Poster Presentation

LiteMol: web-based 3D visualization of macromolecular structure data

<u>Matthew J Conroy</u>¹, David Sehnal², Mandar Deshpande¹, Radka Svobodova², Saqib Mir¹, Karel Berka³, Adam Midlik², Sameer Velankar¹, Jaroslav Koca²

¹Protein Data Bank In Europe EMBL-EBI, Cambridge, United Kingdom, ²CEITEC - Central European Institute of Technology, Brno, Czech Republic, ³Univerzita Palackeho v Olomouci, Olomouci, Czech Republic

E-mail: conroy@ebi.ac.uk

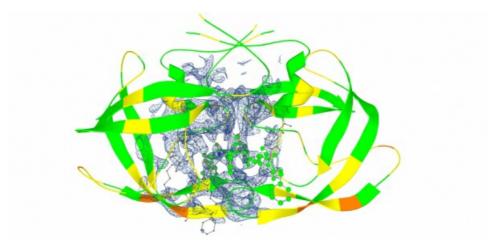
LiteMol is a unique and comprehensive macromolecular structure viewer which through real-time data delivery enables even large macromolecular structures to be visualised in the browser in a platform independent manner. LiteMol is fully integrated into the webpages at the Protein Data Bank in Europe (PDBe.org), a founder member of the wwPDB.

LiteMol is composed of a 3D molecular viewer LiteMol Viewer, data delivery services CoordinateServer and DensityServer, and a data format called BinaryCIF. LiteMol Viewer provides interactive web-browser based visualisation of 3D structures together with maps and annotation of biological context. CoordinateServer and DensityServer enable a dramatic reduction of data transfer size by sending only what is currently relevant to the user instead of whole files. Finally, the BinaryCIF format provides very high compression ratios while retaining compatibility with existing standards used by the wwPDB consortium. As shown by our benchmarks, it is the fastest 3D viewer currently available.

LiteMol is able to display 3D coordinate data in standard representations (cartoons, balls and sticks, etc.) and overlay them with additional annotations (e.g., sequence annotation from Uniprot, annotated assemblies or data quality assessment from wwPDB validation reports) accessed from the PDBe API. Moreover, it readily displays experimental evidence (i.e., electron density maps derived from deposited structure factors for X-ray diffraction data, and electric potential maps for Cryo-EM derived models).

LiteMol and its components are freely available for integration into other online services and, in addition to PDBe, it is currently integrated into Glycopedia and integration to UniProt and Open Targets is in progress.

LiteMol web pages are available at http://ncbr.muni.cz/LiteMol



Keywords: LiteMol, 3D visualisation, PDB