

## 7 Concluding Remarks

The aim of the presented thesis was to investigate the interactions of aromatic groups and their role in the processes of chemical and biological recognition. In particular, the role of aromatic residues in the protein hydrophobic core for the stability of the protein native fold was investigated using high-level quantum chemical calculations. We showed that the interactions of aromatic residues not only with other aromatic and aliphatic sidechains but also with the peptide

bond portion of the protein backbone can provide a substantial contribution to the protein stabilisation. Two more specific examples of the aromatic interactions, the interaction of aromatic residue with proline and the aromatic-peptide bond interaction were both examined in more detail.

The chapter on the IEM focused on aromatic interactions from the perspective of all the pairwise residue interactions in protein. The aromatic residues were shown to play a key role in the stabilisation of the Trp-cage model protein. It was also shown that the IEM can be used as a reliable method for the identification of these key residues. Several computational methods were tested and it was shown that when used with the Amber parm94 force field and GB solvent model, the IEM gives satisfactory results while being computationally feasible for even large proteins. This makes several possible applications of this method useful tools for the analysis of the protein structure.

In the last chapter, the aromatic interactions were dealt with in two examples of reactions catalysed by aromatic organic catalysts. It was shown that the interactions between the catalyst and the aromatic portion of the substrate play a significant role in the TS of these reactions. Moreover, in the Quinox-catalysed reaction, the differences in the Gibbs free energy between the two TS structures were calculated which lead to the two different enantiomers. Our theoretical predictions are in very good agreement with the experimental results.

The six original research papers <sup>[1-6]</sup> that complement the thesis are enclosed in the Appendix.