

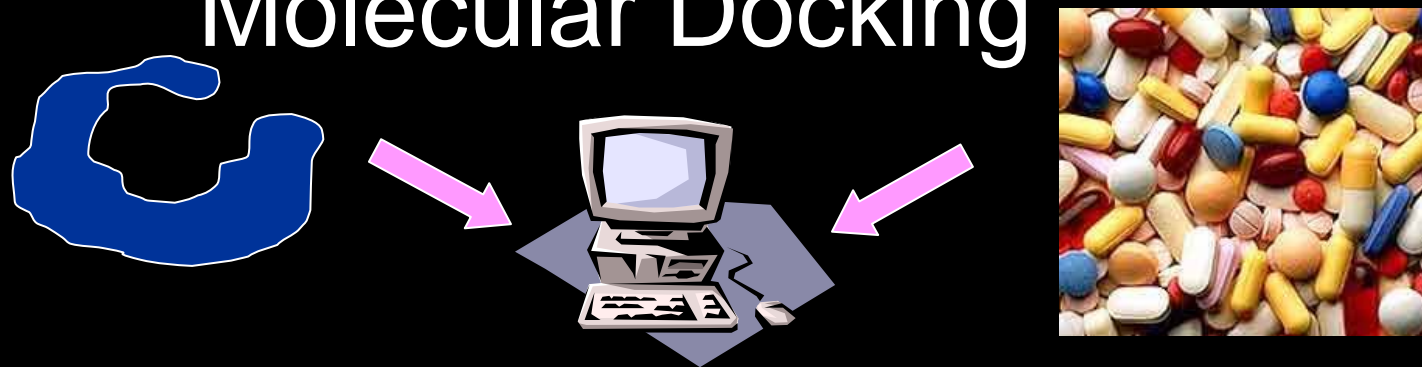
Molecular Docking Workshop with DOCK Blaster

John Irwin
Monday 3pm

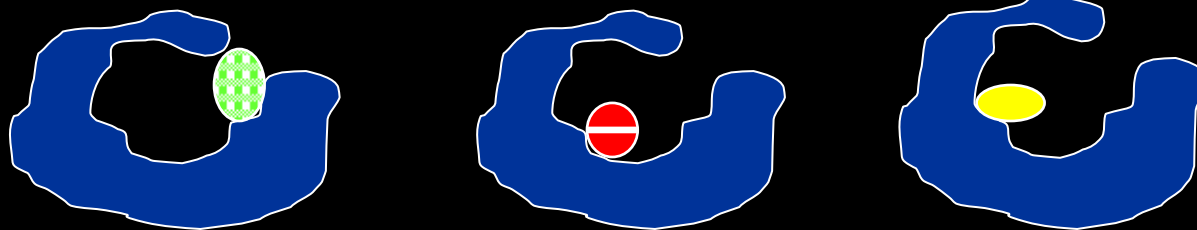
Outline

- 1. Very Brief Introduction to docking
- 2. A DOCK Blaster run
- 3. A hit picking party
- 4. Example presentation
- 5. Introduction to set problems

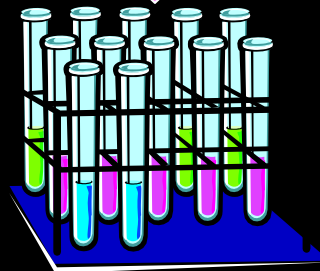
Screening for Novel Inhibitors by Molecular Docking



dock



**Test high-scoring
molecules**



Why is docking so difficult?

