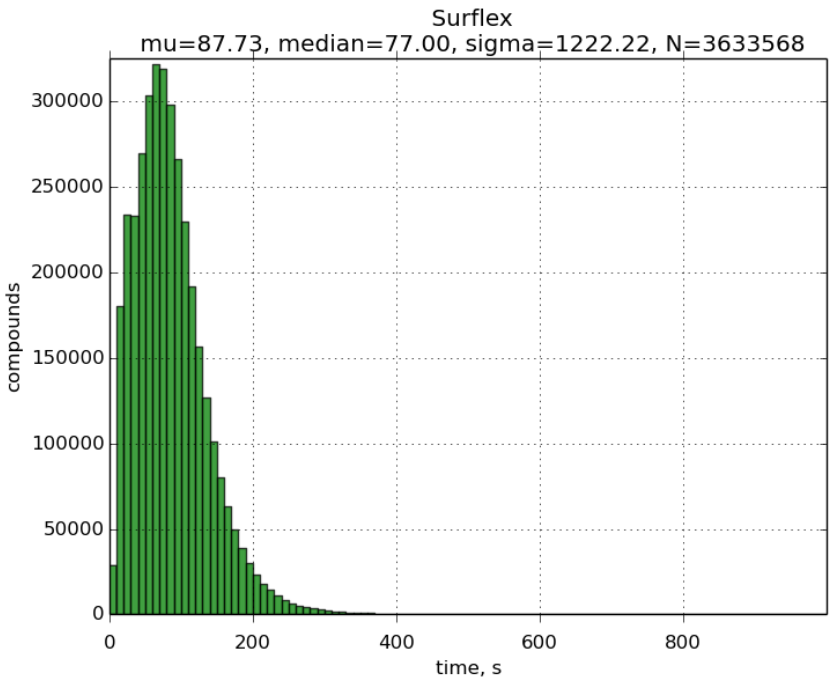


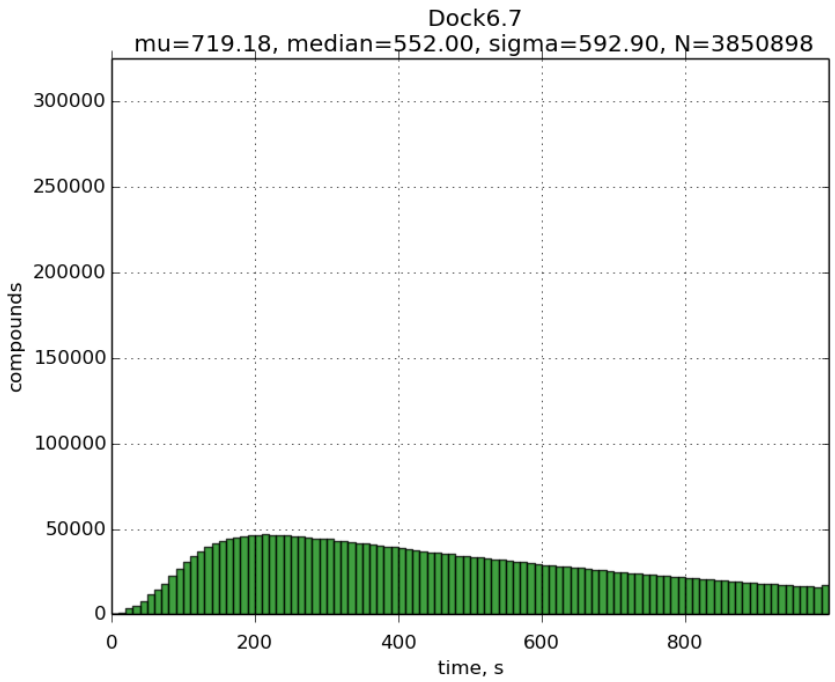




Docking Compute Expense

- Compute time for docking depends the search space, search quality, and complexity of the scoring function.
- To dock millions of compounds, we cut corners.
- Docking time varies between programs (~1 minute/compound).

