Table 1: Simulation parameters

	Equilibration	**Ensemble**
Coarse Grain	**MARTINI**[1]	
dt [ps]	0.02	0.02
Thermostat	v-rescale	v-rescale
Barostat	Berendsen	Parrinello-Rahman
Type of barostat[2]	Anisotropic	Anisotropic
All-atom	**CHARMM**	
dt [ps]	0.002 (bond constraints)	0.002 (bond constraints)
Thermostat	Berendsen	Nose-Hoover
Barostat	Berendsen	Parrinello-Rahman
Type of barostat[3]	Semiisotropic	Semiisotropic
Molecular Dynamics package	GROMACS	

[1] The plain MARTINI water model is known to have issues regarding crystallization at temperatures well above the melting point. To avoid such phenomenon antifreeze particles was introduced at 10%, according to MARTINI protocol.
[2] In CG simulations the initial configuration consist of random arrangement of lipids and water molecules, thus, Anisotropic barostat type is chosen in order to leave all the possible degrees of freedom to the system to formate a more complex structure.
[3] In AA simulations the bilayer structure is formed and the 2 out of 3 degrees of freedom, concerning the volume deviations of the simulation box, change the same way (isotropic). Hence, the Semiisotropic type of barostat was chosen.

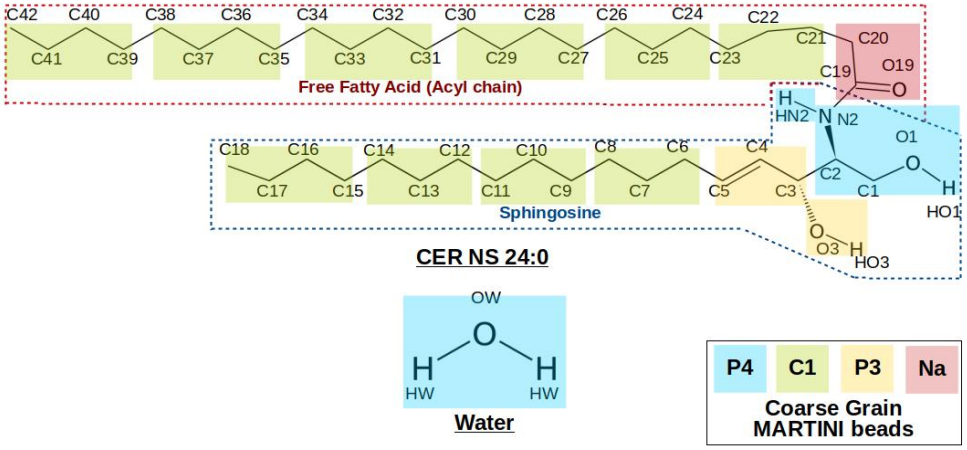

Figure 1: All-atom and Coarse Grain mapping of CER NS 24:0 and Water molecules

Table 2: Atoms abbreviations for CHARMM forcefield

CER NS 24:0

	atom	type	charge
1	C1	CTO2	0.49
2	H1a	HAL2	-0.05
3	H1b	HAL2	-0.05
4	O1	OHL	-0.69
5	HO1	H	0.3
6	C2	CTL1	0.3
7	H2	HAL1	0.05
8	N2	NHL	-0.7
9	HN2	H	0.35
10	C3	CTO1	0.5
11	H3	HAL1	-0.11
12	O3	OHL	-0.69
13	HO3	H	0.3
14	C4	CEL1	-0.15
15	H4	HEL1	0.15
16	C5	CEL1	-0.15
17	H5	HEL1	0.15
18	C6	CTL2	-0.18
19	H6a	HAL2	0.09
20	H6b	HAL2	0.09
21	C7	CTL2	-0.18
22	H7a	HAL2	0.09
23	H7b	HAL2	0.09
24	C8	CTL2	-0.18
25	H8a	HAL2	0.09
26	H8b	HAL2	0.09
27	C9	CTL2	-0.18
28	H9a	HAL2	0.09
29	H9b	HAL2	0.09
30	C10	CTL2	-0.18
31	H10a	HAL2	0.09
32	H10b	HAL2	0.09
33	C11	CTL2	-0.18
34	H11a	HAL2	0.09
35	H11b	HAL2	0.09
36	C12	CTL2	-0.18
37	H12a	HAL2	0.09
38	H12b	HAL2	0.09
39	C13	CTL2	-0.18
40	H13a	HAL2	0.09
41	H13b	HAL2	0.09

42	C14	CTL2	-0.18
43	H14a	HAL2	0.09
44	H14b	HAL2	0.09
45	C15	CTL2	-0.18
46	H15a	HAL2	0.09
47	H15b	HAL2	0.09
48	C16	CTL2	-0.18
49	H16a	HAL2	0.09
50	H16b	HAL2	0.09
51	C17	CTL2	-0.18
52	H17a	HAL2	0.09
53	H17b	HAL2	0.09
54	C18	CTL3	-0.27
55	H18a	HAL3	0.09
56	H18b	HAL3	0.09
57	H18c	HAL3	0.09
58	C19	C	0.55
59	O19	O	-0.6
60	C20	CTL2	-0.07
61	H20a	HAL2	0.06
62	H20b	HAL2	0.06
63	C21	CTL2	-0.18
64	H21a	HAL2	0.09
65	H21b	HAL2	0.09
66	C22	CTL2	-0.18
67	H22a	HAL2	0.09
68	H22b	HAL2	0.09
69	C23	CTL2	-0.18
70	H23a	HAL2	0.09
71	H23b	HAL2	0.09
72	C24	CTL2	-0.18
73	H24a	HAL2	0.09
74	H24b	HAL2	0.09
75	C25	CTL2	-0.18
76	H25a	HAL2	0.09
77	H25b	HAL2	0.09
78	C26	CTL2	-0.18
79	H26a	HAL2	0.09
80	H26b	HAL2	0.09
81	C27	CTL2	-0.18
82	H27a	HAL2	0.09
83	H27b	HAL2	0.09

