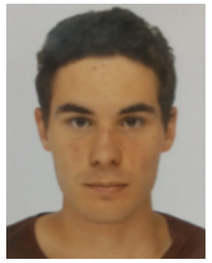
The MArtini Database (MAD) and web server

Luca Monticelli
CNRS & University of Lyon, France

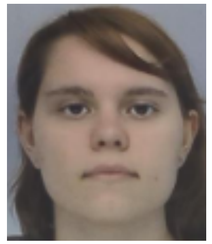
The people behind MAD

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?

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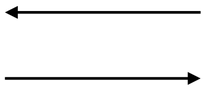
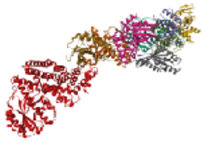
The answer: a database!

Hardware/software infrastructure

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



NGL viewer



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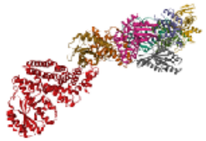
React

NGL viewer



Web server

Hardware/software infrastructure

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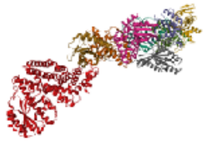
NGL viewer



Web server

Computation & storage

CouchDB

slurm
workload manager

Hardware/software infrastructure

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

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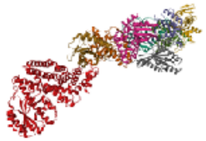
NGL viewer



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https://github.com/MMSB-MOBI

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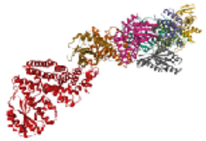


Web server

Computation & storage

CouchDB

slurm
workload manager

https://github.com/MMSB-MOBI

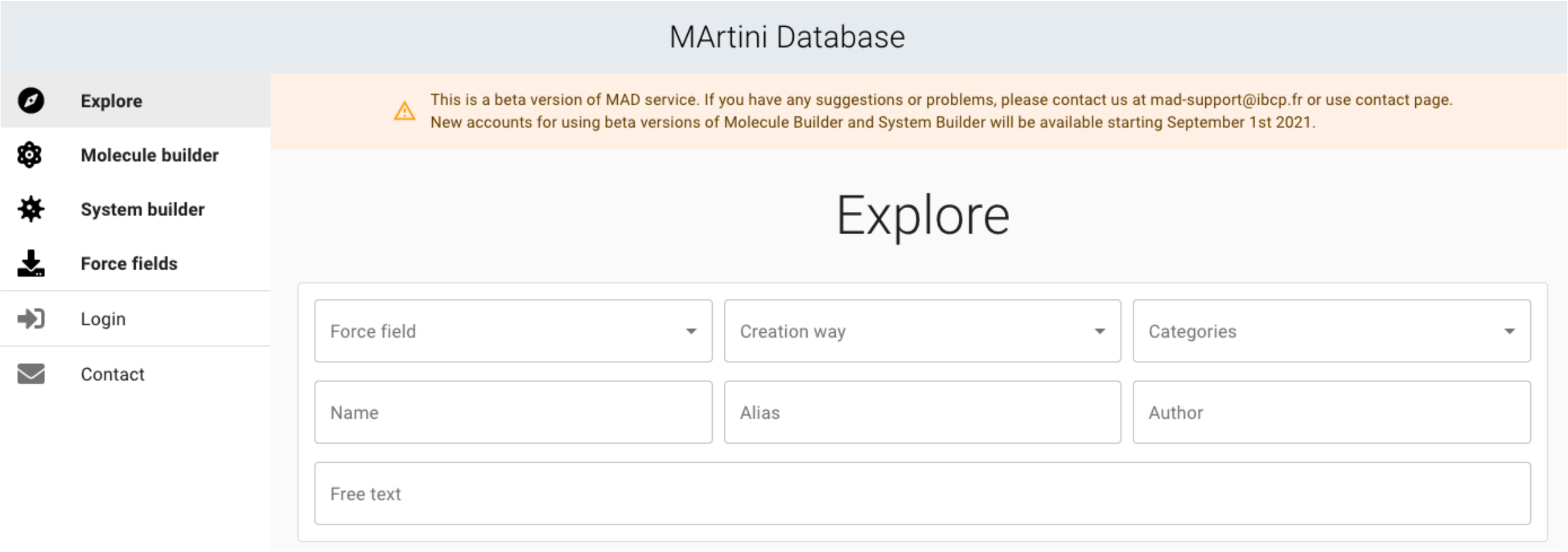
100+ physical cores (more coming soon)

Two high performance storage units

Local backup + remote backup

How does it look like?

https://mad.ibcp.fr



How does it look like?

