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Supporting Material

Improved ligand-protein binding affinity predictions using multiple binding modes

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Supplementary Material

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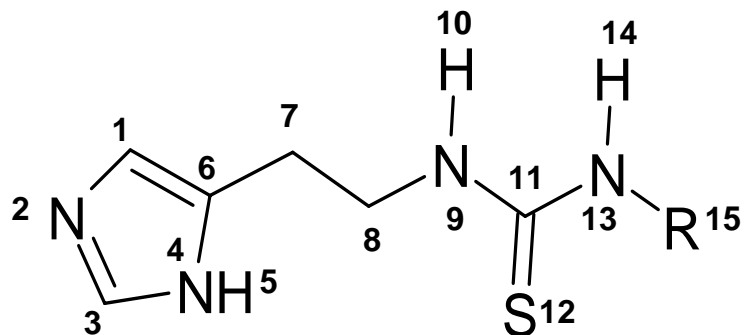
Improved ligand-protein binding affinity predictions using multiple binding modes

GROMOS 45a4 force-field parameters for the scaffold of the thiourea containing compounds

Description of the parameters is available in:

van Gunsteren, W. F., Billeter, S. R., Eising, A. A., Hünenberger, P. H., Krüger, P., Mark, A. E., Scott, W. R. P., Tironi, I. G., Biomolecular simulation: The GROMOS96 manual and user guide, Vdf Blochschulverlag AG an der ETH Zürich: Zürich 1996.

Scaffold of thiourea containing compounds



For the example below R=CH₃

MTBUILDBLSOLUTE

#

N-methyl-N'-(4-imidazole-ethyl)thiourea

#

#

building block (residue, nucleotide, etc.)

RNME

TH1

number of atoms, number of preceding exclusions

NMAT,NLIN

15 0

preceding exclusions

#ATOM

MAE MSAE

atoms

#ATOM ANM IACM MASS CGMICGM MAE MSAE

1 C1 16 3 0.13000 0 6 2 3 4 5 6 7

2 N3 8 14 -0.58000 0 5 3 4 5 6 7

3 C5 16 3 0.26000 0 4 4 5 6 7

4 N7 8 14 0.00000 0 3 5 6 7

5 H6 18 1 0.19000 0 2 6 7

6 C8 11 12 0.00000 1 2 7 8

7 C9 13 4 0.00000 0 2 8 9

8 C12 13 4 0.00000 1 3 9 10 11

9 N15 5 14 -0.28000 0 4 10 11 12 13

10 H16 18 1 0.28000 1 1 11

11 C17 11 12 0.20000 0 4 12 13 14 15

12 S20 20 32 -0.20000 1 1 13

13 N18 5 14 -0.28000 0 2 14 15

```

14 H19 18 1 0.28000 1 1 15
15 C21 14 5 0.00000 1 0
# bonds
# NB
15
# IB JB MCB
1 2 9
1 6 9
2 3 9
3 4 9
4 5 2
4 6 9
6 7 26
7 8 26
8 9 20
9 10 2
9 11 9
11 12 4
11 13 9
13 14 2
13 15 15
# bond angles
# NBA
20
# IB JB KB MCB
2 1 6 6
1 2 3 6
2 3 4 6
3 4 5 35
3 4 6 6
5 4 6 35
1 6 4 6
1 6 7 36
4 6 7 36
6 7 8 14
7 8 9 12
8 9 10 17
8 9 11 30
10 9 11 31
9 11 12 26
9 11 13 26
12 11 13 26
11 13 14 31
11 13 15 30
14 13 15 17

```

```
# improper dihedrals
# NIDA
10
# IB JB KB LB MCB
1 2 3 4 1
2 1 6 4 1
2 3 4 6 1
3 4 6 1 1
4 3 5 6 1
6 1 2 3 1
6 1 4 7 1
9 8 10 11 1
11 9 12 13 1
13 11 14 15 1
# dihedrals
# NDA
5
# IB JB KB LB MCB
1 6 7 8 20
6 7 8 9 17
7 8 9 10 19
8 9 11 12 2
9 11 13 14 2
END
```