

Electronic Supplementary Information to
“The role of solvent in the self-assembly of m-
aminobenzoic acid: a density functional theory and
molecular dynamics study”

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SI.1 GAFF parameters for mABA and DMSO

mABA

Table SI.1.1

Topology file used in Gromacs containing the GAFF atom types and partial charges used to model mABA.

```
; MBA_GMX.top created by acpype (Rev: 403) on Thu Jul 9 22:34:48 2015

[ 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
ca         ca              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
nh         nh              0.00000    0.00000    A          3.25000e-01  7.11280e-01 ; 1.82  0.1700
hn         hn              0.00000    0.00000    A          1.06908e-01  6.56888e-02 ; 0.60  0.0157
c          c              0.00000    0.00000    A          3.39967e-01  3.59824e-01 ; 1.91  0.0860
oh         oh              0.00000    0.00000    A          3.06647e-01  8.80314e-01 ; 1.72  0.2104
ho         ho              0.00000    0.00000    A          0.00000e+00  0.00000e+00 ; 0.00  0.0000
o          o              0.00000    0.00000    A          2.95992e-01  8.78640e-01 ; 1.66  0.2100

[ moleculetype ]
;name      nrexcl
MBA        3

[ atoms ]
;  nr  type  resi  res  atom  cgnr      charge      mass      ; qtot  bond_type
;  1   ca    1    MBA   C2    1      -0.185783    12.01000 ; qtot -0.186
;  2   ha    1    MBA   H2    2       0.172356     1.00800 ; qtot -0.013
;  3   ca    1    MBA   C1    3       0.297382    12.01000 ; qtot  0.284
;  4   nh    1    MBA   N1    4      -0.890198    14.01000 ; qtot -0.606
;  5   hn    1    MBA   H5    5       0.379769     1.00800 ; qtot -0.226
;  6   hn    1    MBA   H6    6       0.379769     1.00800 ; qtot  0.153
;  7   ca    1    MBA   C6    7      -0.178160    12.01000 ; qtot -0.025
;  8   ha    1    MBA   H1    8       0.160780     1.00800 ; qtot  0.136
;  9   ca    1    MBA   C5    9      -0.218354    12.01000 ; qtot -0.082
; 10   ha    1    MBA   H4   10       0.169120     1.00800 ; qtot  0.087
; 11   ca    1    MBA   C4   11      -0.118964    12.01000 ; qtot -0.032
; 12   ha    1    MBA   H3   12       0.157379     1.00800 ; qtot  0.125
; 13   ca    1    MBA   C3   13      -0.112371    12.01000 ; qtot  0.013
; 14   c     1    MBA   C7   14       0.773096    12.01000 ; qtot  0.786
; 15   oh    1    MBA   O2   15      -0.641122    16.00000 ; qtot  0.145
; 16   ho    1    MBA   H7   16       0.451189     1.00800 ; qtot  0.596
; 17   o     1    MBA   O1   17      -0.595890    16.00000 ; qtot  0.000

[ bonds ]
;  ai  aj  funct  r      k
;  1   2   1      1.0870e-01  2.8811e+05 ; C2 - H2
;  1   3   1      1.3870e-01  4.0033e+05 ; C2 - C1
;  1  13   1      1.3870e-01  4.0033e+05 ; C2 - C3
;  3   4   1      1.3640e-01  3.7572e+05 ; C1 - N1
;  3   7   1      1.3870e-01  4.0033e+05 ; C1 - C6
;  4   5   1      1.0140e-01  3.3572e+05 ; N1 - H5
;  4   6   1      1.0140e-01  3.3572e+05 ; N1 - H6
;  7   8   1      1.0870e-01  2.8811e+05 ; C6 - H1
;  7   9   1      1.3870e-01  4.0033e+05 ; C6 - C5
;  9  10   1      1.0870e-01  2.8811e+05 ; C5 - H4
;  9  11   1      1.3870e-01  4.0033e+05 ; C5 - C4
; 11  12   1      1.0870e-01  2.8811e+05 ; C4 - H3
; 11  13   1      1.3870e-01  4.0033e+05 ; C4 - C3
; 13  14   1      1.4870e-01  2.9263e+05 ; C3 - C7
; 14  15   1      1.3060e-01  3.9028e+05 ; C7 - O2
; 14  17   1      1.2140e-01  5.4225e+05 ; C7 - O1
; 15  16   1      9.7400e-02  3.0928e+05 ; O2 - H7

[ pairs ]
;  ai  aj  funct
;  1   5   1 ; C2 - H5
;  1   6   1 ; C2 - H6
;  1   8   1 ; C2 - H1
```

1	9	1 ;	C2 - C5
1	12	1 ;	C2 - H3
1	15	1 ;	C2 - O2
1	17	1 ;	C2 - O1
2	4	1 ;	H2 - N1
2	7	1 ;	H2 - C6
2	11	1 ;	H2 - C4
2	14	1 ;	H2 - C7
3	10	1 ;	C1 - H4
3	11	1 ;	C1 - C4
3	14	1 ;	C1 - C7
4	8	1 ;	N1 - H1
4	9	1 ;	N1 - C5
5	7	1 ;	H5 - C6
6	7	1 ;	H6 - C6
7	12	1 ;	C6 - H3
8	10	1 ;	H1 - H4
8	11	1 ;	H1 - C4
9	14	1 ;	C5 - C7
10	12	1 ;	H4 - H3
10	13	1 ;	H4 - C3
11	15	1 ;	C4 - O2
11	17	1 ;	C4 - O1
12	14	1 ;	H3 - C7
13	4	1 ;	C3 - N1
13	7	1 ;	C3 - C6
13	16	1 ;	C3 - H7
16	17	1 ;	H7 - O1

[angles]

;	ai	aj	ak	funct	theta	cth			
	1	3	4	1	1.2013e+02	5.8024e+02 ;	C2 - C1	-	N1
	1	3	7	1	1.1997e+02	5.6216e+02 ;	C2 - C1	-	C6
	1	13	11	1	1.1997e+02	5.6216e+02 ;	C2 - C3	-	C4
	1	13	14	1	1.2014e+02	5.4091e+02 ;	C2 - C3	-	C7
	2	1	3	1	1.2001e+02	4.0551e+02 ;	H2 - C2	-	C1
	2	1	13	1	1.2001e+02	4.0551e+02 ;	H2 - C2	-	C3
	3	1	13	1	1.1997e+02	5.6216e+02 ;	C1 - C2	-	C3
	3	4	5	1	1.1613e+02	4.1070e+02 ;	C1 - N1	-	H5
	3	4	6	1	1.1613e+02	4.1070e+02 ;	C1 - N1	-	H6
	3	7	8	1	1.2001e+02	4.0551e+02 ;	C1 - C6	-	H1
	3	7	9	1	1.1997e+02	5.6216e+02 ;	C1 - C6	-	C5
	4	3	7	1	1.2013e+02	5.8024e+02 ;	N1 - C1	-	C6
	5	4	6	1	1.1485e+02	3.3514e+02 ;	H5 - N1	-	H6
	7	9	10	1	1.2001e+02	4.0551e+02 ;	C6 - C5	-	H4
	7	9	11	1	1.1997e+02	5.6216e+02 ;	C6 - C5	-	C4
	8	7	9	1	1.2001e+02	4.0551e+02 ;	H1 - C6	-	C5
	9	11	12	1	1.2001e+02	4.0551e+02 ;	C5 - C4	-	H3
	9	11	13	1	1.1997e+02	5.6216e+02 ;	C5 - C4	-	C3
	10	9	11	1	1.2001e+02	4.0551e+02 ;	H4 - C5	-	C4
	11	13	14	1	1.2014e+02	5.4091e+02 ;	C4 - C3	-	C7
	12	11	13	1	1.2001e+02	4.0551e+02 ;	H3 - C4	-	C3
	13	14	15	1	1.1344e+02	5.8668e+02 ;	C3 - C7	-	O2
	13	14	17	1	1.2344e+02	5.7463e+02 ;	C3 - C7	-	O1
	14	15	16	1	1.0737e+02	4.2836e+02 ;	C7 - O2	-	H7
	15	14	17	1	1.2288e+02	6.4752e+02 ;	O2 - C7	-	O1

[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	3	4	5	3	8.78640	0.00000	-8.78640	0.00000	0.00000	
0.00000 ;		C2-	C1-	N1-	H5						
	1	3	4	6	3	8.78640	0.00000	-8.78640	0.00000	0.00000	
0.00000 ;		C2-	C1-	N1-	H6						
	1	3	7	8	3	30.33400	0.00000	-30.33400	0.00000	0.00000	
0.00000 ;		C2-	C1-	C6-	H1						
	1	3	7	9	3	30.33400	0.00000	-30.33400	0.00000	0.00000	
0.00000 ;		C2-	C1-	C6-	C5						
	1	13	11	9	3	30.33400	0.00000	-30.33400	0.00000	0.00000	
0.00000 ;		C2-	C3-	C4-	C5						
	1	13	11	12	3	30.33400	0.00000	-30.33400	0.00000	0.00000	
0.00000 ;		C2-	C3-	C4-	H3						
	1	13	14	15	3	8.36800	0.00000	-8.36800	0.00000	0.00000	
0.00000 ;		C2-	C3-	C7-	O2						
	1	13	14	17	3	8.36800	0.00000	-8.36800	0.00000	0.00000	
0.00000 ;		C2-	C3-	C7-	O1						

2	1	3	4	3	30.33400	0.00000	-30.33400	0.00000	0.00000
0.00000 ;	H2-	C2-	C1-	N1					
2	1	3	7	3	30.33400	0.00000	-30.33400	0.00000	0.00000
0.00000 ;	H2-	C2-	C1-	C6					
2	1	13	11	3	30.33400	0.00000	-30.33400	0.00000	0.00000
0.00000 ;	H2-	C2-	C3-	C4					
2	1	13	14	3	30.33400	0.00000	-30.33400	0.00000	0.00000
0.00000 ;	H2-	C2-	C3-	C7					
3	1	13	11	3	30.33400	0.00000	-30.33400	0.00000	0.00000
0.00000 ;	C1-	C2-	C3-	C4					
3	1	13	14	3	30.33400	0.00000	-30.33400	0.00000	0.00000
0.00000 ;	C1-	C2-	C3-	C7					
3	7	9	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000
0.00000 ;	C1-	C6-	C5-	H4					
3	7	9	11	3	30.33400	0.00000	-30.33400	0.00000	0.00000
0.00000 ;	C1-	C6-	C5-	C4					
4	3	7	8	3	30.33400	0.00000	-30.33400	0.00000	0.00000
0.00000 ;	N1-	C1-	C6-	H1					
4	3	7	9	3	30.33400	0.00000	-30.33400	0.00000	0.00000
0.00000 ;	N1-	C1-	C6-	C5					
5	4	3	7	3	8.78640	0.00000	-8.78640	0.00000	0.00000
0.00000 ;	H5-	N1-	C1-	C6					
6	4	3	7	3	8.78640	0.00000	-8.78640	0.00000	0.00000
0.00000 ;	H6-	N1-	C1-	C6					
7	9	11	12	3	30.33400	0.00000	-30.33400	0.00000	0.00000
0.00000 ;	C6-	C5-	C4-	H3					
7	9	11	13	3	30.33400	0.00000	-30.33400	0.00000	0.00000
0.00000 ;	C6-	C5-	C4-	C3					
8	7	9	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000
0.00000 ;	H1-	C6-	C5-	H4					
8	7	9	11	3	30.33400	0.00000	-30.33400	0.00000	0.00000
0.00000 ;	H1-	C6-	C5-	C4					
9	11	13	14	3	30.33400	0.00000	-30.33400	0.00000	0.00000
0.00000 ;	C5-	C4-	C3-	C7					
10	9	11	12	3	30.33400	0.00000	-30.33400	0.00000	0.00000
0.00000 ;	H4-	C5-	C4-	H3					
10	9	11	13	3	30.33400	0.00000	-30.33400	0.00000	0.00000
0.00000 ;	H4-	C5-	C4-	C3					
11	13	14	15	3	8.36800	0.00000	-8.36800	0.00000	0.00000
0.00000 ;	C4-	C3-	C7-	O2					
11	13	14	17	3	8.36800	0.00000	-8.36800	0.00000	0.00000
0.00000 ;	C4-	C3-	C7-	O1					
12	11	13	14	3	30.33400	0.00000	-30.33400	0.00000	0.00000
0.00000 ;	H3-	C4-	C3-	C7					
13	1	3	4	3	30.33400	0.00000	-30.33400	0.00000	0.00000
0.00000 ;	C3-	C2-	C1-	N1					
13	1	3	7	3	30.33400	0.00000	-30.33400	0.00000	0.00000
0.00000 ;	C3-	C2-	C1-	C6					
13	14	15	16	3	19.24640	0.00000	-19.24640	0.00000	0.00000
0.00000 ;	C3-	C7-	O2-	H7					
16	15	14	17	3	27.19600	-7.94960	-19.24640	0.00000	0.00000
0.00000 ;	H7-	O2-	C7-	O1					

[dihedrals] ; impropers

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

i	j	k	l	func	phase	kd	pn				
1	7	3	4	1	180.00	4.60240	2 ;	C2-	C6-	C1-	N1
2	1	13	3	1	180.00	4.60240	2 ;	H2-	C2-	C3-	C1
3	5	4	6	1	180.00	4.60240	2 ;	C1-	H5-	N1-	H6
3	9	7	8	1	180.00	4.60240	2 ;	C1-	C5-	C6-	H1
7	11	9	10	1	180.00	4.60240	2 ;	C6-	C4-	C5-	H4
9	13	11	12	1	180.00	4.60240	2 ;	C5-	C3-	C4-	H3
13	17	14	15	1	180.00	43.93200	2 ;	C3-	O1-	C7-	O2
14	1	13	11	1	180.00	4.60240	2 ;	C7-	C2-	C3-	C4

[system]

MBA

[molecules]

; Compound nmols
MBA 1

DMSO

Table SI.1.2

Topology file used in Gromacs containing the GAFF atom types and partial charges used to model DMSO.

```
; DMS_GMX.top created by acpype (Rev: 403) on Mon Jul 20 12:30:57 2015

[ 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
o          o              0.00000   0.00000    A          2.95992e-01  8.78640e-01 ; 1.66  0.2100
s4         s4              0.00000   0.00000    A          3.56359e-01  1.04600e+00 ; 2.00  0.2500
c3         c3              0.00000   0.00000    A          3.39967e-01  4.57730e-01 ; 1.91  0.1094
h1         h1              0.00000   0.00000    A          2.47135e-01  6.56888e-02 ; 1.39  0.0157

[ moleculetype ]
;name      nrexcl
DMS        3

[ atoms ]
;  nr  type  resi  res  atom  cgnr      charge      mass      ; qtot  bond_type
;  1   o    1    DMS  O1    1      -0.508933    16.00000 ; qtot -0.509
;  2   s4    1    DMS  S1    2       0.316100    32.06000 ; qtot -0.193
;  3   c3    1    DMS  C2    3      -0.282583    12.01000 ; qtot -0.475
;  4   h1    1    DMS  H4    4       0.126333     1.00800 ; qtot -0.349
;  5   h1    1    DMS  H5    5       0.126333     1.00800 ; qtot -0.223
;  6   h1    1    DMS  H6    6       0.126333     1.00800 ; qtot -0.096
;  7   c3    1    DMS  C1    7      -0.282583    12.01000 ; qtot -0.379
;  8   h1    1    DMS  H1    8       0.126333     1.00800 ; qtot -0.253
;  9   h1    1    DMS  H2    9       0.126333     1.00800 ; qtot -0.126
; 10   h1    1    DMS  H3   10       0.126333     1.00800 ; qtot -0.000

[ bonds ]
;  ai  aj  funct  r      k      ;
;  1   2   1      1.4970e-01  3.7547e+05 ; O1 - S1
;  2   3   1      1.8070e-01  1.9564e+05 ; S1 - C2
;  2   7   1      1.8070e-01  1.9564e+05 ; S1 - C1
;  3   4   1      1.0930e-01  2.8108e+05 ; C2 - H4
;  3   5   1      1.0930e-01  2.8108e+05 ; C2 - H5
;  3   6   1      1.0930e-01  2.8108e+05 ; C2 - H6
;  7   8   1      1.0930e-01  2.8108e+05 ; C1 - H1
;  7   9   1      1.0930e-01  2.8108e+05 ; C1 - H2
;  7  10   1      1.0930e-01  2.8108e+05 ; C1 - H3

[ pairs ]
;  ai  aj  funct      ;
;  1   4   1 ; O1 - H4
;  1   5   1 ; O1 - H5
;  1   6   1 ; O1 - H6
;  1   8   1 ; O1 - H1
;  1   9   1 ; O1 - H2
;  1  10   1 ; O1 - H3
;  3   8   1 ; C2 - H1
;  3   9   1 ; C2 - H2
;  3  10   1 ; C2 - H3
;  4   7   1 ; H4 - C1
;  5   7   1 ; H5 - C1
;  6   7   1 ; H6 - C1

[ angles ]
;  ai  aj  ak  funct  theta      cth      ;
;  1   2   3   1      1.0621e+02  3.4359e+02 ; O1 - S1 - C2
;  1   2   7   1      1.0621e+02  3.4359e+02 ; O1 - S1 - C1
;  2   3   4   1      1.0866e+02  4.5422e+02 ; S1 - C2 - H4
;  2   3   5   1      1.0866e+02  4.5422e+02 ; S1 - C2 - H5
;  2   3   6   1      1.0866e+02  4.5422e+02 ; S1 - C2 - H6
;  2   7   8   1      1.0866e+02  4.5422e+02 ; S1 - C1 - H1
;  2   7   9   1      1.0866e+02  4.5422e+02 ; S1 - C1 - H2
;  2   7  10   1      1.0866e+02  4.5422e+02 ; S1 - C1 - H3
```

3	2	7	1	9.6820e+01	3.2501e+02 ;	C2 - S1	- C1
4	3	5	1	1.0955e+02	3.2786e+02 ;	H4 - C2	- H5
4	3	6	1	1.0955e+02	3.2786e+02 ;	H4 - C2	- H6
5	3	6	1	1.0955e+02	3.2786e+02 ;	H5 - C2	- H6
8	7	9	1	1.0955e+02	3.2786e+02 ;	H1 - C1	- H2
8	7	10	1	1.0955e+02	3.2786e+02 ;	H1 - C1	- H3
9	7	10	1	1.0955e+02	3.2786e+02 ;	H2 - C1	- H3

[dihedrals] ; props

; 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	3	4	3	0.83680	2.51040	0.00000	-3.34720	0.00000
0.00000 ;		O1-	S1-	C2-	H4					
0.00000 ;	1	2	3	5	3	0.83680	2.51040	0.00000	-3.34720	0.00000
0.00000 ;		O1-	S1-	C2-	H5					
0.00000 ;	1	2	3	6	3	0.83680	2.51040	0.00000	-3.34720	0.00000
0.00000 ;		O1-	S1-	C2-	H6					
0.00000 ;	1	2	7	8	3	0.83680	2.51040	0.00000	-3.34720	0.00000
0.00000 ;		O1-	S1-	C1-	H1					
0.00000 ;	1	2	7	9	3	0.83680	2.51040	0.00000	-3.34720	0.00000
0.00000 ;		O1-	S1-	C1-	H2					
0.00000 ;	1	2	7	10	3	0.83680	2.51040	0.00000	-3.34720	0.00000
0.00000 ;		O1-	S1-	C1-	H3					
0.00000 ;	3	2	7	8	3	0.83680	2.51040	0.00000	-3.34720	0.00000
0.00000 ;		C2-	S1-	C1-	H1					
0.00000 ;	3	2	7	9	3	0.83680	2.51040	0.00000	-3.34720	0.00000
0.00000 ;		C2-	S1-	C1-	H2					
0.00000 ;	3	2	7	10	3	0.83680	2.51040	0.00000	-3.34720	0.00000
0.00000 ;		C2-	S1-	C1-	H3					
0.00000 ;	4	3	2	7	3	0.83680	2.51040	0.00000	-3.34720	0.00000
0.00000 ;		H4-	C2-	S1-	C1					
0.00000 ;	5	3	2	7	3	0.83680	2.51040	0.00000	-3.34720	0.00000
0.00000 ;		H5-	C2-	S1-	C1					
0.00000 ;	6	3	2	7	3	0.83680	2.51040	0.00000	-3.34720	0.00000
0.00000 ;		H6-	C2-	S1-	C1					

[system]

DMS

[molecules]

; Compound nmols

DMS 1

SI.2 Molecular dynamics simulations of mABA solutions

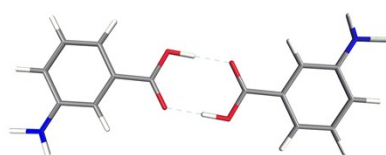
Table SI.2. Details of classical molecular dynamics simulation of mABA solutions.

	solvent	no. of mABA molecules	no. of solvent molecules	Box length (Å)	[mABA] (mol/L)	Simulation time (ns)
1	DMSO	8	3003	70.66	0.04	200
2	DMSO	16	3002	70.74	0.08	200
3	DMSO	32	3036	70.84	0.15	200
4	DMSO	64	3004	71.22	0.29	200
5	DMSO	128	3012	71.92	0.57	200
6	DMSO	256	3030	73.23	1.08	200
7	water	8	11480	70.25	0.04	30
8	water	16	11426	70.13	0.08	30
9	water	32	11314	69.95	0.16	30
10	water	64	11419	70.70	0.30	30
11	water	128	11430	71.27	0.59	30
12	water	256	11075	72.03	1.14	30

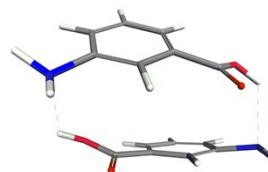
SI.3 Dimers

Structure of the mABA dimers

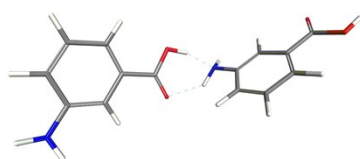
Figure SI.3.1. Structures of (mABA)₂ dimers as computed at the M06-2X/6-31+G(d,p) level of theory.