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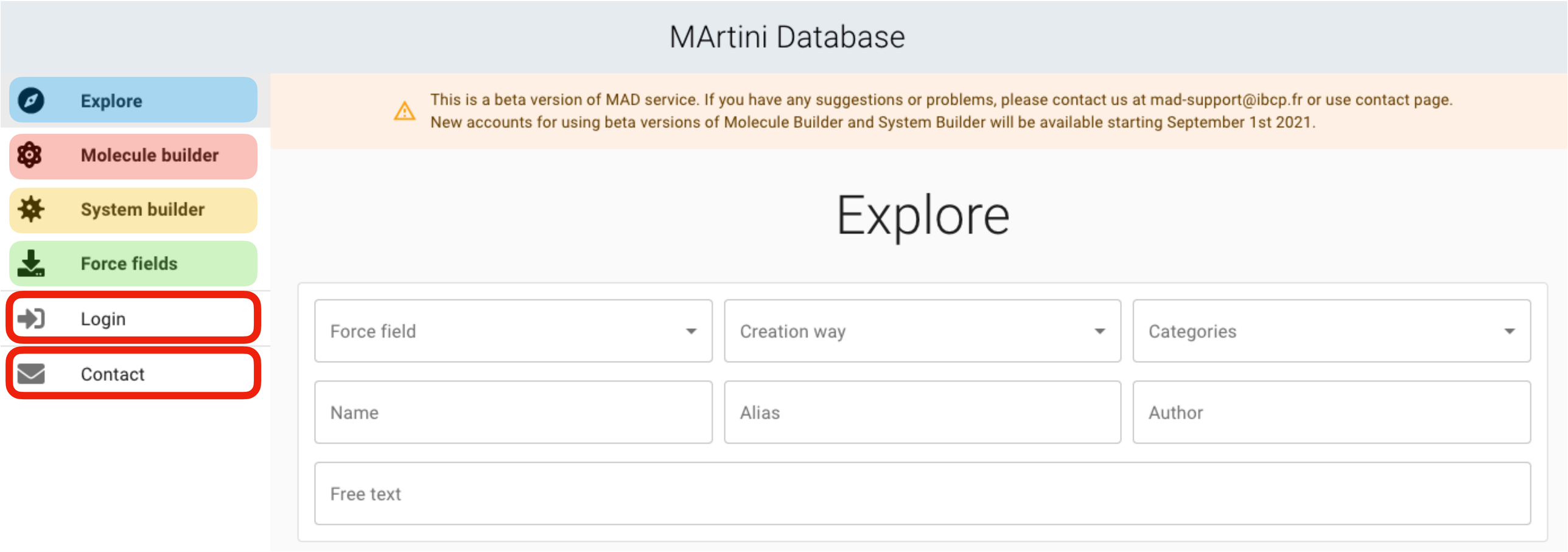
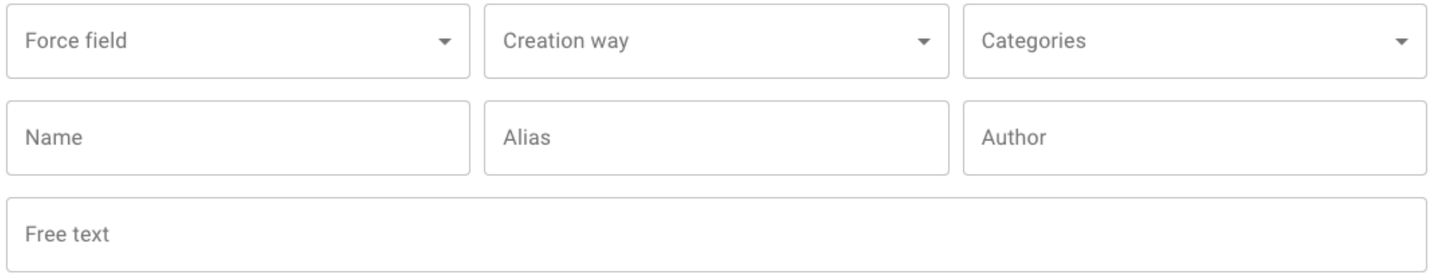


Explore the database

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



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 where 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.jpcb.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

