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Molécules Thérapeutiques In silico

Plotly: interactive plots using JavaScript

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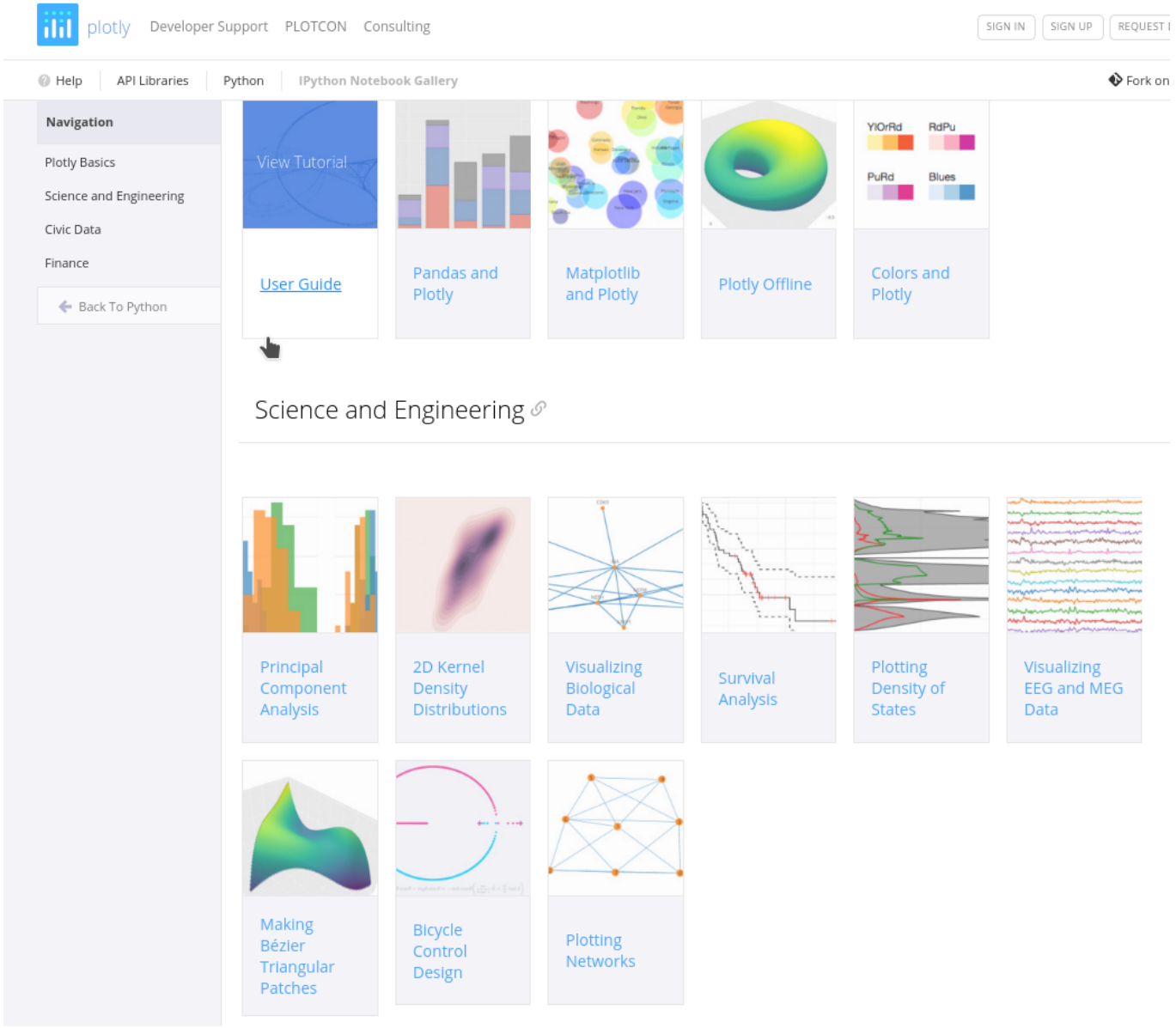
INSERM, UMR-S 973, Molécules Thérapeutiques In silico (MTI)

Plotly

JavaScript library to generate plots in the browser



Why JavaScript?
Why Plotly?