Binding sites are complicated

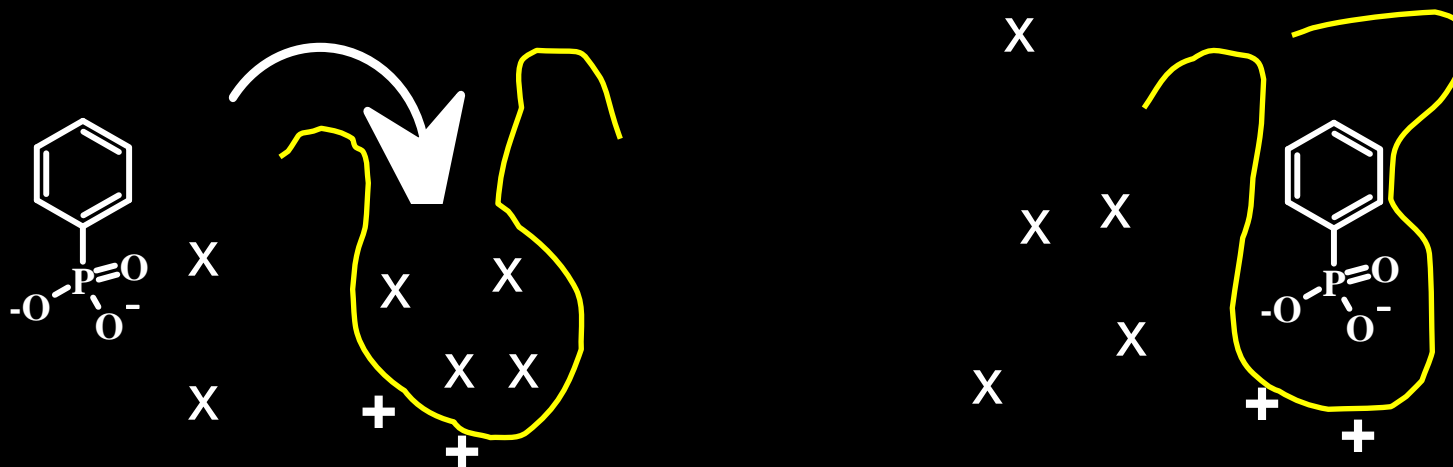
Lots of interactions to consider

Everything in competition with water

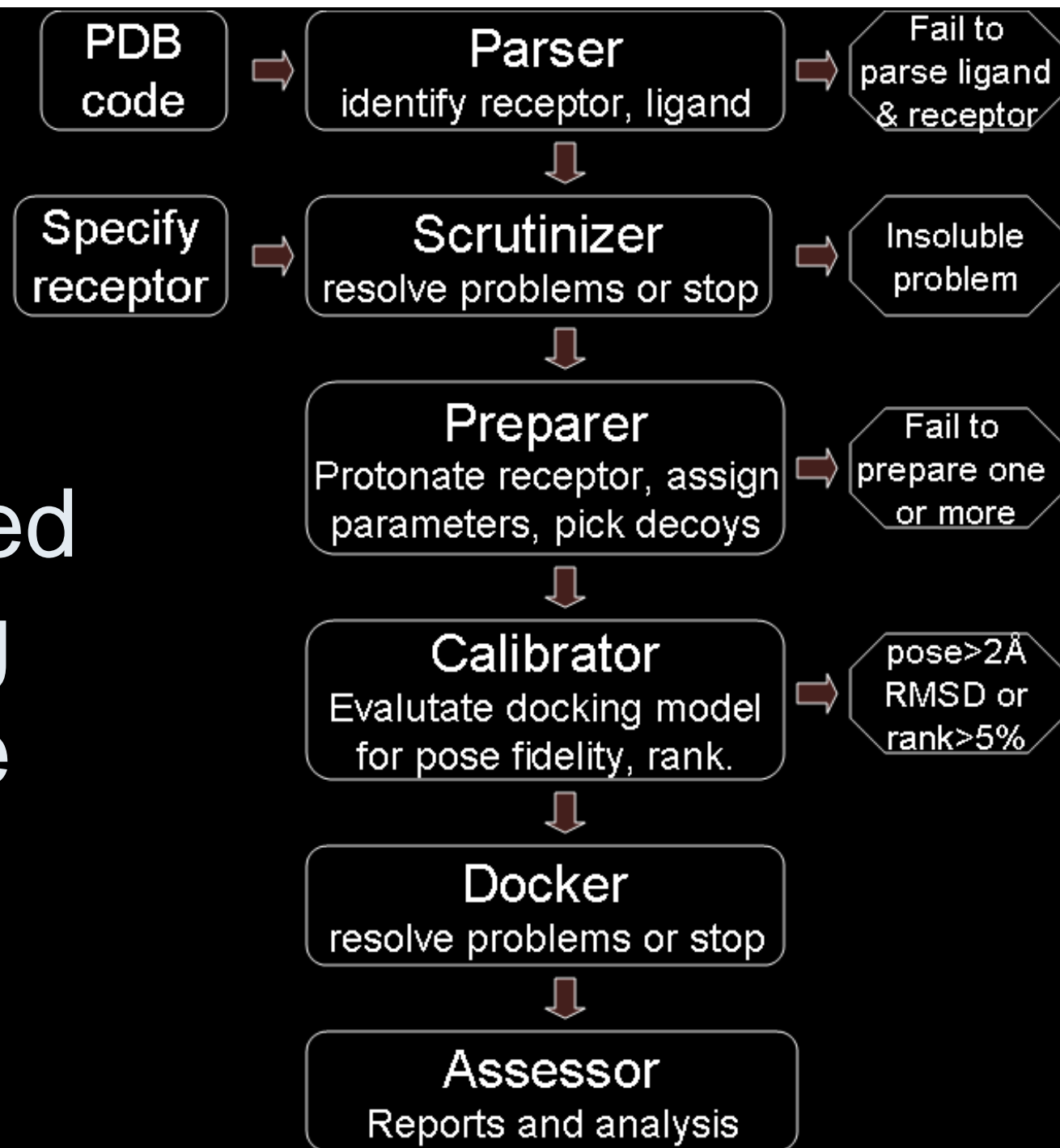
$$K_d = e^{-\Delta G/RT}$$

$$\Delta G_{\text{bind}} = \Delta G_{\text{inter}} - \Delta G_{\text{solv}}$$

small large large

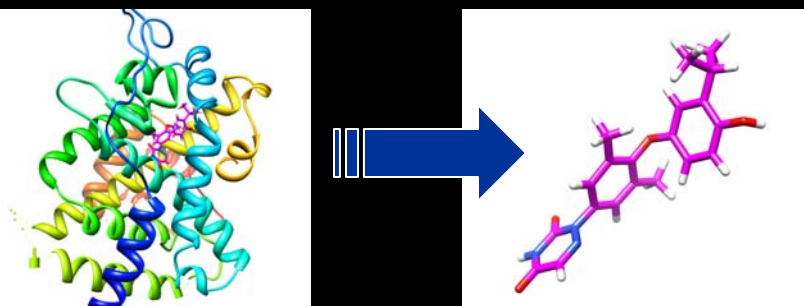


Automated docking pipeline

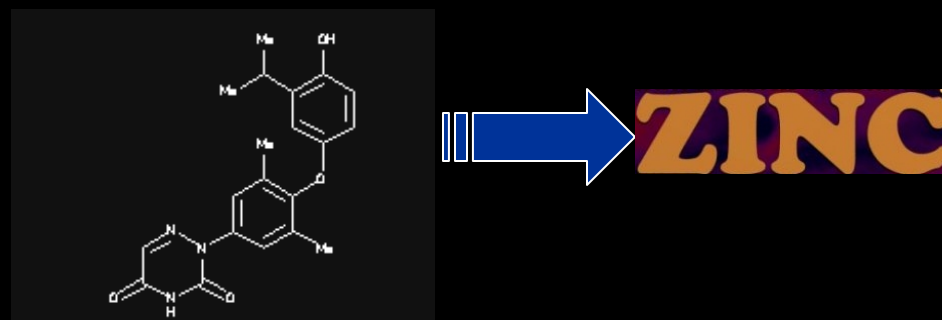


Automatic self-assessment

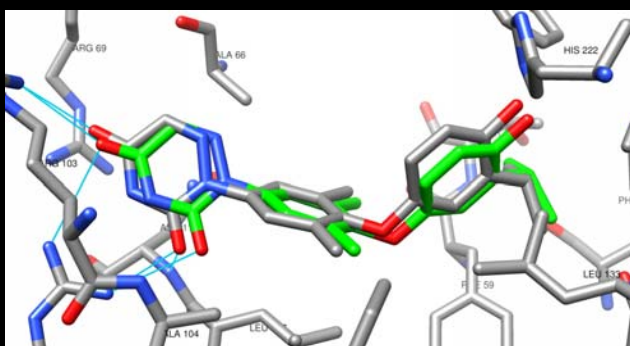
1. Remove ligand from receptor



2. Rebuild ligand without bias



3. Dock ligand and 100 physically-matched decoys using 4 parameter sets



4. Evaluate pose-fidelity, enrichment

| | | Scoring | |
|----------|----------------|------------------|---------------|
| Sampling | | <i>Polarized</i> | <i>Normal</i> |
| | <i>Coarser</i> | 3.61 Å / 1% | 1.32 Å / 9% |
| | <i>Finer</i> | 1.32 Å / 2 % | 2.02 Å / 3% |

Starting point: <http://blaster.docking.org>
Choose: Start with a PDB code

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DOCK Blaster v1.0.1

Home | DOCK | Documentation | Mailing Lists

Welcome to... answer the... which I have...

