

HPRC Laboratory for Molecular Simulation (LMS)

<https://lms.hprc.tamu.edu/>

Subscription Rates for TAMU Researchers FY22



Subscription Type	Number of Users with Access to LMS Software and Hardware	Consulting Hours Included	Cost per year
1	PI & 1 researcher	5	\$500
2	PI & 2 researchers	10	\$1000
3	PI & 3 researchers	15	\$1500
4	PI & 4+ researchers	20	\$2000

Consulting Fee for non-subscribers and additional hours for subscribers: \$65/hour

In addition to the consulting hours, an annual subscription to the LMS gives the PI and designated researcher(s) access to the licensed software and hardware outlined below.

Licensed Software	
Company	Software
Dassault Systèmes	BIOVIA Materials Studio Visualizer, Conformers, Forcite Plus, Gaussian Interface, QSAR+, Reflex, VAMP, MS Pipeline Pilot Collection, Adsorption Locator, Amorphous Cell, Blends, Compass, GULP, Mesocite, Mesodyn, Sorption, Synthia, CASTEP, DFTB+, DMOL3, NMR CASTEP, ONETEP, QMERA
Dassault Systèmes	BIOVIA Discovery Studio Visualizer, Analysis, Biopolymer, Catalyst (Conformation, Score DB Build, Search, Hypothesis, SBP & Shape), CHARMM, DMOL3, MMFF, Protein Refine, QUANTUMm, CFF FF, De Novo Evolution, De Novo Ligand Builder, Flexible Docking, LibDock, LigandFit, LigandScore, Ludi, MCSS, MODELER, Protein Docking: ZDOCK and RDOCK, Protein Families, Protein Health, Sequence Analysis, X-ray.
Materials Design	MedeA Software MedeA Environment (includes MedeA GUI, MedeA Analysis, MedeA Builders, MedeA JobServer and TaskServer, MedeA InfoMaticA, MedeA COD GUI, MedeA LAMMPS GUI, and MedeA Forcefield)
Schrödinger	Schrödinger suite of software: Maestro, CombiGlide, Glide, Liaison, Strike, QikProp, Canvas, LigPrep, BioLuminate GUI, Prime, Qsite, MacroModel, ConfGen, Jaguar, pKa Predictor, Epik, SiteMap, and PIPER.
CCG	MOE: Molecular Operating Environment. A fully integrated drug discovery software package, including structure-based design, fragment-based design, pharmacophore discovery, medicinal and biologics applications, protein and antibody modeling, molecular mechanics/dynamics, cheminformatics and QSAR.
Gaussian	Gaussian (09 & 16)
GaussView	GaussView 6 with GMMX add-on
AMBER	AMBER
Molpro	Molpro
SCM	ADF & ADF-GUI
TK Gristmill	AIMALL Professional
NBO	NBO7
Chemissian	Chemissian
Hardware:	
Computer	Configuration
LMS	2 Dell Precision T3420 workstations NVIDIA Quadro K620 GPU
VIDI	312-core cluster (Mix of 8 and 12-core nodes)
MM	Cluster to be deployed Fall 21 with 20-core compute nodes.