Supplementary Material (ESI) for PCCP

The R.E.D. Tools: Advances in RESP and ESP charge derivation and force field library building

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(A)

```
REMARK TITLE Ethanol
REMARK CHARGE-VALUE 0
REMARK MULTIPLICITY-VALUE 1
REMARK
REMARK REORIENT 1 5 8 | 8 5 1
REMARK
ATOM      1 CT1  EOH     1       1.218  -0.218  -0.000       C1
ATOM      2  H1  EOH     1       2.059   0.469  -0.000       H11
ATOM      3  H1  EOH     1       1.287  -0.849   0.879       H12
ATOM      4  H1  EOH     1       1.287  -0.849  -0.879       H13
ATOM      5 CT2  EOH     1      -0.092   0.543   0.000       C2
ATOM      6  H2  EOH     1      -0.152   1.184   0.878       H21
ATOM      7  H2  EOH     1      -0.152   1.184  -0.878       H22
ATOM      8  O3  EOH     1      -1.139  -0.394   0.000       O3
ATOM      9  H3  EOH     1      -1.971   0.058  -0.000       H3
CONECT    1    2    3    4    5
CONECT    2    1
CONECT    3    1
CONECT    4    1
CONECT    5    1    6    7    8
CONECT    6    5
CONECT    7    5
CONECT    8    5    9
CONECT    9    8
END
```

(B)

```
REMARK TITLE g,g_Dimethylphosphate
REMARK CHARGE-VALUE -1
REMARK MULTIPLICITY-VALUE 1
REMARK
REMARK REORIENT 1 6 10 | 10 6 1 | 7 6 8 | 8 6 7
REMARK
REMARK INTER-MCC 0.0 | 1 2 | 10 11 12 13 | 1 2
REMARK INTER-MCC 0.0 | 1 2 | 1 2 3 4 | 3 4
REMARK
REMARK INTER-MEQA 2 3 4 5 | 1 2 3 4  7 8 9 10 11 12 13 14 15 16 17
REMARK
ATOM      1  C1  DMP     1       1.100   0.000   0.000          C1
ATOM      2  H11 DMP     1       0.000   0.000   0.000          H11
ATOM      3  H12 DMP     1       1.476   1.034   0.000          H12
ATOM      4  H13 DMP     1       1.476  -0.484   0.913          H13
ATOM      5  O2  DMP     1       1.524  -0.687  -1.135          O3'
ATOM      6  P3  DMP     1       3.138  -0.847  -1.398          P
ATOM      7  O4  DMP     1       3.811   0.378  -0.942          O1P
ATOM      8  O4  DMP     1       3.281  -1.435  -2.738          O2P
ATOM      9  O6  DMP     1       3.475  -2.001  -0.280          O5'
ATOM     10  C7  DMP     1       3.096  -3.315  -0.544          C2
ATOM     11  H71 DMP     1       2.018  -3.403  -0.661          H21
ATOM     12  H72 DMP     1       3.568  -3.689  -1.444          H22
ATOM     13  H73 DMP     1       3.401  -3.925   0.302          H23
CONECT    1    2    3    4    5
CONECT    2    1
CONECT    3    1
CONECT    4    1
CONECT    5    1    6
CONECT    6    5    7    8    9
CONECT    7    6
CONECT    8    6
CONECT    9    6   10
CONECT   10    9   11   12   13
CONECT   11   10
CONECT   12   10
CONECT   13   10
END
```

(C1)

```
REMARK TITLE O-methyl-tyrosine-dipeptide
REMARK CHARGE-VALUE 0
REMARK MULTIPLICITY-VALUE 1
REMARK
REMARK REORIENT 5 11 12 | 12 11 5 | 6 12 31 | 31 12 6
REMARK
REMARK conformation close to that found in an alpha-helix structure
ATOM      1  CT1 ACE     1      -5.084  -1.603  -0.248          C1
ATOM      2  H1  ACE     1      -4.983  -2.676  -0.108          H11
ATOM      3  H1  ACE     1      -5.962  -1.270   0.287          H12
ATOM      4  H1  ACE     1      -5.206  -1.410  -1.308          H13
ATOM      5  C2  ACE     1      -3.867  -0.910   0.325          C
ATOM      6  O3  ACE     1      -3.846  -0.454   1.432          O
ATOM      7  N4  TYM     2      -2.788  -0.838  -0.506          N
ATOM      8  H4  TYM     2      -2.817  -1.380  -1.341          H
ATOM      9  C5  TYM     2      -1.474  -0.461  -0.004          CA
ATOM     10  H5  TYM     2      -1.267  -0.984   0.919          HA
ATOM     11  C6  TYM     2      -1.377   1.027   0.346          C
ATOM     12  O7  TYM     2      -0.642   1.399   1.215          O
ATOM     13 CT8  TYM     2      -0.430  -0.846  -1.074          CB
ATOM     14  H8  TYM     2      -0.614  -1.883  -1.343          HB1
ATOM     15  H8  TYM     2      -0.614  -0.254  -1.966          HB2
ATOM     16  C9  TYM     2       1.015  -0.703  -0.652          CG
ATOM     17 C100 TYM     2       1.773   0.391  -1.021          CD1
ATOM     18 H100 TYM     2       1.329   1.172  -1.614          HD1
ATOM     19 C100 TYM     2       1.633  -1.689   0.117          CD2
ATOM     20 H100 TYM     2       1.073  -2.559   0.418          HD2
ATOM     21 C111 TYM     2       3.105   0.521  -0.643          CE1
ATOM     22 H111 TYM     2       3.652   1.390  -0.951          HE1
ATOM     23 C111 TYM     2       2.948  -1.579   0.503          CE2
ATOM     24 H111 TYM     2       3.421  -2.340   1.096          HE2
ATOM     25 C14  TYM     2       3.697  -0.466   0.125          CZ
ATOM     26 O15  TYM     2       4.978  -0.448   0.547          OZ
ATOM     27 CT16 TYM     2       5.784   0.658   0.261          CM
ATOM     28 H16  TYM     2       6.742   0.460   0.719          HM1
ATOM     29 H16  TYM     2       5.370   1.569   0.681          HM2
ATOM     30 H16  TYM     2       5.921   0.785  -0.808          HM3
ATOM     31 N17  NME     3      -2.081   1.873  -0.442          N
ATOM     32 H17  NME     3      -2.830   1.482  -0.965          H
ATOM     33 CT18 NME     3      -2.150   3.283  -0.119          C2
ATOM     34 H18  NME     3      -1.152   3.669   0.027          H21
ATOM     35 H18  NME     3      -2.722   3.465   0.785          H22
ATOM     36 H18  NME     3      -2.614   3.808  -0.944          H23
CONECT    1    2    3    4    5
CONECT    2    1
CONECT    3    1
CONECT    4    1
CONECT    5    1    6    7
CONECT    6    5
CONECT    7    5    8    9
CONECT    8    7
CONECT    9    7   10   11   13
CONECT   10    9
CONECT   11    9   12   31
CONECT   12   11
CONECT   13    9   14   15   16
CONECT   14   13
CONECT   15   13
CONECT   16   13   17   19
CONECT   17   16   18   21
CONECT   18   17
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To be continued on the next page...