84	C28	CTL2	-0.18
85	H28a	HAL2	0.09
86	H28b	HAL2	0.09
87	C29	CTL2	-0.18
88	H29a	HAL2	0.09
89	H29b	HAL2	0.09
90	C30	CTL2	-0.18
91	H30a	HAL2	0.09
92	H30b	HAL2	0.09
93	C31	CTL2	-0.18
94	H31a	HAL2	0.09
95	H31b	HAL2	0.09
96	C32	CTL2	-0.18
97	H32a	HAL2	0.09
98	H32b	HAL2	0.09
99	C33	CTL2	-0.18
100	H33a	HAL2	0.09
101	H33b	HAL2	0.09
102	C34	CTL2	-0.18
103	H34a	HAL2	0.09
104	H34b	HAL2	0.09
105	C35	CTL2	-0.18
106	H35a	HAL2	0.09
107	H35b	HAL2	0.09
108	C36	CTL2	-0.18
109	H36a	HAL2	0.09
110	H36b	HAL2	0.09
111	C37	CTL2	-0.18
112	H37a	HAL2	0.09
113	H37b	HAL2	0.09
114	C38	CTL2	-0.18
115	H38a	HAL2	0.09
116	H38b	HAL2	0.09
117	C39	CTL2	-0.18
118	H39a	HAL2	0.09
119	H39b	HAL2	0.09
120	C40	CTL2	-0.18
121	H40a	HAL2	0.09
122	H40b	HAL2	0.09
123	C41	CTL2	-0.18
124	H41a	HAL2	0.09
125	H41b	HAL2	0.09

126	C42	CTL3	-0.27
127	H42a	HAL3	0.09
128	H42b	HAL3	0.09
129	H42c	HAL3	0.09

Table 3: CHARMM parameters for GROMACS input

CHARMM

[atomtypes]

atomtype	atomnr	atommass	charge	ptype	σ	ϵ
CTL3	6	12.0107	0	A	0.363487	0.326352
CTL2	6	12.0107	0	A	0.358141	0.234304
CTO2	6	12.0107	0	A	0.358141	0.234304
CTL1	6	12.0107	0	A	0.405359	0.08368
CTO1	6	12.0107	0	A	0.405359	0.08368
CEL1	6	12.0107	0	A	0.372396	0.284512
C	6	12.0107	0	A	0.356359	0.46024
OHL	8	15.9994	0	A	0.315378	0.636386
O	8	15.9994	0	A	0.302906	0.50208
NHL	7	14.0067	0	A	0.329633	0.8368
HAL3	1	1.0079	0	A	0.238761	0.100416
HAL2	1	1.0079	0	A	0.238761	0.117152
HAL1	1	1.0079	0	A	0.235197	0.092048
HEL1	1	1.0079	0	A	0.222725	0.129704
H	1	1.0079	0	A	0.040001	0.192464
CRL2	6	12.0107	0	A	0.359923	0.25104
CRL1	6	12.0107	0	A	0.358141	0.150624
HGA2	1	1.0079	0	A	0.238761	0.14644
HGA1	1	1.0079	0	A	0.238761	0.18828
CL	6	12.0107	0	A	0.356359	0.29288
OBL	8	15.9994	0	A	0.302906	0.50208
CG2R61	6	12.0107	0	A	0.355005	0.29288
CG2O2	6	12.0107	0	A	0.302906	0.410032
CG331	6	12.0107	0	A	0.365268	0.326352
OG2D1	8	15.9994	0	A	0.302906	0.50208
HGR61	1	1.0079	0	A	0.242004	0.12552
HGA3	1	1.0079	0	A	0.238761	0.100416
CG311	6	12.0107	0	A	0.356359	0.133888
CG321	6	12.0107	0	A	0.358141	0.234304
CG2O3	8	12.0107	0	A	0.356359	0.29288
OG311	8	15.9994	0	A	0.314487	0.803746
OG2D2	8	15.9994	0	A	0.302906	0.50208

HGP1	1	1.0079	0	A	0.040001	0.192464
OW	8	15.9994	0	A	0.315066	0.636272
HW	1	1.0079	0	A	0	0
Na	11	22.9898	0	A	0.258361	0.131838

[nonbond_params]

atom1	atom2	func	σ	ϵ
CRL1	HAL2	1	0.298451	0.134306
HGA1	HAL2	1	0.238761	0.150206
CRL2	HAL2	1	0.299342	0.173636
HGA2	HAL2	1	0.238761	0.132633
CRL1	HAL1	1	0.298451	0.122591
HGA1	HAL1	1	0.238761	0.137654
CRL2	HAL1	1	0.299342	0.158574
HGA2	HAL1	1	0.238761	0.120918
CRL1	CTL1	1	0.35725	0.11506
HGA1	CTL1	1	0.29756	0.128867
CRL2	CTL1	1	0.358141	0.148532
HGA2	CTL1	1	0.29756	0.113386

[bondtypes]

atom1	atom2	func	b_0	K_b
CTL3	CTL2	1	0.1528	186188
CTL3	HAL3	1	0.1111	269449.6
CTL2	CTL2	1	0.153	186188
CTL2	CEL1	1	0.1502	305432
CTL2	C	1	0.149	209200
CTL2	HAL2	1	0.1111	258571.2
CTO2	CTL1	1	0.1538	186188
CTO2	OHL	1	0.142	358150.4
CTO2	HAL2	1	0.1111	258571.2
CTL1	CTO1	1	0.15	186188
CTL1	NHL	1	0.143	267776
CTL1	HAL1	1	0.1111	258571.2
CTO1	CEL1	1	0.149	209200
CTO1	OHL	1	0.142	358150.4
CTO1	HAL1	1	0.1111	258571.2
CEL1	CEL1	1	0.134	368192
CEL1	HEL1	1	0.11	301666.4
C	O	1	0.123	518816
C	NHL	1	0.1345	309616
OHL	H	1	0.096	456056
NHL	H	1	0.0997	368192
CTL3	CTL1	1	0.1538	186188

CTL3	CRL1	1	0.1538	186188
CTL2	CTL1	1	0.1538	186188
CRL2	CRL2	1	0.153	186188
CRL2	CRL1	1	0.1538	186188
CRL2	CEL1	1	0.1502	305432
CRL2	HGA2	1	0.1111	258571.2
CTL1	CRL1	1	0.15	186188
CRL1	CRL1	1	0.15	186188
CRL1	CEL1	1	0.1502	200832
CRL1	OHL	1	0.142	358150.4
CRL1	HGA1	1	0.1111	258571.2
CTL2	CL	1	0.1522	167360
CL	OHL	1	0.14	192464
CL	OBL	1	0.122	627600
CG2R61	CG2R61	1	0.1375	255224
CG2R61	HGR61	1	0.108	284512
CG2O2	OG2D1	1	0.122	627600
CG331	HGA3	1	0.1111	269449.6
CG331	CG311	1	0.1538	186188
CG321	CG311	1	0.1538	186188
CG321	CG2R61	1	0.149	192464
CG321	HGA2	1	0.1111	258571.2
CG311	CG2O2	1	0.1522	167360
CG311	CG2O3	1	0.1522	167360
CG311	CG2R61	1	0.149	192464
CG311	HGA1	1	0.1111	258571.2
CG2O2	OG311	1	0.14	192464
CG2O3	OG2D2	1	0.126	439320
OG311	HGP1	1	0.096	456056

