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Volume 6 of the successful series 'Reviews in Computational Chemistry' contains articles of interest to pharmaceutical chemists, biological chemists, chemical engineers, inorganic and organometallic chemists, synthetic organic chemists, polymer chemists, and theoretical chemists. The series is designed to help the chemistry community keep current with the many new developments in computational techniques. The writing style is refreshingly pedagogical and non-mathematical, allowing students and researchers access to computational methods outside their immediate area of expertise.