DOCK Blaster... University of... al., "Autom...

Get started
Start with a structure
Start with a PDB code
I'm Feeling Lucky
Query a Job
Browse Jobs

service for [structure-based ligand discovery](#). DOCK Blaster aims to... should I purchase and test for activity against my biological target for...

laboratory in the Department of Pharmaceutical Chemistry at the... (SF). To cite DOCK Blaster, please reference Irwin, Shoichet, Mysinger et al., "Automated... study.", *J. Med. Chem.* **2009**, 52(18), pp 5712-5720.

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.

A product of [BCIRC](#), the Bioinformatics and Chemical Informatics Research Center @ UCSF. Last updated Aug 6, 2009. Please direct correspondence as follows: questions and discussion to [blaster-fans at docking.org](#); bug reports to [support at docking.org](#); any other correspondence to comments at [docking.org](#). [Terms of use](#). [Privacy policy](#).

Pick a PDB Code for docking. Click DOCK! We will give you a list of codes to try

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Dock PDB target

Home | **DOCK!** | Documentation | Mailing Lists

Preparer Scrutinizer Target Prep Calibration Docking Results
Q'd Run Done Q'd Run Done Q'd Run

Welcome to the DOCK Blaster Parser, where you can start docking with just a PDB code*
To start you need a target (and sometimes a ligand). To get a PDB code: (* restrictions apply)

- To find a PDB code, you may [search the PDB](#).
- For a demonstration that will work, try human thyroid receptor beta (PDB code 1N46).
- You may pick from a list of 9870 eligible structures containing a ligand
- Or if you want to take your chances, try clicking: "I'm Feeling Lucky" (below)

Some [documentation](#) is available.

PDB Code : ([9870 eligible PDB structures with ligand](#), PDB 2008-08)

Ligand : (optional)

Email : (optional)

The aim of this experiment is :

By clicking "DOCK!" you agree to the [Terms and Conditions](#)

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Check OK, and click DOCK! to confirm

The screenshot shows a web browser window with the URL `http://blaster.docking.org/cgi-bin/parser.pl`. The page header includes the UCSF logo and navigation links. The main content area is titled 'Parser' and features a large 'DOCK Blaster' logo. Below the logo, there are tabs for 'Home', 'DOCK!', 'Documentation', and 'Mailing Lists'. The 'DOCK!' tab is selected. The page displays a summary of a docking job with the following details:

- PDB code: 1N46
- Ligand to be used: PFA
- Resolution: 2.20
- ion:
- coef
- name THYROID HORMONE RECEPTOR BETA-1

Below the summary, a message states: 'Looks OK... If you would like to proceed, please click "DOCK!" below:'. The 'DOCK!' button is highlighted with a red circle. At the bottom, the report date is 'Tue Dec 8 15:01:34 PST 2009' and a warning message says: 'Please do not reload this page or you will attempt to launch an identical job!'.

The preliminary calculation has started.
Take a note of the Job number. Wait.

Still running... Wait 40 minutes or so....
(if everything looks ok, perhaps try SEA while waiting...)

The screenshot shows a web browser window with the URL http://blaster.docking.org/cgi-bin/jobwatch.pl?job_id=39669&pin=. The page header includes the UCSF logo and navigation links. The main content area displays 'Watching Job #39669' and a progress bar with stages: Preparer, Scrutinizer, Target Prep (highlighted in yellow), Calibration, Docking, and Results. Below the progress bar, it shows 'Files supplied: Receptor, Ligand' and 'Status: Target preparation in progress'. A 'Time in this state: 15s. (typically 1800s)' is shown, along with 'Cancel request' and 'Reload page' buttons. The 'Reload page' button is circled. On the right, there is a 'Leave A Message' button and a 'Live Help Offline' button. At the bottom, there is a footer with contact information and links to 'Get Chimera!' and 'Get Pymol!'.

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Watching Job #39669

Home DOCK! Documentation Mailing Lists

Preparer Scrutinizer **Target Prep** Calibration Docking Results

Q'd Run Done Q'd Run Done Qd Run

Files supplied: [Receptor](#), [Ligand](#).

Status: Target preparation in progress

Time in this state: 15s. (typically 1800s) [Cancel request](#) [Reload page](#)

Report date: Tue Dec 8 15:02:20 PST 2009

[Leave A Message](#)

[Live Help Offline](#)

[Get Chimera!](#) [Get Pymol!](#)

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Wait 40 minutes or so...

Target preparation finished, now doing calibration (watch the yellow highlight move right...)

The screenshot shows a web browser window with the URL `http://blaster.docking.org/cgi-bin/jobwatch.pl?job_id=39669&pin=`. The page header includes the UCSF logo and navigation links. The main content area displays the job status for "Job #39669". A progress bar at the top of the job status section shows the following stages: "Preparer", "Scrutinizer", "Target Prep", "Calibration", "Docking", and "Results". The "Calibration" stage is highlighted in yellow and circled with a black oval. Below the progress bar, the text "Files supplied: [Receptor](#), [Ligand](#)." is visible. The status is "Calibration docking queued". A "Time in this state: 45s. (typically 7200s)" is shown, with "45s." circled. Below this, there are "Cancel Job" and "Reload page" buttons. The report date is "Tue Dec 8 15:18:14 PST 2009". At the bottom, there is a footer with contact information and links to "Get Chimera!" and "Get Pymol!".

Watching Job #39669

Home DOCK! Documentation Mailing Lists

Preparer Scrutinizer Target Prep Calibration Docking Results

Files supplied: [Receptor](#), [Ligand](#).

Status: Calibration docking queued

Time in this state: 45s. (typically 7200s) Calibration docking queued. You are first in the queue.

Cancel Job Reload page

Report date: Tue Dec 8 15:18:14 PST 2009

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20 minutes later.....

Calibration done. Are the results any good?

Watching Job #39669

Home DOCK! Documentation Mailing Lists

Preparer Scrutinizer Target Prep Calibration Docking Results
Q'd Run Done Q'd Run Done Q'd Run

Files supplied: [Receptor](#), [Ligand](#).