Things I don't know about

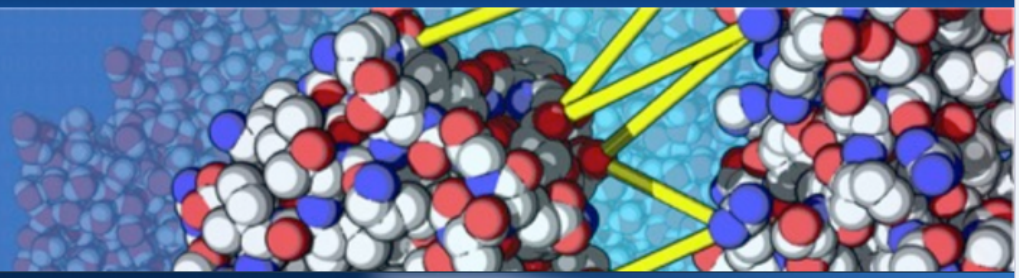
- JavaScript
- Browser DOM
- Plotly

Things I do know about

- Data-driven protein-protein docking
- HADDOCK server
  - 9334 registered users
  - 169004 jobs served
  - 671 citations

    SJ De Vries, M Van Dijk, AMJJ Bonvin - Nature protocols, 2010

HADDOCK2.2
@BonvinLab



HADDOCK server status for docking run E2A-HPR

Status: FINISHED

Your HADDOCK run has successfully completed. The complete run can be downloaded as a gzipped tar file **here**. The file containing your docking parameters is **here**.

Please cite the following paper in your work:
G.C.P van Zundert, J.P.G.L.M. Rodrigues, M. Trellet, C. Schmitz, P.L. Kastritis, E. Karaca, A.S.J. Melquiond, M. van Dijk, S.J. de Vries and (2016). "The HADDOCK2.2 webserver: User-friendly integrative modeling of biomolecular complexes."
J. Mol. Biol., **428**, 720-725 (2015).

Questions / feedback ? ask.bioexcel.eu

Please also consider giving us some feedback by filling our online survey.

Summary

HADDOCK clustered **193** structures in **6** cluster(s), which represents **96.5 %** of the water-refined models HADDOCK generated. Note that currently the maximum number of models considered for clustering is 200.

The statistics of the top 10 clusters are shown below. The top cluster is the most reliable according to HADDOCK. Its Z-score indicates how many standard deviations from the average this cluster is located in terms of score (the more negative the better).

A graphical representation of the results is also provided at the bottom of the page.

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Cluster 1

HADDOCK score	-137.4 +/- 2.7
Cluster size	114
RMSD from the overall lowest-energy structure	0.7 +/- 0.6
Van der Waals energy	-40.7 +/- 6.5
Electrostatic energy	-440.8 +/- 82.6
Desolvation energy	-9.6 +/- 12.4
Restraints violation energy	11.2 +/- 2.23
Buried Surface Area	1556.0 +/- 31.9
Z-Score	-1.8

View the docking solutions in a Jmol structure viewer. Your browser must be Java enabled:

Nr 1 best structure Download structure
Nr 2 best structure Download structure
Nr 3 best structure Download structure
Nr 4 best structure Download structure

CLUSTER 2

HADDOCK score	-112.8 +/- 2.3
Cluster size	33
RMSD from the overall lowest-energy structure	10.9 +/- 0.1
Van der Waals energy	-40.5 +/- 2.5
Electrostatic energy	-311.2 +/- 22.8
Desolvation energy	-11.3 +/- 3.8
Restraints violation energy	11.8 +/- 3.29
Buried Surface Area	1597.7 +/- 60.2
Z-Score	-0.4

View the docking solutions in a Jmol structure viewer. Your browser must be Java enabled:

Nr 1 best structure Download structure
Nr 2 best structure Download structure
Nr 3 best structure Download structure
Nr 4 best structure Download structure