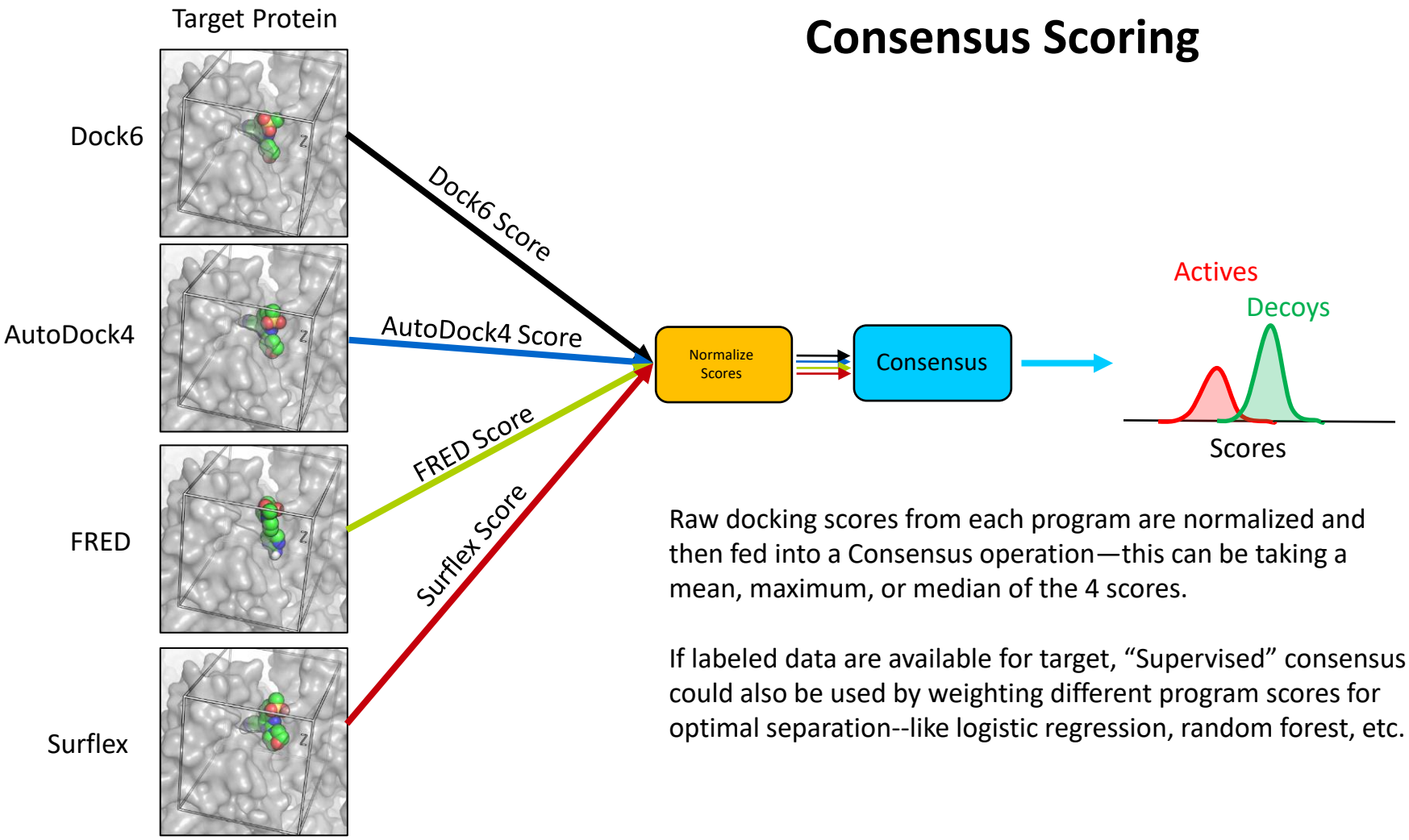




(seconds)

Program	Time	Std. Dev.
AD4	435.6	197.1
Dock	719.2	592.9
Fred	15.6	5.7
Hybrid	9.3	2.9
Plants	43.4	20.5
rDock	49.3	26.7
Smina	250.1	172.8
Surflex	78.9	1159.6