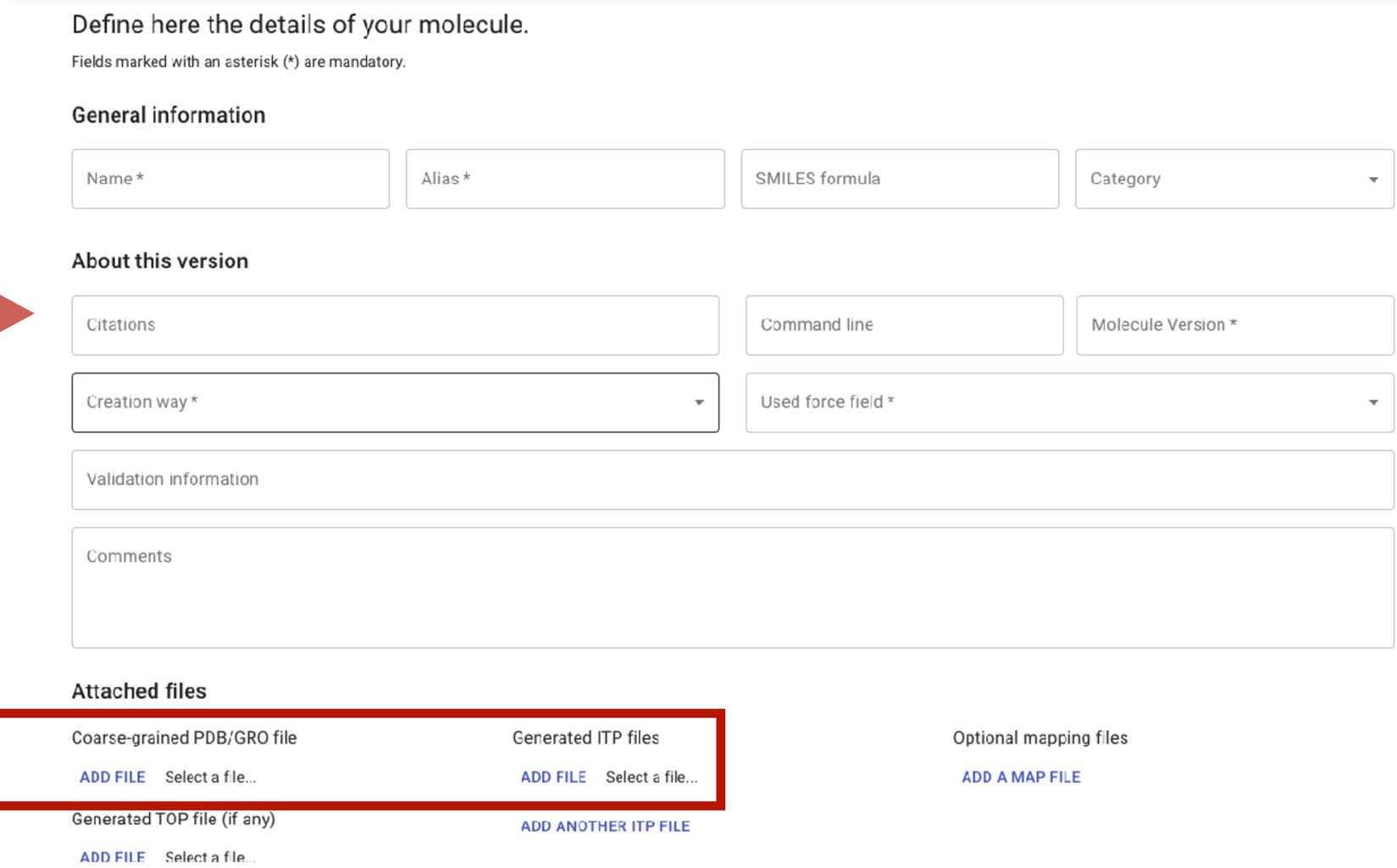
➡ **Interactive uploading in the browser**
Submitted by standard users, approved by admins

Batch of molecules

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

Database: individual insertion

https://mad.ibcp.fr/explore



publication ID / doi

Mandatory

Database: individual insertion

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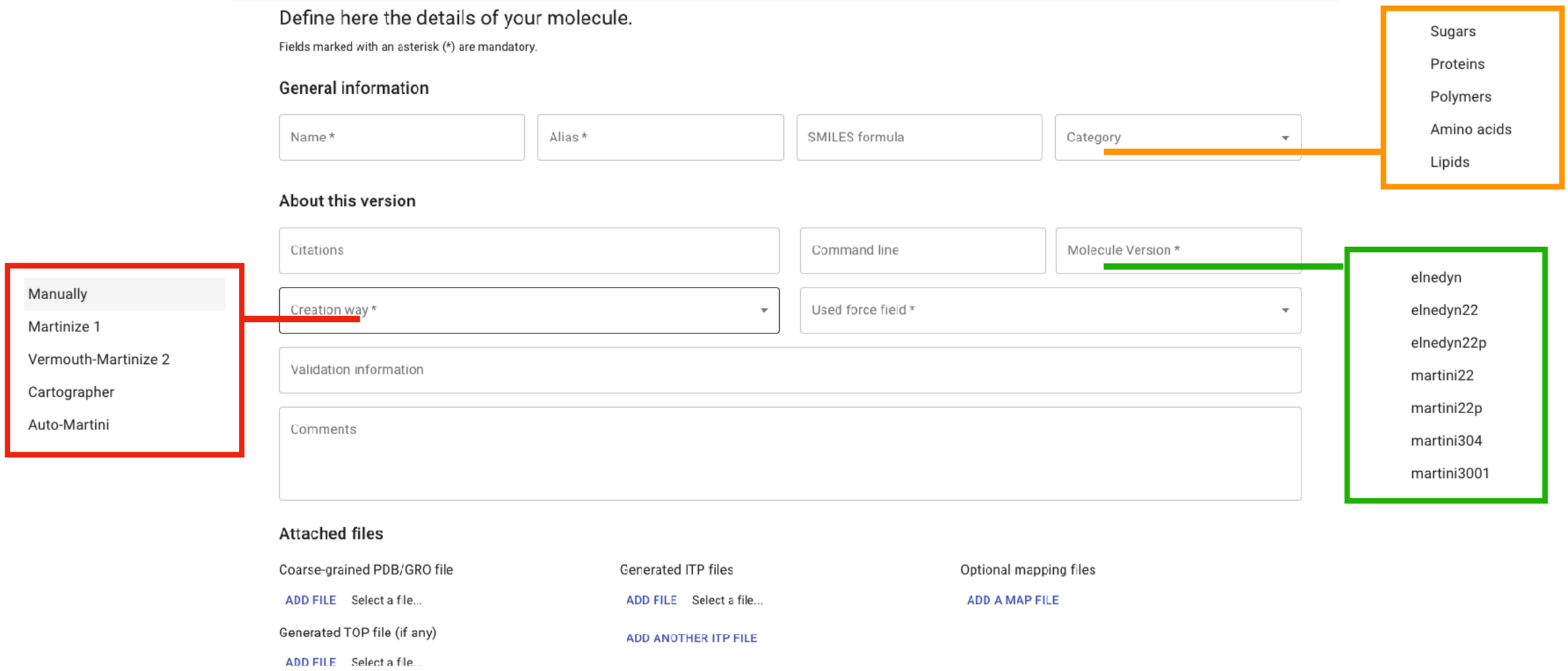
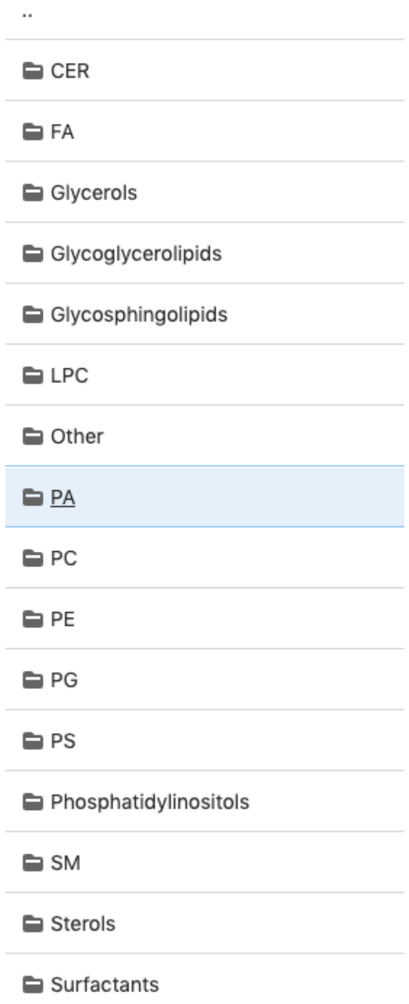
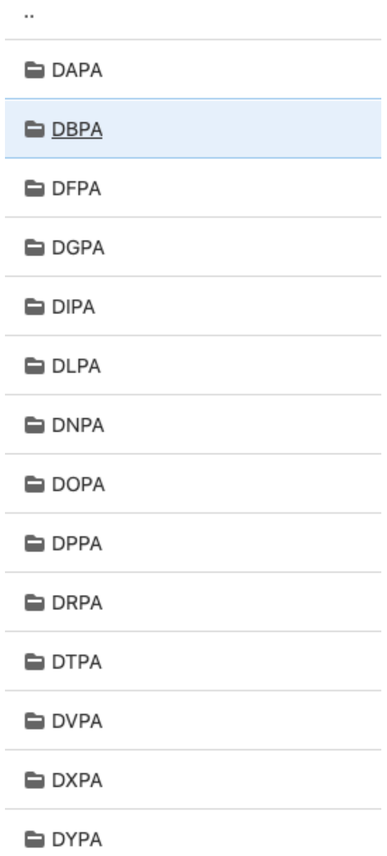


