

ChemBioServer

- Uploading and Browsing Compounds in 2D and 3D
- Filtering of compounds based on ***physicochemical properties***
- ***Substructure filtering*** of compounds based on custom sdf files
- ***Van der Waals filtering*** using distance and energy tests
- ***Toxicity filtering*** using specific organic toxic roots
- ***Hierarchical clustering*** with 4 different distances
- ***Affinity Propagation clustering***, providing exemplars for each cluster
- Creating custom pipeline filtering
- Visualization of compounds' properties

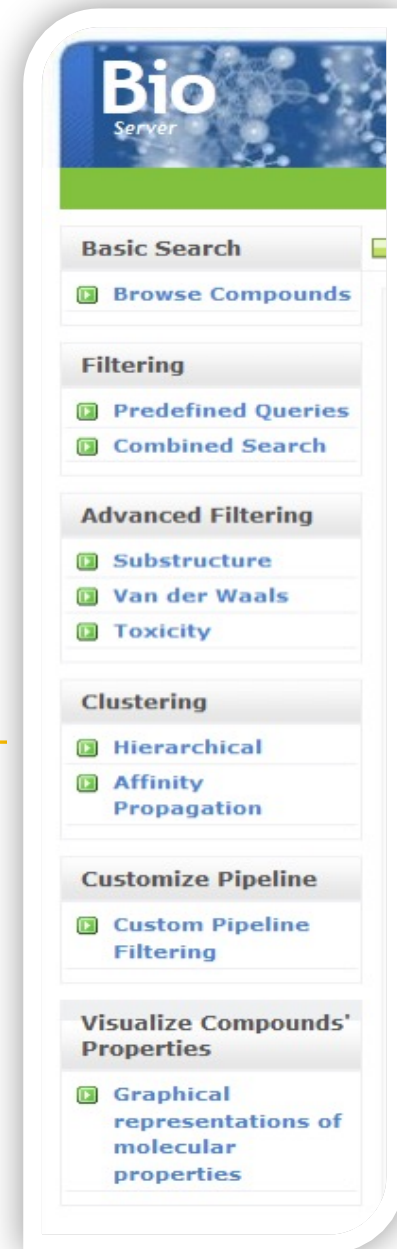
Filtering of chemical compounds

Computational methods can predict important physicochemical properties.

- *LogP*, a lipophilicity measure
- Solubility
- Permeability

Conformation of ligand inside the protein (e.g. bad van der Waals contacts)

Identification of unwanted or toxic moieties on a compound



Physicochemical Properties

ChemBioServer Performs filtering to discard molecules with undesired physicochemical properties

The screenshot shows the ChemBioServer web interface. The top navigation bar includes 'Home', 'Help', and 'Contact us'. The left sidebar contains sections for 'Basic Search', 'Filtering', 'Advanced Filtering', 'Clustering', 'Customize Pipeline', and 'Visualize Compounds' Properties. The main content area is titled 'Combined Search' and includes a 'Step 1' section for uploading an SDF file, an 'Optional Step' for uploading search parameters, and a 'Combined Search Results' section. The 'Combined Search Results' section shows a list of compounds that pass or fail search criteria. A large blue arrow points from the 'Combined Search Results' section to the table on the right.

Basic Search

- Browse Compounds

Filtering

- Predefined Queries
- Combined Search

Advanced Filtering

- Substructure
- Van der Waals
- Toxicity

Clustering

- Hierarchical
- Affinity Propagation

Customize Pipeline

- Custom Pipeline Filtering

Visualize Compounds' Properties

- Graphical representations of molecular properties

Combined Search

Step 1. Please, Upload an sdf* file.
In this step user is able to upload an sdf File that used for further processing.
Note: Maximum allowed upload size is 10MB (~2000 compounds)

Optional Step. Please, Upload Searchings Parametres file.
In this step user is able to upload a file with custom searching criteria.
Please note that each time process data button is pressed, the user is able to download an additional txt file that stores used searching settings to repeat searches. Your file "test2.sdf" was successfully uploaded.

