SCIENCESPRINGDAY

FACULDADE DE CIÊNCIAS E TECNOLOGIA
UNIVERSIDADE NOVA DE LISBOA

Chemistry Department

Modelling and Molecular Interactions

Molecular Structure & Interactions NMR group

MSI NMR group

PTNMR

requimte
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2010 – Post-Doc in Molecular Modelling (Universidade Aveiro

2009 – PhD in Organic Chemistry (FCUL and Université Pierre et Marie Curie – Paris VI)

2003 – Graduation in Chemsitry (FCUL)

Objectives

- Separation of gas mixtures, particularly CO_2 from other gases, remains a major challenge due to its implication on global warming. Seeking a more energy-efficient method for CO_2 sequestration, we are committed to understand at atomistic level the interactions occurring between the CO_2 and Ionic liquids (ILs), which have been suggested as possible materials for CO_2 capture, due to their high capacities and selectivities for CO_2 compared to other gases.
- Non-catalytic cellulosomal CBMs (carbohydrate-binding modules) are responsible for increasing the catalytic efficiency of cellulosic enzymes by selectively putting the substrate and enzyme into close contact. Molecular docking and dynamics simulations were used to obtain structural models of cellotetraose and cellohexaose bound to CtCBM11

Methodology

The molecular interaction studies were performed by means of Molecular Mechanics (MM), Molecular Dynamics (MD) and Docking. The Liu *et al* force field (LWH-FF) was used to parameterize the ILs. The RESP atomic charges were derived from the electrostatic potential obtained at the HF/6-31G(d) level using Gaussian09. The initial configuration was obtained by randomly placed the molecular entities in a cubic box using PACKMOL. The MD simulations were performed using AMBER 12 package. Each system was equilibrated under periodic boundary conditions. Then NPT data production runs were carried out for 30 ns. The molecular diagrams were drawn with PyMOL.
The Haddock software was used to dock the carbohydrate motifs to CtCBM11. Further MD simulation studies were carried out using the ff99SB and GLYCAM06 force fields to parameterized both protein and carbohydrates, respectively.

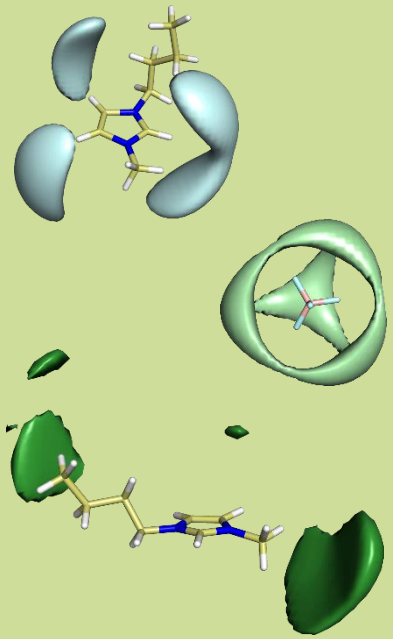

Figure 1: Spatial distribution functions of BF_4^- around $BMIM^+$ (top), $BMIM^+$ around BF_4^- (center) and CO_2 around $BMIM^+$

Expected Results

- Study the influence of the anions on the strength of hydrogen bonding and the orientation relative to the cations within the framework (Figure 1).
- Correlate how the size of the anion influence the preferred positions around the cation.
- Demonstrate the role of both cation and anion on CO_2 solubility and which one control the interaction (Figure 1).
- Study how the polar contacts, CH-π and Van der Waals interactions are important for the stability of the *Ct*CBM11 – Ligand complexes and to the specificity of the protein (Figure 2).
- Rationalization of the mechanism by which *Ct*CBM11 is able to distinguish and select its ligands

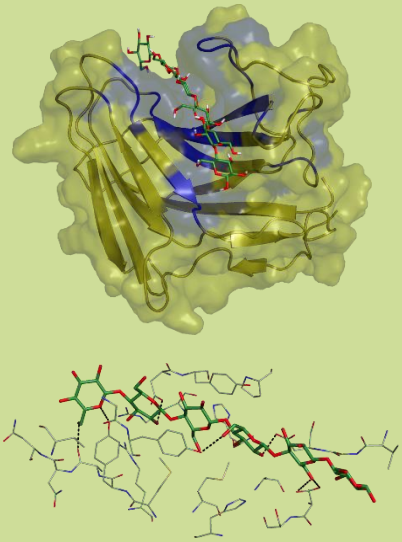

Figure 2: Molecular Dynamics models of *Ct*CBM11 with cellohexaose at 25 ºC

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