Database: batch insertion

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 :

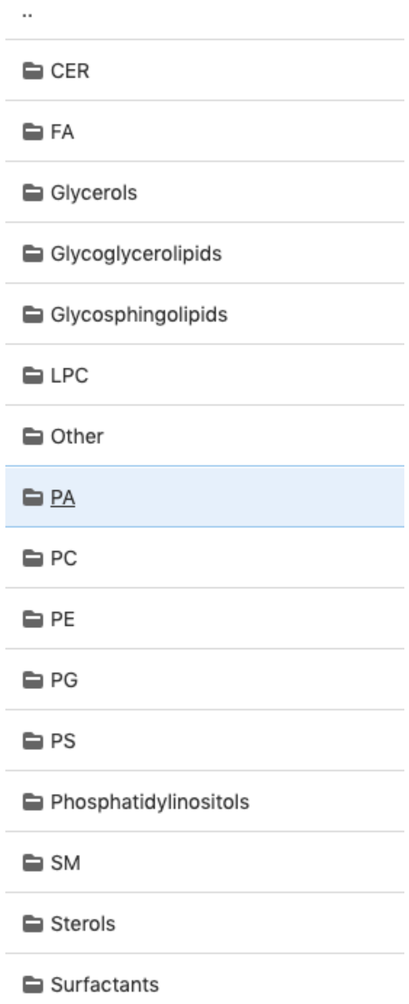
One coordinates file

Potentially many parameter version files

Optional mapping files

Database: batch insertion

https://mad.ibcp.fr/explore



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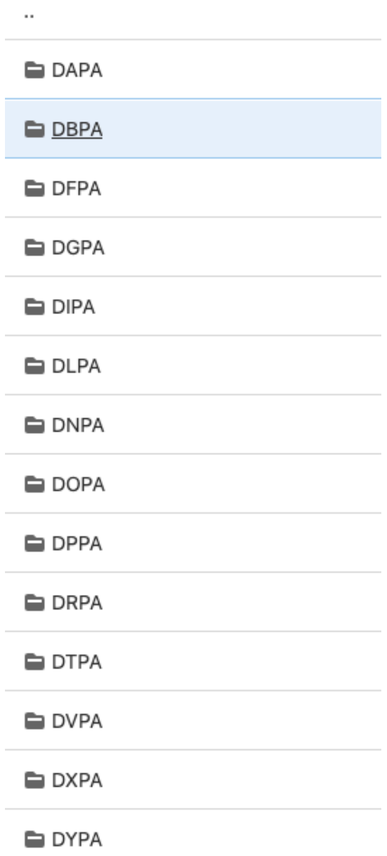

