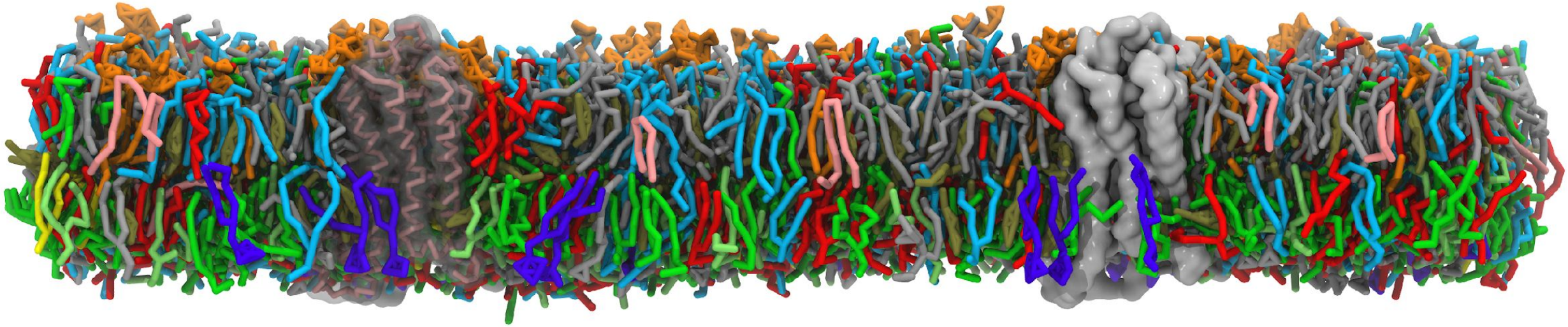
ProLint: Automated analysis and visualization of lipid – protein interactions



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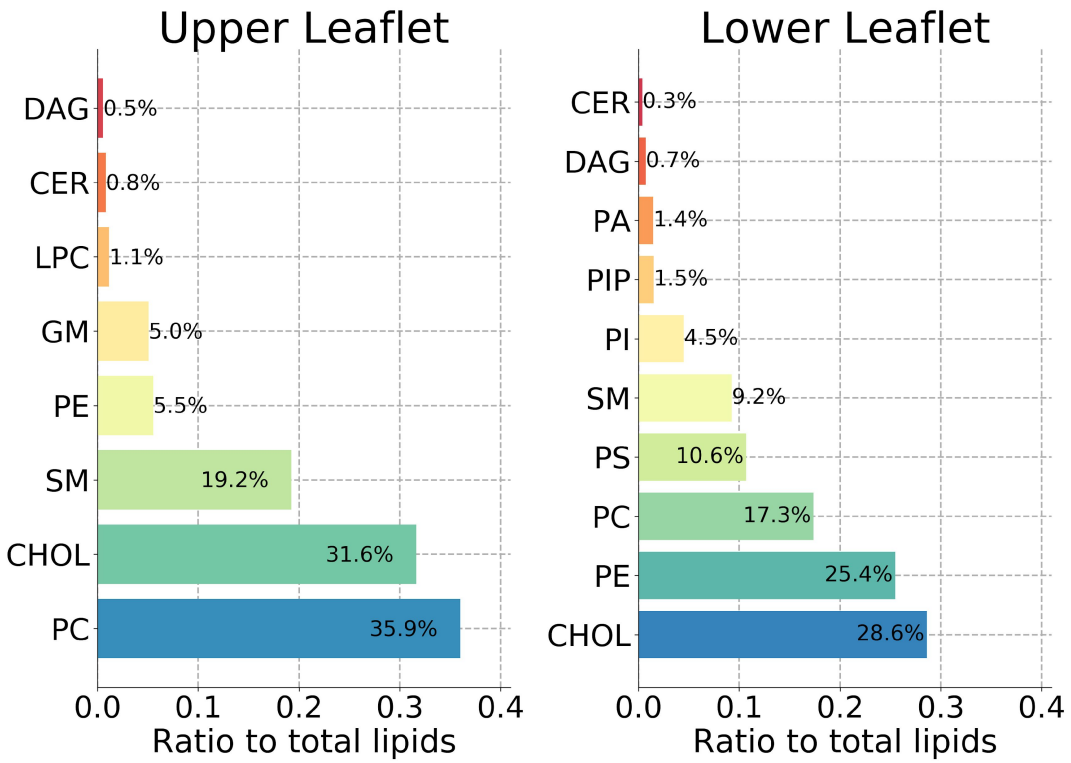
Motivation