Combined Search Results

[click here to Download Searching Parametres](#)
Compounds that PASS searching criteria ZINC00486904
Compounds that FAIL searching criteria ZINC02534226
[click here to Download SDF with Compounds that Pass searching criteria](#)

Final Step.
(*Warning: .sdf files are temporary saved on the server and deleted after processing)

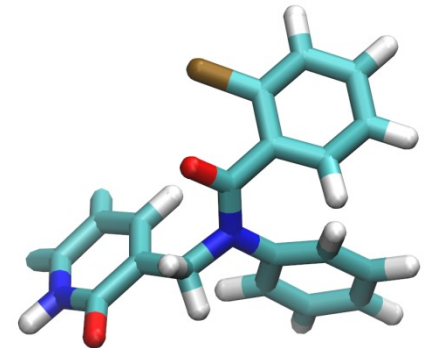
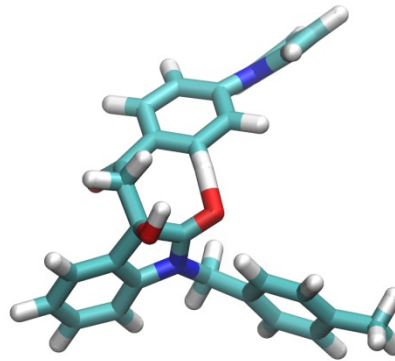
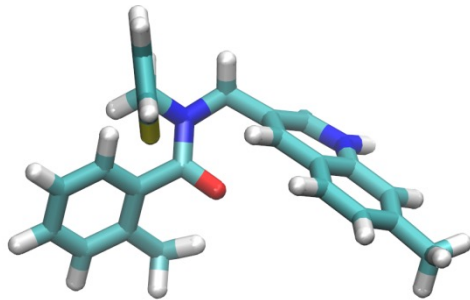
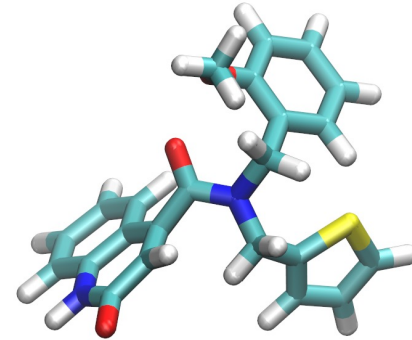
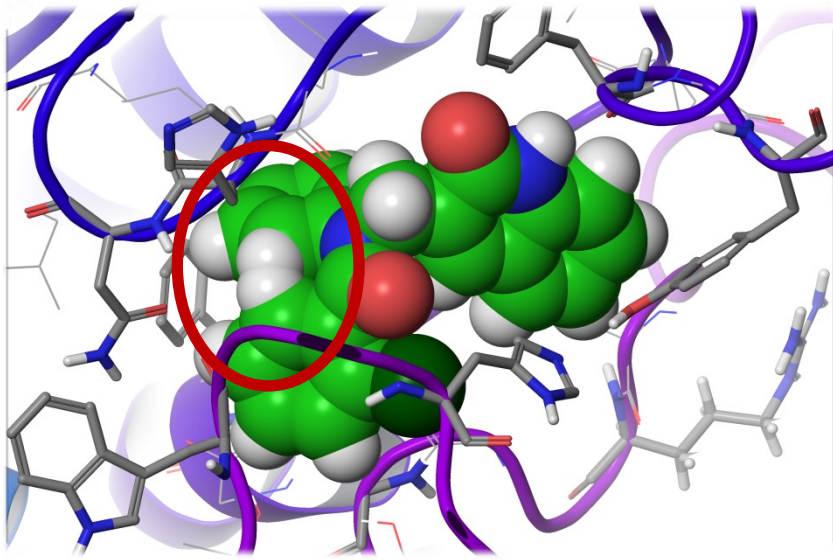
Customize Pipeline