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Optional mapping files

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

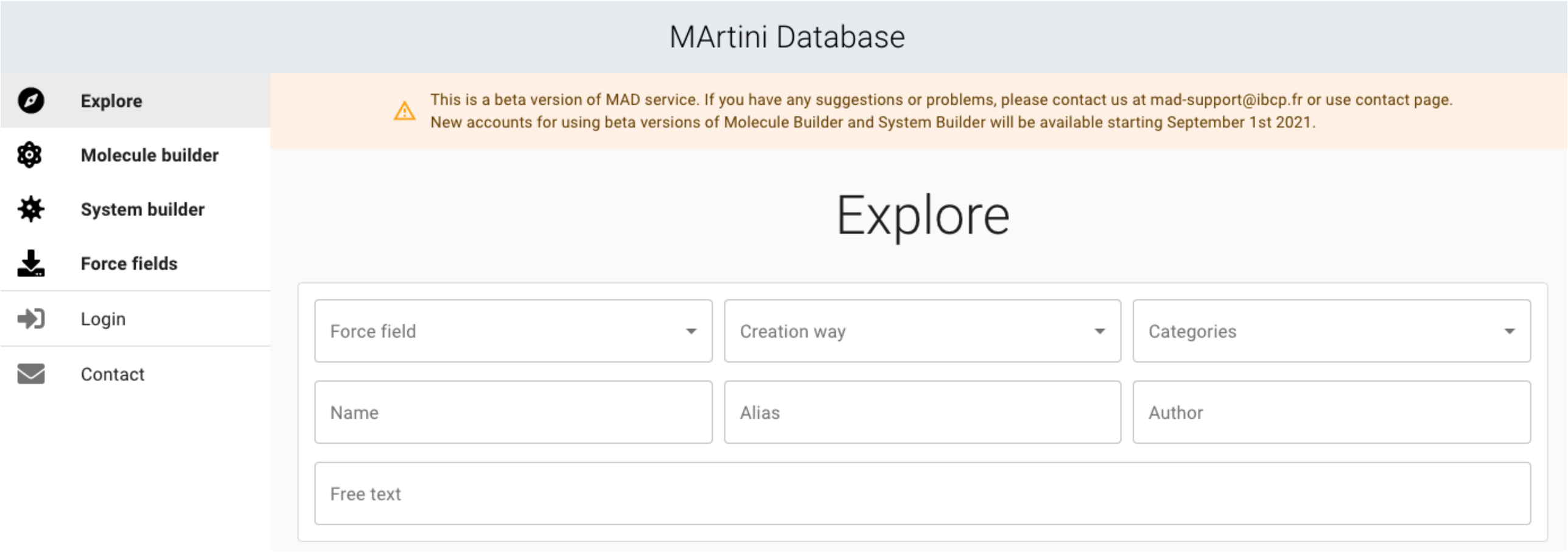
System builder

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

Using the servers requires authentication!

MAD: the *Molecule builder*

https://mad.ibcp.fr/builder



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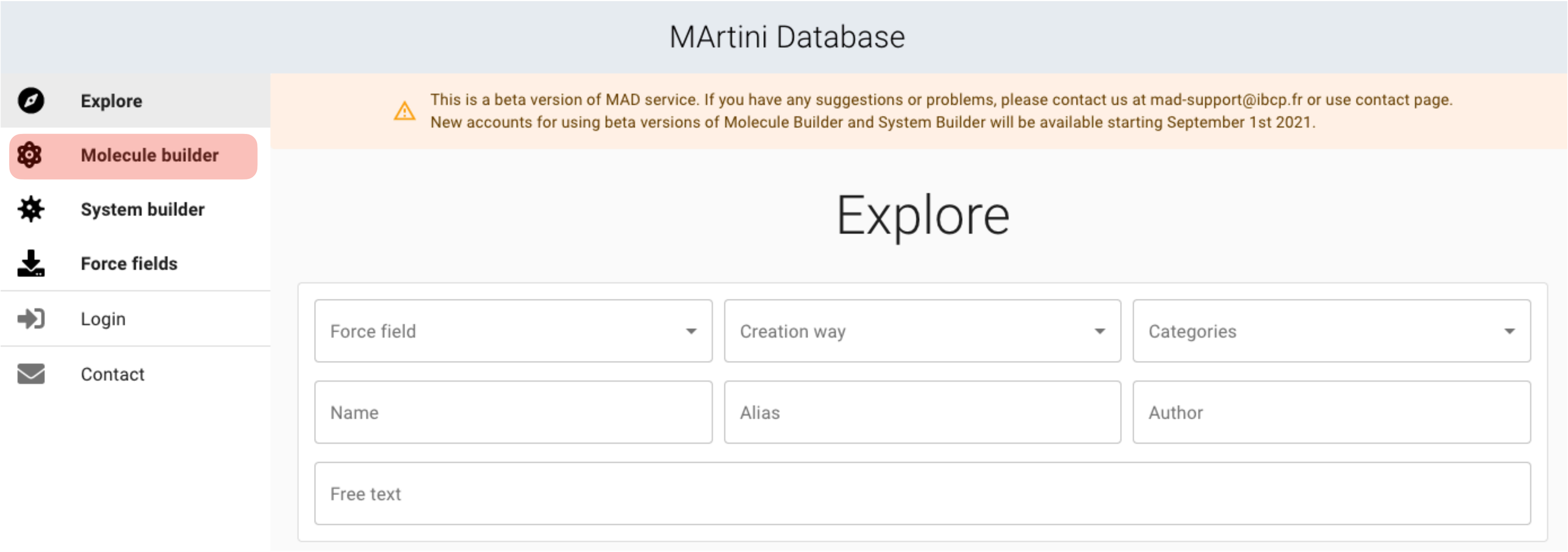

