

Wavefunction, Inc. © 1991-2016 - Spartan Comparison Chart 5/1/2016

Graphical User Interface	Student V6	Spartan'16	Parallel Suite
<b>Available Platforms:</b>	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	✓	✓	✓
<b>File Compatibility - Import/Export</b>	<b>Student V6</b>	<b>Spartan'16</b>	<b>Parallel Suite</b>
Spartan Files	✓	✓	✓
SYBYL MOL and MOL2	✓	✓	✓
PDB	✓	✓	✓
MACROMODEL	✓	✓	✓
MDL SKC, TGF, and SDF	✓	✓	✓
InChI	import	import	import
SMILES	✓	✓	✓
CIF	import	import	import
XYZ	✓	✓	✓
JCAMP (.dx) for IR .CML for NMR	JCAMP only	✓	✓
ChemDraw (.CDX)	import	import	import
<b>Graphics Export/Save as</b>	<b>Student V6</b>	<b>Spartan'16</b>	<b>Parallel Suite</b>
JPEG	✓	✓	✓
PNG	✓	✓	✓
BMP	Win Only	Win Only	Win Only
QuickTime Recording	✓	Mac Only	Mac Only
<b>Tasks - Calculations</b>	<b>Student V6</b>	<b>Spartan'16</b>	<b>Parallel Suite</b>
Energies	✓	✓	multi-core
Equilibrium Geometries	✓	✓	multi-core
Transition State Geometries	✓	✓	multi-core
Intrinsic Reaction Coordinate (IRC)	—	✓	✓
Equilibrium Conformer	✓	✓	multi-threaded
Conformation Distribution	—	✓	multi-threaded
Similarity Library	—	✓	✓
Energy Profiles	✓	✓	multi-threaded
Similarity Analysis	—	✓	✓
QSAR calculations	—	✓	✓
Thermodynamics and Vibrational Modes	Vibrational Modes	✓	✓
Orbitals & Energies, Charges & Bond Orders	✓	✓	✓

Spectra Calculations	Student V6	Spartan'16	Parallel Suite
Infrared/Raman	IR Only	✓	multi-core
UV/vis	—	✓	✓
NMR Chemical Shifts	✓	✓	multi-core
HH Splitting	✓	✓	✓
Display of COSY, HSQC, & HMBC NMR Plots	—	✓	✓
Properties	Student V6	Spartan'16	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	Student V6	Spartan'16	Parallel Suite
SYBYL	—	✓	✓
MMFF94	✓	✓	✓
MMFF94(aq)	—	✓	✓
MNDO, MNDO(d)	—	✓	✓
AM1	—	✓	✓
RM1	—	✓	✓
PM3, PM3 Transition Metal Extensions	to 75 atoms	✓	✓
PM6	—	✓	✓
Hartree Fock	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<30	✓	multi-core
RSH-GGA: ωB97X-D, ωB97X-V, ωB97X, CAM-B3LYP, N12-SX, LC-VV10	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	—	✓	✓
CIS, CISD, QCIS, QCIS(D)	—	✓	✓
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	✓	multi-core
G3, G3(MP2), G4, G4(MP2)	—	✓	multi-core
G3elect, G3(MP2)elect	—	✓	✓
G4elect, G4(MP2)elect	—	✓	✓

Basis Sets	Student V6	Spartan'16	Parallel Suite
<b>Pople basis sets:</b> 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**	✓	✓
<b>Dunning basis sets:</b> cc-pVDZ, cc-pVTZ, cc-pVQZ	6-311+G**	✓	✓
aug-cc-pVDZ, aug-cc-pVTZ, aug-cc-pVQZ	—	✓	✓
<b>Alrichs/Weigend basis sets:</b> 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 V6	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 V6	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	—	✓	✓
Computational Server	—	—	✓
Included Databases*	Student V6	Spartan'16	Parallel Suite
Spartan Spectra & Properties Database (# molecules)	≈ 6000	≈ 6000	>300,000
Spartan Molecular Database (# molecules)	≈ 6000	≈ 6000	>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

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Contact support@wavefun.com with any Questions.



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