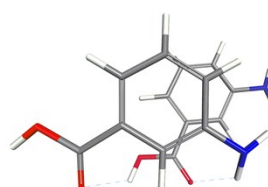
(mABA)₂ - type I



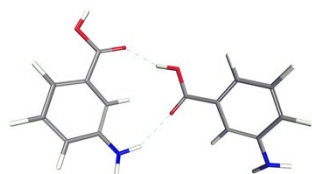
(mABA)₂ - type II



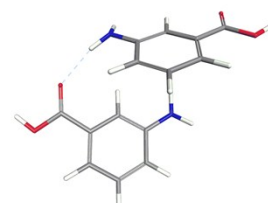
(mABA)₂ - type III



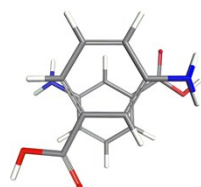
(mABA)₂ - type IV



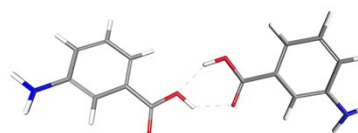
(mABA)₂ - type V



(mABA)₂ - type VI



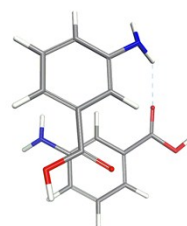
(mABA)₂ - type VII



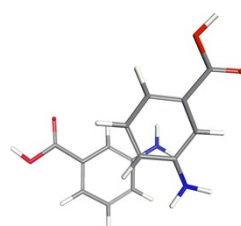
(mABA)₂ - type VIII



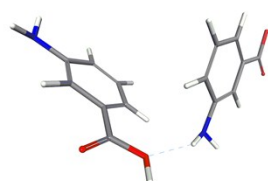
(mABA)₂ - type IX



(mABA)₂ - type X



(mABA)₂ - type XI



(mABA)₂ - type XI

Coordinates of the optimised geometries of the mABA dimers

Table SI.3.1. Geometries [in Angstrom] of the dimeric structures of *m*-aminobenzoic acid as computed at the M06-2X/6-31+G(d,p) level of theory. XYZ format.

```
34
config_1032
H      3.4870490      0.7480040      0.7053900
C      1.3450030      0.8758520      0.9035180
N      1.2206110     -0.2742270      1.6706970
C      0.2189020      1.6452060      0.5915970
H     -0.7660750      1.3268200      0.9186090
C      0.3482430      2.8235910     -0.1401870
C      1.5993070      3.2808860     -0.5629270
H      1.6840800      4.2009080     -1.1286600
C      2.7205920      2.5158500     -0.2499130
H      3.7038120      2.8428510     -0.5728130
C      2.6008560      1.3311750      0.4696040
H      1.9637130     -0.9501640      1.5601360
H      0.3073240     -0.7135180      1.6470280
C     -0.9015730      3.5454780     -0.4889520
O     -2.0213630      3.0867700     -0.3732510
O     -0.6932850      4.7797850     -0.9762020
H     -1.5617460      5.1538630     -1.1895090
H     -3.0254350     -0.2401850      0.6865770
C     -1.5137880     -0.7970220     -0.7444370
N     -1.7955100      0.2467160     -1.6078740
C     -0.5188650     -1.7375630     -1.0443390
H      0.0829330     -1.6426970     -1.9437150
C     -0.2811620     -2.8096780     -0.1869780
C     -1.0179670     -2.9769170      0.9897220
H     -0.8212540     -3.8171780      1.6443890
C     -2.0035880     -2.0378510      1.2914220
H     -2.5890290     -2.1421700      2.1995210
C     -2.2516590     -0.9634850      0.4417480
H     -2.1962360      1.0772710     -1.1840930
H     -1.0550360      0.4755120     -2.2568240
C      0.8032040     -3.7575490     -0.5668130
O      1.4952600     -3.6581720     -1.5534290
O      0.9594050     -4.7651510      0.3165790
H      1.6736490     -5.3268400     -0.0201060
```

```
34
config_1086
H      3.3639430      1.2439770      0.6242860
C      1.2405170      1.0404580      0.9300960
N      1.3307610     -0.1343530      1.6637830
C     -0.0031670      1.6380500      0.6988960
H     -0.9106030      1.1666540      1.0632820
C     -0.0911540      2.8405130      0.0009160
C      1.0528780      3.4925010     -0.4670310
H      0.9685590      4.4286550     -1.0057030
C      2.2912920      2.8986540     -0.2340510
H      3.1958170      3.3789700     -0.5932500
C      2.3889890      1.6917540      0.4510170
H      2.1600100     -0.6867730      1.4950950
H      0.4936160     -0.7059990      1.6693500
C     -1.4519950      3.3734280     -0.2617970
O     -2.4827610      2.7489340     -0.1027540
```

O	-1.4574600	4.6353900	-0.7219730
H	-2.3824210	4.8784030	-0.8802220
H	-2.9101060	-0.7349800	0.9203840
C	-1.4257690	-1.0101260	-0.6172760
N	-1.9188240	0.0001830	-1.4235970
C	-0.3193470	-1.7758020	-1.0100660
H	0.2020510	-1.5634720	-1.9390910
C	0.1338940	-2.8217970	-0.2091890
C	-0.4914510	-3.1339330	1.0019910
H	-0.1269860	-3.9515290	1.6119340
C	-1.5876670	-2.3677660	1.3963800
H	-2.0906020	-2.5867040	2.3330610
C	-2.0515520	-1.3217680	0.6035560
H	-2.4114900	0.7489820	-0.9476550
H	-1.2665020	0.3555040	-2.1091410
C	1.3232180	-3.5798140	-0.6882980
O	1.9250980	-3.3489350	-1.7113340
O	1.6897600	-4.5735820	0.1472690
H	2.4577380	-5.0088300	-0.2524380

34

config_1132

H	-2.9189110	1.0764770	0.0468140
C	-1.0446710	1.7342070	0.8818700
N	-1.5186040	1.7965970	2.1906000
C	0.2989200	2.0007680	0.6005490
H	0.9888270	2.2757400	1.3934920
C	0.7816510	1.8728840	-0.7006940
C	-0.0565080	1.4827200	-1.7477340
H	0.3419860	1.3691990	-2.7487290
C	-1.3904950	1.2036970	-1.4614760
H	-2.0551860	0.8662090	-2.2505600
C	-1.8816050	1.3224960	-0.1653290
H	-2.5159640	1.9227050	2.2868870
H	-0.9926640	2.3916930	2.8146930
C	2.2411230	2.0662690	-0.9122080
O	3.0620350	2.1425460	-0.0184790
O	2.5903300	2.1378680	-2.2037500
H	3.5583460	2.1713700	-2.2349950
H	-3.1613350	-2.6883460	0.7537400
C	-1.4872420	-2.3721480	-0.5649860
N	-2.1667600	-2.7946630	-1.7112910
C	-0.1744090	-1.9027380	-0.6502870
H	0.3558100	-1.8901350	-1.5986680
C	0.4665610	-1.4018340	0.4810010
C	-0.1779750	-1.3654280	1.7186140
H	0.3237320	-0.9465020	2.5825890
C	-1.4835920	-1.8404090	1.8032600
H	-2.0065540	-1.8114110	2.7539270
C	-2.1357330	-2.3352770	0.6776640
H	-2.9219270	-3.4453020	-1.5448100
H	-1.5702470	-3.0995920	-2.4680510
C	1.8310710	-0.8334670	0.2912880
O	2.4226330	-0.8241300	-0.7675750
O	2.3388080	-0.2791440	1.4026820
H	3.1042320	0.2584860	1.1323870

34

config_1163

H	1.9463910	-6.5596090	-0.5227790
C	-0.0401220	-5.7403930	-0.3559290

N	-0.6799330	-6.9302300	-0.6904560
C	-0.7800490	-4.5996030	-0.0296810
H	-1.8656790	-4.6074730	-0.0667050
C	-0.1320770	-3.4277980	0.3556870
C	1.2610790	-3.3653080	0.4290410
H	1.7543120	-2.4530240	0.7420900
C	1.9965510	-4.5037320	0.1073450
H	3.0803150	-4.4797830	0.1607740
C	1.3598590	-5.6771750	-0.2809590
H	-0.1387820	-7.5821720	-1.2395040
H	-1.6299770	-6.8386350	-1.0201000
C	-0.9917440	-2.2536820	0.6809550
O	-2.1987500	-2.2703650	0.6936930
O	-0.2848690	-1.1389580	0.9661650
H	-0.8925000	-0.3899990	1.1528340
H	0.8988100	7.1181310	-0.6024860
C	-0.3862330	5.6392510	0.2944260
N	-1.3486440	6.5591280	0.6997960
C	-0.5634790	4.2717460	0.5256470
H	-1.4342990	3.9036160	1.0603150
C	0.3798540	3.3550750	0.0649360
C	1.5151650	3.7719280	-0.6330760
H	2.2378610	3.0449970	-0.9829080
C	1.6886710	5.1345900	-0.8624290
H	2.5625080	5.4845540	-1.4025990
C	0.7537300	6.0585840	-0.4086430
H	-1.0259460	7.5070670	0.8285590
H	-1.9630520	6.2532080	1.4404130
C	0.1306110	1.9168440	0.3498680
O	-0.8380350	1.5107280	0.9687460
O	1.0723870	1.1027160	-0.1360370
H	0.8398860	0.1819420	0.0889360

34

config_1182

H	-1.6842020	-5.9366520	0.6749410
C	-1.1931220	-4.4375860	-0.7929490
N	-2.0113230	-4.9791410	-1.7821410
C	-0.4733310	-3.2619550	-1.0266440
H	-0.5053090	-2.7692410	-1.9942010
C	0.2957680	-2.6963390	-0.0118960
C	0.3666510	-3.2830980	1.2531370
H	0.9692600	-2.8276030	2.0294580
C	-0.3500260	-4.4548510	1.4834470
H	-0.3105380	-4.9301300	2.4585130
C	-1.1222210	-5.0273060	0.4781280
H	-2.2020430	-5.9673110	-1.7007300
H	-1.7904130	-4.7039230	-2.7282810
C	1.0441820	-1.4464120	-0.3307320
O	1.0405420	-0.9269810	-1.4344030
O	1.7210270	-0.9475730	0.7020100
H	2.1727220	-0.1146270	0.4049230
H	3.1782470	3.5145060	0.9182590
C	1.7257650	2.3907030	-0.2065630
N	2.6316070	1.3661750	-0.5619150
C	0.3890400	2.3081870	-0.6000940
H	0.0424560	1.4864730	-1.2217210
C	-0.5126530	3.2889910	-0.1876770
C	-0.1035690	4.3556660	0.6153770
H	-0.8187970	5.1087690	0.9236070
C	1.2310720	4.4286110	1.0048540

H	1.5694770	5.2495090	1.6286740
C	2.1398110	3.4545680	0.6025030
H	3.5944540	1.6773030	-0.6127850
H	2.3572000	0.8697650	-1.4076230
C	-1.9242050	3.1568590	-0.6463600
O	-2.3373950	2.2779410	-1.3648370
O	-2.7256500	4.1357020	-0.1772480
H	-3.6127770	3.9633280	-0.5267760

34

config_1280

H	-2.6486490	-1.3955080	2.2301520
C	-0.6291820	-0.9961250	1.5994740
N	-0.4238310	0.0143430	2.5373330
C	0.3810580	-1.3639590	0.7062950
H	1.3387330	-0.8504360	0.7085710
C	0.1566720	-2.3666770	-0.2350640
C	-1.0648240	-3.0403200	-0.2970530
H	-1.2235810	-3.8159200	-1.0366810
C	-2.0659370	-2.6841770	0.6059130
H	-3.0230920	-3.1963050	0.5811670
C	-1.8561970	-1.6766130	1.5419570
H	-1.2620710	0.5450300	2.7439650
H	0.3374690	0.6385590	2.2987380
C	1.2502740	-2.6441400	-1.2041850
O	2.2759640	-2.0064890	-1.2901600
O	0.9905730	-3.6885540	-2.0163860
H	1.7496810	-3.7774790	-2.6118820
H	3.1904320	3.4717550	-0.3594920
C	1.1957340	3.5239370	0.4556240
N	1.4203120	4.6653430	1.2207640
C	-0.0577380	2.9042940	0.4436950
H	-0.8683220	3.2699910	1.0686650
C	-0.2890550	1.8041270	-0.3832360
C	0.7166140	1.2941710	-1.2057160
H	0.5300980	0.4232370	-1.8227160
C	1.9705220	1.9012810	-1.1785210
H	2.7725420	1.5026950	-1.7911460
C	2.2101620	3.0022570	-0.3639510
H	2.3816470	4.8475520	1.4699070
H	0.7832650	4.8129630	1.9900830
C	-1.6266410	1.1536920	-0.3016030
O	-2.4678590	1.4196350	0.5310250
O	-1.8117850	0.2082530	-1.2355470
H	-2.6447700	-0.2439750	-1.0299930

34

config_1373

H	3.0246660	0.2833130	0.4404300
C	1.4713920	1.0197050	-0.8589670
N	1.7283500	0.1000510	-1.8595220
C	0.4680990	1.9880710	-1.0017890
H	-0.1578970	2.0136830	-1.8891640
C	0.2537140	2.9335330	-0.0007890
C	1.0218830	2.9425260	1.1675510
H	0.8415630	3.6845850	1.9356950
C	2.0171660	1.9763510	1.3119440
H	2.6263440	1.9586590	2.2101010
C	2.2435110	1.0294320	0.3174990
H	2.1506770	-0.7737420	-1.5622900
H	0.9721670	-0.0459520	-2.5137890

C	-0.8393640	3.9213210	-0.2209580
O	-1.5576660	3.9531780	-1.1932060
O	-0.9694680	4.8019590	0.7924520
H	-1.6918010	5.4020050	0.5533730
H	-3.4449960	-1.0199370	0.6652280
C	-1.2904720	-0.9849790	0.7071540
N	-1.1954530	0.1235710	1.5372180
C	-0.1351010	-1.6416180	0.2698350
H	0.8432160	-1.2676400	0.5538190
C	-0.2268710	-2.7792930	-0.5284080
C	-1.4667820	-3.3099110	-0.8943390
H	-1.5223540	-4.1976590	-1.5127870
C	-2.6171350	-2.6587450	-0.4547990
H	-3.5934740	-3.0445270	-0.7302210
C	-2.5362060	-1.5136750	0.3314490
H	-1.9946710	0.7418610	1.5277820
H	-0.3223260	0.6350060	1.4749320
C	1.0466510	-3.3748130	-1.0056650
O	2.1339410	-2.8359420	-0.9304460
O	0.9000580	-4.5885100	-1.5616090
H	1.7777030	-4.8770240	-1.8551720

34

config_148

H	-3.4410210	1.4660740	-0.9230410
C	-1.4391200	0.8490870	-1.4136200
N	-1.8575210	-0.1092140	-2.3338880
C	-0.0820850	1.0736760	-1.1678330
H	0.6798270	0.4794440	-1.6652510
C	0.3135460	2.0372670	-0.2433360
C	-0.6256320	2.8112320	0.4424400
H	-0.3006240	3.5539650	1.1612400
C	-1.9779970	2.5976220	0.1834660
H	-2.7266520	3.1905600	0.7001330
C	-2.3843020	1.6295010	-0.7289980
H	-2.6970160	-0.5958050	-2.0397720
H	-1.1323020	-0.7628330	-2.6020370
C	1.7709460	2.1566140	0.0257250
O	2.6323830	1.4974970	-0.5105820
O	2.0658900	3.0820870	0.9642050
H	3.0298580	3.0817090	1.0617340
H	-2.1339960	-0.0115250	2.2405820
C	-1.6723090	-1.4573130	0.7116520
N	-3.0036550	-1.6192270	0.2953730
C	-0.6442290	-2.1247130	0.0442320
H	-0.8594860	-2.8171880	-0.7656080
C	0.6850480	-1.8891690	0.3934600
C	1.0155910	-0.9988470	1.4160610
H	2.0551580	-0.8167880	1.6618560
C	-0.0138220	-0.3361200	2.0805280
H	0.2186180	0.3765110	2.8658440
C	-1.3424630	-0.5567110	1.7327810
H	-3.6873140	-1.3210790	0.9792980
H	-3.2174360	-2.5501610	-0.0405870
C	1.7311830	-2.5843710	-0.4051940
O	1.5126920	-3.2272730	-1.4081020
O	2.9704180	-2.4266970	0.0913470
H	3.5802810	-2.8719330	-0.5158740

34

config_1656

H	-2.9935650	-3.9730690	-0.8164600
C	-1.6230650	-2.6754440	0.2274360
N	-2.5803990	-1.7969140	0.7087350
C	-0.2792950	-2.4787760	0.5632480
H	-0.0112730	-1.6312900	1.1821170
C	0.7000990	-3.3501440	0.1010440
C	0.3737290	-4.4682340	-0.6726560
H	1.1474710	-5.1405290	-1.0235930
C	-0.9667300	-4.6750750	-0.9886050
H	-1.2510510	-5.5315980	-1.5916620
C	-1.9544250	-3.7945480	-0.5525660
H	-3.4500820	-1.7632140	0.1978290
H	-2.2234540	-0.8833160	0.9669010
C	2.1010490	-3.0026860	0.4327380
O	2.4589180	-1.9315150	0.8927280
O	2.9844470	-3.9753290	0.1740940
H	3.8634670	-3.6352110	0.4015520
H	-0.3291160	6.2299980	-1.0007430
C	-1.1999910	4.5422990	0.0173370
N	-2.4306660	5.1622620	0.2290300
C	-0.9855510	3.2237100	0.4292390
H	-1.7581570	2.6727920	0.9578250
C	0.2296420	2.5935700	0.1682910
C	1.2551250	3.2585430	-0.5068710
H	2.1944940	2.7546570	-0.6984110
C	1.0378990	4.5704850	-0.9211500
H	1.8198360	5.1067200	-1.4494870
C	-0.1717290	5.2077870	-0.6665020
H	-2.4124380	6.1719740	0.2410990
H	-2.9830850	4.7802610	0.9833910
C	0.3919700	1.1863730	0.6398490
O	-0.4940710	0.5633430	1.1975770
O	1.5995430	0.6891690	0.3906500
H	1.6931570	-0.2394210	0.6950370

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config_1698

H	0.3222650	-6.6193700	0.4610760
C	-0.8785950	-4.8619300	0.1260780
N	-2.0941390	-5.5396490	0.2089260
C	-0.8456910	-3.4782250	-0.0707980
H	-1.7634680	-2.9124810	-0.2025630
C	0.3714030	-2.8003340	-0.0999810
C	1.5789970	-3.4811140	0.0674710
H	2.5160260	-2.9387430	0.0395790
C	1.5441410	-4.8589890	0.2674890
H	2.4702460	-5.4091370	0.4008100
C	0.3345730	-5.5447460	0.2984180
H	-2.0569950	-6.5267520	-0.0013230
H	-2.8758870	-5.0819320	-0.2376810
C	0.3347440	-1.3243080	-0.3208170
O	-0.6993400	-0.6948080	-0.4560480
O	1.5442760	-0.7733910	-0.3573780
H	1.5102610	0.1965410	-0.5027430
H	-3.3703530	4.1981660	0.6301830
C	-1.9743900	2.7022110	-0.0526910
N	-2.9080810	1.6961550	-0.2447490
C	-0.6316690	2.4588070	-0.3589340
H	-0.3457210	1.4750720	-0.7089260
C	0.3236660	3.4546730	-0.1966260
C	-0.0276710	4.7339090	0.2463920

H	0.7264490	5.5023400	0.3669370
C	-1.3670190	4.9796280	0.5379470
H	-1.6697000	5.9617490	0.8871980
C	-2.3310690	3.9836000	0.3952720
H	-3.7561200	1.7620510	0.2980920
H	-2.5210040	0.7601660	-0.2892140
C	1.7266390	3.0766590	-0.4837790
O	2.1084050	1.9439070	-0.7236560
O	2.5873500	4.1027490	-0.4539340
H	3.4696970	3.7445990	-0.6361210