```
CONECT   19   16   20   23
CONECT   20   19
CONECT   21   17   22   25
CONECT   22   21
CONECT   23   19   24   25
CONECT   24   23
CONECT   25   21   23   26
CONECT   26   25   27
CONECT   27   26   28   29   30
CONECT   28   27
CONECT   29   27
CONECT   30   27
CONECT   31   11   32   33
CONECT   32   31
CONECT   33   31   34   35   36
CONECT   34   33
CONECT   35   33
CONECT   36   33
TER
REMARK conformation close to that found in an beta-sheet structure
ATOM      1  CT1 ACE     1      -0.937   3.565   0.075          C1
ATOM      2  H1  ACE     1       0.045   3.673   0.526          H11
ATOM      3  H1  ACE     1      -1.034   4.295  -0.715          H12
ATOM      4  H1  ACE     1      -1.684   3.750   0.839          H13
ATOM      5  C2  ACE     1      -1.048   2.179  -0.521          C
ATOM      6  O3  ACE     1      -0.766   1.955  -1.667          O
ATOM      7  N4  TYM     2      -1.444   1.214   0.346          N
ATOM      8  H4  TYM     2      -1.825   1.476   1.228          H
ATOM      9  C5  TYM     2      -1.636  -0.160  -0.047          CA
ATOM     10  H5  TYM     2      -1.392  -0.221  -1.096          HA
ATOM     11  C6  TYM     2      -3.093  -0.538   0.205          C
ATOM     12  O7  TYM     2      -3.641  -0.216   1.228          O
ATOM     13 CT8  TYM     2      -0.735  -1.124   0.754          CB
ATOM     14  H8  TYM     2      -1.002  -1.044   1.802          HB1
ATOM     15  H8  TYM     2      -0.973  -2.140   0.450          HB2
ATOM     16  C9  TYM     2       0.744  -0.865   0.574          CG
ATOM     17 C100 TYM     2       1.424  -1.325  -0.540          CD1
ATOM     18 H100 TYM     2       0.897  -1.889  -1.292          HD1
ATOM     19 C100 TYM     2       1.473  -0.148   1.520          CD2
ATOM     20 H100 TYM     2       0.980   0.219   2.403          HD2
ATOM     21 C111 TYM     2       2.779  -1.084  -0.727          CE1
ATOM     22 H111 TYM     2       3.260  -1.461  -1.608          HE1
ATOM     23 C111 TYM     2       2.818   0.101   1.356          CE2
ATOM     24 H111 TYM     2       3.377   0.652   2.090          HE2
ATOM     25 C14  TYM     2       3.483  -0.365   0.225          CZ
ATOM     26 O15  TYM     2       4.799  -0.074   0.151          OZ
ATOM     27 CT16 TYM     2       5.535  -0.480  -0.966          CM
ATOM     28 H16  TYM     2       6.543  -0.124  -0.809          HM1
ATOM     29 H16  TYM     2       5.142  -0.046  -1.880          HM2
ATOM     30 H16  TYM     2       5.552  -1.561  -1.060          HM3
ATOM     31 N17  NME     3      -3.687  -1.285  -0.744          N
ATOM     32 H17  NME     3      -3.237  -1.377  -1.625          H
ATOM     33 CT18 NME     3      -5.073  -1.692  -0.634          C2
ATOM     34 H18  NME     3      -5.751  -0.864  -0.807          H21
ATOM     35 H18  NME     3      -5.257  -2.085   0.355          H22
ATOM     36 H18  NME     3      -5.267  -2.467  -1.363          H23
END
```

(C2)

