

The MArtini Database (MAD) and web server

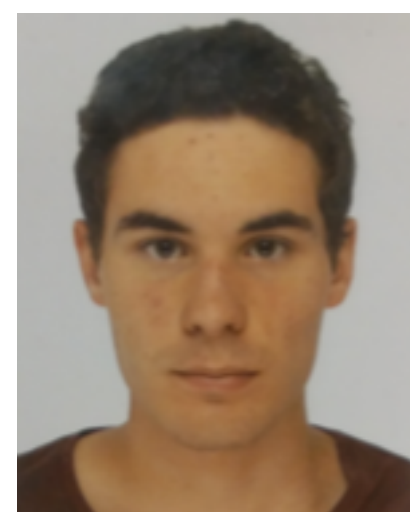


Luca Monticelli
CNRS & University of Lyon, France

The people behind MAD

Permanent staff

Master Degree Internships



Louis Beranger
M2 - 2020



Anaïs Chopin
M2 - 2021

Bioinformatics



Cécile Hilpert
Study Engineer



Guillaume Launay
Assistant Professor

Molecular simulations



Luca Monticelli
Research Director



Paulo CT Souza
Researcher



Keeping up the physical infrastructure: Alexis Michon and Samuel Bosquin (sysadmins, permanent CNRS staff)

The question

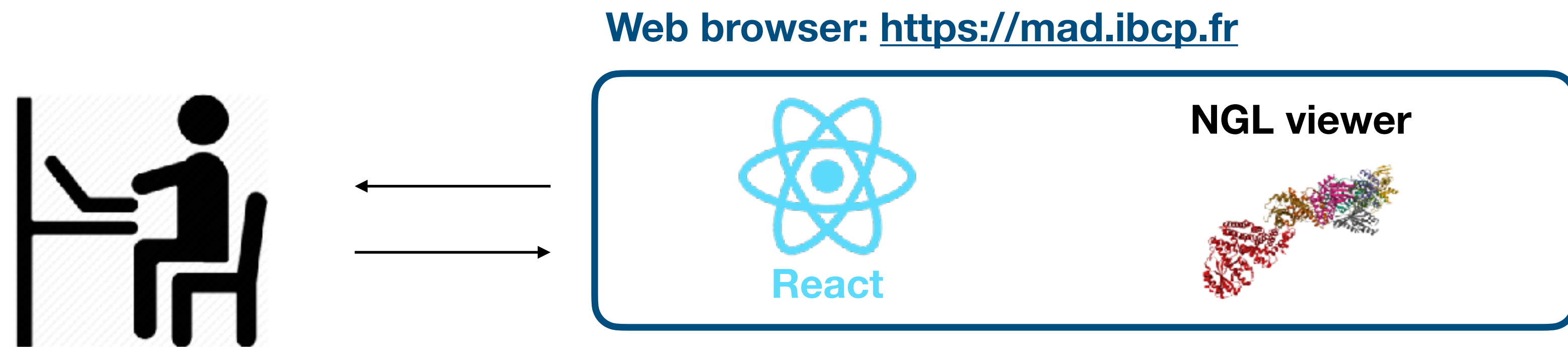
- Where do I find such and such Martini file?
- Which version is this DOPC? Who wrote it? Who modified it? When?
- Why is the DOPC used in this paper different from the one I just downloaded?

The question

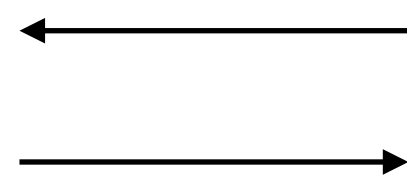
- Where do I find such and such Martini file?
- Which version is this DOPC? Who wrote it? Who modified it? When?
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The answer: a database!