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config_1746

H	0.7817390	-7.1894250	-0.3377160
C	-0.5817440	-5.5212780	-0.3169160
N	-1.7272350	-6.3136870	-0.3197730
C	-0.6786520	-4.1274130	-0.2639680
H	-1.6466650	-3.6349610	-0.2641210
C	0.4741940	-3.3465920	-0.2051560
C	1.7432910	-3.9286730	-0.1965780
H	2.6263710	-3.3029930	-0.1514470
C	1.8370230	-5.3170120	-0.2478700
H	2.8120440	-5.7937000	-0.2421180
C	0.6934330	-6.1065750	-0.3058190
H	-1.6180020	-7.2406840	-0.7049030
H	-2.5705020	-5.8592410	-0.6394380
C	0.3130590	-1.8678910	-0.1553480
O	-0.7989870	-1.3367570	-0.1710100
O	1.4347710	-1.1927920	-0.0956940
H	1.2491930	-0.2002900	-0.0648490
H	-0.6219970	7.2024650	0.1642730
C	0.7416350	5.5345320	0.1375800
N	1.8836500	6.3225420	0.2594320
C	0.8383270	4.1404120	0.0913800
H	1.8058070	3.6472510	0.1094790
C	-0.3143390	3.3598690	0.0255600
C	-1.5830880	3.9424010	0.0053750
H	-2.4659880	3.3170200	-0.0468010
C	-1.6766950	5.3308820	0.0530780
H	-2.6514700	5.8078990	0.0390410
C	-0.5333520	6.1200910	0.1198280
H	1.7947450	7.2757710	-0.0615320
H	2.7450100	5.8912860	-0.0437050
C	-0.1531420	1.8812600	-0.0267430
O	0.9591130	1.3504000	-0.0184230
O	-1.2749600	1.2060080	-0.0825260
H	-1.0892940	0.2136090	-0.1161340

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config_1840

H	-1.7767690	-3.6190740	0.6623540
C	-1.2584310	-2.0077820	-0.6691380
N	-2.5851710	-1.7510120	-1.0534300
C	-0.2197300	-1.2059460	-1.1459820
H	-0.4094800	-0.4235900	-1.8778160
C	1.0695350	-1.3608720	-0.6425300
C	1.3567760	-2.3353590	0.3164070
H	2.3641390	-2.4390550	0.7017210
C	0.3251760	-3.1555840	0.7642910
H	0.5271320	-3.9240590	1.5037470
C	-0.9725100	-2.9919340	0.2843100

H	-3.1704540	-2.5751090	-1.1122530
H	-2.6653290	-1.1918230	-1.8943490
C	2.1074580	-0.4219370	-1.1458690
O	1.9126590	0.4486010	-1.9643020
O	3.3209330	-0.6227640	-0.5942250
H	3.9146360	0.0402430	-0.9774270
H	-0.3069240	-0.3202230	3.3577800
C	-1.4164270	0.3153050	1.6237820
N	-2.5694870	-0.4021160	1.9311620
C	-1.3700580	1.0963100	0.4635080
H	-2.2182410	1.1210040	-0.2152990
C	-0.2160830	1.7997230	0.1340080
C	0.9032070	1.7823870	0.9700910
H	1.7966830	2.3296220	0.6922770
C	0.8492830	1.0227560	2.1360020
H	1.7124740	0.9796200	2.7929650
C	-0.2902470	0.2910580	2.4589870
H	-2.4262420	-1.1545390	2.5911420
H	-3.0747070	-0.7176280	1.1089830
C	-0.1823940	2.4669410	-1.1951620
O	-0.9969330	2.2800610	-2.0730880
O	0.8584560	3.3030770	-1.3469740
H	0.8445660	3.6047890	-2.2675110

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config_1979

H	1.0086630	0.0724200	-0.9327620
C	-0.4581200	1.6450540	-0.8041430
N	-1.3074350	1.0791390	-1.7496400
C	-0.8019440	2.8352790	-0.1549580
H	-1.7173630	3.3640170	-0.4052130
C	0.0289280	3.3612150	0.8325770
C	1.2126980	2.7175940	1.2006910
H	1.8469400	3.1402330	1.9703830
C	1.5518660	1.5317210	0.5536450
H	2.4675730	1.0132960	0.8196750
C	0.7331410	0.9987570	-0.4361690
H	-0.8904490	0.3951910	-2.3680660
H	-1.9376090	1.7164670	-2.2143050
C	-0.3988610	4.6344600	1.4735940
O	-1.4063680	5.2446110	1.1974050
O	0.4589790	5.0676030	2.4204000
H	0.0943060	5.8937220	2.7714200
H	-0.8862790	-3.4123780	2.8169010
C	0.2982690	-4.1064050	1.1555830
N	0.8543360	-5.1738730	1.8545050
C	0.6095510	-3.8931710	-0.1898180
H	1.3209280	-4.5311100	-0.7063930
C	0.0032030	-2.8520020	-0.8940750
C	-0.9261480	-2.0076290	-0.2829210
H	-1.3978570	-1.1988780	-0.8301300
C	-1.2320060	-2.2232470	1.0593420
H	-1.9452250	-1.5741580	1.5569040
C	-0.6327860	-3.2549200	1.7717860
H	0.8802940	-5.0766130	2.8591350
H	1.7144160	-5.5448960	1.4774040
C	0.4055860	-2.6852790	-2.3145680
O	1.1412110	-3.4249620	-2.9232790
O	-0.1254450	-1.5843140	-2.9101450
H	0.1913870	-1.5999920	-3.8268150

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config_2017

H	-2.4279850	-0.5756730	-1.6718510
C	-0.5583310	0.4965460	-1.6702870
N	-0.0048430	-0.1988950	-2.7390510
C	0.1717360	1.5123940	-1.0444490
H	1.1757100	1.7515210	-1.3829580
C	-0.3580310	2.1886010	0.0513190
C	-1.6472420	1.9151840	0.5154040
H	-2.0465360	2.4499960	1.3690060
C	-2.3860260	0.9256770	-0.1306840
H	-3.3847690	0.6837040	0.2192280
C	-1.8518850	0.2176040	-1.2020580
H	-0.4362070	-1.0964490	-2.9181300
H	1.0061180	-0.2737960	-2.6923380
C	0.5361360	3.1481220	0.7479960
O	1.7337960	3.2365110	0.5649990
O	-0.0994800	3.9235050	1.6441290
H	0.5714400	4.4874900	2.0577770
H	-2.2503020	-3.6737260	1.0508990
C	-0.5146400	-3.2707300	-0.1621440
N	-0.7913560	-4.2728610	-1.0963580
C	0.5903950	-2.4334490	-0.3285380
H	1.2742160	-2.5702580	-1.1621580
C	0.8171380	-1.3842710	0.5612210
C	-0.0355480	-1.1581580	1.6422950
H	0.1464230	-0.3274730	2.3135450
C	-1.1351240	-1.9971010	1.8087990
H	-1.8194420	-1.8330360	2.6352440
C	-1.3803240	-3.0357130	0.9172540
H	-1.3789060	-5.0225090	-0.7584310
H	0.0155370	-4.6260900	-1.5922820
C	1.9317110	-0.4469950	0.2467280
O	2.5552790	-0.4628610	-0.7956710
O	2.1470370	0.4563350	1.2100720
H	2.6988660	1.1749350	0.8549070

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config_2124

H	-3.6935630	-3.3787850	-0.1048830
C	-1.9366380	-2.3255920	0.5700930
N	-2.6107510	-1.3258060	1.2527330
C	-0.5376930	-2.3397080	0.5769430
H	-0.0067460	-1.5575020	1.1056440
C	0.1627020	-3.3363840	-0.0928520
C	-0.5010880	-4.3746220	-0.7535780
H	0.0580560	-5.1461890	-1.2692280
C	-1.8937040	-4.3715900	-0.7415530
H	-2.4376080	-5.1613960	-1.2500090
C	-2.6068060	-3.3639580	-0.0958130
H	-3.5611870	-1.1516510	0.9613290
H	-2.0705410	-0.4811350	1.4060120
C	1.6381580	-3.2092470	-0.1075280
O	2.2507600	-2.2121270	0.2354030
O	2.2793460	-4.2984630	-0.5499440
H	3.2279210	-4.0977860	-0.5431790
H	0.1486740	6.2171380	-1.3391620
C	-0.6196720	4.6987630	-0.0173660
N	-1.6507300	5.4946960	0.4797660
C	-0.4747620	3.3738440	0.4044770
H	-1.1359890	2.9534910	1.1567340

C	0.5268620	2.5689510	-0.1348870
C	1.4031520	3.0620500	-1.1036480
H	2.1780550	2.4235520	-1.5096870
C	1.2537520	4.3805710	-1.5269380
H	1.9218750	4.7850020	-2.2806770
C	0.2567800	5.1916800	-0.9954100
H	-1.4976990	6.4912320	0.4205730
H	-2.0168790	5.2163690	1.3789990
C	0.6272620	1.1654470	0.3641050
O	-0.1465590	0.6888610	1.1755280
O	1.6462570	0.4955660	-0.1655270
H	1.6967370	-0.4292050	0.1600080

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config_2296

H	0.8555580	-6.5364880	-1.5361700
C	-0.5605810	-5.2229010	-0.5809950
N	-1.6119670	-6.1364670	-0.6327320
C	-0.7314960	-3.9715490	0.0186940
H	-1.6951180	-3.6708060	0.4199890
C	0.3410890	-3.0875250	0.1175080
C	1.6027360	-3.4257170	-0.3756210
H	2.4238690	-2.7243920	-0.2908800
C	1.7709260	-4.6726540	-0.9729830
H	2.7422280	-4.9579990	-1.3644750
C	0.7075880	-5.5633620	-1.0751210
H	-1.5480540	-6.8350230	-1.3591570
H	-2.5370800	-5.7375380	-0.5624940
C	0.0907870	-1.7679300	0.7669310
O	-1.0034100	-1.4267400	1.1875970
O	1.1699460	-0.9955960	0.8458360
H	0.9148570	-0.1418510	1.2908310
H	-1.7460250	0.7169050	0.0871370
C	-0.3644260	2.1022700	0.9782140
N	-0.0133240	1.2167200	2.0238430
C	0.2479210	3.3489830	0.8686380
H	0.9695530	3.6901500	1.6058140
C	-0.0637750	4.1840390	-0.2043600
C	-0.9794820	3.7878700	-1.1803220
H	-1.2110450	4.4484760	-2.0073040
C	-1.5823660	2.5371720	-1.0661660
H	-2.2963010	2.2112270	-1.8155560
C	-1.2817100	1.6958280	0.0005170
H	-0.7646290	0.5735130	2.2647860
H	0.3421100	1.6895840	2.8467390
C	0.6157520	5.5075120	-0.2574820
O	1.4062280	5.9097480	0.5646740
O	0.2632340	6.2417590	-1.3313840
H	0.7527370	7.0761620	-1.2755660

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config_2311

H	2.9685270	-0.3500000	-1.8375810
C	2.1975260	0.1439500	0.1103250
N	2.9872920	-0.7928150	0.7778720
C	1.3170030	0.9684510	0.8155140
H	1.2047330	0.8749410	1.8921910
C	0.5315690	1.8970360	0.1357940
C	0.6245490	2.0477510	-1.2499400
H	-0.0065090	2.7616070	-1.7644690
C	1.5170220	1.2377960	-1.9462510

H	1.6037580	1.3322590	-3.0243710
C	2.2927850	0.2933810	-1.2804190
H	3.2568300	-1.5879420	0.2131470
H	2.6378230	-1.0732390	1.6847180
C	-0.4330760	2.6883590	0.9427660
O	-0.5453180	2.6345820	2.1469310
O	-1.2147370	3.5000910	0.1963950
H	-1.7819920	3.9807840	0.8174720
H	-3.1645630	0.9618410	0.3636400
C	-1.8523030	-0.1715810	-0.9157080
N	-2.2202650	0.4995850	-2.0749690
C	-0.8600080	-1.1570860	-0.9466990
H	-0.3745730	-1.4313800	-1.8790310
C	-0.4592430	-1.7827410	0.2314120
C	-1.0261850	-1.4442330	1.4631930
H	-0.6996670	-1.9374730	2.3709230
C	-2.0015590	-0.4511870	1.4936540
H	-2.4382030	-0.1490680	2.4398230
C	-2.4122890	0.1778290	0.3231500
H	-3.1244410	0.9479600	-2.0638080
H	-2.0219250	0.0256130	-2.9437960
C	0.6306160	-2.7871250	0.1301040
O	1.2522030	-3.0449040	-0.8774730
O	0.8979840	-3.4062380	1.3013120
H	1.5945560	-4.0557300	1.1227920

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config_2479

H	2.0438760	-6.4946510	0.0754060
C	0.1083090	-5.7151700	-0.4640310
N	-0.3649120	-6.9256790	-0.9615930
C	-0.7129910	-4.5835780	-0.4404980
H	-1.7214290	-4.6157980	-0.8430520
C	-0.2492250	-3.3896890	0.1080400
C	1.0354000	-3.2954590	0.6474470
H	1.3816280	-2.3661100	1.0832710
C	1.8509010	-4.4246110	0.6266170
H	2.8518330	-4.3759700	1.0434310
C	1.3988440	-5.6199340	0.0790370
H	0.3385120	-7.5783880	-1.2753950
H	-1.1476580	-6.8620590	-1.5963090
C	-1.1826880	-2.2270720	0.0890210
O	-2.3222090	-2.2687330	-0.3071680
O	-0.6275900	-1.0915590	0.5645790
H	-1.2702880	-0.3507470	0.5142710
H	1.0429910	7.1550190	-0.5381120
C	-0.4801810	5.6812960	-0.1494010
N	-1.5214910	6.6039010	-0.1133590
C	-0.7313100	4.3149290	0.0085220
H	-1.7359270	3.9499730	0.2016480
C	0.3116250	3.3952600	-0.0857240
C	1.6214620	3.8079070	-0.3385730
H	2.4191840	3.0785580	-0.4079450
C	1.8684450	5.1693950	-0.4961260
H	2.8777540	5.5162160	-0.6932880
C	0.8358560	6.0964020	-0.4051210
H	-1.2622920	7.5523000	0.1161090
H	-2.3577320	6.3023270	0.3655580
C	-0.0255200	1.9584250	0.0983570
O	-1.1513400	1.5554010	0.3353630
O	1.0259380	1.1418760	-0.0182900

H	0.7268760	0.2226240	0.1159440
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config_2499

H	-2.8664960	-2.1146630	-1.3182480
C	-1.3927240	-1.6082000	0.1693570
N	-2.2725430	-0.9120520	0.9938160
C	-0.0517520	-1.7527590	0.5387610
H	0.3101670	-1.3207280	1.4675610
C	0.8383910	-2.4248670	-0.2941580
C	0.4094260	-3.0249170	-1.4814420
H	1.1152640	-3.5422410	-2.1199480
C	-0.9337740	-2.9123870	-1.8285100
H	-1.2926100	-3.3626650	-2.7485120
C	-1.8246770	-2.2084110	-1.0224150
H	-3.0875190	-0.5411090	0.5247120
H	-1.8320230	-0.2073320	1.5754030
C	2.2711770	-2.4011150	0.0912270
O	2.7488530	-1.6744040	0.9415290
O	3.0342420	-3.2552040	-0.6104920
H	3.9481280	-3.1336470	-0.3116600
H	-0.4846880	2.1496610	3.5695850
C	0.5235540	1.3198820	1.8521950
N	1.4232260	0.5748380	2.5856800
C	0.5222120	1.2545900	0.4513030
H	1.2808490	0.6824190	-0.0746270
C	-0.4731320	1.8944830	-0.2815410
C	-1.4675280	2.6494230	0.3473320
H	-2.2306510	3.1460870	-0.2396230
C	-1.4426850	2.7486340	1.7371720
H	-2.1966260	3.3370530	2.2507590
C	-0.4718420	2.0871250	2.4845370
H	1.6446280	0.8711910	3.5226220
H	2.1474380	0.0667550	2.0918510
C	-0.4346150	1.7249590	-1.7608200
O	0.4253800	1.1301850	-2.3666430
O	-1.4796160	2.3062460	-2.3879840
H	-1.3621920	2.1418380	-3.3356230

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config_2501

H	0.8458820	-0.8839540	2.9258130
C	1.2214660	-1.1591210	0.8212450
N	2.2413310	-0.2266310	0.7599830
C	0.8438470	-1.8835550	-0.3187390
H	1.3250350	-1.7015860	-1.2760740
C	-0.1517410	-2.8573440	-0.2373530
C	-0.7972070	-3.1363830	0.9709450
H	-1.5651320	-3.8989800	1.0165850
C	-0.4222530	-2.4135890	2.1030950
H	-0.9076180	-2.6106860	3.0540110
C	0.5675530	-1.4397670	2.0343460
H	2.2374790	0.4618590	1.4999310
H	2.4051830	0.1990980	-0.1465550
C	-0.4972620	-3.5852000	-1.4916990
O	0.0232420	-3.3946350	-2.5654800
O	-1.4725250	-4.5004910	-1.3194580
H	-1.6237570	-4.9163130	-2.1815710
H	-2.9564680	2.2111190	1.7383900
C	-1.5224890	1.3016040	0.4113660
N	-2.1957850	0.0928230	0.3059820

C	-0.3383690	1.5167890	-0.3028010
H	0.0761010	0.7265310	-0.9211810
C	0.3152320	2.7448820	-0.2332970
C	-0.1988970	3.7981220	0.5282130
H	0.3188400	4.7488770	0.5684610
C	-1.3795690	3.5847990	1.2357290
H	-1.7983460	4.3837220	1.8394020
C	-2.0336310	2.3577960	1.1832690
H	-2.8120990	-0.1294170	1.0748950
H	-1.6208520	-0.6996920	0.0443270
C	1.6001600	2.8721700	-0.9678550
O	2.2223000	1.9418920	-1.4404370
O	2.0466100	4.1363820	-1.0569220
H	2.8901470	4.1082880	-1.5337760

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config_2670

H	-0.7376520	3.8279740	-2.5566280
C	0.3606280	3.6007980	-0.7161090
N	1.0914430	4.7747740	-0.8799210
C	0.5290050	2.8044890	0.4210720
H	1.2676880	3.0578190	1.1771410
C	-0.2618330	1.6695950	0.6060820
C	-1.2267070	1.3007840	-0.3323970
H	-1.8148900	0.4026160	-0.1873820
C	-1.3802180	2.0846010	-1.4737240
H	-2.1046710	1.7968980	-2.2284530
C	-0.6021690	3.2207290	-1.6654280
H	1.1962440	5.0999750	-1.8300660
H	1.9479880	4.8389140	-0.3491760
C	0.0115110	0.8293400	1.8051160
O	0.9458480	0.9955350	2.5608990
O	-0.8730160	-0.1674470	1.9635090
H	-0.5511800	-0.7286790	2.6858330
H	2.6633400	-1.8285490	2.0768960
C	1.8224290	-1.0526830	0.2531250
N	2.7365430	-0.0050600	0.1523900
C	0.8266950	-1.2323760	-0.7112740
H	0.7270390	-0.5400720	-1.5431300
C	-0.0862930	-2.2786050	-0.5929740
C	-0.0198670	-3.1794140	0.4717670
H	-0.7390660	-3.9858280	0.5504020
C	0.9832610	-3.0081580	1.4249130
H	1.0588790	-3.6983800	2.2597190
C	1.8933410	-1.9610180	1.3216990
H	3.0242680	0.3619630	1.0521330
H	2.4214790	0.7474460	-0.4481710
C	-1.1636830	-2.3590290	-1.6151910
O	-1.3547080	-1.5386890	-2.4849630
O	-1.9460720	-3.4490270	-1.4802190
H	-2.6160610	-3.4023970	-2.1785620

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config_2671

H	-3.2917590	-1.4485900	-1.6709720
C	-2.1081550	-0.7290390	-0.0209960
N	-2.9871680	0.2936240	0.3196990
C	-0.9429310	-0.9419580	0.7233760
H	-0.6891860	-0.2929110	1.5566370
C	-0.0779840	-1.9818390	0.3909490
C	-0.3566080	-2.8475230	-0.6707540