```
REMARK TITLE O-methyl-tyrosine-dipeptide
REMARK CHARGE-VALUE 0
REMARK MULTIPLICITY-VALUE 1
REMARK
REMARK REORIENT 5 11 12 | 12 11 5 | 6 12 31 | 31 12 6
REMARK
REMARK INTRA-MCC 0.0 |  1  2  3  4  5  6 | R
REMARK INTRA-MCC 0.0 | 31 32 33 34 35 36 | R
REMARK INTRA-MCC -.4157 |  7 | K
REMARK INTRA-MCC  .2719 |  8 | K
REMARK INTRA-MCC  .5973 | 11 | K
REMARK INTRA-MCC -.5679 | 12 | K
REMARK
REMARK conformation close to that found in an alpha-helix structure
ATOM      1  C1  ACE     1      -5.084  -1.603  -0.248           C1
ATOM      2  H11 ACE     1      -4.983  -2.676  -0.108           H11
ATOM      3  H12 ACE     1      -5.962  -1.270   0.287           H12
ATOM      4  H13 ACE     1      -5.206  -1.410  -1.308           H13
ATOM      5  C2  ACE     1      -3.867  -0.910   0.325           C
ATOM      6  O3  ACE     1      -3.846  -0.454   1.432           O
ATOM      7  N4  TYM     2      -2.788  -0.838  -0.506           N
ATOM      8  H4  TYM     2      -2.817  -1.380  -1.341           H
ATOM      9  C5  TYM     2      -1.474  -0.461  -0.004           CA
ATOM     10  H5  TYM     2      -1.267  -0.984   0.919           HA
ATOM     11  C6  TYM     2      -1.377   1.027   0.346           C
ATOM     12  O7  TYM     2      -0.642   1.399   1.215           O
ATOM     13 CT8  TYM     2      -0.430  -0.846  -1.074           CB
ATOM     14  H8  TYM     2      -0.614  -1.883  -1.343           HB1
ATOM     15  H8  TYM     2      -0.614  -0.254  -1.966           HB2
ATOM     16  C9  TYM     2       1.015  -0.703  -0.652           CG
ATOM     17 C100 TYM     2       1.773   0.391  -1.021           CD1
ATOM     18 H100 TYM     2       1.329   1.172  -1.614           HD1
ATOM     19 C100 TYM     2       1.633  -1.689   0.117           CD2
ATOM     20 H100 TYM     2       1.073  -2.559   0.418           HD2
ATOM     21 C111 TYM     2       3.105   0.521  -0.643           CE1
ATOM     22 H111 TYM     2       3.652   1.390  -0.951           HE1
ATOM     23 C111 TYM     2       2.948  -1.579   0.503           CE2
ATOM     24 H111 TYM     2       3.421  -2.340   1.096           HE2
ATOM     25 C14  TYM     2       3.697  -0.466   0.125           CZ
ATOM     26 O15  TYM     2       4.978  -0.448   0.547           OZ
ATOM     27 CT16 TYM     2       5.784   0.658   0.261           CM
ATOM     28 H16  TYM     2       6.742   0.460   0.719           HM1
ATOM     29 H16  TYM     2       5.370   1.569   0.681           HM2
ATOM     30 H16  TYM     2       5.921   0.785  -0.808           HM3
ATOM     31 N17  NME     3      -2.081   1.873  -0.442           N
ATOM     32 H17  NME     3      -2.830   1.482  -0.965           H
ATOM     33 C18  NME     3      -2.150   3.283  -0.119           C2
ATOM     34 H181 NME     3      -1.152   3.669   0.027           H21
ATOM     35 H182 NME     3      -2.722   3.465   0.785           H22
ATOM     36 H183 NME     3      -2.614   3.808  -0.944           H23
CONECT    1    2    3    4    5
CONECT    2    1
CONECT    3    1
CONECT    4    1
CONECT    5    1    6    7
CONECT    6    5
CONECT    7    5    8    9
CONECT    8    7
CONECT    9    7   10   11   13
CONECT   10    9
CONECT   11    9   12   31
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To be continued on the next page...

```
CONECT   12   11
CONECT   13    9   14   15   16
CONECT   14   13
CONECT   15   13
CONECT   16   13   17   19
CONECT   17   16   18   21
CONECT   18   17
CONECT   19   16   20   23
CONECT   20   19
CONECT   21   17   22   25
CONECT   22   21
CONECT   23   19   24   25
CONECT   24   23
CONECT   25   21   23   26
CONECT   26   25   27
CONECT   27   26   28   29   30
CONECT   28   27
CONECT   29   27
CONECT   30   27
CONECT   31   11   32   33
CONECT   32   31
CONECT   33   31   34   35   36
CONECT   34   33
CONECT   35   33
CONECT   36   33
TER
REMARK conformation close to that found in an beta-sheet structure
ATOM      1  C1  ACE     1      -0.937   3.565   0.075           C1
ATOM      2  H11 ACE     1       0.045   3.673   0.526           H11
ATOM      3  H12 ACE     1      -1.034   4.295  -0.715           H12
ATOM      4  H13 ACE     1      -1.684   3.750   0.839           H13
ATOM      5  C2  ACE     1      -1.048   2.179  -0.521           C
ATOM      6  O3  ACE     1      -0.766   1.955  -1.667           O
ATOM      7  N4  TYM     2      -1.444   1.214   0.346           N
ATOM      8  H4  TYM     2      -1.825   1.476   1.228           H
ATOM      9  C5  TYM     2      -1.636  -0.160  -0.047           CA
ATOM     10  H5  TYM     2      -1.392  -0.221  -1.096           HA
ATOM     11  C6  TYM     2      -3.093  -0.538   0.205           C
ATOM     12  O7  TYM     2      -3.641  -0.216   1.228           O
ATOM     13 CT8  TYM     2      -0.735  -1.124   0.754           CB
ATOM     14  H8  TYM     2      -1.002  -1.044   1.802           HB1
ATOM     15  H8  TYM     2      -0.973  -2.140   0.450           HB2
ATOM     16  C9  TYM     2       0.744  -0.865   0.574           CG
ATOM     17 C100 TYM     2       1.424  -1.325  -0.540           CD1
ATOM     18 H100 TYM     2       0.897  -1.889  -1.292           HD1
ATOM     19 C100 TYM     2       1.473  -0.148   1.520           CD2
ATOM     20 H100 TYM     2       0.980   0.219   2.403           HD2
ATOM     21 C111 TYM     2       2.779  -1.084  -0.727           CE1
ATOM     22 H111 TYM     2       3.260  -1.461  -1.608           HE1
ATOM     23 C111 TYM     2       2.818   0.101   1.356           CE2
ATOM     24 H111 TYM     2       3.377   0.652   2.090           HE2
ATOM     25 C14  TYM     2       3.483  -0.365   0.225           CZ
ATOM     26 O15  TYM     2       4.799  -0.074   0.151           OZ
ATOM     27 CT16 TYM     2       5.535  -0.480  -0.966           CM
ATOM     28 H16  TYM     2       6.543  -0.124  -0.809           HM1
ATOM     29 H16  TYM     2       5.142  -0.046  -1.880           HM2
ATOM     30 H16  TYM     2       5.552  -1.561  -1.060           HM3
ATOM     31 N17  NME     3      -3.687  -1.285  -0.744           N
ATOM     32 H17  NME     3      -3.237  -1.377  -1.625           H
ATOM     33 C18  NME     3      -5.073  -1.692  -0.634           C2
ATOM     34 H181 NME     3      -5.751  -0.864  -0.807           H21
ATOM     35 H182 NME     3      -5.257  -2.085   0.355           H22
ATOM     36 H183 NME     3      -5.267  -2.467  -1.363           H23
END
```

Figure S1. Examples of P2N input files used by the R.E.D. program. (A) P2N input file used in charge derivation of the ethanol molecule (two molecular orientations and a single molecule conformation). (B) P2N input file used in charge derivation of the dimethylphosphate molecule (four molecular orientations and a single molecule conformation) involved in the FFTopDB building for deoxyribonucleic acid. (C1) P2N input file used in charge derivation of the *N*-acetyl-*O*-methyl-*L*-tyrosine-*N'*-methylamide dipeptide (four molecular orientations and two molecule conformations). (C2) P2N input file used in charge derivation of the central fragment of *N*-acetyl-*O*-methyl-*L*-tyrosine-*N'*-methylamide dipeptide (four molecular orientations and two molecular conformations). Detailed descriptions of the P2N file format associated with the R.E.D. Tools is available in a specific tutorial.[64]

