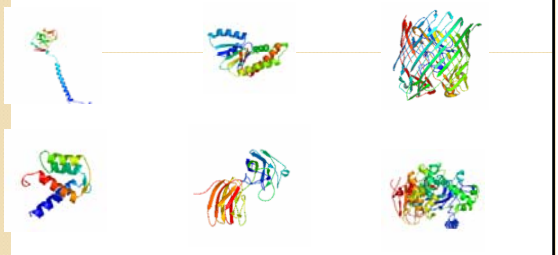
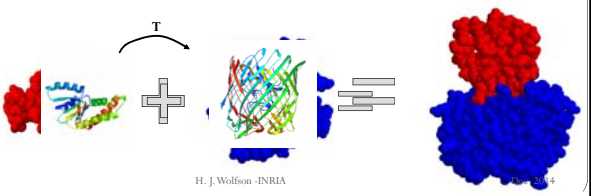
Molecular Docking – Part II

Flexible Docking



Docking Problem

- **Input**: A pair of molecules in their native conformation
- **Goal**: Find their correct association as it appears in nature



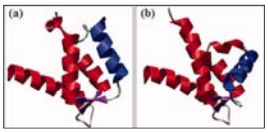
Small Molecule Flexibility

Docking and Flexibility

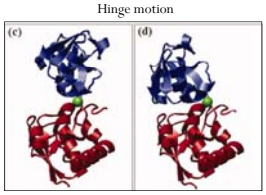
- Which types of molecules are docked?
  - Protein + small molecule
  - Protein + protein
  - …
- Which types of flexibility are taken into account?
  - Large-scale hinge-bent motions
  - Small-scale side-chain motions
  - Small molecule torsional flexibility
  - …
- Which molecules are considered as flexible?
  - Receptor, ligand or both

Handling Protein Backbone Flexibility in Docking

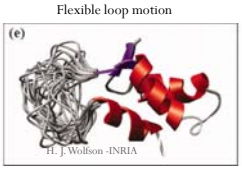
Shear motion



Hinge motion



Flexible loop motion

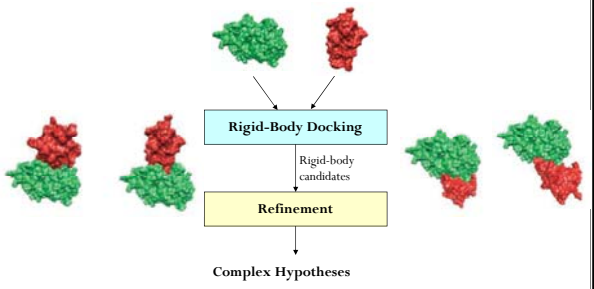


FireDock

Fast Interaction REfinement in molecular DOCKing

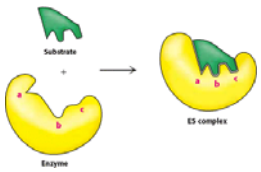
N. Andrusier, R. Nussinov, H. J. Wolfson, *FireDock: Fast Interaction Refinement in Molecular Docking*, Proteins, 69, 139—159, (2007).

General Docking Flow



Flexible Refinement Motivation

- Proteins are in constant motion
- Both backbone and side-chains change conformation
- The induced-fit model:
- Correct docking of the 'unbound' proteins may cause steric clashes
- Refine and re-score rigid-docking solutions



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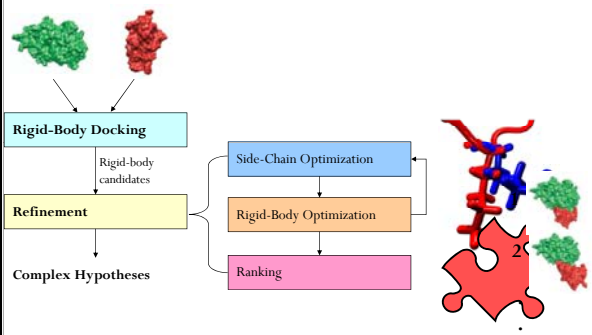
Refinement Flow



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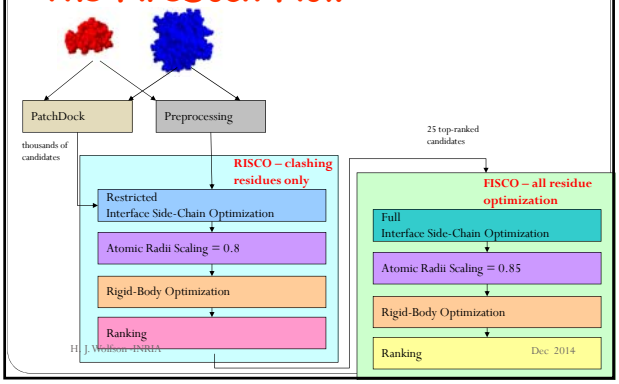
Goals