[pairtypes]

atom1	atom2	func	$\sigma 1-4$	$\epsilon 1-4$
CTL3	CTL2	1	0.338542	0.04184
CTL3	HAL2	1	0.288651	0.070012
CTL2	CTL2	1	0.338542	0.04184
CTL2	CTL1	1	0.338542	0.04184
CTL2	CEL1	1	0.355469	0.109105
CTL2	C	1	0.347451	0.138768
CTL2	OHL	1	0.32696	0.163176
CTL2	O	1	0.293997	0.144938
CTL2	NHL	1	0.30736	0.187114
CTL2	HAL3	1	0.288651	0.064818
CTL2	HAL2	1	0.288651	0.070012

CTL2	HAL1	1	0.286869	0.062059
CTL2	HEL1	1	0.280633	0.073667
CTL2	H	1	0.189271	0.089737
CTO2	CEL1	1	0.355469	0.109105
CTO2	C	1	0.347451	0.138768
CTO2	OHL	1	0.32696	0.163176
CTO2	HAL1	1	0.286869	0.062059
CTO2	H	1	0.189271	0.089737
CTL1	HAL2	1	0.288651	0.070012
CTL1	HEL1	1	0.280633	0.073667
CTL1	H	1	0.189271	0.089737
CTL1	CEL1	1	0.355469	0.109105
CTL1	O	1	0.293997	0.144938
CTO1	CTL2	1	0.338542	0.04184
CTO1	C	1	0.347451	0.138768
CTO1	OHL	1	0.32696	0.163176
CTO1	HAL2	1	0.288651	0.070012
CTO1	HEL1	1	0.280633	0.073667
CTO1	H	1	0.189271	0.089737
CEL1	OHL	1	0.343887	0.425511
CEL1	NHL	1	0.324287	0.487934
CEL1	HAL2	1	0.305578	0.182568
CEL1	HAL1	1	0.303796	0.161829
CEL1	H	1	0.206199	0.234005
C	HAL2	1	0.29756	0.232203
C	HAL1	1	0.295778	0.205826
OHL	NHL	1	0.295778	0.729745
OHL	HAL1	1	0.275288	0.242029
OHL	HEL1	1	0.269051	0.287301
O	HAL2	1	0.244106	0.242528
O	H	1	0.144726	0.310857
NHL	HAL2	1	0.25747	0.313102
NHL	HAL1	1	0.255688	0.277535
HAL3	HAL2	1	0.238761	0.108462
HAL2	HAL2	1	0.238761	0.117152
HAL2	HAL1	1	0.236979	0.103844
HAL2	HEL1	1	0.230743	0.123268
HAL2	H	1	0.139381	0.150158
HAL1	HAL1	1	0.235197	0.092048
HAL1	HEL1	1	0.228961	0.109266
HAL1	H	1	0.137599	0.133101
HEL1	HEL1	1	0.222725	0.129704

CTL3	CRL2	1	0.338542	0.04184
CTL3	CTL1	1	0.338542	0.04184
CTL3	CRL1	1	0.338542	0.04184
CTL3	CEL1	1	0.355469	0.109105
CTL3	HAL3	1	0.288651	0.064818
CTL3	HGA2	1	0.288651	0.078275
CTL3	HGA1	1	0.288651	0.088756
CTL2	CRL2	1	0.338542	0.04184
CTL2	CRL1	1	0.338542	0.04184
CTL2	HGA1	1	0.288651	0.088756
CRL2	CRL2	1	0.338542	0.04184
CRL2	CTL1	1	0.338542	0.04184
CRL2	CRL1	1	0.338542	0.04184
CRL2	CEL1	1	0.355469	0.109105
CRL2	OHL	1	0.32696	0.163176
CRL2	HAL3	1	0.288651	0.064818
CRL2	HGA2	1	0.288651	0.078275
CRL2	HAL1	1	0.286869	0.062059
CRL2	HGA1	1	0.288651	0.088756
CRL2	HEL1	1	0.280633	0.073667
CRL2	H	1	0.189271	0.089737
CTL1	CRL1	1	0.338542	0.04184
CTL1	HGA2	1	0.288651	0.078275
CRL1	CRL1	1	0.338542	0.04184
CRL1	CEL1	1	0.355469	0.109105
CRL1	HAL3	1	0.288651	0.064818
CRL1	HAL2	1	0.288651	0.070012
CRL1	HGA2	1	0.288651	0.078275
CRL1	HAL1	1	0.286869	0.062059
CRL1	HGA1	1	0.288651	0.088756
CRL1	HEL1	1	0.280633	0.073667
CEL1	HAL3	1	0.305578	0.169025
CEL1	HGA2	1	0.305578	0.204117
CEL1	HGA1	1	0.305578	0.231447
OHL	HGA2	1	0.27707	0.305274
HAL3	HAL1	1	0.236979	0.096141
HGA2	HGA2	1	0.238761	0.14644
HGA2	HGA1	1	0.238761	0.166047
HGA2	HEL1	1	0.230743	0.137818
HAL1	HGA1	1	0.236979	0.131646
HGA1	HGA1	1	0.238761	0.18828
HGA1	H	1	0.139381	0.190361

