

Supporting Information

New basis sets for the prediction of specific rotation in flexible biological molecules

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TABLE I: B3LYP/6-311G** optimized geometrical parameters of investigated systems. All values in Å.

Conformer 1A		
C	-0.684259	0.625518 0.726602
C	-1.377910	-0.563125 0.018325
C	0.739639	0.227774 1.171514
C	1.624038	-0.024666 -0.043884
N	-0.775072	1.815560 -0.131224
N	1.868637	-1.330688 -0.332788
O	-2.195092	-0.189148 -0.963674
O	-1.202449	-1.712512 0.341244
O	2.053441	0.902812 -0.717721
H	-1.281721	0.806487 1.626455
H	0.674315	-0.649999 1.814456
H	1.181902	1.049674 1.737207
H	-2.057320	0.785705 -1.039065
H	2.319461	-1.526575 -1.214641
H	1.271331	-2.043664 0.059640
H	-0.905554	2.658275 0.415525
H	0.086379	1.923773 -0.665638
Conformer 1B		
C	0.528608	0.276660 -0.214397
C	1.882618	-0.453672 -0.118235
C	-0.613063	-0.594895 0.311025
C	-1.980196	-0.026223 -0.060686
N	0.652474	1.613599 0.382107
N	-3.034880	-0.839664 0.220708
O	2.918686	0.379019 0.039908
O	2.002578	-1.647053 -0.210891

O -2.124941 1.079585 -0.557898
H 0.364205 0.435514 -1.285889
H -0.549560 -0.680605 1.403029
H -0.497890 -1.608907 -0.081180
H 2.518128 1.272801 0.127350
H -3.960482 -0.525131 -0.024630
H -2.912014 -1.781327 0.552521
H 0.529746 1.565398 1.390744
H -0.093683 2.201087 0.023160

Conformer **1C**

C 0.515688 0.183886 -0.446275
C 1.891369 -0.421545 -0.086840
C -0.533831 -0.477530 0.468442
C -1.958887 -0.054708 0.132080
N 0.552856 1.641228 -0.256300
N -2.847017 -1.066007 -0.050123
O 2.697418 0.435311 0.546467
O 2.181923 -1.563204 -0.329804
O -2.282120 1.121685 0.042796
H 0.308503 -0.111406 -1.481635
H -0.340493 -0.174475 1.503618
H -0.400635 -1.558589 0.408310
H 2.176269 1.272375 0.598258
H -3.807382 -0.831377 -0.248731
H -2.583313 -2.033837 0.017565
H 0.820339 2.104186 -1.119217
H -0.377963 1.975623 -0.013320

Conformer **1D**

C -0.684458 0.629193 0.411239
C -1.510332 -0.583165 -0.091889

C 0.603768 0.831465 -0.426753
C 1.763034 -0.061060 -0.014183
N -1.456362 1.867353 0.406810
N 2.999071 0.410822 -0.292991
O -0.932047 -1.780532 0.014389
O -2.613511 -0.443578 -0.557107
O 1.605516 -1.148494 0.539460
H -0.377516 0.417642 1.440226
H 0.882022 1.882697 -0.324397
H 0.403897 0.659366 -1.491294
H -0.003846 -1.684982 0.340729
H 3.796526 -0.164203 -0.068954
H 3.146080 1.308962 -0.720843
H -2.061686 1.855967 -0.412030
H -2.096173 1.859550 1.195394

Conformer **1E**

C 0.585309 -0.624415 0.233582
C 1.408825 0.666106 0.017450
C -0.682194 -0.687433 -0.652903
C -1.944621 -0.062160 -0.038065
N 1.500603 -1.772545 0.095451
N -1.889311 1.277093 0.162623
O 2.719756 0.496439 0.168561
O 0.918067 1.739316 -0.241908
O -2.911951 -0.751396 0.237137
H 0.281409 -0.593361 1.286077
H -0.940040 -1.734098 -0.812518
H -0.478276 -0.228619 -1.625396
H 2.834625 -0.472390 0.308501
H -2.684423 1.724404 0.590214

H -1.039254 1.795268 -0.026727
H 1.533284 -2.097600 -0.866727
H 1.202737 -2.552894 0.669346

Conformer **2A**

C -2.425192 -1.132394 -0.464560
C -3.063505 0.097213 -0.312031
C -2.360711 1.172353 0.226687
C -1.029248 1.018444 0.609442
C -0.374268 -0.209890 0.459950
C -1.094781 -1.281683 -0.081429
C 1.079463 -0.370769 0.845320
C 2.063209 -0.173345 -0.328550
C 3.504502 -0.408605 0.123751
N 1.942673 1.199691 -0.836425
H -2.965924 -1.977531 -0.876542
H -4.100642 0.214180 -0.605630
H -2.850072 2.131780 0.354703
H -0.486627 1.858921 1.029017
H -0.608789 -2.245840 -0.196180
H 1.237221 -1.371958 1.259495
H 1.339077 0.351909 1.624959
H 1.816237 -0.928129 -1.095227
H 4.199856 -0.292861 -0.713695
H 3.632855 -1.417161 0.525829
H 3.781816 0.316467 0.893731
H 2.596698 1.344294 -1.600005
H 1.012780 1.350142 -1.216964

