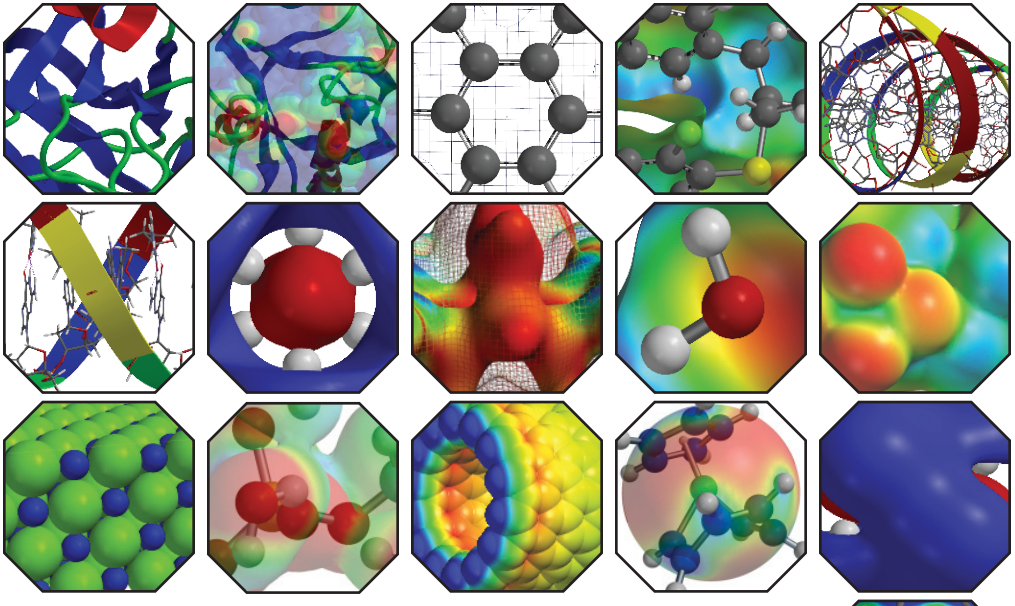
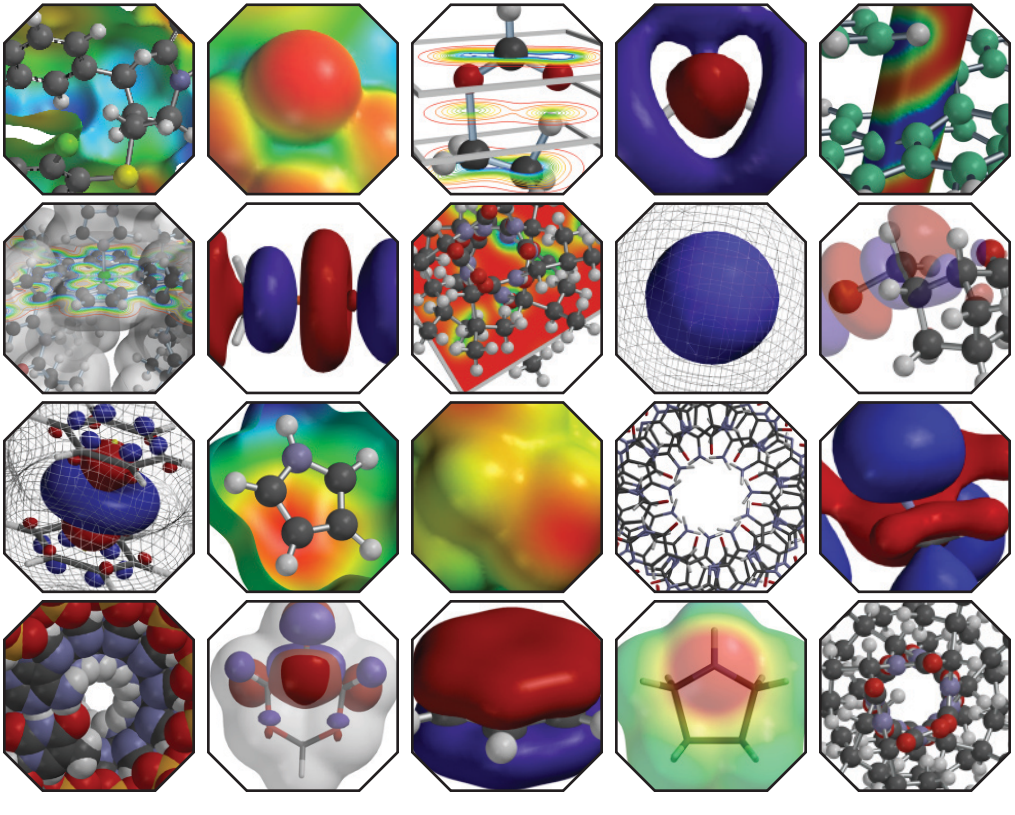
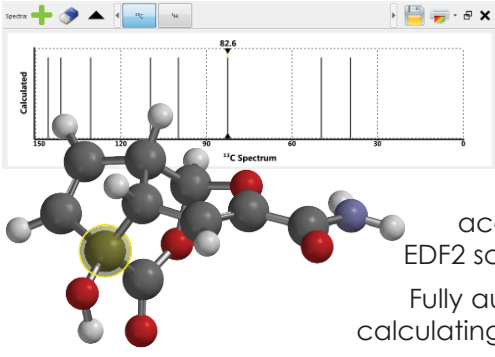


