**MSMS algorithms for building protein surfaces**

The area of computational biology has been growing exponentially for the last decade or maybe even more. Proteins are one of a few key classes of molecules crucial for any live organism, so studying them can be quite rewarding. The surface of a protein is especially critical for understanding its behaviour since it is what mostly interacts with the outer world and thus defines a protein’s functions. Moving closely to Mathematica, the bio-direction is a priority now as I understand it. It’s especially true because of the ongoing pandemic. I found that although Mathematica has a “Protein” entity, it lacks such an important property as the surface of a protein. Nowadays surfaces of proteins are used [1-3] for studying protein-protein, protein-ligand and other interactions via advanced optimization techniques, particularly NNs. So I thought I could implement the first step on the way of bringing sophisticated protein analysis to Mathematica - implement a function for building a mesh of a 3d protein structure given the atoms of the protein. There is an article [4] with a thorough description of algorithms to build such a mesh and also to build different types of more physical types of surfaces given the mesh. So the idea is to implement the algorithm to the WL.

[1] Gainza, P., Sverrisson, F., Monti, F. *et al.* Deciphering interaction fingerprints from protein molecular surfaces using geometric deep learning. *Nat Methods* 17, 184–192 (2020).

doi.org/10.1038/s41592-019-0666-6

[2] Yoichi Murakami, Kenji Mizuguchi, Applying the Naïve Bayes classifier with kernel density estimation to the prediction of protein–protein interaction sites, *Bioinformatics*, Volume 26, Issue 15, 1 August 2010, Pages 1841–1848,

[doi.org/10.1093/bioinformatics/btq302](https://doi.org/10.1093/bioinformatics/btq302)

[3] Porollo A, Meller J. Prediction-based fingerprints of protein-protein interactions. *Proteins*. 2007;66(3):630-645.

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[4] Sanner MF, Olson AJ, Spehner JC. Reduced surface: an efficient way to compute molecular surfaces. *Biopolymers*. 1996;38(3):305-320. doi:10.1002/(SICI)1097-0282(199603)38:3%3C305::AID-BIP4%3E3.0.CO;2-Y