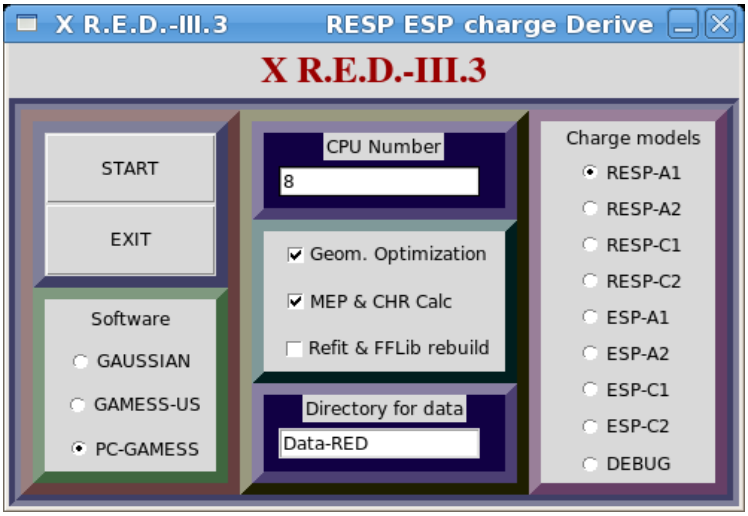

Figure S2. Screen snapshot of the X R.E.D. graphical interface.

Molecule	Proc. [a]	QM P. [b]	Step 1 [c]	Step 2 [d]	Step 2	Step 2	Step 3 [e]	R.E.DD.B.
name			T.L. [f]	T.L.	Surf. [g]	R.A. [h]	Fit [i]	code [j]
Dimethylsulfoxide	1 conf - 1 orient	GAMESS	HF/6-31G*	HF/6-31G*	Connolly	QMRA	2 RESP stg	W-1
Dimethylsulfoxide	1 conf - 1 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	QMRA	2 RESP stg	W-2
Dimethylsulfoxide	1 conf - 1 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-3
Dimethylsulfoxide	1 conf - 2 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-4
Ethanol	1 conf[a1] - 1 orient	GAMESS	HF/6-31G*	HF/6-31G*	Connolly	QMRA	2 RESP stg	W-5
Ethanol	1 conf[a1] - 1 orient	GAMESS	HF/6-31G*	HF/6-31G*	Connolly	QMRA	2 RESP stg	W-6
Ethanol	1 conf[a1] - 1 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	QMRA	2 RESP stg	W-7
Ethanol	1 conf[a1] - 1 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	QMRA	2 RESP stg	W-8
Ethanol	1 conf[a1] - 2 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-9
Ethanol	2 conf[a2] - 4 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-10
Dimethylphosphate	1 conf[a3] - 1 orient	GAMESS	HF/6-31G*	HF/6-31G*	Connolly	QMRA	2 RESP stg	W-11
Dimethylphosphate	1 conf[a3] - 1 orient	GAMESS	HF/6-31G*	HF/6-31G*	Connolly	QMRA	2 RESP stg	W-12
Dimethylphosphate	1 conf[a3] - 1 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	QMRA	2 RESP stg	W-13
Dimethylphosphate	1 conf[a3] - 1 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	QMRA	2 RESP stg	W-14
Trifluoroethanol	1 conf[a1] - 2 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-15
Trifluoroethanol	2 conf[a2] - 4 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-16
Methoxyethane	1 conf[a1] - 2 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-17
Methoxyethane	1 conf[a4] - 2 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-18
Methoxyethane	2 conf[a2] - 4 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-19
N-Methylacetamide	1 conf[a5] - 2 orient	g98	B3LYP/6-311++G**	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-20
N-Methylacetamide	1 conf[a6] - 2 orient	g98	B3LYP/6-311++G**	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-21
N-Methylacetamide	2 conf[a7] - 4 orient	g98	B3LYP/6-311++G**	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-22
1,4-Dioxane	1 conf[a8] - 2 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-23
1,4-Dioxane	1 conf[a9] - 2 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-24
1,4-Dioxane	2 conf[a10] - 4 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-25
Ethane-1,2-diol	1 conf[a11] - 2 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-26
Ethane-1,2-diol	1 conf[a12] - 2 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-27
Ethane-1,2-diol	1 conf[a13] - 2 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-28
Ethane-1,2-diol	1 conf[a14] - 2 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-29
Ethane-1,2-diol	1 conf[a15] - 2 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-30
Ethane-1,2-diol	5 conf[a16] - 4 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-31

Molecule	**Proc.** [a]	**QM P.** [b]	**Step 1** [c]	**Step 2** [d]	**Step 2**	**Step 2**	**Step 3** [e]	**R.E.DD.B.**
name			**T.L.** [f]	**T.L.**	**Surf.** [g]	**R.A.** [h]	**Fit** [i]	**code** [j]
Methanol	1 conf - 2 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-32
Propanone	1 conf - 4 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-33
Ethanoic acid	1 conf - 4 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-34
Acetonitrile	1 conf - 2 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-35
Formamide	1 conf - 2 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-36
Methanal	1 conf - 2 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-37
Furane	1 conf - 4 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-38
Pyrrole	1 conf - 4 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-39
Benzene	1 conf - 4 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-40
Toluene	1 conf - 4 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-41
Choroforme	1 conf - 2 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-42
Cyclohexane	1 conf[a8] - 2 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-43
Cyclohexane	1 conf[a9] - 2 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-44
Cyclohexane	2 conf[a10] - 4 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-45
Organic solvent 10 molecules[m1]	1 conf - 2 & 4 orient[a17]	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-46
Organic solvent 10 molecules[m1]	1 conf - 2 & 4 orient[a17]	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	2 RESP stg	W-47
Organic solvent 10 molecules[m1]	1 conf - 2 & 4 orient[a17]	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	ESP	W-48
Organic solvent 10 molecules[m1]	1 conf - 2 ; 4 orient[a17]	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	ESP	W-49
N-ACE-*L*-ALA-*N'*-NME	1 conf [a18]- 1 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-50
N-ACE-*L*-ALA-*N'*-NME	1 conf [a18]- 1 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-51
N-ACE-*L*-ALA-*N'*-NME	1 conf [a18]- 1 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-52
N-ACE-*L*-ALA-*N'*-NME	1 conf [a18]- 1 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-53
N-ACE-*L*-ALA-*N'*-NME	1 conf [a18]- 4 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-54
N-ACE-*L*-ALA-*N'*-NME	1 conf [a18]- 10 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-55
N-ACE-*L*-ALA-*N'*-NME	1 conf [a19]- 10 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-56
N-ACE-*L*-ALA-*N'*-NME	1 conf [a20]- 10 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-57