Spartan'16

for Windows, Macintosh and Linux



Spartan'16 is the latest addition to Wavefunction's line of molecular modeling software for research and education. It represents a significant leap forward in access to modern computational methods while new interface developments add to ***Spartan's*** legacy of user-friendliness. Easy access to research quality methods in today's increasingly mobile computer environment remains a primary emphasis. New and improved features include:



NMR PREDICTIONS

A 3rd generation parameterization scheme based on the ωB97X-D functional with both 6-31G* and 6-311G* basis sets offers increased accuracy over the previous B3LYP and EDF2 schemes and uses fewer parameters.

Fully automated procedure for accurately calculating NMR spectra of flexible molecules.

Both calculated and empirical NMR coupling constants now available.

CONFORMATIONAL ANALYSIS

A new procedure for establishing accurate Boltzmann weights of flexible molecules is available. This combines molecular mechanics, HF/3-21G, ωB97X-D/6-31G* and choice of a high-order correlated model, for example, the ωB97X-V/6-311+G(2df,2p) model.

SOLVATION METHODS

A new default solvent method (C-PCM) includes recent refinements[1,2]. This allows calculation of equilibrium and transition-state geometries as well as infrared spectra in the presence of solvent. SM5.0R, SM5.4, SM8 solvent approaches remain available and have been joined by SM12[3].

EXCITED STATES

Analytical gradients for time-dependent density functional (TDDFT) models, enabling calculation of equilibrium and transition-state geometries for molecules in excited states are now available and have been parallelized. Excited-state geometry calculations were previously restricted to CIS models (Hartree-Fock theory).

PARALLEL PROCESSING

A shared memory parallel procedure has been implemented, significantly reducing memory requirements for jobs run in parallel (up to **12 cores** per job). Overall performance has improved by ~25%.

MODERN COMPUTATIONAL METHODS

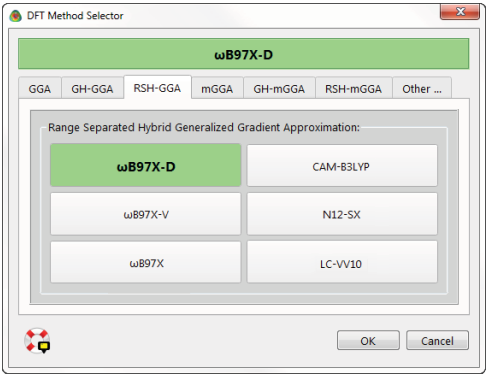
Spartan'16 provides convenient access to a number of important correlated methods, with emphasis on density functional models including:

GGA functionals. B86PW91, BLYP, BPW91, B97-D2, SOGGA11, PBE-D3, VV10

GH-GGA functionals. B3LYP, B3LYP-D3, EDF2, B3PW91, B97-3, MPW3LYP, SOGGA11-X

RSH-GGA functionals. ωB97X-D, ωB97X-V, ωB97X, CAM-B3LYP, N12-SX, LC-VV10

mGGA functionals. B97M-V, M06-L, BMK, M11-L, TPSS-D3



GH-mGGA functionals. M06-2X, M06, M08-HX, M08-SO, MPW1B95

RSH-mGGA functionals. M11, ωB97M-V, MN12-SX

Among the wave-function based correlated models are G3(MP2)elect, G3elect, G4(MP2)elect, G4elect, QCISD, QCISD(T), CCSD and CCSD(T).

