Laboratory for Molecular Simulation

Subscription Rates for TAMU Researchers FY19

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
BIOVIA	**Materials Studio** Visualizer and the following modules: Conformers, Forcite Plus Parallel, 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
BIOVIA	**Discovery Studio** Visualizer and the following modules: Analysis, Biopolymer, Catalyst Conformation, Catalyst Score, CHARMm, DMOL3 Molecular, MMFF (Merk Molecular Force Field), Protein Refine, QUANTUMm (QM/MM - DMOL3/CHARMm), Catalyst DB Build, Catalyst DB Search, Catalyst Hypothesis, Catalyst SBP, Catalyst Shape, CFF (Consistent Force-Field), De Novo Evolution, De Novo Lignad Builder, Flexible Docking, LibDock, LigandFit, LigandScore, Ludi, MCSS (Multiple Copy Simultaneous Search), MODELER, Protein Docking: ZDOCK and RDOCK, Protein Families, Protein Health, Sequence Analysis, X-ray.
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, One 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** (16 & 09)
Semichem	**AMPAC**
Semichem	**Ampac** GUI (aka **GaussView**)
AMBER	**AMBER**
Molpro	**Molpro**
SCM	**ADF**
TK Gristmill Software	**AIMALL Professional**
NBO	**NBO6**
Chemissian	**Chemissian**
Hardware: LMS hardware can host ITAR and Export Controlled Software (EAR)	
Computer	Configuration
LMS	17 Dell Precision T3420 workstations NVIDIA Quadro K620 GPU
VICI	1088-core cluster (768 core of 16-core nodes and 320 core of 8-core nodes)
MEDUSA	176-core cluster (2 64-core and 1 48-core Altix 450s)