

**Method C:** <http://www.scfbio-iitd.res.in/software/drugdesign/raspdzip.jsp>

The screenshot shows the RASPD web interface. At the top, there is a header for the Supercomputing Facility for Bioinformatics & Computational Biology, IIT Delhi, with logos and navigation links (Home, Group, Publications, Resources, Contact Us). The main title is "RASPD - A Rapid Scoring Methodology Based on Physico-Chemical Descriptors of Small Molecules". The interface includes three input fields: "Input Protein file" with a "Browse..." button, "Enter HetID[Identifier]:" with the value "DRG", and "Input tar file" 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, the HetID field, and the "Get Status" button, providing additional information.

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 tar file  Browse... **Ziped format of the input 3D coordinates of the molecules.**

**Another Query** **User can track the job by Entering the jobid here.**


Enter Job Id:

**\*The input zipped file can be in any of the following formats (\*.rar, \*.zip, \*.tar,\*.gz).**

An representative user design dataset is given upon clicking **Customized Dataset** option



## Supercomputing Facility for Bioinformatics & Computational Biology, IIT Delhi



Home | Drug Design Software

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### RASPD for Preliminary Screening of Drugs

The challenge for computer aided drug discovery is to identify potential drug candidates - in binding to target proteins, at reduced cost and with proper ADMET profiles. RASPD is a computational methodology that takes as input target protein structure, binding pocket, hydrogen bond acceptors, number of hydrophobic groups and other mentioned properties of the target protein and generates a list of potential drug candidates. The methodology is that it takes fraction of a second to generate a list of million molecule complexes as opposed to several weeks for traditional methods. Whereas the accuracy of this method in sorting out potential hits is higher than traditional methods. We have also created million molecules database with various properties like molecular weight, topological index, number of hydrogen bond donors, number of hydrogen bond acceptors, logP values for each of the million molecules to identify hits for a particular protein target is

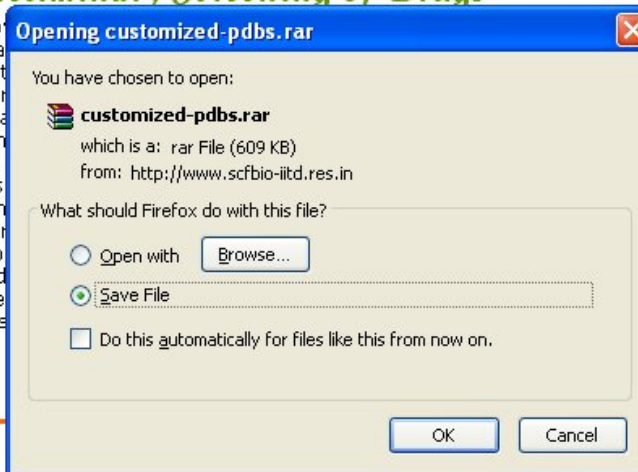
[Click here to see 'How to Use Tool'.](#)

- Method A** [Protein-Ligand Complex]
- Method B** [Protein 3D Structure Without Ligand]
- Method C** [Customized Dataset]
- Method D** [Customized Molecule]

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**Step 2: Click on 'Submit' to submit your job**


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User can track Job status by the Job ID (Say here Job ID is 21353688Method3)



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## RASPD - A Rapid Scoring Methodology Based on Physico-Chemical Descriptors of Small Molecules

Your job has been submitted successfully.  
And the Jobid is

**21353688Method3**

[Another Query](#)

Enter Job Id:

## Current Job Status

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### STATUS PAGE

For any exception/problem, kindly contact [goutam@scfbio-iitd.res.in](mailto:goutam@scfbio-iitd.res.in).

Your Job has been successfully completed.

[View Result](#)

[Download The Result in .xls Format](#)

[Another Query](#)

**Job Status**

Enter Job Id:

## Result

<b>Pred. BE</b>	<b>Ligand ID</b>
-11	10GSligand
-2	182Lligand
-4	184Lligand
-7	1a30ligand
-11	1a4kligand
-10	1a4qligand
-13	1a4wligand
-6	1A50ligand
-5	1A69ligand
-11	1a9mligand
-14	1aaqligand
-1	1ABELligand
-2	1ABFligand
-2	1ac4ligand
-5	1acjligand
-3	1acmligand
-1	1acoligand
-6	1ADDligand
-7	1ADLligand
-10	1ae8ligand
-2	1aeblligand
-2	1aeelligand
-9	1afkligand
-9	1afllligand
-3	1ai4ligand
-4	1ai5ligand
-4	1ai6ligand
-4	1ajnligand
-3	1ajpligand
-13	1ajvligand
-12	1ajxligand

**THANK YOU**