Hardware/software infrastructure



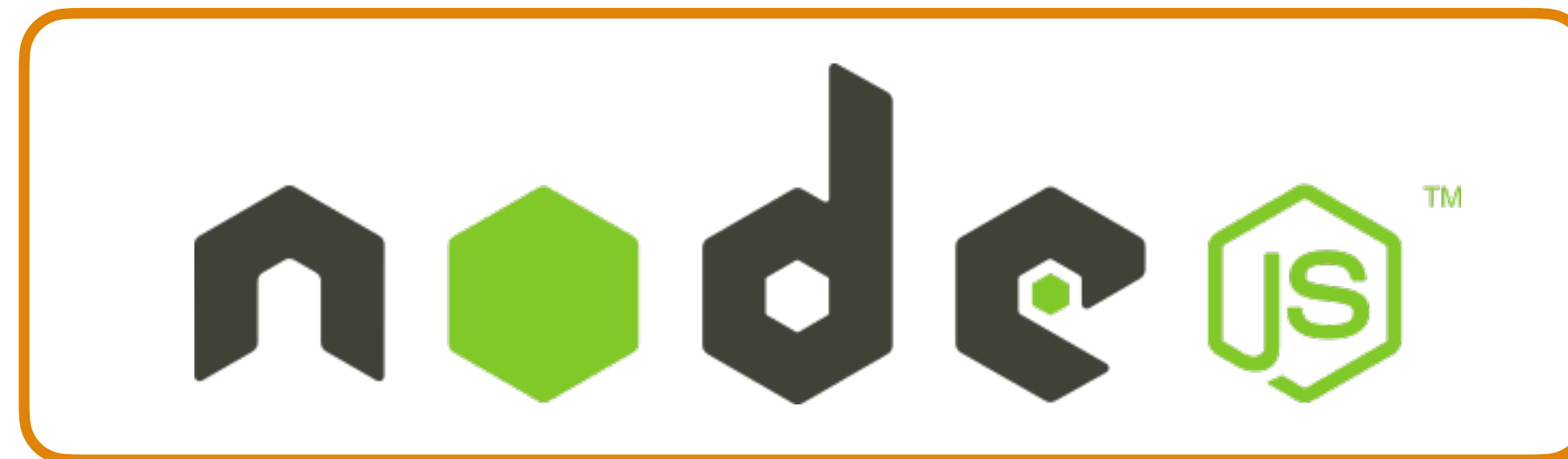
Hardware/software infrastructure



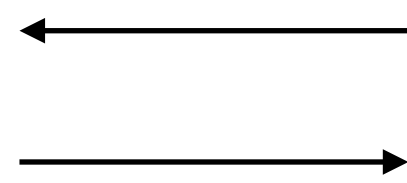
Web browser: <https://mad.ibcp.fr>



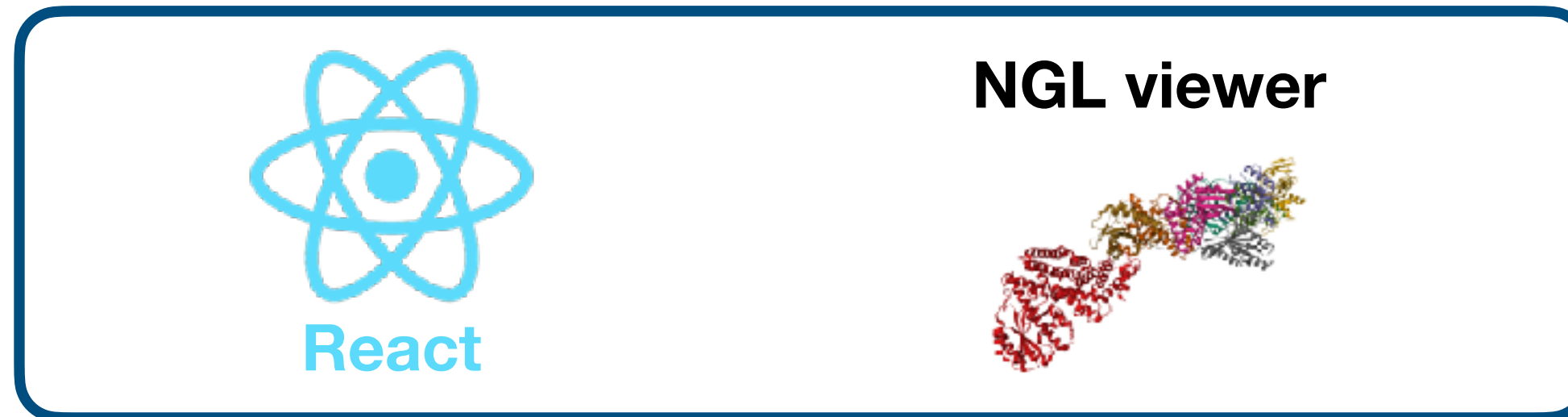
Web server



Hardware/software infrastructure



Web browser: <https://mad.ibcp.fr>



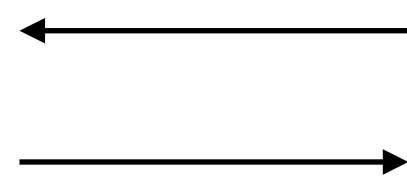
Web server



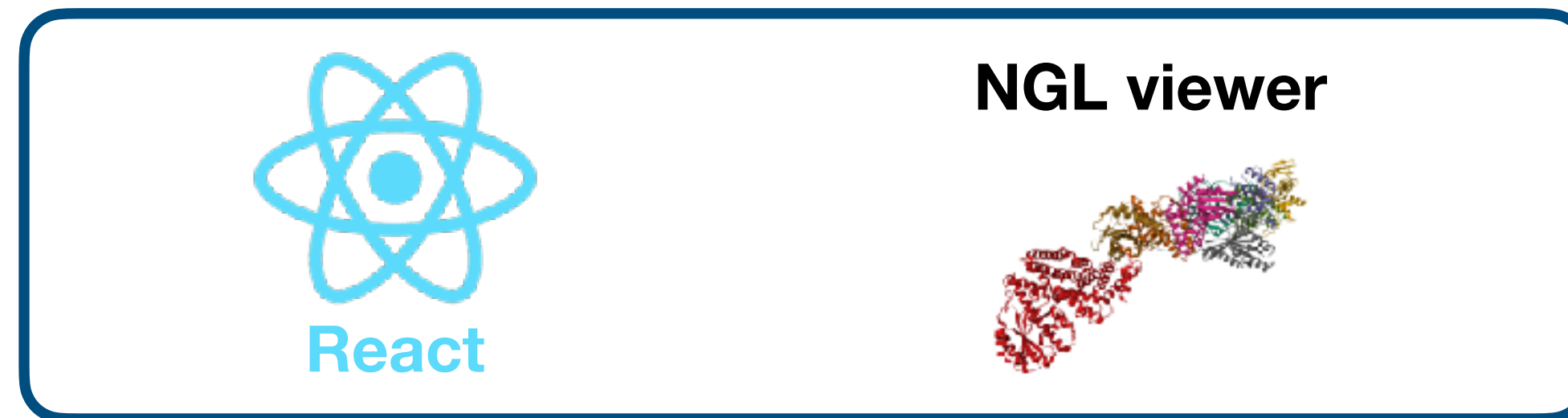
Computation & storage



Hardware/software infrastructure



Web browser: <https://mad.ibcp.fr>



Web server

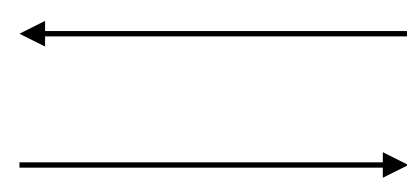


Computation & storage

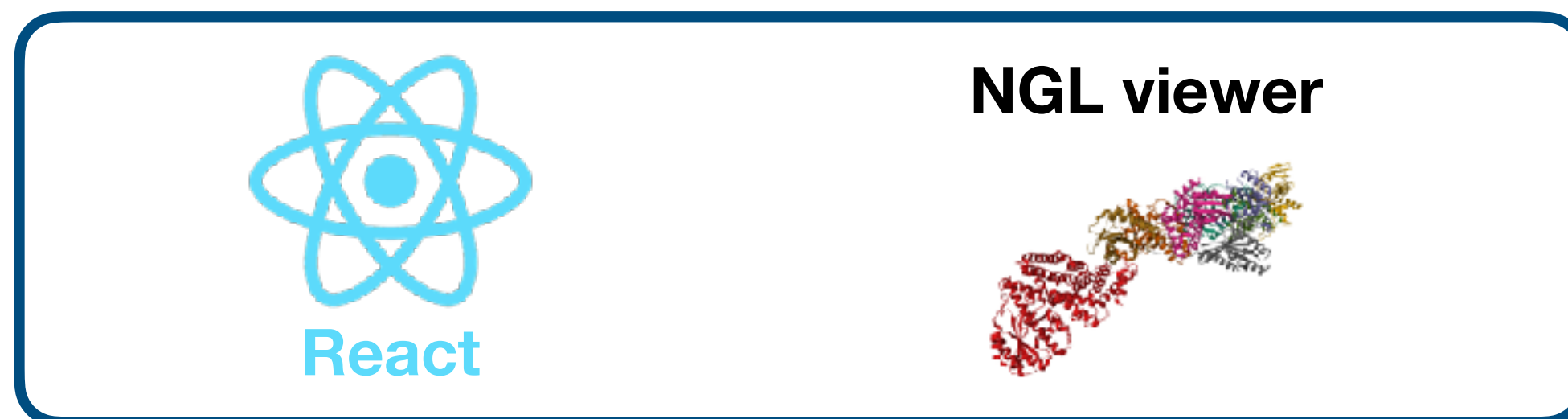


<https://github.com/MMSB-MOBI>

Hardware/software infrastructure



Web browser: <https://mad.ibcp.fr>



Web server



Computation & storage



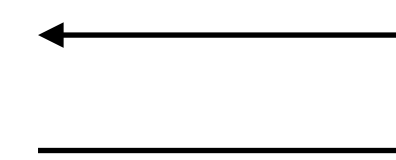
<https://github.com/MMSB-MOBI>



100+ physical cores (more coming soon)

Two high performance storage units

Local backup + remote backup



How does it look like?

<https://mad.ibcp.fr>

MArtini Database



This is a beta version of MAD service. If you have any suggestions or problems, please contact us at mad-support@ibcp.fr or use contact page. New accounts for using beta versions of Molecule Builder and System Builder will be available starting September 1st 2021.