- Molecular Weight: 500
- Number of Charges: ALL VALUES
- Number of C Atoms: ALL VALUES
- Number of RNH2: 2
- Number of R2NH: 4
- Number of R3N: 1
- Number of ROPO3: 1
- Number of ROH: 1
- Number of RCHO: 2
- Number of RCOR: 5
- Number of RCOOH: 3
- Number of RCOOR: 2
- Number of ROR: 5
- Number of RINGS: ALL VALUES
- Number of AROMATIC: ALL VALUES
- Hydrogen Bond Donors: 1
- Hydrogen Bond Acceptors: 2
- Partition coefficient log P: 5
- Polar surface Area: 150



Compound ID	VDW Energy Test	VDW Distance Test
Compound: 1 AW 00785	- PASS AW 00785 - Browse List For Details...	- FAIL AW 00785 - Browse List For Details...
Compound: 2 AW 00788	- PASS AW 00788 - Browse List For Details...	- FAIL AW 00788 - Browse List For Details...
Compound: 3 AW 00785	- PASS AW 00785 - Browse List For Details...	- FAIL AW 00785 - Browse List For Details...
Compound: 4 AW 00939	- PASS AW 00939 - Browse List For Details...	- FAIL AW 00939 - Browse List For Details...
Compound: 5 AW 00694	- PASS AW 00694 - Browse List For Details...	- FAIL AW 00694 - Browse List For Details...
Compound: 6 CD 10205	- PASS CD 10205 - Browse List For Details...	- PASS CD 10205 - Browse List For Details...
Compound: 7 GK 02096	- PASS GK 02096 - Browse List For Details...	- FAIL GK 02096 - Browse List For Details...
Compound: 8 HTS 01561	- PASS HTS 01561 - Browse List For Details...	- FAIL HTS 01561 - Browse List For Details...
Compound: 9 MWP 00404	- PASS MWP 00404 - Browse List For Details...	- FAIL MWP 00404 - Browse List For Details...
Compound: 10 NRB 02577	- PASS NRB 02577 - Browse List For Details...	- FAIL NRB 02577 - Browse List For Details...

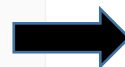
Bad van der Waals contacts



Bad van der Waals contacts

ChemBioServer Performs filtering to discard molecules with steric clashes by means of van der Waals energy and radii tolerance (*OPLS parameters**)

The screenshot shows the ChemBioServer web interface. The header includes the 'Bio Server' logo and 'ChemBioServer' text. Navigation links for 'Home', 'Help', and 'Contact us' are present. The left sidebar contains sections for 'Basic Search' (Browse Compounds), 'Filtering' (Predefined Queries, Combined Search), 'Advanced Filtering' (Substructure, Van der Waals, Toxicity), and 'Clustering' (Hierarchical, Affinity Propagation). The main content area is titled 'van der Waals Filtering' and displays a three-step process: Step 1 (uploading an sdf file), Step 2 (selecting vdW parameters: 50 Kcal/mol and 75%), and Step 3 (Process Data). A warning note states that sdf files are temporary. A 3D molecular model with a red circle highlighting a specific contact is shown at the bottom.