1. Top ranking of near native solutions
2. High-accuracy solution
3. Fast

FireDock

The FireDock Flow



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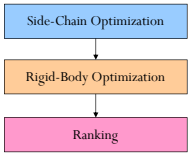
The Refinement Stages



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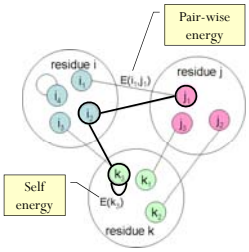
Interface Side-Chain Optimization

Graph Representation:

Choosing one node per residue

to minimize the weight of the induced sub graph

$$E_{GMEC} = \min_{r,s}\left(\sum_{i} E(i_r) + \sum_{i,j} E(i_r, j_s)\right)$$



GMEC = Global Minimal Energy Conformation

The Side Chain Optimization Problem was proven to be **NP-hard**

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The Linear Programming (LP) Technique

- A technique for optimization of a **linear function**
- Subject to **linear** equality and inequality **constraints**.
- Can be solved by a fast (polynomial time) method, supported by an efficiently implemented software package (CPLEX).

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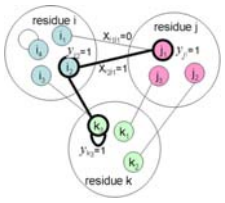
Formulation of ISCO as LP

$$y_{i_r} = \begin{cases} 1 & \text{rotamer } r \text{ was selected for residue } i \\ 0 & \text{rotamer } r \text{ was not selected for residue } i \end{cases}$$

$$x_{i_r j_s} = \begin{cases} 1 & \text{the edge } (i_r, j_s) \text{ is in the induced graph} \\ 0 & \text{the edge } (i_r, j_s) \text{ is not in the induced graph} \end{cases}$$



$$\text{Minimize} \sum_{(i,r)} E(i_r) y_{i_r} + \sum_{(i,r,j,s):i<j, j\in N(i)} E(i_r, j_s) x_{i_r j_s}$$

subject to:

$$\sum_r y_{i_r} = 1, \quad i \in V$$

$$\sum_r x_{i_r j_s} = y_{j_s}, \quad i \in V, j \in N(i)$$

$$0 \le x_{i_r} \le 1 \quad i, j \in V$$

$$0 \le y_{i_r} \le 1 \quad i \in V$$

Not linear!

V – set of movable residues

$N(i)$ – interacting residues of residue i

In 99.9% the LP solution is integral

FireDock

Rigid-Body Optimization

Side-Chain Optimization

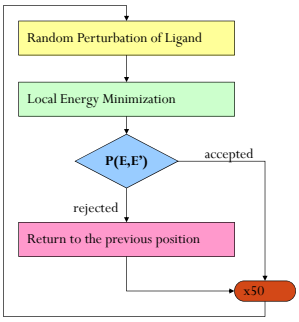
Rigid-Body Optimization

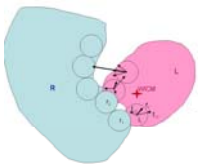
Ranking

- Why?
  - Soft rigid-body docking
  - Unresolved clashes
  - Surface was changed after ISCO
- How?
  - Energy Minimization
  - 6 Degrees of freedom

FireDock

Monte Carlo Minimization





Metropolis Criterion:

$$P(E,E') = \min\{\exp(\frac{E-E'}{C_b T}),1\}$$

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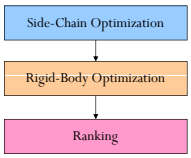
The Refinement Stages



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The Binding Model

- Binding score:
  - ACE
  - Electrostatics
  - Hydrophobic interactions
  - van der Waals
  - …

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Atomic Contact Energy

- ACE - desolvation free energies required to transfer atoms from water to a protein's interior.
- Estimated from known crystal structures.
- Introduced by *Miyazawa & Jernigan 96'. Zhang et al. 97'* extended this approach to the atomic contacts.
- Calculated over atoms pairs within 6Å distance:

$$\Delta G_{ACE} = \sum_i \sum_j e_{ij}$$

e_{ij} - effective free energy change when a bond between two atoms of type i and j is replaced by solute-solvent bonds.

$$e_{ij} \propto -\frac{n_{ij} n_{00}}{n_{i0} n_{j0}}$$

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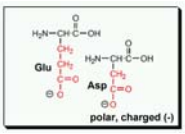
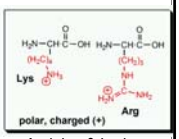
Electrostatics