Conformer **2B**

C -2.410111 -1.147687 -0.446631

C -3.059616 0.079375 -0.320929
C -2.370227 1.168594 0.205425
C -1.040380 1.030671 0.600682
C -0.373522 -0.193889 0.478802
C -1.082088 -1.279890 -0.050628
C 1.080163 -0.337374 0.862069
C 2.060320 -0.175630 -0.335347
C 3.503036 -0.421232 0.108868
N 1.986958 1.118299 -1.020228
H -2.940408 -2.003828 -0.849144
H -4.094879 0.183131 -0.625556
H -2.868239 2.125886 0.314247
H -0.515162 1.882348 1.020849
H -0.587457 -2.241601 -0.146983
H 1.241761 -1.321927 1.315124
H 1.340281 0.407841 1.623170
H 1.795607 -0.935455 -1.080424
H 4.179044 -0.330658 -0.743251
H 3.621626 -1.414366 0.550054
H 3.807231 0.316145 0.860709
H 1.038672 1.299371 -1.335852
H 2.227776 1.867392 -0.375203

Conformer **2C**

C -2.188916 -1.213268 -0.206275
C -2.866639 -0.028965 -0.488893
C -2.252957 1.192295 -0.220046
C -0.970256 1.226081 0.323141
C -0.273685 0.045436 0.607507
C -0.907179 -1.175417 0.338311
C 1.124073 0.078008 1.187885

C 2.271487 -0.043009 0.152822
C 2.360288 1.172898 -0.782774
N 2.169223 -1.331915 -0.547284
H -2.661725 -2.169437 -0.402951
H -3.866442 -0.057665 -0.907413
H -2.775018 2.120140 -0.427263
H -0.506017 2.183058 0.539297
H -0.384831 -2.099578 0.559867
H 1.238996 -0.747715 1.894922
H 1.263295 1.007821 1.748383
H 3.197505 -0.086826 0.737899
H 3.209002 1.065636 -1.465023
H 2.497159 2.104940 -0.224059
H 1.454013 1.271212 -1.387531
H 2.995072 -1.478337 -1.120214
H 1.377139 -1.314198 -1.184989

Conformer **2D**

C -2.433556 1.138115 -0.213469
C -3.071767 0.027158 0.332260
C -2.368313 -1.168127 0.470861
C -1.038148 -1.247415 0.067731
C -0.380720 -0.137643 -0.478155
C -1.101257 1.053747 -0.613561
C 1.072464 -0.231669 -0.885290
C 2.086277 -0.214454 0.293734
C 2.060339 1.105687 1.063426
N 3.466802 -0.487849 -0.126082
H -2.973318 2.071381 -0.331541
H -4.108758 0.089824 0.642285
H -2.858129 -2.041185 0.888158

H -0.503375 -2.186775 0.170722
H -0.613892 1.924015 -1.041514
H 1.322576 0.590255 -1.566471
H 1.229912 -1.161220 -1.444719
H 1.804274 -1.018050 0.984463
H 2.773745 1.069229 1.888649
H 1.066802 1.317905 1.462553
H 2.344141 1.938259 0.408611
H 3.514998 -1.366186 -0.634779
H 3.781494 0.235095 -0.769074

Conformer **2E**

C -2.435467 1.133142 -0.217880
C -3.071299 0.025860 0.337727
C -2.365405 -1.166743 0.486871
C -1.035055 -1.246584 0.084275
C -0.379851 -0.140427 -0.471237
C -1.102894 1.047937 -0.617548
C 1.070136 -0.232209 -0.888724
C 2.077906 -0.205572 0.281829
C 2.067742 1.125223 1.032732
N 3.421849 -0.421581 -0.276114
H -2.977087 2.064246 -0.344216
H -4.108514 0.089033 0.647056
H -2.853556 -2.037184 0.911605
H -0.498247 -2.183859 0.195034
H -0.616847 1.914561 -1.053922
H 1.324915 0.583177 -1.572042
H 1.223972 -1.165023 -1.444809
H 1.783772 -0.998161 0.990553
H 2.782965 1.105568 1.861281

