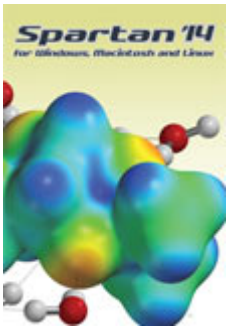

Spartan'14 for Windows

The latest release of the ultimate desktop application for chemistry research in industry and academia. A full range of theoretical models are available from the most intuitive user interface in the business. Enhanced, Refined, and Faster than ever. Also available in a Parallel Suite including the Spartan Molecular Database, the Spartan Spectra and Properties Database, Parallel Processing features and the ability to act as a Computational Server for jobs submitted from other ***Spartan'14*** licenses or from ***iSpartan*** on the iPad, iPhone, or iPod Touch.

Computational chemistry like never before.

Minimum System Requirements

- Intel Pentium III or higher; AMD Athlon
- Windows Vista, Win 7, or 8
- 1024 x 768 (or higher) graphics resolution

2 GB

60 GB disk space

Click on one of the following links to learn more:

- **Graphical User Interface**
- **Tasks Performed**
- Database Access
- **New to Spartan'14**
- **Pricing**
- **Computational Methods**
- **Properties Calculated**
- Additional Features
- **User's Guide and Tutorial (15 MB pdf)**
- **Maintenance**

Click on one of the following links to learn more:
Main Page | Graphical User Interface | **Computational Methods**
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The Spartan Computational Methods. ***Spartan'14*** provides a full range of computational methods, addressing the needs of educators, bench chemists, and professional modelers. All methods are easily accessed via Spartan's seamless graphical interface.

Methods: (Items in BLUE are available in Parallel with the Spartan'14 Parallel Suite)

Molecular Mechanics	Molecular mechanics is presently the only practical method for calculations on very large molecules or for conformational searching on highly flexible molecules. MMFF94, in particular, has proven to be a reliable and fast tool for conformational analysis. There are no atom limits for molecular mechanics calculations. Both the SYBYL and MMFF94 force fields are supported. SYBYL extends throughout the entire Periodic Table while MMFF94 has been specifically parameterized to reproduce geometries and conformations of organic molecules and biopolymers. Additionally, an MMFFaq option applies an aqueous solvent energy correction to energy data, of special utility in ranking conformers.
Semi-Empirical Molecular Orbital	Semi-empirical models are the simplest of the quantum chemical schemes, and are useful for equilibrium and transition-state structure calculations. PM3, in particular, has proven to be a reliable tool for geometry calculations on transition metal inorganic and organometallic compounds. MNDO, AM1, RM1, PM3, and PM6 methods are supported. MNDO/d extensions for heavy main-group elements have been implemented and PM3 parameters for most transition metals are available. The RM1 (Recife Model 1) reparameterization of AM1 is new in Spartan'06. In most cases RM1 yields superior results to both AM1 and PM3 (for organic molecules).
Hartree-Fock Molecular Orbital	Hartree-Fock models useful for predicting structure, energy and property calculations, in particular for organic molecules. A variety of standard basis sets are supported: STO-3G, 3-21G, 6-31G*, 6-311G*, cc-pVDZ, cc-pVTZ and cc-pVQZ, with extensions including (d), (d,p), (2d), (2d,2p), (2df, 2dp), (3d, 3p), (3df, 3dp) and diffuse functions and/or additional polarization functions. Also supported are a variety of pseudopotentials for calculations on molecules incorporating heavy elements. Spartan allows for the import of additional basis sets, and for the construction of user-created basis sets. Additionally, a new dual basis set procedure is is available, allowing the approximation of basis set extension using perturbation theory (for improved precision and performance).

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Methods:

Density Functional	Density functional models typically provide results of a quality comparable to conventional correlated models such as MP2, but at a cost only slightly greater than that of Hartree-Fock models. As such, they are particularly useful for high-quality structure, energy and property calculations, including calculations on transition-metal inorganic and organometallic compounds. Local density models and BP, BLYP, EDF1, EDF2, and B3LYP models are supported with the same basis sets and pseudopotentials as available for Hartree-Fock models. The non-empirical GGA functional PBE has been implemented. Five Minnesota hybrid meta-GGA functionals from Zhao and Truhlar have also been implemented, in particular, M05, M05-2X, M06, M06-2X, and M06-HF; and the local meta-GGA from that group, namely M06-L, is also available. Additionally, a wider range of functionals is available as calculation options with the ability to specify model and percentages for exchange and correlation (these include Slater-Dirac), Vokso-Wilk-Nusair, Perdew-Zunger, Wigner, Becke88, Gill96, Gilbert-Gill99, Lee-Yang-Parr, Perdew86, GGA91, BMK, EDF1 and EDF2).
Møller-Plesset	MP2 is perhaps the simplest model to take reasonable account of electron correlation, and generally provides accurate descriptions of equilibrium structure, conformation and energetics of a variety of chemical reactions, including reactions where chemical bonds are broken. MP methods are supported for the same basis sets and pseudopotentials available for Hartree-Fock and density functional models. The RI-MP2 model, providing nearly identical results to MP2 but with significant performance improvements: energy calculations an order of magnitude faster and structure calculations a factor of 3 times faster than conventional MP2. MP3 and MP4 models are available for single-point energy calculations only, as is a fast localized orbital variant of MP2. The same basis sets and pseudopotentials supported for Hartree-Fock are available.
Thermochemical Recipes	Several recipes for obtaining highly accurate heats of formation are available, including the T1 recipe that provides results within 2 kJ/mol of the (also available) G3(MP2) approach, but with performance several orders of magnitude faster than G3(MP2). Additional recipes include G2, G3.
Advanced Correlated	A number of high-order correlated models are available for energy calculations only. These include CCSD, CCSD(T), OD, OD(T), QCISD, QCISD(T), QCCD, and QCCD(T) models, with the same basis sets and pseudopotentials available for Hartree-Fock, density functional and Møller-Plesset calculations.

Excited-State Methods	Calculations on excited states may be performed using CIS, CIS(D), RI-CIS(D) and TDDFT models in addition to the entire range of density functional models. The same basis sets and pseudopotentials supported for ground-state calculations are available.

Click on one of the following links to learn more:
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Spartan includes access to a number of highly useful molecular databases, including: The Spartan Molecular Database, Spartan Reaction Database, Cambridge Structural Database* and Protein Data Bank**. **(Items in BLUE are available in Parallel with the Spartan'14 Parallel Suite)**

*CSD must be licensed separately. **PDB access requires internet connectivity.

Databases:

SMD	Access and retrieve/replace constructed or imported structures from a library of 150,000* molecules, pre-calculated at up to 5 quantum theory levels: HF/3-21G, HF/6-31G*, EDF1/6-31G*, B3LYP/6-31G*, and MP2/6-31G* models. Retrieved data includes: the name, equilibrium geometry, gas-phase energy, estimated (aqueous) solvation energy, HOMO and LUMO energies, dipole moments, electrostatic-fit atomic charges, surface area, polar surface area, volume, weight, symmetry, and spectra data. *Spartan'14 includes a subset of >6,000 molecules. The full SMD (and SSPD) is available for purchase. Customers with Maintenance receive the full SMD at no additional charge.
SSPD	The SSPD is a collection of >75,000 molecules that includes highly accurate structures, energies, properties, and IR and NMR spectra as well as the molecule's wavefunction for auto-generation of graphical surfaces.
SRD	Access to exact and substructure searching of the Spartan Reaction Database of more than 1500 reaction types for providing initial structure guesses for transition state geometry calculations.
CSD	Accesses the Cambridge Structural Database (CSD)* of over 500,000 experimental X-ray crystal structures for organic and organometallic molecules, together with their literature references. Spartan optionally adds hydrogens and refines hydrogen positions. *CSD may be licensed from the Cambridge Crystallographic Data Centre or one of its distributors.
PDB	Spartan can retrieve (based on PDB ID) entries from RCSB PDB (provided your computer has current internet connectivity). The Protein Data Bank includes more than 90,000 x-ray crystal and NMR structures of proteins and nucleic acids. Band ligands may be extracted.

Click on one of the following links to learn more:
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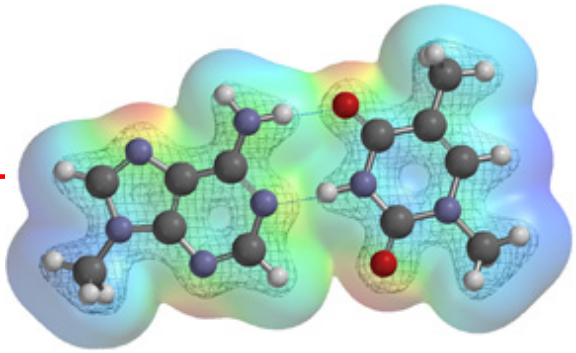
Additional *Spartan'14* Features:

List processing	Spartan automatically processes files comprising lists of molecules. In general, operations applicable to a single molecule may be applied to lists of molecules. Spartan is optimized to operate on lists of hundreds of molecules (not thousands or tens of thousands).
NOEs	NOE data can be applied to conformational searching as a post-processing filter.
On-line Infrared and UV/vis data	If your computer has internet connectivity, ***Spartan'14*** can retrieve and plot experimental IR (~ 14,000 molecules) and UV/Vis (~ 1,500) spectra from the NIST Chemistry Webbook.
On-line NMR Chemical Shift data	If your computer has internet connectivity, ***Spartan'14*** can retrieve and plot experimental NMR Chemical Shifts (~ 15,000 molecules) from the NMR database maintained by the University of Cologne.
Ligand and Binding Site Extraction	***Spartan'14*** can optionally extract bound ligands and their environment from protein (PDB) files, along with customizable chemical function descriptors (CFD's).
Constraints and Frozen Atoms	Geometry optimization and conformational analysis are available subject to user specified constraints (of distance, angle, or torsion angle) and/or frozen atoms.
User Generated Database	Extend the Spartan Molecular Database (SMD) and Spartan Specta and Properties Database (SSPD). Users can save Spartan data in the .spentry format (Spartan Database format) and construct custom databases, extend the computational models, and the number of molecules available from within Spartan.



Spartan'10 **conveniently delivers:**

Equilibrium Geometry Structures

Molecular Properties

Calculated Electronic Surfaces

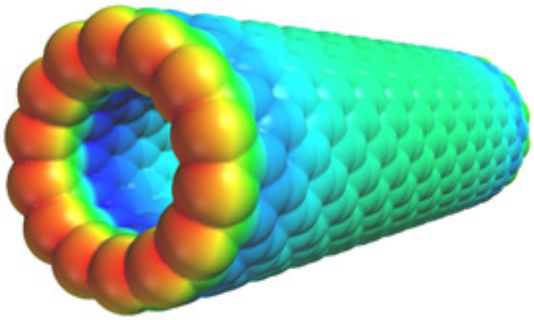
Linear Regression Analysis

Conformational Analysis

3D Alignment & Superposition

3D Similarity Analysis

Spartan'10 maintains compatibility with previously released versions of Spartan (and Trident) software. The strenth of the Spartan application for use in both education and research is the well designed and easy-to-use graphical interface. With very little exposure, new users can be up and running calculations in no time at all.



For more information on available graphical models, review Chapter 4 in Wavefunction's ***A Guide to Molecular Mechanics and Quantum Chemical Calculations***. Click here to download this reference (pdf file).

Click on one of the following links to learn more:
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The Spartan Graphical User Interface. A single, integrated, easy-to-use GUI. In little time, one can build/import/and augment molecules and systems, run molecular mechanics and quantum chemical calculations, and analyze results with Spartan graphics, property dialogs, integrated spreadsheets, data and spectra plots, and text output. Completely re-imagined for ***Spartan'14***, fully supported for touch devices.

Click here for a gallery of Spartan **screen shots**.

Build / Import / Export / Embed

New Sketch Builder	Borrowing from iSpartan, a brand new 2D building panel for easy construction of organic molecules.
Organic	Accesses a builder for common organic fragments (e.g., "sp^3 carbon"), functional groups and rings for easy construction of organic molecules.
Inorganic	Extends building throughout the entire *Periodic Table*. Includes groups, rings and a library of common ligands.
Peptide	Accesses a builder with amino acids for construction of polypeptides as helices, sheets or in user-defined conformations.
Nucleotide	Accesses a builder of nucleotide bases for construction of single or double stranded DNA or RNA as A or B helices or in user-defined conformations.
Substituent	For generating groups of substituted molecules and virtual libraries.
2D Building	Seamless access to 2-D building via ChemDraw (must be licensed separately from CambridgeSoft). Requires ChemDraw 10 or later. *Windows only*
Custom	Access an included (and customizable) library of additional functional groups, rings and ligands.
Clipboard	Access to any molecule or molecular fragment which has previously been constructed.
Import	Spartan, SYBYL MOL and MOL2, PDB, MacroModel, smiles, XYZ, SDF, TGF, SKC, CIF, CDX, and JCAMP files.
Export	Spartan, SYBYL MOL and MOL2, PDB, MacroModel, smiles, and XYZ molecule files, graphics as JPG, PNG, BMP files, and animations, and Spectra as JCAMP files.
Embed	Spartan can embed external files (Word, Excel, PDF, JCAMP, etc.) into native Spartan files for improved organization of molecular data.