CTL2	CL	1	0.347451	0.110698
CTL2	OBL	1	0.293997	0.144938
CL	HAL2	1	0.29756	0.185234
OHL	HAL2	1	0.27707	0.273046
OBL	HAL2	1	0.244106	0.242528
OBL	H	1	0.144726	0.310857
CG331	CG2R61	1	0.346773	0.110698
CG331	OG2D1	1	0.320724	0.144938
CG2R61	CG2R61	1	0.355005	0.29288
CG2O2	CG2R61	1	0.328955	0.34654
CG2O2	HGA3	1	0.270833	0.202913
CG2R61	OG2D1	1	0.328955	0.38347
CG2R61	HGR61	1	0.298505	0.191735
HGR61	HGR61	1	0.242004	0.12552
CG331	OG311	1	0.326514	0.183381
CG331	OG2D2	1	0.320724	0.144938
CG331	HGA3	1	0.288651	0.064818
CG331	HGA2	1	0.288651	0.078275
CG321	CG2R61	1	0.346773	0.110698
CG321	HGA3	1	0.288651	0.064818
CG321	HGR61	1	0.290273	0.072469
CG311	CG2R61	1	0.346773	0.110698
CG311	HGR61	1	0.290273	0.072469
CG311	HGP1	1	0.189271	0.089737
CG2O3	CG2R61	1	0.355682	0.29288
CG2O3	HGA3	1	0.29756	0.171493
CG2R61	CG331	1	0.346773	0.110698
CG2R61	OG311	1	0.334746	0.485182
CG2R61	OG2D2	1	0.328955	0.38347
CG2R61	HGA3	1	0.296883	0.171493
CG2R61	HGA2	1	0.296883	0.207097
CG2R61	HGA1	1	0.296883	0.234826
OG2D1	HGA1	1	0.270833	0.30746
OG2D1	HGP1	1	0.171453	0.310857
OG2D2	HGA1	1	0.270833	0.30746
OG311	HGA1	1	0.276624	0.389011
HGA3	HGA1	1	0.238761	0.1375
HGA2	HGA1	1	0.238761	0.166047

[angletypes]

atom1	atom2	atom3	func	θ_o	K_θ	s_0	K_s
CTL2	CTL3	HAL3	5	110.1	289.5328	0.2179	18853.1
HAL3	CTL3	HAL3	5	108.4	297.064	0.1802	4518.72

CTL3	CTL2	CTL2	5	115	485.344	0.2561	6694.4
CTL2	CTL2	CTL2	5	113.6	488.2728	0.2561	9338.69
CTL2	CTL2	CEL1	5	112.2	267.776	0	0
CTL2	CTL2	C	5	108	435.136	0	0
CTL3	CTL2	HAL2	5	110.1	289.5328	0.2179	18853.1
CTL2	CTL2	HAL2	5	110.1	221.752	0.2179	18853.1
CEL1	CTL2	HAL2	5	111.5	376.56	0	0
C	CTL2	HAL2	5	109.5	276.144	0.2163	25104
HAL2	CTL2	HAL2	5	109	297.064	0.1802	4518.72
CTL1	CTO2	OHL	5	110.1	633.4576	0	0
CTL1	CTO2	HAL2	5	110.1	221.752	0.2179	18853.1
OHL	CTO2	HAL2	5	108.89	384.0912	0	0
HAL2	CTO2	HAL2	5	109	297.064	0.1802	4518.72
CTO2	CTL1	CTO1	5	113.5	488.2728	0.2561	9338.69
CTO2	CTL1	NHL	5	113.5	585.76	0	0
CTO2	CTL1	HAL1	5	110.1	288.696	0.2179	18853.1
CTO1	CTL1	HAL1	5	110.1	288.696	0.2179	18853.1
CTO1	CTL1	NHL	5	113.5	585.76	0	0
NHL	CTL1	HAL1	5	108	401.664	0	0
CTL1	CTO1	CEL1	5	108	435.136	0	0
CTL1	CTO1	OHL	5	110.1	633.4576	0	0
CTL1	CTO1	HAL1	5	110.1	288.696	0.2179	18853.1
CEL1	CTO1	OHL	5	110.1	633.4576	0	0
CEL1	CTO1	HAL1	5	109.5	276.144	0.2163	25104
OHL	CTO1	HAL1	5	108.89	384.0912	0	0
CTL2	CEL1	CEL1	5	123.5	401.664	0	0
CTO1	CEL1	CEL1	5	123.5	401.664	0	0
CTL2	CEL1	HEL1	5	116	334.72	0	0
CTO1	CEL1	HEL1	5	116	334.72	0	0
CEL1	CEL1	HEL1	5	119.5	435.136	0	0
CTL2	C	O	5	121	669.44	0	0
CTL2	C	NHL	5	116.5	669.44	0	0
O	C	NHL	5	122.5	669.44	0	0
CTO2	OHL	H	5	106	481.16	0	0
CTO1	OHL	H	5	106	481.16	0	0
CTL1	NHL	C	5	120	418.4	0	0
CTL1	NHL	H	5	117	292.88	0	0
C	NHL	H	5	123	284.512	0	0
CTL1	CTL3	HAL3	5	110.1	279.7422	0.2179	18853.1
CRL1	CTL3	HAL3	5	110.1	279.7422	0.2179	18853.1
CTL2	CTL2	CTL1	5	113.5	488.2728	0.2561	9338.69
CTL1	CTL2	HAL2	5	110.1	221.752	0.2179	18853.1

