Graphical User Interface	SpartanModel	Student V5	Spartan'14	Parallel Suite
Available Platforms:	Win/Mac	Win/Mac	Win/Mac	Win/Mac/Linux
Organic Builder	—	✓	✓	✓
Inorganic Builder	—	✓	✓	✓
Peptide Builder	—	✓	✓	✓
Nucleotide Builder	—	✓	✓	✓
Sustituent Builder	—	—	✓	✓
Sketch (2-D) Builder	—	—	✓	✓
2-D Builder (Requires ChemDraw Access)	—	Win Only	Win Only	Win Only
Transition State Library	—	✓	✓	✓
Clipboard Access	—	✓	✓	✓
Cambridge Structural Database Access	—	—	✓	✓
Spartan Spectra & Properties Database Access*	IR and H of F	✓	✓	✓
Protein Databank Access	✓	✓	✓	✓
National Cancer Institute (CACTUS) Database Access	—	✓	—	—
NIST Infrared Database Access	—	—	✓	✓
Automatic Tautomer Detection	—	—	✓	✓
Extraction of bound Ligands	—	—	✓	✓
Chemical Functional Descriptors	—	—	✓	✓
Reaction Calculator	—	✓	✓	✓
Display molecules in multiple model styles	✓	✓	✓	✓
Display/Manipulation of structural models	✓	✓	✓	✓
Measures distance, angle, dihedrals	✓	✓	✓	✓
Normal-mode animations	✓	✓	✓	✓
Spreadsheet and Data Plots (2D & 3D)	—	2D Only	✓	✓
Ramachandron Plots	✓	✓	✓	✓
Molecular Alignment and scoring	—	✓	✓	✓
Linear Regression Analysis	—	—	✓	✓
File Compatibility - Import/Export	**SpartanModel**	**Student V5**	**Spartan'14**	**Parallel Suite**
Spartan Files	import	✓	✓	✓
SYBYL MOL and MOL2	—	✓	✓	✓
PDB	import	✓	✓	✓
MACROMODEL	—	✓	✓	✓
MDL SKC, TGF, and SDF	—	✓	✓	✓
SMILES	—	✓	✓	✓
CIF	—	import	import	import
XYZ	—	✓	✓	✓
JCAMP	—	✓	✓	✓
ChemDraw (.CDX)	—	import	import	import
Graphics Export/Save as	**SpartanModel**	**Student V5**	**Spartan'14**	**Parallel Suite**
JPEG	—	✓	✓	✓
PNG	✓	✓	✓	✓
BMP	—	Win Only	Win Only	Win Only
QuickTime Recording	—	✓	✓	Win/Mac
Tasks - Calculations	**SpartanModel**	**Student V5**	**Spartan'14**	**Parallel Suite**
Energies	✓	✓	✓	✓
Equilibrium Geometries	✓	✓	✓	✓
Transition State Geometries	—	✓	✓	✓
Intrinsic Reaction Coordinate (IRC)	—	—	✓	✓
Equilibrium Conformer	—	✓	✓	✓
Conformation Distribution	—	—	✓	✓
Conformer Library	—	—	✓	✓
Energy Profiles	—	✓	✓	multi-threaded
Similarity Analysis	—	—	✓	✓
Spectra Calculations	**SpartanModel**	**Student V5**	**Spartan'14**	**Parallel Suite**
Infrared/Raman	from DB	IR	✓	multi-core
UV/vis	—	—	✓	✓
NMR Chemical Shifts	—	✓	✓	✓
HH Splitting	—	✓	✓	✓
Display of COSY, HSQC, & HMBC NMR Plots	—	—	✓	✓
Properties	**SpartanModel**	**Student V5**	**Spartan'14**	**Parallel Suite**
Weight, Area, Volume	✓	✓	✓	✓
Solvation Energy SM5.4, SM5.0R	—	✓	✓	✓
Solvation Energy SM8, SS(V)PE	—	—	✓	✓
Enthalpy, Entropy, Gibbs Free Energy	—	✓	✓	✓
Heat Capacity & Zero Point Energy	—	✓	✓	✓
LogP	—	✓	✓	✓
Acidity and Basicity from SSPD database	—	—	✓	✓
Polar Surface Area	✓	✓	✓	✓
Polar Area from Electrostatic Potential Map	—	✓	✓	✓
Mulliken Charges & Natural Charges	—	—	✓	✓

