NATIONAL COMPUTATIONAL SCIENCE INSTITUTE	acd/ChemSketch	BioRad	CAChe	Chem3D	GAMESS	GaussView/Gaussian	HyperChem	PC Model	Spartan
WIN mac linux/unix	1	1	✓ ✓ U	> >	✓ LU	✓ ✓ LU	√ (√)	✓ ✓ L	✓ ✓ LU
Methods molecular mechanics MM2/MM3/MM+/etc. Amber other semi-empirical AM1/PM3/etc. Extended Hückel ZINDO ab initio HF dft MP2/MP4/G1/G2/CBS-?/etc.	1	/	/ / / * / *	* * *	<i>y y y y</i>	\\ \\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\	\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\	\frac{\sqrt{\sqrt{\sqrt{\sqrt{\sqrt{\sqrt{\sqrt{\sqrt{\sqrt{\color{\sqrt{\sq}}}}}}}}}}}}} \signtimes\signtifta}\signtifta}\signtifta}\signtifta}\signtifta}\signtifta}\signtifta\sintitita}\signtifta}\signtifta}\signtifta\sintitita\sintitita}\signtifta}\signtifta\sintitita\sintitita\sintiin}\signtifta\sintitita\signtifta}\signtifta\sintiin}\signtifta\sintiin}\signtifta\sintiin}\signtifta\sintiit	\ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \
Features various molecular properties conformer searching crystals data base developer kit and scripting molecular dynamics molecular interactions movies/animations naming software nmr polymers proteins and biomolecules QSAR scientific graphical objects spectral and thermodynamic transition and excited state web plugin	\ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \	,	\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\	\\ \\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\		\ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \	\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\	\ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \	>> > >> >> >> >>
Input 2D editor 3D editor text conversion editor protein/sequence editor various file formats	1	1	√ √ √	> > > > >	**	√ √ √	1	✓ ✓	>> >>
Output various renderings various file formats animation graphs spreadsheet	<i>'</i>	<i>y y</i>	\ \ \ \ \ \	<i>y y</i>	**	<i>y y y</i>	1	<i>y y y</i>	>>>>

^{*} GAMESS and/or GAUSSIAN interface
** Text only. Optional interface required for input, viewing, etc.

ACD/ChemSketch/3DViewer (acdlabs)

http://www.acdlabs.com/products

WIN v 8

pricing: free academic license

free download

comments/optional addons: front end for many programs

BioRad KnowItAll

http://www.knowitall.com/academic

WIN v 4.1 Academic

pricing: free academic license

free download

comments/optional addons: front end for many programs

CAChe WorkSystem Pro (Fujitsu)

http://www.CACheSoftware.com

WIN v 6.1, mac v 4.9, unix

pricing: Annual Academic Site License

comments/optional addons: several flavors

Chem3D Ultra (CambridgeSoft)

http://www.cambridgesoft.com

WIN v 9, mac v 9 pricing: site license

comments/optional addons: includes ChemDraw Std.

> several flavors ChemOffice Ultra

ChemOffice Active X Net 2004 Download Ed

GAMESS

http://www.msg.ameslab.gov/GAMESS

DOS(via WIN), linux

pricing: free

comments/optional addons: interfaces available include Chem3D, PC Model, WebMo, pcgRun, RUNpcg

Gaussian 03 (Gaussian)

http://www.gaussian.com

WIN 03W, mac 03M, linux/unix

pricing: site license

comments/optional addons: interfaces available include CAChe, Chem3D, GaussView W, PC Model

HyperChem (Hypercube)

http://www.hyper.com/products

WIN v 7.5 (runs on mac) pricing: site license

comments/optional addons:

hardware lock several flavors

> HyperChem Web Viewer Student HyperChem

PCModel (Serena Software)

http://www.serenasoft.com

WIN v 8, mac v 8, linux pricing: site license

comments/optional addons: OrbDraw and Vibrate

Spartan (Wavefunction)

http://www.wavefun.com

WIN v '04, mac v '04, linux/unix

comments/optional addons: hardware lock

Spartan Student Ed