

## DATA AND SOFTWARE AVAILABILITY

Server/Software	Function	Website
Gaussian09	Optimization, frequency and Gibbs free energy calculation	<a href="https://gaussian.com/glossary/g09/">https://gaussian.com/glossary/g09/</a>
Biovia Discovery Studio 2024	Visualization of compound models and interactions	<a href="https://www.3ds.com/products/biovia/discovery-studio/">https://www.3ds.com/products/biovia/discovery-studio/</a>
Origin Pro (2021)	Plotting data, PCA	<a href="https://www.originlab.com/2021">https://www.originlab.com/2021</a>
Microsoft Excel	Plotting data	<a href="https://www.microsoft.com/en-us/microsoft-365/microsoft-office">https://www.microsoft.com/en-us/microsoft-365/microsoft-office</a>
YASARA Dynamics	Molecular Dynamics Simulation And data analysis	<a href="#">YASARA - Yet Another Scientific Artificial Reality Application</a>

Any additional data will be provided by the corresponding author upon request.