Status: Calibration docking complete

Summary Report of Calibration Docking ([What is this?](#))

| | | Scoring | |
|----------|---------|-----------|-----------|
| | | Polarized | AMBER |
| Sampling | Coarser | 0.703 / 0 | 0.742 / 0 |
| | Finer | 0.704 / 0 | 0.876 / 0 |

Detailed reports: [plots](#) and [poses and scores](#)

RMDS / % RANK

Congratulations! You are now eligible for database docking ([How to use this](#))

| Sampling | Scoring | Database type | Database (#) number of molecules |
|----------|-----------|---------------|----------------------------------|
| Coarser | Polarized | By Property | clean-fragments (#12) 120727 |

If you have any doubts, please consider screening the "clean fragments" (subset 12) first. Three reasons: 1. it will be done faster. 2. fragments are less complex, and therefore more efficient than leads for sampling chemical space. 3. you can still dock the leads afterwards. Still not convinced? Fragments dock in hours, leads can take days, even a week.

When you are ready to start docking, click Only one database at a time, please!

4 ways to dock: which one is best?

Calibration runs for job 41412 × ZINC - A Free database for... × DOCK Blaster - A Free Virtu... ×

http://blaster.docking.org/results/02/41412/browseprelim.html

zinc blog blaster Raphael livehelp otrs disi logs IP Address Locator - ... Google Apps 401 Authorization Re... Other bookmarks

Browse calibration runs to pick best sampling (coarser, finer) and scoring (Polarized, AMBER)

Number of molecules in each list given in (parentheses).

| Coarser/Polarized | Coarser/AMBER | Finer/Polarized | Finer/AMBER |
|-----------------------------|-----------------------------|-----------------------------|-----------------------------|
| ligand (1) | ligand (1) | ligand (1) | ligand (1) |
| similar (1) | similar (1) | similar (1) | similar (1) |
| decoys (1) | decoys (1) | decoys (1) | decoys (1) |
| extrema (1) | extrema (1) | extrema (1) | extrema (1) |
| random (1) | random (1) | random (1) | random (1) |

All preliminary docking subtasks appear to have ended cleanly...

Review calibration data

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Watching Job #39669

Home DOCK! Documentation Mailing Lists

Preparer Scrutinizer Target Prep Calibration Docking Results

Files supplied: Receptor, Ligand

Status: Calibration docking complete

Summary Report of Calibration Docking (What is this?)

| | Scoring | |
|---------|-----------|---------|
| | Polarized | AMBER |
| Coarser | 0.75215 | 0.75215 |
| Finer | 0.75475 | 0.63615 |

Detailed reports: [plots](#) and [poses and scores](#).

Congratulations! You are now eligible for database docking ([How to use this?](#))

| Sampling | Scoring | Database type | Database (#) number of molecules |
|----------|-----------|---------------|----------------------------------|
| Coarser | Polarized | By Property | clean fragments (12) 120727 |

If you have any doubts, please consider screening the "clean fragments" (subset 12) first. Three reasons: 1. it will be done faster. 2. fragments are less complex, and therefore more efficient than leads for sampling chemical space. 3. you can still dock the leads afterwards. Still not convinced?

[Get Chimeral](#) [Get Pymol](#)

DOCK Blaster - A Free Virtu... ZINC - A free database for... DOCK Blaster - A Free Virtu...

http://blaster.docking.org/cgi-bin/resultsbrowser.pl?job_id=41412&i=decoys&j=1&k=A&pin=

zinc blog blaster Raphael livehelp otrs disi logs IP Address Locator - ... Google Apps 401 Authorization Re... Other bookmarks

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Results Browser Job #41412

Home DOCK! Documentation Mailing Lists

Preparer Scrutinizer Target Prep Calibration Docking Results

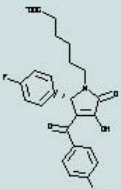
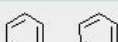
Files supplied: [Receptor](#), [Ligand](#)

Visualize using: [CHIMERA](#) [PYMOL](#) [Important note about broken molecules.](#)

Download hits: [PDB](#) [SDF](#) [CEL1](#) [mol2](#)

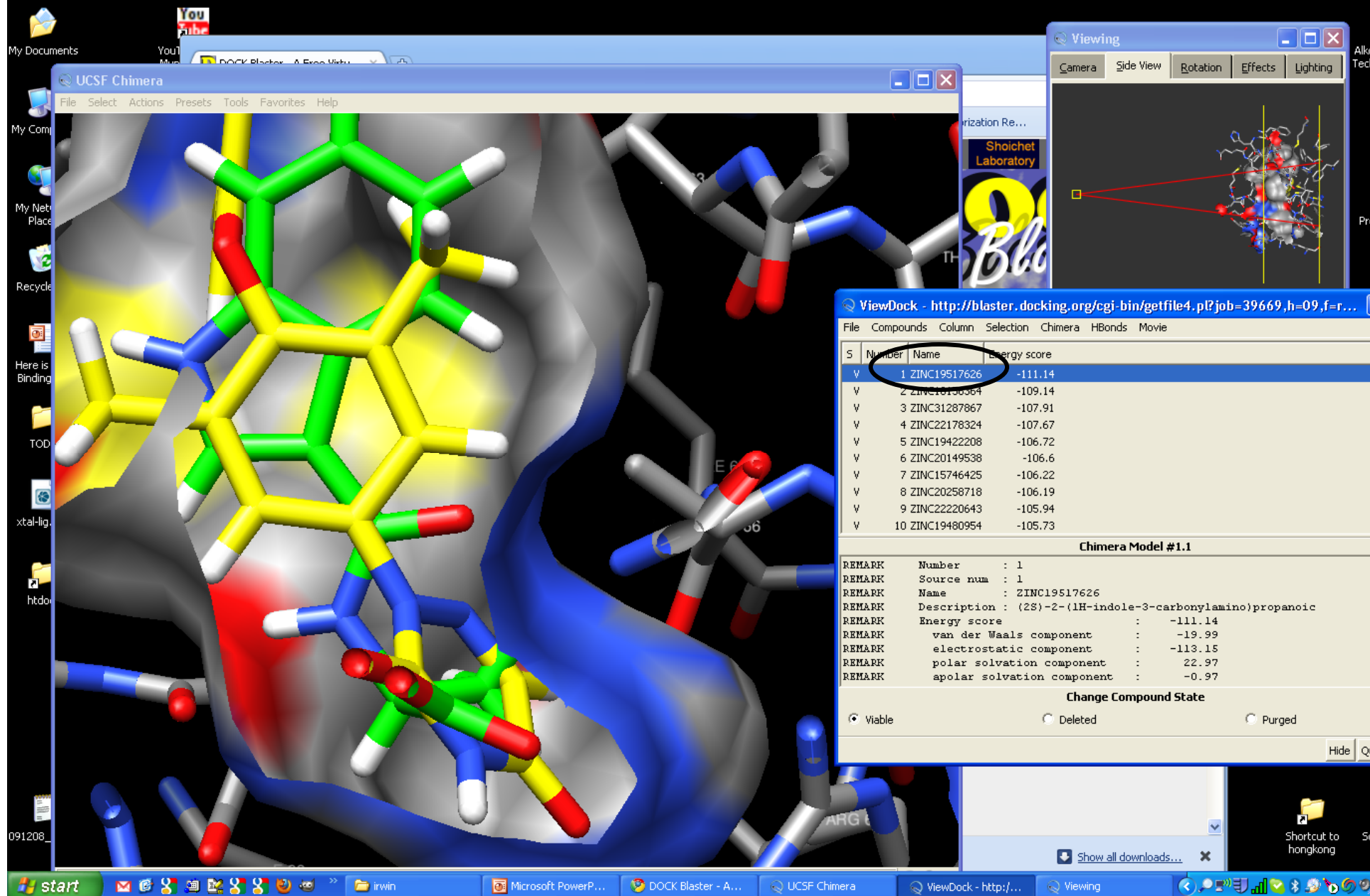
[Leave A Message](#)
[Live Help Offline](#)

