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CHOPIN, MABELLINI and HANSEN: Enabling combatting emerging antibiotic resistance in mycobacteria through multi-dimensional structural proteome data resources

Marcin J Skwark
University of Cambridge, UK

Here we propose a set of computational resources to inform experiments and facilitate drug discovery against *Mycobacterium* spp. Mycobacteria are etiological agents of some of the most notorious hazards to public health-tuberculosis *(M. tuberculosis)* and leprosy *(M. leprae)*. They are also responsible for opportunistic infections in Cystic Fibrosis (CF) patients (*M. abscessus*). Finally, they are conjectured to be the underlying cause of ulcerative colitis and Crohn's disease *(M. avium* subsp. *paratuberculosis)*. Despite their importance for public health, there are very few successful treatment strategies against Mycobacteria, due to their intrinsic resistance to antimicrobials, as well as inherent experimental difficulties in testing drug candidates *in vitro*. Our resources (CHOPIN: *M. tuberculosis*, MABELLINI: *M. abscessus*, HANSEN: *M. leprae*) provide comprehensive set of high-confidence structural models for the entire bacterial proteome. Models are generated using Vivace pipeline, using Fugue for template identification and Modeller for model building-both developed in-house. On contrary to typical protein structure prediction approaches (e.g. I-TASSER or HHpred), our approach aims to produce models that inform experiments and not necessarily maximize the stereo chemical quality and superposition to crystal structure. As our models are not over-optimized, they can be readily used for analysis of drug ability, effects of mutations and assessing interactions. By combining the results of state-of-art methods developed locally, with comprehensive survey of local and publicly available experimental results, CHOPIN, MABELLINI and HANSEN form resources of unprecedented utility-delivering results of rigorous computational analysis in a user-friendly, approachable and understandable way. The resources are free to use, constantly updated and produced in close collaboration with mycobacterial research community. All the software developed and used is open source and all the data is open access.

Biography

Marcin J Skwark has completed his PhD in Biochemistry from Stockholm University. He is currently working as a Research Associate in the Department of Chemistry at University of Cambridge, UK.

mjs294@cam.ac.uk

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