Click on one of the following links to learn more:
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Refinement and Analysis:

Structure Refinement	Energy (strain energy) minimization with MMFF94 molecular mechanics force field, provides fast structure clean-up and assists in building molecules.
Chirality Inversion	Assignment of R/S chirality and user specified inversion of both chiral centers and absolute configuration.
Structure Query	Measure, post to spreadsheet (and optionally constrain) any distance, angle or dihedral (torsion) angle. Surface area, polar surface area, and molecular volumes may be measured and data posted to Spartan's spreadsheet.
Align Molecules	Instant alignment of multiple conformers or molecules based on either molecular structure or chemical function descriptors with alignment scores (rms values) available in dialoques and the Spartan Spreadsheet.
Data Organization	Post a full range of calculated molecular properties, or, optionally copy/paste directly to/from other cell-based data organization tools. Tabulated data in Spartan Spreadsheets is available for Linear Regression Analysis.
Plotting	2D and 3D plots are available for all data tabulated in Spartan's spreadsheet.
Spectra	Calculated spectra plots for IR, Raman, Proton and ^{13}C NMR, and UV/vis. Additional NMR representations for COSY, HSQC, and HMBC plots.

Graphical Displays:

Molecular Models	Structures may be displayed in several styles, including: line, wire, ball-and-wire, tube, ball-and-spoke, and space-filling models. User-defined points and planes may be added to the models. Atoms, bonds, and molecules may be custom colored to emphasize specific features, or for highlighting superposition. An arrow may be displayed with the model, indicating the sign and direction of the calculated dipole moment.
Biopolymer Models	Display options for polypeptides and polynucleotides, include: ribbons, lines, or beads, with the option to customize color based on secondary structure, strand or residue type. PDB files with explicitly specified ligands will be automatically rendered in ribbon style with ligands displayed. Ligands are available for extraction, along with their environment.
Hydrogen Bonds	Optionally displays graphical indicator of inter/intra molecular hydrogen bonds.

Click on one of the following links to learn more:
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Graphical Displays: con't

Surfaces and Maps	Electron densities, van der Waals surfaces, spin densities, molecular orbitals, electrostatic potentials (and esp from charges) and local ionization potentials may be displayed as isosurfaces or color mapped on top of isosurfaces. Maps are available with continuous color gradient, or discrete bands. Additional clipping features provide a view beneath the calculated surface. Surfaces and maps may be displayed as opaque or translucent solids, meshes, or as a series of "dots". Area and volume of a displayed surface may be measured and property value at a selected surface location may be measured and posted to Spartan's spreadsheet. Accessible surface regions may be optionally highlighted, and an alternate definition of polar surface area (termed polar area) based on the value of the electrostatic potential above and below a user-defined lipophilic range is also provided.
Slices	Electron densities, spin densities, molecular orbitals, electrostatic potentials and local ionization potentials may be displayed as contour plots.
Animations	Molecular models and associated surfaces, maps and slices for molecules contained within a list may be displayed in sequence. This allows visualizing changes in property throughout a chemical reaction or conformational motion. A "special case", involving motion along the normal mode, is useful for establishing whether a transition state smoothly connects reactants and products. Animations can be exported.
Multiple Molecules	As many molecules as desired may be displayed simultaneously on screen, together with any associated graphics.
Chemical Function Desctiptors	Spartan optionally displays and makes use of CFDs in either alignment or similarity analysis. CFD's are based on standard pharmacophore definitions (hydrogen bond acceptors/donors, positive/negative ionizable centers, aromatic centers, hydrophobic centers, and excluded volume centers, but may also be further customized or user-defined.

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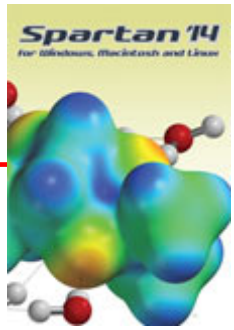
Dialogs:

Calculations	A single dialog allows for easy specification of all aspects of a molecular mechanics or quantum chemical calculation. A "surface" dialog allows specification of surfaces, property maps and slices.
Output	Individual dialogs are available for standard text output.
Properties	Dialogs display calculated properties (energies, dipole moments and atomic charges, among other quantities) without having to examine "text" output.
Spreadsheet	A spreadsheet is available to collect calculated quantities for molecules contained in a list. 2D and 3D plots are available using this data.
Surfaces	A single, user friendly dialog for requesting and displaying graphical indicators as molecular surfaces.
Similarities	A dialog for screening and review of similarity analysis results, includes similarity score (rms value), visualization of aligned and superimposed similarity pair (template and library entry), conformer number (from conformer libraries) as well indication of enantiomer. Includes the ability to retrieve any 'hit' to main Spartan interface.
Reactions	A reactions dialog provides an easy-to-use tool for calculation of user-defined reaction energies from either calculated data of the Spartan Molecular Database.
Database	Provides GUI tool for screening results from searches of the Spartan Molecular Database (SMD), Spartan Reaction Database (SRD), Spartan Infrared Database (SIRD), Cambridge Structural Database (CSD), and Spartan Spectra and Properties Database (SSPD).

Spartan'14 for Windows



All Spartan purchases include 60 days of full maintenance, offering Technical Support through e-mail, and providing all minor and major version updates. In order to provide ongoing prioirity support and access to the latest Spartan updates, Wavefunction offers Desktop Maintenance Contracts.

Click on one of the following links to learn more:

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Three-Year Maintenance Pricing for Spartan'14 for Windows (per license)	Commercial	Government	Academic
Global Pricing	$1,800	$1,200	$ 600

Three-Year Maintenance Pricing for Spartan'14 Parallel Suite* for Windows (per license)	Commercial	Government	Academic
Global Pricing	$2,100	$1,400	$ 700

* Includes all updates to the Spartan Spectra and Properties Database (SSPD)

Click on one of the following links to learn more:
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Spartan'14 is the latest release of Wavefunction's flagship Spartan line. In addition to the performance, stability, and functionality provided by more than 20 years of professional software development, the following **New Features** have been added.

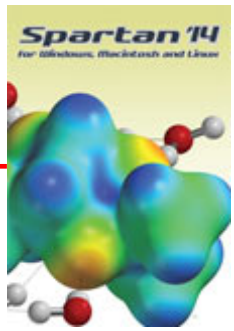
Click here for itemized **New Feature List (pdf file)**

New Graphical User Interface Features:

- Completely reimagined icons and toolbar display. Fully supports touch devices.
- Tab-based visualization option for multiple open documents
- Orbital Energy Diagram provides display of occupied and unoccupied molecular orbitals, accessible from a single and convenient energy diagram table
- Refined Surfaces Dialogue, with a new menu for most commonly used graphical models
- Surface Clipping feature accessed via Surface Properties Dialogue allows for visualization inside calculated graphical models
- Calculation of Selected Area feature for composite maps accessed via the Surface Propertied Dialogue
- QSAR and Thermodynamic properties available in the Molecule Properties Dialogue
- Access to the Spartan Spectra and Propertied Database (SSPD) including IR and NMR spectra, molecular and atomic properties, and QSAR descriptors
- NMR Spectra Display now includes COSY, HSQC, and HMBC
- Datamining, Statistical Analysis, and Plotting features available for the Spartan Molecular Database (SMD) and Spartan Spectra and Propertied Database (SSPD)
- Formula Editor Dialogue allows user to easily specify custom queries of the Spartan Molecular Database (SMD) and Spartan Spectra and Propertied Database (SSPD)
- Automatic Name Search of Wikipedia available from the Database Preview Dialogue

New Computational Enhancements:

- Calculation of Raman frequencies and intensities, Display of Raman Spectra for Hartree-Fock and DFT models
- Correction scheme for calculated NMR chemical shifts (EDF2 model) provides accuracy to ~ 1.4-1.6 ppm. For ^{13}C, .1 to .15 ppm for ^{1}H, and 3.4 for ^{19}F.
- The T1 thermochemical recipe has been extended to incorporate molecules containing silicon and phosphorous
- Gradients have been implemented for RI-CIS(D) allowing for equilibrium geometries of excited states
- Vibrational frequencies have been parallelized for Hartree-Fock and DFT (parallel suite only)
- Raman spectra can be calculated for Hartree-Fock and DFT
- Full 64-bit implementation has been completed and is available for Windows and Linux



Spartan'14 for Windows

Single User License Pricing is listed below. In addition, Wavefunction also offers software leases, discounted lab licensing, academic, government, and commercial site licensing, and commercial enterprise licensing. For more information, please contact our sales department.

