Supporting Information

Photophysics of BODIPY-Based Photosensitizer for Photodynamic Therapy: Surface Hopping and Classical Molecular Dynamics

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Table S1. Vertical excitation energies of BODIPY at TD-DFT (B3LYP/cc-pVDZ) level of theory

1) First 5 excited singlets RPAS (eV)	1) Oscillator strength	2) First 5 excited singlets URPA (eV)	2) Oscillator strength	3) First 5 excited triplets (RPAT) (eV)	4) First 5 excited triplets (close shell) URPA (eV)	4) Oscillator strength	5) First 5 excited triplets (open shell) URPA (eV)
3.129	0.343	3.129	0.343	1.576	1.576	0.118×10^{-14}	1.701
3.631	0.230	3.631	0.230	2.691	2.691	0.584×10^{-14}	2.914
3.745	0.260×10^{-01}	3.745	0.260×10^{-01}	2.893	2.893	0.355×10^{-15}	3.115
5.183	0.771×10^{-04}	5.183	0.771×10^{-04}	3.551	3.551	0.363×10^{-16}	3.853
5.210	0.324×10^{-01}	5.210	0.324×10^{-01}	4.871	4.871	0.935×10^{-14}	5.070

Table S2. Vertical excitation energies of 1-BODIPY at TD-DFT (B3LYP/cc-pVDZ) level of theory

1) First 5 excited singlets RPAS (eV)	1) Oscillator strength	2) First 5 excited singlets URPA (eV)	2) Oscillator strength	3) First 5 excited triplets (RPAT) (eV)	4) First 5 excited triplets (close shell) URPA (eV)	4) Oscillator strength	5) First 5 excited triplets (open shell) URPA (eV)
2.844	0.342	2.844	0.342	1.491	1.491	0.933×10^{-13}	1.617
3.158	0.347	3.158	0.347	2.431	2.431	0.178×10^{-11}	2.647
3.372	0.750×10^{-01}	3.372	0.750×10^{-01}	2.603	2.603	0.659×10^{-12}	2.811
4.332	0.396×10^{-05}	4.332	0.396×10^{-05}	3.399	3.399	0.525×10^{-11}	3.669
4.466	0.762×10^{-05}	4.466	0.760×10^{-05}	4.306	4.306	0.282×10^{-11}	4.410

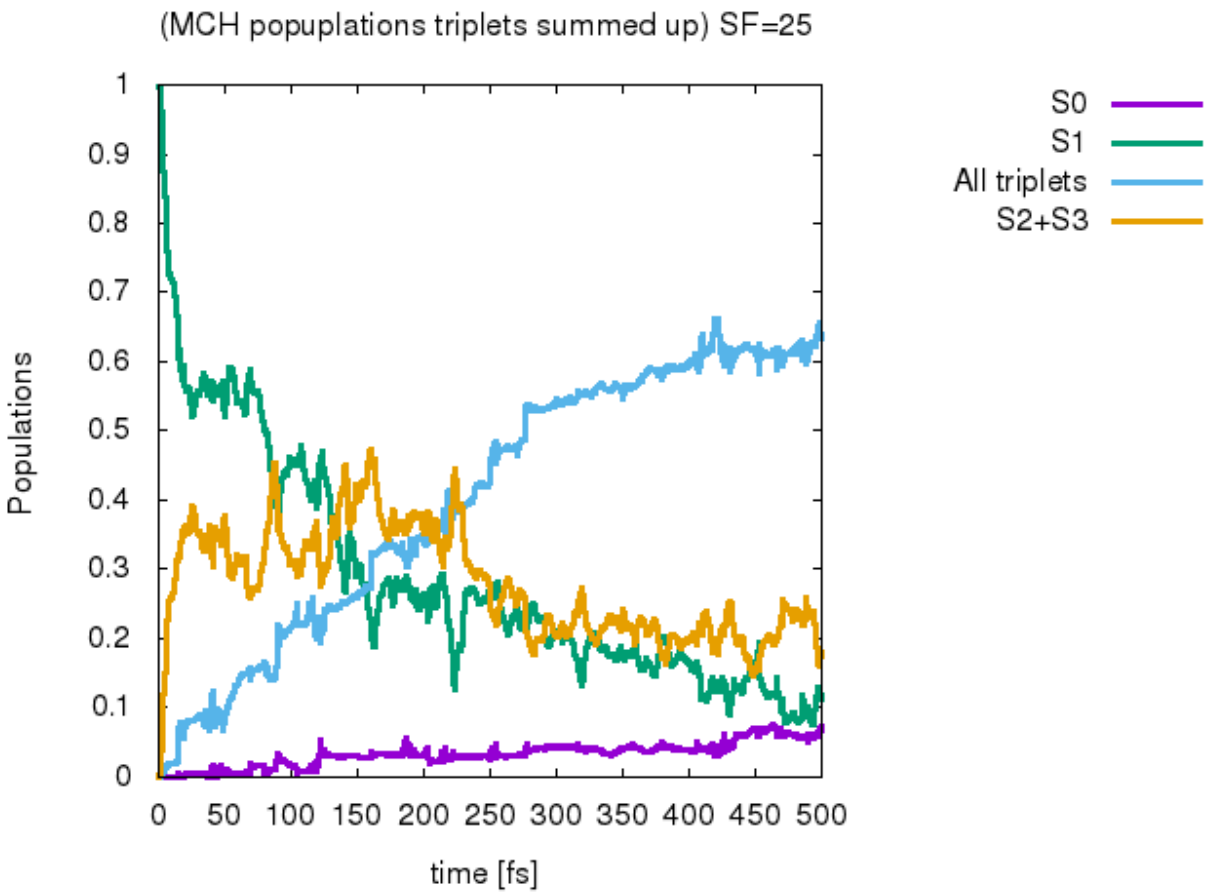

Fig. S1. Average adiabatic populations in benchmark trajectories using four singlet and three triplet states with scaling factor 25. When comparing with Fig. S2 it is evident that the additional states do not significantly alter the dynamics.

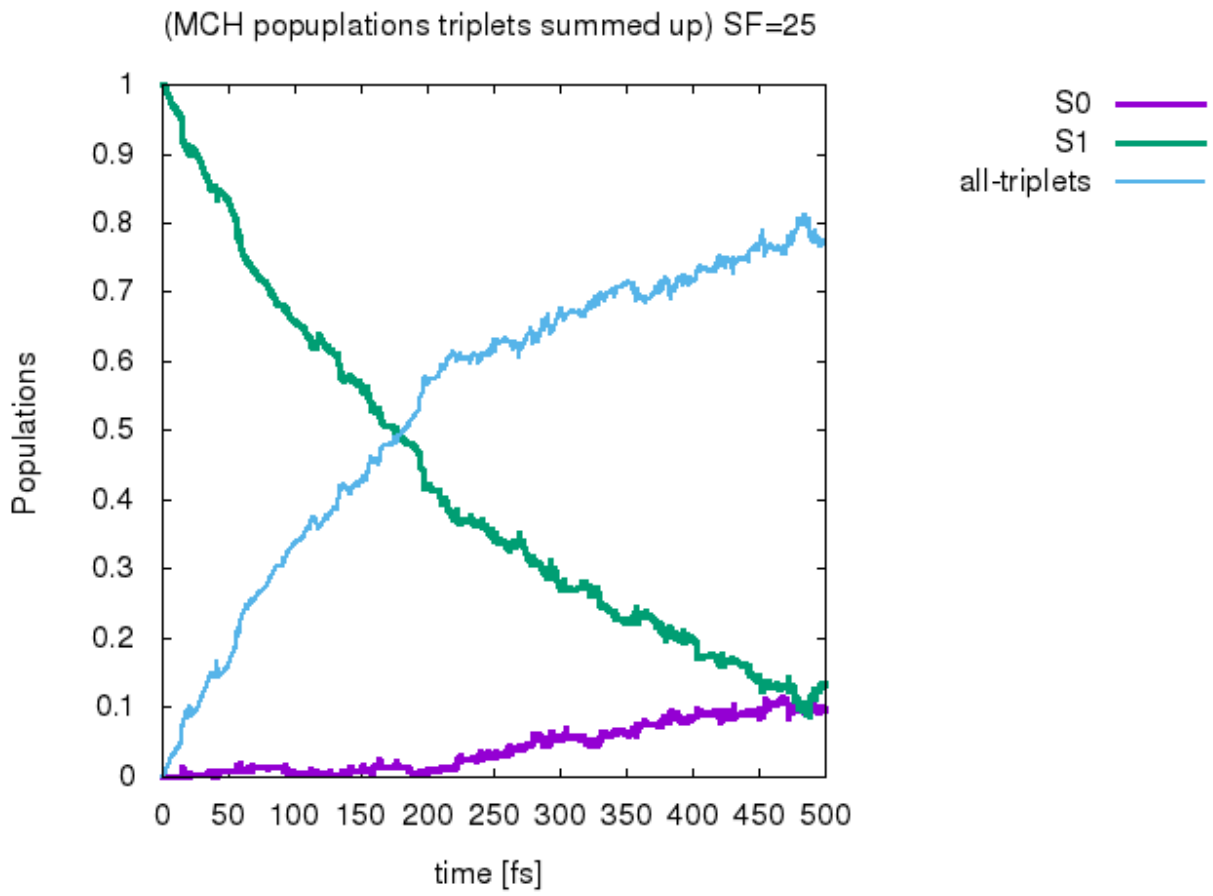

Fig. S2. Average adiabatic populations in singlets and triplets with scaling factor 25.

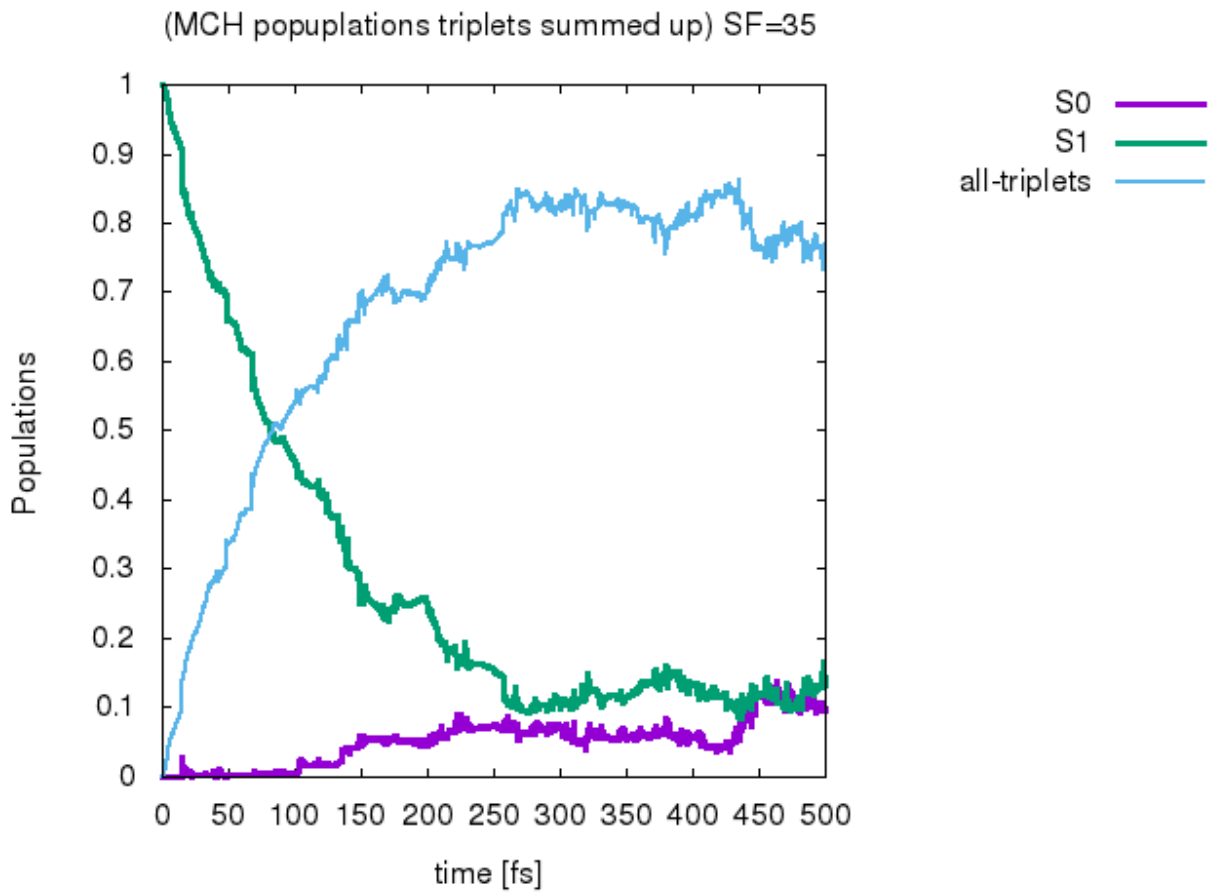

Fig. S3. Average adiabatic populations in singlets and triplets with scaling factor 35.

