The degree of molecular quantum similarity (MQS) between different quantum objects can be expressed in different ways, depending on the operator used in the MQS equation. The most intuitive one is based on the integrated overlap between the electron densities of both quantum objects. The evaluation of the MQS requires the quantum objects to be placed in the same coordinate system; in other words the molecules must be aligned in some way. Up to now this was mostly done via topogeometrical methods. It will, however, be shown that molecular alignments based on maximization of the QSM offer important advantages.

References