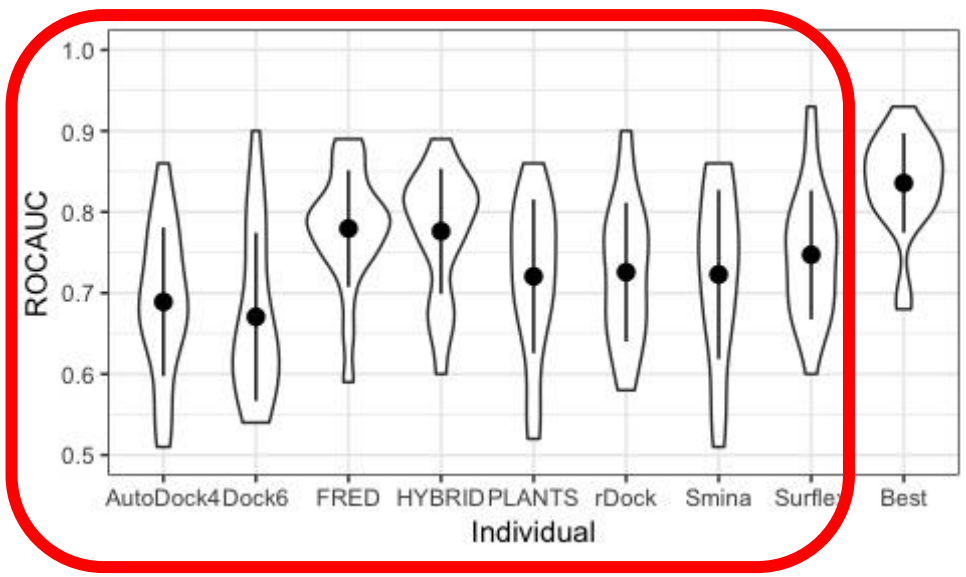
Consensus Scoring

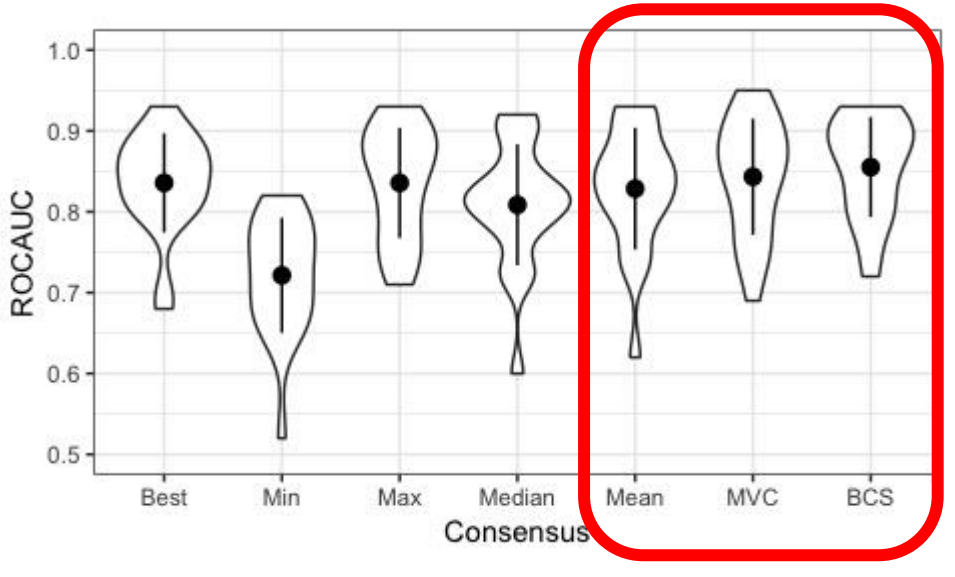


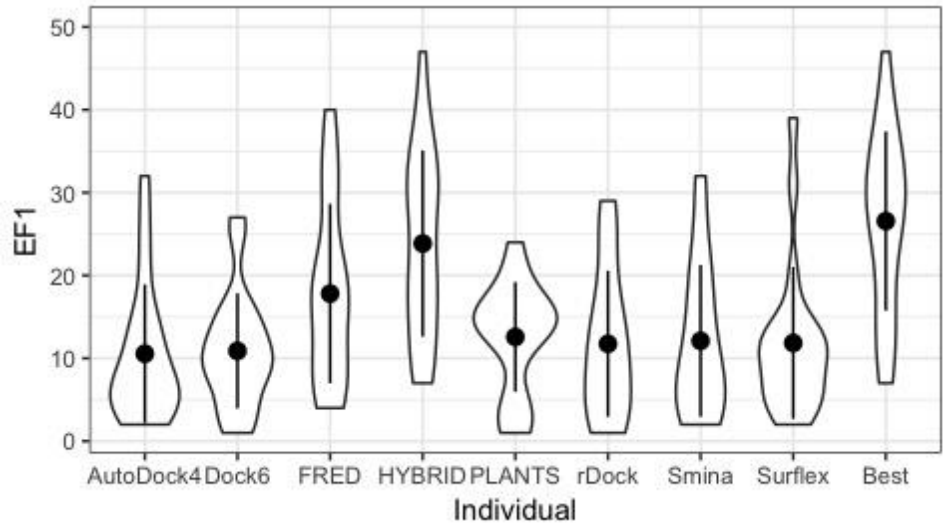
Raw docking scores from each program are normalized and then fed into a Consensus operation—this can be taking a mean, maximum, or median of the 4 scores.

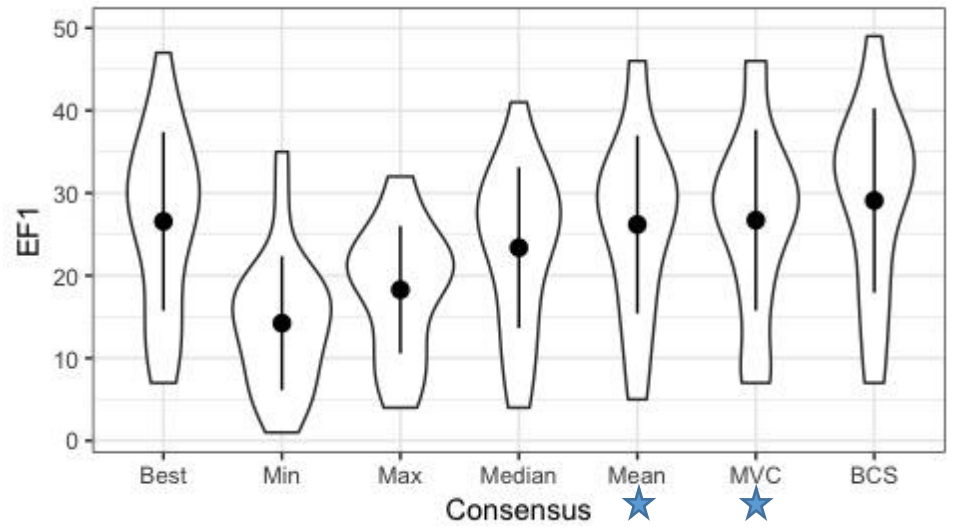
If labeled data are available for target, “Supervised” consensus could also be used by weighting different program scores for optimal separation--like logistic regression, random forest, etc.

Virtual screening performance on N=21 benchmark targets









Ericksen et al., J. Chem. Inf. Model. **2017**, 57, 7, 1579-1590 DOI: 10.1021/acs.jcim.7b00153

How do we scale to HTC resources?

- Each docking run is independent--*pleasantly parallelizable*!
- Typical docking codes don't benefit from specialized hardware or multiple cores.

- To maximize throughput:
    - Enable "Flock" and "Glide" to access more nodes.
    - Split compound library up into small chunks.
        - Number of compounds should run in ~2hr for a given docking program.
        - Chunk size varies from 5—500 compounds!
    - Dock each chunk on a single slot to scavenge ANY open slots. Dock compounds in chunk serially.
    - Checkpointing is enabled and a wrapper script is used to track the compounds completed in case job is evicted and migrates to another node.

