# Checkmymetal 2.0: A Macromolecular Metal-Binding Validation And Modeling Tool

**Michal Gucwa[1], Joanna Lenkiewicz[2], Heping Zheng[3], Marcin Cymborowski[4], David Cooper[5], Krzysztof Murzyn[6], Wladek Minor[7]**

*[1]University of Virginia [2]University of Virginia, [3]Hunan University College of Biology, Bioinformatics Center, Hunan 410082, People's Republic of China, [4]University of Virginia, [5]University of Virginia, Department of Computational Biophysics and Bioinformatics, [7]Jagiellonian University, Kraków, Poland, University of Virginia*

*michal_g@iwonka.med.virginia.edu*

CheckMyMetal is a server used to validate the metal binding sites of macromolecular structures. An easy-to-use interface allows the evaluation of structures in the PDB or uploaded by the user. The new version incorporates electron density maps, which expands the number of parameters used for validation. The structure and maps are now displayed using the NGL viewer and provide a more informative and intuitive experience. One of the most important new features is the ability to conduct a fast refinement of the vicinity around alternate metal candidates. CheckMyMetal guides the metal selection process in two ways. First, it evaluates the substitution of several metals in the current environment, re-scores the binding sites, and displays a ranked list of candidate metals. Second, the researcher is alerted to potential metals from the crystallization conditions when they are available. The refined metal binding site containing the newly selected metals can be downloaded. CheckMyMetal is available at cmm.minorlab.org.