Electronic Supplementary Information to

"Solvation and aggregation of meta-aminobenzoic acid in water: density functional theory and molecular dynamics study"

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SI.1 GAFF parameters for mABA and mABA±

mABA

Table SI.1. General AMBER forcefield parameters used to model mABA in GROMACS (topology file)

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; 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
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```
     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
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     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
```

mABA±

Table SI.2. General AMBER forcefield parameters used to model mABA± in GROMACS (topology file).

```
; ZMB_GMX.top created by acpype (Rev: 403) on Sun Sep  4 21:51:21 2016

[ 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
 n4       n4          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
 o        o           0.00000  0.00000   A     2.95992e-01   8.78640e-01 ; 1.66  0.2100

[ moleculetype ]
;name            nrexcl
 ZMB              3

[ atoms ]
;   nr  type  resi  res  atom  cgnr     charge      mass       ; qtot   bond_type
     1   ca     1   ZMB    C2    1    -0.201672     12.01000 ; qtot -0.202
     2   ha     1   ZMB    H2    2     0.168307      1.00800 ; qtot -0.033
     3   ca     1   ZMB    C1    3     0.126418     12.01000 ; qtot 0.093
     4   n4     1   ZMB    N1    4    -0.389661     14.01000 ; qtot -0.297
     5   hn     1   ZMB    H5    5     0.335820      1.00800 ; qtot 0.039
     6   hn     1   ZMB    H6    6     0.335820      1.00800 ; qtot 0.375
     7   hn     1   ZMB    H7    7     0.335820      1.00800 ; qtot 0.711
     8   ca     1   ZMB    C6    8    -0.233164     12.01000 ; qtot 0.478
     9   ha     1   ZMB    H1    9     0.161128      1.00800 ; qtot 0.639
    10   ca     1   ZMB    C5   10    -0.204098     12.01000 ; qtot 0.435
    11   ha     1   ZMB    H4   11     0.174390      1.00800 ; qtot 0.609
    12   ca     1   ZMB    C4   12    -0.057139     12.01000 ; qtot 0.552
    13   ha     1   ZMB    H3   13     0.159004      1.00800 ; qtot 0.711
    14   ca     1   ZMB    C3   14    -0.022851     12.01000 ; qtot 0.688
    15    c     1   ZMB    C7   15     0.797939     12.01000 ; qtot 1.486
    16    o     1   ZMB    O2   16    -0.743031     16.00000 ; qtot 0.743
    17    o     1   ZMB    O1   17    -0.743031     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     14   1    1.3870e-01    4.0033e+05 ;     C2 - C3
     3      4   1    1.4650e-01    2.7246e+05 ;     C1 - N1
     3      8   1    1.3870e-01    4.0033e+05 ;     C1 - C6
     4      5   1    1.0330e-01    3.0878e+05 ;     N1 - H5
     4      6   1    1.0330e-01    3.0878e+05 ;     N1 - H6
     4      7   1    1.0330e-01    3.0878e+05 ;     N1 - H7
     8      9   1    1.0870e-01    2.8811e+05 ;     C6 - H1
     8     10   1    1.3870e-01    4.0033e+05 ;     C6 - C5
    10     11   1    1.0870e-01    2.8811e+05 ;     C5 - H4
    10     12   1    1.3870e-01    4.0033e+05 ;     C5 - C4
    12     13   1    1.0870e-01    2.8811e+05 ;     C4 - H3
    12     14   1    1.3870e-01    4.0033e+05 ;     C4 - C3
    14     15   1    1.4870e-01    2.9263e+05 ;     C3 - C7
    15     16   1    1.2140e-01    5.4225e+05 ;     C7 - O2
    15     17   1    1.2140e-01    5.4225e+05 ;     C7 - O1

