Graphical User Interface	SpartanModel	Student V5	Spartan'10
Available Platforms:	**Win/Mac**	**Win/Mac**	**Win/Mac/Linux**
Organic Builder	—	✓	✓
Inorganic Builder	—	✓	✓
Peptide Builder	—	✓	✓
Nucleotide Builder	—	✓	✓
Sustituent Builder	—	—	✓
2-D Builder (Requires ChemDraw Access)	—	**Win Only**	**Win Only**
Automatic Transition State Guess	—	✓	✓
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	—	✓	—
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'10
Spartan Files	**import**	✓	✓
SYBYL MOL and MOL2	—	✓	✓
PDB	**import**	✓	✓
MACROMODEL	—	✓	✓
MDL SKC, TGF, and SDF	—	✓	✓
SMILES	—	**export**	**export**
CIF	—	**import**	**import**
XYZ	—	✓	✓
JCAMP	—	✓	✓
ChemDraw (.CDX)	—	**import**	**import**

Graphics Export/Save as	SpartanModel	Student V5	Spartan'10
JPEG	—	✓	✓
PNG	✓	✓	✓
BMP	—	**win only**	✓
QuickTime Recording	—	✓	**Win/Mac**

Tasks - Calculations	SpartanModel	Student V5	Spartan'10
Energies	✓	✓	✓
Equilibrium Geometries	✓	✓	✓
Transition State Geometries	—	✓	✓
Intrinsic Reaction Coordinate (IRC)	—	—	✓
Conformation Distribution	—	—	✓
Conformer Library	—	—	✓
Energy Profiles	—	✓	✓
Similarity Analysis	—	—	✓

Spectra Calculations	SpartanModel	Student V5	Spartan'10
Infrared/Raman	from DB	IR	✓
UV/vis	—	—	✓
NMR Chemical Shifts	—	✓	✓
HH Splitting	—	✓	✓

Properties	SpartanModel	Student V5	Spartan'10
Weight, Area, Volume	✓	✓	✓
Solvation Energy SM5.4, SM5.0R	—	✓	✓
Solvation Energy SM8, SS(V)PE	—	—	✓
LogP	—	✓	✓
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	—	✓	✓
Molecular area and volume	—	✓	✓
Ovality	—	✓	✓
Enthalpy, entropy, free energy	—	✓	✓
HBA & HBD, +/- Ionizable Center Count	—	✓	✓

Methods/Basis Sets	SpartanModel	Student V5	Spartan'10
SYBYL	—	—	✓
MMFF94	✓	✓	✓
MMFF94(aq)	—	—	✓
MNDO, MNDO(d)	—	—	✓
AM1	—	—	✓
RM1	—	—	✓
PM3, PM3 Transition Metal Extensions	**PM3/HF**	**to 75 atoms**	✓
Hartree Fock	**PM3/HF**	**to 30 atoms**	✓
DFT local/BP/BLYP/B3LYP	—	**B3LYP<30 atoms**	✓
DFT EDF1/EDF2/M06/ωB97X-D	—	**EDF2<30 atoms**	✓
DFT Slater-Dirac/Vokso-Wilk-Nusair	—	—	✓
DFT Perdew-Zunger/Wigner/Becke88/Gill96	—	—	✓
DFT Gilbert-Gill99/Lee-Yang-Parr/Perdew86	—	—	✓
DFT GGA91/BMK/M05/M05-2X	—	—	✓
DFT M06/M06-2X/M06-L/M06-HF	—	—	✓
Non-empirical GGA Functional PBE	—	—	✓
Customize Exchange and Correlation	—	—	✓
TDDFT	—	—	✓
MP2, MP3, MP4	—	**MP2<20 atoms**	✓
Resolution of the Identity - RI-MP2	—	—	✓
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**	✓
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'10
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, planes	✓	✓	✓
Chemical Function Descriptors	—	—	✓
Hydrogen bonds	✓	✓	✓

Additional Features	SpartanModel	Student V5	Spartan'10
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 EBI	—	✓	✓
Draw NOESY, COSY, DEPT, HSQC, HMBC plots	—	—	✓
Boltzmann Averaged NMR spectra	—	—	✓

Included Databases*	SpartanModel	Student V5	Spartan'10
Spartan Molecular Database (# molecules)	**5000**	**5000**	**5000**
Spartan Spectra & Properties Database (# molecules)	—	**5000**	**5000**
Name Search	✓	✓	✓
Substructure Search	—	—	✓
Formula Search	—	—	✓
Weight Search	—	—	✓
Isomer Search	—	—	✓
Substituent directed searching	—	—	✓
Searching by IR Spectra	—	—	✓
Spartan Reaction Database	—	—	✓
Spartan IR Database	—	—	✓

*Available for purchase:
Spartan Spectra & Properties Database (SSPD) includes more than 170,000 Molecules Conformationally searched and optimized with the DFT EDF2 functional, and includes calculated IR spectra and proton and 13C NMR spectra as well as the T1 heat of formation and atomic and molecular properties.

Spartan Molecular Database (SMD) includes
more than 15,000 conformationally searched molecules
optimized at up to 10 different QM Models
select entries include calcualted IR and NMR
spectra, all entries include atomic and molecular properties

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