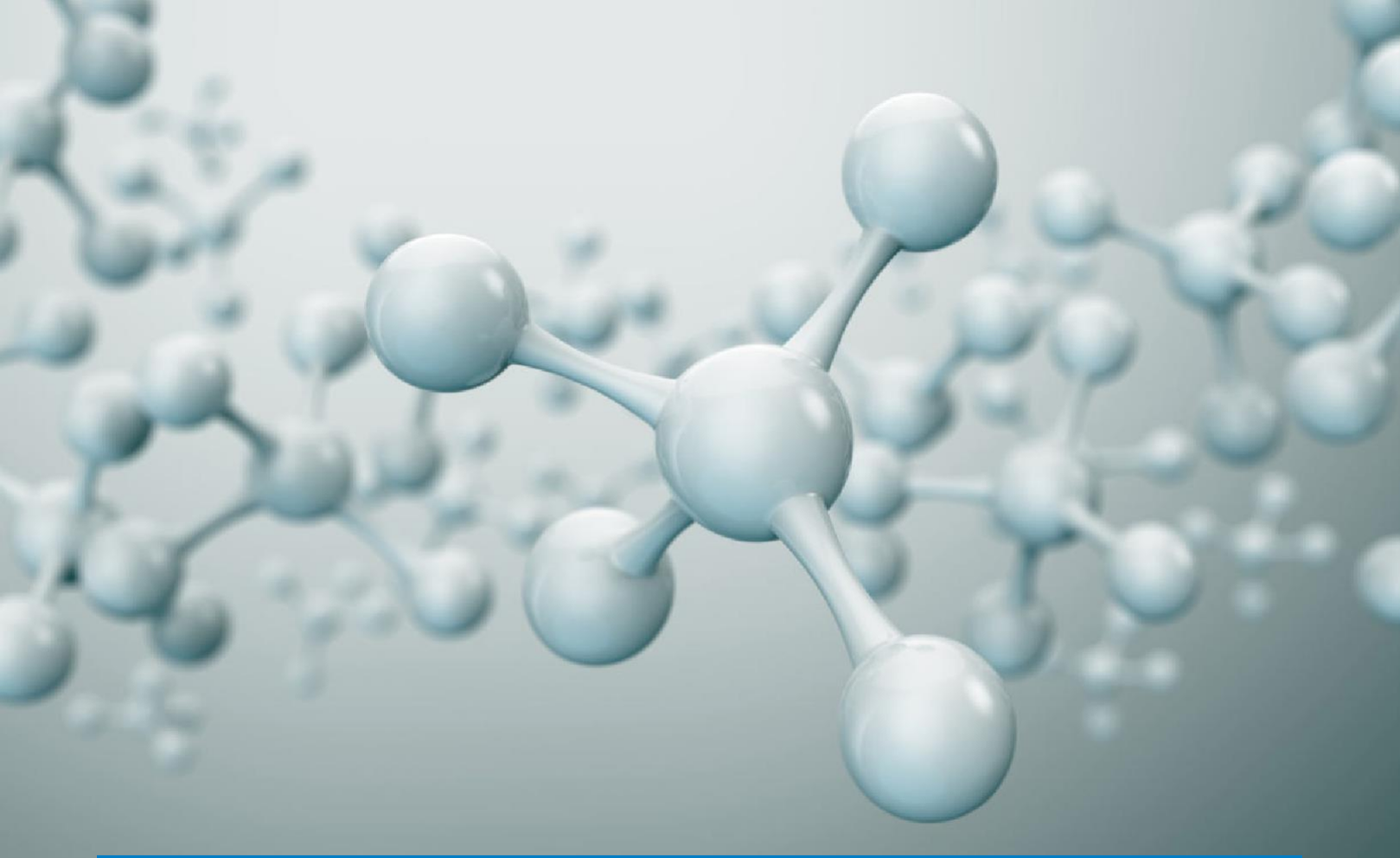

MOLECULAR DESIGN FOR ACHIEVING SPECTRAL PROPERTIES

Characterisation of chemical systems can be achieved using spectroscopies. In cases when the spectroscopic properties of a chemical species cannot be measured for technical reasons its spectral properties can be calculated and predicted. Due to the robustness of quantum chemical calculations, the calculated spectrum is suitable for structural identification and for predicting the spectral properties of molecules.

COMPETENCIES

Identifying predictable spectra properties:

- Gas-phase microwave spectra
- IR-, Raman-, UV/Vis-, VCD -spectra

SERVICES

- High-precision prediction of thermodynamic parameters of multicomponent systems
- Identifying principles of possible measurements

TOOLS

- Gaussian software packages
- AMS software packages
- Dalton software packages
- ORCA software

REFERENCES

- Femtonics Kft. – Theoretical design of highly efficient two-photon caging of neurotransmitter for neurobiological application
- BorsodChem Zrt. – Exploring main and by- product formation reaction pathways for MDI and TDI products. Characterisation of online measurable spectral properties for the important intermediates, main and by-products.

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