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Computational Chemistry in Nuclear Magnetic Resonance

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Message from the Guest Editor

Dear Colleague,

Accurate quantum chemical modeling of NMR spectra is deeply involved in the NMR structural assignment of compounds that are currently of utmost importance in both organic and inorganic chemistry. The development of new effective approaches and computational tools capable of providing very accurate NMR chemical shifts and spin–spin coupling constants is at the cutting edge of modern computational NMR spectroscopy. Since the first application of perturbation theory to NMR properties by Ramsey over 70 years ago, computational methodology has taken a great strides due to both the accelerated progress of computer techniques and the development of electronic theory.

This Special Issue entitled *Computational Chemistry in Nuclear Magnetic Resonance* will provide researchers with the opportunity to publish their most recent discoveries in the field of high-quality computational methodologies relating to NMR spectral parameters.

Dr. Irina L. Rusakova
Guest Editor