SCIENCESPRINGDAY

FACULDADE DE CIÊNCIAS E TECNOLOGIA
UNIVERSIDADE NOVA DE LISBOA

Chemistry Department

Chemoinformatics

REQUIMTE and Centro de Química Fina e Biotecnologia Unit / Organic Chemistry group

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Team member

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Objectives

The research developed during 2008-2013 period focused mainly on:

(1) Software solutions for the processing of chemical data by blind and visually impaired (BVI) users;

(2) 1D ^{13}C NMR data as molecular descriptors in spectra–structure relationship analysis of carbohydrates;

(3) Estimation of Mayr electrophilicity and nucleophilicity with a Quantitative Structure−Property Relationship (QSPR) approach using empirical and density functional theory (DFT) descriptors.

Methodology

(1) Computer interfaces for BVI users enable the proficient manipulation of non-graphical applications and data. A significant obstacle to the access of BVI students to chemical courses is the requirement of processing graphic information. Chemoinformatics can greatly assist in this task since computers can store chemical structures not only as drawings but rather as graphs.

(2) The application of pattern recognition techniques to NMR data can greatly assist in the structure elucidation of specific classes of compounds. NMR data can be seen as fingerprints of 3D chemical structures.

(3) The Mayr's database of Reactivity Parameters contains a compilation of the published reactivity parameters. Computer-assisted predictions of reactivity are desirable, particularly those based on fast algorithms, for the development of new products by chemical and pharmaceutical industries.

Figure 1

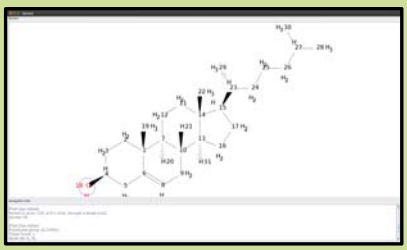

Figure 2

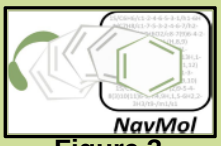

Figure 3

Expected Results

(1) We have developed strategies to teach chemistry to BVI people, which can be found in the web portal MOLinsight at www.molinsight.net. (Figure 1). A second generation of the *NavMol* program was released specially designed to enable BVI users the navigation, editing and saving of molecular structures (Figure 2 and 3). The conversion of cartographic IR data into non-speech audio sounds, a strategy for the identification of functional groups in a molecule using sonified infrared spectra (SIRS), and teaching activities for the interpretation of SIRS by BIV students were developed (Figure 4). (2) The structural elucidation of pyranosyl disaccharides and linear/branched trisaccharides was successfully accomplished using Random Forests from the ^{13}C NMR chemical shifts (Figure 5). (3) The combination of empirical and DFT reactivity descriptors enabled to build QSPR models to estimate Mayr electrophilicty and nucleophilicity parameters with high accuracies for an independent test set (Figure 6).

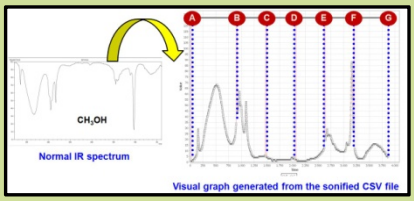

Figure 4

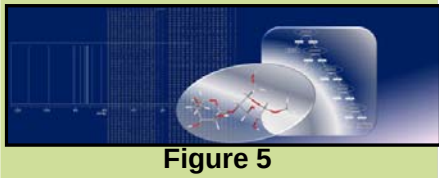

Figure 5

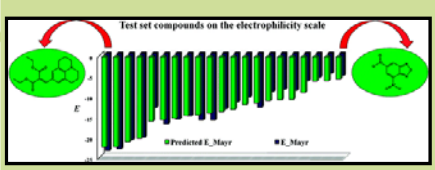

Figure 6

Funding: CHEM4ALL – ICT tools for teaching chemistry to blinds and visually impaired students.

FCT Fundação para a Ciência e a Tecnologia
MINISTÉRIO DA EDUCAÇÃO E CIÊNCIA

ICT as Gateway to Scientific Education of Blind and People with Visual Disabilities

Education and Culture
Lifelong learning programme
LEONARDO DA VINCI