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

[ angles ]
;   ai     aj     ak    funct   theta         cth
     1      3      4      1    1.1841e+02    5.6300e+02 ;     C2 - C1     - N1
     1      3      8      1    1.1997e+02    5.6216e+02 ;     C2 - C1     - C6
     1     14     12      1    1.1997e+02    5.6216e+02 ;     C2 - C3     - C4
     1     14     15      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     14      1    1.2001e+02    4.0551e+02 ;     H2 - C2     - C3
     3      1     14      1    1.1997e+02    5.6216e+02 ;     C1 - C2     - C3
     3      4      5      1    1.0852e+02    3.9781e+02 ;     C1 - N1     - H5
     3      4      6      1    1.0852e+02    3.9781e+02 ;     C1 - N1     - H6
     3      4      7      1    1.0852e+02    3.9781e+02 ;     C1 - N1     - H7
     3      8      9      1    1.2001e+02    4.0551e+02 ;     C1 - C6     - H1
     3      8     10      1    1.1997e+02    5.6216e+02 ;     C1 - C6     - C5
     4      3      8      1    1.1841e+02    5.6300e+02 ;     N1 - C1     - C6
     5      4      6      1    1.0811e+02    3.3907e+02 ;     H5 - N1     - H6
     5      4      7      1    1.0811e+02    3.3907e+02 ;     H5 - N1     - H7
     6      4      7      1    1.0811e+02    3.3907e+02 ;     H6 - N1     - H7
     8     10     11      1    1.2001e+02    4.0551e+02 ;     C6 - C5     - H4
     8     10     12      1    1.1997e+02    5.6216e+02 ;     C6 - C5     - C4
     9      8     10      1    1.2001e+02    4.0551e+02 ;     H1 - C6     - C5
    10     12     13      1    1.2001e+02    4.0551e+02 ;     C5 - C4     - H3
    10     12     14      1    1.1997e+02    5.6216e+02 ;     C5 - C4     - C3
    11     10     12      1    1.2001e+02    4.0551e+02 ;     H4 - C5     - C4
    12     14     15      1    1.2014e+02    5.4091e+02 ;     C4 - C3     - C7
    13     12     14      1    1.2001e+02    4.0551e+02 ;     H3 - C4     - C3
    14     15     16      1    1.2344e+02    5.7463e+02 ;     C3 - C7     - O2
    14     15     17      1    1.2344e+02    5.7463e+02 ;     C3 - C7     - O1
    16     15     17      1    1.3038e+02    6.5413e+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     0.00000     0.00000    14.64400     0.00000     0.00000
0.00000 ;     C2-    C1-    N1-    H5
     1      3      4      6      3     0.00000     0.00000    14.64400     0.00000     0.00000
0.00000 ;     C2-    C1-    N1-    H6
     1      3      4      7      3     0.00000     0.00000    14.64400     0.00000     0.00000
0.00000 ;     C2-    C1-    N1-    H7
     1      3      8      9      3    30.33400     0.00000   -30.33400     0.00000     0.00000
0.00000 ;     C2-    C1-    C6-    H1
     1      3      8     10      3    30.33400     0.00000   -30.33400     0.00000     0.00000
0.00000 ;     C2-    C1-    C6-    C5
     1     14     12     10      3    30.33400     0.00000   -30.33400     0.00000     0.00000
0.00000 ;     C2-    C3-    C4-    C5
     1     14     12     13      3    30.33400     0.00000   -30.33400     0.00000     0.00000
0.00000 ;     C2-    C3-    C4-    H3
     1     14     15     16      3     8.36800     0.00000    -8.36800     0.00000     0.00000
0.00000 ;     C2-    C3-    C7-    O2
     1     14     15     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      8      3    30.33400     0.00000   -30.33400     0.00000     0.00000