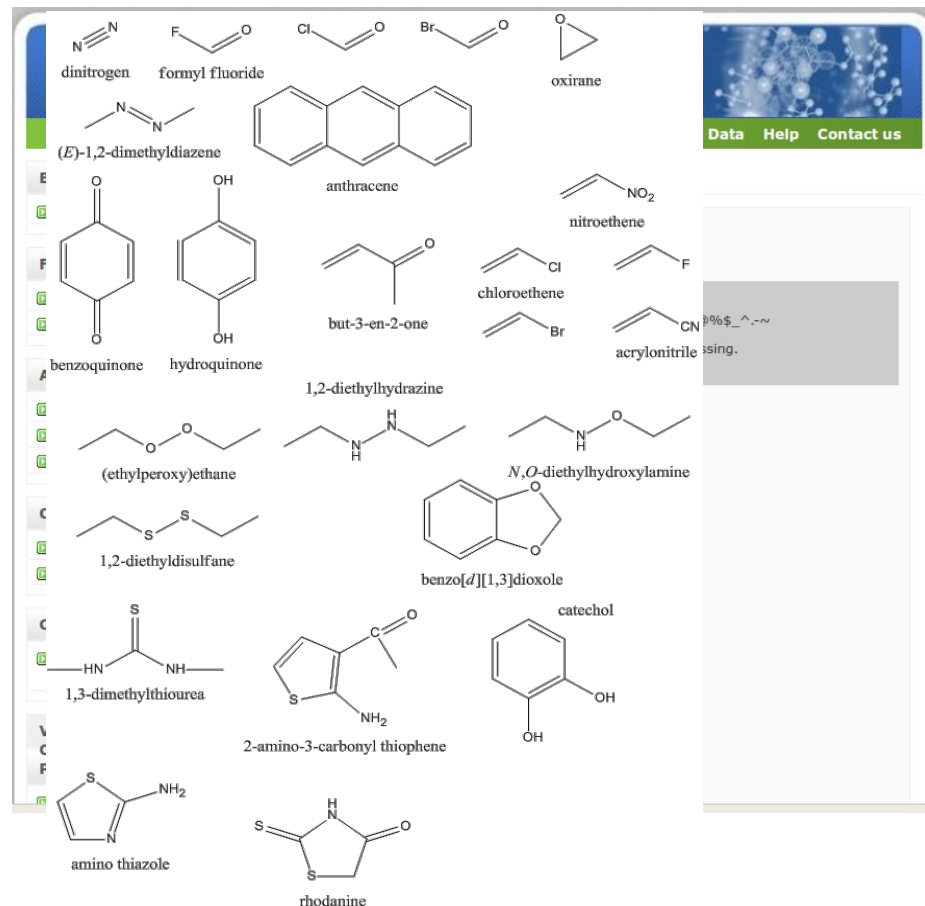
Compound ID	VDW Energy Test	VDW Distance Test
Compound: 1 AW 00785	- PASS AW 00785 - Browse List For Details...	- FAIL AW 00785 - Browse List For Details...
Compound: 2 AW 00788	- PASS AW 00788 - Browse List For Details...	- FAIL AW 00788 - Browse List For Details...
Compound: 3 AW 00785	- PASS AW 00785 - Browse List For Details...	- FAIL AW 00785 - Browse List For Details...
Compound: 4 AW 00939	- PASS AW 00939 - Browse List For Details...	- FAIL AW 00939 - Browse List For Details...
Compound: 5 AW 00694	- PASS AW 00694 - Browse List For Details...	- FAIL AW 00694 - Browse List For Details...
Compound: 6 CD 10205	- PASS CD 10205 - Browse List For Details...	- PASS CD 10205 - Browse List For Details...
Compound: 7 GK 02096	- PASS GK 02096 - Browse List For Details...	- FAIL GK 02096 - Browse List For Details...
Compound: 8 HTS 01561	- PASS HTS 01561 - Browse List For Details...	- FAIL HTS 01561 - Browse List For Details...
Compound: 9 MWP 00404	- PASS MWP 00404 - Browse List For Details...	- FAIL MWP 00404 - Browse List For Details...
Compound: 10 NRB 02577	- PASS NRB 02577 - Browse List For Details...	- FAIL NRB 02577 - Browse List For Details...

* Jorgensen *et al.*, JACS, 1996.

Toxicity filtering

ChemBioServer Performs filtering to discard molecules with undesired toxic moieties