Basis sets have been expanded to include both the widely-used Dunning correlation consistent sets and Ahlrich/Weigend def2 sets. Triple-ζ basis sets are now available for transition metals and lanthanides, allowing improved reaction energy calculations. The dual basis set approximation may be employed with double-ζ and larger basis sets, leading to an order of magnitude reduction in computation time.

Pople: STO-3G, 3-21G, 6-31G*, 6-31G**, 6-31+G**, 6-311G**, 6-311+G**, 6-311G(2d,p), 6-311+G(2d,p), 6-311+G(2df,2p), 6-311+G(3df,2p); additional variations on 6-31G and 6-311G may be specified

Dunning: cc-pVDZ, aug-cc-pVDZ, cc-pVTZ, aug-cc-pVTZ, cc-pVQZ, aug-cc-pVQZ

Ahlrichs/Weigend: def2-SV(P), def2-SVPD, def2-TZVP, def2-TZVPPD, def2-QZVP, def2-QZVPPD

Available thermochemical recipes now include **G4(MP2)** and **G4** in addition to G3, G3(MP2), and T1[4].

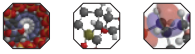
REMOTE SUBMISSION

Spartan'16 Parallel Suite can be used as a server for both remotely submitted calculations and the ***Spartan Spectra and Properties Database***, extending access to computational tools from remote devices. Remote access is available from computers running ***Spartan'14*** and ***Spartan'16***, as well as iOS devices (iPad and iPhone) running the ***iSpartan***[5] app.

SPARTAN'16 FEATURE SET

Items in bold are new, or enhanced in the *Spartan'16* release.

GRAPHICAL INTERFACE



Sketch (2D) organic, **inorganic**, **organometallic** molecules in 2D and automatically convert to 3D structures. **Groups**, **rings** and **ligands** templates now available

Build (3D) organic, inorganic and organometallic molecules, peptides and nucleotides

Fuse rings when 3D building

Link seamlessly to ChemDraw®[6]

Build libraries of substituted molecules

Display and query molecules using a variety of model styles

Display dipole vector, hydrogen bonds, points and planes

Display and customize chemical function descriptors

IUPAC names and 2D structures for all molecules in the *SSPD*

Display user-defined annotations

Align molecules using structure, chemical function descriptors, or **atom labels**

Align molecules to pharmacophores

Enhanced visualization models for polypeptides and proteins

Generate transition states from an extensive reaction library

Define transition states using reaction arrows in 2D

Generate and display molecular orbitals, electron densities, spin densities electrostatic potentials, local ionization potentials, electrostatic potential maps, orbital maps, and local ionization potential maps

Orbital Energy Diagram **with single click posting of orbital energies to spreadsheet**

Optionally view property maps in Red-White-Blue color scale

Toggle between default and absolute property ranges for property maps

Display electron density based on % enclosure

Display solvent accessible regions on surfaces and property maps

Single click/tap access to R/S chirality display

Determine reaction energies with integrated reaction energy calculator and **automatically balance reactions**

Organize data in spreadsheets, **improved add properties feature in spreadsheets**

Perform regression analysis and make, save and print 2D or 3D plots

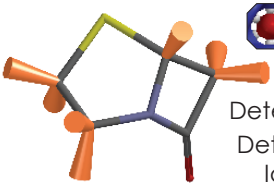
Embed external files such as MS® Office and Adobe® PDF files in ***Spartan*** files

Plot, print, and save calculated and experimental[7] IR, Raman, and UV/vis spectra

Calculated 1D (proton, ^{13}C, DEPT) and 2D (COSY, HSQC, HMBC) and experimental proton and ^{13}C NMR spectra

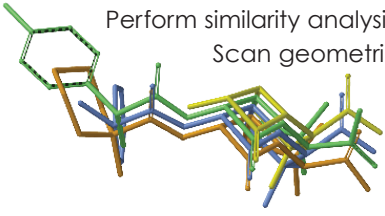
Improved SDF file export includes *Spartan* spreadsheet data

Full support of touch interface commands and gestures for Windows PCs and tablet computers



TASKS

Calculate strain energy, total energy and heat of formation
Determine gas-phase equilibrium and transition-state geometries
Determine geometries and IR spectra in the presence of solvent
Identify global minimum; establish conformer distributions with **improved estimation of Boltzmann weights**
Build libraries of diverse conformers for use in similarity analysis