Explore

Force field

Creation way

Categories

Name

Alias

Author

Free text



Explore



Molecule builder



System builder



Force fields



Login



Contact

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Explore the database

<https://mad.ibcp.fr/explore>

- Browsing the DB and downloading files does not require authentication
- Organized by molecular classes (Glycolipids, peptides, ...)
- At the moment: 174 biomolecules (Lipids subset from Martini website)
- Per molecule **Version Tracking** system:
 - Subsequent versions of parameter files
 - Force field versions
 - Submission author

Multiple search fields

Force field	Creation way	Categories
Name	Alias	Author
Free text		

Explore the database

<https://mad.ibcp.fr/molecule/DPG3>

C(d18:1/18:0)GM3(DPG3)

DPG3

General information

Name : C(d18:1/18:0)GM3(DPG3)

Alias : DPG3

Categories : Lipids

Comments :

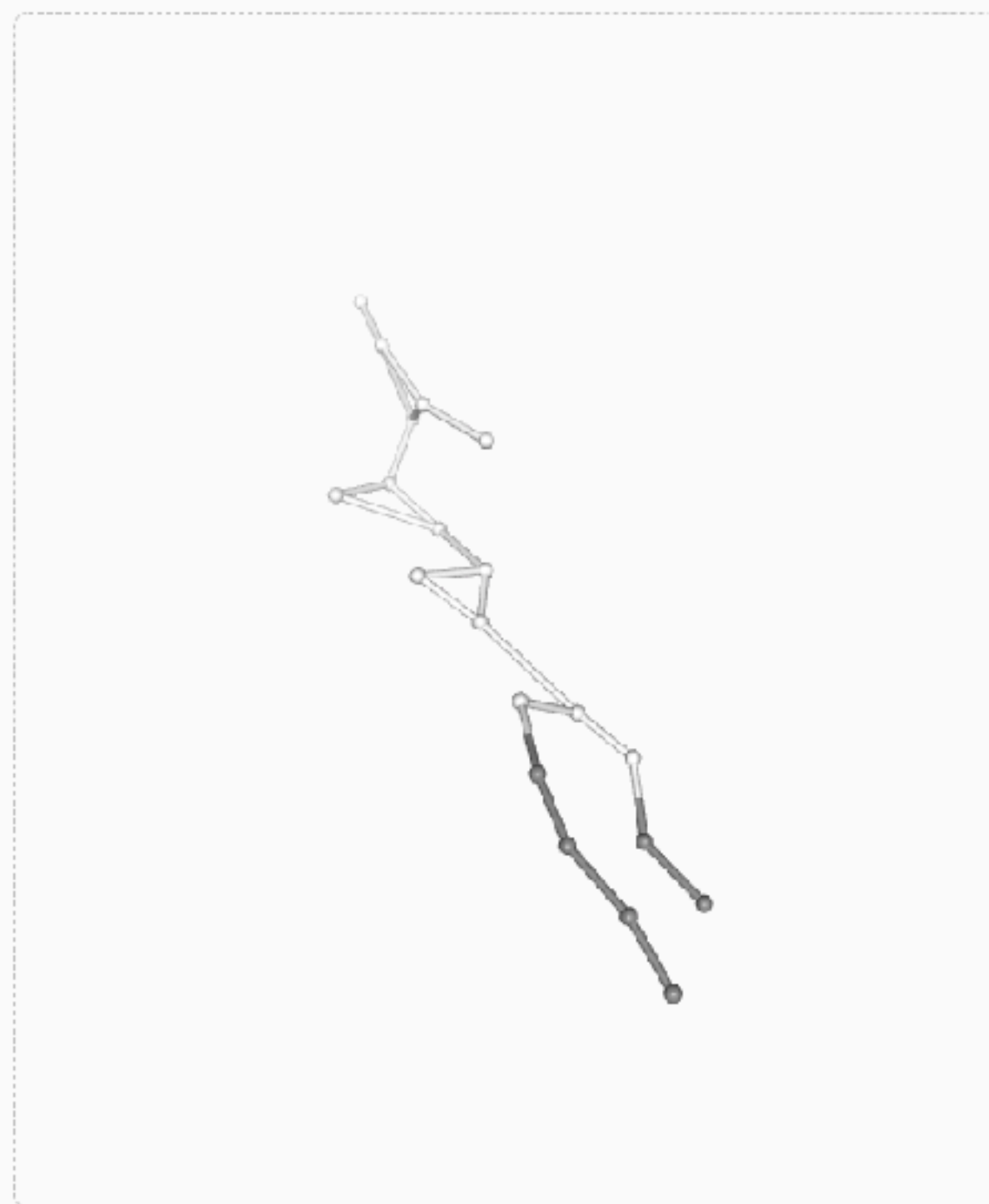
; Description:

; A general model monosialodihexosylganglioside (GM3) lipid corresponding to atomistic e.g. C(d18:1/18:0); N-stearoyl-D-erythro tails.