CRL2	CRL2	CRL1	5	113.5	488.2728	0.2561	9338.69
CRL1	CRL2	CEL1	5	112.2	267.776	0	0
CRL2	CRL2	HGA2	5	110.1	221.752	0.2179	18853.1
CRL1	CRL2	HGA2	5	110.1	221.752	0.2179	18853.1
CEL1	CRL2	HGA2	5	111.5	376.56	0	0
HGA2	CRL2	HGA2	5	109	297.064	0.1802	4518.72
CTL3	CTL1	CTL3	5	113.5	488.2728	0.2561	9338.69
CTL3	CTL1	CTL2	5	113.5	488.2728	0.2561	9338.69
CTL3	CTL1	CRL1	5	108.5	446.4328	0.2561	6694.4
CTL2	CTL1	CRL1	5	113.5	488.2728	0.2561	9338.69
CTL3	CTL1	HAL1	5	110.1	288.696	0.2179	18853.1
CTL2	CTL1	HAL1	5	110.1	288.696	0.2179	18853.1
CRL1	CTL1	HAL1	5	110.1	288.696	0.2179	18853.1
CTL3	CRL1	CRL2	5	113.5	488.2728	0.2561	9338.69
CTL3	CRL1	CRL1	5	108.5	446.4328	0.2561	6694.4
CTL3	CRL1	CEL1	5	112.2	267.776	0	0
CRL2	CRL1	CRL2	5	113.5	488.2728	0.2561	9338.69
CRL2	CRL1	CTL1	5	113.5	488.2728	0.2561	9338.69
CRL2	CRL1	CRL1	5	113.5	488.2728	0.2561	9338.69
CRL2	CRL1	CEL1	5	112.2	267.776	0	0
CRL2	CRL1	OHL	5	110.1	633.4576	0	0
CRL1	CRL1	CTL1	5	111	446.4328	0.2561	6694.4
CRL1	CRL1	CRL1	5	111	446.4328	0.2561	6694.4
CRL1	CRL1	CEL1	5	112.2	267.776	0	0
CRL2	CRL1	HGA1	5	110.1	288.696	0.2179	18853.1
CTL1	CRL1	HGA1	5	110.1	288.696	0.2179	18853.1
CRL1	CRL1	HGA1	5	110.1	288.696	0.2179	18853.1
OHL	CRL1	HGA1	5	108.89	384.0912	0	0
CRL2	CEL1	CRL1	5	113	418.4	0	0
CRL2	CEL1	CEL1	5	123.5	401.664	0	0
CRL1	CEL1	CEL1	5	123.5	401.664	0	0
CRL2	CEL1	HEL1	5	116	334.72	0	0
CRL1	OHL	H	5	106	481.16	0	0
CTL2	CTL2	CL	5	108	435.136	0	0
CL	CTL2	HAL2	5	109.5	276.144	0.2163	25104
CTL2	CL	OHL	5	110.5	460.24	0	0
CTL2	CL	OBL	5	125	585.76	0.2442	16736
OHL	CL	OBL	5	123	418.4	0.2262	175728
CL	OHL	H	5	115	460.24	0	0
HGA3	CG331	HGA3	5	108.4	297.064	0.1802	4518.72
CG2R61	CG2R61	CG2R61	5	120	334.72	0.2416	29288
CG2R61	CG2R61	HGR61	5	120	251.04	0.2153	18409.6

CG311	CG331	HGA3	5	110.1	279.7422	0.2179	18853.1
CG311	CG321	CG2R61	5	107.5	433.4624	0	0
CG311	CG321	HGA2	5	110.1	279.7422	0.2179	18853.1
CG2R61	CG321	HGA2	5	107.5	412.5424	0	0
HGA2	CG321	HGA2	5	109	297.064	0.1802	4518.72
CG331	CG311	CG331	5	114	446.4328	0.2561	6694.4
CG331	CG311	CG321	5	114	446.4328	0.2561	6694.4
CG331	CG311	CG2O2	5	108	435.136	0	0
CG331	CG311	CG2O3	5	108	435.136	0	0
CG331	CG311	CG2R61	5	107.5	433.4624	0	0
CG331	CG311	HGA1	5	110.1	288.696	0.2179	18853.1
CG321	CG311	HGA1	5	110.1	288.696	0.2179	18853.1
CG2O2	CG311	CG2R61	5	107.5	433.4624	0	0
CG2O2	CG311	HGA1	5	109.5	418.4	0	0
CG2O3	CG311	CG2R61	5	107.5	433.4624	0	0
CG2O3	CG311	HGA1	5	109.5	418.4	0	0
CG2R61	CG311	HGA1	5	111	359.824	0	0
CG311	CG2O2	OG2D1	5	125	585.76	0.2442	16736
CG311	CG2O2	OG311	5	110.5	460.24	0	0
OG2D1	CG2O2	OG311	5	123	418.4	0.2262	175728
CG311	CG2O3	OG2D2	5	116	334.72	0.2353	41840
OG2D2	CG2O3	OG2D2	5	128	836.8	0.2259	58576
CG321	CG2R61	CG2R61	5	120	383.2544	0	0
CG311	CG2R61	CG2R61	5	120	383.2544	0	0
CG2O2	OG311	HGP1	5	115	460.24	0	0

[dihedraltypes]

atom1	atom2	atom3	atom4	func	d_ϕ	K_ϕ	n
HAL3	CTL3	CTL2	X	9	0	0.6694	3
CTL3	CTL2	CTL2	CTL2	9	0	0.6778	2
CTL3	CTL2	CTL2	CTL2	9	180	0.1966	3
CTL3	CTL2	CTL2	CTL2	9	0	0.4393	4
CTL3	CTL2	CTL2	CTL2	9	0	0.7406	5
CTL2	CTL2	CTL2	CTL2	9	0	0.4226	2
CTL2	CTL2	CTL2	CTL2	9	180	0.5941	3
CTL2	CTL2	CTL2	CTL2	9	0	0.3096	4
CTL2	CTL2	CTL2	CTL2	9	0	0.4058	5
CTL2	CTL2	CTL2	CEL1	9	180	0.5858	1
CTL2	CTL2	CTL2	CEL1	9	0	0.7113	2
CTL2	CTL2	CTL2	CEL1	9	180	0.2092	3
CTL2	CTL2	CTL2	C	9	180	0	5
CTL2	CTL2	CTL2	C	9	180	1.3263	3
CTL2	CTL2	CTL2	C	9	0	2.3305	2

