

AD2



OpenBabelGUI

File View Plugins Help

INPUT FORMAT

gom -- PCModel format

Use this format for all input files (ignore file extensions)

E:\Workspace\ashutosh\lgend.pdb

Input below (ignore input file)

COMPND	UNPAIRED
AUTHOR	GENERATED BY OPEN BABEL 2.3.0
HETATM	1 C UNL 1 -1.851 2.263 -0.058 1.00
0.00	C
HETATM	2 C UNL 1 -2.999 1.482 0.024 1.00
0.00	C
HETATM	3 C UNL 1 -0.582 1.657 -0.052 1.00
0.00	C
HETATM	4 C UNL 1 -2.885 0.097 0.118 1.00
0.00	C
HETATM	5 C UNL 1 -0.473 0.264 0.037 1.00
0.00	C
HETATM	6 C UNL 1 -1.624 -0.522 0.126 1.00
0.00	C
HETATM	7 C UNL 1 -1.585 -1.898 0.236 1.00
0.00	C
HETATM	8 C UNL 1 -0.355 -2.845 -0.004 1.00
0.00	C
HETATM	9 C UNL 1 -1.055 -4.179 -0.305 1.00
0.00	C
HETATM	10 H UNL 1 0.236 -2.861 0.916 1.00
0.00	H
HETATM	11 H UNL 1 0.240 -2.484 -0.846 1.00
0.00	H
HETATM	12 N UNL 1 -2.643 -2.688 0.545 1.00
0.00	N
HETATM	13 N UNL 1 -2.205 -3.881 0.513 1.00
0.00	N
HETATM	14 C UNL 1 -0.397 -5.525 -0.066 1.00
0.00	C
HETATM	15 H UNL 1 -1.302 -4.194 -1.364 1.00
0.00	H
HETATM	16 C UNL 1 -1.233 -0.682 0.044 1.00
0.00	C
HETATM	17 C UNL 1 0.981 -5.767 -0.267 1.00
0.00	C

Start input at molecule # specified

End input at molecule # specified

Continue with next object after error, if possible

Attempt to translate keywords

Delete hydrogens (make implicit)

Add hydrogens (make explicit)

Add hydrogens appropriate for this pH

Convert dative bonds e.g. [N+]=[O-] to N=[O]

Remove all but the largest contiguous fragment

Center Coordinates

Combine mols in first file with others by name

Convert only if match SMARTS or mols in file

Filter: convert only when tests are true:

Add properties from descriptors

Delete properties in list

Append properties or descriptors in list to title:

Join all input molecules into a single output molecule

Output disconnected fragments separately

add or replace a property (SOP)

Add or replace molecule title

Append text to title

Output multiple conformers separately

Append output index to title

Additional file output

Append input filename to title

Append input index to title

Add balloons to only atoms ask

OUTPUT FORMAT

mol -- MOL MOL format

Output file

lg

Output below only (no output file) Display in preview

1 molecule converted

E:\Workspace\ashutosh\lgend.pdb
OpenBabel33220492730

```
33 35 0 0 1 0 0 0 0 099942000
-1.8510 2.2630 -0.0580 C 0 0 0 0 0 0 0 0 0 0
-2.9990 1.4820 0.0240 C 0 0 0 0 0 0 0 0 0 0
-0.5820 1.6570 -0.0520 C 0 0 0 0 0 0 0 0 0 0
-2.8850 0.0970 0.1180 C 0 0 0 0 0 0 0 0 0 0
-0.4730 0.2640 0.0370 C 0 0 0 0 0 0 0 0 0 0
-1.6240 -0.5220 0.1260 C 0 0 0 0 0 0 0 0 0 0
-1.5850 -1.8980 0.2360 C 0 0 2 0 0 0 0 0 0 0
-0.3550 -2.8450 -0.0040 C 0 0 0 0 0 0 0 0 0 0
-1.0550 -4.1790 -0.3050 C 0 0 0 0 0 0 0 0 0 0
-1.2330 -0.6820 0.0440 C 0 0 0 0 0 0 0 0 0 0
0.2360 -2.8610 0.9160 H 0 0 0 0 0 0 0 0 0 0
0.2400 -2.4840 -0.8460 H 0 0 0 0 0 0 0 0 0 0
-2.6430 -2.6880 0.5450 N 0 0 0 0 0 0 0 0 0 0
-2.2050 -3.8810 0.5130 N 0 0 0 0 0 0 0 0 0 0
-0.3970 -5.5250 -0.0660 C 0 0 0 0 0 0 0 0 0 0
-1.3020 -4.1940 -1.3640 H 0 0 0 0 0 0 0 0 0 0
-1.2330 -0.6820 0.0440 H 0 0 0 0 0 0 0 0 0 0
0.9810 -5.7670 -0.2670 C 0 0 0 0 0 0 0 0 0 0
-2.5150 -0.5800 0.0390 H 0 0 0 0 0 0 0 0 0 0
-1.3940 -0.8260 0.2230 H 0 0 0 0 0 0 0 0 0 0
2.5820 -7.2090 -0.0590 H 0 0 0 0 0 0 0 0 0 0
```