; Parameterization:

; GM3 version 2 is based on version 1 but reoptimized to reproduce the strengths of ganglioside aggregations at the atomistic level, see Gu et al. 2016.; GM3 version 1 headgroup is based on Cesar Lopez's GM3 see Lopez et al. 2013 with bonded parameters modified by Manuel Melo; for increased stability and faithfulness to AA. Top two galactose groups were cut off and the branching bead in; GM1 (Nda) was changed to an SP1 type.; The lipid tail follows the standard Martini 2.0 lipid definitions and building block rules. The DP tail (x2 palmitoyl or; stearoyl) has a tail string -altail "TCC CCCC".
; Created: 2016.07.15

Version **02** created at 2021-06-04 18:06.



Details

Created for force field **martini22** (Manually).

For using this molecule, please cite:

; R.X. Gu, H.I. Ingolfsson, A.H. de Vries, S.J. Marrink, D.P. Tieleman. Ganglioside-lipid and ganglioside-protein interactions; revealed by coarse-grained and atomistic molecular dynamics simulations. JPC-B, 2016, Accepted. doi:10.1021/acs.jpcc.6b07142; C.A. Lopez, Z. Sovova, F.J. van Eerden, A.H. de Vries, S.J. Marrink. Martini force field parameters for glycolipids. JCTC.; 9:1694-1708, 2013. doi:10.1021/ct3009655; H.I. Ingolfsson, M.N. Melo, F.J. van Eerden, C. Arnarez, C.A. Lopez, T.A. Wassenaar, X. Periole, A.H. De Vries, D.P. Tieleman, S.J. Marrink. Lipid organization of the plasma membrane. JACS, 136:14554-14559, 2014. doi:10.1021/ja507832e; S.J. Marrink, A.H. de Vries, A.E. Mark. Coarse grained model for semi-quantitative lipid simulations. JPC-B, 108:750-760, 2004. doi:10.1021/jp036508g; S.J. Marrink, H.J. Risselada, S. Yefimov, D.P. Tieleman, A.H. de Vries. The MARTINI force field: coarse grained model for; biomolecular simulations. JPC-B, 111:7812-7824, 2007. doi:10.1021/jp071097f

[Download files](#)

Versions

01 • (Manually, martini22)

02 • (Manually, martini22)

Database: insertion of molecules

- Submission of new biomolecules requires authentication
- Two types of user accounts: standard and administrator

Two modes of molecule insertion:

Individual molecule

- ➔ **Interactive uploading in the browser**
Submitted by standard users, approved by admins

Batch of molecules

- ➔ **Takes a folders bundle as input**
Performed in command line by administrators

Database: individual insertion

<https://mad.ibcp.fr/explore>

Define here the details of your molecule.

Fields marked with an asterisk (*) are mandatory.

General information

<input type="text" value="Name *"/>	<input type="text" value="Alias *"/>	<input type="text" value="SMILES formula"/>	<input type="text" value="Category"/>
-------------------------------------	--------------------------------------	---	---------------------------------------

About this version

<input type="text" value="Citations"/>	<input type="text" value="Command line"/>	<input type="text" value="Molecule Version *"/>
<input type="text" value="Creation way *"/>	<input type="text" value="Used force field *"/>	

Validation information

Comments

Attached files

Coarse-grained PDB/GRO file

[ADD FILE](#) Select a file...

Generated ITP files

[ADD FILE](#) Select a file...

Optional mapping files

[ADD A MAP FILE](#)

Generated TOP file (if any)

[ADD FILE](#) Select a file...

[ADD ANOTHER ITP FILE](#)

publication ID / doi →

Mandatory

Database: individual insertion

<https://mad.ibcp.fr/explore>

Define here the details of your molecule.

Fields marked with an asterisk (*) are mandatory.

General information

Name * Alias * SMILES formula Category

- Sugars
- Proteins
- Polymers
- Amino acids
- Lipids

About this version

Citations Command line Molecule Version *
Creation way * Used force field *

- Manually
- Martinize 1
- Vermouth-Martinize 2
- Cartographer
- Auto-Martini

- elnedyn
- elnedyn22
- elnedyn22p
- martini22
- martini22p
- martini304
- martini3001

Validation information

Comments

Attached files

Coarse-grained PDB/GRO file

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Generated ITP files

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[ADD A MAP FILE](#)

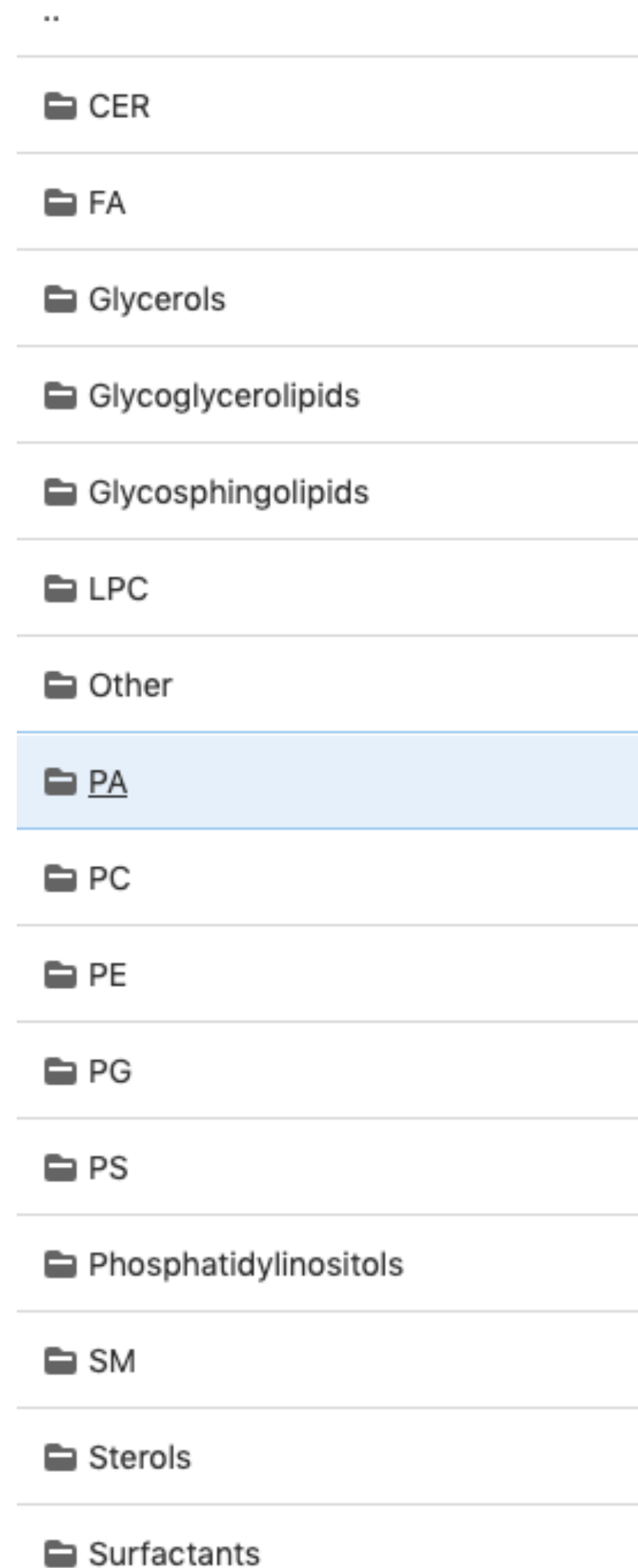
Generated TOP file (if any)

