Wavefunction, Inc. © 1991-2020 - Spartan Comparison - Chart 6 Jan 2020

Graphical User Interface	Student V8	Spartan'18	18 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	✓	✓	✓
Chem Draw Builder (requires ChemDraw v. 12 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 V8**	**Spartan'18**	**18 Parallel Suite**
All Spartan formats	✓	✓	✓
SYBYL MOL and MOL2	✓	✓	✓
PDB and standard XYZ file	✓	✓	✓
MACROMODEL	✓	✓	✓
MDL SKC, TGF, and SDF	✓	✓	✓
InChI	**import**	**import**	**import**
SMILES	✓	✓	✓
CIF	**import**	**import**	**import**
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 V8**	**Spartan'18**	**18 Parallel Suite**
JPEG	✓	✓	✓
PNG	✓	✓	✓
BMP	✓	✓	✓
QuickTime Recording	**Mac Only**	**Mac Only**	**Mac Only**
Tasks - Calculations	**Student V8**	**Spartan'18**	**18 Parallel Suite**
Energies	**multi-core**	✓	**multi-core**
Equilibrium Geometries	**multi-core**	✓	**multi-core**
Transition State Geometries	**multi-core**	✓	**multi-core**
Intrinsic Reaction Coordinate (IRC)	—	✓	**multi-core**
Equilibrium Conformer	**MMFF only**	✓	**multi-threaded**
Conformation Distribution	**MMFF only**	✓	**multi-threaded**
Similiarity Library	—	✓	✓
Energy Profiles	✓	✓	**multi-threaded**
Similarity Analysis	—	✓	✓
QSAR calculations	**subset**	✓	✓
Thermodynamics and Vibrational Modes	✓	✓	✓
Orbitals & Energies, Charges & Bond Orders	✓	✓	✓

Spectra Calculations	Student V8	Spartan'18	18 Parallel Suite
Infrared/Raman	IR Only	✓	multi-core
UV/vis	—	✓	multi-core
NMR Chemical Shifts	✓	✓	multi-core
Calculated HH Splitting	Emiprical only	✓	✓
Display of COSY, HSQC, & HMBC NMR Plots	—	✓	✓
Properties	**Student V8**	**Spartan'18**	**18 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	✓	✓	✓
Orbitals & Energies, Charges & Bond Orders	✓	✓	✓
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	✓	✓	✓
Methods/Basis Sets	**Student V8**	**Spartan'18**	**18 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	and ωB97X-D	✓	multi-core
mGGA: B97M-V, M06-L, BMK, M11-L, TPSS-D3	up to 30 atoms	✓	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	up to 20 atoms	✓	multi-core
G3, G3(MP2), G4, G4(MP2)	—	✓	multi-core
G3elect, G3(MP2)elect, G4elect, G4(MP2)elect	—	✓	✓

Basis Sets	Student V8	Spartan'18	18 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 V8**	**Spartan'18**	**18 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 V8**	**Spartan'18**	**18 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	—	✓	✓
Import 2D NMR spectra (image)	—	✓	✓
Remote Submission to Spartan'18 Parallel Suite	—	✓	✓
Included Computational Server (receives remotely submitted jobs)	—	—	✓
Included Databases*	**Student V8**	**Spartan'18**	**18 Parallel Suite**
Spartan Spectra & Properties Database (# molecules)	**≈ 6000**	**≈ 6000**	**>300,000**
Name Search	✓	✓	✓
Structure / Substructure Search	**Structure Only**	✓	✓
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 note: Beginning with the 2018 release:
parallel processing with up to 16 cores per calculation (default)
may also be licensed with unlimited cores per calcualtion
Spartan Student 8 note: Parallelized up to 16 cores per calcualtion
Contact support@wavefun.com with any Questions.

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