H 1.081293 1.339581 1.448329
H 2.354151 1.939058 0.360428
H 4.113833 -0.401425 0.467449
H 3.481530 -1.342260 -0.702216

Conformer **2F**

C -2.437390 1.139399 -0.190617
C -3.071318 0.017000 0.335658
C -2.363428 -1.178186 0.453201
C -1.033042 -1.245712 0.049154
C -0.379728 -0.124053 -0.476926
C -1.104570 1.066323 -0.592442
C 1.070215 -0.211181 -0.897086
C 2.081104 -0.228272 0.270271
C 2.053237 1.068391 1.092361
N 3.404958 -0.556402 -0.283532
H -2.980427 2.072696 -0.292470
H -4.108618 0.070360 0.646535
H -2.850469 -2.060421 0.854185
H -0.493967 -2.184258 0.134237
H -0.620702 1.945293 -1.006466
H 1.312587 0.631159 -1.556622
H 1.238087 -1.123170 -1.476736
H 1.808269 -1.060028 0.930450
H 2.772090 1.015517 1.915584
H 1.065408 1.261062 1.519413
H 2.324508 1.925893 0.465782
H 4.085089 -0.627029 0.468363
H 3.722960 0.205492 -0.878970

Conformer **2G**

C -2.194035 -1.205789 -0.234478

C -2.858729 -0.009161 -0.491272
C -2.235649 1.199258 -0.186219
C -0.956189 1.208146 0.363932
C -0.269843 0.014912 0.621993
C -0.914765 -1.191246 0.318054
C 1.130510 0.025221 1.189114
C 2.277496 -0.025852 0.129928
C 2.304307 1.208821 -0.772545
N 2.291123 -1.226601 -0.711296
H -2.674383 -2.152587 -0.456139
H -3.855938 -0.018034 -0.916531
H -2.748273 2.136714 -0.372252
H -0.484259 2.155165 0.604669
H -0.415215 -2.130252 0.532228
H 1.256801 -0.834935 1.856069
H 1.270022 0.920163 1.805399
H 3.211864 -0.040570 0.703663
H 3.162785 1.154419 -1.444429
H 2.375346 2.129086 -0.185998
H 1.399515 1.269844 -1.384515
H 2.331256 -2.064985 -0.139166
H 1.434001 -1.283687 -1.254970

Conformer **2H**

C -2.602746 -1.088905 -0.308807
C -3.111333 0.206722 -0.288451
C -2.272404 1.266585 0.052966
C -0.937675 1.034778 0.373971
C -0.413042 -0.264146 0.358103
C -1.265874 -1.317910 0.012451
C 1.036574 -0.540375 0.696177

C 2.059302 -0.043490 -0.351418
C 3.414641 -0.746802 -0.173940
N 2.146733 1.423608 -0.291503
H -3.245054 -1.922711 -0.570949
H -4.151410 0.389815 -0.534775
H -2.659929 2.279653 0.070483
H -0.282617 1.862386 0.613308
H -0.879593 -2.332709 -0.001060
H 1.166627 -1.619057 0.824117
H 1.292949 -0.084288 1.661349
H 1.666979 -0.291687 -1.343845
H 4.140995 -0.374946 -0.902729
H 3.330458 -1.830310 -0.304915
H 3.819295 -0.559686 0.827282
H 2.685917 1.777427 -1.075924
H 2.643588 1.702121 0.551855

Conformer **2I**

C -1.980947 1.372068 0.234945
C -2.886313 0.328634 0.423050
C -2.496989 -0.975154 0.129836
C -1.212327 -1.228211 -0.348360
C -0.293600 -0.191413 -0.543936
C -0.699451 1.116658 -0.245526
C 1.091917 -0.492088 -1.077649
C 2.277625 -0.233821 -0.115189
C 2.078416 -0.872992 1.258583
N 2.477120 1.215306 0.048346
H -2.274978 2.391314 0.461800
H -3.885188 0.531060 0.793458
H -3.191607 -1.796269 0.270439

H -0.919465 -2.248278 -0.577669
H 0.008895 1.926063 -0.365754
H 1.269539 0.092371 -1.989170
H 1.131831 -1.543159 -1.380626
H 3.154103 -0.714155 -0.582388
H 2.971450 -0.739626 1.877670
H 1.894131 -1.946597 1.167619
H 1.231244 -0.419298 1.776759
H 3.199894 1.393740 0.739238
H 2.800331 1.623594 -0.824314

Conformer **3A**

C 2.294240 1.880860 -0.214781
C 1.564141 0.734492 -0.497917
C 0.232414 0.627858 -0.165912
C -0.417909 1.569398 0.610727
C 0.306439 2.732885 0.913281
C 1.623688 2.894976 0.480659
C -0.291452 -0.719380 -0.595705
C -1.135935 -1.254375 0.587097
C -2.274265 -0.223996 0.816146
C -1.757637 1.198677 1.213521
C 1.039620 -1.467613 -0.888472
C 1.469962 -2.450586 0.230586
C 0.963769 -2.053002 1.600780
C -0.249585 -1.530885 1.775354
C -1.187405 -0.631387 -1.851372
C -2.455442 0.185852 -1.597013
C -4.431572 0.368206 -0.204719
N -3.133667 -0.261920 -0.381093