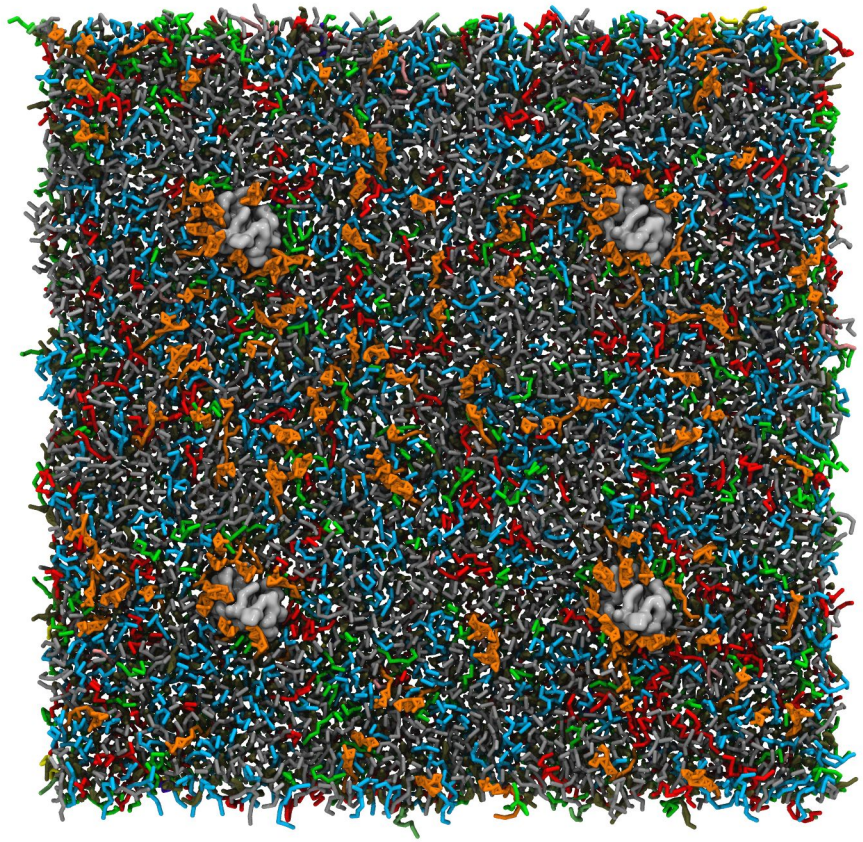
- Biologically important interactions
- Growing and exciting field
- Amenable to MD simulations