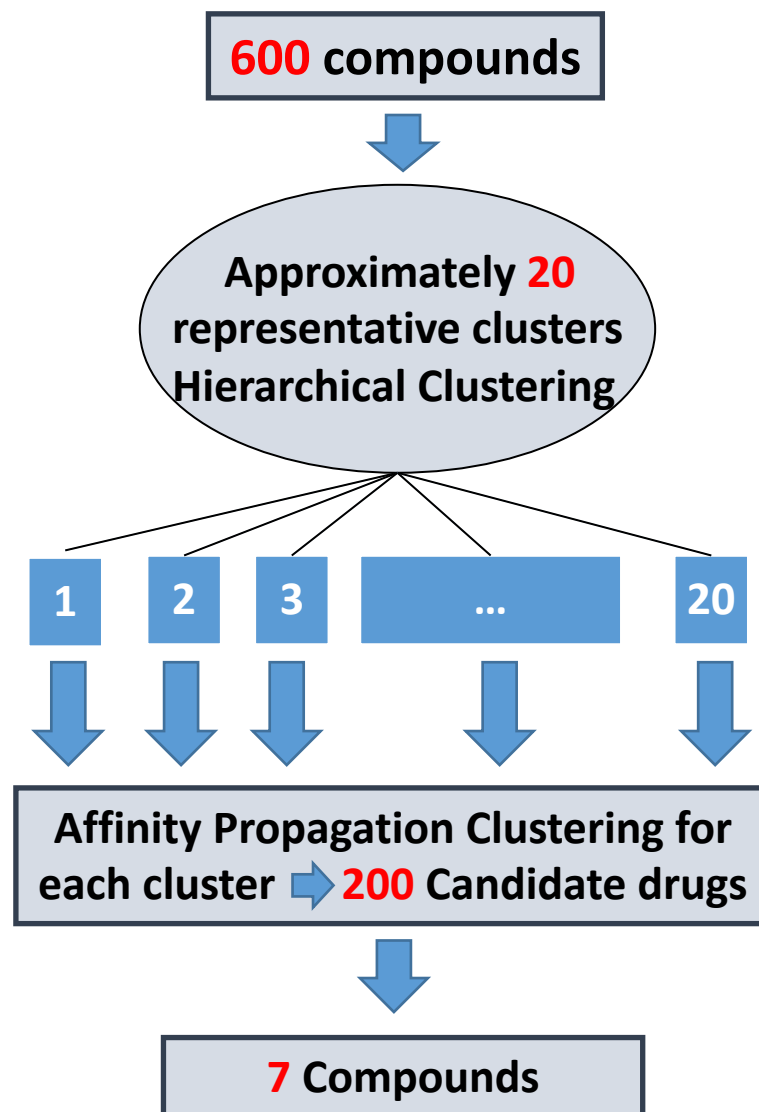
The screenshot displays the ChemBioServer web interface. The top navigation bar includes 'Home', 'Example Data', 'Help', and 'Contact us'. The left sidebar contains sections for 'Basic Search', 'Filtering' (with links to 'Browse Compounds', 'Predefined Queries', and 'Combined Search'), 'Advanced Filtering' (with links to 'Substructure', 'Van der Waals', and 'Toxicity'), 'Clustering' (with links to 'Hierarchical' and 'Affinity Propagation'), 'Customize Pipeline' (with links to 'Custom Pipeline' and 'Filtering'), and 'Visualize Compounds' Properties'. The main content area is titled 'van der Waals Filtering' and shows a two-step process. Step 1 involves uploading files in .sdf or .mol format, with a warning about special characters and a 10MB limit. Step 2 involves selecting vdW parameters, with 'van der Waals Energy Threshold' set to 50 Kcal/mol and 'van der Waals Radii Tolerance' set to 75%. A 'Process' button is visible at the bottom of the steps. A small image of a mouse is shown at the bottom right of the interface.



Athanasiadis, Cournia, Spyrou (2012) Bioinformatics

Clustering and molecular similarity

The screenshot displays the ChemBioServer web interface. The top navigation bar includes 'Home', 'Example Data', 'Help', and 'Contact us'. The left sidebar contains sections for 'Basic Search', 'Filtering', 'Advanced Filtering', 'Clustering', 'Customize Pipeline', and 'Visualize Compounds' Properties. The main content area is titled 'Hierarchical Clustering' and shows a two-step process. Step 1 involves uploading files, with a warning about filename restrictions and file size limits. Step 2 involves selecting parameters for clustering, including Distance Selection (Soergel/Tanimoto Coefficient), Clustering Linkage Selection (Complete), and Clustering Threshold (0.8). A 'Process Data' button is visible at the bottom of the main content area.



Back to the example....

Basic Search

Browse Compounds

Filtering

Predefined Queries

Combined Search

Advanced Filtering

Substructure

Van der Waals

Toxicity

Clustering

Hierarchical

Affinity Propagation

van der Waals Filtering

Step 1.

