SUPPORTING INFORMATION

Exposing the flexibility of human parainfluenza virus haemagglutinin-neuraminidase.

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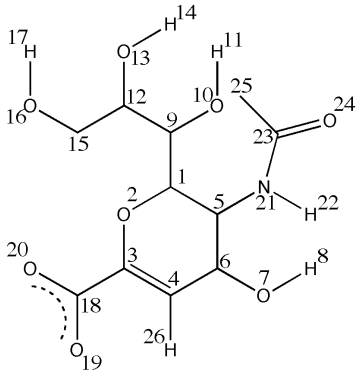
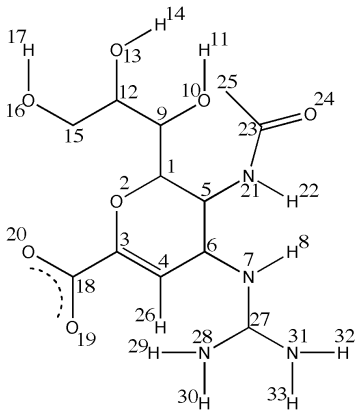
PAREMETERS USED IN MD SIMULATIONS

Parameters for the inhibitors Neu5Ac2en (**1**) and zanamivir (**2**) and have been based on the GROMOS 54A7 and 53A6 force fields. Atom and mass codes, as well as covalent bond-, angle-, dihedral-, and improper dihedral constants are available in the reported literature.[S1]



Neu5Ac2en (**1**)



Zanamivir (**2**)

(1) Non-bonded parameters for (1):

Atom index	Atom code[S1]	Mass code[S1]	Charge
1	14	3	0.267
2	4	16	-0.348
3	12	12	0.080
4	12	12	-0.419
5	14	3	0.223
6	14	3	0.417
7	3	16	-0.641
8	21	1	0.421
9	14	3	0.232
10	3	16	-0.642
11	21	1	0.410
12	14	3	0.232
13	3	16	-0.642
14	21	1	0.410
15	14	4	0.232
16	3	16	-0.642
17	21	1	0.410
18	12	12	0.270
19	2	16	-0.635
20	2	16	-0.635
21	6	14	-0.310
22	21	1	0.310
23	12	12	0.450
24	1	16	-0.450
25	16	5	0.000
26	20	1	0.222

(2) Covalent bonds for (1):

Atom *i*	Atom *j*	Bond constant[S1]
1	2	20
2	3	13
3	4	10

4	6	26	
5	6	27	
1	5	27	
1	9	27	
9	10	18	
10	11	1	
9	12	27	
12	13	18	
13	14	1	
12	15	27	
15	16	20	
16	17	1	
5	21	21	
21	22	2	
21	23	45	
23	24	6	
23	25	26	
6	7	18	
7	8	1	
3	18	26	
18	19	6	
18	20	6	
4	26	3	

(3) Bond angles for (1):

Atom *i*	Atom *j*	Atom *k*	Angle constant[S1]
1	2	3	9
2	1	9	19
2	1	5	15
5	1	9	15
1	9	10	9
1	9	12	9
10	9	12	9
9	10	11	12
9	12	13	9
9	12	15	9
13	12	15	9
12	13	14	12
12	15	16	9
15	16	17	12
2	3	4	35
2	3	18	19
4	3	18	27
3	18	19	22
3	18	20	22
19	18	20	38
3	4	6	35
1	5	6	15
1	5	21	8
6	5	21	15
4	6	5	15
4	6	7	9
5	6	7	15
6	7	8	12
5	21	22	18

5	21	23	31
22	21	23	32
21	23	25	22
21	23	24	33
24	23	25	33
3	4	26	25
6	4	26	25

(4) Improper dihedrals for (1):

Atom *i*	Atom *j*	Atom *k*	Atom *l*	Improper-dihedral constant[S1]
21	5	22	23	1
4	3	26	6	1
3	2	4	18	1
18	3	20	19	1
23	21	24	25	1
1	2	5	9	2
5	1	21	6	2
6	7	5	4	2
9	1	10	12	2
12	9	13	15	2