Perform similarity analysis on the basis of structure or chemical functionality
Scan geometrical coordinates and generate reaction sequences
Calculate reaction and activation energies
Calculate IR, Raman, UV/vis, and NMR spectra
Determine NMR spectra for flexible molecules
Match calculated and experimental NMR spectra[7]
Search SSPD and NIST[7] experimental database for match to IR spectra
Mine databases of calculated molecular, atomic, and reaction properties

COMPUTATIONAL METHODS

Molecular Mechanics. SYBYL, MMFF94, MMFF(aq)
Semi-Empirical. MNDO, AM1, RM1, PM3 (with transition metal parameters), PM6
Hartree-Fock molecular orbital theory
Density Functional Theory (available from menus):
GGA functionals: **B86PW91**, BLYP, **BPW91**, **B97-D2**, **SOGGA11**, **PBE-D3**, **VV10**
GH-GGA functionals: B3LYP, **B3LYP-D3**, EDF2, **B3PW91**, **B97-3**, **MPW3LYP**, **SOGGA11-X**
RSH-GGA functionals: ωB97X-D, **ωB97X-V**, **ωB97X**, **CAM-B3LYP**, **N12-SX**, **LC-VV10**
mGGA functionals: **B97M-V**, **M06-L**, **BMK**, **M11-L**, **TPSS-D3**
GH-mGGA functionals: **M06-2X**, M06, **M08-HX**, **M08-SO**, **MPW1B95**
RSH-mGGA functionals: **M11**, **ωB97M-V**, **MN12-SX**
Functionals may be customized and additional functionals specified via keyword(s)
Møller Plesset. MP2, MP3, MP4, and RI-MP2
Wave-function based advanced correlated models:
G3(MP2)elect, **G3elect**, **G4(MP2)elect**, **G4elect**, **QCISD**, **QCISD(T)**, **CCSD**, **CCSD(T)**
Additional wave-function based advanced correlated methods are available from keywords and include CCSD, CCSD(T), OD, OD(T), QCCD, VOD, and VQCCD
Excited-state methods. CIS, CIS(D), RI-CIS(D), QCIS(D), QCISD(T) and TDDFT
Gradients available for CIS, CIS(D) and **TDDFT**
Thermochemical Recipes. T1[4], G3(MP2), G3, **G4(MP2)**, **G4**
Basis Sets (available from menus):
Pople: STO-3G, 3-21G, 6-31G*, 6-31G**, 6-31+G**, 6-311G**, 6-311+G**, **6-311G(2d,p)**, **6-311+G(2d,p)**, 6-311+G(2df,2p), **6-311+G(3df,2p)**; other variations on 6-31G and 6-311G may be specified
Dunning: **cc-pVDZ**, **aug-cc-pVDZ**, cc-pVTZ, **aug-cc-pVTZ**, **cc-pVQZ**, **aug-cc-pVQZ**
Ahlrichs/Weigend: **def2-SV(P)**, **def2-SVPD**, **def2-TZVP**, **def2-TZVPPD**, **def2-QZVP**, **def2-QZVPPD**
Automatic use of pseudopotentials for elements >Kr (including lanthanides).
Dual basis set approximation available with double-ζ and larger basis sets.
Import and use of custom basis sets available via keyword(s).

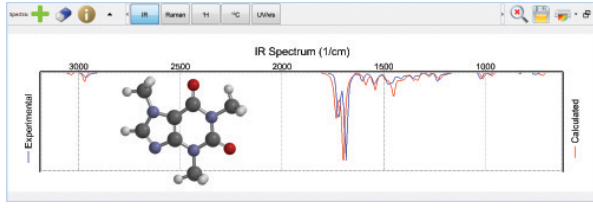
PROPERTIES AND QSAR DESCRIPTORS

Mulliken, natural, and electrostatic-fit charges
Dipole and higher moments, polarizabilities and hyperpolarizabilities
Enthalpies, entropies and free energies
Aqueous solvation energies from **C-PCM**[1,2], as well as SM5.4, SM8, **SM12**[3], and **SS(V)PE**
HOMO, LUMO and SOMO energies
Areas, polar surface areas and volumes based on space-filling models
Areas, accessible areas, polar areas, and volumes based on the electron density
Min/Max of electrostatic potential and Min of local ionization potential
Number of conformers and tautomers
Number Hydrogen Bond acceptors and donors
Empirical and **calculated** NMR HH coupling constants

SPECTRA

NMR, IR, Raman and UV/visible spectra may be calculated using a variety of theoretical models: Hartree-Fock and density functional models for NMR, semi-empirical, Hartree-Fock, density functional and MP2 models for IR, Hartree- Fock, density functional models for Raman, and UV/visible.