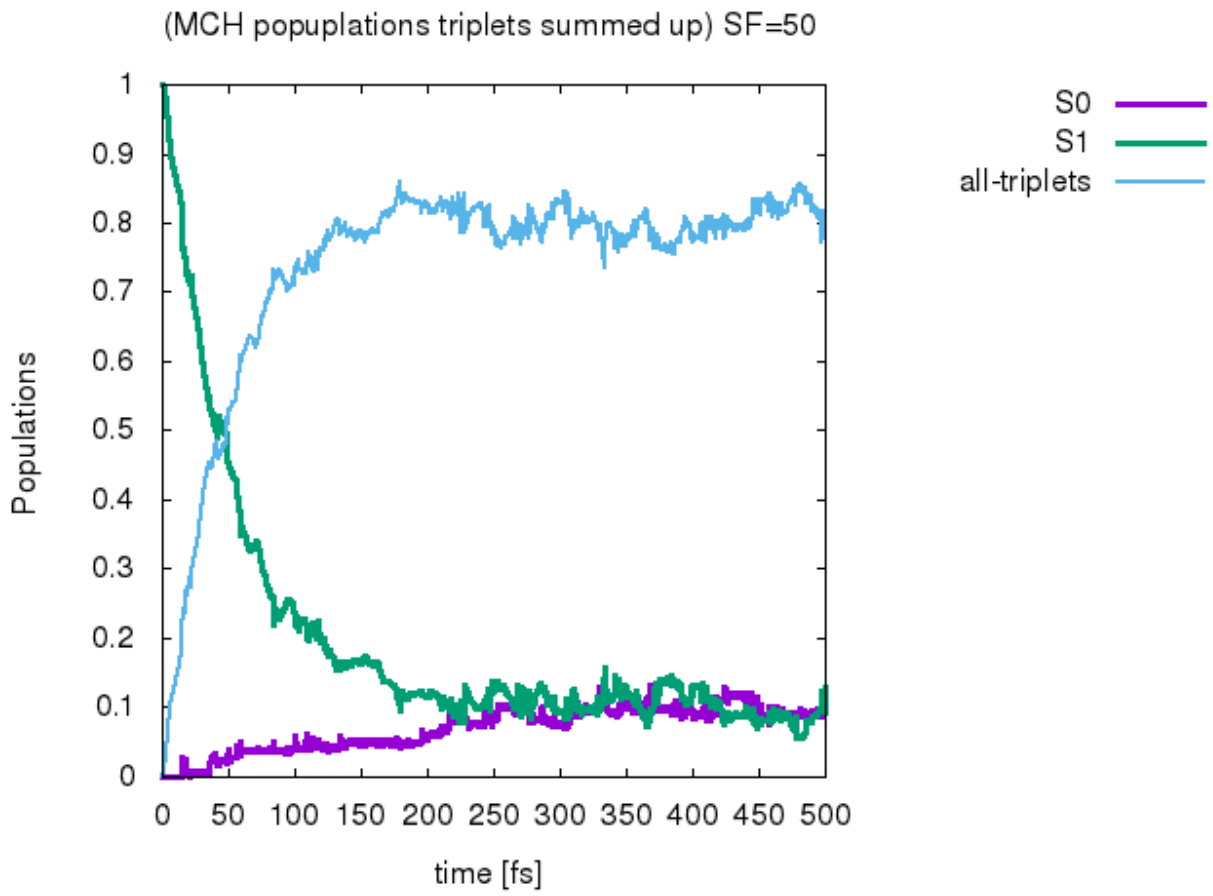

Fig. S4. Average adiabatic populations in singlets and triplets with scaling factor 50

Force field parameters for BODIPY

; by Lukasz Cwiklik, 2019, cwiklik.net

;[defaults]

;; nbfunc comb-rule gen-pairs fudgeLJ fudgeQQ

;1 2 yes 0.5 0.8333

[atomtypes]

;name bond_type mass charge ptype sigma epsilon Amb

f f 0.00000 0.00000 A 3.11815e-01 2.55224e-01; tzv: F params from ffnonbonded.itp fpr Amber

b b 0.00000 0.00000 A 3.56359e-01 1.04600e+00; tzv: S params here, as S similar in radius to B

na na 0.00000 0.00000 A 3.25000e-01 7.11280e-01 ; 1.82 0.1700

c2 c2 0.00000 0.00000 A 3.39967e-01 3.59824e-01 ; 1.91 0.0860

h4 h4 0.00000 0.00000 A 2.51055e-01 6.27600e-02 ; 1.41 0.0150

ha ha 0.00000 0.00000 A 2.59964e-01 6.27600e-02 ; 1.46 0.0150

[moleculetype]

;name nrexcl

BPS0 3

[atoms]

; nr type resi res atom cgnr charge mass ; qtot bond_type

1 f 1 BPS0 F1 1 -0.427675 18.99800 ; qtot -0.722 ;tzv - F atomic mass

2 b 1 BPS0 B1 2 0.765198 10.81000 ; qtot 1.190 ;tzv - B atomic mass

```
    3    f     1   BDS0    F2    3   -0.427675   18.99800 ; qtot 0.468  ;tzv - F atomic mass
    4   na     1   BPS0    N1    4    -0.122556     14.01000 ; qtot -0.272
    5   c2     1   BPS0    C1    5    -0.074172     12.01000 ; qtot -0.347
    6   h4     1   BPS0    H6    6     0.188072      1.00800 ; qtot -0.159
    7   c2     1   BPS0    C4    7    -0.192540     12.01000 ; qtot -0.351
    8   ha     1   BPS0    H1    8     0.165426      1.00800 ; qtot -0.186
    9   c2     1   BPS0    C3    9    -0.234936     12.01000 ; qtot -0.421
   10   ha     1   BPS0    H5   10     0.177426      1.00800 ; qtot -0.243
   11   c2     1   BPS0    C2   11     0.231841     12.01000 ; qtot -0.011
   12   c2     1   BPS0    C5   12    -0.343287     12.01000 ; qtot -0.355
   13   ha     1   BPS0    H7   13     0.216022      1.00800 ; qtot -0.139
   14   c2     1   BPS0    C9   14     0.231841     12.01000 ; qtot 0.093
   15   na     1   BPS0    N2   15    -0.122556     14.01000 ; qtot -0.029
   16   c2     1   BPS0    C6   16    -0.074172     12.01000 ; qtot -0.103
   17   h4     1   BPS0    H4   17     0.188072      1.00800 ; qtot 0.085
   18   c2     1   BPS0    C7   18    -0.192540     12.01000 ; qtot -0.108
   19   ha     1   BPS0    H2   19     0.165426      1.00800 ; qtot 0.058
   20   c2     1   BPS0    C8   20    -0.234936     12.01000 ; qtot -0.177
   21   ha     1   BPS0    H3   21     0.177426      1.00800 ; qtot 0.000


[ bonds ]
;   ai     aj funct   r             k
    1      2   1    2.4300e-01    1.4652e+05 ;     S1 - I1
    2      3   1    2.4300e-01    1.4652e+05 ;     I1 - S2
    2      4   1    2.1290e-01    2.1799e+05 ;     I1 - N1
    2     15   1    2.1290e-01    2.1799e+05 ;     I1 - N2
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```
    4     5   1    1.3910e-01    3.4401e+05 ;     N1 - C1
    4    11   1    1.3910e-01    3.4401e+05 ;     N1 - C2
    5     6   1    1.0840e-01    2.9171e+05 ;     C1 - H6
    5     7   1    1.3240e-01    4.9346e+05 ;     C1 - C4
    7     8   1    1.0870e-01    2.8811e+05 ;     C4 - H1
    7     9   1    1.3240e-01    4.9346e+05 ;     C4 - C3
    9    10   1    1.0870e-01    2.8811e+05 ;     C3 - H5
    9    11   1    1.3240e-01    4.9346e+05 ;     C3 - C2
   11    12   1    1.3240e-01    4.9346e+05 ;     C2 - C5
   12    13   1    1.0870e-01    2.8811e+05 ;     C5 - H7
   12    14   1    1.3240e-01    4.9346e+05 ;     C5 - C9
   14    15   1    1.3910e-01    3.4401e+05 ;     C9 - N2
   14    20   1    1.3240e-01    4.9346e+05 ;     C9 - C8
   15    16   1    1.3910e-01    3.4401e+05 ;     N2 - C6
   16    17   1    1.0840e-01    2.9171e+05 ;     C6 - H4
   16    18   1    1.3240e-01    4.9346e+05 ;     C6 - C7
   18    19   1    1.0870e-01    2.8811e+05 ;     C7 - H2
   18    20   1    1.3240e-01    4.9346e+05 ;     C7 - C8
   20    21   1    1.0870e-01    2.8811e+05 ;     C8 - H3

[ pairs ]
;   ai     aj    funct
    1      5      1 ;     S1 - C1
    1     11      1 ;     S1 - C2
    1     14      1 ;     S1 - C9
    1     16      1 ;     S1 - C6
```

2 6 1 ; I1 - H6

2 7 1 ; I1 - C4

2 9 1 ; I1 - C3

2 12 1 ; I1 - C5

2 17 1 ; I1 - H4

2 18 1 ; I1 - C7

2 20 1 ; I1 - C8

3 5 1 ; S2 - C1

3 11 1 ; S2 - C2

3 14 1 ; S2 - C9

3 16 1 ; S2 - C6

4 8 1 ; N1 - H1

4 10 1 ; N1 - H5

4 13 1 ; N1 - H7

4 14 1 ; N1 - C9

4 16 1 ; N1 - C6

5 10 1 ; C1 - H5

5 12 1 ; C1 - C5

5 15 1 ; C1 - N2

6 8 1 ; H6 - H1

6 9 1 ; H6 - C3

6 11 1 ; H6 - C2

7 12 1 ; C4 - C5

8 10 1 ; H1 - H5

8 11 1 ; H1 - C2

9 13 1 ; C3 - H7

```
    9    14     1 ;    C3 - C9
   10    12     1 ;    H5 - C5
   11    15     1 ;    C2 - N2
   11    20     1 ;    C2 - C8
   12    16     1 ;    C5 - C6
   12    18     1 ;    C5 - C7
   12    21     1 ;    C5 - H3
   13    15     1 ;    H7 - N2
   13    20     1 ;    H7 - C8
   14    17     1 ;    C9 - H4
   14    19     1 ;    C9 - H2
   15    19     1 ;    N2 - H2
   15    21     1 ;    N2 - H3
   16    21     1 ;    C6 - H3
   17    19     1 ;    H4 - H2
   17    20     1 ;    H4 - C8
   19    21     1 ;    H2 - H3

[ angles ]
;   ai    aj    ak    funct   theta         cth
    1     2     3      1    1.1000e+02    5.2894e+02 ;    S1 - I1    - S2
    1     2     4      1    1.1000e+02    5.2894e+02 ;    S1 - I1    - N1
    1     2    15      1    1.1000e+02    5.2894e+02 ;    S1 - I1    - N2
    2     4     5      1    1.0674e+02    4.9354e+02 ;    I1 - N1    - C1
    2     4    11      1    1.0674e+02    4.9354e+02 ;    I1 - N1    - C2
    2    15    14      1    1.0674e+02    4.9354e+02 ;    I1 - N2    - C9
```

2 15 16 1 1.0674e+02 4.9354e+02 ; I1 - N2 - C6

3 2 4 1 1.1000e+02 5.2894e+02 ; S2 - I1 - N1

3 2 15 1 1.1000e+02 5.2894e+02 ; S2 - I1 - N2

4 2 15 1 1.0700e+02 5.6216e+02 ; N1 - I1 - N2

4 5 6 1 1.1322e+02 4.2702e+02 ; N1 - C1 - H6

4 5 7 1 1.2138e+02 5.8434e+02 ; N1 - C1 - C4

4 11 9 1 1.2138e+02 5.8434e+02 ; N1 - C2 - C3

4 11 12 1 1.2138e+02 5.8434e+02 ; N1 - C2 - C5

5 4 11 1 1.1037e+02 5.6735e+02 ; C1 - N1 - C2

5 7 8 1 1.2094e+02 4.1873e+02 ; C1 - C4 - H1

5 7 9 1 1.2181e+02 5.8442e+02 ; C1 - C4 - C3

6 5 7 1 1.2254e+02 4.1631e+02 ; H6 - C1 - C4

7 9 10 1 1.2094e+02 4.1873e+02 ; C4 - C3 - H5

7 9 11 1 1.2181e+02 5.8442e+02 ; C4 - C3 - C2

8 7 9 1 1.2094e+02 4.1873e+02 ; H1 - C4 - C3

9 11 12 1 1.2181e+02 5.8442e+02 ; C3 - C2 - C5

10 9 11 1 1.2094e+02 4.1873e+02 ; H5 - C3 - C2

11 12 13 1 1.2094e+02 4.1873e+02 ; C2 - C5 - H7

11 12 14 1 1.2181e+02 5.8442e+02 ; C2 - C5 - C9

12 14 15 1 1.2138e+02 5.8434e+02 ; C5 - C9 - N2

12 14 20 1 1.2181e+02 5.8442e+02 ; C5 - C9 - C8

13 12 14 1 1.2094e+02 4.1873e+02 ; H7 - C5 - C9

14 15 16 1 1.1037e+02 5.6735e+02 ; C9 - N2 - C6

14 20 18 1 1.2181e+02 5.8442e+02 ; C9 - C8 - C7

14 20 21 1 1.2094e+02 4.1873e+02 ; C9 - C8 - H3

15 14 20 1 1.2138e+02 5.8434e+02 ; N2 - C9 - C8

15 16 17 1 1.1322e+02 4.2702e+02 ; N2 - C6 - H4

15 16 18 1 1.2138e+02 5.8434e+02 ; N2 - C6 - C7

16 18 19 1 1.2094e+02 4.1873e+02 ; C6 - C7 - H2

16 18 20 1 1.2181e+02 5.8442e+02 ; C6 - C7 - C8

17 16 18 1 1.2254e+02 4.1631e+02 ; H4 - C6 - C7

18 20 21 1 1.2094e+02 4.1873e+02 ; C7 - C8 - H3

19 18 20 1 1.2094e+02 4.1873e+02 ; H2 - C7 - C8

[dihedrals] ; propers

; treated as RBs in GROMACS to use combine multiple AMBER torsions per quartet

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2 4 5 6 3 5.23000 0.00000 -5.23000 0.00000 0.00000 0.00000 ; I1- N1- C1- H6