CTL2	CTL2	CTL2	C	9	0	3.1506	1
CTL3	CTL2	CTL2	HAL2	9	0	0.795	3
CTL2	CTL2	CTL2	HAL2	9	0	0.795	3
CEL1	CTL2	CTL2	HAL2	9	0	0.795	3
C	CTL2	CTL2	HAL2	9	0	0.795	3
HAL2	CTL2	CTL2	HAL2	9	0	0.795	3
CTL2	CTL2	CEL1	CEL1	9	180	3.8074	1
CTL2	CTL2	CEL1	CEL1	9	180	0.7531	2
CTL2	CTL2	CEL1	CEL1	9	180	0.7113	3
CTL2	CTL2	CEL1	HEL1	9	0	0.5021	3
HAL2	CTL2	CEL1	CEL1	9	180	1.2552	3
HAL2	CTL2	CEL1	HEL1	9	0	0	3
CTL2	CTL2	C	O	9	0	5.8576	1
CTL2	CTL2	C	NHL	9	0	8.3262	1
CTL2	CTL2	C	NHL	9	180	2.6778	2
CTL2	CTL2	C	NHL	9	180	1.1715	3
HAL2	CTL2	C	O	9	180	0	3
HAL2	CTL2	C	NHL	9	0	0	3
OHL	CTO2	CTL1	CTO1	9	0	0.8368	3
OHL	CTO2	CTL1	NHL	9	0	2.3012	1
OHL	CTO2	CTL1	NHL	9	180	6.8199	2
OHL	CTO2	CTL1	NHL	9	180	5.9831	3
OHL	CTO2	CTL1	HAL1	9	0	0.8368	3
HAL2	CTO2	CTL1	CTO1	9	0	0.8368	3
HAL2	CTO2	CTL1	NHL	9	0	0.8368	3
HAL2	CTO2	CTL1	HAL1	9	0	0.8368	3
X	CTO2	OHL	H	9	0	0.5858	3
CTO2	CTL1	CTO1	CEL1	9	0	0	1
CTO2	CTL1	CTO1	OHL	9	0	0.8368	3
CTO2	CTL1	CTO1	HAL1	9	0	0.8368	3
NHL	CTL1	CTO1	CEL1	9	0	3.933	1
NHL	CTL1	CTO1	CEL1	9	180	3.6819	2
NHL	CTL1	CTO1	CEL1	9	0	8.7446	3
NHL	CTL1	CTO1	OHL	9	0	1.7573	1
NHL	CTL1	CTO1	OHL	9	180	6.4015	2
NHL	CTL1	CTO1	OHL	9	180	6.6107	3
NHL	CTL1	CTO1	HAL1	9	0	0.8368	3
HAL1	CTL1	CTO1	CEL1	9	0	0.8368	3
HAL1	CTL1	CTO1	OHL	9	0	0.8368	3
HAL1	CTL1	CTO1	HAL1	9	0	0.8368	3
CTO2	CTL1	NHL	C	9	0	17.0707	1
CTO2	CTL1	NHL	C	9	180	6.527	2

CTO2	CTL1	NHL	C	9	0	7.5312	3
CTO2	CTL1	NHL	H	9	0	0	1
CTO1	CTL1	NHL	C	9	0	17.0707	1
CTO1	CTL1	NHL	C	9	180	6.527	2
CTO1	CTL1	NHL	C	9	0	7.5312	3
CTO1	CTL1	NHL	H	9	0	0	1
HAL1	CTL1	NHL	C	9	0	0	1
HAL1	CTL1	NHL	H	9	0	0	1
CTL1	CTO1	CEL1	CEL1	9	0	3.5982	1
CTL1	CTO1	CEL1	CEL1	9	0	7.9914	2
CTL1	CTO1	CEL1	CEL1	9	180	6.3597	3
CTL1	CTO1	CEL1	HEL1	9	0	0.5021	3
OHL	CTO1	CEL1	CEL1	9	180	5.7739	1
OHL	CTO1	CEL1	CEL1	9	0	2.4267	2
OHL	CTO1	CEL1	CEL1	9	0	4.3095	3
OHL	CTO1	CEL1	HEL1	9	180	0.5021	3
HAL1	CTO1	CEL1	CEL1	9	0	0.1255	3
HAL1	CTO1	CEL1	HEL1	9	0	0	3
CTL1	CTO1	OHL	H	9	180	20.92	1
CTL1	CTO1	OHL	H	9	0	0.9205	2
CTL1	CTO1	OHL	H	9	180	4.6442	3
CEL1	CTO1	OHL	H	9	0	5.5647	1
HAL1	CTO1	OHL	H	9	0	0.5858	3
CTL2	CEL1	CEL1	CTO1	9	0	0.6276	1
CTL2	CEL1	CEL1	CTO1	9	180	35.564	2
CTL2	CEL1	CEL1	HEL1	9	180	0.6276	1
CTL2	CEL1	CEL1	HEL1	9	180	35.564	2
HEL1	CEL1	CEL1	CTO1	9	180	0.6276	1
HEL1	CEL1	CEL1	CTO1	9	180	35.564	2
HEL1	CEL1	CEL1	HEL1	9	180	4.184	2
CTL2	C	NHL	CTL1	9	0	0	1
CTL2	C	NHL	H	9	180	10.46	2
O	C	NHL	CTL1	9	180	10.46	2
O	C	NHL	H	9	0	2.2175	1
O	C	NHL	H	9	180	5.3137	2
O	C	NHL	H	9	0	0.5858	3
O	C	NHL	H	9	0	3.2635	4
X	CTL3	CTL1	X	9	0	0.8368	3
X	CTL3	CRL1	X	9	0	0.8368	3
CTL2	CTL2	CTL2	CTL1	9	0	0.795	3
CTL1	CTL2	CTL2	HAL2	9	0	0.795	3
CTL2	CTL2	CTL1	CTL3	9	0	0.8368	3

CTL2	CTL2	CTL1	HAL1	9	0	0.8368	3
HAL2	CTL2	CTL1	CTL3	9	0	0.8368	3
HAL2	CTL2	CTL1	CRL1	9	0	0.8368	3
CTL2	CTL2	CTL1	CRL1	9	180	0.5096	3
CTL2	CTL2	CTL1	CRL1	9	180	0.91	2
CTL2	CTL2	CTL1	CRL1	9	180	1.0033	1
HAL2	CTL2	CTL1	HAL1	9	0	0.8368	3
X	CRL2	CRL2	X	9	0	0.795	3
X	CRL2	CRL1	X	9	0	0.8368	3
CRL1	CRL2	CEL1	CRL1	9	180	1.2552	3
CRL1	CRL2	CEL1	CEL1	9	180	2.092	1
CRL1	CRL2	CEL1	CEL1	9	180	5.4392	3
CRL1	CRL2	CEL1	HEL1	9	0	0	3
HGA2	CRL2	CEL1	CRL1	9	0	0.1255	3
HGA2	CRL2	CEL1	CEL1	9	180	1.2552	3
HGA2	CRL2	CEL1	HEL1	9	0	0	3
CTL3	CTL1	CRL1	CRL2	9	0	0.8368	3
CTL3	CTL1	CRL1	CRL1	9	0	0.8368	3
CTL3	CTL1	CRL1	HGA1	9	0	0.8368	3
CTL2	CTL1	CRL1	CRL2	9	0	0.8368	3
CTL2	CTL1	CRL1	CRL1	9	0	0	3
CTL2	CTL1	CRL1	HGA1	9	0	0.8368	3
HAL1	CTL1	CRL1	CRL2	9	0	0.8368	3
HAL1	CTL1	CRL1	CRL1	9	0	0.8368	3
HAL1	CTL1	CRL1	HGA1	9	0	0.8368	3
CTL2	CTL1	CRL1	CRL1	9	0	0	3
X	CRL1	CRL1	X	9	0	0.8368	3
CTL3	CRL1	CEL1	CEL1	9	180	2.092	1
CTL3	CRL1	CEL1	CEL1	9	180	5.4392	3
CRL2	CRL1	CEL1	CEL1	9	180	2.092	1
CRL2	CRL1	CEL1	CEL1	9	180	5.4392	3
CRL1	CRL1	CEL1	CEL1	9	180	2.092	1
CRL1	CRL1	CEL1	CEL1	9	180	5.4392	3
CTL3	CRL1	CEL1	CRL2	9	180	0	3
CRL2	CRL1	CEL1	CRL2	9	180	1.2552	3
CRL1	CRL1	CEL1	CRL2	9	180	0	3
X	CRL1	OHL	X	9	0	0.5858	3
CRL2	CEL1	CEL1	CRL2	9	180	1.8828	1
CRL2	CEL1	CEL1	CRL2	9	180	35.564	2
CRL2	CEL1	CEL1	CRL1	9	180	1.8828	1
CRL2	CEL1	CEL1	CRL1	9	180	35.564	2
CRL2	CEL1	CEL1	HEL1	9	180	1.8828	1