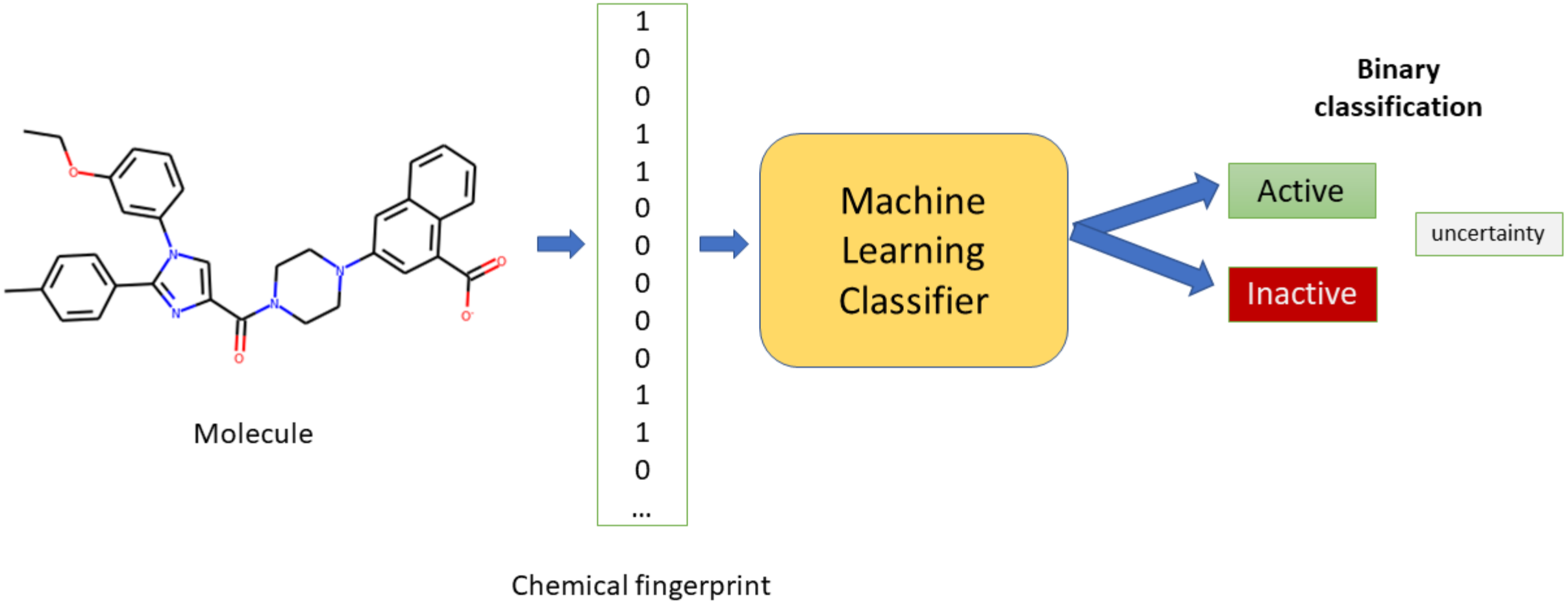
How does SBVS benefit from HTC?

- Can’t really see how docking-based VS works without proper testing/validation!
- Examine performance over many targets
- Benchmarking of different docking programs
- Extensive docking parameter testing/validation
- Dock large compound sets
  - Recently performed SBVS on 8 million and 40 million cpd in-stock libraries
- Hypothetical 100 node cluster = 3.5 million/day
- ~~100s of millions to~~ BILLIONS of dockings!

ligand-based virtual screening

LBVS

Ligand-Based VS—a ML hit-finding model



Gitter Lab: Liu, et al., "**Practical Model Selection for Prospective Virtual Screening.**" *J. Chem. Inf. Model.* 2019, 59, 1, 282–293. https://doi.org/10.1021/acs.jcim.8b00363

LBVS on Ultra-Large Virtual Chemical Library

Train RF model on prior screening data (PriA-SSB interaction)

- LifeChem Diversity Sets 1-3: 74,763 cpds (primary and retest)
- LifeChem Diversity Set 4: 25,278 cpds (primary only)
- MLPCN (NIH probe set): 337,104 cpds (primary and retest)

Total: 427,300 cpds, number of actives: 554 (hit rate = 0.13%)

VS Procedure

- Download Enamine REAL database 1.077 billion cpds (Oct 11, 2019)—SMILES format.
- Split library up into 18 batches (each 60.3 million)
- Run each batch as a single job on generic CPU compute node on HTCondor
  - Single core, ~5GB RAM, 32 GB disk
  - SMILES canonicalized/de-salted and converted to ECFP4 fingerprints
  - ECFP4 fingerprints scored by pre-trained random forest classifier.
  - Average compute time of **3.24 ms per compound**
  - Mean run time per 60 million cpd batch = 53.2 hours (standard deviation=6.4 hr)

Gitter Lab: Alnammi M. et al., “Scalable supervised learning for synthesize-on-demand chemical libraries.” manuscript in prep