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



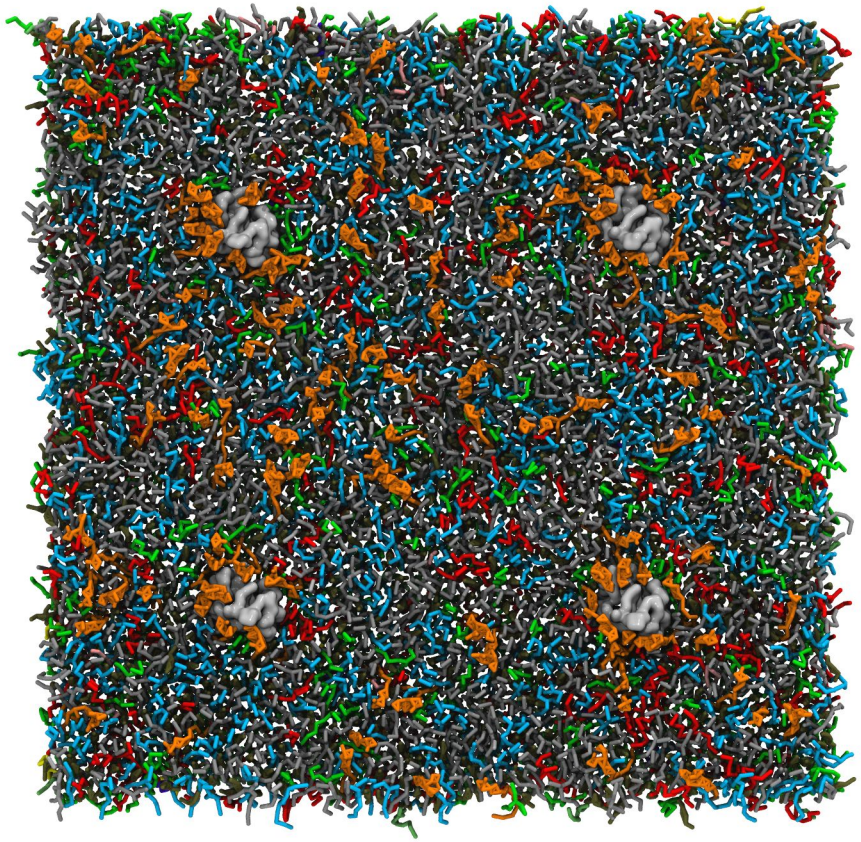


Sejdiu, B. I. & Tieleman D. P. Biophysical Journal. 118(8):1887-1900

Common MD system

- 28 different GPCRs
- 63 different lipid species

4 x 28 x 63 (30 µs)



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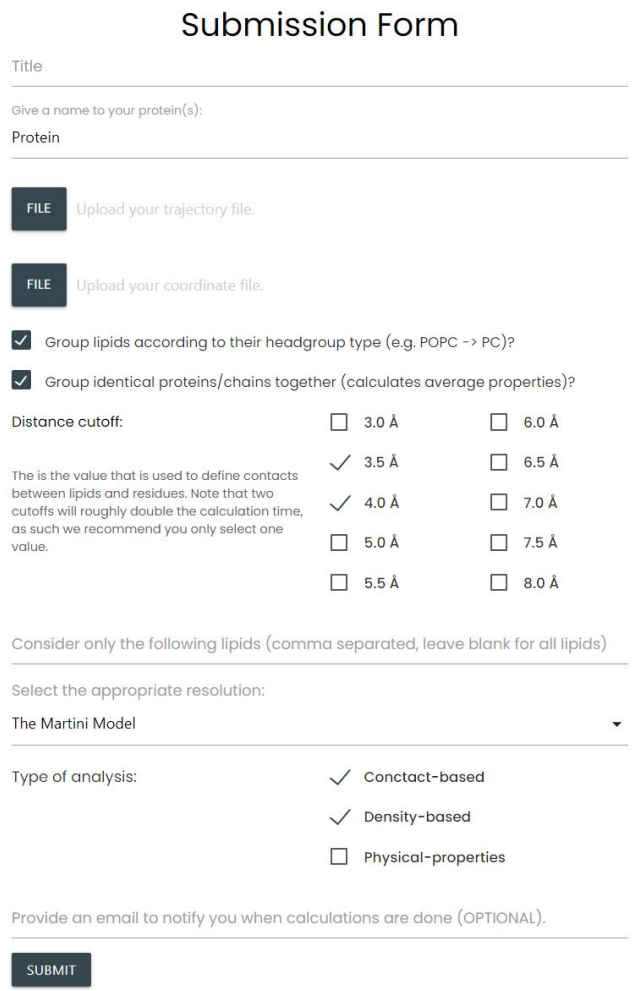
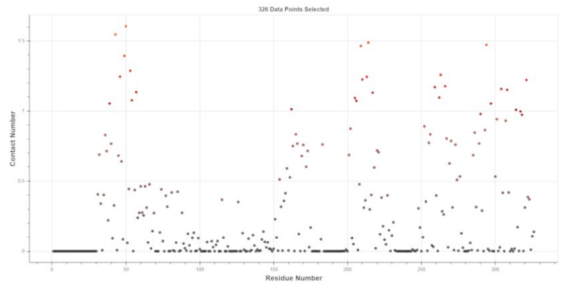
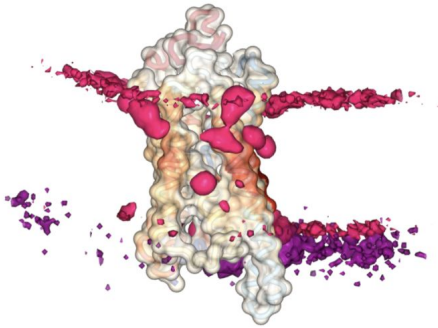
ProLint Components