Electrostatic Fit Charges	✓	✓	✓	✓
Bond Orders	—	✓	✓	✓
Dipole Moments	✓	✓	✓	✓
Higher Moments	—	—	✓	✓
Polarizabilities	—	—	✓	✓
Hyperpolarizabilities	—	—	✓	✓
Electronegativity	—	—	✓	✓
Hardness	—	—	✓	✓
Q-minus and Q-plus	—	—	✓	✓
Ovality	—	—	✓	✓
HBA & HBD, +/- Ionizable Center Count	—	—	✓	✓
Methods/Basis Sets	**SpartanModel**	**Student V5**	**Spartan'14**	**Parallel Suite**
SYBYL	—	—	✓	✓
MMFF94	✓	✓	✓	✓
MMFF94(aq)	—	—	✓	✓
MNDO, MNDO(d)	—	—	✓	✓
AM1	—	—	✓	✓
RM1	—	—	✓	✓
PM3, PM3 Transition Metal Extensions	**PM3/HF**	**to 75 atoms**	✓	✓
PM6	—	—	✓	✓
Hartree Fock	**PM3/HF**	**to 30 atoms**	✓	**multi-core**
DFT local/BP/BLYP/B3LYP	—	**B3LYP<30 atoms**	✓	**multi-core**
DFT EDF1/EDF2/M06/ωB97X-D	—	**EDF2<30 atoms**	✓	**multi-core**
DFT Slater-Dirac/Vokso-Wilk-Nusair	—	—	✓	**multi-core**
DFT Perdew-Zunger/Wigner/Becke88/Gill96	—	—	✓	**multi-core**
DFT Gilbert-Gill99/Lee-Yang-Parr/Perdew86	—	—	✓	**multi-core**
DFT GGA91/BMK/M05/M05-2X	—	—	✓	**multi-core**
DFT M06/M06-2X/M06-L/M06-HF	—	—	✓	**multi-core**
Non-empirical GGA Functional PBE	—	—	✓	**multi-core**
Customize Exchange and Correlation	—	—	✓	✓
TDDFT	—	—	✓	✓
MP2, MP3, MP4	—	**MP2<20 atoms**	✓	✓
Resolution of the Identity - RI-MP2	—	—	✓	**multi-core**
CCSD, CCSD(T), OD, OD(T)	—	—	✓	✓
QCCSD, QCCSD(T)	—	—	✓	✓
CIS, CISD	—	—	✓	✓
QCIS, QCIS(D)	—	—	✓	✓
Resolution of the Identity - RI-CIS(D)	—	—	✓	✓
T1	**from Database**	**from Database**	✓	**multi-core**
G2, G3, G3(MP2)	—	—	✓	✓
Basis Sets:				
STO-3G	—	—	✓	✓
3-21G	✓	✓	✓	✓
6-31G, 6-31G*, 6-31G**, 6-31+G*	—	**6-31G***	✓	✓
6-311G*/6-311G**/6-311+G**/6-311++G**	—	**6-311+G****	✓	✓
6-311++G(2df,2p), cc-pVTZ	—	—	✓	✓
additional and custom basis sets	—	—	✓	✓
polarization and diffuse functions	—	✓	✓	✓
dual basis sets	—	—	✓	✓
pseudopotentials for heavy elements	—	✓	✓	✓
Graphical Models	**SpartanModel**	**Student V5**	**Spartan'14**	**Parallel Suite**
Orbital Energy Diagram	✓	✓	✓	✓
Orbital surface, contours, maps	—	✓	✓	✓
Density surfaces and contours	—	✓	✓	✓
vdW surfaces	—	—	✓	✓
Spin density surfaces and contours	—	✓	✓	✓
Local ionization potential maps	—	✓	✓	✓
ESP surfaces, contours, maps	**ESP Map**	✓	✓	✓
Emphasize Accessible Regions	—	✓	✓	✓
Graphical Animations	✓	✓	✓	✓
Ribbon Style Display for biopolymers	✓	✓	✓	✓
Defined points, plains	✓	✓	✓	✓
Chemical Function Descriptors	—	—	✓	✓
Hydrogen bonds	✓	✓	✓	✓
Additional Features	**SpartanModel**	**Student V5**	**Spartan'14**	**Parallel Suite**
Automatic use of symmetry	—	✓	✓	✓
Use of constraints and/or frozen atoms	—	✓	✓	✓
Automatic inversion of chiral centers	✓	✓	✓	✓
Automatic inversion of absolute chirality	✓	✓	✓	✓
Automatic filling of open valences w/ H's	✓	✓	✓	✓
Screen centering	✓	✓	✓	✓
Cut/Paste Clipboard Access	**Graphics**	✓	✓	✓

Remote Submission Capabilities	—	—	✓	✓
Experimental IR & UV/vis access via NIST	—	IR Only	✓	✓
Experimental NMR access from NMR Shift DB	—	✓	✓	✓
Boltzmann Averaged NMR spectra	—	—	✓	✓
Included Databases*	**SpartanModel**	**Student V5**	**Spartan'14**	**Parallel Suite**
Spartan Molecular Database (# molecules)	5000	5000	5000	>142,000
Spartan Spectra & Properties Database (# molecules)	—	5000	5000	>250,000
Name Search	✓	✓	✓	✓
Substructure Search	—	—	✓	✓
Formula Search	—	—	✓	✓
Weight Search	—	—	✓	✓
Isomer Search	—	—	✓	✓
Substituent directed searching	—	—	✓	✓
Searching by IR Spectra	—	—	✓	✓
Spartan Reaction Database	—	—	✓	✓
Spartan IR Database	—	—	✓	✓
Regression Analysis from SMD / SSPD	—	—	✓	✓

***Available for purchase:**

Spartan Spectra & Properties Database (SSPD) includes more than 250,000 Molecules Conformationally searched and optimized with the DFT EDF2 functional, and includes calculated IR spectra and proton and 13C NMR spectra and T1 heat of formation, also included are the wave functions for generation of graphical surfaces.

Spartan Molecular Database (SMD) includes more than 142,000 conformationally searched molecules optimized with up to 10 QM models

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