CLUSTER 3

HADDOCK score	-111.8 +/- 4.4
Cluster size	19
RMSD from the overall lowest-energy structure	8.8 +/- 0.7
Van der Waals energy	-38.4 +/- 3.6
Electrostatic energy	-290.9 +/- 53.9
Desolvation energy	-16.2 +/- 6.7
Restraints violation energy	9.6 +/- 7.69

Cluster 3

HADDOCK score	-111.8 +/- 4.4
Cluster size	19
RMSD from the overall lowest-energy structure	8.8 +/- 0.7
Van der Waals energy	-38.4 +/- 3.6
Electrostatic energy	-290.9 +/- 53.9
Desolvation energy	-16.2 +/- 6.7
Restraints violation energy	9.6 +/- 7.69
Buried Surface Area	1462.3 +/- 81.2
Z-Score	-0.3

View the docking solutions in a Jmol structure viewer. Your browser must be Java enabled:

Nr 1 best structure Download structure
Nr 2 best structure Download structure
Nr 3 best structure Download structure
Nr 4 best structure Download structure

Cluster 6

HADDOCK score	-102.2 +/- 7.8
Cluster size	5
RMSD from the overall lowest-energy structure	7.4 +/- 1.3
Van der Waals energy	-35.1 +/- 2.7
Electrostatic energy	-307.7 +/- 18.0
Desolvation energy	-8.7 +/- 2.3
Restraints violation energy	30.6 +/- 28.43
Buried Surface Area	1357.4 +/- 34.0
Z-Score	0.2

View the docking solutions in a Jmol structure viewer. Your browser must be Java enabled:

Cluster 6

HADDOCK score	-102.2 +/- 7.8
Cluster size	5
RMSD from the overall lowest-energy structure	7.4 +/- 1.3
Van der Waals energy	-35.1 +/- 2.7
Electrostatic energy	-307.7 +/- 18.0
Desolvation energy	-8.7 +/- 2.3
Restraints violation energy	30.6 +/- 28.43
Buried Surface Area	1357.4 +/- 34.0
Z-Score	0.2

View the docking solutions in a Jmol structure viewer. Your browser must be Java enabled:

Nr 1 best structure	Download structure
Nr 2 best structure	Download structure
Nr 3 best structure	Download structure
Nr 4 best structure	Download structure

Cluster 4

HADDOCK score	-90.6 +/- 3.6
Cluster size	16
RMSD from the overall lowest-energy structure	6.0 +/- 0.4
Van der Waals energy	-26.9 +/- 2.1
Electrostatic energy	-290.1 +/- 18.8
Desolvation energy	-9.6 +/- 4.4
Restraints violation energy	39.2 +/- 36.29
Buried Surface Area	1220.9 +/- 96.9
Z-Score	0.9

View the docking solutions in a Jmol structure viewer. Your browser must be Java enabled:

View the docking solutions in a Jmol structure viewer. Your browser must be Java enabled:

Nr 1 best structure Download structure
Nr 2 best structure Download structure
Nr 3 best structure Download structure
Nr 4 best structure Download structure

CLUSTER 5

HADDOCK score	-82.8 +/- 12.5
Cluster size	6
RMSD from the overall lowest-energy structure	7.9 +/- 1.7
Van der Waals energy	-35.8 +/- 4.1
Electrostatic energy	-186.5 +/- 44.7
Desolvation energy	-13.0 +/- 3.9
Restraints violation energy	33.9 +/- 15.09
Buried Surface Area	1291.2 +/- 102.8
Z-Score	1.3

View the docking solutions in a Jmol structure viewer. Your browser must be Java enabled:

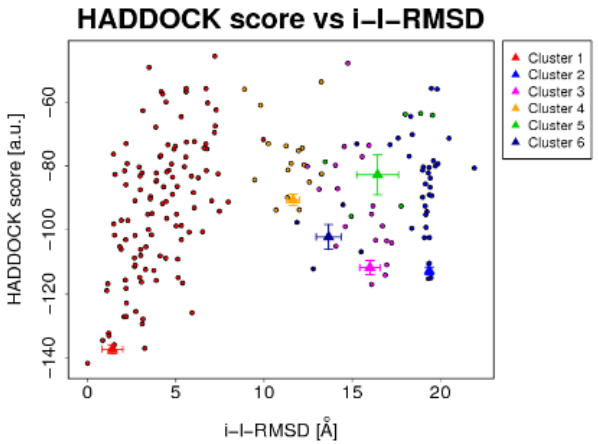
Nr 1 best structure Download structure
Nr 2 best structure Download structure
Nr 3 best structure Download structure
Nr 4 best structure Download structure