2 4 5 7 3 5.23000 0.00000 -5.23000 0.00000 0.00000 0.00000 ; I1- N1- C1- C4

2 4 11 9 3 5.23000 0.00000 -5.23000 0.00000 0.00000 0.00000 ; I1- N1- C2- C3

2 4 11 12 3 5.23000 0.00000 -5.23000 0.00000 0.00000 0.00000 ; I1- N1- C2- C5

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2 15 14 20 3 5.23000 0.00000 -5.23000 0.00000 0.00000 0.00000 ; I1- N2- C9- C8

2 15 16 17 3 5.23000 0.00000 -5.23000 0.00000 0.00000 0.00000 ; I1- N2- C6- H4

2 15 16 18 3 5.23000 0.00000 -5.23000 0.00000 0.00000 0.00000 ; I1- N2- C6- C7

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4 2 15 16 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N1- I1- N2- C6

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4 11 12 13 3 55.64720 0.00000 -55.64720 0.00000 0.00000 0.00000 ; N1- C2- C5- H7

4 11 12 14 3 55.64720 0.00000 -55.64720 0.00000 0.00000 0.00000 ; N1- C2- C5- C9

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5 4 11 12 3 5.23000 0.00000 -5.23000 0.00000 0.00000 0.00000 ; C1- N1- C2- C5

5 7 9 10 3 55.64720 0.00000 -55.64720 0.00000 0.00000 0.00000 ; C1- C4- C3- H5

5 7 9 11 3 55.64720 0.00000 -55.64720 0.00000 0.00000 0.00000 ; C1- C4- C3- C2

6 5 4 11 3 5.23000 0.00000 -5.23000 0.00000 0.00000 0.00000 ; H6- C1- N1- C2

6 5 7 8 3 55.64720 0.00000 -55.64720 0.00000 0.00000 0.00000 ; H6- C1- C4- H1

6 5 7 9 3 55.64720 0.00000 -55.64720 0.00000 0.00000 0.00000 ; H6- C1- C4- C3

7 5 4 11 3 5.23000 0.00000 -5.23000 0.00000 0.00000 0.00000 ; C4- C1- N1- C2

7 9 11 12 3 55.64720 0.00000 -55.64720 0.00000 0.00000 0.00000 ; C4- C3- C2- C5

8 7 9 10 3 55.64720 0.00000 -55.64720 0.00000 0.00000 0.00000 ; H1- C4- C3- H5

8 7 9 11 3 55.64720 0.00000 -55.64720 0.00000 0.00000 0.00000 ; H1- C4- C3- C2

9 11 12 13 3 55.64720 0.00000 -55.64720 0.00000 0.00000 0.00000 ; C3- C2- C5- H7

9 11 12 14 3 55.64720 0.00000 -55.64720 0.00000 0.00000 0.00000 ; C3- C2- C5- C9

10 9 11 12 3 55.64720 0.00000 -55.64720 0.00000 0.00000 0.00000 ; H5- C3- C2- C5

11 4 2 15 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C2- N1- I1- N2

11 12 14 15 3 55.64720 0.00000 -55.64720 0.00000 0.00000 0.00000 ; C2- C5- C9- N2

11 12 14 20 3 55.64720 0.00000 -55.64720 0.00000 0.00000 0.00000 ; C2- C5- C9- C8

12 14 15 16 3 5.23000 0.00000 -5.23000 0.00000 0.00000 0.00000 ; C5- C9- N2- C6

12 14 20 18 3 55.64720 0.00000 -55.64720 0.00000 0.00000 0.00000 ; C5- C9- C8- C7

12 14 20 21 3 55.64720 0.00000 -55.64720 0.00000 0.00000 0.00000 ; C5- C9- C8- H3

13 12 14 15 3 55.64720 0.00000 -55.64720 0.00000 0.00000 0.00000 ; H7- C5- C9- N2

13 12 14 20 3 55.64720 0.00000 -55.64720 0.00000 0.00000 0.00000 ; H7- C5- C9- C8

14 15 16 17 3 5.23000 0.00000 -5.23000 0.00000 0.00000 0.00000 ; C9- N2- C6- H4

14 15 16 18 3 5.23000 0.00000 -5.23000 0.00000 0.00000 0.00000 ; C9- N2- C6- C7

14 20 18 16 3 55.64720 0.00000 -55.64720 0.00000 0.00000 0.00000 ; C9- C8- C7- C6

14 20 18 19 3 55.64720 0.00000 -55.64720 0.00000 0.00000 0.00000 ; C9- C8- C7- H2

15 14 20 18 3 55.64720 0.00000 -55.64720 0.00000 0.00000 0.00000 ; N2- C9- C8- C7

15 14 20 21 3 55.64720 0.00000 -55.64720 0.00000 0.00000 0.00000 ; N2- C9- C8- H3

15 16 18 19 3 55.64720 0.00000 -55.64720 0.00000 0.00000 0.00000 ; N2- C6- C7- H2

15 16 18 20 3 55.64720 0.00000 -55.64720 0.00000 0.00000 0.00000 ; N2- C6- C7- C8

16 15 14 20 3 5.23000 0.00000 -5.23000 0.00000 0.00000 0.00000 ; C6- N2- C9- C8

16 18 20 21 3 55.64720 0.00000 -55.64720 0.00000 0.00000 0.00000 ; C6- C7- C8- H3

17 16 18 19 3 55.64720 0.00000 -55.64720 0.00000 0.00000 0.00000 ; H4- C6- C7- H2

17 16 18 20 3 55.64720 0.00000 -55.64720 0.00000 0.00000 0.00000 ; H4- C6- C7- C8

19 18 20 21 3 55.64720 0.00000 -55.64720 0.00000 0.00000 0.00000 ; H2- C7- C8- H3

; treated as usual propers in GROMACS since Phase angle diff from 0 or 180 degrees

; i j k l func phase kd pn

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1 2 4 11 1 60.00 0.00000 2 ; S1- I1- N1- C2

1 2 15 14 1 60.00 0.00000 2 ; S1- I1- N2- C9

1 2 15 16 1 60.00 0.00000 2 ; S1- I1- N2- C6

3 2 4 5 1 60.00 0.00000 2 ; S2- I1- N1- C1

3 2 4 11 1 60.00 0.00000 2 ; S2- I1- N1- C2

3 2 15 14 1 60.00 0.00000 2 ; S2- I1- N2- C9

```
    3     2    15    16     1    60.00   0.00000   2 ;    S2-   I1-   N2-   C6

[ dihedrals ] ; impropers
; treated as propers in GROMACS to use correct AMBER analytical function
;   i     j     k     l  func   phase     kd      pn
    5     9     7     8     1   180.00   4.60240   2 ;    C1-   C3-   C4-   H1
    5    11     4     2     1   180.00   4.60240   2 ;    C1-   C2-   N1-   I1
    7     6     5     4     1   180.00   4.60240   2 ;    C4-   H6-   C1-   N1
    7    11     9    10     1   180.00   4.60240   2 ;    C4-   C2-   C3-   H5
    9    12    11     4     1   180.00   4.60240   2 ;    C3-   C5-   C2-   N1
   11    14    12    13     1   180.00   4.60240   2 ;    C2-   C9-   C5-   H7
   12    20    14    15     1   180.00   4.60240   2 ;    C5-   C8-   C9-   N2
   14    16    15     2     1   180.00   4.60240   2 ;    C9-   C6-   N2-   I1
   14    18    20    21     1   180.00   4.60240   2 ;    C9-   C7-   C8-   H3
   16    20    18    19     1   180.00   4.60240   2 ;    C6-   C8-   C7-   H2
   18    17    16    15     1   180.00   4.60240   2 ;    C7-   H4-   C6-   N2
```

Force field parameters for 1-BODIPY S_0

```
; by Lukasz Cwiklik, 2019, cwiklik.net

;[ defaults ]
;; nbfunc        comb-rule       gen-pairs       fudgeLJ fudgeQQ
;1               2               yes             0.5     0.8333

[ atomtypes ]
;name   bond_type     mass     charge   ptype   sigma         epsilon       Amb
 f       f          0.00000  0.00000   A     3.11815e-01   2.55224e-01; tzv: F params from ffnonbonded.itp fpr Amber
 b       b          0.00000  0.00000   A     3.56359e-01   1.04600e+00; tzv: S params here, as S similar in radius to B
 na      na         0.00000  0.00000   A     3.25000e-01   7.11280e-01 ; 1.82  0.1700
 cc      cc         0.00000  0.00000   A     3.39967e-01   3.59824e-01 ; 1.91  0.0860
 c3      c3         0.00000  0.00000   A     3.39967e-01   4.57730e-01 ; 1.91  0.1094
 hc      hc         0.00000  0.00000   A     2.64953e-01   6.56888e-02 ; 1.49  0.0157
 cd      cd         0.00000  0.00000   A     3.39967e-01   3.59824e-01 ; 1.91  0.0860
 ce      ce         0.00000  0.00000   A     3.39967e-01   3.59824e-01 ; 1.91  0.0860
 ha      ha         0.00000  0.00000   A     2.59964e-01   6.27600e-02 ; 1.46  0.0150
 h4      h4         0.00000  0.00000   A     2.51055e-01   6.27600e-02 ; 1.41  0.0150
 br      br         0.00000  0.00000   A     3.59923e-01   1.75728e+00 ; 2.02  0.4200

[ moleculetype ]
;name            nrexcl
 BDS0             3
```

```
[ atoms ]
;   nr  type  resi  res  atom  cgnr     charge      mass       ; qtot   bond_type
     1    f     1   BDS0    F1    1  -0.418096     18.99800 ; qtot -0.722 ;tzv - F atomic mass
     2    b     1   BDS0    B1    2   0.708382     10.81000 ; qtot 1.190  ;tzv - B atomic mass
     3    f     1   BDS0    F2    3  -0.418096     18.99800 ; qtot 0.468  ;tzv - F atomic mass
     4   na     1   BDS0    N1    4  -0.360335     14.01000 ; qtot -0.577
     5   cc     1   BDS0    C1    5   0.512793     12.01000 ; qtot 0.038
     6   c3     1   BDS0   C13    6  -0.537274     12.01000 ; qtot -0.617
     7   hc     1   BDS0    H1    7   0.173528      1.00800 ; qtot -0.407
     8   hc     1   BDS0    H2    8   0.173528      1.00800 ; qtot -0.197
     9   hc     1   BDS0   H13    9   0.173528      1.00800 ; qtot 0.014
    10   cc     1   BDS0    C4   10  -0.401483     12.01000 ; qtot -0.292
    11   c3     1   BDS0   C11   11   0.212327     12.01000 ; qtot -0.204
    12   c3     1   BDS0   C12   12  -0.189140     12.01000 ; qtot -0.426
    13   hc     1   BDS0    H9   13   0.050740      1.00800 ; qtot -0.357
    14   hc     1   BDS0   H10   14   0.050740      1.00800 ; qtot -0.288
    15   hc     1   BDS0   H11   15   0.050740      1.00800 ; qtot -0.219
    16   hc     1   BDS0    H8   16  -0.003402      1.00800 ; qtot -0.186
    17   hc     1   BDS0   H12   17  -0.003402      1.00800 ; qtot -0.153
    18   cd     1   BDS0    C3   18   0.247818     12.01000 ; qtot -0.063
    19   c3     1   BDS0   C10   19  -0.354686     12.01000 ; qtot -0.502
    20   hc     1   BDS0    H3   20   0.118225      1.00800 ; qtot -0.354
    21   hc     1   BDS0    H4   21   0.118225      1.00800 ; qtot -0.205
    22   hc     1   BDS0    H5   22   0.118225      1.00800 ; qtot -0.056
    23   cd     1   BDS0    C2   23  -0.012684     12.01000 ; qtot 0.444
```

```
    24   ce     1   BDS0    C5   24  -0.157088     12.01000 ; qtot -0.180
    25   ha     1   BDS0    H7   25   0.154681      1.00800 ; qtot 0.070
    26   cc     1   BDS0    C6   26   0.198056     12.01000 ; qtot 0.712
    27   na     1   BDS0    N2   27  -0.061846     14.01000 ; qtot 0.028
    28   cc     1   BDS0    C7   28  -0.090009     12.01000 ; qtot 0.080
    29   h4     1   BDS0    H6   29   0.180866      1.00800 ; qtot 0.266
    30   cd     1   BDS0    C8   30  -0.049703     12.01000 ; qtot 0.134
    31   br     1   BDS0   BR1   31  -0.038126     79.90000 ; qtot 0.190
    32   cd     1   BDS0    C9   32  -0.134757     12.01000 ; qtot -0.070
    33   br     1   BDS0   BR2   33  -0.012274     79.90000 ; qtot 0.000

[ bonds ]
;   ai     aj funct   r             k
     1      2   1    1.9220e-01    2.0987e+05 ;     S1 - P1
     2      3   1    1.9220e-01    2.0987e+05 ;     P1 - S2
     2      4   1    1.7150e-01    2.7221e+05 ;     P1 - N1
     2     27   1    1.7150e-01    2.7221e+05 ;     P1 - N2
     4      5   1    1.3710e-01    3.6719e+05 ;     N1 - C1
     4     23   1    1.3710e-01    3.6719e+05 ;     N1 - C2
     5      6   1    1.4990e-01    2.8225e+05 ;     C1 - C13
     5     10   1    1.4290e-01    3.5003e+05 ;     C1 - C4
     6      7   1    1.0920e-01    2.8225e+05 ;    C13 - H1
     6      8   1    1.0920e-01    2.8225e+05 ;    C13 - H2
     6      9   1    1.0920e-01    2.8225e+05 ;    C13 - H13
    10     11   1    1.4990e-01    2.8225e+05 ;     C4 - C11
    10     18   1    1.3710e-01    4.2175e+05 ;     C4 - C3
```

```
    11     12   1    1.5350e-01    2.5363e+05 ;    C11 - C12
    11     16   1    1.0920e-01    2.8225e+05 ;    C11 - H8
    11     17   1    1.0920e-01    2.8225e+05 ;    C11 - H12
    12     13   1    1.0920e-01    2.8225e+05 ;    C12 - H9
    12     14   1    1.0920e-01    2.8225e+05 ;    C12 - H10
    12     15   1    1.0920e-01    2.8225e+05 ;    C12 - H11
    18     19   1    1.4990e-01    2.8225e+05 ;     C3 - C10
    18     23   1    1.4290e-01    3.5003e+05 ;     C3 - C2
    19     20   1    1.0920e-01    2.8225e+05 ;    C10 - H3
    19     21   1    1.0920e-01    2.8225e+05 ;    C10 - H4
    19     22   1    1.0920e-01    2.8225e+05 ;    C10 - H5
    23     24   1    1.3666e-01    4.2786e+05 ;     C2 - C5
    24     25   1    1.0890e-01    2.8577e+05 ;     C5 - H7
    24     26   1    1.4532e-01    3.2459e+05 ;     C5 - C6
    26     27   1    1.3710e-01    3.6719e+05 ;     C6 - N2
    26     32   1    1.3710e-01    4.2175e+05 ;     C6 - C9
    27     28   1    1.3710e-01    3.6719e+05 ;     N2 - C7
    28     29   1    1.0830e-01    2.9296e+05 ;     C7 - H6
    28     30   1    1.3710e-01    4.2175e+05 ;     C7 - C8
    30     31   1    1.8847e-01    2.3230e+05 ;     C8 - BR1
    30     32   1    1.4290e-01    3.5003e+05 ;     C8 - C9
    32     33   1    1.8847e-01    2.3230e+05 ;     C9 - BR2

[ pairs ]

;   ai     aj    funct

     1      5      1 ;     S1 - C1
```

```
1    23     1 ;    S1 - C2
1    26     1 ;    S1 - C6
1    28     1 ;    S1 - C7
2     6     1 ;    P1 - C13
2    10     1 ;    P1 - C4
2    18     1 ;    P1 - C3
2    24     1 ;    P1 - C5
2    29     1 ;    P1 - H6
2    30     1 ;    P1 - C8
2    32     1 ;    P1 - C9
3     5     1 ;    S2 - C1
3    23     1 ;    S2 - C2
3    26     1 ;    S2 - C6
3    28     1 ;    S2 - C7
4     7     1 ;    N1 - H1
4     8     1 ;    N1 - H2
4     9     1 ;    N1 - H13
4    11     1 ;    N1 - C11
4    19     1 ;    N1 - C10
4    25     1 ;    N1 - H7
4    26     1 ;    N1 - C6
4    28     1 ;    N1 - C7
5    12     1 ;    C1 - C12
5    16     1 ;    C1 - H8
5    17     1 ;    C1 - H12
5    19     1 ;    C1 - C10
```