H	0.3243660	-3.6547760	-0.9123030
C	-1.5236640	-2.6430320	-1.4017330
H	-1.7644500	-3.3004410	-2.2312410
C	-2.3877220	-1.5992370	-1.0862030
H	-3.6310380	0.5597890	-0.4124610
H	-2.5605560	1.1078190	0.7467680
C	1.1688770	-2.1113530	1.1874570
O	1.5295980	-1.3422210	2.0513660
O	1.9123810	-3.1873920	0.8468850
H	2.6758300	-3.2008300	1.4434810
H	1.4703870	-0.3934810	-2.6912500
C	1.8522100	0.4951120	-0.7658810
N	3.0305710	-0.2115240	-0.5440120
C	1.3880560	1.4126050	0.1818470
H	1.9177880	1.5593040	1.1186710
C	0.2028900	2.1092310	-0.0464290
C	-0.5250090	1.9385300	-1.2267340
H	-1.4441970	2.4899590	-1.3876020
C	-0.0465400	1.0412440	-2.1779730
H	-0.5959300	0.8858880	-3.1011390
C	1.1223790	0.3233020	-1.9519190
H	3.1197140	-1.0746600	-1.0628410
H	3.2726400	-0.3232260	0.4321860
C	-0.2808290	3.0019020	1.0381370
O	0.3822080	3.4225600	1.9544640
O	-1.6050830	3.2877900	0.9285110
H	-1.8209230	3.8874750	1.6592530

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config_2701

H	-0.2862850	-0.0341600	1.6212160
C	0.7871860	1.7126290	0.9514690
N	1.9594870	1.4048400	1.6566700
C	0.7386180	2.8379700	0.1249540
H	1.5776920	3.5258590	0.0635130
C	-0.3946320	3.0904780	-0.6470080
C	-1.4920250	2.2262740	-0.6203500
H	-2.3615460	2.4306580	-1.2333320
C	-1.4400320	1.1070250	0.2067060
H	-2.2761660	0.4152980	0.2361030
C	-0.3192210	0.8527200	0.9914290
H	1.8242360	0.7558530	2.4215770
H	2.4960550	2.2119850	1.9478980
C	-0.3781900	4.3099610	-1.5009030
O	0.5434760	5.0903810	-1.5709620
O	-1.5113410	4.4749190	-2.2112620
H	-1.4045340	5.2866070	-2.7296280
H	3.0817060	-1.4080850	1.2554850
C	1.5756820	-1.3234850	-0.2777360
N	2.2591110	-0.3784390	-1.0340840
C	0.3503440	-1.8473130	-0.7047950
H	-0.1083130	-1.5061430	-1.6288170
C	-0.3238160	-2.7846950	0.0743280
C	0.2053340	-3.2331300	1.2880490
H	-0.3333860	-3.9603890	1.8833070
C	1.4368740	-2.7286170	1.7008200
H	1.8756550	-3.0726570	2.6324520
C	2.1191130	-1.7924220	0.9292290
H	2.7849120	0.2788850	-0.4685860
H	1.6832150	0.1054760	-1.7111240
C	-1.6428510	-3.2624440	-0.4238700

O	-2.1896790	-2.8633090	-1.4263630
O	-2.2003620	-4.2027150	0.3665210
H	-3.0466220	-4.4444420	-0.0387890

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config_2783

H	-2.7777490	-2.8480010	0.2721370
C	-1.4970440	-1.4628760	-0.7678780
N	-2.5430000	-0.6795330	-1.2359740
C	-0.1681370	-1.1162130	-1.0325710
H	0.0658620	-0.2531430	-1.6498080
C	0.8736760	-1.8523560	-0.4713300
C	0.6227310	-2.9612800	0.3390130
H	1.4439710	-3.5166460	0.7747510
C	-0.7006730	-3.3152660	0.5875700
H	-0.9210550	-4.1693840	1.2198910
C	-1.7487470	-2.5757850	0.0507040
H	-3.4291810	-1.1399690	-1.3794630
H	-2.3147760	-0.0028260	-1.9495920
C	2.2592920	-1.3843040	-0.7267580
O	2.5517990	-0.3468410	-1.2883990
O	3.2023740	-2.2215900	-0.2627060
H	4.0622600	-1.8181160	-0.4540010
H	-0.0369450	4.0713440	-2.0096690
C	0.8530690	2.5804120	-0.7324050
N	2.1441860	2.7191020	-1.2345590
C	0.6025210	1.6746420	0.3041020
H	1.4059750	1.0665360	0.7077590
C	-0.6885650	1.5019560	0.7944090
C	-1.7558910	2.2588450	0.3039880
H	-2.7566690	2.1009410	0.6871060
C	-1.4989390	3.1946380	-0.6950720
H	-2.3086810	3.8022220	-1.0876430
C	-0.2159270	3.3514860	-1.2147730
H	2.1978420	3.1882990	-2.1280820

H	2.6659820	1.8492130	-1.2385370
C	-0.8847380	0.4392190	1.8186340
O	-0.0021830	-0.2500850	2.2776730
O	-2.1706710	0.2966020	2.2009340
H	-2.1863920	-0.4317280	2.8396350

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config_337

H	0.1657000	6.6166310	1.3711770
C	-0.9051650	5.2058980	0.1438080
N	-1.9716050	6.0666360	-0.1100890
C	-0.8660910	3.9304090	-0.4274650
H	-1.6823520	3.5700950	-1.0471020
C	0.2315130	3.0986860	-0.2146310
C	1.3107920	3.5141280	0.5676310
H	2.1543600	2.8526260	0.7229370
C	1.2700070	4.7851840	1.1358270
H	2.0969300	5.1304350	1.7483180
C	0.1801400	5.6240690	0.9283830
H	-2.1226340	6.7897700	0.5783990
H	-2.8315410	5.6200060	-0.3945730
C	0.2089730	1.7495820	-0.8512030
O	-0.7256180	1.3434720	-1.5237110
O	1.3010710	1.0281370	-0.6185370
H	1.2024810	0.1497400	-1.0774980

H	-1.6435420	-0.7897040	-0.5598680
C	-0.0317800	-2.1404380	-1.0066010
N	0.5457640	-1.2746480	-1.9646610
C	0.5744580	-3.3543350	-0.6900680
H	1.4729300	-3.6872160	-1.2024280
C	0.0260020	-4.1667400	0.3024270
C	-1.1233350	-3.7799810	0.9933190
H	-1.5370510	-4.4227660	1.7611500
C	-1.7194330	-2.5618480	0.6745630
H	-2.6131490	-2.2435470	1.2013350
C	-1.1835420	-1.7435200	-0.3149710
H	-0.1406490	-0.6755340	-2.4187080
H	1.1184520	-1.7578060	-2.6470950
C	0.7143750	-5.4560810	0.5849860
O	1.7040640	-5.8489860	0.0116350
O	0.1219250	-6.1702040	1.5625710
H	0.6381140	-6.9831290	1.6705200

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config_401

H	1.2632080	-6.5513900	1.1754260
C	0.6372550	-5.2304570	-0.4076880
N	0.8999160	-6.1452520	-1.4258250
C	0.0976800	-3.9739880	-0.6990550
H	-0.0904860	-3.6707000	-1.7250400
C	-0.2152190	-3.0880730	0.3300340
C	0.0000600	-3.4295900	1.6665740
H	-0.2481130	-2.7267710	2.4525290
C	0.5375370	-4.6818200	1.9548120
H	0.7144750	-4.9697860	2.9862560
C	0.8520070	-5.5742710	0.9354410
H	1.5904230	-6.8504620	-1.2123200
H	1.0271540	-5.7470210	-2.3451110
C	-0.7851340	-1.7625230	-0.0492210
O	-0.9685000	-1.4201650	-1.2067050
O	-1.0749800	-0.9859510	0.9901550
H	-1.4458260	-0.1270740	0.6484570
H	0.2847450	0.6956670	-1.7179140
C	-0.8404730	2.1041440	-0.5465610
N	-1.9515800	1.2391570	-0.4116020
C	-0.8332280	3.3521410	0.0729620
H	-1.6940060	3.7104510	0.6308650
C	0.2958250	4.1662880	-0.0179330
C	1.4285680	3.7478840	-0.7177210
H	2.2973820	4.3923450	-0.7791510
C	1.4148100	2.4961050	-1.3289790
H	2.2863220	2.1529240	-1.8768980
C	0.2940890	1.6754990	-1.2476200
H	-2.0477050	0.5960900	-1.1948170
H	-2.8203910	1.7286370	-0.2308360
C	0.2355620	5.4920420	0.6565520
O	-0.7214900	5.9130910	1.2643030
O	1.3721230	6.2048250	0.5271240
H	1.2349570	7.0422160	0.9950030

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config_48

H	0.6062450	-0.6051330	2.9823270
C	1.1561440	-1.0067330	0.9372540
N	2.1530110	-0.0487570	0.8925060
C	0.8897700	-1.8161710	-0.1766880

H	1.4409790	-1.6826900	-1.1037880
C	-0.0834880	-2.8131420	-0.1070260
C	-0.8160490	-3.0320190	1.0633910
H	-1.5650250	-3.8136750	1.1008850
C	-0.5517380	-2.2247510	2.1694600
H	-1.1065290	-2.3736640	3.0907140
C	0.4147030	-1.2270380	2.1118870
H	2.0718900	0.6864720	1.5813390
H	2.3776270	0.3215850	-0.0252800
C	-0.3087190	-3.6320950	-1.3322090
O	0.2896980	-3.4951150	-2.3730690
O	-1.2692050	-4.5654120	-1.1743150
H	-1.3403710	-5.0411310	-2.0155330
H	-3.1772230	2.2912680	1.2867930
C	-1.6142710	1.3378580	0.1498210
N	-2.2432370	0.1029810	0.0806220
C	-0.3819790	1.5411750	-0.4814770
H	0.1034630	0.7232220	-1.0048180
C	0.2292760	2.7924970	-0.4514060
C	-0.3745910	3.8795400	0.1866410
H	0.1113990	4.8476920	0.1973660
C	-1.6028930	3.6776910	0.8116600
H	-2.0919230	4.5032170	1.3190190
C	-2.2162390	2.4288310	0.7980240
H	-2.9123850	-0.0854460	0.8135280
H	-1.6281080	-0.6864700	-0.0788510
C	1.5655310	2.9105610	-1.0895290
O	2.2493450	1.9707280	-1.4429210
O	1.9826530	4.1796010	-1.2344400
H	2.8622870	4.1466610	-1.6405060

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config_62

H	-1.0645800	6.0638620	-1.1461820
C	-1.2799570	4.4716010	0.2894400
N	-2.4433670	4.9893850	0.8550770
C	-0.7466730	3.2594140	0.7380790
H	-1.2036900	2.7173360	1.5610550
C	0.3837350	2.7210500	0.1268600
C	1.0068300	3.3715980	-0.9399500
H	1.8840790	2.9364130	-1.4028680
C	0.4746520	4.5793180	-1.3846840
H	0.9414950	5.1040350	-2.2122840
C	-0.6541710	5.1252740	-0.7827150
H	-2.5686050	5.9870830	0.7633130
H	-2.6615180	4.6556670	1.7828930
C	0.9069690	1.4295290	0.6584980
O	0.4148630	0.8482760	1.6112290
O	1.9665180	0.9674720	-0.0028330
H	2.2370140	0.1045060	0.4077440
H	3.3617160	-3.4897130	0.1013680
C	1.5616860	-2.4104150	0.5837810
N	2.2239190	-1.4422410	1.3718780
C	0.1850060	-2.3173340	0.3734520
H	-0.3982750	-1.5333420	0.8497810
C	-0.4483250	-3.2380200	-0.4611670
C	0.2705250	-4.2540150	-1.0942890
H	-0.2400590	-4.9606560	-1.7374560
C	1.6437430	-4.3374880	-0.8806640
H	2.2207040	-5.1194130	-1.3636100
C	2.2877100	-3.4231840	-0.0526540

H	3.0684550	-1.7880070	1.8120410
H	1.6096530	-0.9948600	2.0496530
C	-1.9209910	-3.0988270	-0.6405340
O	-2.6065320	-2.2636990	-0.1001610
O	-2.4392840	-4.0164390	-1.4830370
H	-3.3914110	-3.8440510	-1.5340150

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config_620

H	-3.2015810	-1.8455520	0.7514980
C	-1.2228780	-1.1132550	1.1809260
N	-1.6726080	-0.0245250	1.9257610
C	0.1434750	-1.3402680	0.9928580
H	0.8817950	-0.6565330	1.4029120
C	0.5782010	-2.4254100	0.2343650
C	-0.3301050	-3.3201960	-0.3349670
H	0.0246190	-4.1572690	-0.9242770
C	-1.6923520	-3.1024630	-0.1318470
H	-2.4186480	-3.7865580	-0.5602740
C	-2.1372670	-2.0156590	0.6140350
H	-2.5562080	0.3482090	1.5984560
H	-0.9880990	0.7169590	2.0136400
C	2.0429800	-2.5523070	0.0097800
O	2.8686440	-1.7380930	0.3582370
O	2.3858210	-3.6775130	-0.6490600
H	3.3486370	-3.6589160	-0.7559740
H	2.3877820	3.9059870	0.7873870
C	0.2820490	3.6132760	0.4321780
N	-0.0945150	4.8266110	1.0019860
C	-0.6724770	2.7555470	-0.1232420
H	-1.7320370	2.9932910	-0.0773760
C	-0.2738610	1.5770160	-0.7554840
C	1.0735590	1.2233430	-0.8419270
H	1.3665420	0.2920850	-1.3120270
C	2.0218650	2.0700240	-0.2712970
H	3.0720420	1.7991290	-0.3058120
C	1.6367180	3.2502670	0.3545940
H	0.5487830	5.2162760	1.6755940
H	-1.0575750	4.8951870	1.2973700
C	-1.3449490	0.6788810	-1.2708070
O	-2.5277730	0.8236640	-1.0438220
O	-0.8714560	-0.3408590	-2.0030490
H	-1.6137770	-0.9378720	-2.1851980

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config_719

H	0.4634290	-7.1394500	-1.0416530
C	0.3793700	-5.5350660	0.3939790
N	0.4375170	-6.3753100	1.5033150
C	0.3379630	-4.1464520	0.5521050
H	0.3103740	-3.6979160	1.5408480
C	0.3362380	-3.3137030	-0.5654020
C	0.3765130	-3.8376890	-1.8589690
H	0.3735540	-3.1723190	-2.7137460
C	0.4192010	-5.2208740	-2.0136940
H	0.4511660	-5.6529240	-3.0088030
C	0.4222040	-6.0618450	-0.9058160
H	0.1158320	-7.3207830	1.3544170
H	0.0932380	-5.9811610	2.3669850
C	0.2857760	-1.8435780	-0.3390800
O	0.2405130	-1.3643100	0.7954990

O	0.2922030	-1.1170830	-1.4298020
H	0.2555880	-0.1340040	-1.1997470
H	-0.0095870	7.1773420	0.9955120
C	0.0689740	5.5726170	-0.4400230
N	0.1301730	6.4163860	-1.5464830
C	0.1171090	4.1841950	-0.5978370
H	0.1626040	3.7360320	-1.5860800
C	0.1116500	3.3513790	0.5196290
C	0.0594910	3.8751580	1.8128330
H	0.0553250	3.2096850	2.6675250
C	0.0130670	5.2582580	1.9673110
H	-0.0274210	5.6901710	2.9621640
C	0.0190910	6.0993450	0.8595530
H	-0.2551250	7.3404250	-1.4151800
H	-0.1463930	6.0033700	-2.4255320
C	0.1593750	1.8811660	0.2934880
O	0.1971230	1.4014520	-0.8411840
O	0.1566490	1.1550670	1.3845100
H	0.1901760	0.1719220	1.1550260

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config_761

H	-1.1082520	0.3351390	-1.8207780
C	-1.6035000	-1.0586290	-0.2534270
N	-2.6656300	-0.3116550	0.2169600
C	-1.2576860	-2.2836510	0.3337070
H	-1.8076850	-2.6674180	1.1884220
C	-0.2020890	-3.0396950	-0.1791030
C	0.5407340	-2.5959160	-1.2753620
H	1.3572750	-3.1944440	-1.6607680
C	0.1997140	-1.3737460	-1.8554860
H	0.7643630	-1.0028300	-2.7051220
C	-0.8542440	-0.6160000	-1.3605560
H	-2.6542420	0.6878720	0.0414250
H	-3.0262180	-0.5601520	1.1260080
C	0.0994980	-4.3319640	0.4969300
O	-0.5097070	-4.7764330	1.4420900
O	1.1464520	-4.9844470	-0.0491890
H	1.2555800	-5.8075560	0.4503560
H	3.6568510	1.4189960	0.2405410
C	1.5661540	1.0751940	0.6333480
N	1.7346650	-0.2133460	1.1210090
C	0.2928920	1.6539460	0.5966000
H	-0.5708650	1.0911570	0.9360740
C	0.1184070	2.9487370	0.1152930
C	1.2069030	3.7198330	-0.3020960
H	1.0556720	4.7269530	-0.6714880
C	2.4768460	3.1511480	-0.2446720
H	3.3396020	3.7255390	-0.5667090
C	2.6588370	1.8482690	0.2101700
H	2.5669600	-0.6891700	0.8017250
H	0.9156270	-0.8073320	1.0494310
C	-1.2751700	3.4490750	0.0116220
O	-2.2698130	2.7593110	0.1275950
O	-1.3594550	4.7634960	-0.2479310
H	-2.3011240	4.9820850	-0.3201090

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config_770

H	1.1439820	4.1227020	0.7759830
C	1.0564150	2.4990090	-0.6366550

N	2.4339900	2.5458900	-0.9325670
C	0.2375650	1.5240950	-1.2084980
H	0.6257610	0.8406030	-1.9579710
C	-1.0748950	1.3645400	-0.7637380
C	-1.6111390	2.2070020	0.2097620
H	-2.6263980	2.0576210	0.5580840
C	-0.8119980	3.2254910	0.7261760
H	-1.2132390	3.9006280	1.4751610
C	0.5126190	3.3622930	0.3235570
H	2.8122030	3.4830780	-0.9967200
H	2.6914460	1.9887860	-1.7397790
C	-1.8319150	0.1973770	-1.3003780
O	-1.4830080	-0.4578710	-2.2603360
O	-2.9149680	-0.1114190	-0.5743790
H	-3.1581330	-1.0266030	-0.8136500
H	-2.2710950	-2.9232280	2.1058920
C	-1.0679710	-2.4279830	0.3891970
N	-2.0079610	-2.9176840	-0.5401940
C	0.1092050	-1.8152980	-0.0433960
H	0.3649990	-1.7834560	-1.0984550
C	0.9363550	-1.1647160	0.8721700
C	0.6395560	-1.1645490	2.2349350
H	1.2825220	-0.6384720	2.9308250
C	-0.4990730	-1.8397420	2.6710920
H	-0.7419540	-1.8635520	3.7285750
C	-1.3553910	-2.4503430	1.7603150
H	-2.4654120	-3.7746440	-0.2541680
H	-1.6408090	-2.9925780	-1.4824360
C	2.0834340	-0.3923660	0.3140720
O	2.4863310	-0.4996400	-0.8255710
O	2.5949610	0.4960280	1.1769560
H	3.1107400	1.1337350	0.6463490

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config_923

H	-0.3870240	7.2289390	0.4937980
C	-0.1790580	5.5315480	-0.8168220
N	-0.0843980	6.2976250	-1.9762360
C	-0.0783830	4.1381050	-0.8718020
H	0.0351590	3.6238080	-1.8216320
C	-0.1187130	3.3858030	0.3006260
C	-0.2579920	3.9965660	1.5484320
H	-0.2879520	3.3926210	2.4471700
C	-0.3566160	5.3845770	1.6005710
H	-0.4652410	5.8833770	2.5583490
C	-0.3167020	6.1457920	0.4371950
H	-0.5065090	7.2138230	-1.9316960
H	-0.2992320	5.8143390	-2.8365170
C	-0.0133860	1.9059500	0.1825240
O	0.0996870	1.3502530	-0.9116930
O	-0.0522140	1.2576290	1.3208810
H	0.0227900	0.2627900	1.1633670
H	0.6121000	-7.1719750	-0.4922430
C	0.4098700	-5.4743020	0.8189020
N	0.4342280	-6.2327040	1.9868050
C	0.3221080	-4.0800100	0.8749020
H	0.2312040	-3.5643040	1.8264060
C	0.3549630	-3.3281200	-0.2980120
C	0.4759230	-3.9399760	-1.5471950
H	0.4984520	-3.3364510	-2.4464330
C	0.5645520	-5.3286360	-1.6001470

H	0.6596310	-5.8282590	-2.5589400
C	0.5339670	-6.0893350	-0.4361550
H	0.1442190	-7.1950930	1.8909280
H	0.0390900	-5.7888870	2.8032840
C	0.2527180	-1.8480560	-0.1795690
O	0.1364680	-1.2926680	0.9144710
O	0.2950410	-1.1994480	-1.3176160
H	0.2200860	-0.2046200	-1.1599520

Energies of the mABA dimers

Table SI.3.2. Energies [in Hartree] of the dimeric structures of acetic acid as computed at the M06-2X/6-31+G(d,p) level of theory using the SMD solvation model to describe DMSO and water.