Browse... top1000.sdf

Please, Upload files* in either ".sdf", or ".mol" format.

*Warning:

Uploaded filename **should not contain any** special character i.e. @%\$_^.-~

Files are temporary saved on the server and deleted after processing.

Maximum allowed upload size is **10MB** (~2000 compounds).

Step 2.

Please, Select vdW Parametres.

van der Waals Energy Threshold:

50 Kcal/mol

van der Waals Radii Tolerance:

75 %

Final Step.

Process Data

Molecular Modeling of Biomolecules (DI440), 11.1.2022

Compound: 7 HTS 05412	- PASS HTS 05412 - Browse List For Details... ▴ ▾	- PASS HTS 05412 - Browse List For Details... ▴ ▾
Compound: 8 HTS 05683	- PASS HTS 05683 - Browse List For Details... ▴ ▾	- PASS HTS 05683 - Browse List For Details... ▴ ▾
Compound: 9 BTB 05835	- PASS BTB 05835 - Browse List For Details... ▴ ▾	- PASS BTB 05835 - Browse List For Details... ▴ ▾
Compound: 10 BTB 14912	- PASS BTB 14912 - Browse List For Details... ▴ ▾	- PASS BTB 14912 - Browse List For Details... ▴ ▾
Compound: 11 HTS 07996	- PASS HTS 07996 - Browse List For Details... ▴ ▾	- PASS HTS 07996 - Browse List For Details... ▴ ▾
Compound: 12 SEW 02809	- PASS SEW 02809 - Browse List For Details... ▴ ▾	- PASS SEW 02809 - Browse List For Details... ▴ ▾
Compound: 13 HTS 05414	- PASS HTS 05414 - Browse List For Details... ▴ ▾	- PASS HTS 05414 - Browse List For Details... ▴ ▾
Compound: 14 JFD 00844	- PASS JFD 00844 - Browse List For Details... ▴ ▾	- FAIL JFD 00844 - Browse List For Details... ▴ ▾
Compound: 15 HTS 05414	- PASS HTS 05414 - Browse List For Details... ▴ ▾	- PASS HTS 05414 - Browse List For Details... ▴ ▾

Basic Search

[Browse Compounds](#)

Filtering

[Predefined Queries](#)

[Combined Search](#)

Advanced Filtering

[Substructure](#)

[Van der Waals](#)

[Toxicity](#)

Clustering

[Hierarchical](#)

[Affinity Propagation](#)

Customize Pipeline

[Custom Pipeline
Filtering](#)

Visualize Compounds' Properties

[Graphical
representations of](#)

Toxicity Filtering Toxicophores

Step 1. `upload_1412609322_vdW_pass.sdf`

Please, Upload files* in either ".sdf", or ".mol" format.

*Warning:



Uploaded filename **should not contain any** special character i.e. @%\$_^.-~



Files are temporary saved on the server and deleted after processing.



Maximum allowed upload size is **10MB** (~2000 compounds).



Custom List of Organic Toxic Compounds

1. N#N dinitrogen
2. C(=O)F formyl fluoride-Michael acceptor
3. C(=O)Cl formyl chloride-Michael acceptor
4. C(=O)Br formyl bromide-Michael acceptor
5. O1CC1 oxirane
6. C/N=N/C diazene
7. c1ccc2c(c1)cc1c(c2)cccc1 anthracene
8. C1=CC(=O)C=CC1=O quinone
9. c1cc(ccc1O)O hydroquinone
10. C=CC(=O)C butenone-Michael acceptor
11. CCOOCC O-O heteroatom
12. CCNNCC hydrazine-N-N heteroatom
13. CCNOCC N-O heteroatom
14. C=CCl chloroethane-Michael acceptor
15. C=CF fluoroethane-Michael acceptor
16. C=CBr bromoethane-Michael acceptor
17. C=CC#N acrylonitrile-Michael acceptor
18. C=C[N+](=O)[O-] nitroethene-Michael acceptor
19. CCSSCC disulfane-S-S heteroatom
20. c1ccc2c(c1)OCO2 benzo-dioxane