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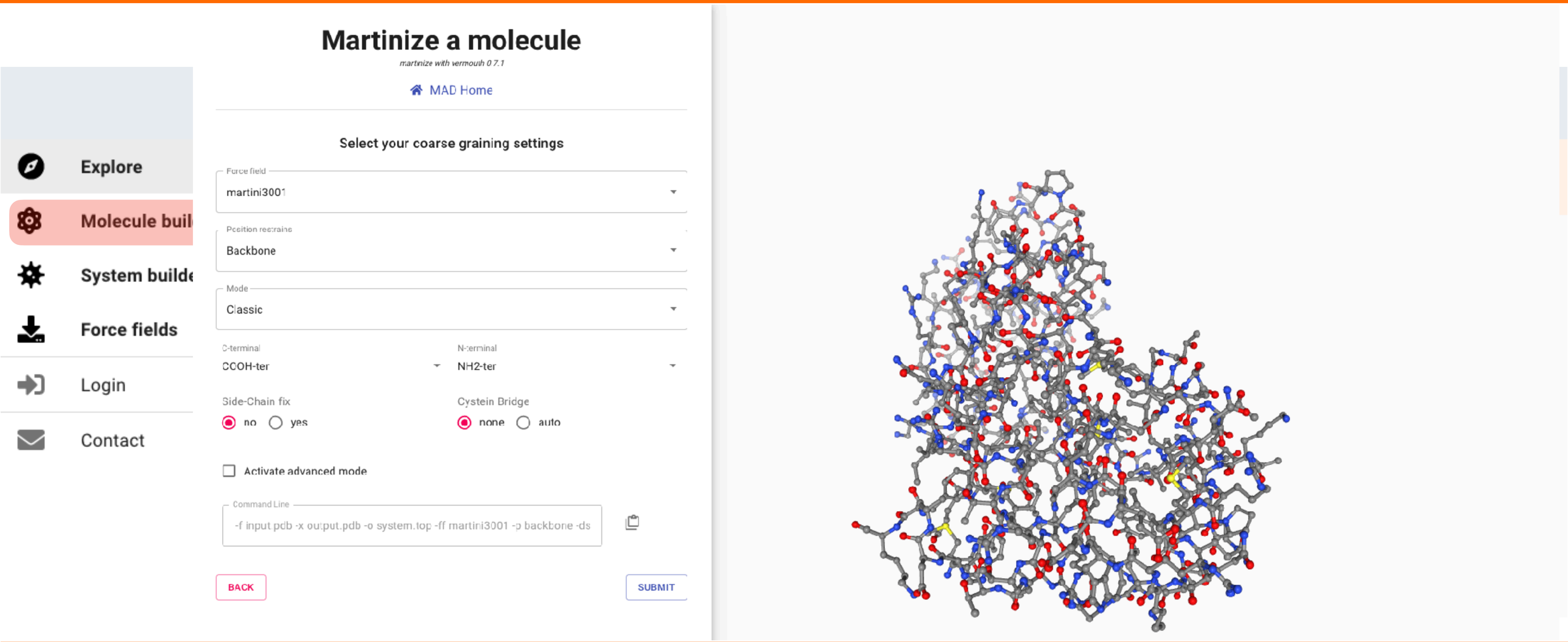