Molecule	**Proc.** [a]	**QM P.** [b]	**Step 1** [c]	**Step 2** [d]	**Step 2**	**Step 2**	**Step 3** [e]	**R.E.DD.B.**
name			**T.L.** [f]	**T.L.**	**Surf.** [g]	**R.A.** [h]	**Fit** [i]	**code** [j]
N-ACE-*L*-ALA-*N'*-NME	3 conf [a21]- 10 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-58
N-ACE-*L*-ALA-*N'*-NME	3 conf [a21]- 10 orient	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	2 RESP stg	W-59
N-ACE-*L*-ALA-*N'*-NME	3 conf [a21]- 10 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	ESP	W-60
N-ACE-*L*-ALA-*N'*-NME	3 conf [a21]- 10 orient	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	ESP	W-61
Deoxyadenosine	1 conf [a22]- 12 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-62
Deoxyadenosine	1 conf [a23]- 12 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-63
Deoxyadenosine	2 conf [a24]- 12 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-64
Deoxyadenosine	2 conf [a24]- 12 orient	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	2 RESP stg	W-65
Deoxyadenosine	2 conf [a24]- 12 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	ESP	W-66
Deoxyadenosine	2 conf [a24]- 12 orient	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	ESP	W-67
Deoxyadenosine	2 conf [a24]- 12 orient	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	1 RESP stg	W-68
DNA Nucleosides[m2] 4 molecules	2 conf [a24]- 6 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-69
DNA Nucleosides[m2] 4 molecules	2 conf [a24]- 6 orient	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	2 RESP stg	W-70
DNA Nucleosides[m2] 4 molecules	2 conf [a24]- 6 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	ESP	W-71
DNA Nucleosides[m2] 4 molecules	2 conf [a24]- 6 orient	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	ESP	W-72
DNA Nucleosides[m2] 4 molecules	2 conf [a24]- 6 orient	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	1 RESP stg	W-73
RNA Nucleosides[m3] 4 molecules	1 conf [a23]- 6 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	W-74
RNA Nucleosides[m3] 4 molecules	1 conf [a23]- 6 orient	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	2 RESP stg	W-75
RNA Nucleosides[m3] 4 molecules	1 conf [a23]- 6 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	ESP	W-76
RNA Nucleosides[m3] 4 molecules	1 conf [a23]- 6 orient	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	ESP	W-77
RNA Nucleosides[m3] 4 molecules	1 conf [a23]- 6 orient	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	1 RESP stg	W-78

Molecule	**Proc.** [a]	**QM P.** [b]	**Step 1** [c]	**Step 2** [d]	**Step 2**	**Step 2**	**Step 3** [e]	**R.E.DD.B.**
name			**T.L.** [f]	**T.L.**	**Surf.** [g]	**R.A.** [h]	**Fit** [i]	**code** [j]
N-ACE-AIB-*N*'-NME[m4]	1 conf [a25]- 4 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	F-1
N-ACE-AIB-*N*'-NME[m4]	1 conf [a26]- 4 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	F-2
N-ACE-AIB-*N*'-NME[m4]	2 conf [a27]- 4 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	F-3
N-ACE-AIB-*N*'-NME[m4]	2 conf [a27]- 4 orient	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	2 RESP stg	F-4
N-ACE-AIB-*N*'-NME[m4]	2 conf [a27]- 4 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	ESP	F-5
N-ACE-AIB-*N*'-NME[m4]	2 conf [a27]- 4 orient	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	ESP	F-6
Methylammonium[m5] *N*-ACE-AIB-*N*'-NME	1 conf - 2 orient 2 conf [a27]- 4 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	F-7
Methylammonium[m5] *N*-ACE-AIB-*N*'-NME	1 conf - 2 orient 2 conf [a27]- 4 orient	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	2 RESP stg	F-8
Methylammonium[m5] *N*-ACE-AIB-*N*'-NME	1 conf - 2 orient 2 conf [a27]- 4 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	ESP	F-9
Methylammonium[m5] *N*-ACE-AIB-*N*'-NME	1 conf - 2 orient 2 conf [a27]- 4 orient	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	ESP	F-10
Ethanoate[m6] *N*-ACE-AIB-*N*'-NME	1 conf - 2 orient 2 conf [a27]- 4 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	F-11
Ethanoate[m6] *N*-ACE-AIB-*N*'-NME	1 conf - 2 orient 2 conf [a27]- 4 orient	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	2 RESP stg	F-12
Ethanoate[m6] *N*-ACE-AIB-*N*'-NME	1 conf - 2 orient 2 conf [a27]- 4 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	ESP	F-13
Ethanoate[m6] *N*-ACE-AIB-*N*'-NME	1 conf - 2 orient 2 conf [a27]- 4 orient	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	ESP	F-14
Methylamine[m7] *N*-ACE-AIB-*N*'-NME	1 conf - 2 orient 2 conf [a27]- 4 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	F-15
Methylamine[m7] *N*-ACE-AIB-*N*'-NME	1 conf - 2 orient 2 conf [a27]- 4 orient	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	2 RESP stg	F-16
Methylamine[m7] *N*-ACE-AIB-*N*'-NME	1 conf - 2 orient 2 conf [a27]- 4 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	ESP	F-17
Methylamine[m7] *N*-ACE-AIB-*N*'-NME	1 conf - 2 orient 2 conf [a27]- 4 orient	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	ESP	F-18