- Electrostatics
  - Coulomb:

$$E_{elec} = \sum_{i,j} 332 \frac{q_i q_j}{d_{ij}^2}$$



Glutamic & Aspartic Acids

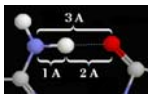


Arginine & Lysine

  - separated to attractive/repulsive and short/long range categories
- Hydrogen Bonds

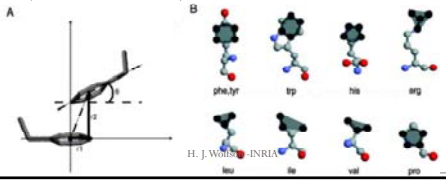
$$E_{HB} = \sum_{ij} \left(5\left(\frac{r_0}{d_{ij}}\right)^{12} - 6\left(\frac{r_0}{d_{ij}}\right)^{10} \right)$$

where 2.74 Å < d_{ij} < 3.5 Å, r_0 = 2.9 Å



π-stacking & Aliphatic Interactions

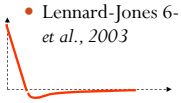
- E_{pipi} - π-π interactions
  (Phenylalanine, Tyrosine, Tryptophan, Histidine, Proline)
- E_{catpi} - cation-π interactions
  (Arginine, Lysine) – (Phenylalanine, Tyrosine, Tryptophan)
- E_{aliph} - aliphatic interactions
  (Leucin, Isoleucin, Valine)



Misura et al., 2004

van der Waals

- Lennard-Jones 6-12 potential with linear repulsion as in *Gray et al., 2003*

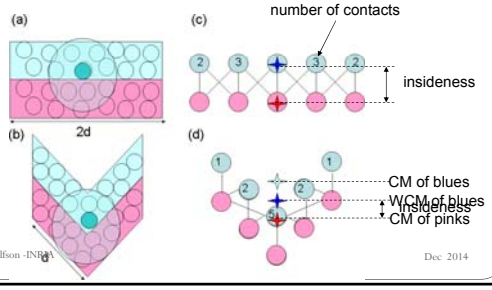


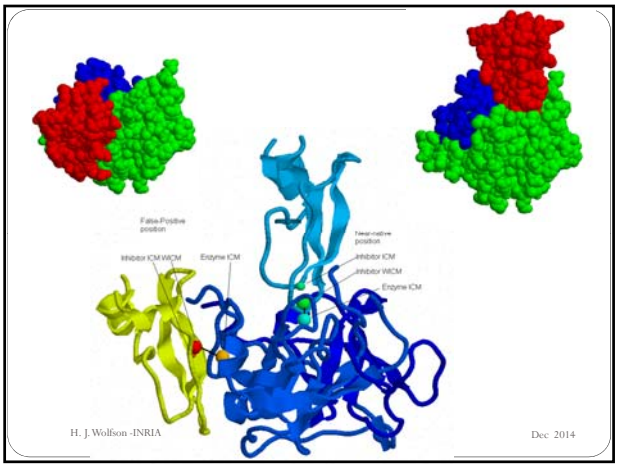
to avoid big penalty for small clashes

- based on CHARMM19

"Insideness" Term

For enzyme/inhibitor concave interfaces





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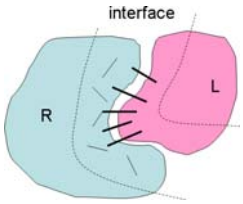
Binding Free Energy

$$\Delta G = G^C - (G^R + G^L)$$

$$\Delta G = G^{C}_{\text{interf\_inter}} + \Delta G^{L}_{\text{interf\_intra}} + \Delta G^{R}_{\text{interf\_intra}}$$



FireDock

Ranking – energy function

Antibody Antigen complex

$$E_{AA} = 1.5E_{s\_attrVdW} + 0.6E_{s\_repVdW} + 1.6E_{ACE} + 0.21E_{attEI} + 0.21E_{repEI} + 0.46E_{l\_attrEI} + 0.69E_{l\_repEI} + 1.2E_{HB+SS} + E_{pipi} + 0.7E_{catpi} + 2.5E_{aliph}$$

Enzyme Inhibitor complex

$$E_{EI} = E_{s\_attrVdW} + 0.95E_{s\_repVdW} + 1.6E_{ACE} + 0.07E_{attEI} + 0.12E_{repEI} + 0.3E_{l\_repEI} + 1.32E_{HB+SS} + E_{pipi} + 0.8E_{catpi} + 0.5E_{aliph} + 1.55E_{insideness}$$

