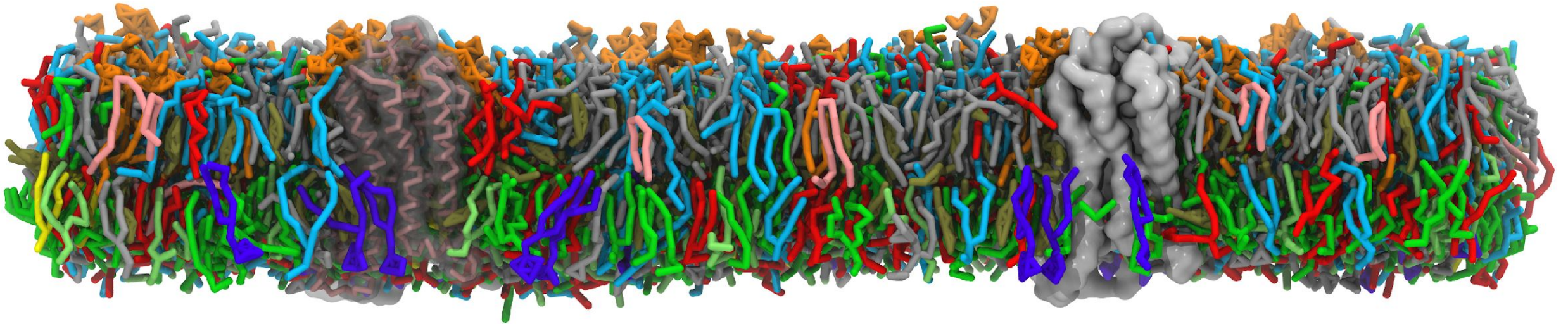


ProLint: Automated analysis and visualization of lipid – protein interactions



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