5 24 1 ; C1 - C5

5 27 1 ; C1 - N2

6 11 1 ; C13 - C11

6 18 1 ; C13 - C3

6 23 1 ; C13 - C2

7 10 1 ; H1 - C4

8 10 1 ; H2 - C4

9 10 1 ; H13 - C4

10 13 1 ; C4 - H9

10 14 1 ; C4 - H10

10 15 1 ; C4 - H11

10 20 1 ; C4 - H3

10 21 1 ; C4 - H4

10 22 1 ; C4 - H5

10 24 1 ; C4 - C5

11 19 1 ; C11 - C10

11 23 1 ; C11 - C2

12 18 1 ; C12 - C3

13 16 1 ; H9 - H8

13 17 1 ; H9 - H12

14 16 1 ; H10 - H8

14 17 1 ; H10 - H12

15 16 1 ; H11 - H8

15 17 1 ; H11 - H12

16 18 1 ; H8 - C3

17 18 1 ; H12 - C3

```
    18     25      1 ;     C3 - H7
    18     26      1 ;     C3 - C6
    19     24      1 ;    C10 - C5
    20     23      1 ;     H3 - C2
    21     23      1 ;     H4 - C2
    22     23      1 ;     H5 - C2
    23     27      1 ;     C2 - N2
    23     32      1 ;     C2 - C9
    24     28      1 ;     C5 - C7
    24     30      1 ;     C5 - C8
    24     33      1 ;     C5 - BR2
    25     27      1 ;     H7 - N2
    25     32      1 ;     H7 - C9
    26     29      1 ;     C6 - H6
    26     31      1 ;     C6 - BR1
    27     31      1 ;     N2 - BR1
    27     33      1 ;     N2 - BR2
    28     33      1 ;     C7 - BR2
    29     31      1 ;     H6 - BR1
    29     32      1 ;     H6 - C9
    31     33      1 ;    BR1 - BR2

[ angles ]
;  ai    aj    ak    funct   theta       cth
    1     2     3     1    1.1413e+02    3.2945e+02 ;     S1 - P1     - S2
    1     2     4     1    1.1135e+02    5.3005e+02 ;     S1 - P1     - N1
```

1 2 27 1 1.1135e+02 5.3005e+02 ; S1 - P1 - N2

2 4 5 1 1.2470e+02 6.4275e+02 ; P1 - N1 - C1

2 4 23 1 1.2470e+02 6.4275e+02 ; P1 - N1 - C2

2 27 26 1 1.2470e+02 6.4275e+02 ; P1 - N2 - C6

2 27 28 1 1.2470e+02 6.4275e+02 ; P1 - N2 - C7

3 2 4 1 1.1135e+02 5.3005e+02 ; S2 - P1 - N1

3 2 27 1 1.1135e+02 5.3005e+02 ; S2 - P1 - N2

4 2 27 1 1.0857e+02 3.3941e+02 ; N1 - P1 - N2

4 5 6 1 1.2278e+02 5.4810e+02 ; N1 - C1 - C13

4 5 10 1 1.0680e+02 6.0425e+02 ; N1 - C1 - C4

4 23 18 1 1.0680e+02 6.0425e+02 ; N1 - C2 - C3

4 23 24 1 1.2371e+02 5.7589e+02 ; N1 - C2 - C5

5 4 23 1 1.2801e+02 5.3455e+02 ; C1 - N1 - C2

5 6 7 1 1.1086e+02 3.9497e+02 ; C1 - C13 - H1

5 6 8 1 1.1086e+02 3.9497e+02 ; C1 - C13 - H2

5 6 9 1 1.1086e+02 3.9497e+02 ; C1 - C13 - H13

5 10 11 1 1.1597e+02 5.4107e+02 ; C1 - C4 - C11

5 10 18 1 1.1419e+02 5.7036e+02 ; C1 - C4 - C3

6 5 10 1 1.1597e+02 5.4107e+02 ; C13 - C1 - C4

7 6 8 1 1.0835e+02 3.2995e+02 ; H1 - C13 - H2

7 6 9 1 1.0835e+02 3.2995e+02 ; H1 - C13 - H13

8 6 9 1 1.0835e+02 3.2995e+02 ; H2 - C13 - H13

10 11 12 1 1.1189e+02 5.3204e+02 ; C4 - C11 - C12

10 11 16 1 1.1086e+02 3.9497e+02 ; C4 - C11 - H8

10 11 17 1 1.1086e+02 3.9497e+02 ; C4 - C11 - H12

10 18 19 1 1.1945e+02 5.4233e+02 ; C4 - C3 - C10

10	18	23	1	1.1419e+02	5.7036e+02 ;	C4 - C3 - C2
11	10	18	1	1.1945e+02	5.4233e+02 ;	C11 - C4 - C3
11	12	13	1	1.1005e+02	3.8802e+02 ;	C11 - C12 - H9
11	12	14	1	1.1005e+02	3.8802e+02 ;	C11 - C12 - H10
11	12	15	1	1.1005e+02	3.8802e+02 ;	C11 - C12 - H11
12	11	16	1	1.1005e+02	3.8802e+02 ;	C12 - C11 - H8
12	11	17	1	1.1005e+02	3.8802e+02 ;	C12 - C11 - H12
13	12	14	1	1.0835e+02	3.2995e+02 ;	H9 - C12 - H10
13	12	15	1	1.0835e+02	3.2995e+02 ;	H9 - C12 - H11
14	12	15	1	1.0835e+02	3.2995e+02 ;	H10 - C12 - H11
16	11	17	1	1.0835e+02	3.2995e+02 ;	H8 - C11 - H12
18	19	20	1	1.1086e+02	3.9497e+02 ;	C3 - C10 - H3
18	19	21	1	1.1086e+02	3.9497e+02 ;	C3 - C10 - H4
18	19	22	1	1.1086e+02	3.9497e+02 ;	C3 - C10 - H5
18	23	24	1	1.2259e+02	5.5128e+02 ;	C3 - C2 - C5
19	18	23	1	1.1597e+02	5.4107e+02 ;	C10 - C3 - C2
20	19	21	1	1.0835e+02	3.2995e+02 ;	H3 - C10 - H4
20	19	22	1	1.0835e+02	3.2995e+02 ;	H3 - C10 - H5
21	19	22	1	1.0835e+02	3.2995e+02 ;	H4 - C10 - H5
23	24	25	1	1.1548e+02	4.1815e+02 ;	C2 - C5 - H7
23	24	26	1	1.3036e+02	5.2953e+02 ;	C2 - C5 - C6
24	26	27	1	1.2422e+02	5.5497e+02 ;	C5 - C6 - N2
24	26	32	1	1.2841e+02	5.3279e+02 ;	C5 - C6 - C9
25	24	26	1	1.1545e+02	3.9773e+02 ;	H7 - C5 - C6
26	27	28	1	1.0990e+02	5.7689e+02 ;	C6 - N2 - C7
26	32	30	1	1.1419e+02	5.7036e+02 ;	C6 - C9 - C8

26 32 33 1 1.2456e+02 5.2099e+02 ; C6 - C9 - BR2

27 26 32 1 1.0942e+02 6.1011e+02 ; N2 - C6 - C9

27 28 29 1 1.1966e+02 4.2024e+02 ; N2 - C7 - H6

27 28 30 1 1.0942e+02 6.1011e+02 ; N2 - C7 - C8

28 30 31 1 1.2456e+02 5.2099e+02 ; C7 - C8 - BR1

28 30 32 1 1.1419e+02 5.7036e+02 ; C7 - C8 - C9

29 28 30 1 1.2911e+02 3.9489e+02 ; H6 - C7 - C8

30 32 33 1 1.2489e+02 5.1731e+02 ; C8 - C9 - BR2

31 30 32 1 1.2489e+02 5.1731e+02 ; BR1 - C8 - C9

[dihedrals] ; propers

; treated as RBs in GROMACS to use combine multiple AMBER torsions per quartet

; i j k l func C0 C1 C2 C3 C4 C5

1 2 4 5 3 6.97333 0.00000 -6.97333 0.00000 0.00000 0.00000 ; S1- P1- N1- C1

1 2 4 23 3 6.97333 0.00000 -6.97333 0.00000 0.00000 0.00000 ; S1- P1- N1- C2

1 2 27 26 3 6.97333 0.00000 -6.97333 0.00000 0.00000 0.00000 ; S1- P1- N2- C6

1 2 27 28 3 6.97333 0.00000 -6.97333 0.00000 0.00000 0.00000 ; S1- P1- N2- C7

2 4 5 6 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; P1- N1- C1- C13

2 4 5 10 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; P1- N1- C1- C4

2 4 23 18 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; P1- N1- C2- C3

2 4 23 24 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; P1- N1- C2- C5

2 27 26 24 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; P1- N2- C6- C5

2 27 26 32 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; P1- N2- C6- C9

2 27 28 29 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; P1- N2- C7- H6

2 27 28 30 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; P1- N2- C7- C8

3 2 4 5 3 6.97333 0.00000 -6.97333 0.00000 0.00000 0.00000 ; S2- P1- N1- C1

3 2 4 23 3 6.97333 0.00000 -6.97333 0.00000 0.00000 0.00000 ; S2- P1- N1- C2

3 2 27 26 3 6.97333 0.00000 -6.97333 0.00000 0.00000 0.00000 ; S2- P1- N2- C6

3 2 27 28 3 6.97333 0.00000 -6.97333 0.00000 0.00000 0.00000 ; S2- P1- N2- C7

4 2 27 26 3 6.97333 0.00000 -6.97333 0.00000 0.00000 0.00000 ; N1- P1- N2- C6

4 2 27 28 3 6.97333 0.00000 -6.97333 0.00000 0.00000 0.00000 ; N1- P1- N2- C7

4 5 6 7 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N1- C1- C13- H1

4 5 6 8 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N1- C1- C13- H2

4 5 6 9 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N1- C1- C13- H13

4 5 10 11 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; N1- C1- C4- C11

4 5 10 18 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; N1- C1- C4- C3

4 23 18 10 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; N1- C2- C3- C4

4 23 18 19 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; N1- C2- C3- C10