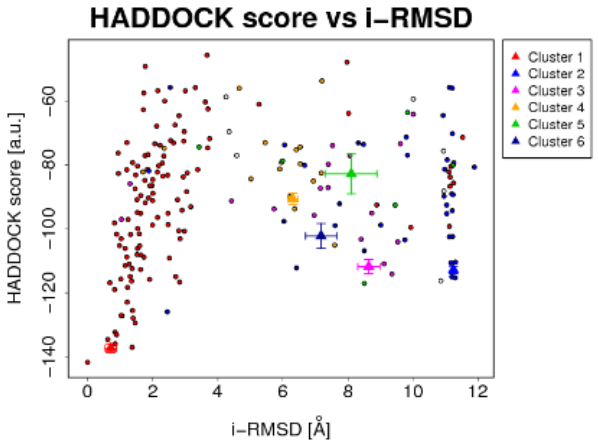
RESULTS ANALYSIS

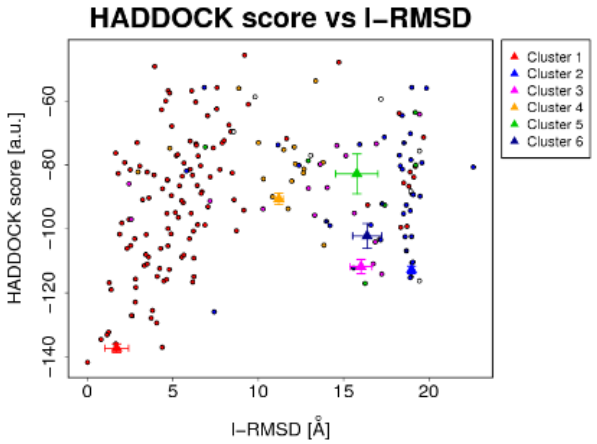
The results and graphics presented below are based on water-refined models generated by HADDOCK. The clusters (indicated in color in the graphs) are calculated based on the interface-ligand RMSDs calculated by HADDOCK, with the interface defined automatically based on all observed contacts. The various structural analysis (FCC, i-RMSD and l-RMSD) are made with respect to the best HADDOCK model (the one with the lowest HADDOCK score).

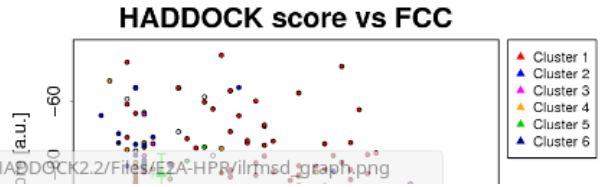
RESULTS ANALYSIS

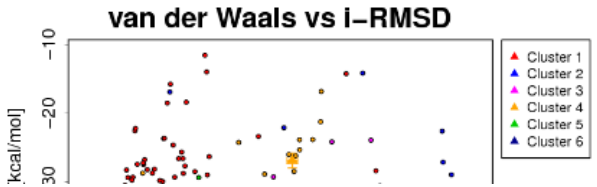
The results and graphics presented below are based on water-refined models generated by HADDOCK. The clusters (indicated in color in the graphs) are calculated based on the interface-ligand RMSDs calculated by HADDOCK, with the interface defined automatically based on all observed contacts. The various structural analysis (FCC, i-RMSD and l-RMSD) are made with respect to the best HADDOCK model (the one with the lowest HADDOCK score).

