A Guidline to use the Application
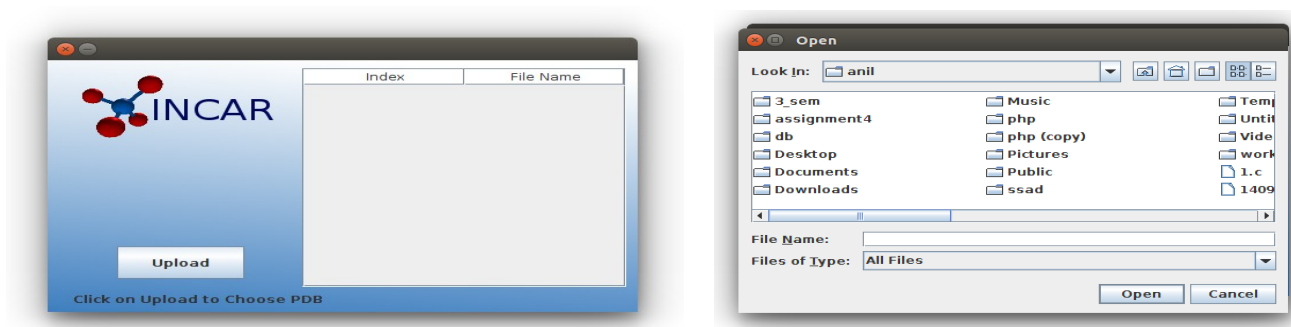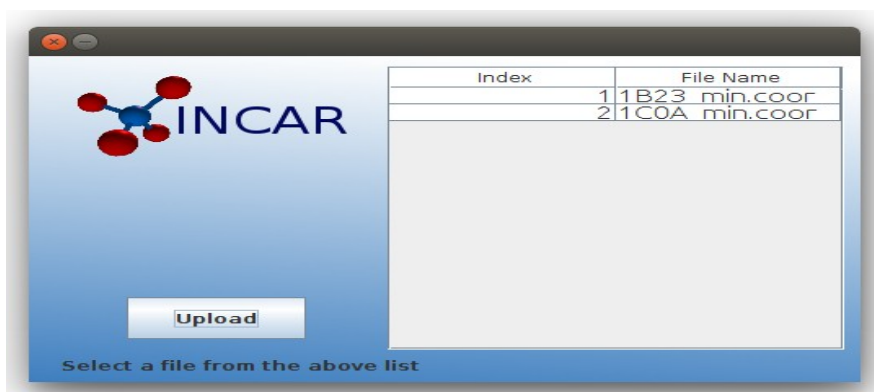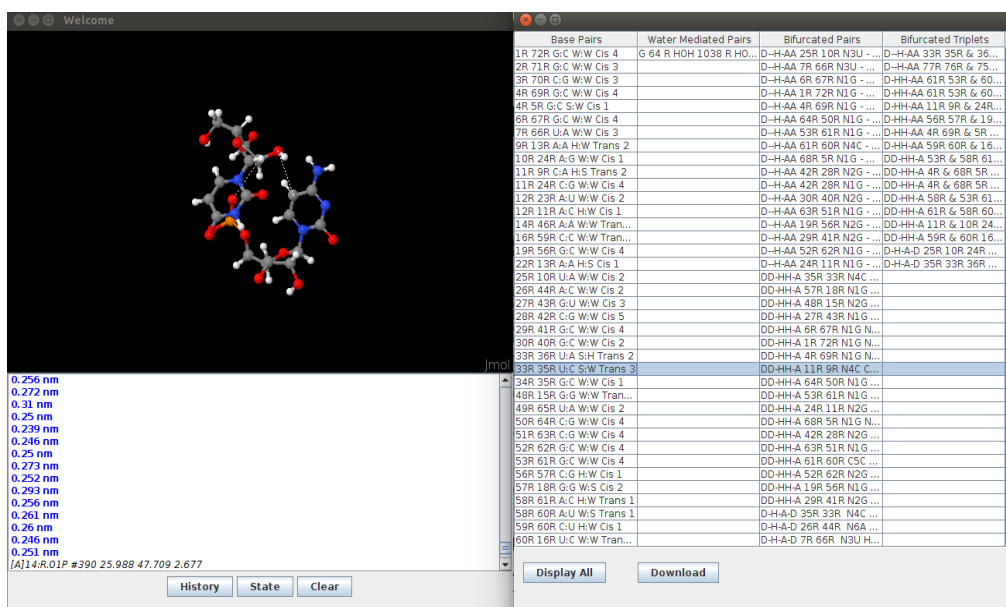
Step 1
Upload the required File

Step 2
Click on the uploaded File for analysing the PDB

Step 3 Analyse specific HBonds of molecule
Click on the Part you want to analyse in the Hbonds Tab

The Format of the Output Data

Output : Contains four parts:

1. Bifuricaed Pairs : It contains 5 types of output

    i). D--H-AA

    Output Format:

        D--H-AA rn+chno of donor , rn+chno of acceptor , at+rt of donor atom , hydrogen atom , at+rt of 1st acceptor , at+rt of 2 nd acceptor.

    ii).DD-HH-A

    Output Format:

        DD-HH-A rn+chno of donor , rn+chno of acceptor , at+rt of 1st donor atom , at+rt of 2nd donor atom , 1 st hydrogen atom , 2 nd hydrogen atom at+rt of acceptor.

    iii).D-H-A-D

    Output Format:

        D-H-A-D rn+chno of donor , rn+chno of acceptor , at+rt of donor atom , 1 st hydrogen atom, at+rt of acceptor , 2 nd hydrogen atom , at+rt of donor

    iv).D-HH-AA

    Output Format:

        D-HH-AA rn+chno of donor , rn+chno of acceptor , at+rt of donor atom , 1 st hydrogen atom , 2 nd hydrogen atom , at+rt of 1st acceptor , at+rt of 2 nd acceptor

    v).D-HH-A

    Output Format:

        D-HH-AA rn+chno of donor , rn+chno of acceptor , at+rt of donor atom , 1 st hydrogen atom , 2 nd hydrogen atom , at+rt of acceptor

2.Bifuricaed Triplets: It contains 4 types of output

    i). D—H-AA

    Output Format:

        D--H-AA rn+chno of donor , rn+chno of 1 st acceptor , rn+chno of 2 nd acceptor , at+rt of donor atom , hydrogen atom , at+rt of 1st acceptor , at+rt of 2 nd acceptor

    ii).DD-HH-A

    Output Format:

        DD-HH-A rn+chno of 1 st donor , rn+chno of 2 nd donor , rn+chno of acceptor , at+rt of 1st donor atom , at+rt of 2nd donor atom , 1st hydrogen atom , 2nd hydrogen atom , at+rt of acceptor

    iii).D-H-A-D

    Output Format:

        D-H-A-D rn+chno of donor , rn+chno of acceptor , at+rt of donor atom , 1 st hydrogenatom , at+rt of acceptor , 2 nd hydrogen atom , at+rt of donor.

    iv).D-HH-AA

    Output Format:

        D-HH-AA rn+chno of donor , rn+chno of 1 st acceptor , rn+chno of 2 nd acceptor , at+rt of donor atom , 1 st hydrogen atom , 2 nd hydrogen atom , at+rt of 1st acceptor , at+rt of 2 nd acceptor.

3.Base Pairs:

    Output Format: rn + chno of donor , rn + chno of acceptor , rt of 1 donor , rt of acceptor , sub-ty , No of such type of H-bonds , Cis or Trans.