BINDING AFFINITY PREDICTION of PROTEIN-LIGAND (BAPPL) server

README FILE
METHOD 1

A SAMPLE PDB FILE IS SHOWN HERE

THE FILE HAS BEEN TRUNCATED TO
HIGHLIGHT THE MAIN FORMAT FEATURES

```
000000000100000000020000000003000000000400000000050000000006000000000700000000
123456789012345678901234567890123456789012345678901234567890123456789012345678
ATOM      1 N    PRO     1      27.687  39.749   6.133 -0.2020  1.8750  0.1700
ATOM      2 H2   PRO     1      26.845  39.527   5.607  0.3120  0.6000  0.0157
ATOM      3 H3   PRO     1      27.701  40.768   6.052  0.3120  0.6000  0.0157
 .
 .
 .
ATOM     29 NE2  GLN     2      29.788  36.842  -2.103 -0.9407  1.8240  0.1700
ATOM     30 HE21 GLN     2      30.228  36.885  -3.003  0.4251  0.6000  0.0157
ATOM     31 HE22 GLN     2      28.925  37.332  -1.868  0.4251  0.6000  0.0157
 .
 .
 .
ATOM   1568 C    PHE    99      23.968  34.664  -9.752  0.7660  1.9080  0.0860
ATOM   1569 O    PHE    99      23.695  35.887  -9.764 -0.8026  1.6612  0.2100
ATOM   1570 OXT  PHE    99      23.666  33.948 -10.733 -0.8026  1.6612  0.2100
ATOM   1571 N    PRO   100      21.136  35.166 -10.482 -0.2020  1.8750  0.1700
ATOM   1572 H2   PRO   100      20.836  34.681  -9.641  0.3120  0.6000  0.0157
ATOM   1573 H3   PRO   100      22.135  34.952 -10.605  0.3120  0.6000  0.0157
 .
 .
 .
ATOM   3136 HD2  PHE   198      23.588  40.185   7.863  0.1408  1.4590  0.0150
ATOM   3137 C    PHE   198      25.733  41.419   4.747  0.7660  1.9080  0.0860
ATOM   3138 O    PHE   198      26.823  41.261   4.144 -0.8026  1.6612  0.2100
ATOM   3139 OXT  PHE   198      25.713  41.819   5.928 -0.8026  1.6612  0.2100
ATOM   3140 O8   DRG   199       2.583  28.101   3.356 -0.7851  1.6612  0.2100
ATOM   3141 C7   DRG   199       2.773  27.608   2.263  0.7886  1.9080  0.0860
ATOM   3142 O9   DRG   199       2.172  28.050   1.304 -0.7851  1.6612  0.2100
ATOM   3143 C6   DRG   199       3.866  26.571   2.062 -0.0834  1.9080  0.1094
ATOM   3144 H15  DRG   199       3.546  25.910   1.254  0.0142  1.4870  0.0157
 .
 .
 .
```

FORMAT DESCRIPTION

COLUMNS	DATA TYPE	DEFINITION
1 - 4	Record Name	"ATOM"
5 - 11	Integer	Atom number
12	Blank space	
13 - 16	Atom	Atom name
17	Blank space	
18 - 20	Residue name	Residue name
21	Blank space	
22 - 26	Integer	Residue number
27	Blank space	
28 - 38	Float	Orthogonal coordinates for X in Å
39 - 46	Float	Orthogonal coordinates for y in Å
47 - 54	Float	Orthogonal coordinates for z in Å
55 - 62	Float	Partial atomic charges
63 - 70	Float	van der Waals parameter (R*)
71 - 78	Float	van der Waals parameter (ε)

SOME IMPORTANT INSTRUCTIONS

1. The Atom number should increase in serial order starting with ‘1’.
2. The Residue number should start with ‘1’ and should increment serially with every next residue.
3. There should be no "TER" records separating two protein chains or a protein chain from the ligand.
4. Atom names with four characters like HE21, HE22 etc. should be represented as such and not like 1HE2, 2HE2 etc.
5. The protein chain should not be specified by any separate variable like ‘A’ ‘B’ etc.
6. The chain termination of a protein should be indicated by "OXT" record in the Atom name column.
7. The ligand / drug should be specified by "DRG" in the Residue name record and should be present as the last residue of the protein-ligand complex file.
8. The PDB file should contain the partial atomic charges and van der Waals parameters for each atom in the format described.