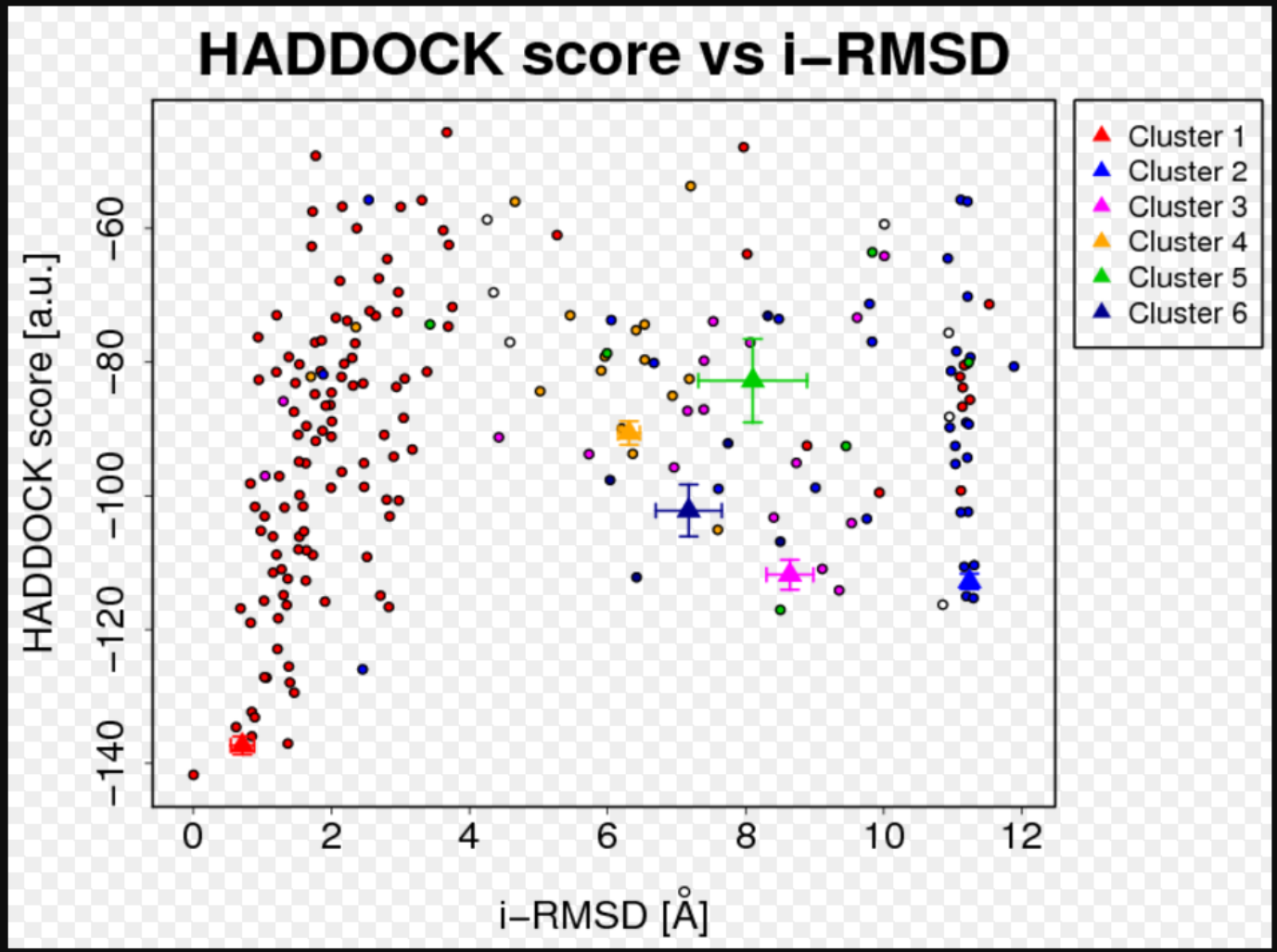


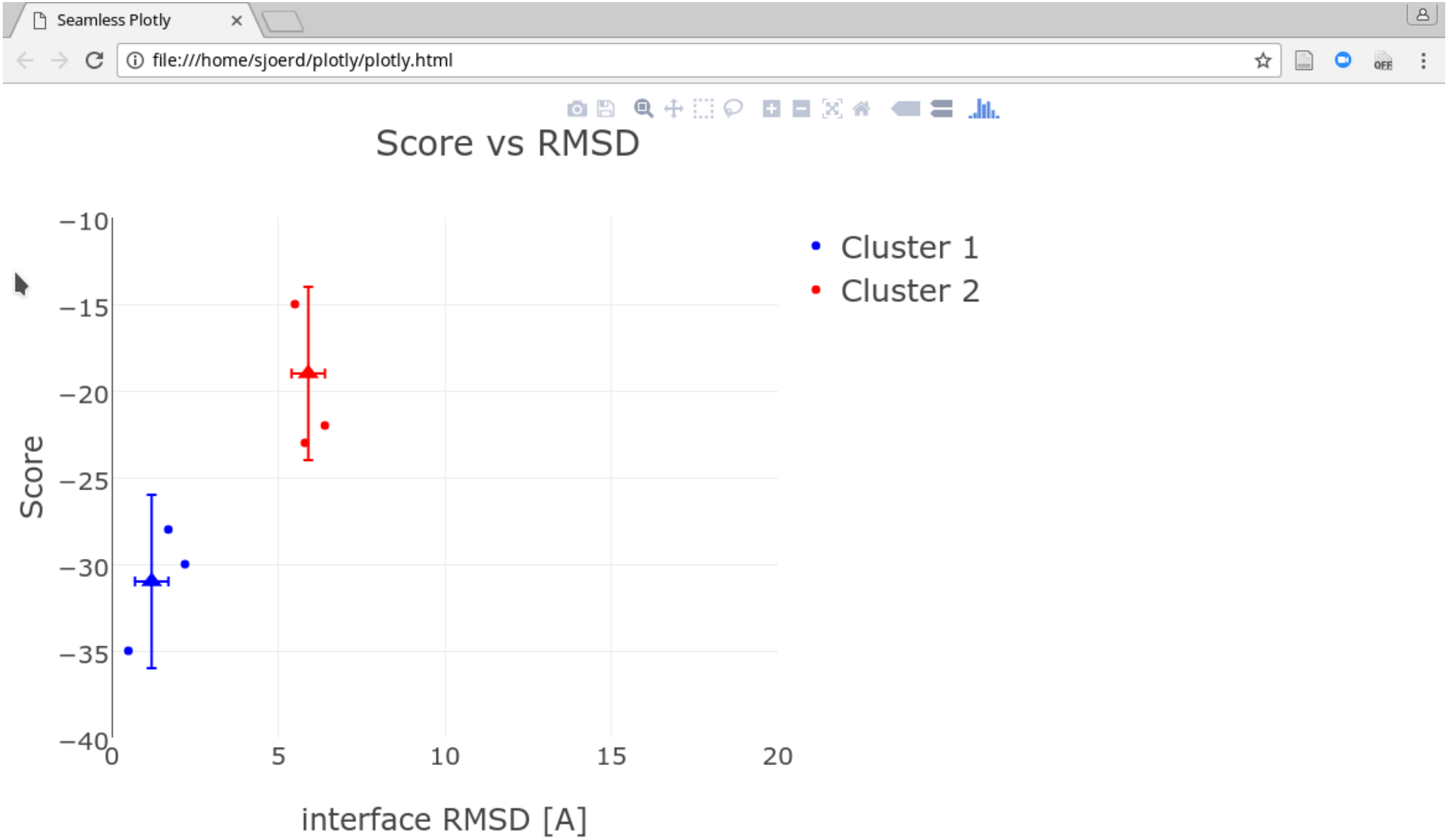











Seamless Plotly
file:///home/sjoerd/plotly/plotly.html
Score vs RMSD
Cluster 1
Cluster 2
Score
−10
−15
−20
−25
−30
−35
−40
0
5
10
15
20
interface RMSD [A]