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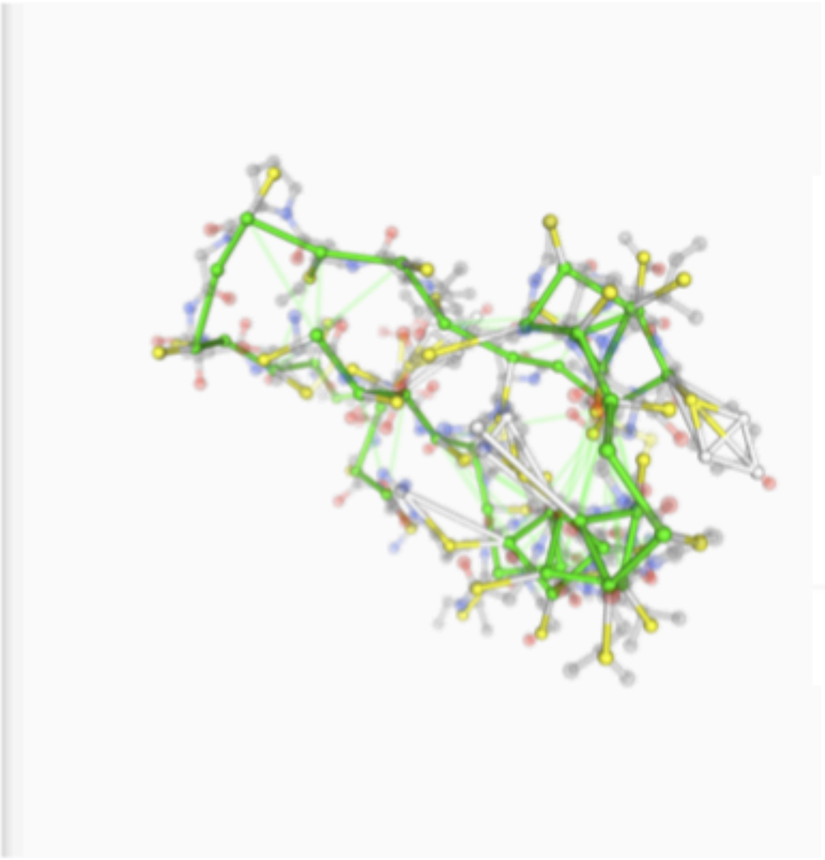
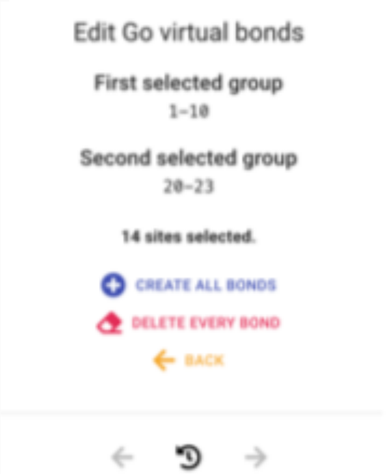
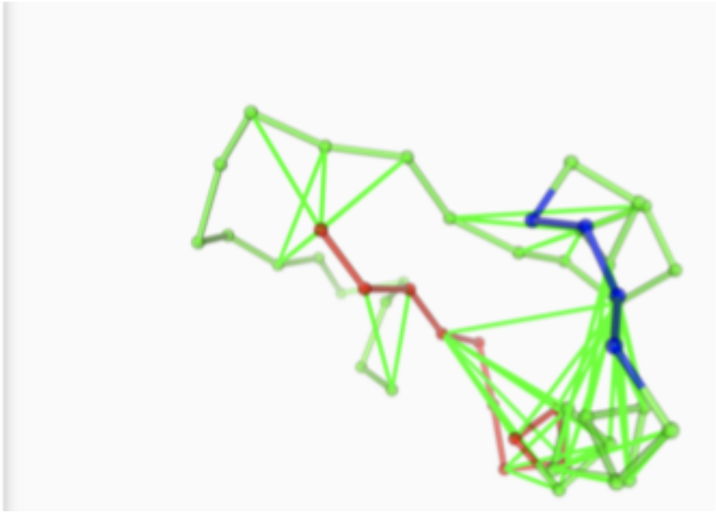
Visualizing and manually editing constraints



