Supplementary Information

MARTINI Force Field Parameters for Compound X

```
[moleculetype]
; molname       nrexcl
  CPX           2

[atoms]
; id    type    resnr   residue  atom    cgnr    charge
    1     P5      1     CPX       P01     1         0
    2     Na      1     CPX       N01     2         0
    3     SP1     1     CPX       S01     3         0
    4     SNa     1     CPX       S02     4         0
    5     Nd      1     CPX       N02     5         0
    6     SP2     1     CPX       S03     6         0
    7     SP1     1     CPX       S04     7         0
    8     SP1     1     CPX       S05     8         0
    9     SN0     1     CPX       S06     9         0
    10    SN0     1     CPX       S07     10        0

[bonds]
; i j     funct     length    force.c.
  1 2       1         0.382     15000
  1 5       1         0.304     15000
  5 6       1         0.280     15000

[constraints]
;  i   j     funct   length
    2   3     1       0.301
    3   4     1       0.125
    2   4     1       0.314
    6   7     1       0.122
    7   8     1       0.210
    6   8     1       0.204
    9  10     1       0.165
    8  9      1       0.245

[angles]
; i j k         funct   angle   force.c.
```

```
39      3 2 1       2       180   125.0
40      4 2 1       2       120   150.0
41      2 1 5       2       95    125.0
42      1 5 6       2       150    60.0
43      5 6 8       2       130    100.0
44      5 6 7       2       160   125.0
45      6 8 9       2       150    250.0
46      7 8 9       2       180    250.0
47      8 9 10      2       180    1000.0
48
49      [dihedrals]
50      ; i    j    k    l   funct   angle  force.c.
```