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Q-Chem Partners with Xperiential Scientific for Distribution in Australia and New Zealand.

Q-Chem, Inc. based in Pleasanton California, USA, brings commercial, academic and government scientists worldwide in pharmaceuticals, materials science, biochemistry and other fields a comprehensive ab initio quantum chemistry program to solve computational problems faster, more accurately and less expensively than they could otherwise. Q-Chem also provides users with the highest level of technical support possible. The company was established in 1993.

Thousands of Q-Chem copies are being used around the world. About 55,000 licensed copies of Q-Chem have been sold up to date through Spartan alone. The citations of the two Q-Chem papers reached 300 per year in 2014, and is growing (as reported by ISI Web of Science).

Harry Traikos, Director of Xperiential Scientific is excited to represent and support the Q-Chem software in Australia and New Zealand.

Q-Chem is a comprehensive ab initio quantum chemistry package for accurate predictions of molecular structures, reactivities, and vibrational, electronic and NMR spectra. The new release of Q-Chem 4 represents the state-of-the-art of methodology from the highest performance DFT/HF calculations to high level post-HF correlation methods:

- Fully integrated graphic interface including molecular builder, input generator, contextual help and visualization toolkit (See amazing image below generated with IQmol; multiple copies available free of charge);
- Dispersion-corrected and double hybrid DFT functionals;
- Faster algorithms for DFT, HF, and coupled-cluster calculations;
- Structures and vibrations of excited states with TD-DFT;
- Methods for mapping complicated potential energy surfaces;
- Efficient valence space models for strong correlation;
- More choices for excited states, solvation, and charge-transfer;
- Effective Fragment Potential and QM/MM for large systems;
- For a complete list of new features, contact Xperiential Scientific.

Regards

Regards

MarySue
Business Marketing Manager
Q-Chem



Harry Traikos, BSc
Director
Xperiential Scientific