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Pricing for Spartan'14 for Windows	Commercial	Government	Academic
Global Pricing	$3,600	$2,400	$1,200

Pricing for Spartan'14 for Windows Parallel Suite	Commercial	Government	Academic
Global Pricing	$4,800	$3,200	$1,500

Exchanges (Worldwide)	Commercial	Government	Academic
From Spartan'04 and older to Spartan'14 Windows	$2,800	$1,400	$ 900
From Spartan'06 to Spartan'14 Windows	$2,200	$1,100	$ 750
From Spartan'08 to Spartan'14 Windows	$2,000	$1,000	$ 650
From Spartan'10 to Spartan'14 Windows	$1,800	$ 900	$ 600
ALL Exchanges to Spartan'14 Parallel Suite Add	$1,200	$ 800	$ 400

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Spartan Molecular Properties: In addition to energies, equilibrium and transition-state geometries and frequencies, Spartan'10 provides a number of valuable properties**.**

Atomic Charges	Mulliken and Natural Bond Orbital Charges are available as are charges based on fits to electrostatic potentials.
Thermodynamics	Enthalpies, entropies and free energies as well as isotope effects, based on calculated geometries and IR vibrational frequencies.
Electrical	Dipole, quadrapole and higher moments, polarizabilities (including alpha, beta, and gamma terms).
Acidity and Basicity	A new feature in ***Spartan'14***, calculated acidities and basicities are available for common carboxylic acids and amines.
Additional Properties	Weight, Area, Volume, Symmetry Group, HOMO and LUMO Energies, Polar Surface Area, LogP, Ovality, Q-Minus, Q-Plus, Electronegativity and Hardness
IR Spectra	Vibrational spectra available from IR calculations including plotting and animation of vibrational modes.
Solvation	Aqueous solvation energies from SM6, SM5.4 or SM50R models. An additional continuum solvation model is also included.
NMR Calculations	Chemical shift calculations for Hartree-Fock and DFT models, and, new in Spartan'10, a correction scheme for the EDF2 model for chemical shifts with accuracy of 1.7-1.8 ppm.
UV/vis Spectra	Vertical excitation spectra based using either CIS/CIS(D) or Time Dependent DFT models is provided.

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Tasks Performed by Spartan'14 for Windows: (Items in BLUE are available in Parallel with the Spartan'14 Parallel Suite.)

Energy	Determine total energy (Hartree-Fock, density functional, Møller-Plesset, advanced correlated), heat of formation (semi-empirical or thermochemical recipes) or strain energy (molecular mechanics).
Equilibrium Geometry	Determines local energy minimum.
Transition State Geometry	Determine transition-state geometry, with the option to calculate the intrinsic reaction coordinate (IRC).
Calculate and Plot IR Spectra	All methods except MP3, MP4 and advanced correlated. Needed to establish validity of transition states.
Calculate and Plot NMR Spectra	Chemical shifts from Hartree-Fock and DFT models.
Calculate and Plot UV/vis Spectra	Hartree-Fock/CIS and DFT/TDDFT models.
Conformational Analysis	Search conformation space to determine either lowest-energy conformer or diverse set of low-energy conformers. Additional procedure for generating a conformational library of the minimal set of conformers required to span conformational space (used in conjunction with Similarity Analysis).
Energy Profile	Define and calculated energies for user specified geometrical coordinates. Useful to locate a transition state along a reaction coordinate and to analyze conformational energy changes. Includes the ability to provide grid scanning to concurrently drive two geometric coordinates.
Similarity Analysis	Assess and quantify similarity between molecules or molecules and pharmacophore models. Similarity based on molecular structure or chemical function descriptors is available. A scoring function based on rms deviations is available (and automatically adjusts to account for unfavorable intramolecualr interactions).

Click on one of the following links to learn more:
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Tasks Performed by Spartan'14 for Windows: con't

	Energy	Equilibrium Geometry	Transition State Geometry	Intrinsic Reaction Coordinate (IRC)
Molecular Mechanics	X	X		
Semi-Empirical	X	X	X	
Hartree-Fock	X	X	X	X
Density Functional	X	X	X	X
MP2, RI-MP2	X	X	X	X
MP3, MP4, LMP2	X			
Advanced Correlated	X			
Thermochemical Recipes	X			
Excited States	X	X	X	X

	IR Spectra	NMR Spectra	UV/vis Spectra	Conformation	Energy Profile
Molecular Mechanics	X			X	X
Semi-Empirical	X			X	X
Hartree-Fock	X	X	X	X	X
Density Functional	X	X	X	X	X
MP2, RI-MP2	X			X	X
MP3, MP4, LMP2					
Advanced Correlated	X				
Thermochemical Recipes					
Excited States	X			X	X