

AquaMem Molecular Modeling Services

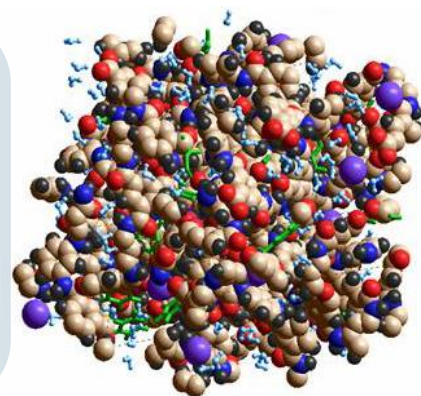


Membrane Modeling Services:

[AquaMem](#) offers expert consultation and learning services for molecular modeling of permselective membrane materials, including aromatic crosslinked polyamides, cellulose-based membranes, ceramics, and hybrid materials. With >20 years of experience in the development of advanced computational

algorithms and powerful modeling protocols for membranes, [AquaMem provides unrivaled expertise](#) in this rapidly evolving discipline. *Our services include:*

- Φ Design of novel polymer and inorganic (ceramic) membranes
- Φ Pore size distribution, fractional free volume, diffusion coefficients
- Φ Visualization of atomic and molecular scale membrane dynamics
- Φ Thermodynamics of organic foulant interaction with membranes
- Φ Nano-scale fluid dynamics at the membrane surface
- Φ Hydrogen-bond network analysis and energy mapping
- Φ Effects of pH on membrane structure and function
- Φ Aging and slow deterioration of membranes by oxidation
- Φ **NEW: Pharmacophore discovery by virtual ligand-receptor screening**



Authoritative Seminars and Workshops: [AquaMem](#)

offers beginning and advanced seminars and intensive workshops to quickly bring scientists and engineers up to speed in all aspects of molecular modeling, especially related to membrane separations and other water treatment processes. Our hands-on seminars are held onsite or as immersive retreat-style workshops at locations across the US and abroad.

Whether you're involved in basic scientific inquiry or commercial applications, please feel free to contact me to learn how molecular simulations can be successfully applied in your research to unleash the full potential of your new membrane materials.