CONFIGURATION	$E_{e,gas}$	δG_{VRT}	$E_{e,dmsO}$	$E_{e,water}$
config_1032	-952.04630	0.21331	-952.07447	-952.07490
config_1086	-952.04628	0.21313	-952.07439	-952.07489
config_1132	-952.04664	0.21499	-952.07790	-952.07853
config_1163	-952.04465	0.21070	-952.07458	-952.07123
config_1182	-952.04762	0.21209	-952.07782	-952.07472
config_1280	-952.04398	0.21304	-952.07382	-952.07636
config_1373	-952.04624	0.21268	-952.07419	-952.07465
config_148	-952.04481	0.21391	-952.07624	-952.07712
config_1656	-952.04829	0.21180	-952.07516	-952.07287
config_1698	-952.04824	0.21141	-952.07480	-952.07227
config_1746	-952.05900	0.21252	-952.08676	-952.08067
config_1840	-952.04692	0.21541	-952.07744	-952.07929
config_1979	-952.03759	0.20940	-952.06905	-952.06897
config_2017	-952.04884	0.21553	-952.07739	-952.07837
config_2124	-952.04829	0.21211	-952.07510	-952.07280
config_2296	-952.04915	0.21269	-952.07812	-952.07507
config_2311	-952.04493	0.21320	-952.07662	-952.07946
config_2479	-952.04465	0.21051	-952.07450	-952.07111
config_2499	-952.04551	0.21292	-952.07325	-952.07348
config_2501	-952.04529	0.21257	-952.07423	-952.07461
config_2670	-952.04400	0.21319	-952.07381	-952.07661
config_2671	-952.04478	0.21432	-952.07555	-952.07826
config_2701	-952.04298	0.21235	-952.07331	-952.07276
config_2783	-952.04388	0.21386	-952.07241	-952.07581
config_337	-952.04917	0.21295	-952.07813	-952.07502
config_401	-952.04914	0.21263	-952.07809	-952.07492
config_48	-952.04529	0.21301	-952.07429	-952.07468
config_62	-952.04763	0.21208	-952.07786	-952.07480
config_620	-952.04399	0.21293	-952.07387	-952.07635
config_719	-952.05904	0.21273	-952.08683	-952.08071
config_761	-952.04636	0.21322	-952.07399	-952.07420
config_770	-952.05175	0.21813	-952.07851	-952.07630
config_923	-952.05900	0.21245	-952.08685	-952.08072

Energetics of formation of mABA dimers

Table SI.3.2. Energetics of formation of *m*-aminobenzoic acid dimers in the gas-phase and solution as computed at the M06-2X/6-31+G(d,p) level of theory. Values in kcal mol⁻¹.

species	reaction	type	$\Delta E_{e,gas}$	ΔG_{ass}	ΔG_{ass}	
					H ₂ O	DMSO
dimer	mABA + mABA → (mABA) ₂	I	-18.33	-6.64	-0.20	-3.40
		II	-13.77	1.41	6.06	5.30
		III	-12.03	-0.22	3.36	2.05
		IV	-11.67	1.95	2.70	4.00
		V	-11.59	-0.44	4.35	3.49
		VI	-10.19	1.77	2.97	4.74
		VII	-9.49	2.60	0.98	3.40
		VIII	-9.31	1.14	4.56	3.07
		IX	-8.90	3.09	4.17	6.83
		X	-8.83	3.67	3.68	6.45
		XI	-8.27	3.29	4.65	4.94
		XII	-4.88	4.83	5.18	5.77

SI.3 Trimers

Coordinates of the optimised geometries of the mABA trimers

Table SI.3.1. Geometries [in Angstrom] of the trimeric structures of *m*-aminobenzoic acid as computed at the M06-2X/6-31+G(d,p) level of theory. XYZ format.

Trimers (Tr)_{3M} generated from the random distribution of three isolated mABA

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config_11
H      -0.3742280      4.1430780      2.0825300
C       1.1565980      2.7361830      1.5206470
N       2.2000800      3.6434480      1.6982350
C       1.4052740      1.4183900      1.1270000
H       2.4169670      1.0772470      0.9243480
C       0.3506530      0.5184770      0.9763150
C      -0.9692610      0.9077540      1.2131530
H      -1.7777730      0.1975060      1.0876780
C      -1.2143550      2.2199610      1.6129850
H      -2.2336970      2.5504090      1.7874110
C      -0.1691240      3.1217740      1.7710140
H       1.9704750      4.6064960      1.4831450
H       3.0698300      3.3719410      1.2603350
C       0.6896310     -0.8643010      0.5408460
O       1.8161390     -1.2539310      0.3124680
O      -0.3852370     -1.6609860      0.4142830
H      -0.0705370     -2.5469990      0.1611520
H       1.9765280     -3.4009550     -1.2286650
C       0.5937940     -4.9892590     -1.7346500
N       0.6563550     -4.7728430     -3.1057080
C      -0.1937930     -6.0194750     -1.2089270
H      -0.8043500     -6.6433520     -1.8556450
C      -0.2026140     -6.2663190      0.1623150
C       0.5667000     -5.5016580      1.0428250
H       0.5475270     -5.7075030      2.1060890
C       1.3479000     -4.4738690      0.5186700
H       1.9510240     -3.8490100      1.1707890
C       1.3623960     -4.2144880     -0.8506370
H       0.9755000     -3.8611030     -3.3984510
H      -0.1254610     -5.1128070     -3.6461210
C      -1.0723340     -7.3753930      0.6462410
O      -1.7701600     -8.0640720     -0.0619030
O      -1.0139870     -7.5498480      1.9810690
H      -1.6076280     -8.2848940      2.1957180
H      -1.3485310      1.9468610     -2.0117110
C      -1.8462110      3.8896020     -1.2205410
N      -3.2052990      3.6115440     -1.0966250
C      -1.3273460      5.1122460     -0.7890690
H      -1.9784840      5.8891300     -0.3976150
C       0.0491830      5.3373950     -0.8197290
C       0.9299210      4.3713570     -1.3078480
H       1.9964730      4.5632130     -1.3277690
C       0.4073110      3.1567940     -1.7481630
H       1.0734580      2.3834740     -2.1175100
C      -0.9589210      2.9121220     -1.6984000
H      -3.5575100      2.8776290     -1.6943720
H      -3.8153730      4.4163390     -1.0734140
C       0.5376550      6.6285380     -0.2698000
O      -0.1509380      7.5891970     -0.0195650
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O	1.8708750	6.6253020	-0.0247720
H	2.0958820	7.5068850	0.3099730

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config_14

H	-0.4534490	2.2492700	-0.6051240
C	1.3504470	1.1006250	-0.9016210
N	1.8992710	1.9644260	-1.8413620
C	2.0507910	-0.0435480	-0.4983930
H	3.0015980	-0.3048830	-0.9560210
C	1.5390580	-0.8691140	0.5002350
C	0.3263880	-0.5772280	1.1287950
H	-0.0634270	-1.2355070	1.8968030
C	-0.3797840	0.5500320	0.7136750
H	-1.3328950	0.7914390	1.1751670
C	0.1138930	1.3754270	-0.2934860
H	1.2831990	2.6374430	-2.2826610
H	2.5654590	1.5543150	-2.4796120
C	2.2957510	-2.1139550	0.8145550
O	3.2748780	-2.4913040	0.2089860
O	1.7687560	-2.8034930	1.8394580
H	2.2412180	-3.6481320	1.8956810
H	1.5072900	-4.2865540	-1.8372600
C	-0.1885500	-3.3680620	-0.8766480
N	-0.3074720	-2.3355660	-1.8051140
C	-1.0789230	-3.4622920	0.1987740
H	-1.8528000	-2.7135090	0.3434220
C	-0.9716920	-4.5073590	1.1114820
C	0.0099410	-5.4930330	0.9704790
H	0.0764210	-6.3031910	1.6872320
C	0.8898270	-5.4035540	-0.1056080
H	1.6632840	-6.1539960	-0.2373700
C	0.7973540	-4.3558140	-1.0174410
H	0.5500460	-2.1265770	-2.2997820
H	-0.7131460	-1.4868140	-1.4265910
C	-1.9266820	-4.5128640	2.2520090
O	-2.7653120	-3.6648740	2.4565930
O	-1.7712630	-5.5737600	3.0709120
H	-2.4307640	-5.4833200	3.7749300
H	2.2508930	4.4732020	-0.1428450
C	0.4101230	4.8538970	-1.1959880
N	1.0186490	4.9147990	-2.4586520
C	-0.9767950	4.9564530	-1.0757920
H	-1.6031760	5.1571230	-1.9408790
C	-1.5843720	4.7917220	0.1694540
C	-0.8265380	4.5218050	1.3101550
H	-1.3126520	4.3888930	2.2692870
C	0.5577980	4.4241130	1.1847230
H	1.1648770	4.2013870	2.0560560
C	1.1742220	4.5863480	-0.0509480
H	1.9936540	5.1854250	-2.4382330
H	0.5035800	5.4497720	-3.1458260
C	-3.0681220	4.9166160	0.2217400
O	-3.7696980	5.1725680	-0.7292780
O	-3.5729940	4.7136090	1.4536150
H	-4.5344790	4.8154660	1.3866760

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config_19

H	1.2477940	0.9075880	1.4561100
C	1.1353870	-0.3779100	-0.2656200

N	2.5008310	-0.7031590	-0.2250020
C	0.2857820	-0.9501070	-1.2139460
H	0.6723420	-1.6274130	-1.9733600
C	-1.0854290	-0.7054340	-1.1619800
C	-1.6299540	0.1415490	-0.1933680
H	-2.6977730	0.3246940	-0.1696080
C	-0.7768110	0.7293560	0.7370270
H	-1.1736880	1.4048760	1.4893380
C	0.5888810	0.4600870	0.7151690
H	3.0897260	0.1017450	-0.0288430
H	2.8232900	-1.1873690	-1.0547930
C	-1.9346440	-1.4134600	-2.1556210
O	-1.5202340	-2.1753870	-3.0009930
O	-3.2484320	-1.1354540	-2.0328260
H	-3.7063540	-1.6553140	-2.7101200
H	-1.2471910	-2.4963390	2.8513890
C	0.3433320	-2.9972780	1.4874290
N	1.3662950	-2.4806950	2.2778550
C	0.6436750	-3.5832140	0.2527500
H	1.6696540	-3.6131080	-0.1043260
C	-0.3723670	-4.0764180	-0.5590280
C	-1.7066430	-4.0433440	-0.1455550
H	-2.4860190	-4.4237360	-0.7959100
C	-2.0035730	-3.4832210	1.0943670
H	-3.0345890	-3.4307490	1.4305760
C	-0.9965730	-2.9591800	1.9000650
H	1.0530440	-1.8254550	2.9814210
H	2.1373500	-2.0998100	1.7367810
C	0.0078880	-4.5287400	-1.9240990
O	1.0860770	-4.3202160	-2.4374500
O	-0.9723060	-5.1938490	-2.5590470
H	-0.6624660	-5.3539160	-3.4627980
H	-1.2638740	5.9393480	2.1907850
C	0.6280720	4.9201320	2.0314590
N	1.0639270	5.2944380	3.3002430
C	1.4155810	4.0971970	1.2200530
H	2.3963150	3.7639350	1.5485590
C	0.9467550	3.6860290	-0.0261790
C	-0.3096090	4.0759990	-0.4924710
H	-0.6649920	3.7302330	-1.4555750
C	-1.0939160	4.8918470	0.3195520
H	-2.0764690	5.2055540	-0.0183810
C	-0.6373130	5.3085210	1.5655100
H	0.6416450	6.1298740	3.6789370
H	2.0635100	5.2704650	3.4421380
C	1.8179930	2.7768660	-0.8182220
O	2.8772710	2.3268540	-0.4285180
O	1.3154280	2.4809280	-2.0250970
H	1.9039810	1.8309540	-2.4381490

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config_3

H	-0.1566110	4.5544780	3.1522600
C	1.1090490	3.2260590	2.0247050
N	2.1964010	4.0969390	2.0024960
C	1.1980160	1.9610440	1.4323040
H	2.1005410	1.6577550	0.9083020
C	0.1111490	1.0903660	1.4697820
C	-1.0779490	1.4467150	2.1120500
H	-1.9161620	0.7604180	2.1228400
C	-1.1543200	2.6958060	2.7226220

H	-2.0642210	2.9906100	3.2375190
C	-0.0786840	3.5774420	2.6812190
H	1.9416120	5.0747080	2.0519430
H	2.8374030	3.9322500	1.2372400
C	0.2373120	-0.2050190	0.7511360
O	1.2057700	-0.5037040	0.0636540
O	-0.8010120	-1.0170800	0.9237190
H	-0.6680670	-1.8257240	0.3942710
H	-2.1486120	-8.4235580	-1.1888880
C	-0.1464620	-7.7421200	-0.7734290
N	0.3889790	-9.0235360	-0.6760080
C	0.6694660	-6.6153660	-0.6365560
H	1.7283830	-6.7152730	-0.4153770
C	0.1350280	-5.3374260	-0.7883570
C	-1.2173850	-5.1521030	-1.0825520
H	-1.6198850	-4.1545500	-1.2115580
C	-2.0280220	-6.2761530	-1.2220550
H	-3.0814850	-6.1563680	-1.4546270
C	-1.5051230	-7.5555330	-1.0704080
H	-0.2622180	-9.7544000	-0.4291440
H	1.2623780	-9.0956040	-0.1745460
C	1.0705560	-4.1882040	-0.6256650
O	2.2579260	-4.2929160	-0.4315880
O	0.4610010	-2.9872430	-0.7179250
H	1.1179230	-2.2670020	-0.5937380
H	-0.4882660	7.0577980	0.1708010
C	-1.3998180	5.1194810	-0.0680800
N	-2.6057660	5.4825010	0.5224400
C	-1.2228060	3.8281550	-0.5751960
H	-2.0026790	3.0777870	-0.4801470
C	-0.0147210	3.4681800	-1.1619320
C	1.0299530	4.3871400	-1.2962890
H	1.9644620	4.0857230	-1.7558730
C	0.8380430	5.6822840	-0.8237120
H	1.6282060	6.4201340	-0.9288100
C	-0.3554870	6.0458320	-0.2040820
H	-2.5706680	6.2709930	1.1520330
H	-3.1569250	4.7174830	0.8850160
C	0.1457270	2.0363410	-1.5445900
O	-0.7546700	1.2263650	-1.5487010
O	1.4156230	1.7074890	-1.8309920
H	1.4597010	0.7367480	-1.8588700

Trimers (Tr)_{D+M} generated from the random distribution of the classic carboxylic dimer with one isolated mABA

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config_1339

H	-3.7097130	-4.5505350	1.2374360
C	-1.7344810	-4.1978510	0.4508290
N	-1.7134060	-2.8434040	0.7829390
C	-0.6185130	-4.7980800	-0.1408290
H	0.2487970	-4.2049910	-0.4191280
C	-0.6053820	-6.1704570	-0.3822480
C	-1.7057150	-6.9715970	-0.0697770
H	-1.6816130	-8.0361940	-0.2694930
C	-2.8207390	-6.3689050	0.5081620
H	-3.6879460	-6.9694650	0.7635480
C	-2.8375560	-5.0030380	0.7725410
H	-2.6186750	-2.4009740	0.8634090

H	-1.0579910	-2.2779670	0.2557210
C	0.6441830	-6.7408750	-0.9550540
O	1.6816400	-6.1298660	-1.0861770
O	0.5270810	-8.0337730	-1.3118000
H	1.3891220	-8.3119980	-1.6562390
H	-1.8100780	9.7333480	0.0883720
C	-0.5585540	8.2557320	-0.8562260
N	-0.0252230	9.1416560	-1.7890650
C	-0.1387680	6.9227830	-0.8169850
H	0.5806840	6.5426280	-1.5363250
C	-0.6382720	6.0589520	0.1558160
C	-1.5598970	6.4970100	1.1088100
H	-1.9363790	5.8088370	1.8559480
C	-1.9745720	7.8256940	1.0690010
H	-2.6896380	8.1916390	1.7989910
C	-1.4827070	8.6968930	0.1026300
H	-0.5907640	9.9513230	-1.9988440
H	0.3671270	8.7185870	-2.6176920
C	-0.1601290	4.6495600	0.1449580
O	0.6520110	4.2476120	-0.6901190
O	-0.6688180	3.8865970	1.0816480
H	-0.2989420	2.9496930	1.0108840
H	2.8297490	-3.9771960	0.1907730
C	1.5949830	-2.4912910	1.1522900
N	1.1503590	-3.3352620	2.1649800
C	1.1591190	-1.1619120	1.0978420
H	0.4599220	-0.7787830	1.8358980
C	1.6305530	-0.3080390	0.1005240
C	2.5467330	-0.7505030	-0.8561400
H	2.9024430	-0.0710240	-1.6213430
C	2.9766070	-2.0744220	-0.8017370
H	3.6770420	-2.4476610	-1.5420000
C	2.5081210	-2.9385880	0.1828030
H	1.2892690	-4.3204180	1.9806200
H	0.2020730	-3.1477220	2.4707940
C	1.1251240	1.0912990	0.0867070
O	0.2782930	1.4824350	0.8932500
O	1.6436210	1.8573660	-0.8416080
H	1.2553330	2.7874310	-0.7878610

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config_1730

H	3.6748150	3.9858410	-1.0353330
C	1.8100100	3.9182140	0.0424640
N	1.8240440	2.5449400	0.2436830
C	0.7680380	4.6947000	0.5597720
H	-0.0424570	4.2222760	1.1055640
C	0.7493030	6.0730960	0.3661490
C	1.7873510	6.7242150	-0.3068180
H	1.7608880	7.7980580	-0.4480360
C	2.8368990	5.9536800	-0.8003890
H	3.6542990	6.4331760	-1.3296440
C	2.8508750	4.5715300	-0.6358310
H	2.3695430	2.0164830	-0.4226920
H	0.9126630	2.1267160	0.3949080
C	-0.4463520	6.8062640	0.8520060
O	-1.4746490	6.2808290	1.2332320
O	-0.3116500	8.1415830	0.8196300
H	-1.1482840	8.5222520	1.1275650
H	0.6915360	-9.8394170	1.0057280
C	0.9242870	-8.1735010	-0.3408750

N	1.5246240	-8.9269380	-1.3467880
C	0.6704160	-6.8110240	-0.5244690
H	0.9702720	-6.3055660	-1.4379270
C	0.0201520	-6.0794280	0.4676350
C	-0.3920400	-6.6809550	1.6582050
H	-0.8950020	-6.0937990	2.4170600
C	-0.1399650	-8.0385150	1.8375290
H	-0.4507470	-8.5298280	2.7541810
C	0.5075400	-8.7788690	0.8542920
H	1.9871140	-9.7719500	-1.0443600
H	2.0710240	-8.4047210	-2.0162670
C	-0.2196710	-4.6314690	0.2226980
O	0.1454450	-4.0812420	-0.8185340
O	-0.8391570	-4.0034690	1.1916740
H	-0.9656350	-3.0291860	0.9585000
H	-1.6906410	4.2525980	-1.2518490
C	-1.8977520	2.6029010	0.1175750
N	-2.5248580	3.3593420	1.0892640
C	-1.6532900	1.2351190	0.3009890
H	-1.9381070	0.7372580	1.2235820
C	-1.0432390	0.4864550	-0.7073130
C	-0.6550380	1.0753990	-1.9123930
H	-0.1810560	0.4767220	-2.6810410
C	-0.8966880	2.4369280	-2.0930460
H	-0.6002780	2.9207950	-3.0185590
C	-1.5104530	3.1913660	-1.1010660
H	-2.3491710	4.3588510	1.0895050
H	-2.5817060	2.9545340	2.0116310
C	-0.8056390	-0.9614580	-0.4558730
O	-1.1604400	-1.5040170	0.5921100
O	-0.1920310	-1.5949760	-1.4256770
H	-0.0647930	-2.5699140	-1.1872320

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config_2030

H	-4.1081050	-2.2300560	-0.3306890
C	-2.0357240	-2.6911600	0.0414650
N	-1.7250140	-1.4369880	0.5373530
C	-1.0707260	-3.7056680	-0.0053370
H	-0.0457170	-3.5027680	0.2857510
C	-1.4117380	-4.9850200	-0.4398970
C	-2.7114120	-5.2898700	-0.8521130
H	-2.9600740	-6.2884470	-1.1902650
C	-3.6697800	-4.2801060	-0.8079440
H	-4.6886330	-4.4896990	-1.1185320
C	-3.3439250	-3.0024020	-0.3667290
H	-2.3526130	-0.6842450	0.2976230
H	-0.7542360	-1.1505010	0.5494980
C	-0.3427690	-6.0175020	-0.4275970
O	0.7651080	-5.8718750	0.0489200
O	-0.7123300	-7.1773490	-1.0000300
H	0.0417480	-7.7819040	-0.9312450
H	3.3927340	-4.5556770	0.2720680
C	2.1712230	-3.1012390	1.2799730
N	1.7418520	-3.9972580	2.2525700
C	1.7343540	-1.7734090	1.2667510
H	1.0266490	-1.4185810	2.0125900
C	2.1868700	-0.8921740	0.2822390
C	3.0983940	-1.3015460	-0.6908590
H	3.4394570	-0.6016280	-1.4445960
C	3.5264790	-2.6286690	-0.6802500

