Wavefunction, Inc. © 1991-2017 - Spartan Comparison Chart 5/16/2017

Graphical User Interface	Student V7	Spartan'16	Parallel Suite
Available Platforms:	**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 v. 10 or later)	**Win Only**	**Win Only**	**Win Only**
Transition State Library	✔	✔	✔
Clipboard Access	✔	✔	✔
Cambridge Structural Database Access	—	✔	✔
Spartan Spectra & Properties Database Access*	✔	✔	✔
Protein Databank Access	✔	✔	✔
NIST Infrared Database Access	✔	✔	✔
Automatic Tautomer Detection	—	✔	✔
Extraction of bound Ligands	—	✔	✔
Chemical Functional Descriptors	—	✔	✔
Reactions 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	**Student V7**	**Spartan'16**	**Parallel Suite**
All Spartan formats	✔	✔	✔
SYBYL MOL and MOL2	✔	✔	✔
PDB and standard XYZ file	✔	✔	✔
MACROMODEL	✔	✔	✔
MDL SKC, TGF, and SDF	✔	✔	✔
InChI	✔	✔	✔
SMILES	✔	✔	✔
CIF	✔	✔	✔
ChemDraw (.CDX)	**import**	**import**	**import**
JCAMP (.dx) or CSV for IR .CML for NMR	✔	✔	✔
Export Spreadsheet as Excel, Open Document Spreadsheet or CSV	✔	✔	✔
Graphics Export/Save as	**Student V7**	**Spartan'16**	**Parallel Suite**
JPEG	✔	✔	✔
PNG	✔	✔	✔
BMP	**Win Only**	**Win Only**	**Win Only**
QuickTime Recording	**Mac Only**	**Mac Only**	**Mac Only**
Tasks - Calculations	**Student V7**	**Spartan'16**	**Parallel Suite**
Energies	✔	✔	**multi-core**
Equilibrium Geometries	✔	✔	**multi-core**
Transition State Geometries	✔	✔	**multi-core**
Intrinsic Reaction Coordinate (IRC)	—	✔	✔
Equilibrium Conformer	✔	✔	**multi-threaded**
Conformation Distribution	✔	✔	**multi-threaded**
Similiarity Library	—	✔	✔
Energy Profiles	✔	✔	**multi-threaded**
Similarity Analysis	—	✔	✔
QSAR calculations	✔	✔	✔
Thermodynamics and Vibrational Modes	✔	✔	✔
Orbitals & Energies, Charges & Bond Orders	✔	✔	✔

Spectra Calculations	Student V7	Spartan'16	Parallel Suite
Infrared/Raman	IR Only	✓	multi-core
UV/vis	—	✓	multi-core
NMR Chemical Shifts	✓	✓	multi-core
HH Splitting	✓	✓	✓
Display of COSY, HSQC, & HMBC NMR Plots	—	✓	✓
Properties	**Student V7**	**Spartan'16**	**Parallel Suite**
Weight, Area, Volume	✓	✓	✓
Solvation Energy SM5.4, SM5.0R, SM8, SM12, SMD	SM5.4, SM5.0R	✓	✓
Solvation Energy C-PCM, SS(V)PE	✓	✓	✓
Enthalpy, Entropy, Gibbs Free Energy	✓	✓	✓
Heat Capacity & Zero Point Energy	✓	✓	✓
LogP	✓	✓	✓
QSAR Routines (& QSAR Tab in Properties dialogue)	✓	✓	✓
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	HBA & HBD count	✓	✓
Methods/Basis Sets	**Student V7**	**Spartan'16**	**Parallel Suite**
SYBYL	—	✓	✓
MMFF94	✓	✓	✓
MMFF94(aq)	—	✓	✓
MNDO, MNDO(d)	—	✓	✓
AM1	—	✓	✓
RM1	—	✓	✓
PM3, PM3 Transition Metal Extensions	up to 75 atoms	✓	✓
PM6	—	✓	✓
Hartree Fock	up to 30 atoms	✓	multi-core
GGA: B86PW91, BLYP, BPW91, B97-D2, SOGGA11, PBE-D3, VV10	—	✓	multi-core
GH-GGA: B3LYP, B3LYP-D3, EDF2, B3PW91, MPW3LYP, SOGA11-X	B3LYP & EDF2	✓	multi-core
RSH-GGA: ωB97X-D, ωB97X-V, ωB97X, CAM-B3LYP, N12-SX, LC-VV10	up to 30 atoms	✓	multi-core
mGGA: B97M-V, M06-L, BMK, M11-L, TPSS-D3	—	✓	multi-core
GH-mGGA: M06-2X, M06, M08-HX, M08-SO, MPW1B95	—	✓	multi-core
RSH-mGGA: M11, ωB97M-V, MN12-SX	—	✓	multi-core
Additional functionals	—	✓	multi-core
Customize Exchange and Correlation	—	✓	multi-core
TDDFT	—	✓	multi-core
CIS, CISD, QCIS, QCIS(D)	—	✓	✓
MP2, MP3, MP4	MP2 up to 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	✓	multi-core
G3, G3(MP2), G4, G4(MP2)	—	✓	multi-core
G3elect, G3(MP2)elect	—	✓	✓
G4elect, G4(MP2)elect	—	✓	✓

Basis Sets	Student V7	Spartan'16	Parallel Suite
Pople 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(2df,2p)	**6-311+G****	✓	✓
Dunning basis sets: cc-pVDZ, cc-pVTZ, cc-pVQZ	—	✓	✓
aug-cc-pVDZ, aug-cc-pVTZ, aug-cc-pVQZ	—	✓	✓
Alrichs/Weigend basis sets: def2-SV(p), def2-SVP, def2-SVPD	—	✓	✓
def2-TZVP, def2-TZVPPD, def2-QZVP, def2-QZVPPD	—	✓	✓
Additional polarization and diffuse functions	—	✓	✓
Dual basis sets	—	✓	✓
pseudopotentials for heavy elements	✓	✓	✓
Graphical Models	**Student V7**	**Spartan'16**	**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	✓	✓	✓
Emphasize Accessible Regions	✓	✓	✓
Graphical Animations	✓	✓	✓
Ribbon Style Display for biopolymers	✓	✓	✓
Defined points, plains	✓	✓	✓
Chemical Function Descriptors	—	✓	✓
Hydrogen bonds	✓	✓	✓
Additional Features	**Student V7**	**Spartan'16**	**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	✓	✓	✓
Remote Submission Capabilities	—	✓	✓
Experimental IR & UV/vis access via NIST	**IR Only**	✓	✓
Experimental NMR access from NMR Shift DB	✓	✓	✓
Boltzmann Averaged NMR spectra	—	✓	✓
Remote Submission to Spartan'16 Parallel Suite	—	✓	✓
Included Computational Server (receives remotely submitted jobs)	—	—	✓
Included Databases*	**Student V7**	**Spartan'16**	**Parallel Suite**
Spartan Spectra & Properties Database (# molecules)	**≈ 6000**	**≈ 6000**	**>300,000**
Spartan Molecular Database (# molecules)	—	—	**>142,000**
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 SSPD/SMD	—	✓	✓

Parallel Suite includes:
full SSPD, SMD, embedded server functions and
parallel processing with up to 12 cores per calculation

WAVEFUNCTION

Last Update May 16, 2017
Contact support@wavefun.com with any Questions.