[Get Chimeral](#) [Get Pymol](#)

| Rank | ZINC ID | Compound | Availability | Properties | Annotations |
|------|------------------------------------|---|--|---|-------------|
| 1 | 9370567 -114.34 |  | Asinex: BAS01029113 IBScreen: STOCK2S-66522 Pharmeks: PHAR041448 ChemBridge: 5951033 Aurora Fine Chemicals: kbsb-0079151 | Mwt: 489.317 xLogP: 4.15 Charge: -1 RotBond: 9 # Protomers: 3 Contact: 159 ES: -106.35 VdW: -26.24 Desolv: p=19.61, ap=-1.36 | |
| 2 | 32242205 |  | | Mwt: 486.592 | |

[PDB](#)

Review hits in Chimera...



Calibration done. Are the results any good?

Watching Job #39669

Home DOCK! Documentation Mailing Lists

Preparer Scrutinizer Target Prep Calibration Docking Results
Q'd Run Done Q'd Run Done Qd Run

Files supplied: [Receptor](#), [Ligand](#).

Status: Calibration docking complete

Summary Report of Calibration Docking ([What is this?](#))

| | | Scoring | |
|----------|---------|-----------|-----------|
| | | Polarized | AMBER |
| Sampling | Coarser | 0.703 / 0 | 0.742 / 0 |
| | Finer | 0.704 / 0 | 0.876 / 0 |

Detailed reports: [plots](#) and [poses and scores](#).

Congratulations! You are now eligible for database docking ([How to use this](#))

| Sampling | Scoring | Database type | Database (#) number of molecules |
|----------|-----------|---------------|----------------------------------|
| Coarser | Polarized | By Property | clean-fragments (#17) 120727 |

If you have any doubts, please consider screening the "clean fragments" (subset 12) first. Three reasons: 1. it will be done faster. 2. fragments are less complex, and therefore more efficient than leads for sampling chemical space. 3. you can still dock the leads afterwards. Still not convinced? Fragments dock in hours, leads can take days, even a week.

When you are ready to start docking, click **DOCK** Only one database at a time, please!

Click on DOCK to run a docking calculation.
This may take 8 hours or so, depending...
So it would be ideal to launch docking no
later than Wednesday at 4pm.

The screenshot shows a web browser window with several tabs. The active tab is titled "DOCK Blaster - A Free Virtu...". The address bar shows the URL "http://blaster.docking.org/cgi-bin/jobaction.pl". The browser's toolbar includes a back button, which is circled in red. The page content features the UCSF logo and navigation links. A large banner for "DOCK Blaster" is visible. Below the banner, there are navigation buttons: "Home", "DOCK!", "Documentation", and "Mailing Lists". A progress bar shows the status of various steps: "Preparer", "Scrutinizer", "Target Prep", "Calibration", "Docking", and "Results". The "Calibration" step is highlighted in yellow and marked "Done". Below the progress bar, a message states: "Queuing docking calculation for job 39669" and "paranoia: whew, database subset1 / 12 exists". A bold message reads: "A docking job has been queued on your behalf!". A reminder text says: "We remind you that you may only dock one big database at a time, and that docking can take a while. Please check back again tomorrow to check on your results. Bye!". At the bottom, a footer provides contact information for BCIRC and docking.org.

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Job 39669 Action

Home DOCK! Documentation Mailing Lists

| Preparer | Scrutinizer | Target Prep | Calibration | Docking | Results |
|----------|-------------|--------------|--------------|---------|---------|
| | | Q'd Run Done | Q'd Run Done | Q'd Run | |

Queuing docking calculation for job 39669
paranoia: whew, database subset1 / 12 exists

A docking job has been queued on your behalf!

We remind you that you may only dock one big database at a time, and that docking can take a while. Please check back again tomorrow to check on your results. Bye!

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Leave A Message
Live Help Offline

This is what it looks like when done.

John - Google Wave DOCK Blaster - A Free Virtu...

http://blaster.docking.org/cgi-bin/jobwatch.pl?job_id=39669&pin=

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Watching Job #39669

Home DOCK! Documentation Mailing Lists

Preparer Scrutinizer Target Prep Calibration Docking **Results**

Q'd Run Done Q'd Run Done Qd Run

Files supplied: [Receptor](#), [Ligand](#).

Status: Docking complete

Summary Report of Calibration Docking ([What is this?](#))

| | | Scoring | |
|----------|---------|-----------|-----------|
| | | Polarized | AMBER |
| Sampling | Coarser | 0.703 / 0 | 0.742 / 0 |
| | Finer | 0.704 / 0 | 0.876 / 0 |

Detailed reports: [plots](#) and [poses and scores](#).

Large database docking results available

Browse

[subset 12](#)
(num entries)

[tani 90%](#)
[tani 80%](#)
[tani 70%](#)
[tani 60%](#)

Leave A Message
Live Help Offline

Get Chimera! Get Pymol!