(5) Dihedral angles for (1):

Atom *i*	Atom *j*	Atom *k*	Atom *l*	Dihedral constant[S1]
3	2	1	5	23
1	2	3	4	11
2	1	5	21	29
5	1	9	10	29
2	3	4	6	10
4	3	18	20	10
1	5	21	23	41
1	5	6	7	29
5	21	23	24	14
1	9	10	11	23
1	9	12	13	29
3	4	6	5	39
5	6	7	8	23
9	12	13	14	23
9	12	15	16	29

(1) Non-bonded parameters for (2):

Atom index	Atom code[S1]	Mass code[S1]	Charge
1	14	3	0.267
2	4	16	-0.348
3	12	12	0.080
4	12	12	-0.419
5	14	3	0.223
6	14	3	0.417
7	10	14	-0.310
8	21	1	0.440
9	14	3	0.232
10	3	16	-0.642
11	16	1	0.410
12	14	3	0.232
13	3	16	-0.642
14	21	1	0.410
15	14	4	0.232
16	3	16	-0.642
17	21	1	0.410
18	12	12	0.270
19	2	16	-0.635
20	2	16	-0.635
21	6	14	-0.310
22	21	1	0.310
23	12	12	0.450
24	1	16	-0.450
25	16	5	0.000
26	20	1	0.222
27	12	12	0.340
28	10	14	-0.260
29	21	1	0.240
30	21	1	0.240
31	10	14	-0.260
32	21	1	0.240
33	21	1	0.240

(2) Covalent bonds for (2):

Atom *i*	Atom *j*	Atom *k*	Angle constant[S1]
1	2	3	9
2	1	9	19
2	1	5	15
5	1	9	15
1	9	10	9
1	9	12	9
10	9	12	9
9	10	11	12
9	12	13	9
9	12	15	9

13	12	15	9
12	13	14	12
12	15	16	9
15	16	17	12
2	3	4	35
2	3	18	19
4	3	18	27
3	18	19	22
3	18	20	22
19	18	20	38
3	4	6	35
1	5	6	15
1	5	21	8
6	5	21	15
4	6	5	15
4	6	7	8
5	6	7	15
6	7	8	20
5	21	22	18
5	21	23	31
22	21	23	32
21	23	25	22
21	23	24	33
24	23	25	33
3	4	26	25
6	4	26	25
6	7	27	33
8	7	27	23
7	27	28	28
7	27	31	28
28	27	31	28
27	28	29	23
27	28	30	23
29	28	30	24
27	31	32	23
27	31	33	23
32	31	33	24

(3) Improper dihedrals (**2**):

Atom *i*	Atom *j*	Atom *k*	Atom *l*	Improper-dihedral constant[S1]
21	5	22	23	1
4	3	26	6	1
3	2	4	18	1
18	3	20	19	1
23	21	24	25	1
1	2	5	9	2
5	1	21	6	2
6	7	5	4	2
9	1	10	12	2
12	9	13	15	2
7	6	27	8	1
27	28	31	7	1
28	29	30	27	1
31	32	33	27	1

(4) Dihedral angles (**2**):

Atom *i*	Atom *j*	Atom *k*	Atom *l*	Dihedral constant[S1]
3	2	1	5	23
1	2	3	4	11
2	1	5	21	29
5	1	9	10	29
2	3	4	6	10
4	3	18	20	10
1	5	21	23	41
1	5	6	7	29
5	21	23	24	14
1	9	10	11	23
1	9	12	13	29
3	4	6	5	39
5	6	7	8	23
9	12	13	14	23
9	12	15	16	29
12	15	16	17	23
6	7	27	28	14
7	27	28	29	14
7	27	31	32	14

REFERENCES FOR SUPPORTING INFORMATION

(S1) Oostenbrink, C.; Villa, A.; Mark, A. E.; van Gunsteren, W. F. *J. Comput. Chem.* **2004**, *25*, 1656.