Results

Type	PatchDock Medium Accuracy	PatchDock Acceptable Accuracy	FireDock Medium Accuracy	FireDock Acceptable Accuracy
Unbound Enz/Inh	2/26	7/26	21/26	25/26
Semi-unbound Enz/Inh	2/4	2/4	4/4	4/4
All Enz/Inh	4/30	9/30	25/30	29/30
Unbound Ant/Ant	1/9	1/9	2/9	4/9
Semi-unbound Ant/Ant	3/18	6/18	14/18	16/18
All Ant/Ant	4/27	7/27	16/27	20/27

☺ Significant improvement over PatchDock ranking
☺ Successful for EI and semi-unbound AA cases
☹ Unsuccessful for unbound AA cases
☺ On the benchmark 1.0 cases:

RosettaDock	PatchDock+FireDock
25/43 (3.61 Å)	30/43 (3.35 Å)

☺ Successful ranking in CAPRI "scorers" category.

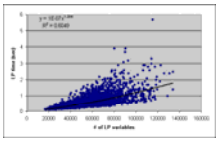
Contribution of Scoring Terms

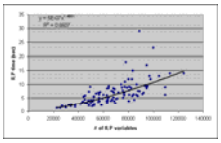
Reduction in Success Rate (%)	Scoring Terms
enzyme-inhibitor	
36	s_attrVdW
32	ACE
16	s_repVdW
8	insideness, attrEl, repEl
4	HB+SS, cstpi, aliph, LrepEl
antibody-antigen	
35	s_attrVdW
29	ACE
24	attrEl, repEl, pipi
18	LattrEl, LrepEl, aliph
12	s_repVdW, HB+SS

Success Rate (%)	Scoring Function
enzyme-inhibitor	
100	E_{El}
25	s_attrVdW
64	ACE
64	$1.6ACE + s\_attrVdW$
64	$1.6ACE + s\_attrVdW + 0.95s\_repVdW$
64	$1.6ACE + 0.05attrEl + 0.12repEl$
72	$1.6ACE + s\_attrVdW + 0.05attrEl + 0.12repEl$
76	$1.6ACE + 1.55insideness$
80	$1.6ACE + s\_attrVdW + 0.95s\_repVdW + 0.05attrEl + 0.12repEl$

Time Efficiency

FISCO LP FISCO ILP





Size (# of interface residues)	Pre-building (sec)	RISCO (sec)	RBO (sec)	All (sec)
60	0.05	0.08	1.28	1.4

- In RISCO LP/ILP is very fast (small number of variables)
- In 99.9 % of the cases the LP solution is integral
- RBO is a bottle-neck
- Pentium 4 CPU 3.2GHz 1GB RAM

FireDock

Conclusions

- Improves both accuracy and ranking of rigid docking solutions (created by PatchDock)
- Typical running time is 4 seconds per candidate
- Assumes rigidity of proteins backbone.

FiberDock

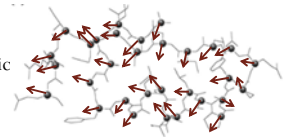
Flexible Induced-fit Backbone Refinement in Molecular Docking

E. Mashiach, R. Nussinov and H. J. Wolfson. FiberDock: Flexible induced-fit backbone refinement in molecular docking. Proteins 2009;78(6):1503-1519.

Normal Modes Analysis (NMA)

- Given a **single** conformation, NMA calculates a set of vectors (3N) which describes the flexibility of a protein.
- NMs span the conformational space
- The coeffic

(3,8,1)
(4,6,2)
(9,1,1)
(7,8,4)



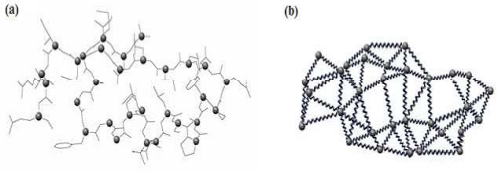
More details…

Tama and Sanejouand (2001)
Hinsen (1998)

Anisotropic Network Model (ANM)

- Simplified spring models of proteins

(a) (b)



$U(R_1, ..., R_N) = \sum_{i,j} U_{ij}(R_i - R_j)$

$U_{ij}(r) = k_{ij}(|r| - |(R_i^0 - R_j^0)|)^2$

$k_{ij} = exp(-\frac{|R_i^0 - R_j^0)|^2}{r_0^2})$

Back…

Figure from Andrusier et al. (2008)

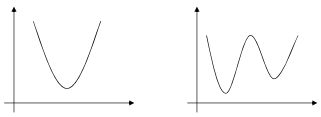
NMA - Advantages

- Similarity to true protein motions
- Conformations can change continuously
- The lowest frequency modes contribute the most to a conformational change (domains rearrangement)

Hinsen (1998)
May, M. Zacharias (2005)
Petrone and Pande (2006)