0.00000 ;     H2-    C2-    C1-    C6
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     2       1      14      12       3   30.33400     0.00000   -30.33400     0.00000     0.00000
0.00000 ;     H2-    C2-     C3-     C4
     2       1      14      15       3   30.33400     0.00000   -30.33400     0.00000     0.00000
0.00000 ;     H2-    C2-     C3-     C7
     3       1      14      12       3   30.33400     0.00000   -30.33400     0.00000     0.00000
0.00000 ;     C1-    C2-     C3-     C4
     3       1      14      15       3   30.33400     0.00000   -30.33400     0.00000     0.00000
0.00000 ;     C1-    C2-     C3-     C7
     3       8      10      11       3   30.33400     0.00000   -30.33400     0.00000     0.00000
0.00000 ;     C1-    C6-     C5-     H4
     3       8      10      12       3   30.33400     0.00000   -30.33400     0.00000     0.00000
0.00000 ;     C1-    C6-     C5-     C4
     4       3       8       9       3   30.33400     0.00000   -30.33400     0.00000     0.00000
0.00000 ;     N1-    C1-     C6-     H1
     4       3       8      10       3   30.33400     0.00000   -30.33400     0.00000     0.00000
0.00000 ;     N1-    C1-     C6-     C5
     5       4       3       8       3    0.00000     0.00000    14.64400     0.00000     0.00000
0.00000 ;     H5-    N1-     C1-     C6
     6       4       3       8       3    0.00000     0.00000    14.64400     0.00000     0.00000
0.00000 ;     H6-    N1-     C1-     C6
     7       4       3       8       3    0.00000     0.00000    14.64400     0.00000     0.00000
0.00000 ;     H7-    N1-     C1-     C6
     8      10      12      13       3   30.33400     0.00000   -30.33400     0.00000     0.00000
0.00000 ;     C6-    C5-     C4-     H3
     8      10      12      14       3   30.33400     0.00000   -30.33400     0.00000     0.00000
0.00000 ;     C6-    C5-     C4-     C3
     9       8      10      11       3   30.33400     0.00000   -30.33400     0.00000     0.00000
0.00000 ;     H1-    C6-     C5-     H4
     9       8      10      12       3   30.33400     0.00000   -30.33400     0.00000     0.00000
0.00000 ;     H1-    C6-     C5-     C4
    10      12      14      15       3   30.33400     0.00000   -30.33400     0.00000     0.00000
0.00000 ;     C5-    C4-     C3-     C7
    11      10      12      13       3   30.33400     0.00000   -30.33400     0.00000     0.00000
0.00000 ;     H4-    C5-     C4-     H3
    11      10      12      14       3   30.33400     0.00000   -30.33400     0.00000     0.00000
0.00000 ;     H4-    C5-     C4-     C3
    12      14      15      16       3    8.36800     0.00000    -8.36800     0.00000     0.00000
0.00000 ;     C4-    C3-     C7-     O2
    12      14      15      17       3    8.36800     0.00000    -8.36800     0.00000     0.00000
0.00000 ;     C4-    C3-     C7-     O1
    13      12      14      15       3   30.33400     0.00000   -30.33400     0.00000     0.00000
0.00000 ;     H3-    C4-     C3-     C7
    14       1       3       4       3   30.33400     0.00000   -30.33400     0.00000     0.00000
0.00000 ;     C3-    C2-     C1-     N1
    14       1       3       8       3   30.33400     0.00000   -30.33400     0.00000     0.00000
0.00000 ;     C3-    C2-     C1-     C6