H	4.2198200	-2.9778560	-1.4388670
C	3.0685520	-3.5192940	0.2829310
H	1.5994740	-4.9346380	1.8921130
H	0.9402200	-3.6841540	2.7844270
C	1.6034260	0.4722700	0.2553700
O	0.5709860	0.7362090	0.8841890
O	2.2350460	1.3426700	-0.4874780
H	1.7543790	2.2320420	-0.4769530
H	-2.0630390	8.8261460	0.0208020
C	-0.5181990	7.5130070	-0.7079520
N	0.1013960	8.4890830	-1.4834360
C	0.0083880	6.2199680	-0.6345120
H	0.8861470	5.9419210	-1.2105430
C	-0.5876060	5.2663750	0.1885340
C	-1.7133550	5.5733060	0.9555980
H	-2.1603730	4.8181210	1.5908160
C	-2.2350060	6.8622250	0.8815310
H	-3.1090830	7.1263010	1.4682400
C	-1.6488420	7.8220810	0.0635110
H	-0.4833160	9.2602250	-1.7709740
H	0.6875850	8.1468180	-2.2308610
C	0.0122130	3.9056590	0.2217380
O	1.0017380	3.6164030	-0.4531310
O	-0.5923570	3.0532860	1.0149530
H	-0.1314820	2.1575400	0.9789350

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config_2397

H	-4.0404250	-4.5591130	-0.0900170
C	-1.9176520	-4.2149900	-0.2367920
N	-1.9925920	-2.8573530	0.0737190
C	-0.6765600	-4.8219310	-0.4532780
H	0.2352180	-4.2304870	-0.4603540
C	-0.5940600	-6.1969760	-0.6624830
C	-1.7399670	-6.9947070	-0.6930470
H	-1.6588420	-8.0617760	-0.8622880
C	-2.9763600	-6.3853390	-0.4921440
H	-3.8818760	-6.9834510	-0.5084620
C	-3.0691310	-5.0165250	-0.2601910
H	-2.8747940	-2.4105710	-0.1351200
H	-1.2010770	-2.2998710	-0.2263030
C	0.7683970	-6.7756290	-0.8151330
O	1.7987570	-6.1708530	-0.6159680
O	0.7596230	-8.0688960	-1.1885450
H	1.6837050	-8.3556200	-1.2439270
H	-1.4889110	9.8229480	-0.3083950
C	-0.0752430	8.3053460	-0.8924710
N	0.7456690	9.1825690	-1.5969590
C	0.2598220	6.9531130	-0.7758410
H	1.1446790	6.5529460	-1.2624200
C	-0.5391740	6.0951450	-0.0224590
C	-1.6829190	6.5581900	0.6306030
H	-2.2900500	5.8752320	1.2124930
C	-2.0132940	7.9058270	0.5145000
H	-2.8971640	8.2909010	1.0132350
C	-1.2228650	8.7716370	-0.2339320
H	0.3006410	10.0222560	-1.9378280
H	1.3496800	8.7572750	-2.2852970
C	-0.1333320	4.6661030	0.0659290
O	0.8730570	4.2430180	-0.5061200
O	-0.9223520	3.9111050	0.7907340

H	-0.5805200	2.9605500	0.8095540
H	2.4947470	-4.0369060	0.8827250
C	1.0577680	-2.5285240	1.4473660
N	0.3151290	-3.3665210	2.2731760
C	0.6826800	-1.1902940	1.2781080
H	-0.1994150	-0.7962930	1.7754490
C	1.4487380	-0.3415990	0.4785260
C	2.6011240	-0.7994130	-0.1637090
H	3.1837210	-0.1245280	-0.7792390
C	2.9688020	-2.1326020	0.0015420
H	3.8518350	-2.5169980	-0.4990590
C	2.2108240	-2.9912720	0.7912470
H	0.4879830	-4.3537240	2.1345620
H	-0.6779640	-3.1635210	2.2823660
C	1.0013450	1.0695660	0.3299950
O	-0.0427320	1.4767350	0.8449100
O	1.7950270	1.8279530	-0.3856650
H	1.4316810	2.7689270	-0.4383150

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config_2530

H	4.4386370	5.4300520	-0.1639390
C	2.3856950	4.7691930	-0.1891430
N	2.6795990	3.4142420	-0.1355870
C	1.0561980	5.2005870	-0.2012340
H	0.2424690	4.4882760	-0.2238330
C	0.7505630	6.5590520	-0.2024470
C	1.7567130	7.5280000	-0.1758710
H	1.5050990	8.5822420	-0.1687380
C	3.0809150	7.0977880	-0.1633870
H	3.8833040	7.8281380	-0.1415720
C	3.3974590	5.7418130	-0.1753670
H	3.5895740	3.1375920	-0.4736890
H	1.9389140	2.7918420	-0.4298510
C	-0.6923640	6.9142070	-0.2605190
O	-1.5992380	6.1063500	-0.3480610
O	-0.9251200	8.2345390	-0.2211880
H	-1.8852450	8.3584210	-0.2679730
H	1.2475090	-10.0707310	-0.4955490
C	0.4471510	-8.5219420	0.7701730
N	0.4212240	-9.3134310	1.9166830
C	0.0488460	-7.1827860	0.8214700
H	-0.3229520	-6.7454300	1.7432570
C	0.1276190	-6.3831310	-0.3178390
C	0.6006160	-6.8929210	-1.5282080
H	0.6501470	-6.2545840	-2.4021430
C	0.9981340	-8.2265500	-1.5762930
H	1.3674320	-8.6486660	-2.5056270
C	0.9257880	-9.0335960	-0.4448370
H	0.3670840	-10.3094830	1.7596760
H	-0.2098230	-9.0036310	2.6418070
C	-0.3053630	-4.9635470	-0.1987320
O	-0.7336480	-4.5073620	0.8625100
O	-0.1916150	-4.2553560	-1.2956640
H	-0.4759890	-3.2969680	-1.1310060
H	-1.9057660	3.9554100	0.7347610
C	-1.4756630	2.3553250	-0.6030120
N	-1.2437800	3.2254520	-1.6728420
C	-1.2830650	0.9766190	-0.7325280
H	-0.9837810	0.5372580	-1.6803130
C	-1.4726340	0.1438990	0.3710890

C	-1.8446020	0.6603930	1.6143390
H	-1.9903830	-0.0082100	2.4543120
C	-2.0127350	2.0368670	1.7449420
H	-2.2900310	2.4613720	2.7042880
C	-1.8250910	2.8760590	0.6536380
H	-1.6142260	4.1599800	-1.5333030
H	-1.4663400	2.8533140	-2.5859860
C	-1.2258920	-1.3128770	0.2029030
O	-0.8575050	-1.7941950	-0.8710590
O	-1.4083890	-2.0287350	1.2863620
H	-1.1727510	-2.9913460	1.1169660

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config_737

H	0.0692770	-2.0020520	1.8168160
C	1.5079070	-2.6823350	0.3627120
N	1.8405820	-1.4073120	-0.0588670
C	2.1264720	-3.8137410	-0.1851260
H	2.8699640	-3.7167980	-0.9715570
C	1.8057070	-5.0897310	0.2814640
C	0.8585400	-5.2734190	1.2910880
H	0.6202720	-6.2702970	1.6424460
C	0.2400650	-4.1463680	1.8328200
H	-0.5035330	-4.2618450	2.6152710
C	0.5585430	-2.8708660	1.3846270
H	1.1313400	-0.6881080	0.0344720
H	2.3576400	-1.3435070	-0.9235440
C	2.5141780	-6.2392690	-0.3465000
O	3.3473350	-6.1438960	-1.2177110
O	2.1343770	-7.4337910	0.1518760
H	2.6528350	-8.1089500	-0.3109710
H	2.2371380	8.8481460	-0.1141720
C	0.4361900	7.7028260	0.1786520
N	-0.3616090	8.8153030	0.4307700
C	-0.1150420	6.4181240	0.1576620
H	-1.1670520	6.2577260	0.3752450
C	0.6844320	5.3187120	-0.1506240
C	2.0413800	5.4678740	-0.4432290
H	2.6449980	4.6001280	-0.6798540
C	2.5871930	6.7485070	-0.4229170
H	3.6394090	6.8919890	-0.6469670
C	1.7992920	7.8532410	-0.1187790
H	0.1201440	9.6336100	0.7735360
H	-1.2218940	8.6344880	0.9273680
C	0.0489670	3.9751000	-0.1588340
O	-1.1431170	3.8152580	0.1093410
O	0.8527960	2.9858410	-0.4723290
H	0.3552690	2.1131800	-0.4481510
H	-3.8440140	-4.2858950	-0.2772520
C	-2.1051770	-3.1143870	-0.7712950
N	-1.3731320	-4.1810330	-1.2779040
C	-1.5681190	-1.8224950	-0.7774250
H	-0.5688070	-1.6513740	-1.1666860
C	-2.3026210	-0.7500990	-0.2771910
C	-3.6032410	-0.9250470	0.2034670
H	-4.1610620	-0.0774120	0.5834740
C	-4.1442910	-2.2075980	0.1920580
H	-5.1501200	-2.3720330	0.5655590
C	-3.4088530	-3.2897480	-0.2828320
H	-1.6486290	-5.0885450	-0.9284140
H	-0.3669810	-4.0622420	-1.2312450

C	-1.6468210	0.5810460	-0.2253120
O	-0.4267930	0.7120740	-0.3967510
O	-2.4417910	1.5857770	0.0291820
H	-1.9259250	2.4565060	0.0681460

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config_73

H	-2.5436200	-3.7202710	3.0564220
C	-1.6807010	-2.7469070	1.3356210
N	-1.6145440	-1.4983450	1.9247490
C	-1.1855710	-2.9489840	0.0403080
H	-0.8228800	-2.1122120	-0.5496850
C	-1.1175810	-4.2327570	-0.4931220
C	-1.5785930	-5.3415890	0.2217690
H	-1.5226370	-6.3329780	-0.2118530
C	-2.1116050	-5.1352040	1.4928390
H	-2.4859730	-5.9782240	2.0654180
C	-2.1537520	-3.8608920	2.0515420
H	-2.2774340	-1.2773810	2.6509500
H	-1.3131890	-0.7192480	1.3526270
C	-0.5191910	-4.3665020	-1.8507380
O	-0.1569520	-3.4427110	-2.5400190
O	-0.4074180	-5.6496300	-2.2562790
H	-0.0121680	-5.6286950	-3.1407020
H	-2.2726230	8.6079720	-0.0259790
C	-0.6712470	7.3513560	-0.7320540
N	-0.0162300	8.3756780	-1.4098680
C	-0.1360310	6.0602390	-0.7009980
H	0.7768640	5.8212240	-1.2387320
C	-0.7701670	5.0562270	0.0283000
C	-1.9442990	5.3093450	0.7402230
H	-2.4228960	4.5143740	1.2992540
C	-2.4754050	6.5959970	0.7074420
H	-3.3874530	6.8188940	1.2519680
C	-1.8506440	7.6062760	-0.0159240
H	-0.5916200	9.1558770	-1.6918230
H	0.6215390	8.0817350	-2.1354140
C	-0.1581550	3.7006670	0.0182450
O	0.8612770	3.4527570	-0.6266190
O	-0.7856560	2.8025960	0.7415680
H	-0.3141090	1.9138060	0.6716280
H	3.4576070	-4.6811420	-0.0454070
C	2.0683640	-3.3282100	0.8917620
N	1.5681640	-4.2645590	1.7932120
C	1.5954190	-2.0121610	0.9095680
H	0.8266530	-1.7165300	1.6186580
C	2.0851680	-1.0773720	0.0009580
C	3.0921280	-1.4094850	-0.9093800
H	3.4605180	-0.6686570	-1.6088200
C	3.5806850	-2.7122220	-0.9068040
H	4.3562880	-2.9994940	-1.6097680
C	3.0748920	-3.6637690	-0.0246010
H	1.6600260	-5.2265080	1.4962970
H	0.6269450	-4.0716070	2.1173490
C	1.4582960	0.2673000	-0.0138140
O	0.3834520	0.4922890	0.5608040
O	2.1100930	1.1800570	-0.6858280
H	1.6171520	2.0605690	-0.6708110

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config_769

H	-0.1845660	5.4189930	3.3695860
C	-0.3631230	4.1049130	1.6703780
N	0.4898440	3.1320840	2.1705500
C	-0.9986170	3.9224510	0.4369660
H	-0.8029870	3.0295710	-0.1480460
C	-1.8924530	4.8751380	-0.0454950
C	-2.1973450	6.0227800	0.6910960
H	-2.8990700	6.7522560	0.3047120
C	-1.5663100	6.2033180	1.9197360
H	-1.7805710	7.0885210	2.5103070
C	-0.6617750	5.2639520	2.4053640
H	1.1638140	3.4475600	2.8531780
H	0.9036250	2.5144760	1.4818940
C	-2.4721260	4.6391590	-1.3922480
O	-2.0571540	3.8215690	-2.1899070
O	-3.5140170	5.4369630	-1.6782350
H	-3.8057290	5.2159670	-2.5758800
H	-1.6631680	-9.1003400	0.3011670
C	-0.1720220	-7.6778110	0.9302900
N	0.5442360	-8.5971810	1.6934680
C	0.2679760	-6.3564630	0.8074080
H	1.1524680	-6.0121520	1.3356350
C	-0.4248890	-5.4599400	-0.0036990
C	-1.5642050	-5.8529100	-0.7085800
H	-2.0883700	-5.1391640	-1.3325550
C	-1.9996680	-7.1695810	-0.5852820
H	-2.8830220	-7.4989560	-1.1232550
C	-1.3156050	-8.0735810	0.2203170
H	0.0196980	-9.3933140	2.0259400
H	1.1393830	-8.2013460	2.4066990
C	0.0825060	-4.0640030	-0.0955270
O	1.0766340	-3.6933720	0.5328060
O	-0.6068410	-3.2789840	-0.8858570
H	-0.2087840	-2.3512290	-0.9013870
H	3.1633170	4.5019910	-0.6909020
C	1.6848760	3.0764920	-1.3455830
N	1.0410110	3.9505830	-2.2031430
C	1.2496730	1.7484960	-1.2249610
H	0.3839640	1.4001720	-1.7823970
C	1.9216410	0.8601000	-0.3869380
C	3.0415620	1.2614950	0.3476210
H	3.5508330	0.5530610	0.9898830
C	3.4762250	2.5800090	0.2235180
H	4.3452650	2.9157710	0.7811620
C	2.8120030	3.4768910	-0.6068080
H	1.1738600	4.9310880	-1.9990440
H	0.0721130	3.7313040	-2.4126700
C	1.4087700	-0.5360390	-0.2930970
O	0.4175920	-0.9022000	-0.9253520
O	2.0904760	-1.3197530	0.5052500
H	1.6909440	-2.2497170	0.5154590

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config_965

H	-3.5622500	-2.9740890	-1.3010250
C	-1.5236330	-3.4663590	-0.7977600
N	-0.9888510	-2.2721250	-1.2469250
C	-0.7010430	-4.4374590	-0.2151490
H	0.3711990	-4.2842980	-0.1756420
C	-1.2453410	-5.6103720	0.3013270
C	-2.6184910	-5.8608160	0.2387080

H	-3.0286620	-6.7795750	0.6401610
C	-3.4360210	-4.8983220	-0.3498440
H	-4.5066540	-5.0661800	-0.4113350
C	-2.9045960	-3.7172270	-0.8577340
H	-1.5111000	-1.7676080	-1.9469560
H	0.0142650	-2.2364340	-1.3784580
C	-0.3020760	-6.5747700	0.9223060
O	0.8842620	-6.3750530	1.0981980
O	-0.8801380	-7.7284480	1.2958730
H	-0.1891020	-8.2774000	1.6962600
H	-1.8254580	9.3367560	0.5813030
C	-0.9697390	7.8313920	-0.7011760
N	-0.9291690	8.6533470	-1.8250320
C	-0.4782790	6.5237630	-0.7551740
H	-0.0921330	6.1108140	-1.6826530
C	-0.4740050	5.7289180	0.3897590
C	-0.9532140	6.2127800	1.6087010
H	-0.9418720	5.5777160	2.4861590
C	-1.4399680	7.5161180	1.6602180
H	-1.8176710	7.9156040	2.5960950
C	-1.4492150	8.3185730	0.5241880
H	-1.5900100	9.4165010	-1.8338300
H	-0.8778270	8.1758630	-2.7132650
C	0.0497890	4.3405100	0.2751350
O	0.4711910	3.8926440	-0.7932770
O	0.0213580	3.6487970	1.3874080
H	0.3825580	2.7172750	1.2365660
H	2.9940390	-4.2685330	-0.4119560
C	2.1330500	-2.7590780	0.8595560
N	2.0360720	-3.5990280	1.9559430
C	1.7241010	-1.4209460	0.9275050
H	1.2995290	-1.0147840	1.8408110
C	1.8321420	-0.5949120	-0.1884800
C	2.3531430	-1.0691650	-1.3962420
H	2.4266430	-0.4089330	-2.2522190
C	2.7737010	-2.3968830	-1.4596330
H	3.1867970	-2.7897020	-2.3835480
C	2.6696550	-3.2324900	-0.3515660
H	1.9174280	-4.5847180	1.7446040
H	1.4102190	-3.2849870	2.6840680
C	1.3456890	0.8068250	-0.0674270
O	0.9385570	1.2615860	1.0020160
O	1.3822890	1.4992500	-1.1806970
H	1.0369240	2.4358120	-1.0257970

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config_980

H	3.1042020	3.9119870	-2.2268550
C	1.5026530	3.8958320	-0.7837700
N	1.2844740	2.5268720	-0.8426530
C	0.7541860	4.6896570	0.0889060
H	-0.0060360	4.2318870	0.7101460
C	0.9640580	6.0642070	0.1592810
C	1.9536930	6.6815220	-0.6097390
H	2.1079750	7.7521490	-0.5483120
C	2.7191810	5.8868880	-1.4618040
H	3.4975040	6.3422280	-2.0662880
C	2.4992450	4.5164120	-1.5543800
H	1.5680940	2.0772250	-1.6997000
H	0.3700010	2.2166790	-0.5329780
C	0.0642330	6.8394120	1.0547050

O	-0.8240320	6.3535760	1.7291260
O	0.2966170	8.1613090	1.0341130
H	-0.3402320	8.5791010	1.6339190
H	-2.5974090	4.1231040	-0.6187850
C	-2.0586790	2.5435600	0.7460490
N	-2.2157490	3.3291320	1.8782790
C	-1.6831710	1.1964980	0.8404710
H	-1.4892360	0.7407380	1.8073950
C	-1.5447380	0.4207560	-0.3112830
C	-1.7844610	0.9569490	-1.5787990
H	-1.6732890	0.3375220	-2.4606650
C	-2.1646120	2.2943120	-1.6715970
H	-2.3539720	2.7353640	-2.6450850
C	-2.3017410	3.0803000	-0.5318890
H	-2.0929550	4.3218900	1.7121520
H	-1.7167170	3.0070650	2.6969750
C	-1.1289650	-1.0000510	-0.1496950
O	-0.8842750	-1.4792080	0.9581570
O	-1.0154120	-1.6712580	-1.2701010
H	-0.7172200	-2.6191420	-1.0850510
H	1.7196020	-9.6178260	0.7691710
C	1.0866270	-8.0668890	-0.5868790
N	1.1857120	-8.8655220	-1.7235640
C	0.6386590	-6.7458700	-0.6801260
H	0.3971240	-6.3053430	-1.6431240
C	0.4937070	-5.9718970	0.4702510
C	0.7839700	-6.4913310	1.7336370
H	0.6645480	-5.8736920	2.6157390
C	1.2285410	-7.8077790	1.8235370
H	1.4636050	-8.2338720	2.7936730
C	1.3781090	-8.5892770	0.6826360
H	1.8232920	-9.6454700	-1.6570690
H	1.2691650	-8.3703580	-2.5992960
C	0.0247790	-4.5687350	0.3129010
O	-0.2209480	-4.0879110	-0.7955310
O	-0.0960170	-3.8999710	1.4335690
H	-0.4153800	-2.9598230	1.2518410

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config_000

H	-0.7213070	7.8225820	-0.4372870
C	0.6005260	6.2093620	-0.9819750
N	1.5664700	7.0197290	-1.5734080
C	0.7975290	4.8248790	-0.9164380
H	1.6970830	4.3759890	-1.3279660
C	-0.1755730	4.0039730	-0.3522720
C	-1.3482150	4.5367930	0.1886550
H	-2.0956820	3.8799640	0.6170510
C	-1.5215930	5.9179290	0.1655090
H	-2.4180120	6.3573520	0.5915540
C	-0.5644000	6.7467830	-0.4132300
H	1.2658750	7.9650760	-1.7671630
H	2.0093030	6.5981220	-2.3826000
C	0.0652130	2.5361290	-0.3583160
O	1.1383130	2.0573590	-0.7299700
O	-0.9416240	1.8080070	0.0655110
H	-0.7239490	0.8330610	-0.0247920
H	1.2651940	-6.4061190	-1.6438610
C	-0.0770670	-4.8537510	-0.9860390
N	-1.1308150	-5.7220960	-0.7234380
C	-0.2014510	-3.4832450	-0.7351420

H	-1.1338570	-3.0652910	-0.3669350
C	0.8791720	-2.6300870	-0.9504740
C	2.1034690	-3.1170390	-1.4143720
H	2.9380460	-2.4414220	-1.5605370
C	2.2260090	-4.4822310	-1.6614720
H	3.1681510	-4.8847820	-2.0194390
C	1.1535170	-5.3421350	-1.4526260
H	-1.1191820	-6.5981640	-1.2249060
H	-2.0488870	-5.3036300	-0.6871770
C	0.6831770	-1.1768640	-0.6877420
O	-0.3757300	-0.7351760	-0.2438260
O	1.7138560	-0.4224490	-0.9902700
H	1.4824700	0.5617180	-0.8582020
H	-0.0598910	-0.6509510	-3.3210640
C	1.1497020	1.0710410	-3.7821990
N	2.3062080	0.3232910	-3.9907660
C	1.1434280	2.4590840	-3.9471170
H	2.0512570	2.9930860	-4.2135200
C	-0.0270270	3.1839350	-3.7333750
C	-1.2141320	2.5505060	-3.3567580
H	-2.1077870	3.1331280	-3.1672330
C	-1.2097530	1.1647720	-3.2112390
H	-2.1161320	0.6490630	-2.9097230
C	-0.0495360	0.4314570	-3.4299920
H	2.3699820	-0.4957500	-3.3983090
H	3.1608220	0.8627930	-3.9595620
C	0.0520990	4.6632240	-3.8527220
O	1.0708140	5.2885450	-4.0704250
O	-1.1319250	5.2742010	-3.6800820
H	-0.9688600	6.2289050	-3.7060010

Energies of the mABA trimers

Table SI.3.2.1 Energies [in Hartree] of the trimeric structures of type (Tr)_{3M} of *m*-aminobenzoic acid as computed at the M06-2X/6-31+G(d,p) level of theory using the SMD solvation model to describe DMSO and water.