NMA - Disadvantages

- Describes only one conformation with minimum energy



Hinsen (1998)
Petrone and Pande (2006)

NMA - Disadvantages

- Describes only one conformation with minimum energy
- Can create distorted conformations
- High complexity in memory ($O(N^2)$) and in CPU time ($O(N^3)$)

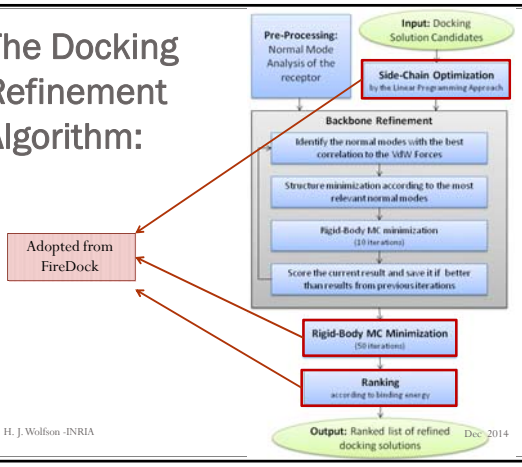
Hinsen (1998)

Petrone and Pande (2006)

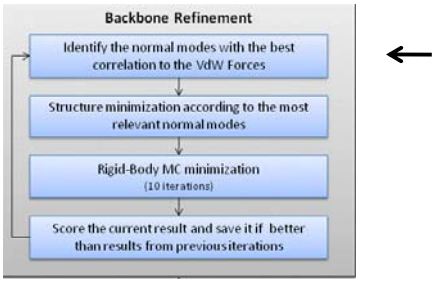
The Main Idea

- Flexible docking refinement which models both **backbone** and **side-chain** flexibility.
- Existing docking methods model backbone flexibility by using only the first few modes. We use an a-priori **unlimited** number of normal modes.
- Iteratively apply the **most relevant** modes on the flexible protein.
- The relevancy of a mode is calculated according to its correlation with the **chemical forces** applied on each atom.

The Docking Refinement Algorithm:



The Backbone Refinement Method:



Correlation Measurement

- The correlation between the forces (F) which are applied on the Cα atoms and a certain normal mode (Vi) is calculated in the following way:

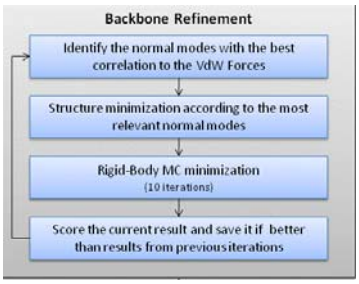
$$\mathrm{corr}(F, V_i) = \left| \frac{1}{m \cdot (V_i^{\mathrm{freq}})^2} \sum_{j=0}^{n} \vec{v_{ij}} \cdot \vec{f_j} \right|$$

Dot product:

$\mathbf{a} \cdot \mathbf{b} = |\mathbf{a}||\mathbf{b}| \cos\theta$

- Good correlation indicates that the directions of the forces suit the directions of the normal mode vectors.

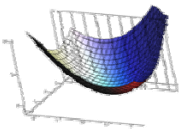
The Backbone Refinement Method:



Structure Minimization

- We use the *BFGS quasi-Newton* algorithm to locate a local energy minimum in the direction of the chosen (most relevant) normal modes.

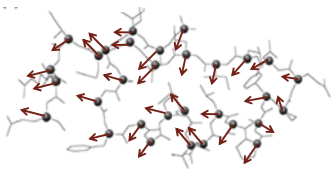
$$E = KE_{intVdW} + E_{repVdW} + \lambda \sum_{i=1}^{M} (V_i^{\mathrm{freq}})^2 |V_i^{\mathrm{amp}}|$$



- Finds the amplitude which produces a local energy minimum.

Changing the Protein Conformation

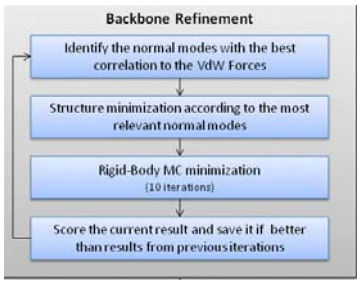
- NMs often distort the protein structure



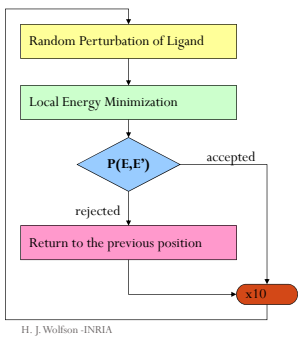
Changing the Protein Conformation

- NMs often distort the protein structure
- Goals:
  - Don't change bonds length and angles
  - Change only φ and ψ torsion angles
- Answer:
  Use a modification of the CCD robotics algorithm by Canutescu and Dunbrack, 2003.