Enamine ID	IC50 (uM)	C 0.5 (% ne	C 1.0	C 2.1	C 4.1	C 8.2	C 16	C 33	C 66	Active
PV-001918010086	0.5	93.2	40.8	21.0	11.6	8.1	6.6	5.9	8.6	1
Z1172208679	2.1	78.2	66.2	45.9	25.2	10.3	7.8	7.1	6.0	1
Z734854148	0.5	116.4	69.3	50.5	24.2	11.4	8.8	7.1	10.3	1
Z3634004206	3.4	79.7	74.1	63.1	33.9	9.9	6.0	6.2	5.3	1
Z3638513333	4.4	85.3	78.5	72.0	47.9	11.8	4.5	3.5	3.4	1
Z71174619	4.8	72.8	63.2	54.6	43.7	33.6	19.4	10.5	8.3	1
Z49571468	4.9	85.7	77.9	70.4	54.4	19.6	8.0	5.6	5.7	1
Z3225506284	6.1	80.1	67.9	67.8	53.2	33.5	15.1	9.0	8.6	1
Z3557629872	6.8	88.1	83.0	81.0	68.8	35.0	10.4	5.5	4.5	1
Z3558428795	9.1	85.0	81.5	81.0	73.0	50.9	14.3	6.5	6.2	1
Z2739840324	3.9	119.8	86.5	82.0	68.2	47.7	15.7	7.3	9.8	1
Z240359708	2.4	126.3	91.8	81.4	72.5	47.3	19.4	7.6	8.5	1
Z3557781825	10.8	86.8	84.3	79.5	76.0	58.9	24.2	8.8	6.2	1
Z1763598930	0.5	132.0	91.3	82.4	73.1	56.0	24.0	9.9	9.5	1
PV-001914484112	12.4	85.5	85.9	85.4	79.8	63.8	30.9	8.0	5.0	1
Z666250890	48.2	81.6	75.7	67.9	60.5	55.0	45.8	30.8	25.8	1
Z2618185084	66.0	121.5	88.3	82.6	75.7	63.1	37.5	9.1	7.2	1
Z3395547714	12.6	87.7	87.0	82.8	83.9	71.1	28.1	8.0	6.1	1
Z3484513235	12.1	89.2	89.7	86.1	80.1	66.8	30.2	10.3	6.7	1
Z3347084877	11.5	91.4	87.2	87.5	84.5	67.7	26.5	10.9	6.3	1
Z109132782	15.5	83.3	88.0	77.3	74.0	62.2	41.1	24.7	12.3	1
Z3242476057	35.4	123.9	94.4	86.1	81.9	68.7	40.8	9.4	8.4	1
Z666485712	13.9	87.7	86.1	87.4	85.7	72.9	38.0	11.4	9.3	1
Z114886052	21.0	86.6	83.3	82.5	75.9	67.8	47.8	24.9	9.2	1
PV-002161956828	15.7	87.8	89.6	89.8	83.9	70.5	43.8	15.8	5.7	1
PV-001915624464	7.0	80.0	78.9	78.9	71.7	53.7	44.8	39.8	36.9	1
Z3652859018	66.0	125.3	92.1	86.0	86.3	74.4	49.5	15.4	10.8	1
Z3557629875	22.2	90.0	90.6	92.1	86.8	76.4	62.5	22.7	7.2	1
Z1741972899	37.8	88.5	87.6	87.0	80.1	77.6	62.3	36.5	11.0	1
PV-002140113355	24.9	84.6	87.5	88.0	89.1	80.0	65.2	29.9	8.9	1
Z3297024656	66.0	140.0	94.7	97.5	91.0	83.1	62.3	25.1	10.1	1
Z734817070	20.2	86.5	85.7	83.3	80.3	80.3	68.4	50.3	43.6	0
Z2976359863	66.0	136.0	100.0	89.3	86.0	86.7	74.1	49.7	28.3	1
Z1101543176	66.0	83.7	86.8	87.7	82.8	76.5	63.1	60.3	65.1	0
Z29466207	66.0	86.9	87.8	85.9	86.7	78.5	78.8	71.7	69.4	0
Z3414110258	7.3	131.5	93.7	90.9	90.4	90.5	82.4	70.5	49.2	0
Z3295052620	66.0	122.0	95.1	90.0	84.9	88.9	84.5	74.2	63.6	0
PV-001915624917	66.0	83.3	83.6	80.6	82.6	82.0	86.1	84.0	86.0	0
PV-002126332674	66.0	84.2	82.1	84.5	83.4	83.3	81.6	84.1	87.9	0
Z2273856428	66.0	134.3	95.6	87.6	85.4	85.2	84.7	77.4	72.8	0
Z314947084	66.0	134.5	97.4	87.2	83.1	84.6	86.1	77.9	74.2	0
Z3075781550	66.0	136.5	93.6	88.8	89.0	87.8	89.4	78.2	63.8	0
Z3559518523	66.0	85.7	86.8	83.5	80.2	87.7	82.1	84.7	87.2	0
Z71173293	66.0	89.4	88.1	89.9	89.3	81.7	82.2	80.6	80.9	0
Z1245633363	66.0	87.3	84.5	88.6	83.2	86.9	81.6	85.0	88.7	0
Z241926076	66.0	86.8	85.6	84.8	86.7	86.2	83.9	88.4	85.0	0
Z3238971184	66.0	134.3	100.4	87.4	88.0	89.0	87.8	77.2	71.0	0
Z3557694708	66.0	89.2	88.1	87.4	89.4	88.2	84.2	82.2	82.8	0
Z339655406	66.0	95.1	87.1	84.9	87.5	87.3	88.0	86.8	81.4	0
Z3559392588	66.0	83.7	85.4	88.7	88.1	86.9	86.8	85.6	84.4	0
Z1407899729	66.0	131.0	93.0	91.7	84.5	87.9	87.0	82.7	79.7	0
Z1443864314	66.0	129.3	95.0	89.2	86.5	90.2	87.5	80.7	78.1	0
Z50106757	66.0	88.1	88.0	83.6	85.4	83.6	89.5	86.7	90.7	0
Z1255380138	66.0	136.3	93.7	92.4	86.6	91.3	81.6	85.5	78.3	0
Z1313381195	66.0	138.0	96.4	92.7	85.1	89.7	82.9	84.5	78.9	0
Z1116571364	66.0	85.0	88.3	91.9	88.0	87.6	88.7	84.8	86.7	0
Z49711282	66.0	87.8	88.8	90.8	88.7	88.9	84.7	89.5	84.7	0
Z56788250	66.0	88.2	88.0	88.1	89.4	88.9	91.0	90.2	87.0	0
Z2998111045	66.0	130.5	94.1	93.9	93.5	93.2	86.5	81.2	81.4	0
Z3295148399	66.0	119.8	91.6	93.1	90.0	88.0	87.7	90.8	84.4	0
Z3649501061	66.0	126.3	96.0	92.6	91.1	92.1	87.8	85.4	81.5	0
PV-002421112068	66.0	89.3	90.8	91.0	89.7	86.5	88.6	88.2	91.7	0
Z202503096	66.0	141.3	99.5	92.2	89.1	91.5	86.7	87.8	82.3	0
Z225905608	66.0	131.5	95.4	94.9	91.6	95.0	88.0	87.6	85.4	0
Z3295209363	66.0	125.3	94.6	94.9	89.9	90.1	93.7	88.5	87.4	0
Z2146195633	66.0	133.0	96.7	92.9	91.7	93.3	91.3	91.6	97.2	0
Z29467739	66.0	85.7	90.2	92.9	92.2	89.1	92.9	96.6	101.8	0
Z285779920	66.0	140.8	101.8	93.2	93.1	97.6	108.8	125.5	170.5	0