CRL2	CEL1	CEL1	HEL1	9	180	35.564	2
CRL1	CEL1	CEL1	HEL1	9	180	1.8828	1
CRL1	CEL1	CEL1	HEL1	9	180	35.564	2
CTL2	CTL2	CTL2	CL	9	180	0	5
CTL2	CTL2	CTL2	CL	9	180	1.3263	3
CTL2	CTL2	CTL2	CL	9	0	2.3305	2
CTL2	CTL2	CTL2	CL	9	0	3.1506	1
CL	CTL2	CTL2	HAL2	9	0	0.795	3
CTL2	CTL2	CL	OHL	9	180	0.2092	6
CTL2	CTL2	CL	OBL	9	180	0.2092	6
HAL2	CTL2	CL	OHL	9	180	0	6
HAL2	CTL2	CL	OBL	9	180	0	6
X	CL	OHL	X	9	180	8.5772	2
CG2R61	CG2R61	CG2R61	CG2R61	9	180	12.9704	2
CG2R61	CG2R61	CG2R61	HGR61	9	180	17.5728	2
HGR61	CG2R61	CG2R61	HGR61	9	180	10.0416	2
HGA3	CG331	CG311	CG331	9	0	0.8159	3
HGA3	CG331	CG311	CG321	9	0	0.8368	3
HGA3	CG331	CG311	CG2O2	9	0	0.8368	3
HGA3	CG331	CG311	CG2O3	9	0	0.6694	3
HGA3	CG331	CG311	CG2R61	9	0	0.1674	3
HGA3	CG331	CG311	HGA1	9	0	0.8159	3
CG2R61	CG321	CG311	CG331	9	0	0.1674	3
CG2R61	CG321	CG311	HGA1	9	0	0.1674	3
HGA2	CG321	CG311	CG331	9	0	0.8368	3
HGA2	CG321	CG311	HGA1	9	0	0.8159	3
CG311	CG321	CG2R61	CG2R61	9	180	0.9623	2
HGA2	CG321	CG2R61	CG2R61	9	0	0.0084	6
CG331	CG311	CG2O2	OG2D1	9	180	0.2092	6
CG331	CG311	CG2O2	OG311	9	180	0.2092	6
CG2R61	CG311	CG2O2	OG2D1	9	180	0.2092	6
CG2R61	CG311	CG2O2	OG311	9	180	0.2092	6
HGA1	CG311	CG2O2	OG2D1	9	0	0	3
HGA1	CG311	CG2O2	OG311	9	180	0.2092	6
CG331	CG311	CG2O3	OG2D2	9	180	0.2092	6
CG2R61	CG311	CG2O3	OG2D2	9	0	0	1
HGA1	CG311	CG2O3	OG2D2	9	180	0.2092	6
CG331	CG311	CG2R61	CG2R61	9	180	0.9623	2
CG2O2	CG311	CG2R61	CG2R61	9	180	0.9623	2
CG2O3	CG311	CG2R61	CG2R61	9	180	0.9623	2
HGA1	CG311	CG2R61	CG2R61	9	180	0.4184	6
CG311	CG2O2	OG311	HGP1	9	180	8.5772	2

OG2D1	CG2O2	OG311	HGP1	9	180	14.4348	2
CG321	CG2R61	CG2R61	CG2R61	9	180	12.9704	2
CG321	CG2R61	CG2R61	HGR61	9	180	10.0416	2
CG311	CG2R61	CG2R61	CG2R61	9	180	12.9704	2
CG311	CG2R61	CG2R61	HGR61	9	180	10.0416	2
CG2R61	CG2R61	CG2R61	CG2R61	9	180	12.9704	2
atom1	atom2	atom3	atom4	func	ϕ_o	K_ϕ	
C	CTL2	NHL	O	2	0	1004.16	
NHL	C	CTL1	H	2	0	167.36	
OBL	CTL2	OHL	CL	2	0	836.8	
CG2O2	CG311	OG2D1	OG311	2	0	543.92	
CG2O3	OG2D2	OG2D2	CG311	2	0	803.33	

Table 4: MARTINI parameters for GROMACS input

MARTINI

[atomtypes]

type	mass	charge	ptype	σ	ϵ
P4	58	0	A	0	0
P3	55	0	A	0	0
Na	41	0	A	0	0
C11	39	0	A	0	0
C21	39	0	A	0	0
C1	56	0	A	0	0
C2	42	0	A	0	0
SP1	55	0	A	0	0
SC1	52	0	A	0	0
SC3	50	0	A	0	0
P4W	72	0	A	0	0
BP4	72	0	A	0	0

[nonbond_params]

B1	B2	func	C6	C12
Na	P4	1	0.17246744	0.00185906363
Na	P4W	1	0.17246744	0.00185906363
Na	P3	1	0.19402587	0.00209144666
Na	SP1	1	0.17246744	0.00185906363
Na	Na	1	0.17246744	0.00185906363
Na	SC3	1	0.11641552	0.001254868
Na	C2	1	0.11641552	0.001254868
Na	C1	1	0.11641552	0.001254868
Na	SC1	1	0.11641552	0.001254868
Na	C11	1	0.11641552	0.001254868