[ADD FILE](#) Select a file...

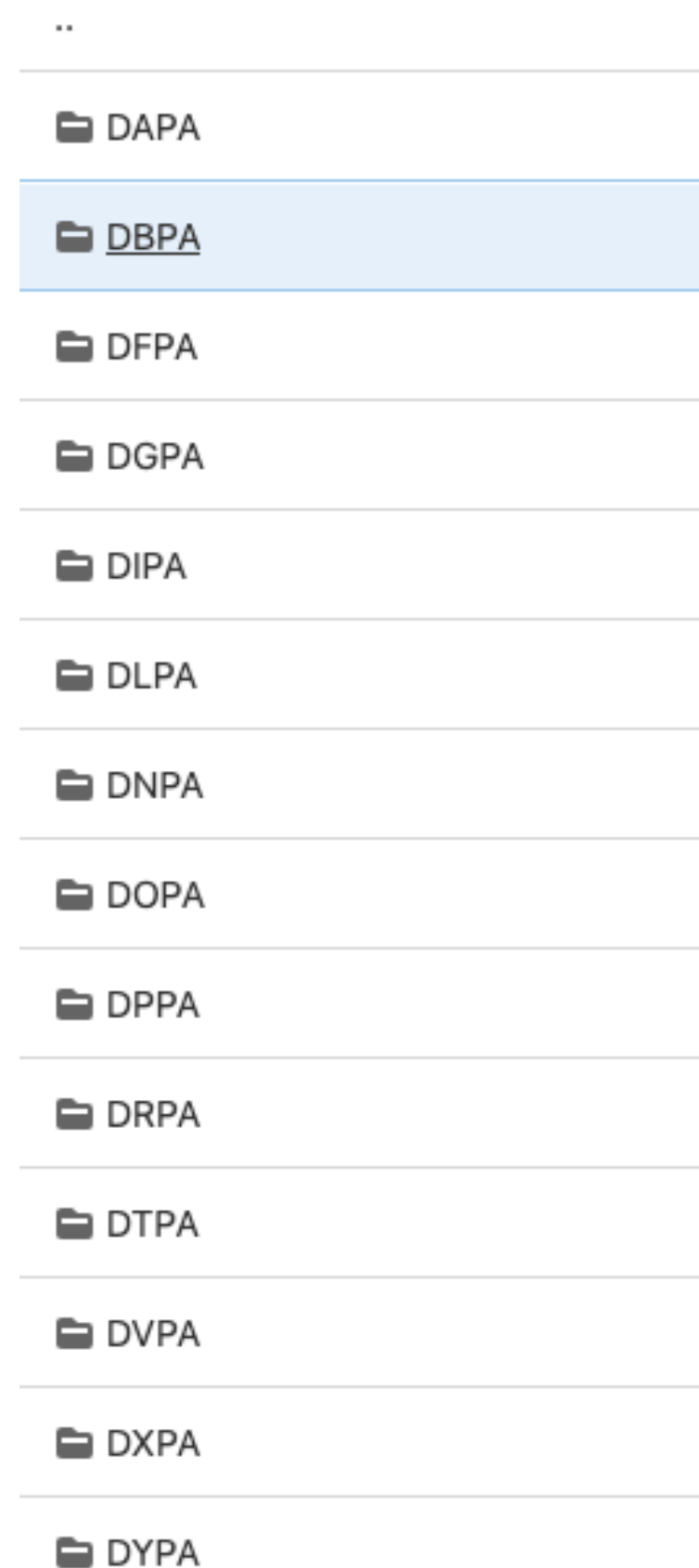
[ADD ANOTHER ITP FILE](#)

Database: batch insertion

<https://mad.ibcp.fr/explore>

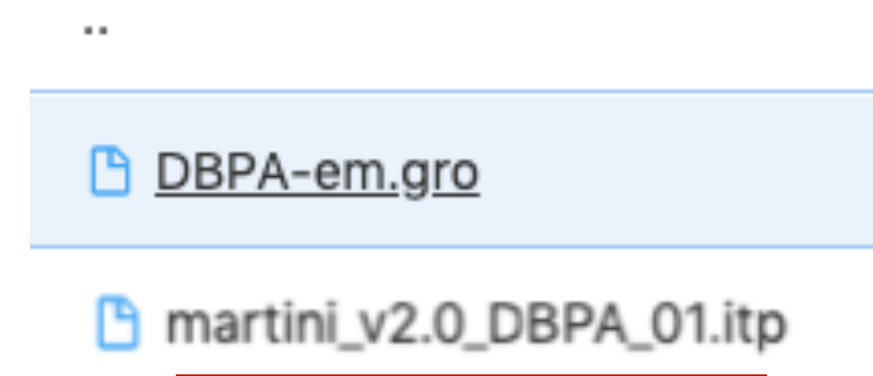


Molecule class is
subdirectory name



- Insert many molecules at the same time
- Used to fill the DB initially
- Inspired from the martini website data layout

Each bottom folder contains a
single molecule information with :