NMR



A 3rd-generation parameterization scheme for NMR chemical shifts for both the ωB97X-D/6-31G* and ωB97X-D/6-311G* models is introduced in ***Spartan'16***. This leads to lower errors in shifts with half the number of parameters. Earlier generation parameterization schemes for use with the B3LYP/6-31G* (^{13}C only) and EDF2/6-31G* are also available.

Calculated (corrected) chemical shifts together with empirical HH coupling constants based on the calculated equilibrium geometry and bond orders allow for presentation of ^{1}H, ^{13}C and DEPT 1D spectra and COSY, HSQC and HMBC 2D spectra. Proton spectra may be displayed with three-bond HH coupling or in an idealized (simplified) form with no HH coupling.

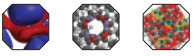
IR AND RAMAN

Infrared (and Raman) frequencies calculated from ωB97X-D/6-31G*, B3LYP/6-31G* and EDF2/6-31G* density functional models are scaled to account for systematic errors associated with the harmonic approximation. Corrected frequencies and intensities are fit to a Lorentzian function with a line width parameter. Alternatively, scale and line width may be adjusted to fit a spectrum calculated using any theoretical model to an experimental spectrum.

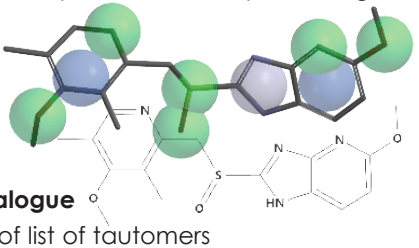
UV/VISIBLE

UV/visible spectra are obtained by explicit calculation of the ground state energies and the low-lying excited states. CIS models are paired with Hartree-Fock models. **TDDFT (time dependent density functional) models are paired with density functional models**.

ADDITIONAL FEATURES



***Spartan'16* Parallel Suite** includes multi-core parallel processing for Hartree-Fock, density functional, RI-MP2, and thermochemical recipes. Automatic processing of groups of molecules



Automatic use of molecular symmetry

View Recent Documents from File menu

Optimize using constraints and/or frozen atoms

Use NOEs for conformational searching

Enhanced Help functions in the Calculations dialogue

Automatic tautomer indicator and generation of list of tautomers

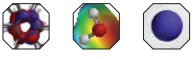
Import experimental IR, Raman, and NMR spectra

Import structures in SMILES, CDX, CIF, SKC, SDF, TGF, XYZ, Macromodel, PDB, SYBYL MOL and MOL2 format

Export as InChI, SMILES, Macromodel, XYZ, PDB, MOL, MOL2 and SDF

Structure retrieval from Cambridge Structural Database[8] and Protein Data Bank[9]

Extract ligands and binding sites from proteins (PDB files)



DATABASES

Spartan Spectra and Properties Database *(SSPD)*®[10] comprises two collections, the first of ≈275,000 organic molecules obtained from the EDF2/6-31G* model and the second of ≈300,000 organic molecules and ≈2,000 organometallic molecules obtained from the ωB97X-D/6-31G* model. Both include the optimized geometry, the energy and a selection of molecular properties, the wave function allowing on-the-fly generation of molecular orbitals, electrostatic potential maps among other graphical surfaces, and the NMR spectrum. The infrared spectrum is also provided for molecules in the EDF2/6-31G* collection.

Systematic (IUPAC) names for all organic molecules in both collections have been provided along with a small (≈4,000 molecule) selection of common (more easily recognized) names. 2D structure drawings have also been provided for organic molecules. IUPAC names and 2D structures generated from Naming[11].

Spartan Molecular Database *(SMD)*® comprises structures, energies and properties for ≈150k molecules obtained using up to 10 quantum chemical models including Hartree-Fock, B3LYP density functional and MP2 models. Limited data have also been provided from the G3(MP2) thermochemical recipe.

Individual SSPD and SMD entries can replace user-built structures, and both databases are searchable by substructure, name, formula, and isomer.

Spartan Reaction Database *(SRD)*® comprises transition states for ≈1,800 reactions searchable by combination of substructure and "reaction arrows" from either **2D** or 3D models.