The Backbone Refinement Method:



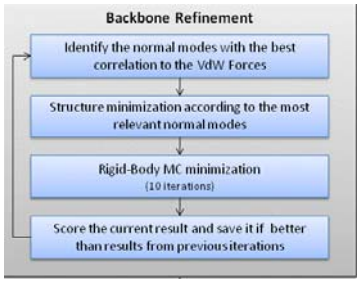
Monte Carlo Minimization



Metropolis Criterion:

$$P(E,E') = \min\{\exp(\frac{E-E'}{k_b T}),1\}$$

The Backbone Refinement Method:



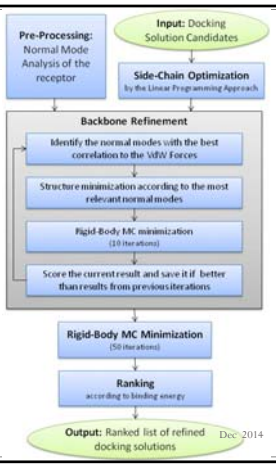
Scoring Function

- Contains the binding Van der Waals energy value (E_{vdw}) and a penalty term which depends on the amount of protein deformation.

$$E = KE_{attrVdW} + E_{repVdW} + \lambda \sum_{i=1}^{M} (V_i^{freq})^2 |V_i^{amp}|$$

- The penalty term prevents the algorithm from returning distorted solutions.

The Docking Refinement Algorithm:



Results

Test III: Docking refinement starting from rigid-body docking candidates

Test III

- For each test case we refined the first 500 rigid docking solutions of PatchDock.
- The results of the refinement with FiberDock and FireDock were compared

Table IV
Refinement of Right-Body Docking Solution Candidates (for Unbound Receptors and Bound Ligands)

	PatchDock		FireDock			FiberDock		
Complex ID	First acceptable[a]	Acceptables in top 20[b]	First acceptable[a]	Original PatchDock result[c]	Acceptables in top 20[b]	First Acceptable[a]	Original PatchDock result[c]	Acceptables in top 20[b]
1A0O	1* (7.66, 3.79)	3[f]	7 (6.34, 2.30)	29 (9.20, 3.15)	3[f]	16 (5.25, 3.33)	108 (5.19, 3.26)	1
1ACB	3 (6.17, 3.12)	2	3 (8.24, 4.31)	259 (8.67, 4.37)	1	2* (6.84, 4.01)	42 (6.12, 3.56)	4[f]
1AY7	14 (9.78, 5.27)	3	5* (1.37, 0.77)	95 (4.19, 1.29)	5[f]	5* (1.37, 0.77)	95 (4.19, 1.29)	5[f]
1BTH	1* (12.10, 3.65)	1	2 (10.11, 3.28)	72 (11.47, 3.63)	2	1* (7.98, 1.97)	403 (14.80, 3.55)	5[f]
1CGI	2 (3.82, 2.31)	1	1* (2.82, 2.25)	2 (3.82, 2.31)	10[f]	1* (5.42, 2.72)	279 (7.50, 2.97)	9
1DFJ	1* (6.84, 2.76)	4	1* (5.55, 2.03)	2 (4.78, 2.33)	6[f]	1* (3.10, 1.53)	5 (4.28, 2.13)	6[f]
1E6E	None	0	474 (6.01, 3.32)	134 (10.20, 4.25)	0	2* (8.38, 3.44)	327 (20.64, 7.46)	2[f]
1FIN	None	0	None	None	0	None	None	0
1GGI	3 (6.06, 3.24)	6[f]	25 (6.83, 3.37)	3 (6.06, 3.24)	0	1* (12.39, 3.77)	281 (11.23, 3.29)	2
1GOT	None	0	None	None	0	None	None	0
1IBR	32 (6.99, 2.78)	0	2* (5.01, 2.50)	208 (6.38, 2.85)	1	2* (6.67, 2.61)	32 (6.99, 2.78)	3[f]
1OAZ	58 (18.47, 3.84)	0	9* (14.41, 3.27)	204 (15.05, 3.59)	1[f]	16 (14.41, 3.27)	204 (15.05, 3.59)	1[f]
1PXV	51 (8.54, 4.03)	0	17 (6.94, 3.49)	54 (5.78, 3.39)	1	1* (8.86, 4.51)	63 (9.86, 4.57)	2[f]
1T6G	4 (8.10, 1.75)	1	1* (6.83, 1.33)	129 (14.78, 3.08)	10	1* (9.61, 1.80)	70 (13.51, 2.33)	11[f]
1TGS	15 (2.69, 1.54)	1	1* (1.94, 1.43)	15 (2.69, 1.54)	10	1* (1.94, 1.43)	15 (2.69, 1.54)	11[f]
1WQ1	6* (2.24, 1.42)	1[f]	20 (5.64, 2.35)	82 (5.40, 2.17)	1[f]	29 (8.92, 4.44)	445 (7.18, 2.95)	0
1ZHI	134 (13.44, 2.81)	0	10 (7.52, 2.73)	311 (8.43, 3.03)	2	4* (7.18, 3.48)	311 (8.43, 3.03)	3[f]
2BUO	1* (9.38, 5.39)	9[f]	3 (5.05, 3.91)	32 (4.87, 3.98)	3	12 (6.3, 4.61)	203 (8.3, 4.71))	2
2KAI	17 (12.46, 3.23)	1	1* (1.94, 0.84)	257 (1.11, 0.77)	3[f]	1* (2.18, 0.94)	257 (1.11, 0.77)	2
3HHR	214* (11.61, 3.27)	0	497 (9.19, 5.51)	420 (9.17, 4.59)	0	214* (13.59, 3.95)	261 (15.38, 3.77)	0
wins[j]	6	4	8		7	14		11