Molecule	Proc. [a]	QM P. [b]	Step 1 [c]	Step 2 [d]	Step 2	Step 2	Step 3 [e]	R.E.DD.B.
name			T.L. [f]	T.L.	Surf. [g]	R.A. [h]	Fit [i]	code [j]
Ethanoic acid[(m8)] *N*-ACE-AIB-*N'*-NME	1 conf - 2 orient 2 conf [(a27)]- 4 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	F-19
Ethanoic acid[(m8)] *N*-ACE-AIB-*N'*-NME	1 conf - 2 orient 2 conf [(a27)]- 4 orient	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	2 RESP stg	F-20
Ethanoic acid[(m8)] *N*-ACE-AIB-*N'*-NME	1 conf - 2 orient 2 conf [(a27)]- 4 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	ESP	F-21
Ethanoic acid[(m8)] *N*-ACE-AIB-*N'*-NME	1 conf - 2 orient 2 conf [(a27)]- 4 orient	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	ESP	F-22
N-ACE-*L*-TYM-*N'*-NME[(m9)]	1 conf [(a25)]- 4 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	F-23
N-ACE-*L*-TYM-*N'*-NME[(m9)]	1 conf [(a26)]- 4 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	F-24
N-ACE-*L*-TYM-*N'*-NME[(m9)]	2 conf [(a27)]- 4 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	F-25
N-ACE-*L*-TYM-*N'*-NME[(m9)]	2 conf [(a27)]- 4 orient	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	2 RESP stg	F-26
N-ACE-*L*-TYM-*N'*-NME[(m9)]	2 conf [(a27)]- 4 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	ESP	F-27
N-ACE-*L*-TYM-*N'*-NME[(m9)]	2 conf [(a27)]- 4 orient	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	ESP	F-28
Methylammonium[(m10)] *N*-ACE-*L*-TYM-*N'*-NME	1 conf - 2 orient 2 conf [(a27)]- 4 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	F-29
Methylammonium[(m10)] *N*-ACE-*L*-TYM-*N'*-NME	1 conf - 2 orient 2 conf [(a27)]- 4 orient	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	2 RESP stg	F-30
Methylammonium[(m10)] *N*-ACE-*L*-TYM-*N'*-NME	1 conf - 2 orient 2 conf [(a27)]- 4 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	ESP	F-31
Methylammonium[(m10)] *N*-ACE-*L*-TYM-*N'*-NME	1 conf - 2 orient 2 conf [(a27)]- 4 orient	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	ESP	F-32
Ethanoate[(m11)] *N*-ACE-*L*-TYM-*N'*-NME	1 conf - 2 orient 2 conf [(a27)]- 4 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	F-33
Ethanoate[(m11)] *N*-ACE-*L*-TYM-*N'*-NME	1 conf - 2 orient 2 conf [(a27)]- 4 orient	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	2 RESP stg	F-34
Ethanoate[(m11)] *N*-ACE-*L*-TYM-*N'*-NME	1 conf - 2 orient 2 conf [(a27)]- 4 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	ESP	F-35
Ethanoate[(m11)] *N*-ACE-*L*-TYM-*N'*-NME	1 conf - 2 orient 2 conf [(a27)]- 4 orient	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	ESP	F-36

Molecule	Proc. [a]	QM P. [b]	Step 1 [c]	Step 2 [d]	Step 2	Step 2	Step 3 [e]	R.E.DD.B.
name			T.L. [f]	T.L.	Surf. [g]	R.A. [h]	Fit [i]	code [j]
Methylamine[m12] *N*-ACE-*L*-TYM-*N*'-NME	1 conf - 2 orient 2 conf [a27]- 4 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	F-37
Methylamine[m12] *N*-ACE-*L*-TYM-*N*'-NME	1 conf - 2 orient 2 conf [a27]- 4 orient	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	2 RESP stg	F-38
Methylamine[m12] *N*-ACE-*L*-TYM-*N*'-NME	1 conf - 2 orient 2 conf [a27]- 4 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	ESP	F-39
Methylamine[m12] *N*-ACE-*L*-TYM-*N*'-NME	1 conf - 2 orient 2 conf [a27]- 4 orient	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	ESP	F-40
Ethanoic acid[m13] *N*-ACE-*L*-TYM-*N*'-NME	1 conf - 2 orient 2 conf [a27]- 4 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	F-41
Ethanoic acid[m13] *N*-ACE-*L*-TYM-*N*'-NME	1 conf - 2 orient 2 conf [a27]- 4 orient	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	2 RESP stg	F-42
Ethanoic acid[m13] *N*-ACE-*L*-TYM-*N*'-NME	1 conf - 2 orient 2 conf [a27]- 4 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	ESP	F-43
Ethanoic acid[m13] *N*-ACE-*L*-TYM-*N*'-NME	1 conf - 2 orient 2 conf [a27]- 4 orient	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	ESP	F-44
DNA FFTopDB 5 molecules[m14]	1 conf [a3]- 4 orient 2 conf [a24]- 6 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	F-45
DNA FFTopDB 5 molecules[m14]	1 conf [a3]- 4 orient 2 conf [a24]- 6 orient	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	2 RESP stg	F-46
DNA FFTopDB 5 molecules[m14]	1 conf [a3]- 4 orient 2 conf [a24]- 6 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	ESP	F-47
DNA FFTopDB 5 molecules[m14]	1 conf [a3]- 4 orient 2 conf [a24]- 6 orient	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	ESP	F-48
DNA FFTopDB 5 molecules[m14]	1 conf [a3]- 4 orient 2 conf [a24]- 6 orient	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	1 RESP stg	F-49
DNA FFTopDB 5 molecules[m15]	1 conf [a3]- 4 orient 2 conf [a24]- 6 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	F-50

Molecule	Proc. [a]	QM P. [b]	Step 1 [c]	Step 2 [d]	Step 2	Step 2	Step 3 [e]	R.E.DD.B.
name			T.L. [f]	T.L.	Surf. [g]	R.A. [h]	Fit [i]	code [j]
RNA FFTopDB 5 molecules[m16]	1 conf [a3]- 4 orient 1 conf [a23]- 6 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	F-51
RNA FFTopDB 5 molecules[m16]	1 conf [a3]- 4 orient 1 conf [a23]- 6 orient	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	2 RESP stg	F-52
RNA FFTopDB 5 molecules[m16]	1 conf [a3]- 4 orient 1 conf [a23]- 6 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	ESP	F-53
RNA FFTopDB 5 molecules[m16]	1 conf [a3]- 4 orient 1 conf [a23]- 6 orient	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	ESP	F-54
RNA FFTopDB 5 molecules[m16]	1 conf [a3]- 4 orient 1 conf [a23]- 6 orient	g98	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	1 RESP stg	F-55
RNA FFTopDB 5 molecules[m17]	1 conf [a3]- 4 orient 1 conf [a23]- 6 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	F-56
NA FFTopDB 9 molecules[m18]	1 conf [a3]- 4 orient 2 conf [a24]- 6 orient 1 conf [a23]- 6 orient	g98	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	F-60
New AA frag 18 molecules[m19]	2 or 4 orient 1 and/or 2 conf [a25,a26,a27]	g03	HF/6-31G*	HF/6-31G*	Connolly	RBRA	1 ESP stg	F-73
New AA frag 18 molecules[m19]	2 or 4 orient 1 and/or 2 conf [a25,a26,a27]	g03	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	F-74
New AA frag 18 molecules[m20]	2 or 4 orient 1 and/or 2 conf [a25,a26,a27]	g03	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	F-75
New AA frag 18 molecules[m21]	2 or 4 orient 1 and/or 2 conf [a25,a26,a27]	g03	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	F-76
New AA frag 18 molecules[m22]	2 or 4 orient 1 and/or 2 conf [a25,a26,a27]	g03	HF/6-31G*	HF/6-31G*	Connolly	RBRA	2 RESP stg	F-77
New AA frag 18 molecules[m19]	2 or 4 orient 1 and/or 2 conf [a25,a26,a27]	g03	HF/6-31G*	B3LYP/cc-pVTZ	Connolly	RBRA	2 RESP stg	F-78
New AA frag 18 molecules[m20]	2 or 4 orient 1 and/or 2 conf [a25,a26,a27]	g03	HF/6-31G*	B3LYP/cc-pVTZ	Connolly	RBRA	2 RESP stg	F-79
New AA frag 18 molecules[m19]	2 or 4 orient 1 and/or 2 conf [a25,a26,a27]	g03	HF/6-31G*	HF/6-31G*	CHELPG	RBRA	2 RESP stg	F-80