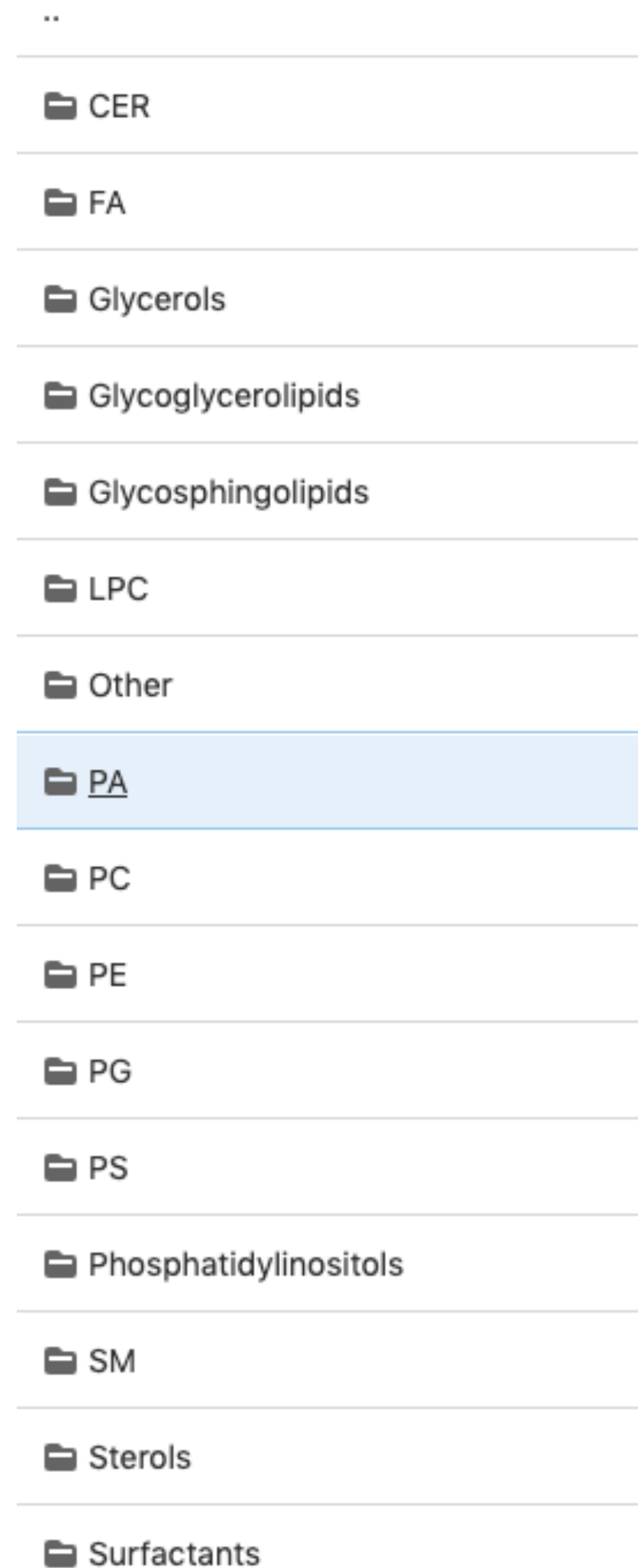
One coordinates file

Potentially many parameter version files

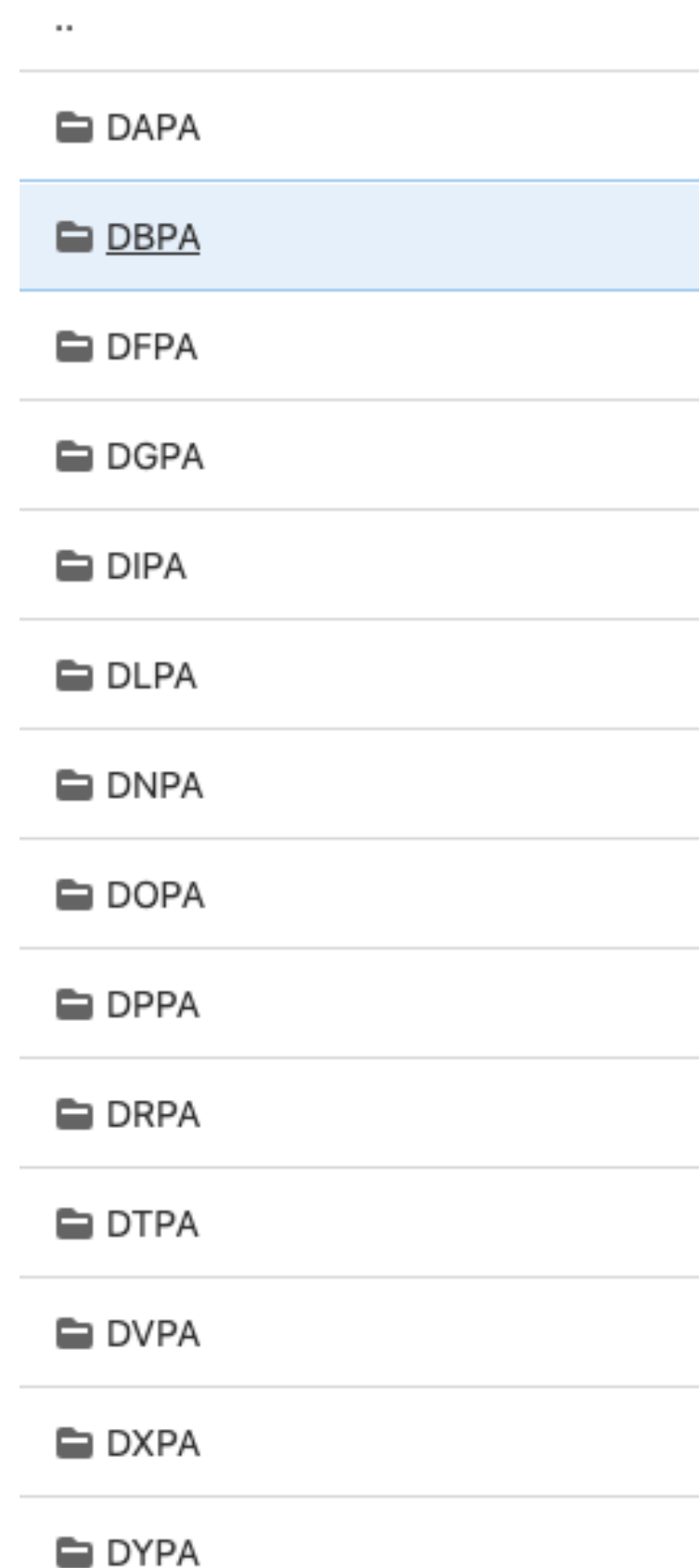
Optional mapping files

Database: batch insertion

<https://mad.ibcp.fr/explore>



Molecule class is
subdirectory name



- ▶ Insert many molecules at the same time
- ▶ Used to fill the DB initially
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Each bottom folder contains a
single molecule information with :



One coordinates file

Potentially many parameter version files

Optional mapping files

The name of the ITP file must fulfil the syntax:

martini_vX.Y_MoleculeName_VersionNumber.itp

where a version number 01 is mandatory

MAD: web servers

Molecule builder

- ▶ GUI for *martinize.py* (vermouth 0.7)
- ▶ *PLUS*: interactive editing of GO and elastic bonds

System builder

- ▶ GUI for *insane.py*
- ▶ *PLUS*: automatic insertion of martinized biomolecules

Using the servers requires authentication!