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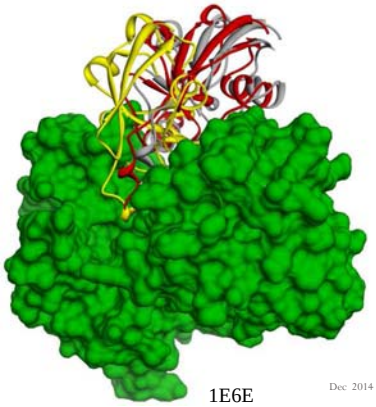
Test III - Results



1E6E

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Test III - Results

Table III: Refinement of rigid-body docking solution candidates (for unbound receptors and bound ligands)

Complex ID	PatchDock	FireDock		FiberDock	
	Best LRMSD in top 10[(a)]	Best LRMSD in top 10[(a)]	PatchDock LRMSD[(b)]	Best LRMSD in top 10[(a)]	PatchDock LRMSD[(b)]
1. 1A0O	7.66(1)	6.21 (10)	5.19 (108)	6.38 (2)	9.61 (179)
2. 1ACB	6.17(3)	8.24 (3)	8.67 (259)	6.58 (8)	6.12 (42)
3. 1AY7	12.46(2)	1.37 (5)	4.19 (95)	1.37 (5)	4.19 (95)
4. 1BTH	12.08 (8)	7.55 (10)	11.02 (232)	4.29 (19)	9.17 (184)
5. 1CGI	3.82 (2)	2.70 (2)	4.65 (107)	1.06 (3)	3.65 (50)
6. 1DFJ	4.28 (5)	1.82 (6)	3.93 (11)	5.58 (2)	7.98 (400)
7. 1E6E	17.01 (5)	12.27 (1)	16.36 (79)	8.01 (2)	16.36 (79)
9. 1GGI	6.06 (3)	12.27 (9)	12.99 (96)	10.57 (2)	11.23 (281)
11. 1IBR	19.11 (9)	3.01 (3)	6.38 (208)	13.06 (1)	11.87 (37)
13. 1PXV	14.63 (1)	10.42 (2)	9.56 (86)	8.36 (1)	11.35 (188)
14. 1T6G	8.10 (4)	3.51 (5)	10.87 (31)	1.76 (7)	3.95 (91)
15. 1TGS	12.16(9)	1.64 (3)	7.02 (458)	1.07 (3)	7.02 (458)
16. 1WQ1	2.42 (6)	11.72 (6)	13.31 (299)	11.68 (4)	12.01 (363)
17. 1ZHI	17.43 (9)	7.52 (9)	8.43 (311)	6.29 (3)	8.43 (311)
18. 2BUO	8.11 (10)	3.01 (3)	4.87 (32)	17.82 (3)	17.40 (381)
19. 2KAI	3.20 (6)	1.06 (3)	1.11 (257)	1.66 (1)	1.11 (257)

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Table IV
Refinement of Right-Body Docking Solution Candidates (for Unbound Receptors and Bound Ligands)

