

Method D: <http://www.scfbio-iitd.res.in/software/drugdesign/raspedmolecule.jsp>

The screenshot shows the RASPD web interface. At the top, there are logos for IIT Delhi and SCFBio, and a navigation bar with links: Home | Group | Publications | Resources | Contact Us. The main heading is "RASPD - A Rapid Scoring Methodology Based on Physico-Chemical Descriptors of Small Molecules". Below this, there is a link: "Click Here to access the 368 Protein-Ligand Complex Dataset." The main form contains three input fields: "Input Protein file" with a "Browse..." button, "Enter HetID [Identifier]:" with a text box containing "DRG", and "Input Molecule" with a "Browse..." button. Below these are "Submit Query" and "Reset" buttons. At the bottom, there is an "Enter Job Id:" field and a "Get Status" button. Annotations with arrows point to the "Browse..." buttons and the "DRG" text box, and a green box highlights the "Get Status" button and the "Enter Job Id:" field.

Click Here to access the 368 Protein-Ligand Complex Dataset.

Input Protein file Browse... ← Input protein Coordinates can be Obtained from RCSB (www.rcsb.org)

Enter HetID [Identifier]: ← Three letter code of the HetID (Identifier) (say for 1NHZ HetID is 486.)

Input Molecule Browse... ← Input 3D coordinates of the ligand molecules (e.g.; Mifepristone.pdb).

Submit Query Reset

Another Query

Enter Job Id: ← User can track the job by Entering the jobid here.

Get Status

Result of the Method D is obtained upon clicking View Result option
The input Molecule file can be in any of the following formats (*.pdb, *.mol, *.xyz, *.sdf).

Thank You