4 23 24 25 3 8.36800 0.00000 -8.36800 0.00000 0.00000 0.00000 ; N1- C2- C5- H7

4 23 24 26 3 8.36800 0.00000 -8.36800 0.00000 0.00000 0.00000 ; N1- C2- C5- C6

5 4 2 27 3 6.97333 0.00000 -6.97333 0.00000 0.00000 0.00000 ; C1- N1- P1- N2

5 4 23 18 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; C1- N1- C2- C3

5 4 23 24 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; C1- N1- C2- C5

5 10 11 12 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C1- C4- C11- C12

5 10 11 16 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C1- C4- C11- H8

5 10 11 17 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C1- C4- C11- H12

5 10 18 19 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C1- C4- C3- C10

5 10 18 23 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C1- C4- C3- C2

6 5 4 23 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; C13- C1- N1- C2

6 5 10 11 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C13- C1- C4- C11

6 5 10 18 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C13- C1- C4- C3

7 6 5 10 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H1- C13- C1- C4

8 6 5 10 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H2- C13- C1- C4

9 6 5 10 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H13- C13- C1- C4

10 5 4 23 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; C4- C1- N1- C2

10 11 12 13 3 0.65084 1.95253 0.00000 -2.60338 0.00000 0.00000 ; C4- C11- C12- H9

10 11 12 14 3 0.65084 1.95253 0.00000 -2.60338 0.00000 0.00000 ; C4- C11- C12- H10

10 11 12 15 3 0.65084 1.95253 0.00000 -2.60338 0.00000 0.00000 ; C4- C11- C12- H11

10 18 19 20 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C4- C3- C10- H3

10 18 19 21 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C4- C3- C10- H4

10 18 19 22 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C4- C3- C10- H5

10 18 23 24 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C4- C3- C2- C5

11 10 18 19 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C11- C4- C3- C10

11 10 18 23 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C11- C4- C3- C2

12 11 10 18 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C12- C11- C4- C3

13 12 11 16 3 0.62760 1.88280 0.00000 -2.51040 0.00000 0.00000 ; H9- C12- C11- H8

13 12 11 17 3 0.62760 1.88280 0.00000 -2.51040 0.00000 0.00000 ; H9- C12- C11- H12

14 12 11 16 3 0.62760 1.88280 0.00000 -2.51040 0.00000 0.00000 ; H10- C12- C11- H8

14 12 11 17 3 0.62760 1.88280 0.00000 -2.51040 0.00000 0.00000 ; H10- C12- C11- H12

15 12 11 16 3 0.62760 1.88280 0.00000 -2.51040 0.00000 0.00000 ; H11- C12- C11- H8

15 12 11 17 3 0.62760 1.88280 0.00000 -2.51040 0.00000 0.00000 ; H11- C12- C11- H12

16 11 10 18 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H8- C11- C4- C3

17 11 10 18 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H12- C11- C4- C3

18 23 24 25 3 8.36800 0.00000 -8.36800 0.00000 0.00000 0.00000 ; C3- C2- C5- H7

18 23 24 26 3 8.36800 0.00000 -8.36800 0.00000 0.00000 0.00000 ; C3- C2- C5- C6

19 18 23 24 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C10- C3- C2- C5

20 19 18 23 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H3- C10- C3- C2

21 19 18 23 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H4- C10- C3- C2

22 19 18 23 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H5- C10- C3- C2

23 4 2 27 3 6.97333 0.00000 -6.97333 0.00000 0.00000 0.00000 ; C2- N1- P1- N2

23 24 26 27 3 8.36800 0.00000 -8.36800 0.00000 0.00000 0.00000 ; C2- C5- C6- N2

23 24 26 32 3 8.36800 0.00000 -8.36800 0.00000 0.00000 0.00000 ; C2- C5- C6- C9

24 26 27 28 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; C5- C6- N2- C7

24 26 32 30 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C5- C6- C9- C8

24 26 32 33 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C5- C6- C9- BR2

25 24 26 27 3 8.36800 0.00000 -8.36800 0.00000 0.00000 0.00000 ; H7- C5- C6- N2

25 24 26 32 3 8.36800 0.00000 -8.36800 0.00000 0.00000 0.00000 ; H7- C5- C6- C9

26 27 28 29 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; C6- N2- C7- H6

26 27 28 30 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; C6- N2- C7- C8

26 32 30 28 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C6- C9- C8- C7

26 32 30 31 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C6- C9- C8- BR1

27 26 32 30 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; N2- C6- C9- C8

27 26 32 33 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; N2- C6- C9- BR2

27 28 30 31 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; N2- C7- C8- BR1

27 28 30 32 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; N2- C7- C8- C9

28 27 26 32 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; C7- N2- C6- C9

28 30 32 33 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C7- C8- C9- BR2

29 28 30 31 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; H6- C7- C8- BR1

29 28 30 32 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; H6- C7- C8- C9

31 30 32 33 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; BR1- C8- C9- BR2

[dihedrals] ; impropers

; treated as propers in GROMACS to use correct AMBER analytical function

; i j k l func phase kd pn

5 23 4 2 1 180.00 4.60240 2 ; C1- C2- N1- P1

6 10 5 4 1 180.00 4.60240 2 ; C13- C4- C1- N1

11 5 10 18 1 180.00 4.60240 2 ; C11- C1- C4- C3

18 24 23 4 1 180.00 4.60240 2 ; C3- C5- C2- N1

19 10 18 23 1 180.00 4.60240 2 ; C10- C4- C3- C2

26 23 24 25 1 180.00 4.60240 2 ; C6- C2- C5- H7

26 28 27 2 1 180.00 4.60240 2 ; C6- C7- N2- P1

30 29 28 27 1 180.00 4.60240 2 ; C8- H6- C7- N2

31 28 30 32 1 180.00 4.60240 2 ; BR1- C7- C8- C9

32 24 26 27 1 180.00 4.60240 2 ; C9- C5- C6- N2

33 26 32 30 1 180.00 4.60240 2 ; BR2- C6- C9- C8

Force field parameters for 1-BODIPY S_1

; by Lukasz Cwiklik, 2019, cwiklik.net

;[defaults]

;; nbfunc comb-rule gen-pairs fudgeLJ fudgeQQ

;1 2 yes 0.5 0.8333

[atomtypes]

;name bond_type mass charge ptype sigma epsilon Amb

f f 0.00000 0.00000 A 3.11815e-01 2.55224e-01; tzv: F params from ffnonbonded.itp fpr Amber

b b 0.00000 0.00000 A 3.56359e-01 1.04600e+00; tzv: S params here, as S similar in radius to B

na na 0.00000 0.00000 A 3.25000e-01 7.11280e-01 ; 1.82 0.1700

cc cc 0.00000 0.00000 A 3.39967e-01 3.59824e-01 ; 1.91 0.0860

c3 c3 0.00000 0.00000 A 3.39967e-01 4.57730e-01 ; 1.91 0.1094

hc hc 0.00000 0.00000 A 2.64953e-01 6.56888e-02 ; 1.49 0.0157

cd cd 0.00000 0.00000 A 3.39967e-01 3.59824e-01 ; 1.91 0.0860

ce ce 0.00000 0.00000 A 3.39967e-01 3.59824e-01 ; 1.91 0.0860

ha ha 0.00000 0.00000 A 2.59964e-01 6.27600e-02 ; 1.46 0.0150

h4 h4 0.00000 0.00000 A 2.51055e-01 6.27600e-02 ; 1.41 0.0150

br br 0.00000 0.00000 A 3.59923e-01 1.75728e+00 ; 2.02 0.4200

[moleculetype]

;name nrexcl

BDS1 3

```
[ atoms ]
;   nr  type  resi  res  atom  cgnr     charge      mass       ; qtot   bond_type
     1    f     1   BDS1    F1    1   -0.423529    18.99800 ; qtot -0.722 ;tzv - F atomic mass
     2    b     1   BDS1    B1    2    0.727143    10.81000 ; qtot 1.190  ;tzv - B atomic mass
     3    f     1   BDS1    F2    3   -0.423529    18.99800 ; qtot 0.468  ;tzv - F atomic mass
     4   na     1   BDS1    N1    4   -0.411372    14.01000 ; qtot -0.577
     5   cc     1   BDS1    C1    5    0.487960    12.01000 ; qtot 0.038
     6   c3     1   BDS1   C13    6   -0.544652    12.01000 ; qtot -0.617
     7   hc     1   BDS1    H1    7    0.171552     1.00800 ; qtot -0.407
     8   hc     1   BDS1    H2    8    0.171552     1.00800 ; qtot -0.197
     9   hc     1   BDS1   H13    9    0.171552     1.00800 ; qtot 0.014
    10   cc     1   BDS1    C4   10   -0.382355    12.01000 ; qtot -0.292
    11   c3     1   BDS1   C11   11    0.227611    12.01000 ; qtot -0.204
    12   c3     1   BDS1   C12   12   -0.184907    12.01000 ; qtot -0.426
    13   hc     1   BDS1    H9   13    0.050405     1.00800 ; qtot -0.357
    14   hc     1   BDS1   H10   14    0.050405     1.00800 ; qtot -0.288
    15   hc     1   BDS1   H11   15    0.050405     1.00800 ; qtot -0.219
    16   hc     1   BDS1    H8   16   -0.004848     1.00800 ; qtot -0.186
    17   hc     1   BDS1   H12   17   -0.004848     1.00800 ; qtot -0.153
    18   cd     1   BDS1    C3   18    0.184138    12.01000 ; qtot -0.063
    19   c3     1   BDS1   C10   19   -0.327258    12.01000 ; qtot -0.502
    20   hc     1   BDS1    H3   20    0.105882     1.00800 ; qtot -0.354
    21   hc     1   BDS1    H4   21    0.105882     1.00800 ; qtot -0.205
    22   hc     1   BDS1    H5   22    0.105882     1.00800 ; qtot -0.056
    23   cd     1   BDS1    C2   23    0.144233    12.01000 ; qtot 0.444
    24   ce     1   BDS1    C5   24   -0.378578    12.01000 ; qtot -0.180
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    25   ha     1   BDS1    H7   25    0.166813     1.00800 ; qtot 0.070
    26   cc     1   BDS1    C6   26    0.361878    12.01000 ; qtot 0.712
    27   na     1   BDS1    N2   27   -0.077110    14.01000 ; qtot 0.028
    28   cc     1   BDS1    C7   28   -0.114710    12.01000 ; qtot 0.080
    29   h4     1   BDS1    H6   29    0.181227     1.00800 ; qtot 0.266
    30   cd     1   BDS1    C8   30   -0.014084    12.01000 ; qtot 0.134
    31   br     1   BDS1   BR1   31    0.039468    79.90000 ; qtot 0.190
    32   cd     1   BDS1    C9   32   -0.191462    12.01000 ; qtot -0.070
    33   br     1   BDS1   BR2   33   -0.020747    79.90000 ; qtot 0.000


[ bonds ]
;   ai     aj funct   r             k
     1      2   1    1.9220e-01    2.0987e+05 ;     S1 - P1
     2      3   1    1.9220e-01    2.0987e+05 ;     P1 - S2
     2      4   1    1.7150e-01    2.7221e+05 ;     P1 - N1
     2     27   1    1.7150e-01    2.7221e+05 ;     P1 - N2
     4      5   1    1.3710e-01    3.6719e+05 ;     N1 - C1
     4     23   1    1.3710e-01    3.6719e+05 ;     N1 - C2
     5      6   1    1.4990e-01    2.8225e+05 ;     C1 - C13
     5     10   1    1.4290e-01    3.5003e+05 ;     C1 - C4
     6      7   1    1.0920e-01    2.8225e+05 ;    C13 - H1
     6      8   1    1.0920e-01    2.8225e+05 ;    C13 - H2
     6      9   1    1.0920e-01    2.8225e+05 ;    C13 - H13
    10     11   1    1.4990e-01    2.8225e+05 ;     C4 - C11
    10     18   1    1.3710e-01    4.2175e+05 ;     C4 - C3
    11     12   1    1.5350e-01    2.5363e+05 ;    C11 - C12
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    11     16   1    1.0920e-01    2.8225e+05 ;    C11 - H8
    11     17   1    1.0920e-01    2.8225e+05 ;    C11 - H12
    12     13   1    1.0920e-01    2.8225e+05 ;    C12 - H9
    12     14   1    1.0920e-01    2.8225e+05 ;    C12 - H10
    12     15   1    1.0920e-01    2.8225e+05 ;    C12 - H11
    18     19   1    1.4990e-01    2.8225e+05 ;     C3 - C10
    18     23   1    1.4290e-01    3.5003e+05 ;     C3 - C2
    19     20   1    1.0920e-01    2.8225e+05 ;    C10 - H3
    19     21   1    1.0920e-01    2.8225e+05 ;    C10 - H4
    19     22   1    1.0920e-01    2.8225e+05 ;    C10 - H5
    23     24   1    1.3666e-01    4.2786e+05 ;     C2 - C5
    24     25   1    1.0890e-01    2.8577e+05 ;     C5 - H7
    24     26   1    1.4532e-01    3.2459e+05 ;     C5 - C6
    26     27   1    1.3710e-01    3.6719e+05 ;     C6 - N2
    26     32   1    1.3710e-01    4.2175e+05 ;     C6 - C9
    27     28   1    1.3710e-01    3.6719e+05 ;     N2 - C7
    28     29   1    1.0830e-01    2.9296e+05 ;     C7 - H6
    28     30   1    1.3710e-01    4.2175e+05 ;     C7 - C8
    30     31   1    1.8847e-01    2.3230e+05 ;     C8 - BR1
    30     32   1    1.4290e-01    3.5003e+05 ;     C8 - C9
    32     33   1    1.8847e-01    2.3230e+05 ;     C9 - BR2

[ pairs ]
;   ai     aj    funct
     1      5      1 ;     S1 - C1
     1     23      1 ;     S1 - C2
```

