

Molecular Structure and Modeling (MSM) Core



Xavier University of Louisiana - RCMI Program

Phone: 504-520-5084 , Email: mmottama@xula.edu



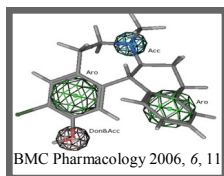
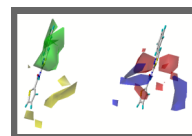
Advanced molecular modeling techniques to support biomedical research • Accelerate new drug design and development • Improve our understanding of the principles underlying biological processes • Small molecule crystallography services

Available Services

Ligand based drug design:

Quantitative Structure Activity Relationship (QSAR) Models:

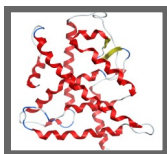
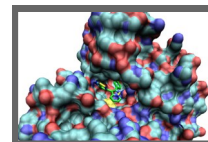
Identify structure patterns related to activity and obtain insights into the nature of interactions between drug molecules and targets.



Pharmacophore Modeling: Determine structure requirements for activity, aids in design of novel ligands/inhibitors and develop pharmacophore based 3D database search strategies.

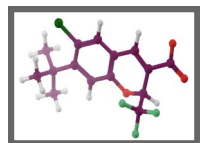
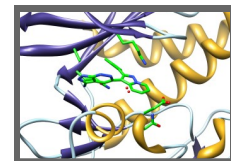
Structure based drug design:

Docking & Virtual Screening: Understand ligand-receptor interactions and identify potential agonists or antagonists through virtual screening of chemical libraries.



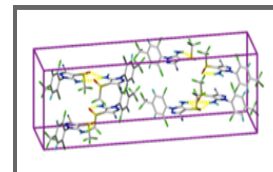
Homology Modeling: Construct a reasonable model of target protein from amino acid sequence and related crystal structures. Find ligand binding sites on homology model, design agonists-antagonists.

Molecular dynamics simulations: Determine time dependent behavior of a molecular system and molecular level insight into structure and function of biological molecules.



DFT calculations: Obtain structural, energetic and electronic properties of isolated small molecules. Very useful for both basic research and structure based drug design.

Small Molecule X-ray Crystallography: Identify structure and reference information useful in the process of drug design and the determination of pharmacophore, QSAR and docking studies.



Service Charges

SERVICES	PRICE*
Docking Crystal Structure or Prepared Homology Model	\$500 (for the first ligand) +\$100 each (for the next 5 ligands) +\$75 each (for the next 15 ligands)
Homology Model or Site Directed Mutant Model	\$500 (for each model)
Virtual Screening of Chemical Libraries	\$1000 (for the first chem library) +\$500 each (for additional libraries)
Quantitative Structure Activity Relationship (QSAR) 3D-QSAR (CoMFA or CoMSIA)	\$1,500 (for the first 25 ligands) +\$500 (for the next 10 ligands) +\$300 (for the next 15 ligands)
2D-QSAR, HQSAR	\$500 (for first 25 ligands) +\$300 (for the next 10 ligands) +\$200 (for the next 15 ligands)
Pharmacophore Modeling	\$1,500 (for the first 25 ligands) +\$500 (for the next 10 ligands) +\$300 (for the next 15 ligands)
Molecular Dynamics Simulation & Analysis	\$4,000 (for each system)
DFT Calculations of Small Compounds	\$200 each (for the first 5 ligands) +\$500 (for the next 10 ligands) +250 (for the next 10 ligands)
X-Ray Crystal Structure	\$200 each (for the first 5 ligands) \$150 each (for the next 10 ligands) \$100 each (for the next 10 ligands)
* Xavier University faculties will be entitled for 50% discount.	

Hardware:

HP-Linux workstations
Bruker Smart X2S benchtop diffractometer.

Chemical Libraries & Databases:

Cambridge Structure Database (CSD), ZINC,
NCI, Chinese Medicine, Natural Product, Asinex,

Software:

Schrodinger Suite 2010
Tripos Sybyl-X 1.3
Chemical Computing Group - MOE
GOLD,
NAMD, AMBER, CHARMM



Core Scientist Contact:

Dr. Madhusoodanan Mottamal, Department of Chemistry
Xavier University of Louisiana, New Orleans, LA 70125
Tele: 504-520-5084, email: mmottama@xula.edu
<http://www.xula.edu/rcmi/molstrucmodcore.php>



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