# MOLEonline and ChannelsDB - Tools and Database for Analysis of Biomacromolecular Channels, Tunnels and Pores

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MOLEonline [1] and ChannelsDB database [2] are interactive, web-based tools for detection and analysis of channels, tunnels and pores in biomacromolecular structures. The updated version of MOLEonline offers easier, simple and fully interactive visualization provided by recently developed LiteMol Viewer which overcomes limitations of the previous version. The application provides two basic modes of calculation: i) computation of the tunnels leading to the specified site within the macromolecule and ii) calculation of transmembrane pores which is available as an automatic pore detection mode. MOLEonline application can use both now obsolete PDB and standard PDBx/mmCIF format and enables analysis of the wide range of biomolecular structures. The tool also brings the connection with other bioinformatics resources – PDBe, OPM, UniProt, CSA and recently developed ChannelsDB database. ChannelsDB contains both channels with the literature reference or channels leading to the biologically important sites (cofactors, active sites) within structures deposited in the Protein Data Bank in Europe [3].

Both MOLEonline and ChannelsDB offer unique analytics for the identification and characterization of channels and pores as well as their geometrical and physico-chemical properties. All is provided free of charge online via internet webpages <https://mole.upol.cz> and <http://ncbr.muni.cz/ChannelsDB/>.

1. Pravda L, et al.: MOLEonline: a web-based tool for analyzing channels, tunnels and pores (2018 update). *Nucleic Acids Res*, gky309, 2018. <https://mole.upol.cz/>
2. Pravda L, et al.: ChannelsDB: database of biomacromolecular tunnels and pores. *Nucleic Acids Res*, 46(D1), D399–D405, 2018. <http://ncbr.muni.cz/ChannelsDB/>
3. Velankar, S. et al.: PDBe: improved accessibility of macromolecular structure data from PDB and EMDB. *Nucleic Acids Res*, 44, D385-D395, 2016. <http://www.ebi.ac.uk>/pdbe