[ dihedrals ] ; impropers
; treated as propers in GROMACS to use correct AMBER analytical function
;    i      j      k      l   func   phase     kd      pn
     1      8      3      4      1   180.00   4.60240   2 ;     C2-    C6-    C1-    N1
     2      1     14      3      1   180.00   4.60240   2 ;     H2-    C2-    C3-    C1
     3     10      8      9      1   180.00   4.60240   2 ;     C1-    C5-    C6-    H1
     8     12     10     11      1   180.00   4.60240   2 ;     C6-    C4-    C5-    H4
    10     14     12     13      1   180.00   4.60240   2 ;     C5-    C3-    C4-    H3
    14     16     15     17      1   180.00   4.60240   2 ;     C3-    O2-    C7-    O1
    15      1     14     12      1   180.00   4.60240   2 ;     C7-    C2-    C3-    C4

[ system ]
 ZMB

[ molecules ]
; Compound        nmols
 ZMB             1
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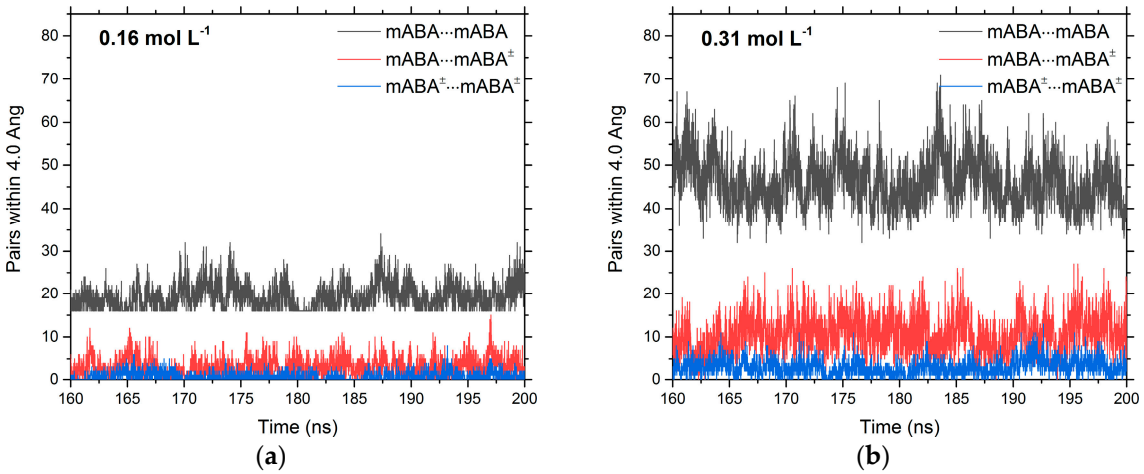
SI.2 Simulations of meta-aminobenzoic acid aqueous solutions

Table SI.2. Details of molecular dynamics simulation.

	Method	no. of mABA molecules	no. of $mABA^+$ molecules	no. of H_2O molecules	Box length (Å)	[mABA] (mol L^{-1})	Simulation time (ps)
1	AIMD	1		210	18.65	0.26	20
2	AIMD	-	1	210	18.7	0.25	20
3	CMD	4	4	11385	69.89	0.04	400000
4	CMD	8	8	11230	69.69	0.08	200000
5	CMD	16	16	11123	69.75	0.16	200000
6	CMD	32	32	11101	69.95	0.31	200000
7	CMD	64	64	11101	70.67	0.60	200000

SI.3 Time evolution of the number of pairs

Figure SI.3.1. Time evolution of the number of pairs between meta-benzoic acid molecules in mixed mABA–mABA± aqueous solutions computed during the last 40 ns of the MD simulations: (**a**) 0.16 mol L^{-1}; (**b**) 0.31 mol L^{-1}.



SI.4 Pairwise interaction matrices of meta-aminobenzoic acid aqueous solutions

Table SI.4.1. Matrix elements p_{ij} of the pairwise interaction matrix for the mixed 0.04 mol L^{-1} mABA–mABA$^{\pm}$ aqueous solutions. Values of p_{ij} expressed as percentage.

	A*	B*	C*	A	B	C
A*	0.2	0.5	7.7	2.0	1.9	2.7
B*		9.4	2.4	0.7	5.7	5.7
C*			0.1	1.9	0.5	3.9
A				6.5	4.7	7.7
B					11.8	15.7
C						8.5

Table SI.4.2. Matrix elements p_{ij} of the pairwise interaction matrix for the mixed 0.16 mol L^{-1} mABA–mABA$^{\pm}$ aqueous solutions. Values of p_{ij} expressed as percentage.

	A*	B*	C*	A	B	C
A*	0.2	0.9	9.3	4.1	3.3	3.6
B*		12.8	3.3	2.4	8.1	6.6
C*			0.3	3.7	1.9	3.0
A				5.0	3.7	6.4
B					6.6	9.1
C						5.6

Table SI.4.3. Matrix elements p_{ij} of the pairwise interaction matrix for the mixed 0.31 mol L^{-1} mABA–mABA$^{\pm}$ aqueous solutions. Values of p_{ij} expressed as percentage.

	A*	B*	C*	A	B	C
A*	0.3	0.7	9.3	4.6	3.5	3.9
B*		9.8	2.8	2.2	7.8	6.9
C*			0.3	3.7	1.7	3.8
A				5.9	4.0	6.3
B					6.5	9.7
C						6.6