Dose-response testing of 68 compounds ordered from Enamine

Rank	Molecule Name	Enamine ID	IC50 (uM)	C 0.5 (% ne	C 1.0	C 2.1	C 4.1	C 8.2	C 16	C 33	C 66	Active
1	SMSSF-0632603	PV-001918010086	0.5	93.2	40.8	21.0	11.6	8.1	6.6	5.9	8.6	1
2	SMSSF-0632555	Z1172208679	2.1	78.2	66.2	45.9	25.2	10.3	7.8	7.1	6.0	1
3	SMSSF-0632596	Z734854148	0.5	116.4	69.3	50.5	24.2	11.4	8.8	7.1	10.3	1
4	SMSSF-0632587	Z3634004206	3.4	79.7	74.1	63.1	33.9	9.9	6.0	6.2	5.3	1
5	SMSSF-0632588	Z3638513333	4.4	85.3	78.5	72.0	47.9	11.8	4.5	3.5	3.4	1
6	SMSSF-0632594	Z71174619	4.8	72.8	63.2	54.6	43.7	33.6	19.4	10.5	8.3	1
7	SMSSF-0632589	Z49571468	4.9	85.7	77.9	70.4	54.4	19.6	8.0	5.6	5.7	1
8	SMSSF-0632536	Z3225506284	6.1	80.1	67.9	67.8	53.2	33.5	15.1	9.0	8.6	1
9	SMSSF-0632580	Z3557629872	6.8	88.1	83.0	81.0	68.8	35.0	10.4	5.5	4.5	1
10	SMSSF-0632584	Z3558428795	9.1	85.0	81.5	81.0	73.0	50.9	14.3	6.5	6.2	1
11	SMSSF-0632567	Z2739840324	3.9	119.8	86.5	82.0	68.2	47.7	15.7	7.3	9.8	1
12	SMSSF-0632565	Z240359708	2.4	126.3	91.8	81.4	72.5	47.3	19.4	7.6	8.5	1
13	SMSSF-0632583	Z3557781825	10.8	86.8	84.3	79.5	76.0	58.9	24.2	8.8	6.2	1
14	SMSSF-0632560	Z1763598930	0.5	132.0	91.3	82.4	73.1	56.0	24.0	9.9	9.5	1
15	SMSSF-0632544	PV-001914484112	12.4	85.5	85.9	85.4	79.8	63.8	30.9	8.0	5.0	1
16	SMSSF-0632542	Z666250890	48.2	81.6	75.7	67.9	60.5	55.0	45.8	30.8	25.8	1
17	SMSSF-0632566	Z2618185084	66.0	121.5	88.3	82.6	75.7	63.1	37.5	9.1	7.2	1
18	SMSSF-0632577	Z3395547714	12.6	87.7	87.0	82.8	83.9	71.1	28.1	8.0	6.1	1
19	SMSSF-0632579	Z3484513235	12.1	89.2	89.7	86.1	80.1	66.8	30.2	10.3	6.7	1
20	SMSSF-0632576	Z3347084877	11.5	91.4	87.2	87.5	84.5	67.7	26.5	10.9	6.3	1
21	SMSSF-0632551	Z109132782	15.5	83.3	88.0	77.3	74.0	62.2	41.1	24.7	12.3	1
22	SMSSF-0632574	Z3242476057	35.4	123.9	94.4	86.1	81.9	68.7	40.8	9.4	8.4	1
23	SMSSF-0632592	Z666485712	13.9	87.7	86.1	87.4	85.7	72.9	38.0	11.4	9.3	1
24	SMSSF-0632554	Z114886052	21.0	86.6	83.3	82.5	75.9	67.8	47.8	24.9	9.2	1
25	SMSSF-0632549	PV-002161956828	15.7	87.8	89.6	89.8	83.9	70.5	43.8	15.8	5.7	1
26	SMSSF-0632545	PV-001915624464	7.0	80.0	78.9	78.9	71.7	53.7	44.8	39.8	36.9	1
27	SMSSF-0632602	Z3652859018	66.0	125.3	92.1	86.0	86.3	74.4	49.5	15.4	10.8	1
28	SMSSF-0632581	Z3557629875	22.2	90.0	90.6	92.1	86.8	76.4	62.5	22.7	7.2	1
29	SMSSF-0632543	Z1741972899	37.8	88.5	87.6	87.0	80.1	77.6	62.3	36.5	11.0	1
30	SMSSF-0632548	PV-002140113355	24.9	84.6	87.5	88.0	89.1	80.0	65.2	29.9	8.9	1
31	SMSSF-0632575	Z3297024656	66.0	140.0	94.7	97.5	91.0	83.1	62.3	25.1	10.1	1
32	SMSSF-0632595	Z734817070	20.2	86.5	85.7	83.3	80.3	80.3	68.4	50.3	43.6	0
33	SMSSF-0632569	Z2976359863	66.0	136.0	100.0	89.3	86.0	86.7	74.1	49.7	28.3	1
34	SMSSF-0632552	Z1101543176	66.0	83.7	86.8	87.7	82.8	76.5	63.1	60.3	65.1	0