MAD: the *Molecule builder*

<https://mad.ibcp.fr/builder>

MArtini Database



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Explore

Force field

Creation way

Categories

Name

Alias

Author

Free text



Explore



Molecule builder



System builder



Force fields



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Contact

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 Explore

 Molecule builder

 System builder

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MAD: the *Molecule builder*

<https://mad.ibcp.fr/builder>

- Explore
- Molecule builder**
- System builder
- Force fields
- Login
- Contact

Martinize a molecule

martinize with vermouth 0.7.1

[MAD Home](#)

Select your coarse graining settings

Force field
martini3001

Position restraints
Backbone

Mode
Classic

C-terminal
CCOH-ter

N-terminal
NH2-ter

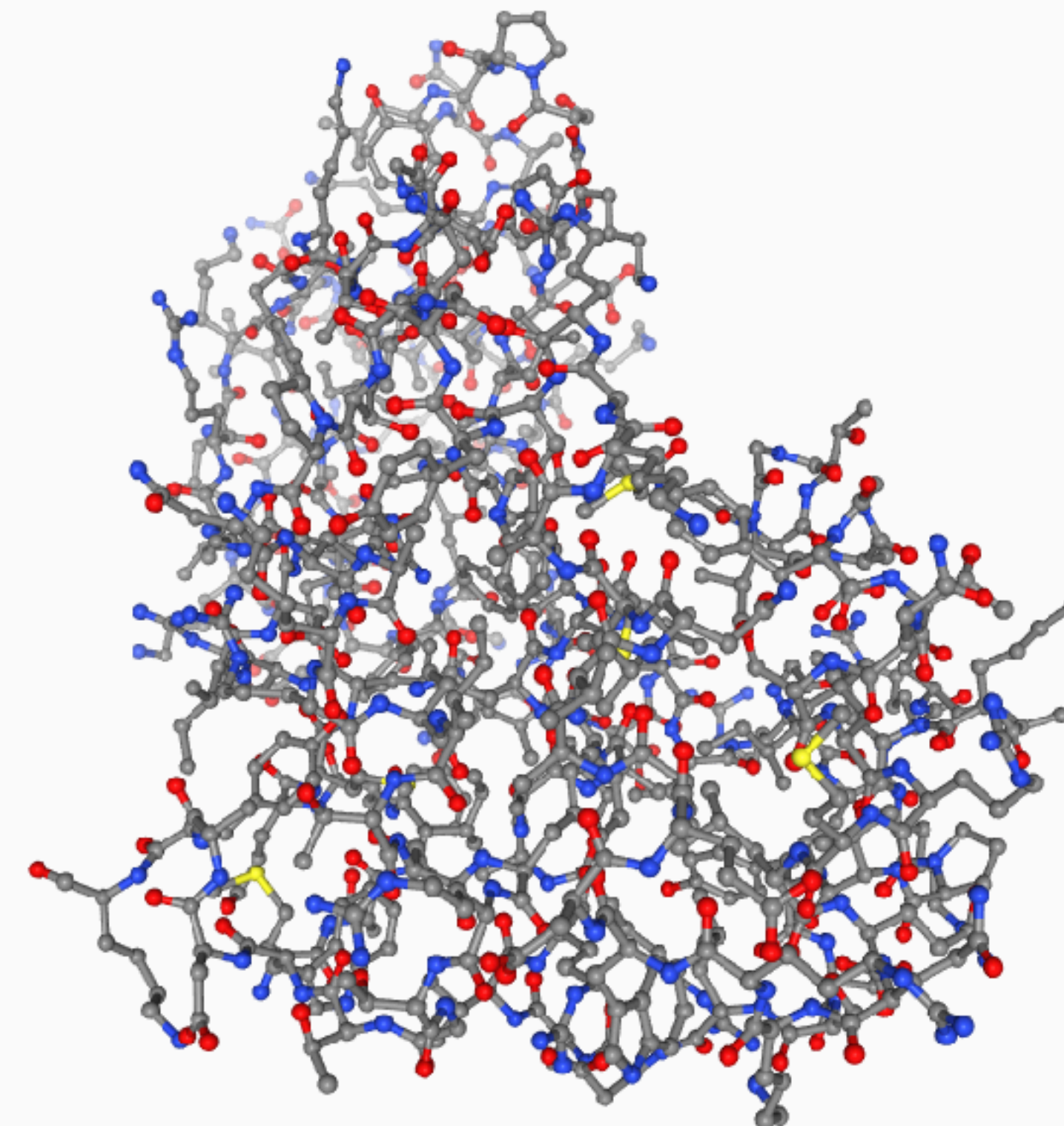
Side-Chain fix
 no yes

Cystein Bridge
 none auto

Activate advanced mode

Command Line
-f input.pdb -x output.pdb -o system.top -ff martini3001 -p backbone -ds

[BACK](#) [SUBMIT](#)



MAD: the *Molecule builder*

<https://mad.ibcp.fr/builder>

Visualizing and manually editing constraints

The screenshot displays the MAD molecule builder interface. On the left is a control panel with the following sections:

- Theme:** A toggle switch for "Dark theme" is currently off.
- All atom Opacity:** A slider set to "Visible" (indicated by a red dot).
- Coarse grained Opacity:** A slider set to "Visible" (indicated by a red dot).
- Virtual Go bonds Opacity:** A slider set to "Visible" (indicated by a red dot).
- Representations:** A row of icons for different visualization modes.
- SAVE** and **DOWNLOAD** buttons at the bottom.