1 26 1 ; S1 - C6

1 28 1 ; S1 - C7

2 6 1 ; P1 - C13

2 10 1 ; P1 - C4

2 18 1 ; P1 - C3

2 24 1 ; P1 - C5

2 29 1 ; P1 - H6

2 30 1 ; P1 - C8

2 32 1 ; P1 - C9

3 5 1 ; S2 - C1

3 23 1 ; S2 - C2

3 26 1 ; S2 - C6

3 28 1 ; S2 - C7

4 7 1 ; N1 - H1

4 8 1 ; N1 - H2

4 9 1 ; N1 - H13

4 11 1 ; N1 - C11

4 19 1 ; N1 - C10

4 25 1 ; N1 - H7

4 26 1 ; N1 - C6

4 28 1 ; N1 - C7

5 12 1 ; C1 - C12

5 16 1 ; C1 - H8

5 17 1 ; C1 - H12

5 19 1 ; C1 - C10

5 24 1 ; C1 - C5

5 27 1 ; C1 - N2

6 11 1 ; C13 - C11

6 18 1 ; C13 - C3

6 23 1 ; C13 - C2

7 10 1 ; H1 - C4

8 10 1 ; H2 - C4

9 10 1 ; H13 - C4

10 13 1 ; C4 - H9

10 14 1 ; C4 - H10

10 15 1 ; C4 - H11

10 20 1 ; C4 - H3

10 21 1 ; C4 - H4

10 22 1 ; C4 - H5

10 24 1 ; C4 - C5

11 19 1 ; C11 - C10

11 23 1 ; C11 - C2

12 18 1 ; C12 - C3

13 16 1 ; H9 - H8

13 17 1 ; H9 - H12

14 16 1 ; H10 - H8

14 17 1 ; H10 - H12

15 16 1 ; H11 - H8

15 17 1 ; H11 - H12

16 18 1 ; H8 - C3

17 18 1 ; H12 - C3

18 25 1 ; C3 - H7

```
    18     26      1 ;     C3 - C6
    19     24      1 ;    C10 - C5
    20     23      1 ;     H3 - C2
    21     23      1 ;     H4 - C2
    22     23      1 ;     H5 - C2
    23     27      1 ;     C2 - N2
    23     32      1 ;     C2 - C9
    24     28      1 ;     C5 - C7
    24     30      1 ;     C5 - C8
    24     33      1 ;     C5 - BR2
    25     27      1 ;     H7 - N2
    25     32      1 ;     H7 - C9
    26     29      1 ;     C6 - H6
    26     31      1 ;     C6 - BR1
    27     31      1 ;     N2 - BR1
    27     33      1 ;     N2 - BR2
    28     33      1 ;     C7 - BR2
    29     31      1 ;     H6 - BR1
    29     32      1 ;     H6 - C9
    31     33      1 ;    BR1 - BR2

[ angles ]
;   ai     aj     ak    funct   theta         cth
      1      2      3       1    1.1413e+02    3.2945e+02 ;     S1 - P1     - S2
      1      2      4       1    1.1135e+02    5.3005e+02 ;     S1 - P1     - N1
      1      2     27       1    1.1135e+02    5.3005e+02 ;     S1 - P1     - N2
```

2 4 5 1 1.2470e+02 6.4275e+02 ; P1 - N1 - C1

2 4 23 1 1.2470e+02 6.4275e+02 ; P1 - N1 - C2

2 27 26 1 1.2470e+02 6.4275e+02 ; P1 - N2 - C6

2 27 28 1 1.2470e+02 6.4275e+02 ; P1 - N2 - C7

3 2 4 1 1.1135e+02 5.3005e+02 ; S2 - P1 - N1

3 2 27 1 1.1135e+02 5.3005e+02 ; S2 - P1 - N2

4 2 27 1 1.0857e+02 3.3941e+02 ; N1 - P1 - N2

4 5 6 1 1.2278e+02 5.4810e+02 ; N1 - C1 - C13

4 5 10 1 1.0680e+02 6.0425e+02 ; N1 - C1 - C4

4 23 18 1 1.0680e+02 6.0425e+02 ; N1 - C2 - C3

4 23 24 1 1.2371e+02 5.7589e+02 ; N1 - C2 - C5

5 4 23 1 1.2801e+02 5.3455e+02 ; C1 - N1 - C2

5 6 7 1 1.1086e+02 3.9497e+02 ; C1 - C13 - H1

5 6 8 1 1.1086e+02 3.9497e+02 ; C1 - C13 - H2

5 6 9 1 1.1086e+02 3.9497e+02 ; C1 - C13 - H13

5 10 11 1 1.1597e+02 5.4107e+02 ; C1 - C4 - C11

5 10 18 1 1.1419e+02 5.7036e+02 ; C1 - C4 - C3

6 5 10 1 1.1597e+02 5.4107e+02 ; C13 - C1 - C4

7 6 8 1 1.0835e+02 3.2995e+02 ; H1 - C13 - H2

7 6 9 1 1.0835e+02 3.2995e+02 ; H1 - C13 - H13

8 6 9 1 1.0835e+02 3.2995e+02 ; H2 - C13 - H13

10 11 12 1 1.1189e+02 5.3204e+02 ; C4 - C11 - C12

10 11 16 1 1.1086e+02 3.9497e+02 ; C4 - C11 - H8

10 11 17 1 1.1086e+02 3.9497e+02 ; C4 - C11 - H12

10 18 19 1 1.1945e+02 5.4233e+02 ; C4 - C3 - C10

10 18 23 1 1.1419e+02 5.7036e+02 ; C4 - C3 - C2

11	10	18	1	1.1945e+02	5.4233e+02	;	C11	- C4	- C3
11	12	13	1	1.1005e+02	3.8802e+02	;	C11	- C12	- H9
11	12	14	1	1.1005e+02	3.8802e+02	;	C11	- C12	- H10
11	12	15	1	1.1005e+02	3.8802e+02	;	C11	- C12	- H11
12	11	16	1	1.1005e+02	3.8802e+02	;	C12	- C11	- H8
12	11	17	1	1.1005e+02	3.8802e+02	;	C12	- C11	- H12
13	12	14	1	1.0835e+02	3.2995e+02	;	H9	- C12	- H10
13	12	15	1	1.0835e+02	3.2995e+02	;	H9	- C12	- H11
14	12	15	1	1.0835e+02	3.2995e+02	;	H10	- C12	- H11
16	11	17	1	1.0835e+02	3.2995e+02	;	H8	- C11	- H12
18	19	20	1	1.1086e+02	3.9497e+02	;	C3	- C10	- H3
18	19	21	1	1.1086e+02	3.9497e+02	;	C3	- C10	- H4
18	19	22	1	1.1086e+02	3.9497e+02	;	C3	- C10	- H5
18	23	24	1	1.2259e+02	5.5128e+02	;	C3	- C2	- C5
19	18	23	1	1.1597e+02	5.4107e+02	;	C10	- C3	- C2
20	19	21	1	1.0835e+02	3.2995e+02	;	H3	- C10	- H4
20	19	22	1	1.0835e+02	3.2995e+02	;	H3	- C10	- H5
21	19	22	1	1.0835e+02	3.2995e+02	;	H4	- C10	- H5
23	24	25	1	1.1548e+02	4.1815e+02	;	C2	- C5	- H7
23	24	26	1	1.3036e+02	5.2953e+02	;	C2	- C5	- C6
24	26	27	1	1.2422e+02	5.5497e+02	;	C5	- C6	- N2
24	26	32	1	1.2841e+02	5.3279e+02	;	C5	- C6	- C9
25	24	26	1	1.1545e+02	3.9773e+02	;	H7	- C5	- C6
26	27	28	1	1.0990e+02	5.7689e+02	;	C6	- N2	- C7
26	32	30	1	1.1419e+02	5.7036e+02	;	C6	- C9	- C8
26	32	33	1	1.2456e+02	5.2099e+02	;	C6	- C9	- BR2

27 26 32 1 1.0942e+02 6.1011e+02 ; N2 - C6 - C9

27 28 29 1 1.1966e+02 4.2024e+02 ; N2 - C7 - H6

27 28 30 1 1.0942e+02 6.1011e+02 ; N2 - C7 - C8

28 30 31 1 1.2456e+02 5.2099e+02 ; C7 - C8 - BR1

28 30 32 1 1.1419e+02 5.7036e+02 ; C7 - C8 - C9

29 28 30 1 1.2911e+02 3.9489e+02 ; H6 - C7 - C8

30 32 33 1 1.2489e+02 5.1731e+02 ; C8 - C9 - BR2

31 30 32 1 1.2489e+02 5.1731e+02 ; BR1 - C8 - C9

[dihedrals] ; propers

; treated as RBs in GROMACS to use combine multiple AMBER torsions per quartet

; i j k l func C0 C1 C2 C3 C4 C5

1 2 4 5 3 6.97333 0.00000 -6.97333 0.00000 0.00000 0.00000 ; S1- P1- N1- C1

1 2 4 23 3 6.97333 0.00000 -6.97333 0.00000 0.00000 0.00000 ; S1- P1- N1- C2

1 2 27 26 3 6.97333 0.00000 -6.97333 0.00000 0.00000 0.00000 ; S1- P1- N2- C6

1 2 27 28 3 6.97333 0.00000 -6.97333 0.00000 0.00000 0.00000 ; S1- P1- N2- C7

2 4 5 6 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; P1- N1- C1- C13

2 4 5 10 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; P1- N1- C1- C4

2 4 23 18 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; P1- N1- C2- C3

2 4 23 24 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; P1- N1- C2- C5

2 27 26 24 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; P1- N2- C6- C5

2 27 26 32 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; P1- N2- C6- C9

2 27 28 29 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; P1- N2- C7- H6

2 27 28 30 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; P1- N2- C7- C8

3 2 4 5 3 6.97333 0.00000 -6.97333 0.00000 0.00000 0.00000 ; S2- P1- N1- C1

3 2 4 23 3 6.97333 0.00000 -6.97333 0.00000 0.00000 0.00000 ; S2- P1- N1- C2

3 2 27 26 3 6.97333 0.00000 -6.97333 0.00000 0.00000 0.00000 ; S2- P1- N2- C6

3 2 27 28 3 6.97333 0.00000 -6.97333 0.00000 0.00000 0.00000 ; S2- P1- N2- C7

4 2 27 26 3 6.97333 0.00000 -6.97333 0.00000 0.00000 0.00000 ; N1- P1- N2- C6

4 2 27 28 3 6.97333 0.00000 -6.97333 0.00000 0.00000 0.00000 ; N1- P1- N2- C7

4 5 6 7 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N1- C1- C13- H1

4 5 6 8 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N1- C1- C13- H2

4 5 6 9 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N1- C1- C13- H13

4 5 10 11 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; N1- C1- C4- C11

4 5 10 18 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; N1- C1- C4- C3

4 23 18 10 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; N1- C2- C3- C4

4 23 18 19 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; N1- C2- C3- C10

4 23 24 25 3 8.36800 0.00000 -8.36800 0.00000 0.00000 0.00000 ; N1- C2- C5- H7

4 23 24 26 3 8.36800 0.00000 -8.36800 0.00000 0.00000 0.00000 ; N1- C2- C5- C6

5 4 2 27 3 6.97333 0.00000 -6.97333 0.00000 0.00000 0.00000 ; C1- N1- P1- N2

5 4 23 18 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; C1- N1- C2- C3

5 4 23 24 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; C1- N1- C2- C5

5 10 11 12 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C1- C4- C11- C12

5 10 11 16 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C1- C4- C11- H8

5 10 11 17 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C1- C4- C11- H12

5 10 18 19 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C1- C4- C3- C10

5 10 18 23 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C1- C4- C3- C2

6 5 4 23 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; C13- C1- N1- C2

6 5 10 11 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C13- C1- C4- C11

6 5 10 18 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C13- C1- C4- C3

7 6 5 10 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H1- C13- C1- C4

8 6 5 10 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H2- C13- C1- C4

9 6 5 10 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H13- C13- C1- C4

10 5 4 23 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; C4- C1- N1- C2

10 11 12 13 3 0.65084 1.95253 0.00000 -2.60338 0.00000 0.00000 ; C4- C11- C12- H9

10 11 12 14 3 0.65084 1.95253 0.00000 -2.60338 0.00000 0.00000 ; C4- C11- C12- H10

10 11 12 15 3 0.65084 1.95253 0.00000 -2.60338 0.00000 0.00000 ; C4- C11- C12- H11

10 18 19 20 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C4- C3- C10- H3

10 18 19 21 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C4- C3- C10- H4

10 18 19 22 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C4- C3- C10- H5

10 18 23 24 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C4- C3- C2- C5

11 10 18 19 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C11- C4- C3- C10

11 10 18 23 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C11- C4- C3- C2

12 11 10 18 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C12- C11- C4- C3

13 12 11 16 3 0.62760 1.88280 0.00000 -2.51040 0.00000 0.00000 ; H9- C12- C11- H8

13 12 11 17 3 0.62760 1.88280 0.00000 -2.51040 0.00000 0.00000 ; H9- C12- C11- H12

14 12 11 16 3 0.62760 1.88280 0.00000 -2.51040 0.00000 0.00000 ; H10- C12- C11- H8

14 12 11 17 3 0.62760 1.88280 0.00000 -2.51040 0.00000 0.00000 ; H10- C12- C11- H12

15 12 11 16 3 0.62760 1.88280 0.00000 -2.51040 0.00000 0.00000 ; H11- C12- C11- H8

15 12 11 17 3 0.62760 1.88280 0.00000 -2.51040 0.00000 0.00000 ; H11- C12- C11- H12

16 11 10 18 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H8- C11- C4- C3

17 11 10 18 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H12- C11- C4- C3

18 23 24 25 3 8.36800 0.00000 -8.36800 0.00000 0.00000 0.00000 ; C3- C2- C5- H7

18 23 24 26 3 8.36800 0.00000 -8.36800 0.00000 0.00000 0.00000 ; C3- C2- C5- C6

19 18 23 24 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C10- C3- C2- C5

20 19 18 23 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H3- C10- C3- C2

21 19 18 23 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H4- C10- C3- C2

22 19 18 23 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H5- C10- C3- C2

23 4 2 27 3 6.97333 0.00000 -6.97333 0.00000 0.00000 0.00000 ; C2- N1- P1- N2

23 24 26 27 3 8.36800 0.00000 -8.36800 0.00000 0.00000 0.00000 ; C2- C5- C6- N2

23 24 26 32 3 8.36800 0.00000 -8.36800 0.00000 0.00000 0.00000 ; C2- C5- C6- C9

24 26 27 28 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; C5- C6- N2- C7

