

## This Site I Like

### The Research Collaboratory for Structural Bioinformatics website: proteins and nucleic acids visualisation for the curious

<http://www.rcsb.org>

“We are now in a position to study the tertiary structure of a single myoglobin molecule separated from its neighbours” wrote John Kendrew in his seminal paper in *Nature* in 1958 “A Three-Dimensional Model of the Myoglobin Molecule Obtained by X-ray Analysis”. His research team discovered the structure of the protein and visualised it using a manual model. A few years later, Kendrew and Perutz received the Nobel Prize for this discovery. Ten years later, Richard E. Dickerson developed a model for predicting the number of protein structures described annually. According to Dickerson’s model, the number of soluble proteins would be 12,066 by 2001. It was a great prediction since the actual figure reached 12,123. It was also clear that the number of protein structures would soon become hard, if not impossible, to handle.

At the end of the 1960s, another great achievement was reported, as eloquently presented by Edgar F. Meyer in his review, “The first years of the Protein Data Bank”. Thanks to the development of software and hardware, and particularly with support of the Brookhaven Raster Display (BRAD), Meyer working with programmers and biologists generated the first 3D images of protein structures. Using Meyer’s approach, the lines of codes that represented the coordinates of protein were handled with computers in a way to help the user surf through the data. To advance this approach, the software SEARCH was developed, which employed a dictionary of protein residues, atom names and molecular properties, facilitating automatic data processing. That was the beginning of the Protein Data Bank, which is a database currently containing information on around 90,000 protein structures.

The Research Collaboratory for Structural Bioinformatics Protein Data Bank (RCSB PDB). Since those early years, the Protein Data Bank has become the largest repository for protein and nucleic acid structures. The bank contains

a total of 87,067 items, with 8,969 of them added only in 2012. The initial collection of codes has evolved into a sophisticated website that allows the user to register a new structure, to search through the database using protein code (PDB code), ligand code, or author name. Once a query is typed in, the user is directed to a page with lots of information about the protein structure and function, with the possibility of obtaining and downloading images.

The RCSB PDB website has become very popular, with the PDB page being accessed by around 140,000 unique visitors monthly from 140 different countries. The website users are students, educators, science writers, editors and professionals from diverse backgrounds, particularly biologists, specialists in bioinformatics, computational chemistry and many other allied fields.

Science editors can benefit from the RCSB PDB website by improving their knowledge on biological topics. The visualisation of biomolecules and retrieval of information on their properties can be especially helpful for editors verifying facts and checking images in manuscripts submitted to biomedical and other journals.

Recently, the RCSB website released a free app for iPhone/iPod/iPad. A version for the Android platform is under development. Perhaps the most impressive feature of the app is the molecule viewer, NDKMol, which allows the user to navigate through the 3D representation of the macromolecule. And all this is on a small screen of Smartphone or Tablet! It is a fantastic tool for researchers, editors and other curious users who want to explore the beauty of the world of molecules.

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The screenshot displays the RCSB PDB website interface. At the top, it features the RCSB PDB logo and a navigation bar with tabs for 'Everything', 'Author', 'Macromolecule', 'Sequence', and 'Ligand'. A search bar is present with a search icon and a placeholder text 'e.g., PDB ID, molecule name, author'. Below the search bar, there are several sections: 'Customize This Page' with links to 'Available on the App Store', 'PDB-101', and 'MvPDB'; 'Biological Macromolecular Resource' with a 'Full Description' section and a 'Learn: Featured Molecules' section; and 'RCSB PDB News' with a 'Create High Resolution Images' section. The 'Molecule of the Month' section highlights 'Dermcidin' with a 3D molecular model and a brief description: 'Bacteria are a constant threat, so our bodies have many defenses to protect us from infection. One of our first lines of defense is a collection of small peptides, termed antimicrobial peptides, that are'.