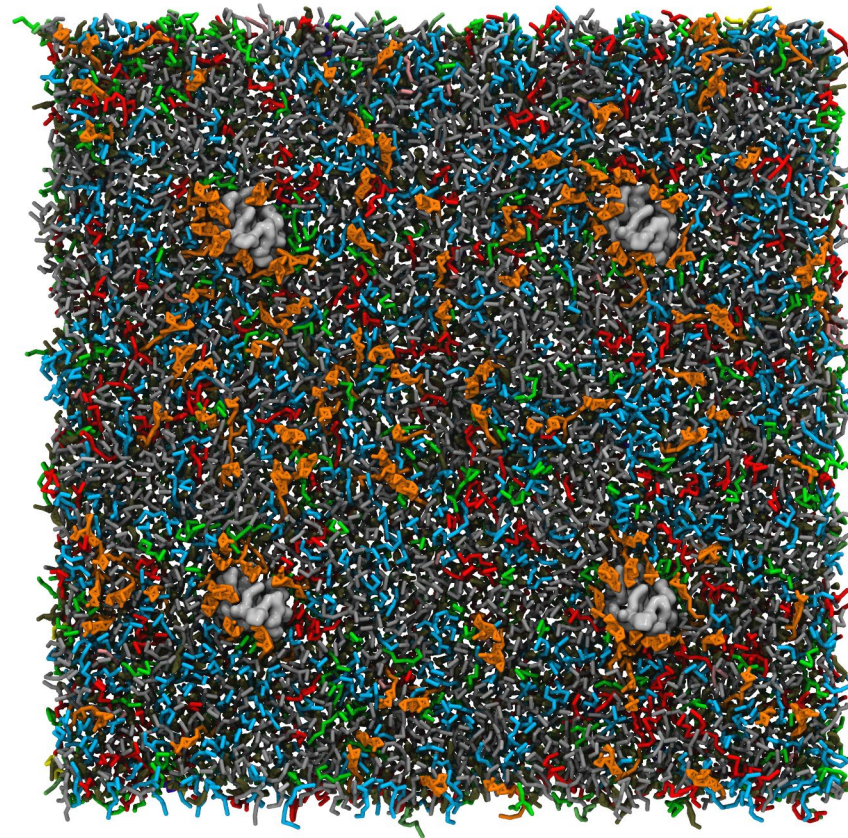
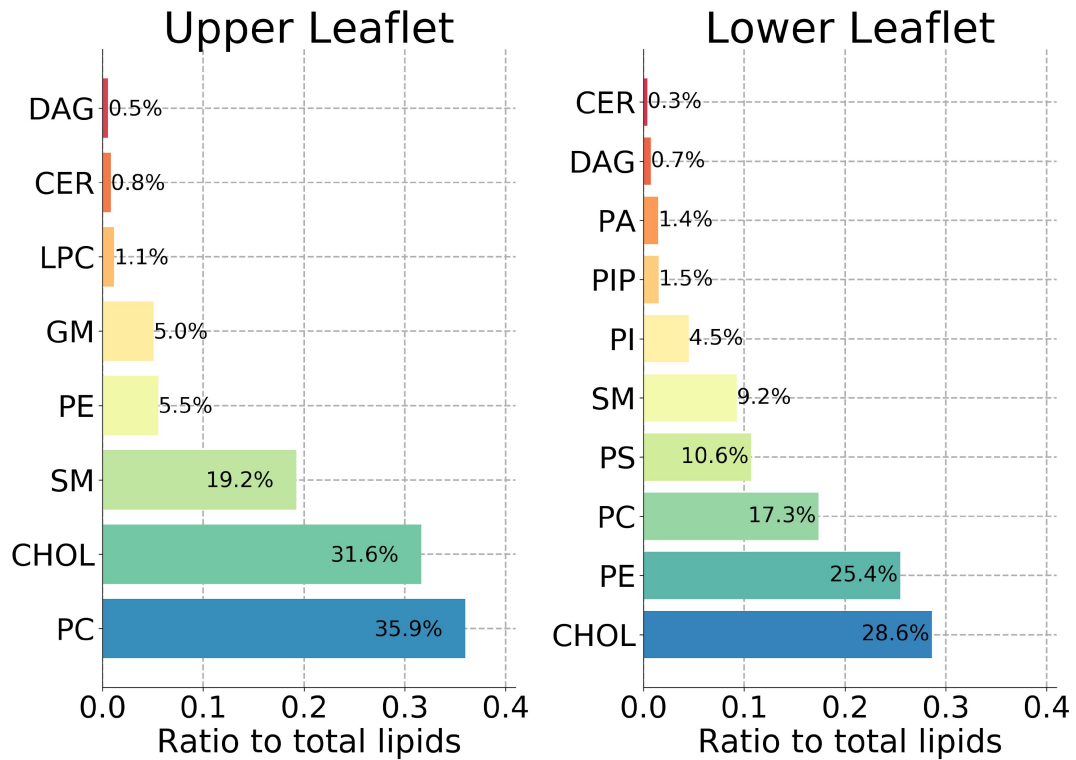
Motivation

- Biologically important interactions
- Growing and exciting field
- Amenable to MD simulations

However:

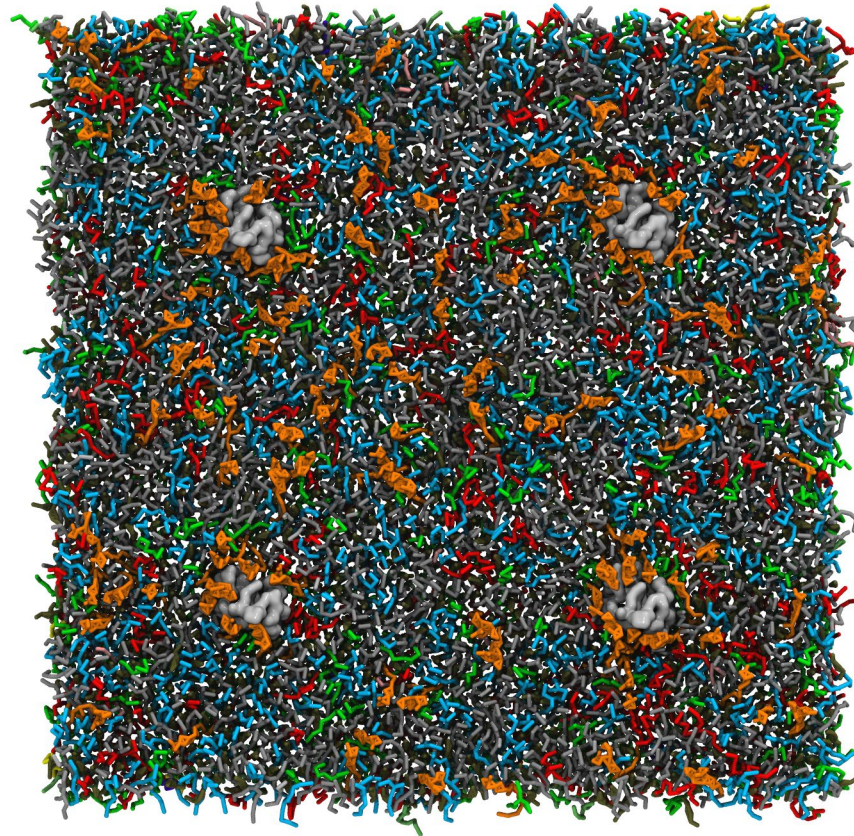
- Analysis and visualization are very time consuming
- Increase in the amount of data generated
- Complex interplay between lipids and proteins.
- Necessity to automate the generation of interaction profiles

Common MD system



Common MD system

- 28 different GPCRs
 - 63 different lipid species
- 4 x 28 x 63 (30 μ s)**



ProLint Components

- ProLint framework:
 - Webservice
 1. Upload & Results
 2. Database
 3. GPCRs page
 - URL: <https://www.prolint.ca>
 - Installable via Docker
 - Standalone python library: prolintpy
 - JupyterLab environment
 - GitHub: <https://github.com/ProLint/prolintpy>
 - g_surf binary

Submission Form

Title

Give a name to your protein(s):

Protein

Upload your trajectory file.

Upload your coordinate file.

Group lipids according to their headgroup type (e.g. POPC -> PC)?

Group identical proteins/chains together (calculates average properties)?

Distance cutoff: 3.0 Å 6.0 Å

3.5 Å 6.5 Å

4.0 Å 7.0 Å

5.0 Å 7.5 Å

5.5 Å 8.0 Å

The is the value that is used to define contacts between lipids and residues. Note that two cutoffs will roughly double the calculation time, as such we recommend you only select one value.

Consider only the following lipids (comma separated, leave blank for all lipids)

Select the appropriate resolution:

The Martini Model ▼

Type of analysis: Contact-based

Density-based

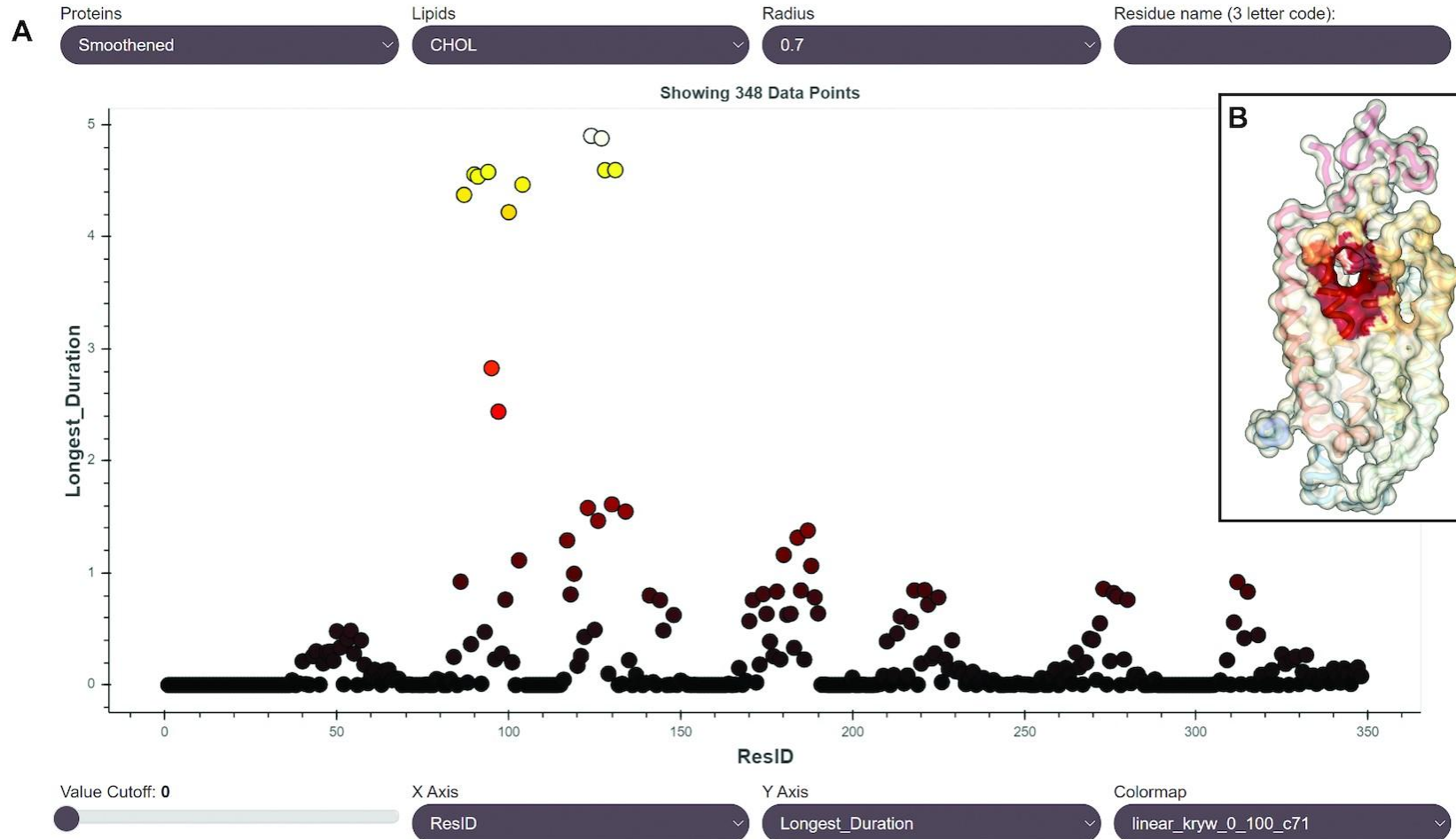
Physical-properties

Provide an email to notify you when calculations are done (OPTIONAL).

