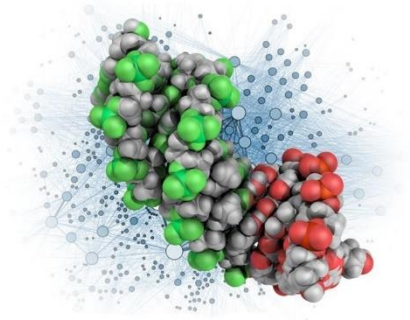

EJIBCE 2017
Encontro de Jovens Investigadores de Biologia Computacional Estrutural
Departamento de Física, Universidade de Coimbra, 22 de Dezembro

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Using the Mechanism and Catalytic Site Atlas (M-CSA) to understand enzyme function and evolution

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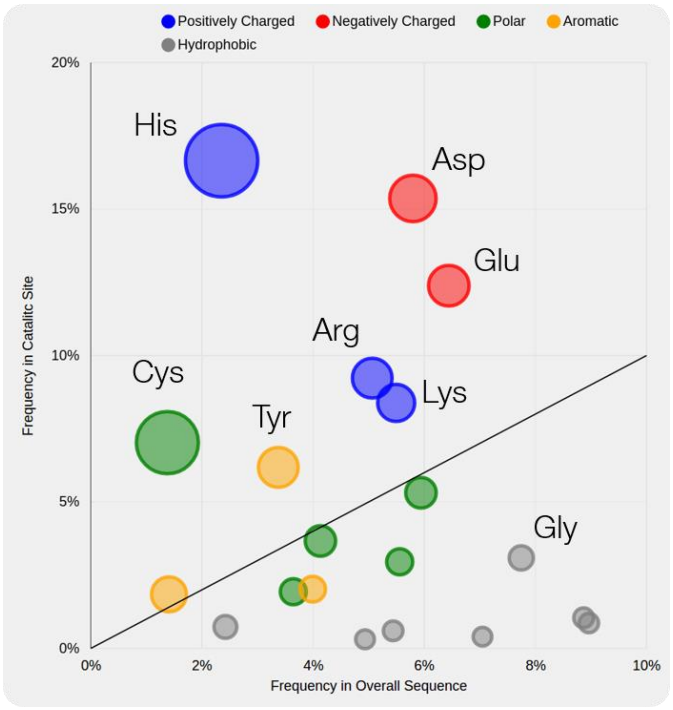

M-CSA (Mechanism and Catalytic Site Atlas) is a database of enzyme mechanisms that can be accessed at www.ebi.ac.uk/thornton-srv/m-csa. Our objectives with M-CSA are to provide an open data resource for the community to browse known enzyme reaction mechanisms and catalytic sites, and to use the dataset to understand enzyme function and evolution. Practical applications that could benefit from this data include the design of new enzymes and inhibitors. M-CSA annotation includes the curly arrow description of the stepwise chemistry, the role of each catalytic residue and any cofactors, and the primary literature that supports such data. We also provide annotation for the associated protein sequences, structures, and their homologues.

M-CSA results from the merging of two previous databases, MACiE (Mechanism, Annotation and Classification in Enzymes), a database of enzyme mechanisms, and CSA (Catalytic Site Atlas), a

	database of catalytic sites of enzymes. In comparison with the parent databases, M-CSA supports the inclusion of several mechanism proposals, better tools for curators, and the creation and edition of new entries through the website. For people consulting the website, we improved the search and browsing tools, as well as the presentation of database statistics. In addition to the changes in the database and website, we are also carrying out a complete revision of existing data. At the moment, M-CSA contains 961 entries, 423 of these with detailed mechanism information, and 538 with information on the catalytic site residues only. In total, these cover 81% (195/241) of third level EC numbers with a PDB structure, and 30% (840/2793) of fourth level EC numbers with a PDB structure, out of 6028 in total.

References

Ribeiro, António J. M., Gemma L. Holliday, Nicholas Furnham, Jonathan D. Tyzack, Katherine Ferris, and Janet M. Thornton. “Mechanism and Catalytic Site Atlas (M-CSA): A Database of Enzyme Reaction Mechanisms and Active Sites.” Nucleic Acids Research. Accessed December 14, 2017. https://doi.org/10.1093/nar/gkx1012.