Conclusion

Concluding Remarks

Within this work, new approaches towards the introduction of flexibility into macrocycles starting from cyclodextrins have been demonstrated: the synthesis and structural evaluation of non-glucose cyclooligosaccharides such as the cycloaltrins, mono-*altro*-cyclodextrins, cyclofructins, cyclogalactofuranosides, and notably the crown acetals. The properties of these compounds have been evaluated in detail and the effects of the increased flexibility on the formation of inclusion complexes have been studied. Multiple examples of macrocycles displaying the phenomenon of pseudorotation were evaluated, clearly demonstrating that lowering the symmetry results in favorable conformations of molecular hosts, that are accessible for inclusion complexation. In contrast to the rather rigid cyclodextrins and their static *lock-and-key*-type host-guest chemistry, the flexible hosts have unequivocally been shown to display a vivid, dynamic *induced-fit*-type formation of inclusion complexes.

The studies on flexible host-guest systems are complemented by approaches towards artificially rigidified hosts such as the intra- and intermolecularly bridged cyclodextrins.

Additional molecular modelling studies were directed towards the evaluation of the chemical and biological properties of some saccharides, amply demonstrating reasons for the atropdiastereoselectivity found in ellagitannins, as well as providing explanations for the enzyme substrate specificity observed in bacterial strains of *Klebsiella pneumoniae* and *Fusobacterium mortiferum*.

The experimental studies were supported by multiple molecular modelling investigations, which required the development of tools for the automated analysis and visualization of the data. With *MolArch*$^{+}$, a software solution has been created that not only supplements many existing tools used in computational chemistry, but also provides access to graphics in unsurpassed quality and resolution. In this work, the usefulness of high-quality visualizations have been demonstrated for scientific and educational purposes.

The combination of experimental and computational studies presented in this work provides a series of principally new insights in the wide field of carbohydrate chemistry.