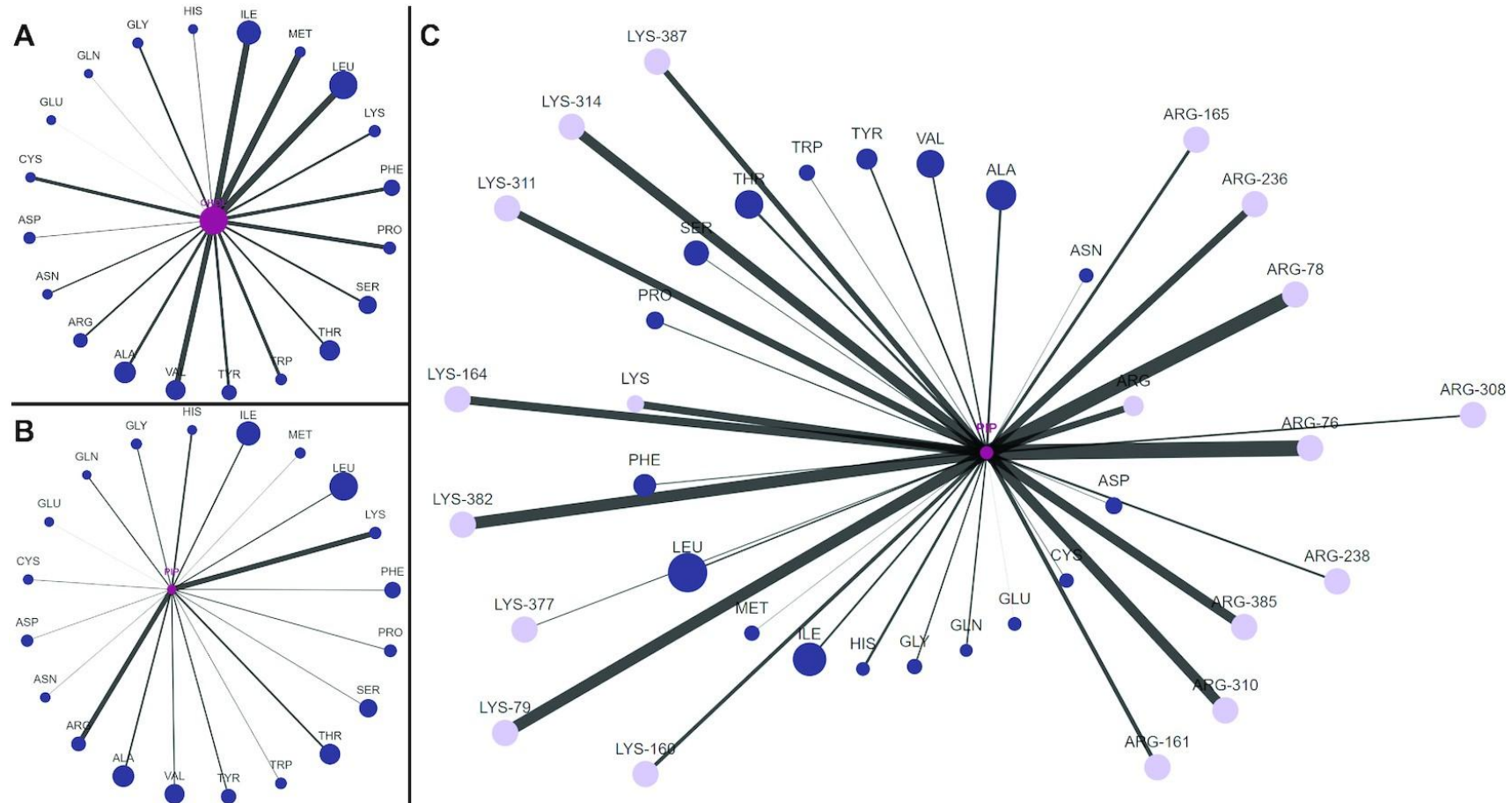
ProLint python library: *prolintpy*

- Features:
 - Automated analysis of lipid-protein interactions
 - Contact-based
 - Densities
 - Physics-based
 - Feature-rich visualization applications
 - User interactivity
- Uses and is optimized for the JupyterLab environment.

