The PDB Format in the 21st Century, a Modest Proposal

Herbert J. Bernstein^a, Frances C. Bernstein^b, ^aMathematics and Computer Science Department, Dowling College, Oakdale, NY 11769, USA. ^bBernstein+Sons, Bellport, NY 11713, USA. E-mail: yaya@bernstein-plus-sons.com

The Protein Data Bank format created in the 1970's is the major user-level interchange format for macromolecular structures but is sorely pressed by the demands of larger structures and the rich detail of information now available for many structures. Newer mmCIF, XML and other formats effectively address these issues, but leave a gap in terms of software support for existing applications. In this presentation we make a modest proposal to help to close this gap and to simplify the adaptation of existing applications to the management of new structures.

Keywords: PDB format, mmCIF, software