Gitter Lab: Alnammi M. et al., “Scalable supervised learning for synthesize-on-demand chemical libraries.” manuscript in prep

VS for ultra-large virtual libraries

- LBVS with RF and fingerprints easily scales to 1.0 billion cpds
- SBVS study required 5 million CPU hours to evaluate 1.3 billion cpds.
  - Gorgulla, C., et al., “An open-source drug discovery platform enables ultra-large virtual screens.” Nature 2020,580, 663–668.
- Another SBVS used 27,612 GPUs to score 1.37 billion in < 24 hours.
  - Glaser, J., et al., “High-throughput virtual laboratory for drug discovery using massive datasets.” The International Journal of High Performance Computing Applications.
- We have applied SBVS in consensus docking screens with 6 programs on libraries up to ~40 million cpds.

TIERED APPROACH FOR SBVS

Synthesized-on-demand virtual library
10 – 100 billion cpds (SMILES)

PROPERTY FILTER

1 – 10 billion cpds (SMILES)

ROCS

0.1 – 5 billion cpds (3D)

Fast Docking

5-200 million cpds

Consensus Docking

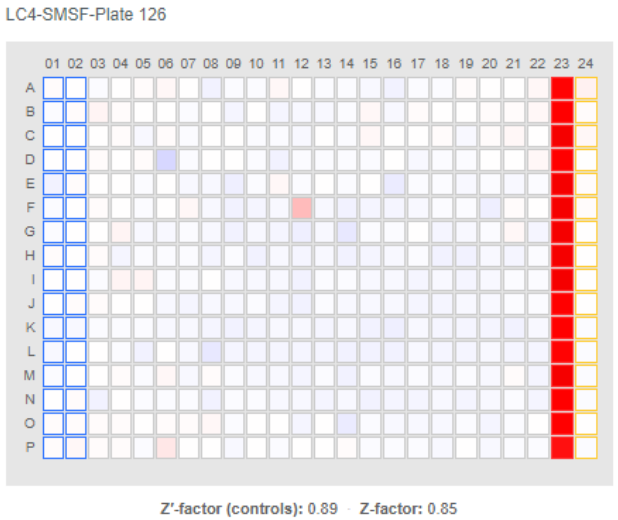
2-20k cpds

clustering

50-500 cpds

$$$

MD/ML-based affinity?



Conclusions

HTC is a fabulous resource for VS.

Rapid cycles of development, testing, validation of VS

Scaling to ultra-large virtual chemical libraries.

Access to large numbers of GPU nodes might enable CNN-based scoring in docking or rigorous MD-based approaches for absolute ligand binding free energy.

Acknowledgments

- CHTC Facilitators:

  Lauren Michael & Christina Koch

- Tony Gitter & Michael Newton

  - “A Machine Learning Platform for Adaptive Chemical Screening.” 1R01GM135631-01A1