24 26 32 30 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C5- C6- C9- C8

24 26 32 33 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C5- C6- C9- BR2

25 24 26 27 3 8.36800 0.00000 -8.36800 0.00000 0.00000 0.00000 ; H7- C5- C6- N2

25 24 26 32 3 8.36800 0.00000 -8.36800 0.00000 0.00000 0.00000 ; H7- C5- C6- C9

26 27 28 29 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; C6- N2- C7- H6

26 27 28 30 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; C6- N2- C7- C8

26 32 30 28 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C6- C9- C8- C7

26 32 30 31 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C6- C9- C8- BR1

27 26 32 30 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; N2- C6- C9- C8

27 26 32 33 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; N2- C6- C9- BR2

27 28 30 31 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; N2- C7- C8- BR1

27 28 30 32 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; N2- C7- C8- C9

28 27 26 32 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; C7- N2- C6- C9

28 30 32 33 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C7- C8- C9- BR2

29 28 30 31 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; H6- C7- C8- BR1

29 28 30 32 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; H6- C7- C8- C9

31 30 32 33 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; BR1- C8- C9- BR2

[dihedrals] ; impropers

; treated as propers in GROMACS to use correct AMBER analytical function

; i j k l func phase kd pn

5 23 4 2 1 180.00 4.60240 2 ; C1- C2- N1- P1

6 10 5 4 1 180.00 4.60240 2 ; C13- C4- C1- N1

11 5 10 18 1 180.00 4.60240 2 ; C11- C1- C4- C3

18 24 23 4 1 180.00 4.60240 2 ; C3- C5- C2- N1

19 10 18 23 1 180.00 4.60240 2 ; C10- C4- C3- C2

26 23 24 25 1 180.00 4.60240 2 ; C6- C2- C5- H7

26 28 27 2 1 180.00 4.60240 2 ; C6- C7- N2- P1

30 29 28 27 1 180.00 4.60240 2 ; C8- H6- C7- N2

31 28 30 32 1 180.00 4.60240 2 ; BR1- C7- C8- C9

32 24 26 27 1 180.00 4.60240 2 ; C9- C5- C6- N2

33 26 32 30 1 180.00 4.60240 2 ; BR2- C6- C9- C8

Force field parameters for 1-BODIPY T_1

; by Lukasz Cwiklik, 2019, cwiklik.net

;[defaults]

;; nbfunc comb-rule gen-pairs fudgeLJ fudgeQQ

;1 2 yes 0.5 0.8333

[atomtypes]

;name bond_type mass charge ptype sigma epsilon Amb

f f 0.00000 0.00000 A 3.11815e-01 2.55224e-01; tzv: F params from ffnonbonded.itp fpr Amber

b b 0.00000 0.00000 A 3.56359e-01 1.04600e+00; tzv: S params here, as S similar in radius to B

na na 0.00000 0.00000 A 3.25000e-01 7.11280e-01 ; 1.82 0.1700

cc cc 0.00000 0.00000 A 3.39967e-01 3.59824e-01 ; 1.91 0.0860

c3 c3 0.00000 0.00000 A 3.39967e-01 4.57730e-01 ; 1.91 0.1094

hc hc 0.00000 0.00000 A 2.64953e-01 6.56888e-02 ; 1.49 0.0157

cd cd 0.00000 0.00000 A 3.39967e-01 3.59824e-01 ; 1.91 0.0860

ce ce 0.00000 0.00000 A 3.39967e-01 3.59824e-01 ; 1.91 0.0860

ha ha 0.00000 0.00000 A 2.59964e-01 6.27600e-02 ; 1.46 0.0150

h4 h4 0.00000 0.00000 A 2.51055e-01 6.27600e-02 ; 1.41 0.0150

br br 0.00000 0.00000 A 3.59923e-01 1.75728e+00 ; 2.02 0.4200

[moleculetype]

;name nrexcl

BDT1 3

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[ atoms ]
;   nr  type  resi  res  atom  cgnr     charge      mass       ; qtot   bond_type
     1    f     1   BDT1    F1    1    -0.420781   18.99800 ; qtot -0.722 ;tzv - F atomic mass
     2    b     1   BDT1    B1    2     0.719660   10.81000 ; qtot 1.190  ;tzv - B atomic mass
     3    f     1   BDT1    F2    3    -0.420781   18.99800 ; qtot 0.468  ;tzv - F atomic mass
     4   na     1   BDT1    N1    4    -0.470933   14.01000 ; qtot -0.577
     5   cc     1   BDT1    C1    5     0.548644   12.01000 ; qtot 0.038
     6   c3     1   BDT1   C13    6    -0.537702   12.01000 ; qtot -0.617
     7   hc     1   BDT1    H1    7     0.170402    1.00800 ; qtot -0.407
     8   hc     1   BDT1    H2    8     0.170402    1.00800 ; qtot -0.197
     9   hc     1   BDT1   H13    9     0.170402    1.00800 ; qtot 0.014
    10   cc     1   BDT1    C4   10    -0.418275   12.01000 ; qtot -0.292
    11   c3     1   BDT1   C11   11     0.226362   12.01000 ; qtot -0.204
    12   c3     1   BDT1   C12   12    -0.196117   12.01000 ; qtot -0.426
    13   hc     1   BDT1    H9   13     0.053702    1.00800 ; qtot -0.357
    14   hc     1   BDT1   H10   14     0.053702    1.00800 ; qtot -0.288
    15   hc     1   BDT1   H11   15     0.053702    1.00800 ; qtot -0.219
    16   hc     1   BDT1    H8   16    -0.001825    1.00800 ; qtot -0.186
    17   hc     1   BDT1   H12   17    -0.001825    1.00800 ; qtot -0.153
    18   cd     1   BDT1    C3   18     0.168325   12.01000 ; qtot -0.063
    19   c3     1   BDT1   C10   19    -0.324847   12.01000 ; qtot -0.502
    20   hc     1   BDT1    H3   20     0.108458    1.00800 ; qtot -0.354
    21   hc     1   BDT1    H4   21     0.108458    1.00800 ; qtot -0.205
    22   hc     1   BDT1    H5   22     0.108458    1.00800 ; qtot -0.056
    23   cd     1   BDT1    C2   23     0.281308   12.01000 ; qtot 0.444
    24   ce     1   BDT1    C5   24    -0.469261   12.01000 ; qtot -0.180
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    25   ha     1   BDT1    H7   25     0.164545    1.00800 ; qtot 0.070
    26   cc     1   BDT1    C6   26     0.368047   12.01000 ; qtot 0.712
    27   na     1   BDT1    N2   27    -0.112535   14.01000 ; qtot 0.028
    28   cc     1   BDT1    C7   28    -0.045067   12.01000 ; qtot 0.080
    29   h4     1   BDT1    H6   29     0.172838    1.00800 ; qtot 0.266
    30   cd     1   BDT1    C8   30    -0.066533   12.01000 ; qtot 0.134
    31   br     1   BDT1   BR1   31    -0.010896   79.90000 ; qtot 0.190
    32   cd     1   BDT1    C9   32    -0.144217   12.01000 ; qtot -0.070
    33   br     1   BDT1   BR2   33    -0.005824   79.90000 ; qtot 0.000

[ bonds ]
;   ai     aj funct   r             k
     1      2   1    1.9220e-01    2.0987e+05 ;     S1 - P1
     2      3   1    1.9220e-01    2.0987e+05 ;     P1 - S2
     2      4   1    1.7150e-01    2.7221e+05 ;     P1 - N1
     2     27   1    1.7150e-01    2.7221e+05 ;     P1 - N2
     4      5   1    1.3710e-01    3.6719e+05 ;     N1 - C1
     4     23   1    1.3710e-01    3.6719e+05 ;     N1 - C2
     5      6   1    1.4990e-01    2.8225e+05 ;     C1 - C13
     5     10   1    1.4290e-01    3.5003e+05 ;     C1 - C4
     6      7   1    1.0920e-01    2.8225e+05 ;    C13 - H1
     6      8   1    1.0920e-01    2.8225e+05 ;    C13 - H2
     6      9   1    1.0920e-01    2.8225e+05 ;    C13 - H13
    10     11   1    1.4990e-01    2.8225e+05 ;     C4 - C11
    10     18   1    1.3710e-01    4.2175e+05 ;     C4 - C3
    11     12   1    1.5350e-01    2.5363e+05 ;    C11 - C12
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    11     16   1    1.0920e-01    2.8225e+05 ;    C11 - H8
    11     17   1    1.0920e-01    2.8225e+05 ;    C11 - H12
    12     13   1    1.0920e-01    2.8225e+05 ;    C12 - H9
    12     14   1    1.0920e-01    2.8225e+05 ;    C12 - H10
    12     15   1    1.0920e-01    2.8225e+05 ;    C12 - H11
    18     19   1    1.4990e-01    2.8225e+05 ;     C3 - C10
    18     23   1    1.4290e-01    3.5003e+05 ;     C3 - C2
    19     20   1    1.0920e-01    2.8225e+05 ;    C10 - H3
    19     21   1    1.0920e-01    2.8225e+05 ;    C10 - H4
    19     22   1    1.0920e-01    2.8225e+05 ;    C10 - H5
    23     24   1    1.3666e-01    4.2786e+05 ;     C2 - C5
    24     25   1    1.0890e-01    2.8577e+05 ;     C5 - H7
    24     26   1    1.4532e-01    3.2459e+05 ;     C5 - C6
    26     27   1    1.3710e-01    3.6719e+05 ;     C6 - N2
    26     32   1    1.3710e-01    4.2175e+05 ;     C6 - C9
    27     28   1    1.3710e-01    3.6719e+05 ;     N2 - C7
    28     29   1    1.0830e-01    2.9296e+05 ;     C7 - H6
    28     30   1    1.3710e-01    4.2175e+05 ;     C7 - C8
    30     31   1    1.8847e-01    2.3230e+05 ;     C8 - BR1
    30     32   1    1.4290e-01    3.5003e+05 ;     C8 - C9
    32     33   1    1.8847e-01    2.3230e+05 ;     C9 - BR2

[ pairs ]
;   ai     aj    funct
     1      5      1 ;     S1 - C1
     1     23      1 ;     S1 - C2
```

1 26 1 ; S1 - C6

1 28 1 ; S1 - C7

2 6 1 ; P1 - C13

2 10 1 ; P1 - C4

2 18 1 ; P1 - C3

2 24 1 ; P1 - C5

2 29 1 ; P1 - H6

2 30 1 ; P1 - C8

2 32 1 ; P1 - C9

3 5 1 ; S2 - C1

3 23 1 ; S2 - C2

3 26 1 ; S2 - C6

3 28 1 ; S2 - C7

4 7 1 ; N1 - H1

4 8 1 ; N1 - H2

4 9 1 ; N1 - H13

4 11 1 ; N1 - C11

4 19 1 ; N1 - C10

4 25 1 ; N1 - H7

4 26 1 ; N1 - C6

4 28 1 ; N1 - C7

5 12 1 ; C1 - C12

5 16 1 ; C1 - H8

5 17 1 ; C1 - H12

5 19 1 ; C1 - C10

5 24 1 ; C1 - C5

5 27 1 ; C1 - N2

6 11 1 ; C13 - C11

6 18 1 ; C13 - C3

6 23 1 ; C13 - C2

7 10 1 ; H1 - C4

8 10 1 ; H2 - C4

9 10 1 ; H13 - C4

10 13 1 ; C4 - H9

10 14 1 ; C4 - H10

10 15 1 ; C4 - H11

10 20 1 ; C4 - H3

10 21 1 ; C4 - H4

10 22 1 ; C4 - H5

10 24 1 ; C4 - C5

11 19 1 ; C11 - C10

11 23 1 ; C11 - C2

12 18 1 ; C12 - C3

13 16 1 ; H9 - H8

13 17 1 ; H9 - H12

14 16 1 ; H10 - H8

14 17 1 ; H10 - H12

15 16 1 ; H11 - H8

15 17 1 ; H11 - H12

16 18 1 ; H8 - C3

17 18 1 ; H12 - C3

18 25 1 ; C3 - H7

```
    18     26      1 ;     C3 - C6
    19     24      1 ;    C10 - C5
    20     23      1 ;     H3 - C2
    21     23      1 ;     H4 - C2
    22     23      1 ;     H5 - C2
    23     27      1 ;     C2 - N2
    23     32      1 ;     C2 - C9
    24     28      1 ;     C5 - C7
    24     30      1 ;     C5 - C8
    24     33      1 ;     C5 - BR2
    25     27      1 ;     H7 - N2
    25     32      1 ;     H7 - C9
    26     29      1 ;     C6 - H6
    26     31      1 ;     C6 - BR1
    27     31      1 ;     N2 - BR1
    27     33      1 ;     N2 - BR2
    28     33      1 ;     C7 - BR2
    29     31      1 ;     H6 - BR1
    29     32      1 ;     H6 - C9
    31     33      1 ;    BR1 - BR2