TOXIC RESULTS

- Compound with NO Toxic Roots: HTS 05684

- TOXIC Compounds: SPB 08304

[click here to Download Results in txt format](#)

[click here to Download SDF file with Compounds that pass the Toxic test](#)

CLICK on the NAME for 3D Display using JMOL APPLET

Compounds	Toxicity Results
Compound: 1 HTS 05684	NOT FOUND dinitrogen
Compound: 2 RH 01155	NOT FOUND dinitrogen
Compound: 3 HTS 05414	NOT FOUND dinitrogen
Compound: 4 RH 01155	NOT FOUND dinitrogen
Compound: 5 HTS 05414	NOT FOUND dinitrogen
Compound: 6 SPB 08304	NOT FOUND dinitrogen
Compound: 7 HTS 05412	NOT FOUND dinitrogen
Compound: 8 HTS 05683	NOT FOUND dinitrogen
Compound: 9 BTB 05835	NOT FOUND dinitrogen
Compound: 10 BTB 14912	NOT FOUND dinitrogen
Compound: 11 HTS 07996	NOT FOUND dinitrogen
Compound: 12 SEW 02809	NOT FOUND dinitrogen
Compound: 13 HTS 05414	NOT FOUND dinitrogen

▶ Step 1. upload_1412609972_tox_pass.sdf

Please, Upload files* in ".sdf", ".mol", or binary fingerprint in ".txt" format.

*Warning:



Uploaded filename **should not contain any** special character i.e. @%\$_^.-~



Files are temporary saved on the server and deleted after processing.



Maximum number of compounds that can be easily distinguished in the plot area is approximately **1000**.



Maximum allowed upload size is **10MB** (~2000 compounds).



fingerprint .txt format should contain two parts separated by a comma (,) character, the binary fingerprint and the name of the compound i.e:

0000011000000101000011110110000000000000111111111111110, Compound 0001

0011111111111111111100000000000000000011011100000000000, Compound 0002

0101111001100100011010010010101110111000000101111001101, Compound 0003

Binary part should not contain any space before comma.

(see [Example Data set 7](#). for more information)



Please notice that a [PDF reader](#) program should be installed in order to display clustering results.

▶ Step 2. Please, select Parametres



Distance Selection:

1. Soergel (Tanimoto Coefficient) ▾



Clustering Linkage Selection:

3. Complete ▾



Clustering Threshold:

0.85 ▾



Final Step.

Process Data

No file selected or the file you attempted to upload is not allowed.

Basic Search

 [Browse Compounds](#)

Filtering

 [Predefined Queries](#)

 [Combined Search](#)

Advanced Filtering

 [Substructure](#)

 [Van der Waals](#)

 [Toxicity](#)

Clustering

 [Hierarchical](#)

 [Affinity Propagation](#)

Customize Pipeline

 [Custom Pipeline
Filtering](#)

Visualize Compounds' Properties

Affinity Propagation Clustering



The affinity propagation algorithm takes as input a set of pairwise similarities among compound fingerprints, considering them as potential representative compounds (exemplars). The clusters and their corresponding representative compounds are calculated by exchanging messages between data points until a maximization process converge. Thus, exemplars for each cluster are proposed to the researcher for further investigation.



Step 1. **1412668473cluster_1_.sdf**

Please, Upload files* in **".sdf"**, **".mol"**, or *binary fingerprint* in **".txt"** format.

*Warning:



Uploaded filename **should not contain any** special character i.e. @%\$^_~



Files are temporary saved on the server and deleted after processing.



Maximum allowed upload size is **10MB** (~2000 compounds).



fingerprint.txt format should contain two parts separated by a comma (,) character, the binary fingerprint and the name of the compound i.e:

0000011000000101000011110110000000000000111111111111110, Compound 0001

0011111111111111111100000000000000000011011100000000000, Compound 0002

0101110011001000110100100101011101110000000101111001101, Compound 0003

Binary part should not contain any space before comma.

(see [Example Data set 7](#) for more information)



Step 2. Please, Select Distance Parametres.



Distance Selection:

1. Soergel (Tanimoto Coefficient)



Final Step.