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Generating predicted models with CCP4

We discuss recent work on making use of deep-learning-based protein structure prediction programs with the CCP4 Software Suite. These programs include AlphaFold2 [1] and OpenFold [2], which use multiple-sequence alignments as input, and ESM-Fold [3], which uses embeddings from protein Language Models. We have developed an adapter script that allows running these programs via a unified interface. The script is distributed with CCP4 and has been integrated in the structure-prediction task of CCP4 Cloud, a front-end of the Suite. We have installed a local mirror of the AFDB database that is used in CCP4 Cloud to find and prepare molecular-replacement models with MrParse [4]. We discuss these developments and related work.
[1] Jumper, John, et al. *Nature* 596, no. 7873 (26 August 2021): 583–89.
[2] Ahdritz, Gustaf, et al. Preprint. Bioinformatics, 22 November 2022.
[3] Lin, Zeming, et al. Preprint. Synthetic Biology, 21 July 2022.
[4] https://mrparse.readthedocs.io/

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