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A Protein's Estimated Net Charge/kDa can be used as a Predictor of the Solution pH for Crystallization. D.S. Dougall¹, V. Gopalakrishnan¹, D. Hennessy², J.M. Rosenberg², ¹Center for Biomedical Informatics, School of Medicine; ²Dept. of Biological Sciences, Univ. of Pittsburgh, Pittsburgh, PA 15260.

It has long been hypothesized that there should be a correlation between the pH at which a protein crystallizes and its isoelectric point (pI). However, this hypothesis has not been supported by the literature. The most widely reported experimental variable in the PDB is the solution pH. This availability of a large amount of data led us to reinvestigate the link between the pI and experimental pH used for crystallization. Similar to other studies, we found no correlation between pI and the reported solution pH. However, since the pI is the pH where the net charge is zero, we examined whether the estimated net charge of the protein could be used as a predictor of pH conditions leading to successful crystallization.

Using a non-redundant PDB dataset (n=4,114), we demonstrate a relationship between a protein's estimated net charge/kDa and the solution pH. Here we show that proteins are usually crystallized at a pH that results in a low estimated net charge/kDa, usually in the range of -0.68 to +0.68 e/kDa. These findings have a reasonable explanation based on physical chemistry and can be exploited for initial crystallization attempts.