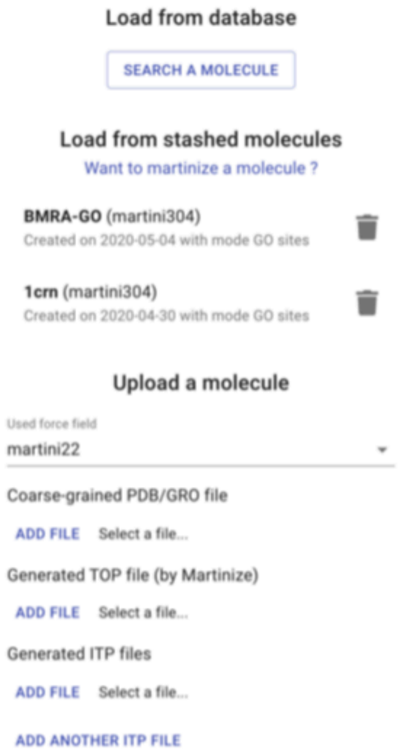




MAD: the *System builder*

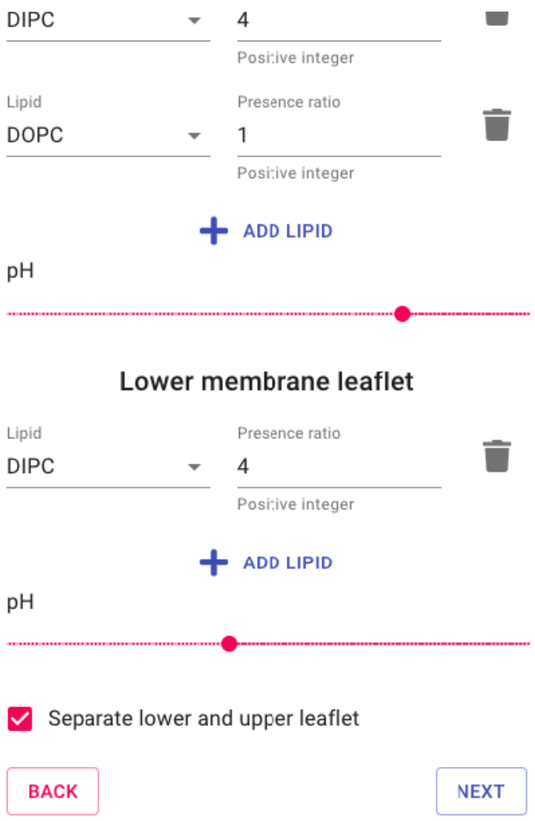
https://mad.ibcp.fr/membrane_builder

Any previously martinized molecule can be inserted in membrane



then

Choose membrane composition

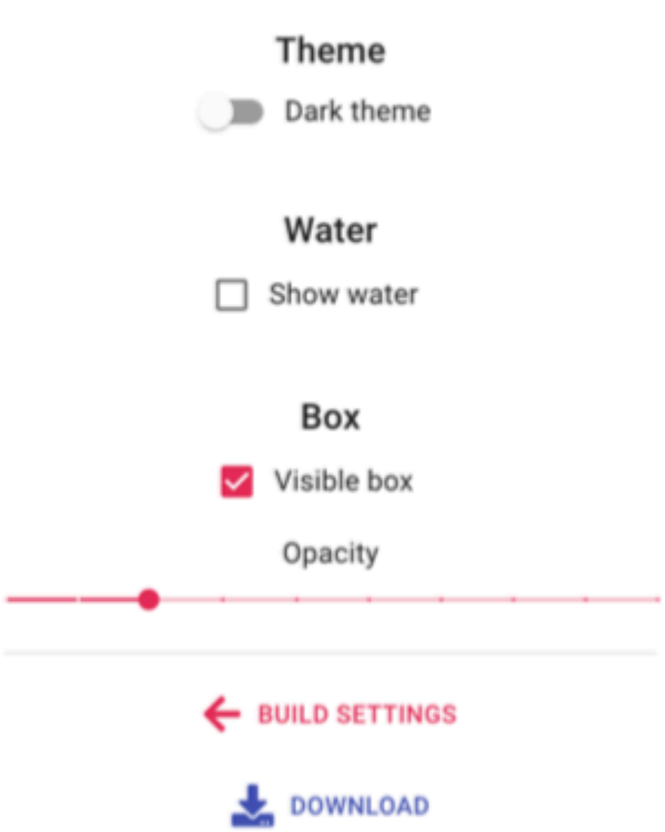


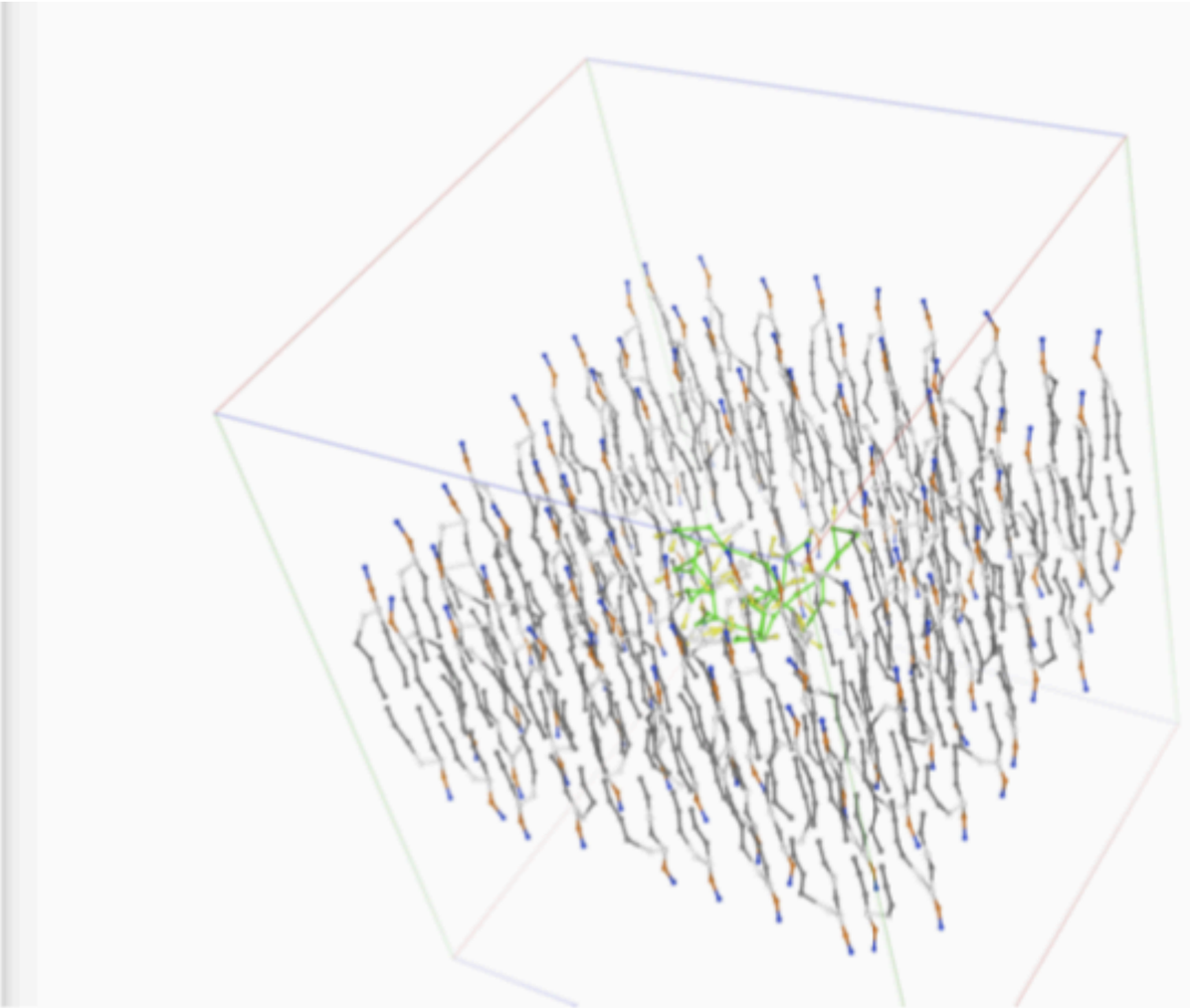
then

Edit Insane membrane parameters

MAD: the *System builder*

https://mad.ibcp.fr/membrane_builder





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*