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| **No.** | **Servers/Tools name** | **References** | **Purposes** |
| 1**.** | **RCSB PDB**: <https://www.rcsb.org/> | N/A | Identification of target viral protein of lujo virus as revealed 3D structure as PDB format. |
| 2. | **CASTp**: <https://sts.bioe.uic.edu/castp/index.html?1bxw> | **Table: Several Tools/Servers name with their specific purposes with references.[Lujo]**  ***Tian et al., Nucleic Acids Res. 2018*** | The CASTp web server additionally referred to as Computed Atlas of floor Topography of proteins is used to predict the active sites of the selected protein. |
| 3. | **PubChem Databases**: <https://pubchem.ncbi.nlm.nih.gov/> | N/A | Pubchem is freely accessible chemical information search chemicals by name, molecular formula, structure, and other identifiers search chemical and physical properties, biological activities, safety and toxicity information etc. It provides unique Pubchem ID, smiles ID and retrieved control ligands as 2D and 3D in SDF format for target viral protein. |
| 4. | **ChemSpider Databases**: <https://www.chemspider.com/> | N/A | ChemSpider is a free chemical structure database providing fast text and structure search and collect molecules as different format. |
| 5. | **Ambinte**r: <https://www.ambinter.com/> | N/A | Ambinter is for searching of similarity compounds of control ligands. It search and Inquire chemicals by online and screening compounds, natural products, building blocs and custom synthesis |
| 6. | **Open Babel**: <https://openbabel.org/> | N/A | Open Babel is a project to facilitate the interconversion of chemical data from one format to another – including file formats of various types |
| 7. | **Biovia Discovery Studio Visulaizer**: <https://discover.3ds.com/discovery-studio-visualizer-download> | N/A | Discovery studio provides a grade graphics visualization tool for **viewing, sharing, and analyzing protein and modeling data with interactive 3D visualization.** |
| 8. | **PyRx**: <https://pyrx.sourceforge.io/> | N/A | PyRx is a Virtual Screening software for Computational Drug Discovery that can be used to screen libraries of compounds against potential drug targets. PyRx enables Medicinal Chemists to run Virtual Screening from any platform and helps users in every step of this process - from data preparation to job submission and analysis of the results |
| 9. | **Molinspiration** : <https://www.molinspiration.com/cgi-bin/properties> | N/A | Molinspiration has capability to predict bioactivity information and data visualization about specific protein. Molinspiration offers [broad range of cheminformatics software tools](https://www.molinspiration.com/products.html) supporting molecule manipulation and processing, including SMILES and SDfile conversion, normalization of molecules, generation of tautomers, molecule fragmentation etc. |
| 10. | **STRING**: <https://string-db.org/> | N/A | String for Protein-Protein Interaction Networks Functional Enrichment Analysis. |
| 11. | **Swiss PDB viewer**: <https://spdbv.vital-it.ch/index.html> | N/A | Swiss-PdbViewer is an application that provides a user friendly interface allowing to analyze several proteins at the same time. The proteins can be superimposed in order to deduce structural alignments and compare their active sites or any other relevant parts. Amino acid mutations, H-bonds, angles and distances between atoms are easy to obtain thanks to the intuitive graphic and menu interface. |
| 12. | **VENN**: <https://bioinformatics.psb.ugent.be/webtools/Venn/> | N/A | It will generate a textual output indicating which elements are in each intersection or are unique to a certain list. If the number of lists is lower than 7 it will also produce a graphical output in the form of a venn/Euler diagram. The graphical output is produced in SVG and PNG format. |
| 13. | **Swiss ADME**: <https://www.swissadme.ch/> | [***SwissADME: a free web tool to evaluate pharmacokinetics, drug-likeness and medicinal chemistry friendliness of small molecules. Sci. Rep. (2017) 7:42717.***](http://www.nature.com/articles/srep42717)  [***iLOGP: a simple, robust, and efficient description of n-octanol/water partition coefficient for drug design using the GB/SA approach. J. Chem. Inf. Model. (2014) 54(12):3284-3301.***](http://pubs.acs.org/doi/abs/10.1021/ci500467k)  [***A BOILED-Egg to predict gastrointestinal absorption and brain penetration of small molecules. ChemMedChem (2016) 11(11):1117-1121.***](http://onlinelibrary.wiley.com/doi/10.1002/cmdc.201600182/abstract) | This website allows you to compute physicochemical descriptors as well as to predict ADME parameters, pharmacokinetic properties, druglike nature and medicinal chemistry friendliness of one or multiple small molecules to support drug discovery. |
| 14. | **pkCSM**: <https://biosig.unimelb.edu.au/pkcsm/> | ***pkCSM: predicting small-molecule pharmacokinetic properties using graph-based signatures***  [***Douglas E. V. Pires***](http://www.dcc.ufmg.br/~dpires)***,***[***Tom L. Blundell***](http://www.bioc.cam.ac.uk/uto/blundell)***,***[***David B. Ascher***](http://scholar.google.co.uk/citations?user=7KrAVc0AAAAJ&hl=en)  ***Journal of Medicinal Chemistry, 58 (9), p. 4066–4072, 2015.*** | pkCSM is a web server to provide an integrated freely available platform to rapidly screen multiple pharmacokinetic properties. The pkCSM signatures were successfully used across five main different pharmacokinetic properties classes to develop predictive regression and classification models. |
| 15. | **GROMACS**: <https://www.gromacs.org/> | N/A | GROMACS is a versatile package to perform molecular dynamics. It is primarily designed for biochemical molecules like proteins, lipids and nucleic acids that have a lot of complicated bonded interactions, but since GROMACS is extremely fast at calculating the non bonded interactions (that usually dominate simulations) many groups are also using it for research on non-biological systems |
| 16. | **CLC-pred**: <https://digitalinsights.qiagen.com/> | N/A | CLC bio develops widely citeddesktop, enterprise and cloud software for analysis of [biological data](https://en.wikipedia.org/wiki/Biological_data). While offering some [open source algorithms](https://en.wikipedia.org/wiki/Open-source_software) with their tools, CLC bio have their own implementations of several popular applications, which have been accelerated using [SIMD](https://en.wikipedia.org/wiki/SIMD) technology |