The central area shows a 3D molecular model with atoms represented by colored spheres (green, blue, yellow, red, grey) and bonds as lines. A panel on the right titled "Edit Go virtual bonds" provides editing options:

- First selected group:** 1-10
- Second selected group:** 20-23
- 14 sites selected.**
- CREATE ALL BONDS** (blue plus icon)
- DELETE EVERY BOND** (red minus icon)
- BACK** (orange left arrow icon)
- Navigation arrows (left, refresh, right) at the bottom.

On the far right, a smaller view of the molecular model shows a specific part of the structure highlighted in blue and red, corresponding to the selected groups in the editing panel.

MAD: the *System builder*

https://mad.ibcp.fr/membrane_builder

Any previously martinized molecule can be inserted in membrane

Load from database

SEARCH A MOLECULE

Load from stashed molecules

Want to martinize a molecule ?

BMRA-GO (martini304)
Created on 2020-05-04 with mode GO sites

1cm (martini304)
Created on 2020-04-30 with mode GO sites

Upload a molecule

Used force field
martini22

Coarse-grained PDB/GRO file

ADD FILE Select a file...

Generated TOP file (by Martinize)

ADD FILE Select a file...

Generated ITP files

ADD FILE Select a file...

ADD ANOTHER ITP FILE

then

Choose membrane composition

DIPC	4	
	Positive integer	
Lipid	Presence ratio	
DOPC	1	
	Positive integer	

+ ADD LIPID

pH



Lower membrane leaflet

Lipid	Presence ratio	
DIPC	4	
	Positive integer	

+ ADD LIPID

pH



Separate lower and upper leaflet

BACK

NEXT

then

Edit Insane membrane parameters

INSANE settings

Periodic boundary conditions

Box type
hexagonal

Box size
7,7,9

3, 6 or 9 positive integers separated by commas

Lipid options

Area per lipid (upper layer, nm ²) 0,6	Area per lipid (lower layer, nm ²) 0,6
Must be greater than 0	Must be greater than 0
Random kick size 0,1	Bead distance (nm) 0,3
Must be greater than 0	Must be greater than 0

Protein options

Center protein in membrane

Orient protein in membrane

Rotate protein
none

MAD: the *System builder*

https://mad.ibcp.fr/membrane_builder

Theme

Dark theme

Water

Show water

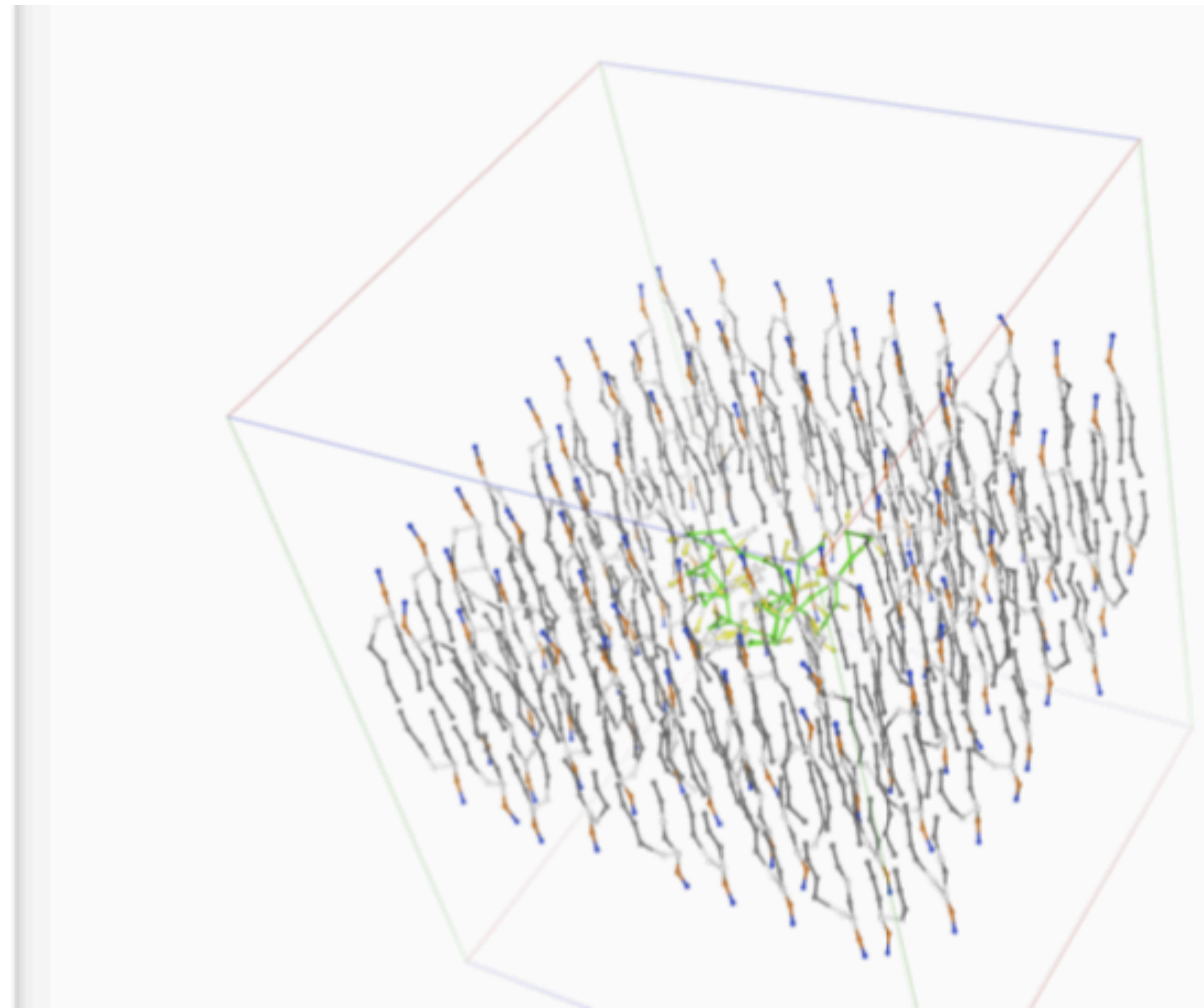
Box

Visible box

Opacity

← BUILD SETTINGS

↓ DOWNLOAD



Perspectives

On the 3 currently existing tools:

- Later retrieval of job results
- Possible: pH slider for *Molecule builder* (and *System builder*?)
- Possible: more changes based on *constructive* feedback from users

Implementation of additional tools:

1. *Mappingbuilder* (designed by J. Barnoud)
2. A GUI for *polyply*
3. A GUI for *TS2CG*