Q. What is RASPD+?

RASPD+ is a virtual screening software for identifying lead-like molecules.

Q. From where I can download standalone version?

To download standalone version, click on below link-

https://github.com/HITS-MCM/RASPDplus

Q. Can I screen target protein against my own dataset?

To screen against own dataset, click on "**Customized Dataset Screening**"

Q. What is reference ligand?

Reference ligands are nonstandard residues that bind non-covalently to a macromolecule and are represented in the PDB file as heteroatoms in a 3-letter code.

Q. What is Scaffolds?

Scaffold refers to the part of the ligand. This part can be a functional group, a metal ion, a repeat of an atom, etc.

Q. What is BIMP database?

BIMP stands for Bio-activity Informatics of Indian Medicinal Plants. It is a database of Indian medicinal plants such as Turmeric, Neem, and Tulsi.

Q. What is active site identifier?

The three-letter code at the end of the PDB file that defines the active site is considered an active site identifier.

Q. Can I screen for multiple protein at a time?

No.

Q. Does it also take protein sequence in fasta format?

It takes protein only in PDB format.

Q. How to site RASPD+?

Holderbach S, Adam L, Jayaram B, Wade RC, Mukherjee G. RASPD+: Fast Protein-Ligand Binding Free Energy Prediction Using Simplified Physicochemical Features. Front Mol Biosci. 2020 Dec 17;7:601065. PMID: 33392260; PMCID: PMC7773945. https://doi.org/10.3389/fmolb.2020.601065

Q. Can I download ZINC dataset on my local machine?

You can only download the results, not the entire dataset.