- ProLint framework:
  - Webserver
    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



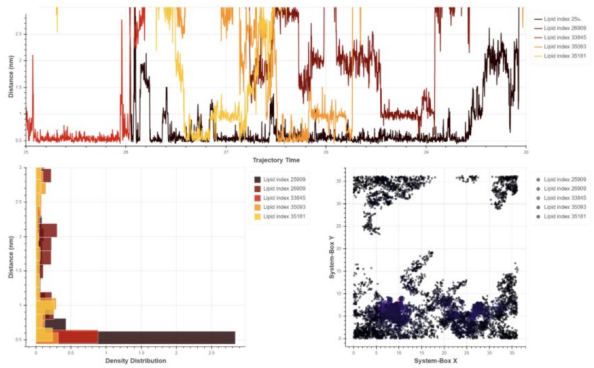


Scatter Application

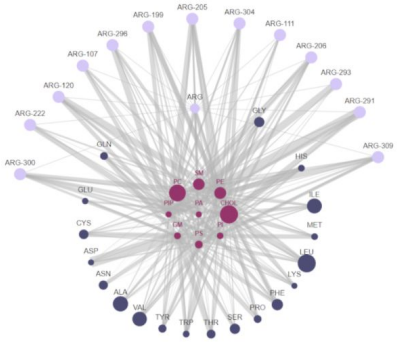


3D Density Application

