At TCG we develop theoretical models and computational simulations of molecular properties and reactivity. We address a wide range of physical chemistry topics, from magnetic and optical spectroscopies to the design of functional molecular structures using molecular dynamics, quantum-statistical and stochastic thermodynamics methods. We investigate also novel approaches, like machine learning techniques and quantum technologies, for theoretical and computational chemistry. Current research subjects are:

- coarse-grained description of biomolecules and supramolecular systems
- deterministic and stochastic kinetics in chemical reaction networks
- computer-guided rational design of bio inspired molecules and catalysts for applications to health and sustainability
- design of quantum nanodevices for molecular logic
- models of quantum dynamics and spectroscopic response

3. Stochastic modelling of C-13 NMR spin relaxation experiments in oligosaccharides. Molecules 2021, 26, 2418