Table S3. Summary of charge derivations reported in this work, and available in R.E.DD.B.[59,60,64,72] Charge values were derived from charge fitting and not arithmetic mean. When not specified all-atom force field libraries were generated. [(a)] Charge derivation procedures involving a fully characterized number of molecular orientation(s) and conformation(s) for each reported molecular system; conf = molecular conformation; orient = molecular orientation. [(b)] QM P. = QM programs used in the geometry optimization and MEP computation steps (GAMESS-US, Gaussian 98 or 03 was interfaced). [(c)] Step 1 = First step of the charge derivation *i. e.* geometry optimization (for each molecule *i* conformations might be considered). [(d)] Step 2 = Second step of the charge derivation *i. e.* MEP computation (for each molecule, *i* conformation * *j* orientation MEP computations might be considered). [(e)] Step 3 = Third and last step of the charge derivation *i. e.* charge fitting. [(f)] T.L. = QM theory levels used in Steps 1 and 2. [(g)] Surface or grid algorithms on which is computed each MEP (the Connolly surface and CHELPG algorithms were both used). [(h)] R.A. = Re-orientation algorithm applied before MEP computation; both QMRA and RBRA approaches were used. [(i)] Fit = Charge fitting approach carried out in Step 3; 2 RESP stg = 2 stage RESP fitting; 1 RESP stg = 1 stage RESP fitting; ESP = 1 stage ESP fitting. [(j)] R.E.DD.B. code. [(a1)] = *anti* conformation. [(a2)] = *anti* and *gauche+* conformations. [(a3)] = *gauche+*, *gauche+* conformation. [(a4)] = *gauche+* conformation. [(a5)] = *cis* conformation. [(a6)] = *trans* conformation. [(a7)] = *cis* and *trans* conformations. [(a8)] = *chair* conformation. [(a9)] = *twist-boat* conformation. [(a10)] = *chair* and *twist-boat* conformations. [(a11)] = *anti anti anti* conformation. [(a12)] = *anti gauche+ anti* conformation. [(a13)] = *gauche+ anti gauche-* conformation. [(a14)] = *gauche+ gauche- gauche+* conformation. [(a15)] = *gauche+ gauche+ gauche+* conformation. [(a16)] = *anti anti anti, anti gauche+ anti, gauche+ anti gauche-, gauche+ gauche- gauche+, gauche+ gauche+ gauche+* conformations. [(a17)] 2 or 4 molecular orientations were used in the charge derivation. [(a18)] = *C5* conformation. [(a19)] = *C7ax* conformation. [(a20)] = *C7eq* conformation. [(a21)] = *C5*, *C7ax* and *C7eq* conformations. [(a22)] = *C2'endo* conformation. [(a23)] = *C3'endo* conformation. [(a24)] = *C2'endo* and *C3'endo* conformations. [(a25)] = conformation close to the alpha helix form. [(a26)] = conformation close to the extended form. [(a27)] = conformations close to the alpha helix and extended forms. [(m1)] = Charge derivation involving 10 solvent molecules (Dimethylsulfoxide, Ethanol, Trifluoroethanol, Methanol, Acetone, Acetic acid, Acetonitrile, Benzene, Toluene and Chloroform). [(m2)] = Charge derivation involving the 4 regular DNA nucleosides (Deoxyadenosine, Deoxycytidine, Deoxyguanosine and Deoxythymidine). [(m3)] = Charge derivation involving the 4 regular RNA nucleosides (Adenosine, Cytidine, Guanosine and Uridine). [(m4)] = Charge derivation of the central fragment of alpha-aminoisobutyric acid. [(m5)] = Charge derivation of the *N*-terminal charged fragment of alpha-aminoisobutyric acid. [(m6)] = Charge derivation of the *C*-terminal charged fragment of alpha-aminoisobutyric acid. [(m7)] = Charge derivation of the *N*-terminal neutral fragment of alpha-aminoisobutyric acid. [(m8)] = Charge derivation of the *C*-terminal neutral fragment of alpha-aminoisobutyric acid. [(m9)] = Charge derivation of the central fragment of *O*-methyl-*L*-tyrosine. [(m10)] = Charge derivation of the *N*-terminal charged fragment of *O*-methyl-*L*-tyrosine. [(m11)] = Charge derivation of the *C*-terminal charged fragment of *O*-methyl-*L*-tyrosine. [(m12)] = Charge derivation of the *N*-terminal neutral fragment of *O*-methyl-*L*-tyrosine. [(m13)] = Charge derivation of the *C*-terminal neutral fragment of *O*-methyl-*L*-tyrosine. [(m14)] = FFTopDB constituted of 16 molecular fragments for deoxyribonucleic acid based on a charge derivation involving the 5 DNA nucleosides and dimethylphosphate. [(m15)] = FFTopDB constituted of 16 molecular fragments for deoxyribonucleic acid based on a charge derivation involving