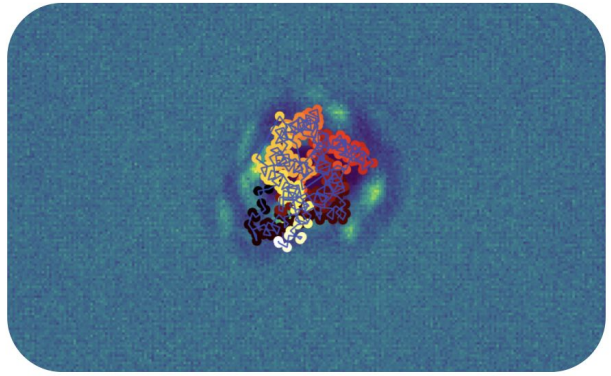
ThickCurv Application



TimeSeries Application



Network Application



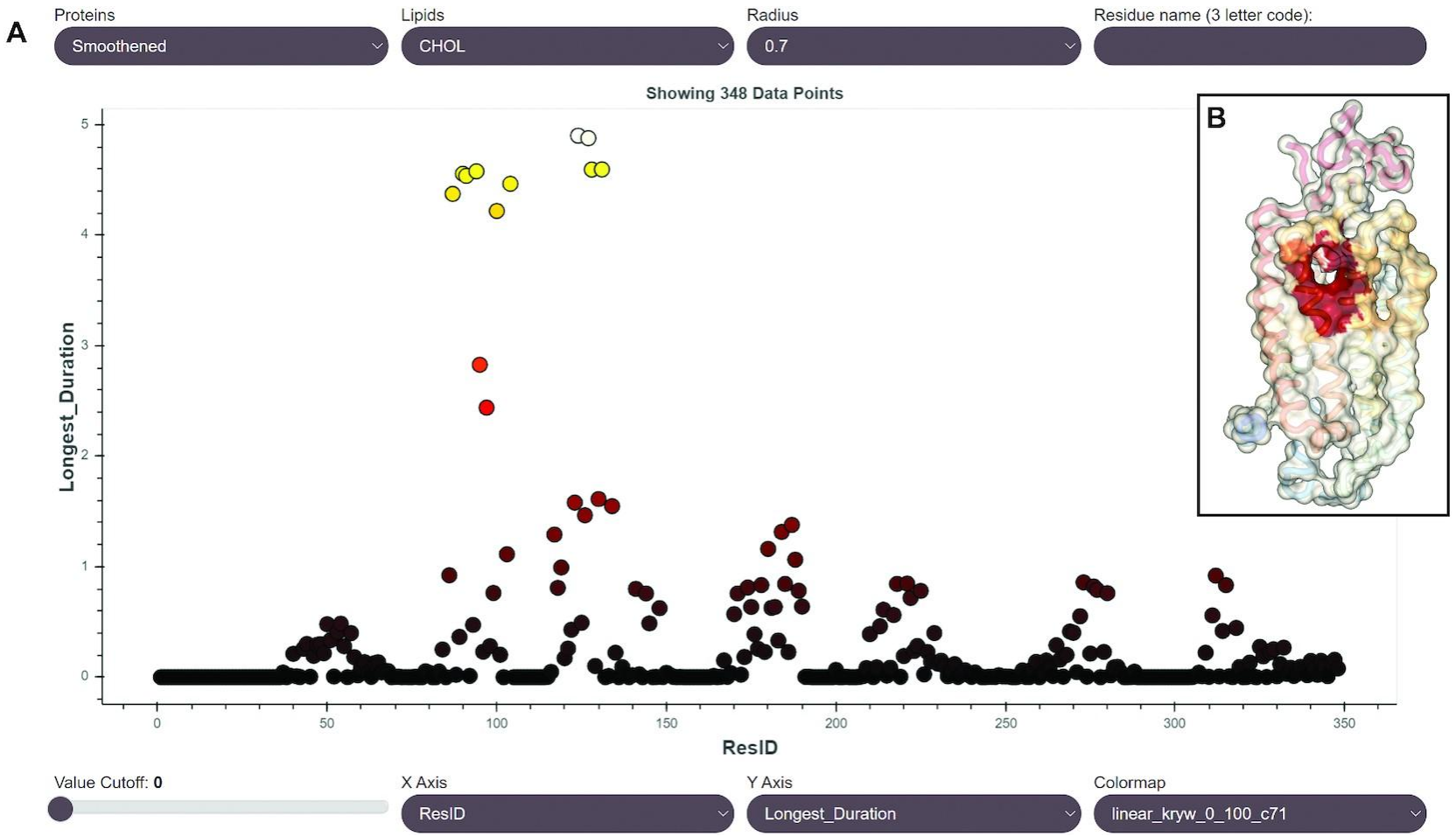
Density Application

ProLint python library: *prolintpy*

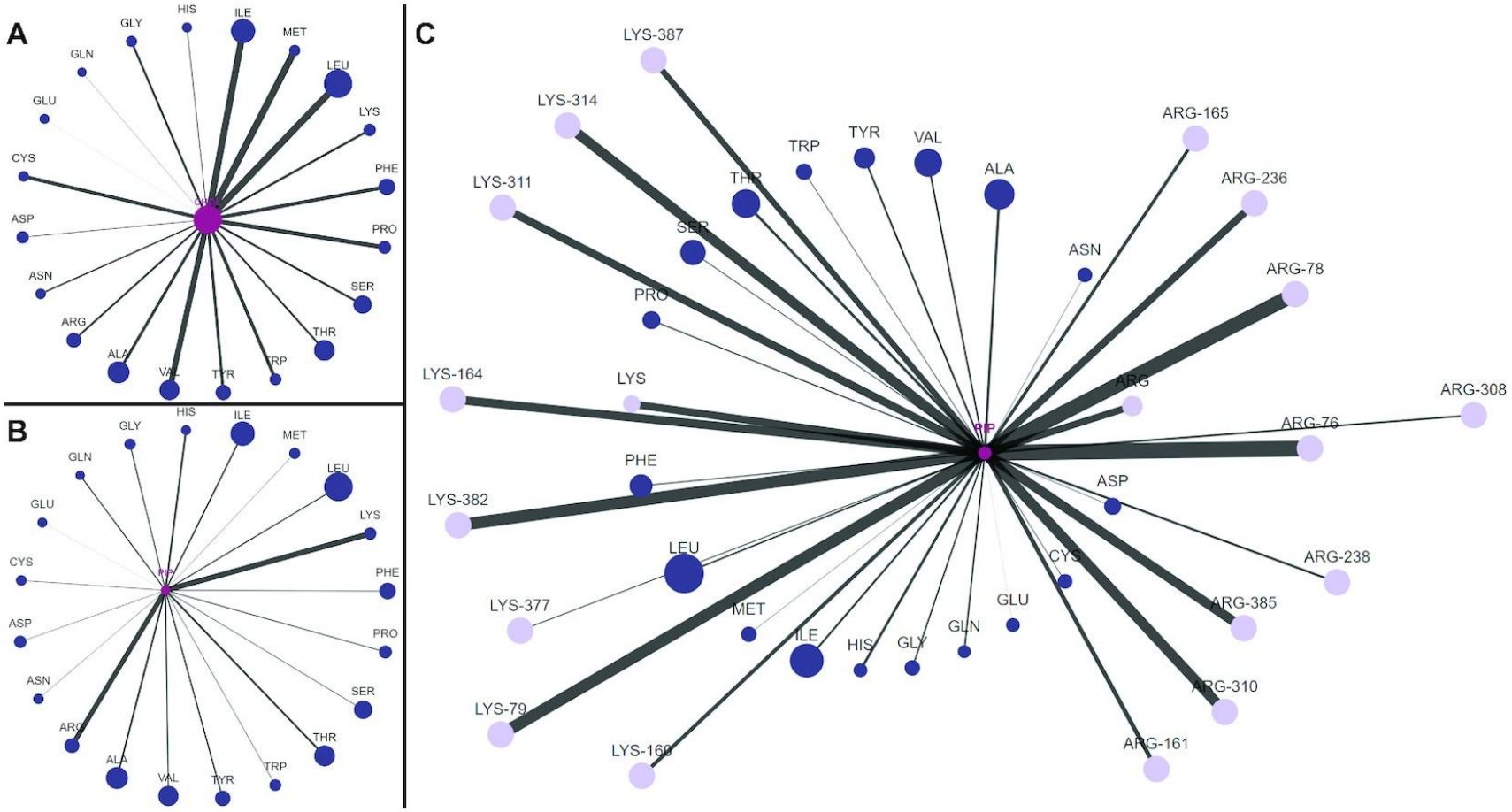
- Features:
  - Automated analysis of lipid-protein interactions
    - Contact-based
    - Densities
    - Physics-based
  - Feature-rich visualization applications
  - User interactivity

- Uses and is optimized for the JupyterLab environment.

