THEORETICAL STUDY OF LOW-MOLECULAR-WEIGHT SULPHUR CONTAINING BIOMOLECULES

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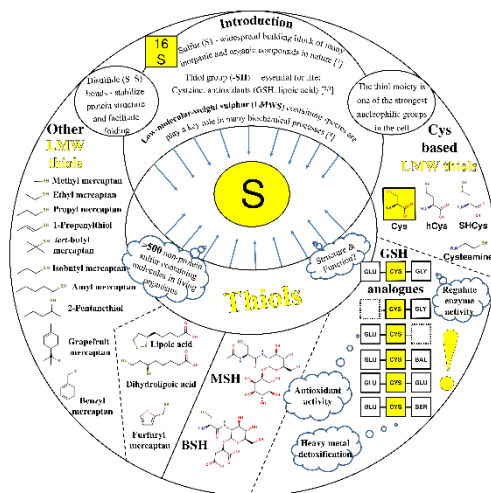
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Abstract

Low-molecular-weight Sulphur (LMWS) containing species play a key role in many biochemical processes and can be found in a wide variety of organisms including prokaryotes, plants and, mammals. These special molecules protect living organisms against free radicals and participate in signal transduction, and the regulation of gene expression. The main purpose of this study is to create a small molecular library with >100 entries and organize the available information in a smart way (**Figure 1**).

Figure 1. Schematic representation of the draft of the poster with the different low-molecular-weight Sulphur (LMWS) containing compounds and their subgroups.

This will serve as the core of our future database and it will contain the most important structural and functional properties of LMWS containing molecules. For a selected set of species, a detailed comparison will be presented based on the calculated properties of the molecules. All in all, the database could serve as a starting point for the design of new LMWS containing compounds.

Keywords: Thiols; Database; Molecular Modelling; Molecular Library.