DEVELOPMENT OF AN ELECTRONIC LABORATORY NOTEBOOK FOR STRUCTURE-BASED DRUG DESIGN.

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Dissection of the 3D-structure of macromolecular targets for the design and synthesis of new drugs with high specificity comprises a series of multi-disciplinary approaches *in vitro*, *in silico* and *in vivo*. Recording and maintaining an up-to-date file with the data derived from the methods applied is of great importance, especially after the advanced instrumentation used nowadays and the vast amount of data generated [1]. Our work focuses on the development of a database and a software tool that follows the individual steps of a structure-based drug design approach for the recording, storage and evaluation of the data produced at each stage. More specifically, the user can store data for compounds to be tested as potential drugs, kinetic and crystallographic experiments, as well as results from toxicological, physiological and clinical studies and background information about drugs already launched in the market. The application is web-based, user friendly and implemented in PHP, HTML and SQL, providing a full user management system. Searching with multiple filters, sorting, exporting and saving results, allow the user to handle efficiently the available records (Figure 1). In addition there exist advanced menu options for editing or deleting data and recording experiments explicitly. The tool includes utilities for routine calculations, on-line help and supports connecting to related online databases for data mining.

All compounds

Sort by: Compound code Sort Export to Excel

#	Compound code	Compound name/description	Sender	Date of arrival	Chemical structure	Chemical type	Molecular weight (g/mol)	Total mass (mg)	Notes	Postition
55	0Beva271	oxadiazole	Sender 2	2009-06-08	chem_structures/Beva271.cdx	C13H14N3O6	309.28	8.5		A
53	0cca59.9	β-D glucopyranosyl guanine	Sender 1	2009-09-15	chem_structures/0cca59.9.cdx	C11H15N5O6	313.27	11		A
54	0KB144	glucopyranosyl urea	Sender 2	2009-06-08	chem_structures/KB144.cdx	C17H16N2O9	394.34	7.8		C

Figure 1. Preview of results for compounds filed in the database

[1] C. Stephan et al. Proteomics 2010, 10, 1230-1249