the 5 DNA nucleosides and dimethylphosphate (fragment topology differs in the phosphate connection). (m16) = FFTopDB constituted of 16 molecular fragments ribonucleic acid based on a charge derivation involving the 5 RNA nucleosides and dimethylphosphate. (m17) = FFTopDB constituted of 16 molecular fragments for ribonucleic acid based on a charge derivation involving the 5 RNA nucleosides and dimethylphosphate (fragment topology differs in the phosphate connection). (m18) = FFTopDB constituted of 32 molecular fragments for nucleic acids based on a charge derivation involving 9 molecules (the regular DNA and RNA nucleosides and dimethylphosphate). (m19) = Simultaneous charge derivation of the central, *N*-terminal and *C*-terminal fragment of *O*-methyl-*L*-tyrosine and the *N*-acetyl-*O*-methyl-*L*-tyrosine-*N'*-methylamide dipeptide involving 18 molecules. (m20) = Simultaneous charge derivation of the central, *N*-terminal and *C*-terminal fragment of *O*-methyl-*L*-tyrosine and the *N*-acetyl-*O*-methyl-*L*-tyrosine-*N'*-methylamide dipeptide involving 18 molecules. United-methylene and methyl carbon force field libraries were generated by setting to a value of zero the charge value of each selected hydrogen atom during the charge fitting step, and by removing the corresponding hydrogen(s) from each force field library. (m21) = Simultaneous charge derivation of the central, *N*-terminal and *C*-terminal fragment of *O*-methyl-*L*-tyrosine and the *N*-acetyl-*O*-methyl-*L*-tyrosine-*N'*-methylamide dipeptide involving 18 molecules. United-carbon force field libraries were generated by summing the charge values of each hydrogen within the charge value of the carbon they are bound to *a posteriori* to the charge fitting step, and by removing the corresponding hydrogen(s) from each force field library. (m22) = Simultaneous charge derivation of the central, *N*-terminal and *C*-terminal fragment of *O*-methyl-*L*-tyrosine and the *N*-acetyl-*O*-methyl-*L*-tyrosine-*N'*-methylamide dipeptide involving 18 molecules. United-methylene and methyl carbon force field libraries were generated by summing the charge values of each hydrogen within the charge value of the carbon they are bound to *a posteriori* to the charge fitting step, and by removing the corresponding hydrogen(s) from each force field library.

Orient.nb [a]	**-A-**	**-B-**	**-C-**	**-D-**	**MCVD**	**-A-**	**-B-**	**-C-**	**-D-**	**MCVD**
Surf [b]	**CS**	**CS**	**CS**	**CS**	**CS**	**CG**	**CG**	**CG**	**CG**	**CG**
ACE-C1	-0.6678	-0.6661	-0.6902	-0.7098	0.044	-0.4875	-0.4998	-0.4841	-0.4835	0.016
ACE-H11	0.1805	0.1783	0.1857	0.1902	-	0.1301	0.1333	0.1288	0.1293	-
ACE-H12	= H11	= H11	= H11	= H11	-	= H11	= H11	= H11	= H11	-
ACE-H13	= H11	= H11	= H11	= H11	-	= H11	= H11	= H11	= H11	-
ACE-C	0.8574	0.8792	0.8736	0.8878	0.030	0.8819	0.8823	0.8841	0.8720	0.012
ACE-O	-0.6257	-0.6284	-0.6281	-0.6303	0.005	-0.6425	-0.6410	-0.6426	-0.6388	0.004
ALA-N	-0.6149	-0.6313	-0.6312	-0.6489	0.034	-0.7077	-0.7021	-0.7147	-0.6936	0.021
ALA-H	0.2920	0.3022	0.2938	0.3010	-	0.3084	0.3086	0.3103	0.3056	-
ALA-CA	0.2248	0.1467	0.2402	0.2448	0.098	0.2583	0.2430	0.2725	0.2437	0.030
ALA-HA	0.0111	0.0289	0.0021	0.0017	-	-0.0033	0.0002	-0.0094	-0.0018	-
ALA-CB	-0.2202	-0.1583	-0.1862	-0.1825	0.062	-0.1064	-0.1173	-0.1033	-0.0987	0.019
ALA-HB1	0.0669	0.0536	0.0564	0.0548	-	0.0331	0.0369	0.0313	0.0315	-
ALA-HB2	= HB1	= HB1	= HB1	= HB1	-	= HB1	= HB1	= HB1	= HB1	-
ALA-HB3	= HB1	= HB1	= HB1	= HB1	-	= HB1	= HB1	= HB1	= HB1	-
ALA-C	0.5651	0.6250	0.5707	0.5799	0.060	0.6519	0.6629	0.6509	0.6520	0.012
ALA-O	-0.5347	-0.5510	-0.5367	-0.5420	0.016	-0.5665	-0.5682	-0.5675	-0.5660	0.002
NME-N	-0.4918	-0.5054	-0.5231	-0.5118	0.031	-0.6298	-0.6325	-0.6260	-0.6263	0.007
NME-H	0.3289	0.3256	0.3345	0.3298	-	0.3369	0.3415	0.3385	0.3386	-
NME-C2	-0.2853	-0.2477	-0.1954	-0.2320	0.090	0.0568	0.0264	0.0288	0.0478	0.030
NME-H21	0.1396	0.1283	0.1165	0.1258	-	0.0533	0.0618	0.0608	0.0554	-
NME-H22	= H21	= H21	= H21	= H21	-	= H21	= H21	= H21	= H21	-
NME-H23	= H21	= H21	= H21	= H21	-	= H21	= H21	= H21	= H21	-
MEP.pts [c]	975	991	992	1017	-	14209	14169	14150	14176	-
RRMS [d]	0.092	0.098	0.097	0.095	-	0.130	0.126	0.130	0.130	-

Table S4. ESP charge derivation and force field library building for the *C5* conformation of the alanine dipeptide automatically carried out using the R.E.D. Tools. Charge values were derived from charge fitting and not arithmetic mean. [a] -i- Accurate geometry optimization, -ii- molecular orientation of the optimized geometry controlled by the RBRA approach implemented in the R.E.D. program. The molecular orientation (named "-A-", "-B-", "-C-", and "-D-") are these reported in Table 4. Each of these orientations was involved in a single orientation ESP fit. The charges reported (charge reproducibility +/- 0.0001 e) were obtained using the Gaussian 03 program for both the geometry optimization and MEP computation steps. MCDV: Maximum charge value difference. [b] The Connolly surface or CHELPG algorithm was used in MEP computation,

while charge equivalencing for chemically equivalent atoms was carried out during charge fitting. [(c)] Number of MEP point generated for the given molecular orientations.[(d)] The RRMS values calculated for the fitting stage were taken directly from the outputs of the RESP program.

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