CONFIGURATION	E _{e,gas}	ΔG _{VRT}	E _{e,dms}	E _{e,water}
config_11	-1428.06430	0.33426	-1428.10942	-1428.11011
config_14	-1428.07002	0.33872	-1428.11437	-1428.11566
config_19	-1428.07480	0.34152	-1428.11758	-1428.12098
config_3	-1428.07678	0.33976	-1428.12014	-1428.11896
config_000	-1428.09563	0.34258	-1428.13332	-1428.13247

Table SI.3.2.2 Energies [in Hartree] of the trimeric structures of type (Tr)_{D+M} of mABA as computed at the M06-2X/6-31+G(d,p) level of theory using the SMD solvation model to describe DMSO and water.

CONFIGURATION	E _{e,gas}	ΔG _{VRT}	E _{e,dms}	E _{e,water}
config_1339	-1428.08731	0.33882	-1428.12549	-1428.11978
config_1730	-1428.09075	0.33950	-1428.12796	-1428.12269
config_2030	-1428.08894	0.33858	-1428.12478	-1428.12029
config_2397	-1428.08713	0.33793	-1428.12521	-1428.11958

config_2530	-1428.07236	0.33905	-1428.12304	-1428.11682
config_73	-1428.08853	0.33852	-1428.12712	-1428.12224
config_737	-1428.08971	0.33898	-1428.12777	-1428.12291
config_769	-1428.08957	0.33853	-1428.12791	-1428.12286
config_965	-1428.08755	0.33741	-1428.12662	-1428.12121
config_980	-1428.05915	0.34125	-1428.12651	-1428.12137

SI.4 Tetramers

Coordinates of the optimised geometries of the mABA tetramers

Table SI.4.1. Geometries [in Angstrom] of the tetrameric structures of *m*-aminobenzoic acid as computed at the M06-2X/6-31+G(d,p) level of theory. XYZ format.

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config_1033
C      0.7989060      -6.1366880      -1.0343850
H      0.9309170      -5.6813230      -2.0123800
C      0.5998500      -7.5150060      -0.9048820
N      0.5124680      -8.3294680      -2.0324620
H      0.7093090      -9.3080480      -1.8789900
H      0.9654350      -7.9731310      -2.8619330
C      0.4245780      -8.0489830      0.3808910
H      0.2579310      -9.1170010      0.4956470
C      0.4623730      -7.2265540      1.5026580
H      0.3280590      -7.6650330      2.4865410
C      0.6659490      -5.8546850      1.3756000
H      0.6833890      -5.1990050      2.2382430
C      0.8286470      -5.3212330      0.0961010
C      1.0115450      -3.8549620      -0.1023230
O      1.1186210      -3.1631580      0.9993020
H      1.1821650      -2.1694240      0.7995380
O      1.0523190      -3.3616390      -1.2335640
C      1.7699320      2.0939930      0.3804250
H      1.6562700      1.6139360      1.3487190
C      2.0219040      3.4665370      0.2848510
N      2.0846830      4.2571420      1.4281050
H      2.5729530      5.1352760      1.3300810
H      2.3029280      3.7739360      2.2871130
C      2.1338210      4.0428940      -0.9895160
H      2.3005220      5.1144340      -1.0743930
C      2.0033600      3.2639130      -2.1343340
H      2.0860760      3.7350520      -3.1088870
C      1.7617280      1.8963130      -2.0428200
H      1.6575860      1.2796570      -2.9275210
C      1.6490470      1.3234620      -0.7745530
C      1.4117760      -0.1343800      -0.6114240
O      1.3279060      -0.8167970      -1.7271160
H      1.2038370      -1.7964440      -1.5295370
O      1.3230600      -0.6511250      0.5058330
C      -1.7876610      -2.0983810      -0.3509060
H      -1.6251280      -1.6370170      -1.3214800
C      -2.0190350      -3.4738890      -0.2425100
N      -2.0703520      -4.2739350      -1.3830410
H      -1.8918180      -5.2552990      -1.2097260
H      -1.4973200      -3.9328970      -2.1450130
C      -2.2280720      -4.0201840      1.0322930
H      -2.4019020      -5.0894570      1.1286120
C      -2.1922860      -3.2137920      2.1660130
H      -2.3465970      -3.6628540      3.1424070
C      -1.9532290      -1.8466170      2.0613310
H      -1.9188760      -1.2087760      2.9364000
C      -1.7567660      -1.3004420      0.7907800
C      -1.5218070      0.1565900      0.6105720
O      -1.4824820      0.8594700      1.7148280
H      -1.3572830      1.8405300      1.5030720
O      -1.3882980      0.6510900      -0.5123540
C      -0.7138570      6.1233540      0.9912660
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H	-0.7881400	5.6586650	1.9701040
C	-0.4720020	7.4944580	0.8575520
N	-0.3930490	8.3139090	1.9829990
H	0.1155850	9.1777840	1.8641280
H	-0.1689060	7.8457260	2.8490060
C	-0.3709240	8.0366160	-0.4315570
H	-0.1918190	9.1025080	-0.5487620
C	-0.5091890	7.2262920	-1.5556040
H	-0.4270330	7.6697150	-2.5431370
C	-0.7495680	5.8619800	-1.4241450
H	-0.8450680	5.2146820	-2.2881920
C	-0.8490740	5.3229220	-0.1391100
C	-1.0756060	3.8642420	0.0623760
O	-1.1405020	3.1648090	-1.0419840
H	-1.2363520	2.1794300	-0.8339240
O	-1.1924790	3.3778920	1.1891580

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config_1100

C	1.4520000	2.0548430	-1.1962480
H	0.7781720	1.6449570	-1.9438440
C	1.7836590	3.4140600	-1.2024300
N	1.2768910	4.2587050	-2.1891670
H	1.2842540	5.2397320	-1.9392640
H	0.3643020	3.9817720	-2.5298470
C	2.6607050	3.8946720	-0.2194320
H	2.9202620	4.9508020	-0.2110080
C	3.1803530	3.0402480	0.7487590
H	3.8511580	3.4382660	1.5039370
C	2.8444150	1.6896450	0.7620410
H	3.2378550	1.0145620	1.5125610
C	1.9789730	1.2086570	-0.2235930
C	1.5998980	-0.2278420	-0.2791500
O	2.1126910	-0.9807120	0.6612310
H	1.8394620	-1.9460970	0.5276140
O	0.8591100	-0.6618530	-1.1664170
C	0.7829840	-6.1644180	0.3504550
H	1.3704030	-5.7430180	1.1608960
C	0.4352850	-7.5193160	0.3381680
N	0.9000820	-8.3796140	1.3322660
H	0.3552190	-9.2162910	1.4815080
H	1.1810650	-7.9378190	2.1955870
C	-0.3392560	-8.0052330	-0.7243470
H	-0.6078850	-9.0584210	-0.7497800
C	-0.7543020	-7.1554750	-1.7468490
H	-1.3519560	-7.5555380	-2.5601180
C	-0.4114330	-5.8068070	-1.7348690
H	-0.7377830	-5.1308110	-2.5165620
C	0.3603600	-5.3238730	-0.6752510
C	0.7336820	-3.8839230	-0.5931600
O	0.2373060	-3.1352480	-1.5447200
H	0.4821250	-2.1641550	-1.3978540
O	1.4564190	-3.4553070	0.3091260
C	-0.9052980	6.1799300	-0.3924590
H	-1.5431490	5.7589530	-1.1652770
C	-0.6024750	7.5452920	-0.3762820
N	-1.0677470	8.3881440	-1.3843830
H	-1.1074330	9.3691270	-1.1473710
H	-1.9021020	8.0753290	-1.8600660
C	0.2348730	8.0341890	0.6377240
H	0.4880150	9.0911900	0.6554550

C	0.7404260	7.1811020	1.6139460
H	1.3833920	7.5843500	2.3900180
C	0.4358340	5.8219910	1.6014640
H	0.8329370	5.1426000	2.3465910
C	-0.3872900	5.3329360	0.5860060
C	-0.7135370	3.8805890	0.4985660
O	-0.2695260	3.1597610	1.4914720
H	-0.4736050	2.1748710	1.3453340
O	-1.3521810	3.4232410	-0.4545310
C	-1.3671680	-2.0473470	1.2705320
H	-0.7233470	-1.6003720	2.0235200
C	-1.6872240	-3.4081610	1.3168440
N	-1.1476120	-4.2314620	2.3011120
H	-1.6567430	-5.0832790	2.4873400
H	-0.8369330	-3.7648580	3.1408700
C	-2.5009990	-3.9423610	0.3064830
H	-2.7298680	-5.0057350	0.3154430
C	-2.9877140	-3.1329250	-0.7146170
H	-3.6081370	-3.5721870	-1.4896450
C	-2.6790370	-1.7764130	-0.7582180
H	-3.0477730	-1.1362990	-1.5507260
C	-1.8662130	-1.2457070	0.2454920
C	-1.5128820	0.1975990	0.2629480
O	-2.0086740	0.9086020	-0.7198650
H	-1.7419850	1.8742220	-0.6227870
O	-0.8143050	0.6776980	1.1601930

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config_170

C	-2.2763760	2.3508900	-0.0367840
H	-2.8324630	1.8429530	-0.8201260
C	-2.2891200	3.7436910	0.0729230
N	-2.9529080	4.5418260	-0.8707740
H	-3.3420340	5.3935060	-0.4875290
H	-3.6397540	4.0451560	-1.4228930
C	-1.5682710	4.3488650	1.1113650
H	-1.5650530	5.4332370	1.1967440
C	-0.8172590	3.5819200	1.9944820
H	-0.2451680	4.0746150	2.7746880
C	-0.7749890	2.1959790	1.8681930
H	-0.1793560	1.5862170	2.5369290
C	-1.5245310	1.5903010	0.8575010
C	-1.5443760	0.1064060	0.7373790
O	-0.6494980	-0.4959520	1.4831510
H	-0.7423760	-1.5020620	1.4205410
O	-2.3436630	-0.4919060	0.0153260
C	-0.3386450	-5.7217900	1.0812690
H	0.1879400	-5.1296650	1.8249170
C	0.0252350	-7.0454770	0.8324610
N	1.1133300	-7.6064830	1.5176540
H	1.1663480	-8.6155110	1.4717710
H	1.2163790	-7.2799770	2.4699900
C	-0.6424530	-7.7500640	-0.1790700
H	-0.3657800	-8.7803540	-0.3884000
C	-1.6478790	-7.1356460	-0.9217000
H	-2.1538520	-7.6994300	-1.6990440
C	-1.9960680	-5.8068850	-0.6899220
H	-2.7513600	-5.3064690	-1.2849350
C	-1.3237680	-5.1086530	0.3127120
C	-1.5234940	-3.6463420	0.5120490
O	-2.3996960	-3.0828460	-0.2804640

H	-2.3983020	-2.0782100	-0.1540020
O	-0.8725030	-3.0356960	1.3603300
C	0.4902750	5.7773650	-0.9528420
H	-0.1380910	5.2123280	-1.6365490
C	0.3534400	7.1624500	-0.8341640
N	-0.5365340	7.8527760	-1.6540400
H	-0.8599290	8.7442020	-1.3079040
H	-1.2746270	7.2926040	-2.0572020
C	1.1613410	7.8412650	0.0908400
H	1.0704620	8.9202450	0.1882680
C	2.0744950	7.1461870	0.8783170
H	2.6867390	7.6934240	1.5883390
C	2.2085830	5.7636390	0.7660540
H	2.9094060	5.2093020	1.3793690
C	1.4057030	5.0930210	-0.1568060
C	1.4470800	3.6118200	-0.2934310
O	2.2828010	2.9920980	0.5040880
H	2.2422680	1.9935660	0.3553490
O	0.7276600	3.0351160	-1.1096520
C	2.1147940	-2.4398230	-0.0708490
H	2.7335860	-1.9924360	0.7022940
C	2.0932890	-3.8258030	-0.2663520
N	2.8718960	-4.6790400	0.5118110
H	2.5514650	-5.6388470	0.5757930
H	3.1693280	-4.3054500	1.4016000
C	1.2984890	-4.3474850	-1.2985320
H	1.2780930	-5.4234700	-1.4596890
C	0.5052810	-3.5131900	-2.0766930
H	-0.1257140	-3.9453980	-2.8474480
C	0.4939800	-2.1383900	-1.8588030
H	-0.1324330	-1.4783260	-2.4463650
C	1.3183340	-1.6117600	-0.8610400
C	1.3587420	-0.1394270	-0.6422430
O	0.4439800	0.5184770	-1.3150970
H	0.5581860	1.5214660	-1.2036810
O	2.1819030	0.4051850	0.0950670

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config_44

C	-2.2824700	2.3478900	-0.2741620
H	-2.7570160	1.8590000	-1.1206880
C	-2.3052900	3.7377880	-0.1352610
N	-2.8738570	4.5588240	-1.1216480
H	-3.2979080	5.4019930	-0.7567730
H	-3.5078590	4.0756040	-1.7445390
C	-1.6885000	4.3184160	0.9812940
H	-1.6887450	5.4009360	1.0876260
C	-1.0340840	3.5297240	1.9202730
H	-0.5398520	4.0031200	2.7630380
C	-0.9867300	2.1462490	1.7720500
H	-0.4654920	1.5207100	2.4866780
C	-1.6292860	1.5648670	0.6766550
C	-1.6425460	0.0829350	0.5278440
O	-0.8774020	-0.5376140	1.3946340
H	-0.9778550	-1.5394890	1.3093710
O	-2.3207910	-0.4991870	-0.3192690
C	-0.4898570	-5.7278190	1.0281670
H	-0.1628480	-5.1388490	1.8806720
C	-0.0279130	-7.0303870	0.8385870
N	0.9099030	-7.5723740	1.7291440
H	1.0012580	-8.5787870	1.6871660

H	0.8076930	-7.2549970	2.6845000
C	-0.4327240	-7.7291240	-0.3069460
H	-0.0736760	-8.7418800	-0.4719050
C	-1.2794650	-7.1303750	-1.2370300
H	-1.5816770	-7.6908430	-2.1160530
C	-1.7216190	-5.8208800	-1.0615590
H	-2.3463770	-5.3303890	-1.7991740
C	-1.3080820	-5.1272140	0.0752380
C	-1.5845700	-3.6747010	0.2533340
O	-2.2903950	-3.1084760	-0.6936280
H	-2.3323040	-2.1109860	-0.5476490
O	-1.1373450	-3.0698630	1.2275440
C	0.5073240	5.7772620	-0.9063660
H	-0.0553010	5.2018200	-1.6369380
C	0.3488930	7.1619470	-0.8119110
N	-0.4788830	7.8355120	-1.7078360
H	-0.8389910	8.7254200	-1.3954990
H	-1.1774740	7.2622400	-2.1602520
C	1.0739720	7.8568080	0.1684570
H	0.9679240	8.9360090	0.2461420
C	1.9237280	7.1768450	1.0360470
H	2.4724000	7.7354360	1.7879270
C	2.0733090	5.7939270	0.9523870
H	2.7225320	5.2510210	1.6293960
C	1.3552100	5.1077330	-0.0275340
C	1.4175910	3.6253610	-0.1419620
O	2.1538760	3.0200750	0.7578280
H	2.1178800	2.0178830	0.6323770
O	0.8032990	3.0355930	-1.0315980
C	2.0792130	-2.4163110	0.2602090
H	2.5427250	-1.9549300	1.1279490
C	2.1183050	-3.8032210	0.0734010
N	2.7627070	-4.6380250	0.9832700
H	2.4470190	-5.6013300	1.0039840
H	2.8936010	-4.2514690	1.9070710
C	1.5273160	-4.3429390	-1.0794250
H	1.5532930	-5.4198580	-1.2346200
C	0.8677800	-3.5261150	-1.9895640
H	0.3895580	-3.9734280	-2.8557690
C	0.7936100	-2.1509070	-1.7867980
H	0.2670190	-1.5054920	-2.4793570
C	1.4201260	-1.6054920	-0.6631950
C	1.4013360	-0.1316330	-0.4513070
O	0.6172440	0.5119250	-1.2831940
H	0.6883370	1.5165690	-1.1529490
O	2.0708250	0.4266930	0.4195350

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config_491

C	1.6044910	3.1352640	-1.4512040
H	0.9579080	2.7074160	-2.2125010
C	1.9015580	4.5009510	-1.4461680
N	1.4259260	5.3440750	-2.4518160
H	1.1455310	6.2660750	-2.1356650
H	0.6995390	4.9302870	-3.0211490
C	2.7113470	5.0048060	-0.4182950
H	2.9504320	6.0651070	-0.4051440
C	3.1902820	4.1676950	0.5847890
H	3.8027640	4.5859900	1.3778430
C	2.8854440	2.8087340	0.5885860
H	3.2368590	2.1493860	1.3733910

C	2.0891660	2.3049610	-0.4418300
C	1.6782470	0.8763170	-0.4735850
O	2.1537320	0.1333610	0.4969420
H	1.8151160	-0.8070720	0.4015870
O	0.9327570	0.4415600	-1.3541000
C	0.6857320	-5.0678450	0.0257890
H	0.9620970	-4.6310220	0.9813180
C	0.3642880	-6.4268800	-0.0678610
N	0.3969610	-7.2218140	1.0766740
H	-0.0632510	-8.1167100	0.9858420
H	0.1188350	-6.7294300	1.9197070
C	0.0362170	-6.9524410	-1.3239380
H	-0.1966960	-8.0107410	-1.4152320
C	-0.0116880	-6.1298390	-2.4484860
H	-0.2726220	-6.5597370	-3.4107980
C	0.2516140	-4.7683600	-2.3458320
H	0.1895050	-4.1122760	-3.2060120
C	0.6040470	-4.2505110	-1.0953570
C	0.8693290	-2.7979830	-0.9134560
O	0.5409660	-2.0501280	-1.9419680
H	0.6882050	-1.0782260	-1.7203320
O	1.3357680	-2.3440320	0.1314770
C	-0.9644110	5.0797930	-0.1345430
H	-1.4496450	4.6254110	-0.9949370
C	-0.7032530	6.4500310	-0.0951920
N	-0.9951020	7.2631790	-1.2032340
H	-1.1329200	8.2399150	-0.9778100
H	-1.7522620	6.9182470	-1.7792940
C	-0.0553620	6.9836370	1.0268440
H	0.1557220	8.0496940	1.0647360
C	0.3277710	6.1594410	2.0803660
H	0.8301330	6.5925940	2.9396180
C	0.0896740	4.7885700	2.0325100
H	0.4105340	4.1304020	2.8311510
C	-0.5595320	4.2595370	0.9165210
C	-0.7944190	2.7921490	0.7916330
O	-0.3425840	2.0844430	1.7995630
H	-0.5189040	1.1014420	1.6488570
O	-1.3577110	2.3028260	-0.1862850
C	-1.5340020	-3.1133580	1.6935430
H	-0.9861940	-2.6253470	2.4949620
C	-1.8846770	-4.4597330	1.7712550
N	-1.4753640	-5.2495250	2.8649880
H	-2.1395020	-5.9757670	3.1059200
H	-1.2429680	-4.7053670	3.6871000
C	-2.5667020	-5.0481210	0.6972000
H	-2.8189030	-6.1054030	0.7401630
C	-2.8748750	-4.3052470	-0.4361670
H	-3.3778210	-4.7867150	-1.2685780
C	-2.5261790	-2.9580240	-0.5189680
H	-2.7506650	-2.3700030	-1.4013230
C	-1.8609430	-2.3717200	0.5573600
C	-1.4689910	-0.9354190	0.5289090
O	-1.8739680	-0.2741250	-0.5282880
H	-1.6071470	0.6890620	-0.4571200
O	-0.8260080	-0.4255940	1.4470620
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config_529			
C	0.6362970	-4.8625240	-0.6206140
H	0.5364890	-4.2979040	-1.5442390

