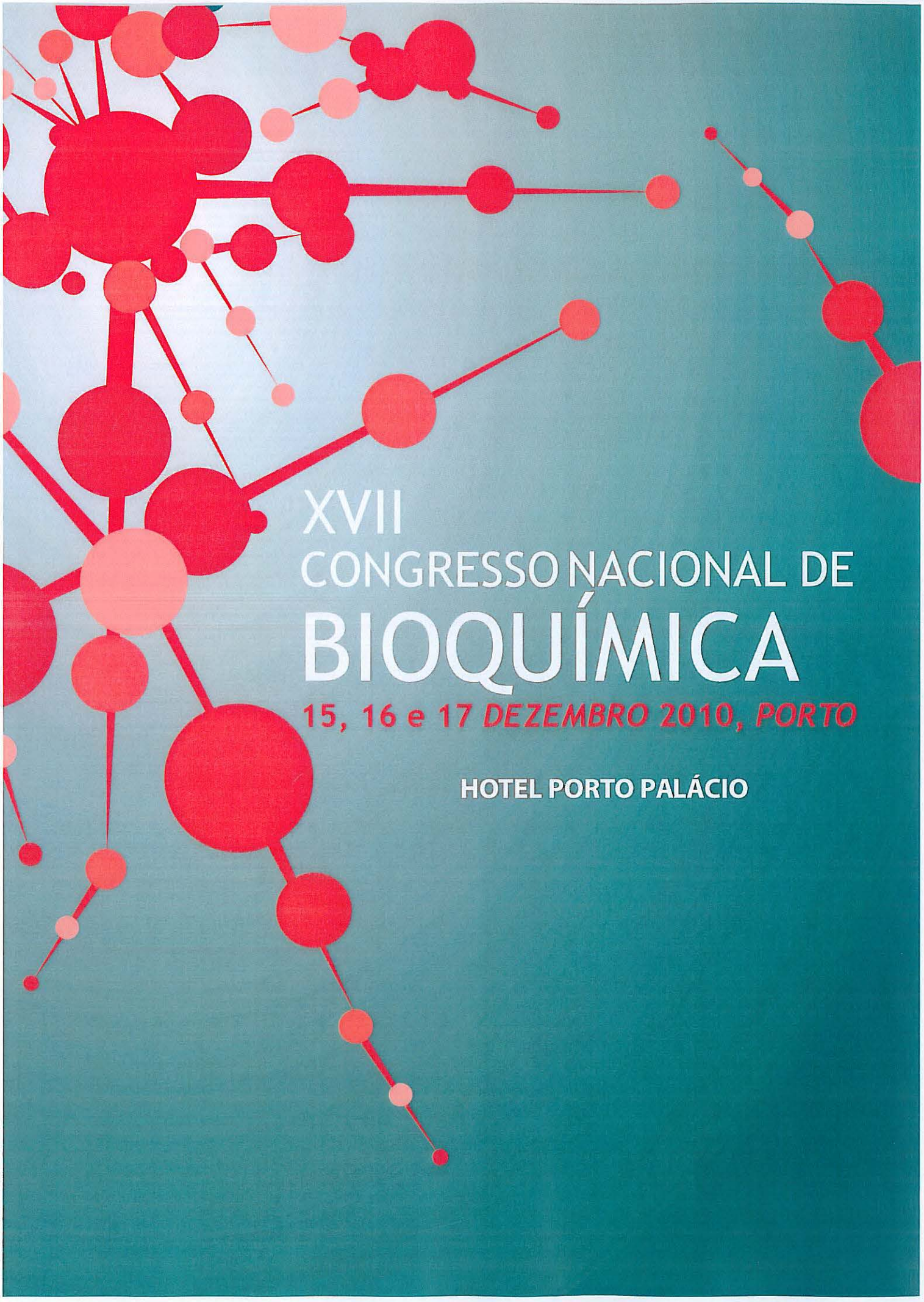
XVII
CONGRESSO NACIONAL DE
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HOTEL PORTO PALÁCIO

Symposium D: Computational Biochemistry

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P D2 Multifractal structure in the heart rate of preeclamptic pregnant women
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P D4 Glycine conjugated bile acid side-chain analogs: molecular modeling of Na+- capturing fluorescent derivatives
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P D11 PrimerIdent 2.0: An improved tool for specific conserved primer design
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P D13 On the mechanism of nitrite reduction by xanthine oxidase family enzymes
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P D14 Evolution and state of art in imaging techniques and representations of the erythrocyte
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P D15 ChemT, a software for building template-based 3D chemical libraries
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ChemT, a software for building template-based 3D chemical libraries

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Abstract

In the modern drug discovery process vast quantities of compounds are generated and there is a need for bioinformatic tools to efficiently create, manage and examine huge chemical compound libraries. Several software tools for drawing and generating chemical compounds structures are available, but they usually lack options for automatic generation of custom-made focused chemical libraries. We have implemented ChemT (Chemical Templates), a free software tool that automates the process of preparing template-based three-dimensional chemical libraries. ChemT accepts several file formats and is able to select compounds by imposing limits according to different physicochemical properties or by applying a Lipinski Rule of Fives filter. The compounds on the library are subject to force field minimization and the resulting three-dimensional structures can be recorded on several file formats more frequently used in Virtual Screening projects. ChemT was developed using C-sharp language and compiled for Windows using SharpDevelop3.5. For file format conversions, properties calculation and compound energy minimization ChemT uses the OpenBabel OBDotNet library. For compound energy minimization ChemT uses the Universal Force Field available with OpenBabel. As supporters of free open-source software ChemT is freely available on his website (www.esa.ipb.pt/~ruiabreu/chemt). ChemT is a fast easy-to-use software that automatically generates three-dimensional chemical libraries by inputting a chemical template and functional groups of interest. A fairly self-explanatory Graphical User Interface is provided and several tools for compound filtering are included. ChemT can be a valuable tool for chemists interested in using virtual screening tools in order to prioritize compounds for further chemical synthesis.

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