Review docking hits, use CHIMERA

DOCK Blaster - A Free Virtu...

http://blaster.docking.org/cgi-bin/resultsbrowser.pl?job_id=39669&i=run.128pin=

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Results Browser

Job #39669

Home DOCK! Documentation Mailing Lists

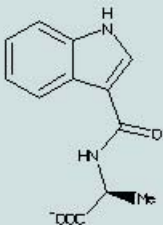
Preparer Scrutinizer Target Prep Calibration **Docking** Results

Q'd Run Done Q'd Run Done Q'd Run

not finished
These incomplete results of a running job are 7 minutes old. Please wait 25 minutes to refresh
Files supplied: [Receptor](#), [Ligand](#),
Visualize using: [CHIMERA](#) [PYMOL](#) [Important note about broken molecules](#).
Download hits: [PDB](#) [SDF](#) [EEL1](#) [mol2](#)

[Leave A Message](#)
[Live Help Offline](#)

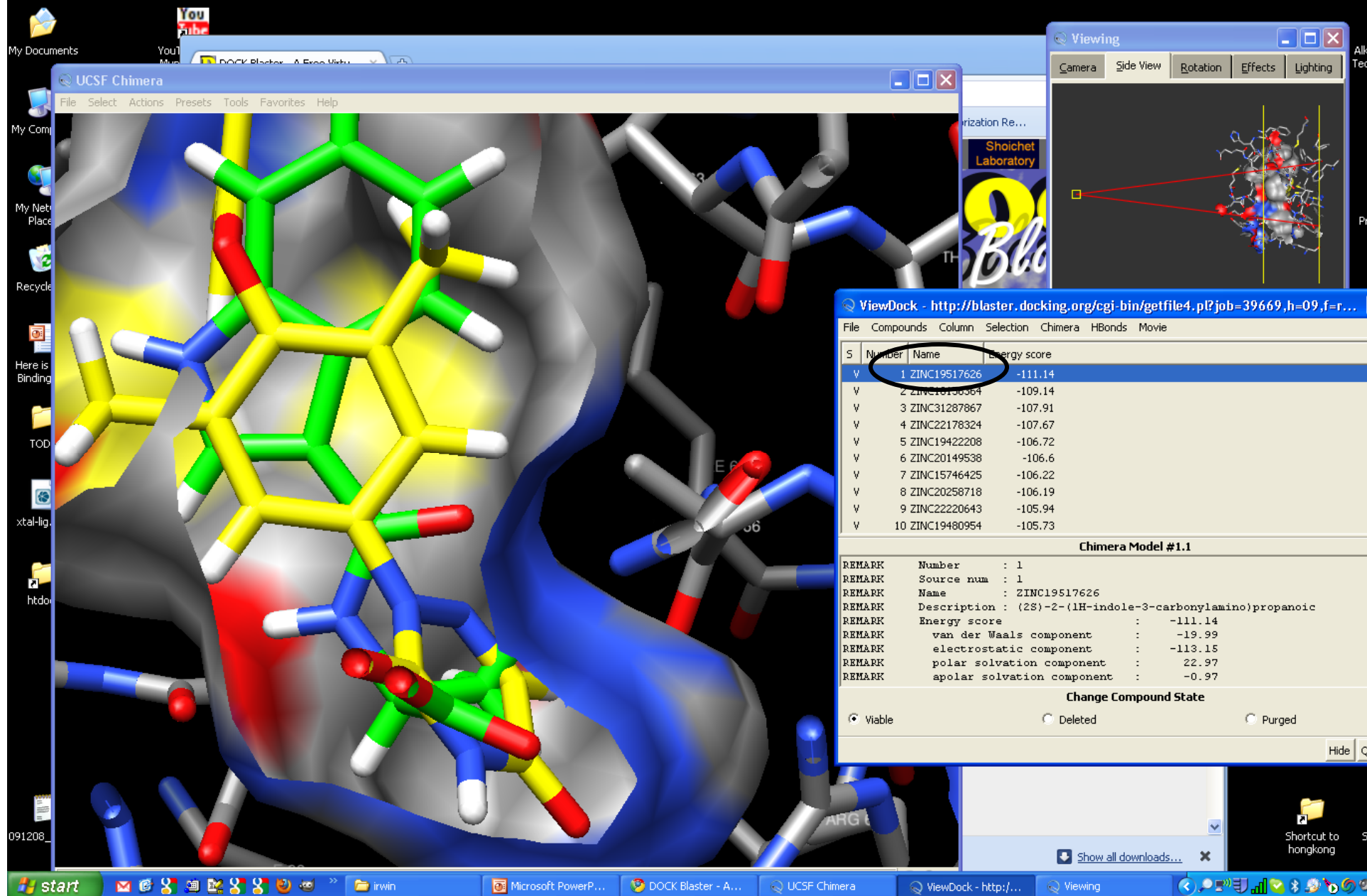
[Get Chimera!](#) [Get Pymol!](#)

| Rank | ZINC ID | Compound | Availability | Properties | Annotations |
|------|-------------------------------------|---|--|--|-------------|
| 1 | 19517626 -111.14 |  | Aurora BuildingBlocks:bb-kuk-083487 UkrOrgSynthesis (Depleted):BBV-087716 Ambinter:BBV-087716 Aurora Feinchemie:bb-kuk-083487 | Mwt: 231.231 xLogP: -0.60 Charge: -1 RotBond: 3 # Protomers: 1 Contact: 160 ES: -113.15 VdW: -19.99 Desolv: p=22.97, ap=-0.97 | |

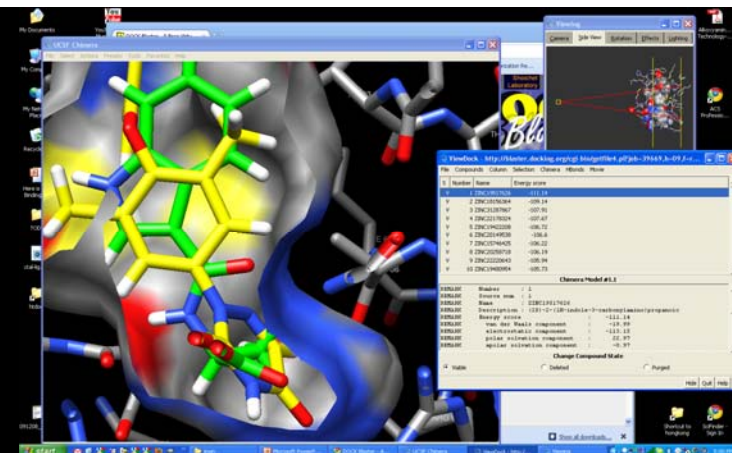
[PDB](#)

TimTec Building Blocks:SBB007469
Asinex:BAS00500340
Enamine (Depleted):T0505-2395

Review hits in Chimera...