Na	C21	1	0.11641552	0.001254868
Na	BP4	1	0.17246744	0.00185906363
P4	P4	1	0.21558431	0.00232382957
P4	P4W	1	0.21558431	0.00232382957
P4	P3	1	0.21558431	0.00232382957
P4	SP1	1	0.17246744	0.00185906363
P4	SC3	1	0.11641552	0.001254868
P4	C2	1	0.0991687775	0.00106896157
P4	C1	1	0.0862337202	0.000929531816
P4	SC1	1	0.0862337202	0.000929531816
P4	C11	1	0.0862337202	0.000929531816
P4	C21	1	0.0862337202	0.000929531816
P4	BP4	1	0.76824045	0.0263479203
P3	P4W	1	0.21558431	0.00232382957
P3	P3	1	0.21558431	0.00232382957
P3	SP1	1	0.17246744	0.00185906363
P3	SC3	1	0.13366227	0.0014407743
P3	C2	1	0.11641552	0.001254868
P3	C1	1	0.0991687775	0.00106896157
P3	SC1	1	0.0991687775	0.00106896157
P3	C11	1	0.0991687775	0.00106896157
P3	C21	1	0.0991687775	0.00106896157
P3	BP4	1	0.21558431	0.00232382957
C1	P4W	1	0.0862337202	0.000929531816
C1	SP1	1	0.11641552	0.001254868
C1	SC3	1	0.15090901	0.00162668072
C1	C2	1	0.15090901	0.00162668072
C1	C1	1	0.15090901	0.00162668072
C1	SC1	1	0.15090901	0.00162668072
C1	C11	1	0.15090901	0.00162668072
C1	C21	1	0.15090901	0.00162668072
C1	BP4	1	0.0862337202	0.000929531816
C2	P4W	1	0.0991687775	0.00106896157
C2	SP1	1	0.13366227	0.0014407743
C2	SC3	1	0.15090901	0.00162668072
C2	C2	1	0.15090901	0.00162668072
C2	SC1	1	0.15090901	0.00162668072
C2	C11	1	0.15090901	0.00162668072
C2	C21	1	0.15090901	0.00162668072
C2	BP4	1	0.0991687775	0.00106896157
BP4	P4W	1	0.76824045	0.0263479203
BP4	SP1	1	0.17246744	0.00185906363

BP4	SC3	1	0.11641552	0.001254868
BP4	SC1	1	0.0862337202	0.000929531816
BP4	C11	1	0.0862337202	0.000929531816
BP4	C21	1	0.0862337202	0.000929531816
BP4	BP4	1	0.21558431	0.00232382957
SP1	P4W	1	0.19402587	0.00209144666
SP1	SP1	1	0.0758563504	0.000479515584
SP1	SC3	1	0.0663743094	0.000419576158
SP1	SC1	1	0.0512030423	0.000323673041
SP1	C11	1	0.11641552	0.001254868
SP1	C21	1	0.11641552	0.001254868
SC1	P4W	1	0.0862337202	0.000929531816
SC1	SC3	1	0.0663743094	0.000419576158
SC1	SC1	1	0.0663743094	0.000419576158
SC1	C11	1	0.15090901	0.00162668072
SC1	C21	1	0.15090901	0.00162668072
SC3	P4W	1	0.11641552	0.001254868
SC3	SC3	1	0.0663743094	0.000419576158
SC3	C11	1	0.15090901	0.00162668072
SC3	C21	1	0.15090901	0.00162668072
P4W	P4W	1	0.21558431	0.00232382957
P4W	C11	1	0.0862337202	0.000929531816
P4W	C21	1	0.0862337202	0.000929531816
C11	C11	1	0.15090901	0.00162668072
C11	C21	1	0.15090901	0.00162668072
C21	C21	1	0.15090901	0.00162668072

Table 5: Atoms abbreviations for Water molecule TIP3P

WaterTIP3P

[atoms]

no	type	resnr	resnm	name	cgnr	charge
1	OW	1	WAT	OW	1	-0.834
2	HW	1	WAT	HW1	1	0.417
3	HW	1	WAT	HW2	1	0.417
#ifdef	WATER_FLEXIBLE					

[bonds]

a1	a2	func	b_o	K_b
1	2	1	0.09572	443169
1	3	1	0.09572	443169

[angles]

a1	a2	a3	func	θ_o	K_θ	d_{HH}	K_{UB}

2	1	3	5	104.52	284.93	0.15193	32007.6
#else							
			[settles]				
OW	func	d_{OH}	d_{HH}				
1	1	0.09572	0.15139				
#endif							

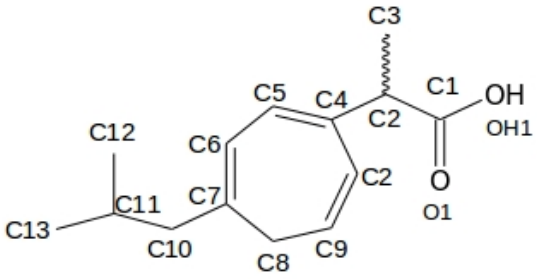

Figure 2: Atomistic representation of ibuprofen molecule

Table 6: Atoms abbreviation for Ibuprofen molecule

	IBU		
	atom	type	charge
1	C1	CG2O2	0.75
2	O1	OG2D1	-0.55
3	OH1	OG311	-0.61
4	HO1	HGP1	0.44
5	C2	CG311	-0.12
6	H2	HGA1	0.09
7	C3	CG331	-0.27
8	H3a	HGA3	0.09
9	H3b	HGA3	0.09
10	H3c	HGA3	0.09
11	C4	CG2R61	0
12	C5	CG2R61	-0.115
13	H5	HGR61	0.115
14	C6	CG2R61	-0.115
15	H6	HGR61	0.115
16	C7	CG2R61	0
17	C8	CG2R61	-0.115
18	H8	HGR61	0.115
19	C9	CG2R61	-0.115
20	H9	HGR61	0.115

21	C10	CG321	-0.18
22	H10a	HGA2	0.09
23	H10b	HGA2	0.09
24	C11	CG311	-0.09
25	H11	HGA1	0.09
26	C12	CG331	-0.27
27	H12a	HGA3	0.09
28	H12b	HGA3	0.09
29	H12c	HGA3	0.09
30	C13	CG331	-0.27
31	H13a	HGA3	0.09
32	H13b	HGA3	0.09
33	H13c	HGA3	0.09