- UWCCC-Drug Development Core

  Tim Bugni, Mike Hoffmann, Weiping Tang

- Computational Chemists

  Scott Wildman, Moayad Alnammi, Ken Satyshur

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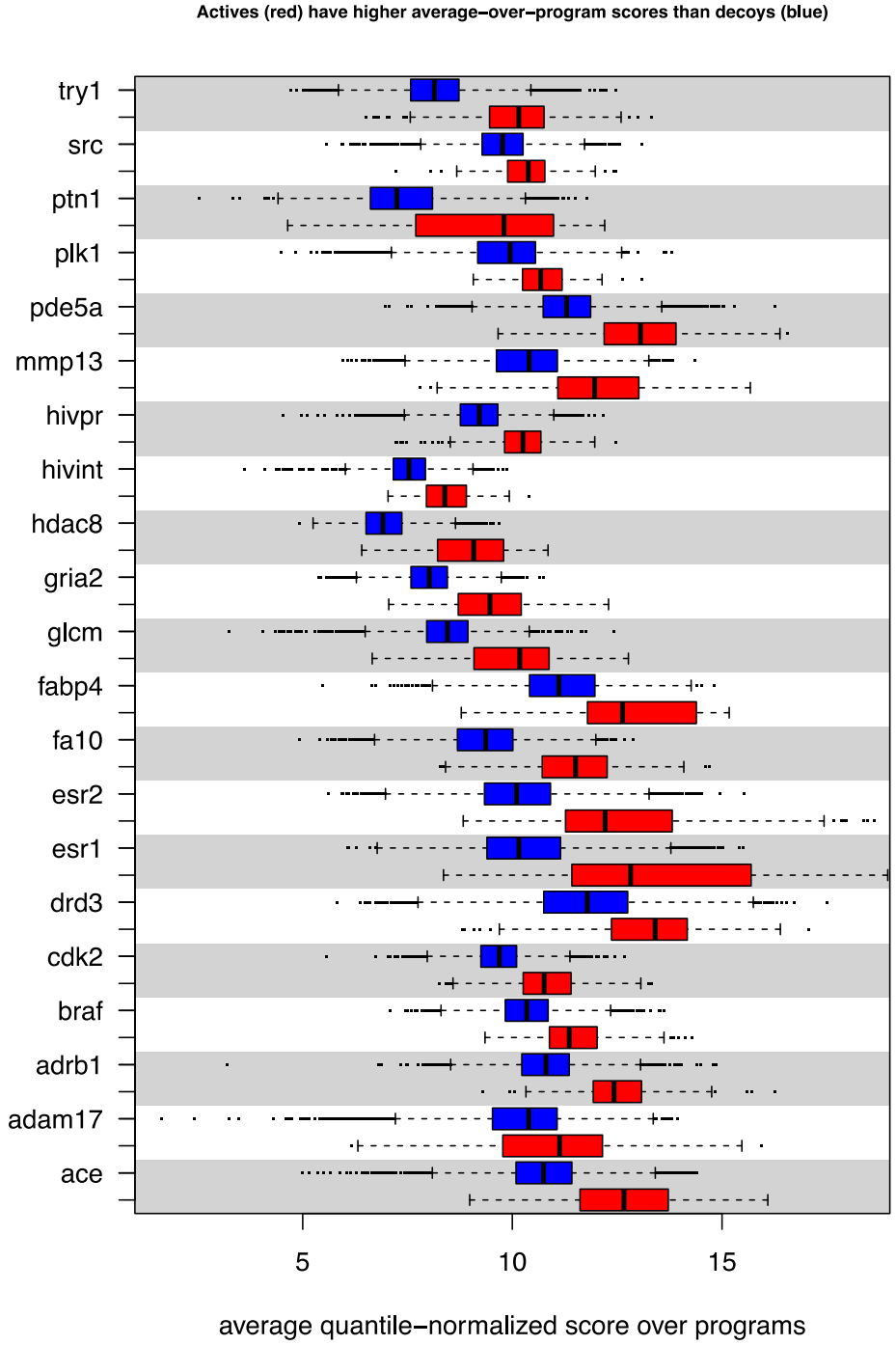
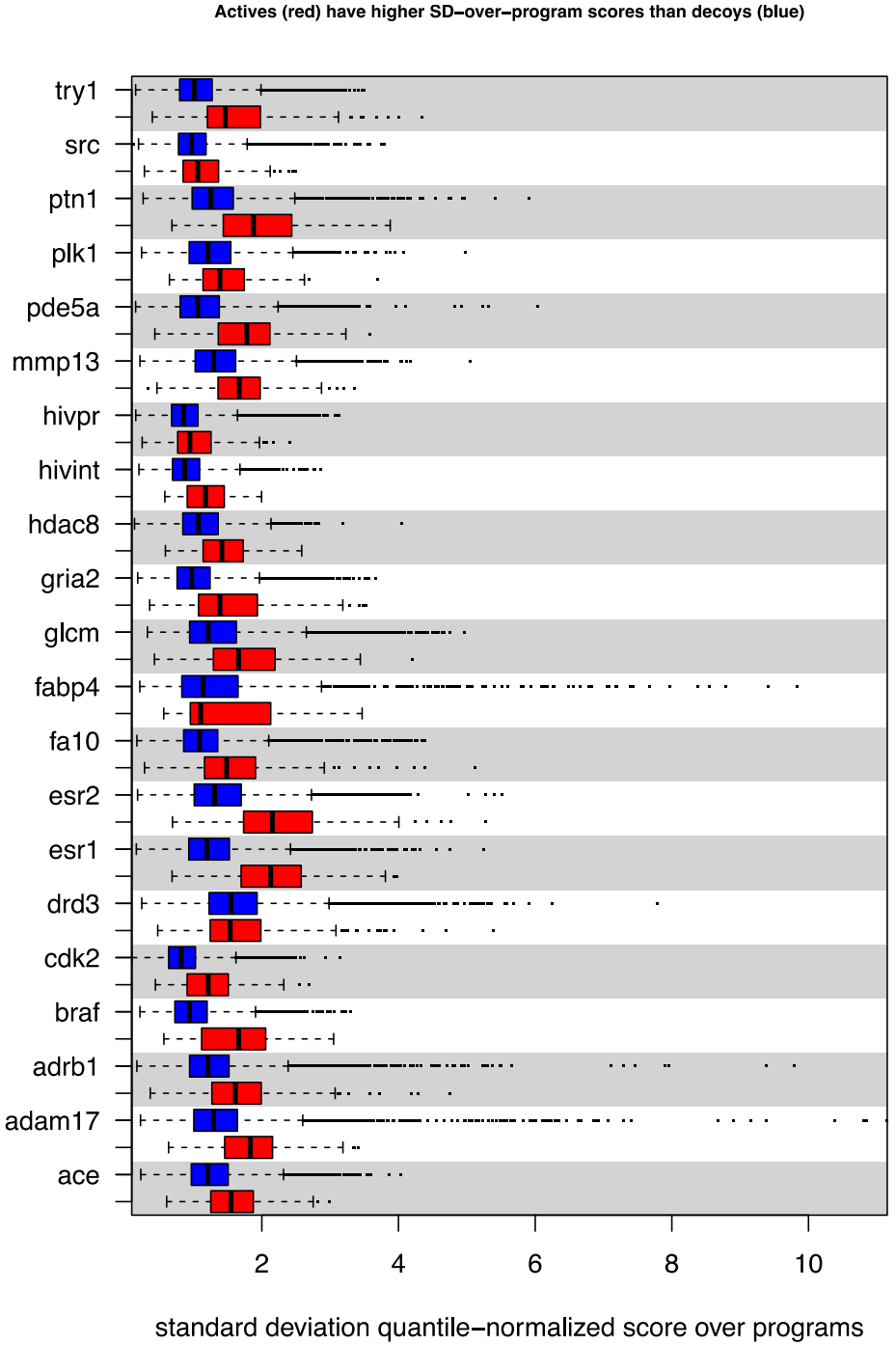
Extras





- Score distribution of actives (red) is shifted relative to inactives (blue).
- Interestingly, the standard deviation in scores was also higher for actives than for decoys

Ericksen et al., J. Chem. Inf. Model. **2017**, 57, 7, 1579-1590
DOI: 10.1021/acs.jcim.7b00153