	PatchDock		FireDock			FiberDock		
Complex ID	First acceptable[a]	Acceptables in top 20[b]	First acceptable[a]	Original PatchDock result[c]	Acceptables in top 20[b]	First Acceptable[a]	Original PatchDock result[c]	Acceptables in top 20[b]
1A0O	1* (7.66, 3.79)	3[f]	7 (6.34, 2.30)	29 (9.20, 3.15)	3[f]	16 (5.25, 3.33)	108 (5.19, 3.26)	1
1ACB	3 (6.17, 3.12)	2	3 (8.24, 4.31)	259 (8.67, 4.37)	1	2* (6.84, 4.01)	42 (6.12, 3.56)	4[f]
1AY7	14 (9.78, 5.27)	3	5* (1.37, 0.77)	95 (4.19, 1.29)	5[f]	5* (1.37, 0.77)	95 (4.19, 1.29)	5[f]
1BTH	1* (12.10, 3.65)	1	2 (10.11, 3.28)	72 (11.47, 3.63)	2	1* (7.98, 1.97)	403 (14.80, 3.55)	5[f]
1CGI	2 (3.82, 2.31)	1	1* (2.82, 2.25)	2 (3.82, 2.31)	10[f]	1* (5.42, 2.72)	279 (7.50, 2.97)	9
1DFJ	1* (6.84, 2.76)	4	1* (5.55, 2.03)	2 (4.78, 2.33)	6[f]	1* (3.10, 1.53)	5 (4.28, 2.13)	6[f]
1E6E	None	0	474 (6.01, 3.32)	134 (10.20, 4.25)	0	2* (8.38, 3.44)	327 (20.64, 7.46)	2[f]
1FIN	None	0	None	None	0	None	None	0
1GGI	3 (6.06, 3.24)	6[f]	25 (6.83, 3.37)	3 (6.06, 3.24)	0	1* (12.39, 3.77)	281 (11.23, 3.29)	2
1GOT	None	0	None	None	0	None	None	0
1IBR	32 (6.99, 2.78)	0	2* (5.01, 2.50)	208 (6.38, 2.85)	1	2* (6.67, 2.61)	32 (6.99, 2.78)	3[f]
1OAZ	58 (18.47, 3.84)	0	9* (14.41, 3.27)	204 (15.05, 3.59)	1[f]	16 (14.41, 3.27)	204 (15.05, 3.59)	1[f]
1PXV	51 (8.54, 4.03)	0	17 (6.94, 3.49)	54 (5.78, 3.39)	1	1* (8.86, 4.51)	63 (9.86, 4.57)	2[f]
1T6G	4 (8.10, 1.75)	1	1* (6.83, 1.33)	129 (14.78, 3.08)	10	1* (9.61, 1.80)	70 (13.51, 2.33)	11[f]
1TGS	15 (2.69, 1.54)	1	1* (1.94, 1.43)	15 (2.69, 1.54)	10	1* (1.94, 1.43)	15 (2.69, 1.54)	11[f]
1WQ1	6* (2.24, 1.42)	1[f]	20 (5.64, 2.35)	82 (5.40, 2.17)	1[f]	29 (8.92, 4.44)	445 (7.18, 2.95)	0
1ZHI	134 (13.44, 2.81)	0	10 (7.52, 2.73)	311 (8.43, 3.03)	2	4* (7.18, 3.48)	311 (8.43, 3.03)	3[f]
2BUO	1* (9.38, 5.39)	9[f]	3 (5.05, 3.91)	32 (4.87, 3.98)	3	12 (6.3, 4.61)	203 (8.3, 4.71))	2
2KAI	17 (12.46, 3.23)	1	1* (1.94, 0.84)	257 (1.11, 0.77)	3[f]	1* (2.18, 0.94)	257 (1.11, 0.77)	2
3HHR	214* (11.61, 3.27)	0	497 (9.19, 5.51)	420 (9.17, 4.59)	0	214* (13.59, 3.95)	261 (15.38, 3.77)	0
wins[j]	6	4	8		7	14		11

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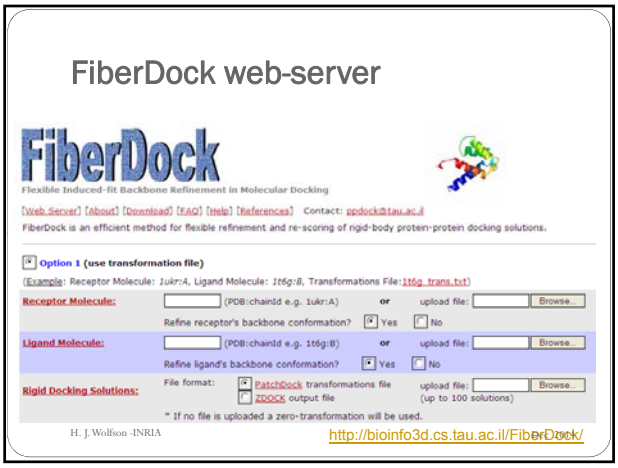
FiberDock web-server



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http://bioinfo3d.cs.tau.ac.il/FiberDock/