[ angles ]
;   ai     aj     ak    funct   theta         cth
      1      2      3      1    1.1413e+02    3.2945e+02 ;     S1 - P1     - S2
      1      2      4      1    1.1135e+02    5.3005e+02 ;     S1 - P1     - N1
      1      2     27      1    1.1135e+02    5.3005e+02 ;     S1 - P1     - N2
```

2 4 5 1 1.2470e+02 6.4275e+02 ; P1 - N1 - C1

2 4 23 1 1.2470e+02 6.4275e+02 ; P1 - N1 - C2

2 27 26 1 1.2470e+02 6.4275e+02 ; P1 - N2 - C6

2 27 28 1 1.2470e+02 6.4275e+02 ; P1 - N2 - C7

3 2 4 1 1.1135e+02 5.3005e+02 ; S2 - P1 - N1

3 2 27 1 1.1135e+02 5.3005e+02 ; S2 - P1 - N2

4 2 27 1 1.0857e+02 3.3941e+02 ; N1 - P1 - N2

4 5 6 1 1.2278e+02 5.4810e+02 ; N1 - C1 - C13

4 5 10 1 1.0680e+02 6.0425e+02 ; N1 - C1 - C4

4 23 18 1 1.0680e+02 6.0425e+02 ; N1 - C2 - C3

4 23 24 1 1.2371e+02 5.7589e+02 ; N1 - C2 - C5

5 4 23 1 1.2801e+02 5.3455e+02 ; C1 - N1 - C2

5 6 7 1 1.1086e+02 3.9497e+02 ; C1 - C13 - H1

5 6 8 1 1.1086e+02 3.9497e+02 ; C1 - C13 - H2

5 6 9 1 1.1086e+02 3.9497e+02 ; C1 - C13 - H13

5 10 11 1 1.1597e+02 5.4107e+02 ; C1 - C4 - C11

5 10 18 1 1.1419e+02 5.7036e+02 ; C1 - C4 - C3

6 5 10 1 1.1597e+02 5.4107e+02 ; C13 - C1 - C4

7 6 8 1 1.0835e+02 3.2995e+02 ; H1 - C13 - H2

7 6 9 1 1.0835e+02 3.2995e+02 ; H1 - C13 - H13

8 6 9 1 1.0835e+02 3.2995e+02 ; H2 - C13 - H13

10 11 12 1 1.1189e+02 5.3204e+02 ; C4 - C11 - C12

10 11 16 1 1.1086e+02 3.9497e+02 ; C4 - C11 - H8

10 11 17 1 1.1086e+02 3.9497e+02 ; C4 - C11 - H12

10 18 19 1 1.1945e+02 5.4233e+02 ; C4 - C3 - C10

10 18 23 1 1.1419e+02 5.7036e+02 ; C4 - C3 - C2

11	10	18	1	1.1945e+02	5.4233e+02	;	C11	- C4	- C3
11	12	13	1	1.1005e+02	3.8802e+02	;	C11	- C12	- H9
11	12	14	1	1.1005e+02	3.8802e+02	;	C11	- C12	- H10
11	12	15	1	1.1005e+02	3.8802e+02	;	C11	- C12	- H11
12	11	16	1	1.1005e+02	3.8802e+02	;	C12	- C11	- H8
12	11	17	1	1.1005e+02	3.8802e+02	;	C12	- C11	- H12
13	12	14	1	1.0835e+02	3.2995e+02	;	H9	- C12	- H10
13	12	15	1	1.0835e+02	3.2995e+02	;	H9	- C12	- H11
14	12	15	1	1.0835e+02	3.2995e+02	;	H10	- C12	- H11
16	11	17	1	1.0835e+02	3.2995e+02	;	H8	- C11	- H12
18	19	20	1	1.1086e+02	3.9497e+02	;	C3	- C10	- H3
18	19	21	1	1.1086e+02	3.9497e+02	;	C3	- C10	- H4
18	19	22	1	1.1086e+02	3.9497e+02	;	C3	- C10	- H5
18	23	24	1	1.2259e+02	5.5128e+02	;	C3	- C2	- C5
19	18	23	1	1.1597e+02	5.4107e+02	;	C10	- C3	- C2
20	19	21	1	1.0835e+02	3.2995e+02	;	H3	- C10	- H4
20	19	22	1	1.0835e+02	3.2995e+02	;	H3	- C10	- H5
21	19	22	1	1.0835e+02	3.2995e+02	;	H4	- C10	- H5
23	24	25	1	1.1548e+02	4.1815e+02	;	C2	- C5	- H7
23	24	26	1	1.3036e+02	5.2953e+02	;	C2	- C5	- C6
24	26	27	1	1.2422e+02	5.5497e+02	;	C5	- C6	- N2
24	26	32	1	1.2841e+02	5.3279e+02	;	C5	- C6	- C9
25	24	26	1	1.1545e+02	3.9773e+02	;	H7	- C5	- C6
26	27	28	1	1.0990e+02	5.7689e+02	;	C6	- N2	- C7
26	32	30	1	1.1419e+02	5.7036e+02	;	C6	- C9	- C8
26	32	33	1	1.2456e+02	5.2099e+02	;	C6	- C9	- BR2

27 26 32 1 1.0942e+02 6.1011e+02 ; N2 - C6 - C9

27 28 29 1 1.1966e+02 4.2024e+02 ; N2 - C7 - H6

27 28 30 1 1.0942e+02 6.1011e+02 ; N2 - C7 - C8

28 30 31 1 1.2456e+02 5.2099e+02 ; C7 - C8 - BR1

28 30 32 1 1.1419e+02 5.7036e+02 ; C7 - C8 - C9

29 28 30 1 1.2911e+02 3.9489e+02 ; H6 - C7 - C8

30 32 33 1 1.2489e+02 5.1731e+02 ; C8 - C9 - BR2

31 30 32 1 1.2489e+02 5.1731e+02 ; BR1 - C8 - C9

[dihedrals] ; propers

; treated as RBs in GROMACS to use combine multiple AMBER torsions per quartet

; i j k l func C0 C1 C2 C3 C4 C5

1 2 4 5 3 6.97333 0.00000 -6.97333 0.00000 0.00000 0.00000 ; S1- P1- N1- C1

1 2 4 23 3 6.97333 0.00000 -6.97333 0.00000 0.00000 0.00000 ; S1- P1- N1- C2

1 2 27 26 3 6.97333 0.00000 -6.97333 0.00000 0.00000 0.00000 ; S1- P1- N2- C6

1 2 27 28 3 6.97333 0.00000 -6.97333 0.00000 0.00000 0.00000 ; S1- P1- N2- C7

2 4 5 6 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; P1- N1- C1- C13

2 4 5 10 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; P1- N1- C1- C4

2 4 23 18 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; P1- N1- C2- C3

2 4 23 24 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; P1- N1- C2- C5

2 27 26 24 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; P1- N2- C6- C5

2 27 26 32 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; P1- N2- C6- C9

2 27 28 29 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; P1- N2- C7- H6

2 27 28 30 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; P1- N2- C7- C8

3 2 4 5 3 6.97333 0.00000 -6.97333 0.00000 0.00000 0.00000 ; S2- P1- N1- C1

3 2 4 23 3 6.97333 0.00000 -6.97333 0.00000 0.00000 0.00000 ; S2- P1- N1- C2

3 2 27 26 3 6.97333 0.00000 -6.97333 0.00000 0.00000 0.00000 ; S2- P1- N2- C6

3 2 27 28 3 6.97333 0.00000 -6.97333 0.00000 0.00000 0.00000 ; S2- P1- N2- C7

4 2 27 26 3 6.97333 0.00000 -6.97333 0.00000 0.00000 0.00000 ; N1- P1- N2- C6

4 2 27 28 3 6.97333 0.00000 -6.97333 0.00000 0.00000 0.00000 ; N1- P1- N2- C7

4 5 6 7 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N1- C1- C13- H1

4 5 6 8 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N1- C1- C13- H2

4 5 6 9 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; N1- C1- C13- H13

4 5 10 11 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; N1- C1- C4- C11

4 5 10 18 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; N1- C1- C4- C3

4 23 18 10 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; N1- C2- C3- C4

4 23 18 19 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; N1- C2- C3- C10

4 23 24 25 3 8.36800 0.00000 -8.36800 0.00000 0.00000 0.00000 ; N1- C2- C5- H7

4 23 24 26 3 8.36800 0.00000 -8.36800 0.00000 0.00000 0.00000 ; N1- C2- C5- C6

5 4 2 27 3 6.97333 0.00000 -6.97333 0.00000 0.00000 0.00000 ; C1- N1- P1- N2

5 4 23 18 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; C1- N1- C2- C3

5 4 23 24 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; C1- N1- C2- C5

5 10 11 12 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C1- C4- C11- C12

5 10 11 16 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C1- C4- C11- H8

5 10 11 17 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C1- C4- C11- H12

5 10 18 19 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C1- C4- C3- C10

5 10 18 23 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C1- C4- C3- C2

6 5 4 23 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; C13- C1- N1- C2

6 5 10 11 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C13- C1- C4- C11

6 5 10 18 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C13- C1- C4- C3

7 6 5 10 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H1- C13- C1- C4

8 6 5 10 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H2- C13- C1- C4

9 6 5 10 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H13- C13- C1- C4

10 5 4 23 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; C4- C1- N1- C2

10 11 12 13 3 0.65084 1.95253 0.00000 -2.60338 0.00000 0.00000 ; C4- C11- C12- H9

10 11 12 14 3 0.65084 1.95253 0.00000 -2.60338 0.00000 0.00000 ; C4- C11- C12- H10

10 11 12 15 3 0.65084 1.95253 0.00000 -2.60338 0.00000 0.00000 ; C4- C11- C12- H11

10 18 19 20 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C4- C3- C10- H3

10 18 19 21 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C4- C3- C10- H4

10 18 19 22 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C4- C3- C10- H5

10 18 23 24 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C4- C3- C2- C5

11 10 18 19 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C11- C4- C3- C10

11 10 18 23 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C11- C4- C3- C2

12 11 10 18 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; C12- C11- C4- C3

13 12 11 16 3 0.62760 1.88280 0.00000 -2.51040 0.00000 0.00000 ; H9- C12- C11- H8

13 12 11 17 3 0.62760 1.88280 0.00000 -2.51040 0.00000 0.00000 ; H9- C12- C11- H12

14 12 11 16 3 0.62760 1.88280 0.00000 -2.51040 0.00000 0.00000 ; H10- C12- C11- H8

14 12 11 17 3 0.62760 1.88280 0.00000 -2.51040 0.00000 0.00000 ; H10- C12- C11- H12

15 12 11 16 3 0.62760 1.88280 0.00000 -2.51040 0.00000 0.00000 ; H11- C12- C11- H8

15 12 11 17 3 0.62760 1.88280 0.00000 -2.51040 0.00000 0.00000 ; H11- C12- C11- H12

16 11 10 18 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H8- C11- C4- C3

17 11 10 18 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H12- C11- C4- C3

18 23 24 25 3 8.36800 0.00000 -8.36800 0.00000 0.00000 0.00000 ; C3- C2- C5- H7

18 23 24 26 3 8.36800 0.00000 -8.36800 0.00000 0.00000 0.00000 ; C3- C2- C5- C6

19 18 23 24 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C10- C3- C2- C5

20 19 18 23 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H3- C10- C3- C2

21 19 18 23 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H4- C10- C3- C2

22 19 18 23 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ; H5- C10- C3- C2

23 4 2 27 3 6.97333 0.00000 -6.97333 0.00000 0.00000 0.00000 ; C2- N1- P1- N2

23 24 26 27 3 8.36800 0.00000 -8.36800 0.00000 0.00000 0.00000 ; C2- C5- C6- N2

23 24 26 32 3 8.36800 0.00000 -8.36800 0.00000 0.00000 0.00000 ; C2- C5- C6- C9

24 26 27 28 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; C5- C6- N2- C7

24 26 32 30 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C5- C6- C9- C8

24 26 32 33 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C5- C6- C9- BR2

25 24 26 27 3 8.36800 0.00000 -8.36800 0.00000 0.00000 0.00000 ; H7- C5- C6- N2

25 24 26 32 3 8.36800 0.00000 -8.36800 0.00000 0.00000 0.00000 ; H7- C5- C6- C9

26 27 28 29 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; C6- N2- C7- H6

26 27 28 30 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; C6- N2- C7- C8

26 32 30 28 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C6- C9- C8- C7

26 32 30 31 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C6- C9- C8- BR1

27 26 32 30 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; N2- C6- C9- C8

27 26 32 33 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; N2- C6- C9- BR2

27 28 30 31 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; N2- C7- C8- BR1

27 28 30 32 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; N2- C7- C8- C9

28 27 26 32 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ; C7- N2- C6- C9

28 30 32 33 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; C7- C8- C9- BR2

29 28 30 31 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; H6- C7- C8- BR1

29 28 30 32 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; H6- C7- C8- C9

31 30 32 33 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ; BR1- C8- C9- BR2

[dihedrals] ; impropers

; treated as propers in GROMACS to use correct AMBER analytical function

; i j k l func phase kd pn

5 23 4 2 1 180.00 4.60240 2 ; C1- C2- N1- P1

6 10 5 4 1 180.00 4.60240 2 ; C13- C4- C1- N1

11 5 10 18 1 180.00 4.60240 2 ; C11- C1- C4- C3

18 24 23 4 1 180.00 4.60240 2 ; C3- C5- C2- N1

19 10 18 23 1 180.00 4.60240 2 ; C10- C4- C3- C2

26 23 24 25 1 180.00 4.60240 2 ; C6- C2- C5- H7

26 28 27 2 1 180.00 4.60240 2 ; C6- C7- N2- P1

30 29 28 27 1 180.00 4.60240 2 ; C8- H6- C7- N2

31 28 30 32 1 180.00 4.60240 2 ; BR1- C7- C8- C9

32 24 26 27 1 180.00 4.60240 2 ; C9- C5- C6- N2

33 26 32 30 1 180.00 4.60240 2 ; BR2- C6- C9- C8