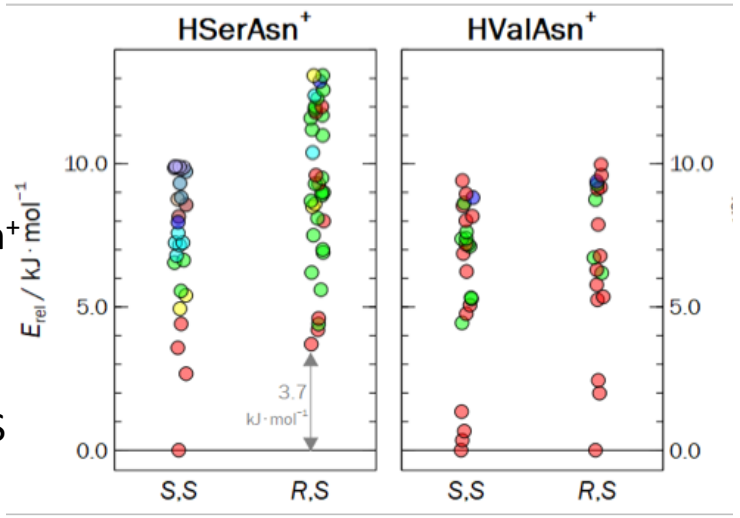
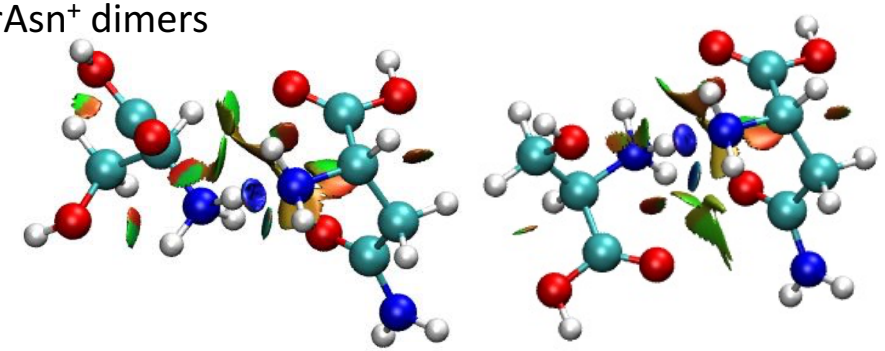
P5389. EXPLORING CONFORMATIONAL SPACES AND AGGREGATION PREFERENCES OF SERINE-ASPARAGINE AND VALINE-ASPARAGINE DIMERS BY IRMPD SPECTROSCOPY AND QUANTUM CHEMISTRY

Haolu Wang, Matthias Heger, Mohamad Al-Jabiri, Yunjie Xu, *Department of Chemistry, University of Alberta*

- conformational space was searched theoretically using a three-tiered computational approach
- 4 types of conformation are classified for SS and RS $HSerAsn^+$ and $HValAsn^+$ based on their binding topologies
- 4.4 kJ/mol energy gap observed only between the SS and RS $HSerAsn^+$ dimers
- strong chirality recognition was observed for $HSerAsn^+$ dimers





SS-$HSerAsn^+$ RS-$HSerAsn^+$