C	0.4732150	-6.2504170	-0.6027660
N	0.1166720	-6.9416310	-1.7753830
H	0.3981790	-7.9141150	-1.7783750
H	0.4239880	-6.4823370	-2.6239590
C	0.5868020	-6.9298730	0.6147960
H	0.4549170	-8.0088940	0.6391940
C	0.8562090	-6.2338790	1.7909850
H	0.9433180	-6.7800800	2.7249960
C	1.0071330	-4.8516040	1.7787710
H	1.2012030	-4.2964980	2.6890270
C	0.8896170	-4.1740960	0.5627800
C	0.9977160	-2.6890640	0.5024450
O	1.1696140	-2.1044190	1.6613470
H	1.2613090	-1.1085470	1.5422590
O	0.9251850	-2.0782970	-0.5653780
C	2.2542170	3.1804110	1.2970290
H	2.1429650	2.6759860	2.2531300
C	2.6324780	4.5210250	1.2268510
N	2.7902280	5.2827120	2.4009580
H	3.4738010	6.0252810	2.3181750
H	2.9730580	4.7251130	3.2261020
C	2.7558540	5.1294330	-0.0296490
H	3.0327390	6.1797170	-0.0891250
C	2.4802180	4.4150340	-1.1896300
H	2.5567400	4.9096230	-2.1526890
C	2.0841640	3.0805290	-1.1232040
H	1.8466750	2.5178680	-2.0189370
C	1.9821280	2.4719360	0.1276210
C	1.5685090	1.0467800	0.2533360
O	1.1675530	0.4963410	-0.8702660
H	1.0146040	-0.4907520	-0.7437760
O	1.6135230	0.4484060	1.3263330
C	-2.3459370	-3.2004820	-1.0766900
H	-2.2928900	-2.7217110	-2.0507110
C	-2.5578610	-4.5748470	-0.9604790
N	-2.7363690	-5.3839600	-2.0857180
H	-2.2563700	-6.2753220	-2.0204400
H	-2.5226010	-4.9222770	-2.9597630
C	-2.6030930	-5.1437310	0.3231510
H	-2.7771860	-6.2122940	0.4201360
C	-2.4031000	-4.3615320	1.4526510
H	-2.4236870	-4.8265590	2.4335020
C	-2.1557480	-2.9934170	1.3378200
H	-1.9673710	-2.3771390	2.2094930
C	-2.1352470	-2.4259560	0.0638790
C	-1.8174680	-0.9854640	-0.1235710
O	-1.3730770	-0.3798570	0.9528370
H	-1.2452930	0.6090270	0.7763460
O	-1.9502120	-0.4250710	-1.2123630
C	-0.5898000	4.8833170	0.4149790
H	-0.4387310	4.3513010	1.3496420
C	-0.3095340	6.2515480	0.3221350
N	0.1585000	6.9445450	1.4356060
H	0.5493160	7.8545970	1.2360450
H	0.7524140	6.4059230	2.0585970
C	-0.5343030	6.8983000	-0.9010920
H	-0.3327130	7.9636070	-0.9852020
C	-0.9983830	6.1896820	-2.0071810
H	-1.1613170	6.7132900	-2.9441980
C	-1.2410450	4.8224740	-1.9263380
H	-1.5814810	4.2552890	-2.7844760

C	-1.0307670	4.1811200	-0.7019080
C	-1.2354900	2.7143830	-0.5625640
O	-1.5686090	2.0931680	-1.6642880
H	-1.6829240	1.1026770	-1.4918500
O	-1.0830340	2.1428310	0.5214210

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config_951

C	-2.2630360	3.4188230	-0.3181070
H	-2.6431910	2.8916540	-1.1891060
C	-2.4399050	4.7943350	-0.1712470
N	-3.0353460	5.5537280	-1.1968210
H	-3.5312720	6.3717870	-0.8646250
H	-3.6241430	5.0107580	-1.8162120
C	-1.9261970	5.4288000	0.9678210
H	-2.0465310	6.5040640	1.0805520
C	-1.2271670	4.7029080	1.9251610
H	-0.8152040	5.2153880	2.7886690
C	-1.0317430	3.3315270	1.7728480
H	-0.4745780	2.7573700	2.5045810
C	-1.5623990	2.6994210	0.6484630
C	-1.3927870	1.2343120	0.4416390
O	-0.5677150	0.6564750	1.2843430
H	-0.5837370	-0.3444680	1.1633200
O	-1.9938350	0.6306450	-0.4453050
C	-0.6943970	-4.7240330	1.1612930
H	-0.0692850	-4.1626860	1.8510300
C	-0.6969900	-6.1212700	1.1668520
N	0.1562150	-6.8323720	2.0306090
H	-0.1735040	-7.7628700	2.2549210
H	0.3858930	-6.3258080	2.8769220
C	-1.4987960	-6.8010390	0.2439660
H	-1.5031580	-7.8883130	0.2378600
C	-2.2798960	-6.0961050	-0.6690300
H	-2.8975780	-6.6428210	-1.3746020
C	-2.2681110	-4.7057540	-0.6877010
H	-2.8575110	-4.1448580	-1.4035020
C	-1.4652110	-4.0286610	0.2335120
C	-1.3811940	-2.5409720	0.2262440
O	-2.0532790	-1.9581560	-0.7340810
H	-1.9686910	-0.9555010	-0.6660150
O	-0.7211520	-1.9273720	1.0671920
C	0.8299670	4.7627610	-0.9111810
H	0.2167000	4.2476670	-1.6447740
C	0.7606470	6.1537140	-0.7742580
N	-0.0941470	6.8935220	-1.5869530
H	-0.2568710	7.8422010	-1.2799970
H	-0.9577560	6.4250090	-1.8434000
C	1.5847220	6.7731980	0.1754310
H	1.5500550	7.8544830	0.2860920
C	2.4337620	6.0194520	0.9831720
H	3.0588990	6.5239170	1.7135830
C	2.4774660	4.6334290	0.8721140
H	3.1176470	4.0321590	1.5065780
C	1.6649420	4.0178860	-0.0843030
C	1.6368000	2.5377730	-0.2274640
O	2.4071300	1.8827520	0.6021910
H	2.3304500	0.8867040	0.4438210
O	0.9194420	1.9871010	-1.0685190
C	2.2913860	-3.4655370	-0.0272760
H	2.8082450	-2.9830560	0.7977060

C	2.2738300	-4.8554670	-0.1528960
N	2.9420420	-5.6798430	0.7567740
H	2.4123940	-6.5071510	1.0097810
H	3.2701770	-5.1957580	1.5819800
C	1.5778470	-5.4263300	-1.2315670
H	1.5656300	-6.5081540	-1.3370470
C	0.8938120	-4.6261750	-2.1367610
H	0.3469670	-5.0908540	-2.9514750
C	0.8841780	-3.2382530	-1.9959470
H	0.3270670	-2.6041190	-2.6760870
C	1.5907630	-2.6718430	-0.9350630
C	1.5613660	-1.2036750	-0.6988080
O	0.6963730	-0.5501140	-1.4385140
H	0.7761490	0.4467410	-1.2797260
O	2.2845480	-0.6625160	0.1387320

Energies of the mABA tetramers

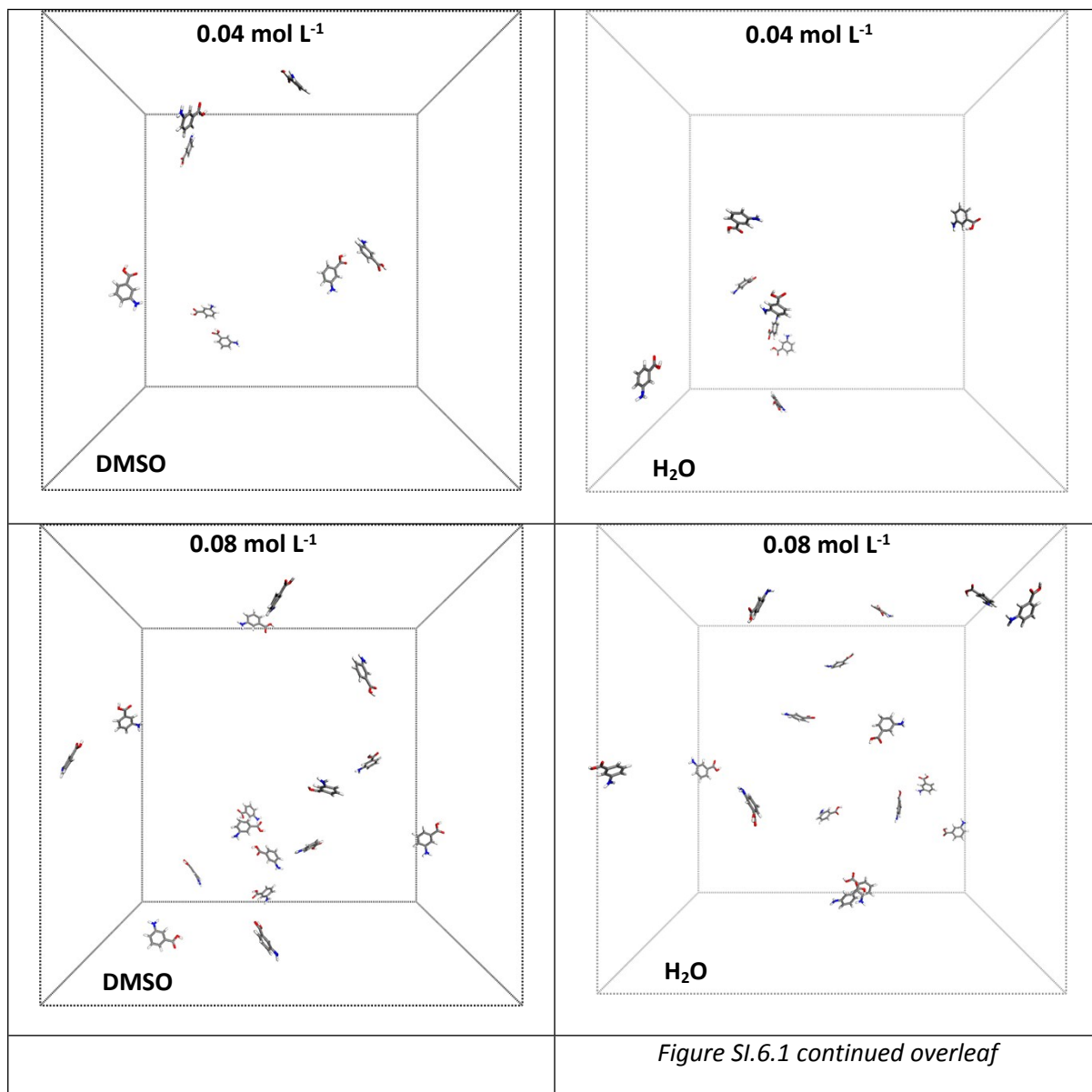
Table SI.4.2. Energies [in Hartree] of the tetrameric structures of *m*-aminobenzoic acid as computed at the M06-2X/6-31+G(d,p) level of theory using the SMD solvation model to describe DMSO and water.

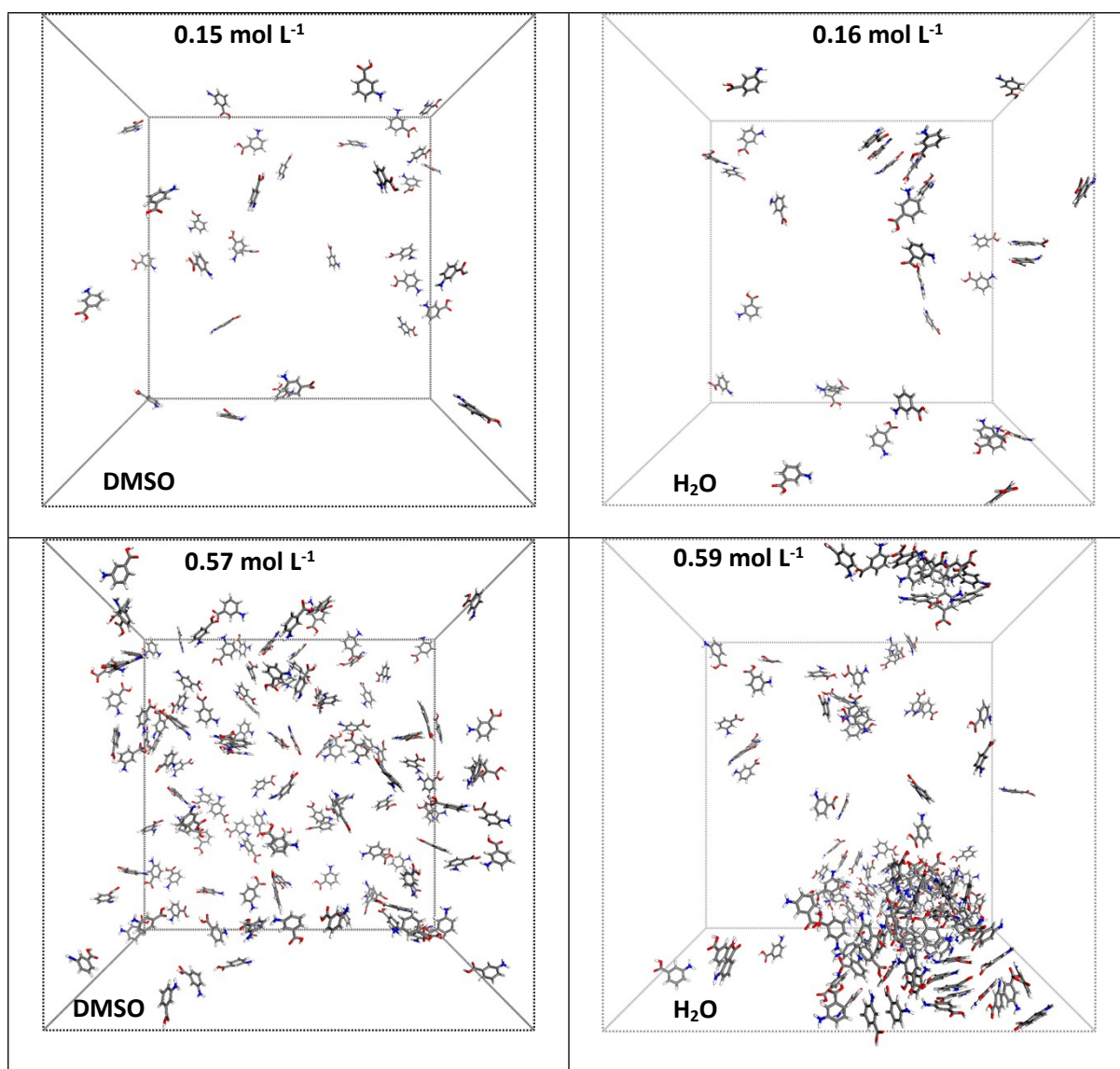
CONFIGURATION	$E_{e,gas}$	δG_{VRT}	$E_{e,dmsO}$	$E_{e,water}$
config_1033	-1904.14605	0.46706	-1904.19518	-1904.19048
config_1100	-1904.14586	0.46601	-1904.19487	-1904.19001
config_170	-1904.14307	0.46539	-1904.19210	-1904.18665
config_44	-1904.14306	0.46470	-1904.19197	-1904.18675
config_491	-1904.14907	0.46611	-1904.19733	-1904.19265
config_529	-1904.15129	0.46961	-1904.19932	-1904.19314
config_951	-1904.15116	0.46913	-1904.19918	-1904.19282
config_1033	-1904.14605	0.46706	-1904.19518	-1904.19048
config_1100	-1904.14586	0.46601	-1904.19487	-1904.19001

SI.5 Classical molecular dynamics

Snapshot of molecular dynamics simulations

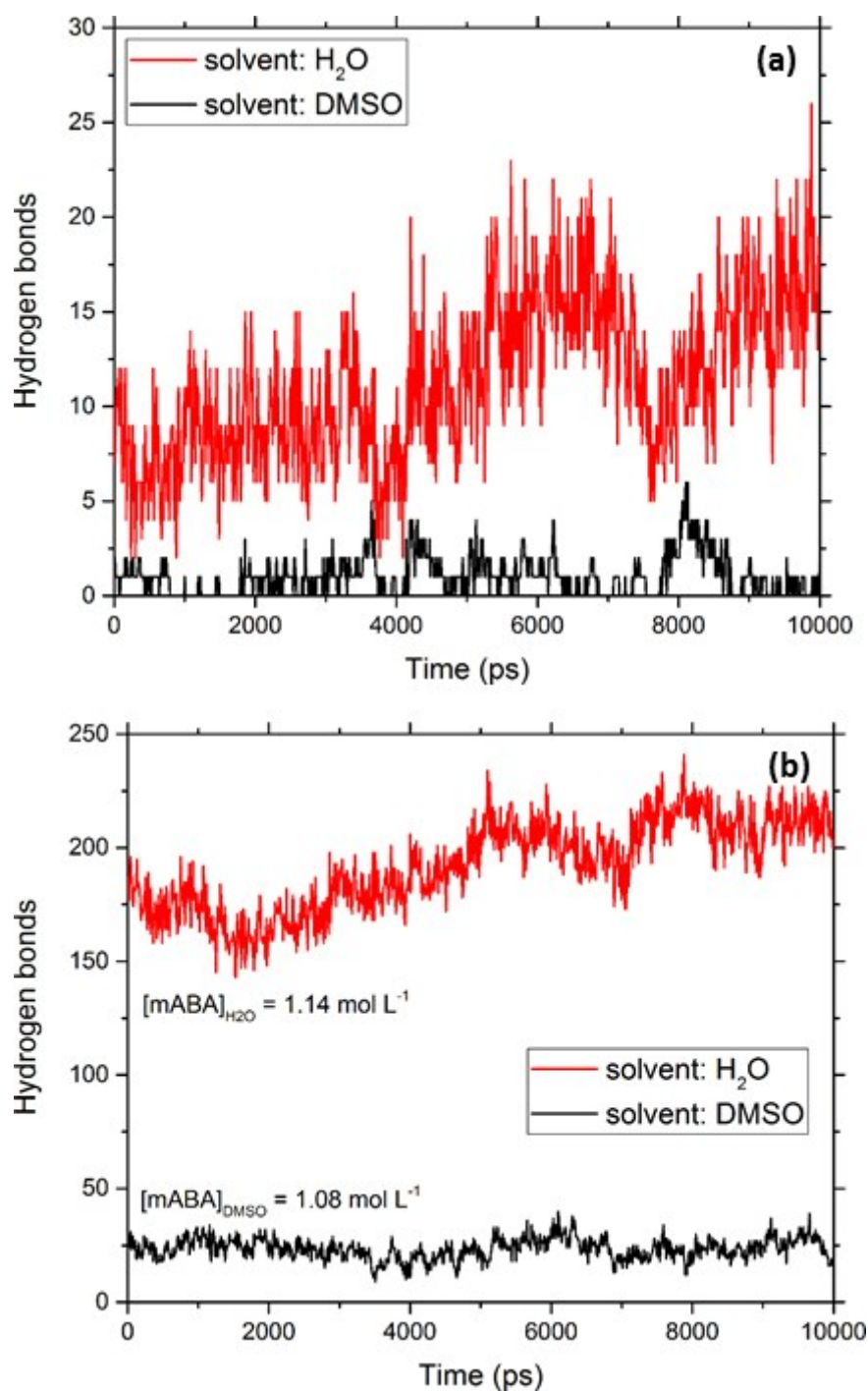
Figure SI.5.1. Last configuration of MD simulations of solutions of mABA in (a) DMSO (200 ns) and (b) water (30 ns). Solvent molecules have been removed for clarity.





Hydrogen bonding analysis

Figure SI.5.2. Time evolution of the hydrogen bond between mABA molecules during the last 10 ns of the MD simulations of (a) 0.3 mol L⁻¹ and (b) 1.1 mol L⁻¹ solutions of mABA in DMSO and water.



SI.6 Metadynamics simulations

Free energy profile for the mABA dimerization

Figure SI.6.1. Free energy profile for the mABA dimerization reaction in water and DMSO obtained by using metadynamics. . The order parameter (OP) used to study the dimerization reaction was the carbon (C=O) carbon (C=O) distance of two mABA molecules.