1. *J. Chem. Phys*. **2010** 133, 24411-1-2441-18.
2. *Chem. Phys. Lett*. **2011** 509, 77-87.
3. *J. Chem. Theory Comput*. **2013** 9 (1), 609-620.
4. *J. Phys. Chem. A*. **2009** 113(10), 2165-2175.
5. ***iSpartan*** is available via the iTunes App Store. www.appstore.com/ispartan.
6. Windows only. ChemDraw® must be licensed from CambridgeSoft®.
7. IR and UV/vis from NIST Chemistry WebBook, NMR from European Bioinformatics Institute. Freely accessible.
8. Cambridge Structural Database® must be licensed from the Cambridge Crystallographic Data Centre®.
9. Protein Data Bank is a freely-acessible on-line resource of biological macromolecules.
10. 6,000 molecules subset included with ***Spartan'16***. Full database included with ***Spartan'16 Parallel Suite***.
11. Naming, 2015, ChemAron (http://www.chemaron.com).

SPARTAN'16 LICENSING*

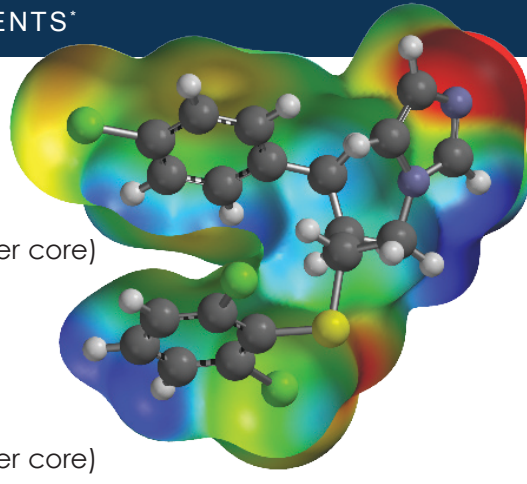
	Academic	Government	Commercial
Spartan'16	$ 1,200	$ 2,400	$ 3,600
Spartan'16* Parallel Suite*	$ 1,600	$ 3,200	$ 4,800

Academic Lab Pricing	***Spartan'16***	***Spartan'16* Parallel Suite**
5 Seat Lab License	$ 5,000	$ 6,500
10 Seat Lab License	$ 9,000	$12,000
20 Seat Lab License	$12,000	$16,000

* *Annual campus-wide site license available. Contact Wavefunction, Inc. for pricing.*

** *Includes parallel processing for select methods and tasks, Spartan'16 Server feature with the ability to act as a computational server from other* ***Spartan'16*** *licenses and the* ***iSpartan app*** *(up to two concurrent clients), and the (≈300,000 molecule) Spartan Spectra and Properties Database and the (≈150,000) molecule Spartan Molecular Database collections.*

MINIMUM SYSTEM REQUIREMENTS*



WINDOWS

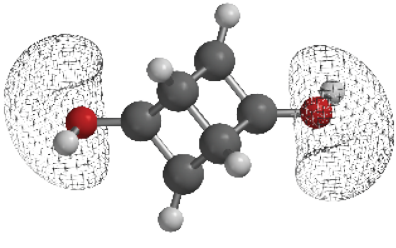
- Intel or AMD only
- Windows 7, 8.1, or 10**
- 128 GB disk space or higher
- 4 GB of RAM (at least 2GB RAM per core)

MACINTOSH

- Intel-based Macintosh only
- OS X 10.9.5, 10.10, or 10.11
- 128 GB disk space or higher
- 4 GB RAM (at least 2GB of RAM per core)

* ***Spartan'16*** *available for Windows and Macintosh only.* ***Spartan'16 Parallel Suite*** *available for Windows, Macintosh, and Linux. Contact Wavefunction for Linux system requirements.*

** *Fully supports Windows 7, 8, and 10 touch screen computers and tablets.*



Spartan'16
for Windows, Macintosh and Linux

is a collaboration with Q-CHEM

WAVEFUNCTION, INC.
18401 Von Karman Ave., Suite 370
Irvine, CA 92612 U.S.A.
(949) 955-2118 fax
sales@wavefun.com
www.wavefun.com

WAVEFUNCTION

WAVEFUNCTION, INC.,
JAPAN BRANCH OFFICE
3-5-2, Kouji-machi, Suite 608
Chiyoda-ku, Tokyo, Japan 102-0083
japan@wavefun.com
www.wavefun.com/japan