How to run a hit picking party



- How ligand docks & in crystal structure
- How actives dock - common interactions, missed opportunities
- Look at the top 10. (watch out for broken)
- Look through the top 200 or so. Use A,B,C to classify your enthusiasm.
- Do this first with one other person, then with a group.

Types of Ligand-Protein Interactions

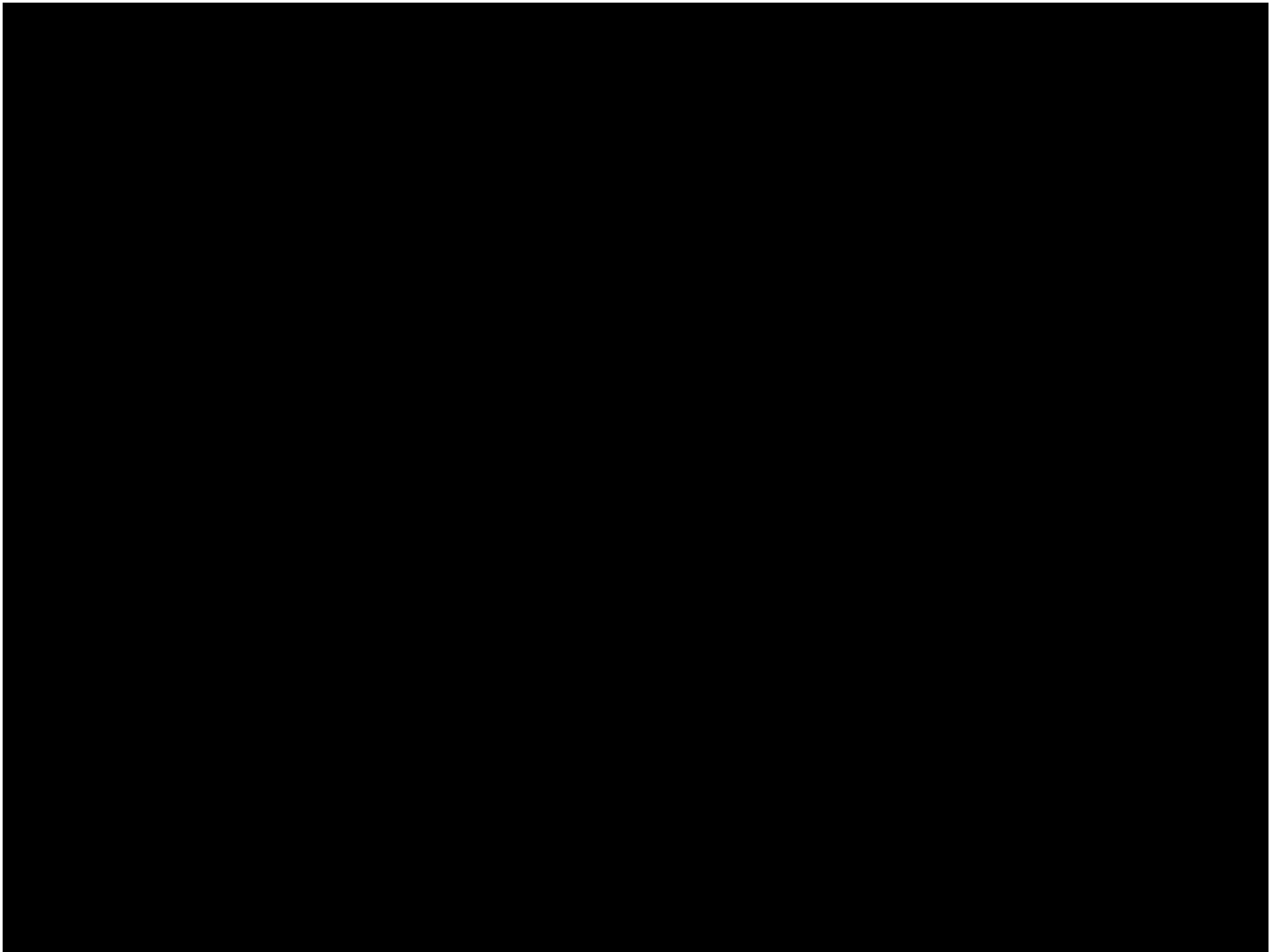
| Types of Interaction | Strength | Effect of Distance |
|----------------------|-------------|-------------------------------|
| Covalent | V. Strong | long range |
| Ionic | V. Strong | $1/r$, long range |
| Ion-Dipole | Strong | $1/r^2$, short range |
| Dipole-Dipole | Moderate | $1/r^3$, short range |
| Hydrogen Bond | Moderate | $1/r^3$ (?) short range |
| Ion-Induced Dipole | Weak | $1/r^4$, v. short range |
| Dispersion | V. Weak | $1/r^6$, ext. short range |
| Repulsion | Ext. Strong | $1/r^{12}$, ext. short range |
| “Hydrophobic” | Weak | ?? |

Example final presentation

- 1: Introduce the protein and binding site
- 2: Show the ligand, discuss how it binds
- 3: Calibration? Controls?
- 4-7. Show the four compounds you liked best. How different are they from precedented compounds? Show in 2D and 3D. Rotate if possible. Purchasable? Properties? likes/dislikes