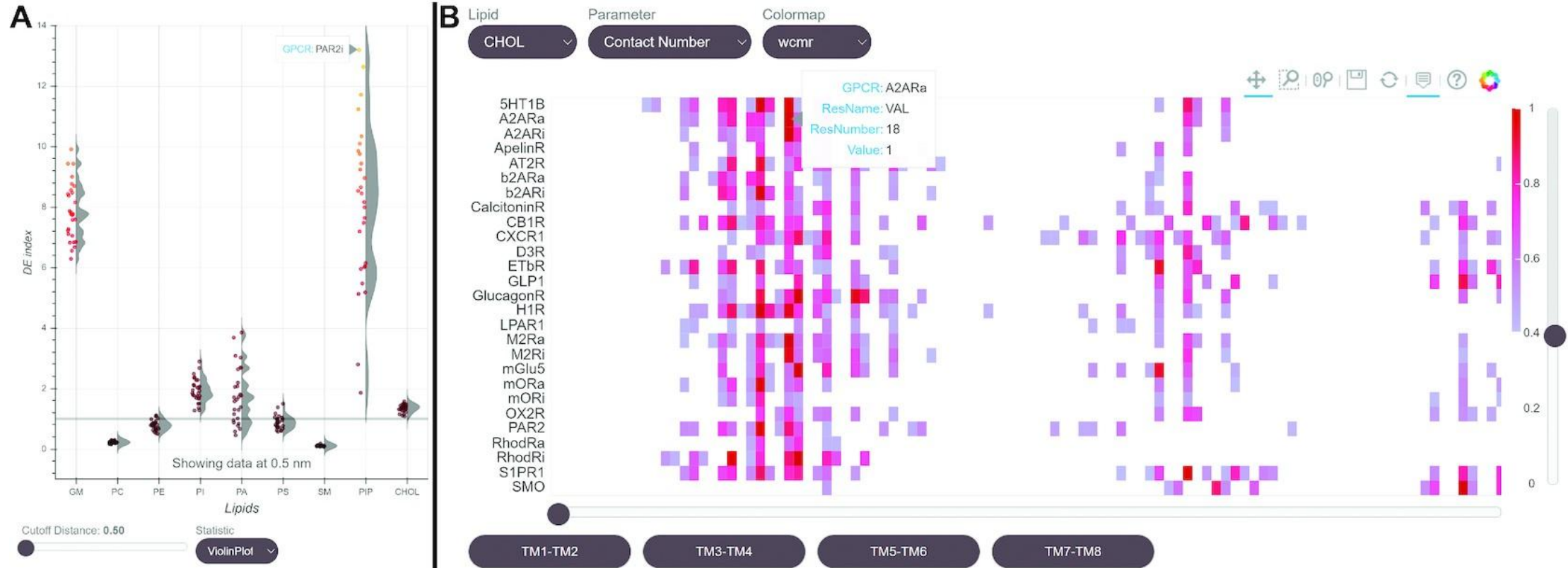
SMO-cholesterol interactions



Protein-lipid contact networks

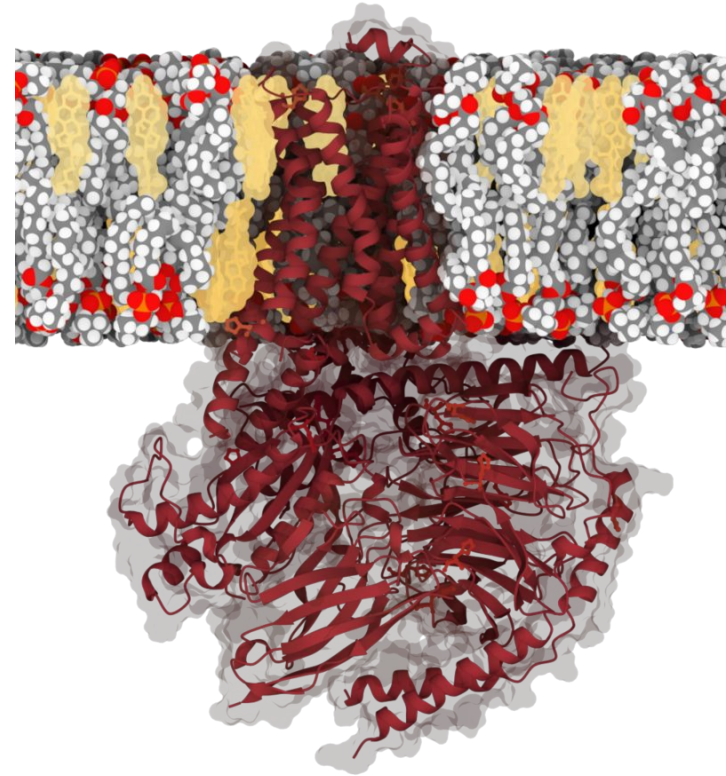


GPCR-wide interactions



Conclusions

1. **Automated and modular analysis**
2. **Interactive visualization**
3. **Automation & scalability**
4. **Accessibility & shareability**



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