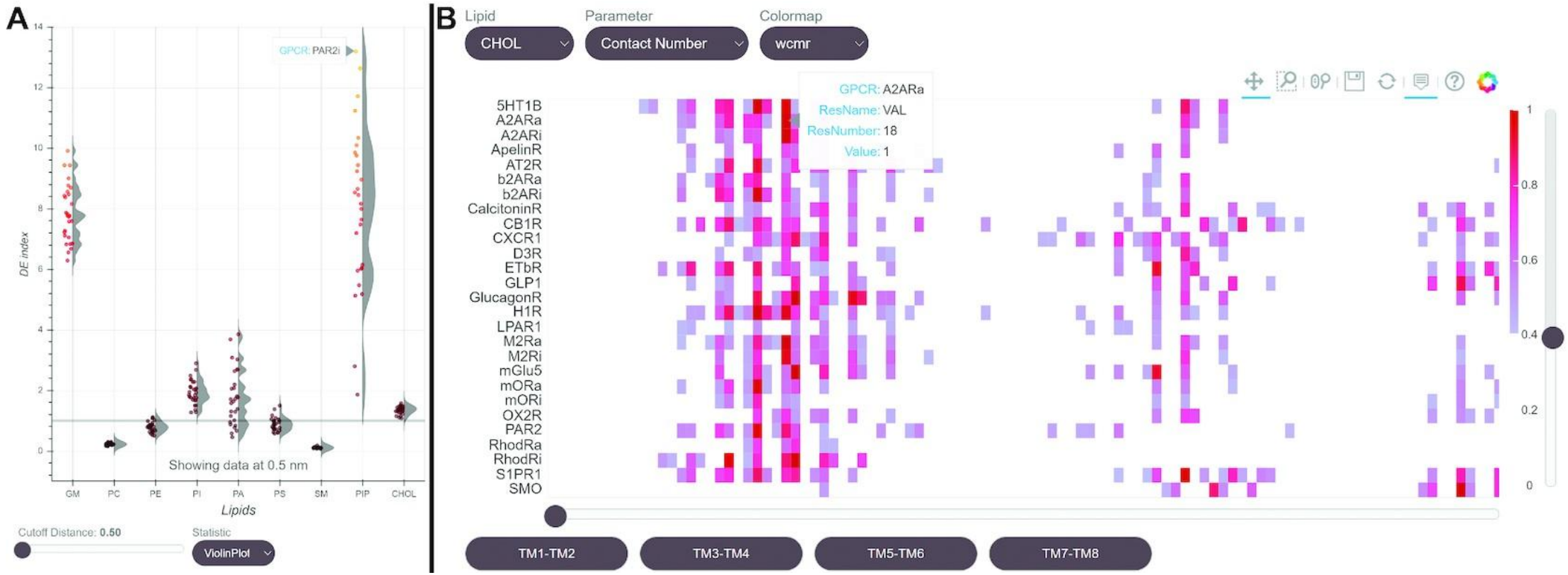
SMO-cholesterol interactions



Protein-lipid contact networks

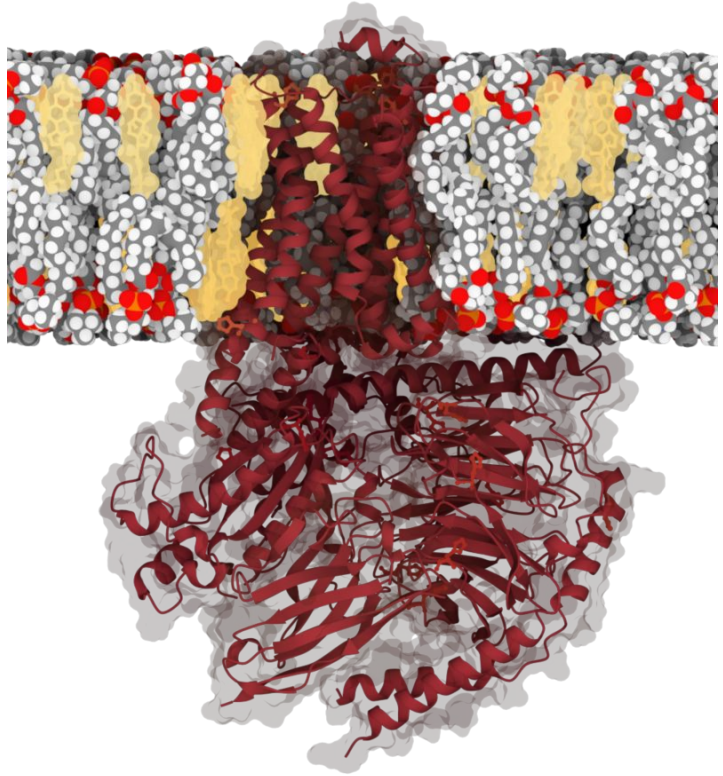


GPCR-wide interactions



Conclusions

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



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