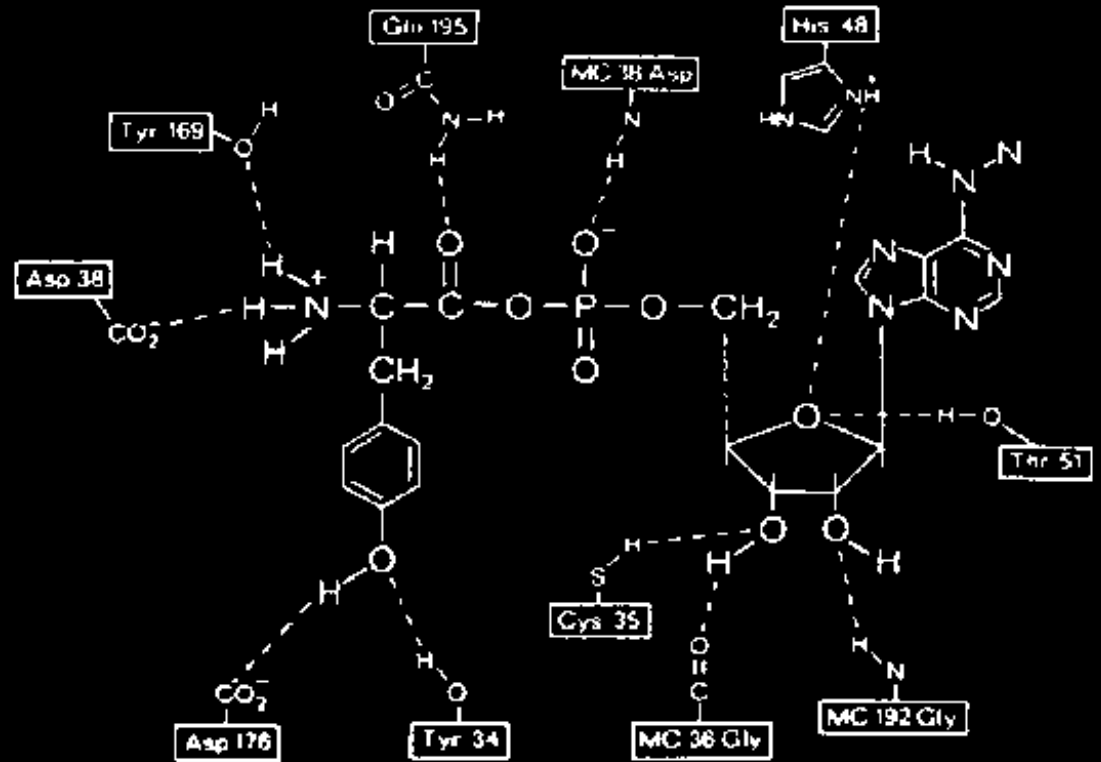
Now it is your turn....

- Monday evening
 - DOCK Blaster Set problems.
 - Work on at most 2 (to avoid overloading the server)
 - Work in groups of 1 or 2
- Wednesday
 - Dock to your own target.
 - Pick something that
 - A. you are interested in / know about
 - B. works with DOCK Blaster
- Thursday
 - Hit picking parties
 - Group presentations



Non-covalent Interactions in Proteins

A.R Fersht, *Nature* (1985)



| Energies in Vacuo | | | Energies in Protein Complexes (binding sites) | | |
|-------------------|----------------|-----------------|---|----------------|-----------------|
| donor | acceptor | energy kcal/mol | donor | acceptor | energy kcal/mol |
| dipole | dipole | ~ -6.5 | dipole | dipole | -0.5 to -1.5 |
| dipole | induced dipole | ~ -3 | dipole | induced dipole | ~ 1 |
| charged | dipole | -13 to -20 | charge | dipole | -3 to -5 |
| charged | charged | ~ -50 | charge | charge | -3 to -5 |

How to run a group hit picking party

- Same as for 1 or 2, except only show specific molecules, not all molecules
- Solicit explanations for why people prefer one molecule or another.
- Disagreements can be interesting, and didactic.

DOCK Blaster - A Free Virtu... Index of /2010/decoyfor78... ZINC - A free database for... DOCK Blaster - A Free Virtu...

http://blaster.docking.org/cgi-bin/jobwatch.pl?job_id=41412&pin=

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Shoichet Laboratory docking

Watching Job #41412

Home DOCK! Documentation Mailing Lists

Preparer Scrutinizer Target Prep Calibration Docking Results

Q'd Run Done Q'd Run Done Q'd Run

Files supplied: [Receptor](#), [Ligand](#).

Status: Calibration docking complete

[Leave A Message](#)

[Live Help Offline](#)

[Get Chimera!](#) [Get F](#)

Summary Report of Calibration Docking ([What is this?](#))

| | | Scoring | |
|----------|---------|-----------|-----------|
| | | Polarized | AMBER |
| Sampling | Coarser | 1.105 / 0 | 1.128 / 0 |
| | Finer | 1.098 / 0 | 1.035 / 0 |

Detailed reports: [plots](#) and [poses and scores](#).

Congratulations! You are now eligible for database docking ([How to use this](#))

| Sampling | Scoring | Database type | Database (#) number of molecules |
|----------|-----------|---------------|----------------------------------|
| Coarser | Polarized | By Property | clean-fragments (#12) 120727 |

If you have any doubts, please consider screening the "clean fragments" (subset 12) first. Three reasons: 1. it will be done faster. 2. fragments less complex, and therefore more efficient than leads for sampling chemical space. 3. you can still dock the leads afterwards. Still not convinced? Fragments dock in hours, leads can take days, even a week.

When you are ready to start docking, click [DOCK](#). Only one database at a time, please!

go (10).chimerax go (9).chimerax NMDZ1_RAT.smi

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Q'd Run Done Q'd Run Done Q'd Run

s supplied: [Receptor](#), [Ligand](#),




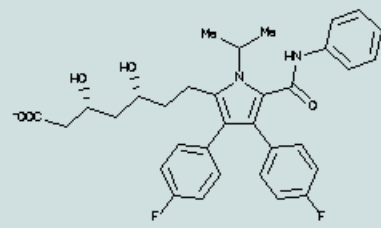
alize using: [CHIMERA](#) [PYMOL](#) [Important note about broken molecules](#).

vnlod hits: [PDB](#) [SDF](#) [EEL1](#) [mol2](#)

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| Rank | Compound | Availability | Properties | Annotations |
|---|---|--|---|-------------|
| ZINC ID re kcal/mol | | | | |
| 1 <input type="checkbox"/> 6052413 -139.01    PDB |  | Individual Suppliers:882_1_3CD7 Individual Suppliers:UNNAMED00000089 Individual Suppliers:882 Individual Suppliers:385219 | Mwt: 575.632 xLogP: 5.75 Charge: -1 RotBond: 12 #Protomers: 1 Contact: 248 ES: -122.64 VdW: -37.27 Desolv: p=23.40, ap=-2.50 | |

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HPP (1) How ligand looks

Ligand poses well

e.G ligand poses badly

HPP (2) How actives look

Actives look good

Actives look bad

HPP (3) Look at the top 10

Examples of good

Examples of bad, broken

Actual example (7 slides)

- So, here it goes....