Plotly

JavaScript library to generate plots in the browser

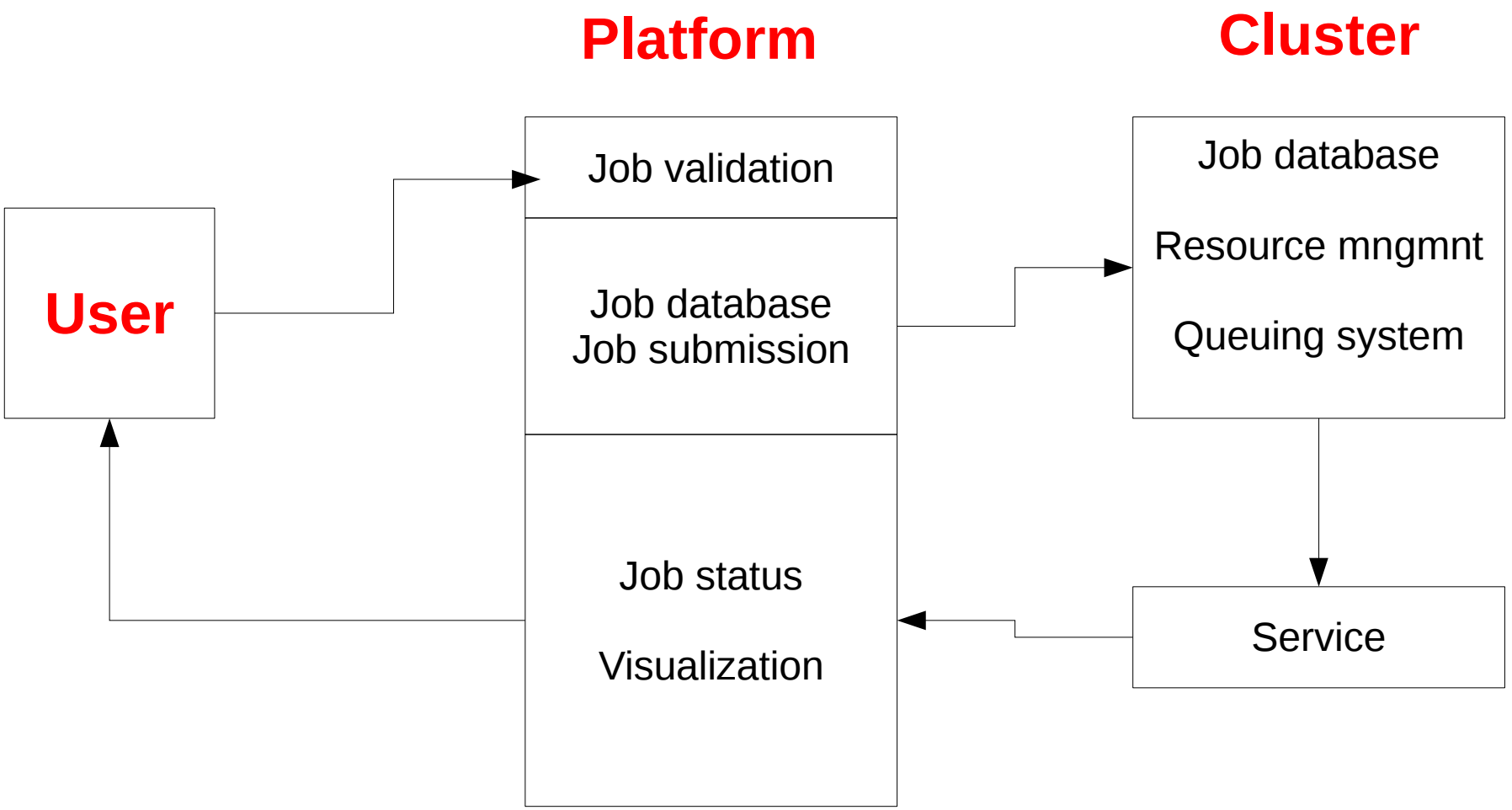
Advantages

- Open source
- Completely declarative
- Browser GUI + APIs for Python, R, Matlab, …
- On top of D3 and SVG

  Very flexible and beautiful

  no dead pixels!

Platform paradigm



Platformless paradigm?