O 2.075786 -0.425475 -1.040405
O 3.614295 2.027100 -0.541044
O 2.870187 -2.670634 0.196593
H -0.147251 3.513905 1.514627
H 2.177620 3.794960 0.720844
H -1.638736 -2.182572 0.285345
H -2.894284 -0.588791 1.641360
H -2.526378 1.937027 0.961644
H -1.660236 1.241441 2.304549
H 1.028669 -1.990716 -1.844478
H 1.018930 -3.419675 -0.021118
H 1.618805 -2.286721 2.433635
H -0.618875 -1.307172 2.772542
H 3.887792 1.255499 -1.049871
H 3.272073 -1.803266 0.062581
H -1.467567 -1.649307 -2.145540
H -0.626375 -0.188654 -2.680284
H -3.145073 0.054678 -2.436307
H -2.205371 1.261261 -1.561458
H -4.394890 1.468706 -0.111017
H -5.066456 0.134117 -1.063677
H -4.917304 -0.031096 0.689557

Conformer **3B**

C 2.318830 1.837569 -0.228002
C 1.576130 0.696964 -0.518167
C 0.243621 0.613657 -0.171886
C -0.395168 1.560833 0.609611
C 0.338749 2.715074 0.911277
C 1.657303 2.855910 0.472296
C -0.306170 -0.725587 -0.597018

C -1.154087 -1.249673 0.587213
C -2.277845 -0.205309 0.820138
C -1.737399 1.207579 1.217904
C 1.011609 -1.490641 -0.894917
C 1.453780 -2.461588 0.232188
C 0.942906 -2.061391 1.600181
C -0.269160 -1.536149 1.774501
C -1.204339 -0.622172 -1.850037
C -2.459771 0.212632 -1.591511
C -4.428431 0.422717 -0.192690
N -3.141291 -0.227112 -0.374419
O 2.052722 -0.465298 -1.070525
O 3.634643 1.886158 -0.595384
O 2.856627 -2.658783 0.200618
H -0.101542 3.501210 1.515682
H 2.209147 3.758792 0.719804
H -1.668859 -2.171301 0.285692
H -2.900998 -0.561515 1.646796
H -2.495165 1.959139 0.971897
H -1.633320 1.245490 2.308462
H 0.983269 -2.027057 -1.843284
H 1.012930 -3.438426 -0.009167
H 1.595974 -2.297344 2.434053
H -0.639219 -1.314741 2.772105
H 4.017384 2.709286 -0.275205
H 3.242784 -1.799622 -0.017125
H -1.499996 -1.635625 -2.144248
H -0.638639 -0.187418 -2.679883
H -3.153529 0.092816 -2.429156
H -2.194719 1.284550 -1.554854

H -4.374357 1.522447 -0.096225
H -5.069385 0.201123 -1.050487
H -4.918017 0.028812 0.701927

Conformer **3C**

C -2.641682 -1.432258 -0.272910
C -1.674343 -0.468235 -0.522683
C -0.359224 -0.657233 -0.163304
C 0.055101 -1.728084 0.608087
C -0.910438 -2.710440 0.876472
C -2.221905 -2.576640 0.416828
C 0.455060 0.548523 -0.562000
C 1.370021 0.872305 0.646316
C 2.255747 -0.395068 0.879376
C 1.432933 -1.667619 1.236044
C -0.676020 1.571666 -0.865053
C -0.909452 2.607141 0.265590
C -0.530862 2.089813 1.637042
C 0.541613 1.321331 1.823955
C 1.339524 0.277094 -1.803088
C 2.365163 -0.836332 -1.521964
C 4.253822 0.256660 -0.402382
N 3.126510 -0.658522 -0.280074
O -1.909368 0.781629 -1.056679
O -3.954804 -1.284320 -0.625911
O -2.228058 3.124823 0.210171
H -0.649641 -3.579912 1.470871
H -2.962703 -3.338218 0.630659
H 2.052071 1.689444 0.373627
H 2.922420 -0.193716 1.723460
H 2.047068 -2.532865 0.968974

H 1.305875 -1.706903 2.323691
H -0.530576 2.094566 -1.810216
H -0.254714 3.459923 0.041187
H -1.141592 2.442795 2.461633
H 0.833779 1.010202 2.823421
H -4.043181 -0.466331 -1.128021
H -2.803947 2.367262 0.047924
H 1.848339 1.209196 -2.077275
H 0.712300 -0.008669 -2.654090
H 3.073559 -0.918090 -2.350265
H 1.838278 -1.793688 -1.468320
H 4.814495 0.267211 0.536237
H 4.926030 -0.106665 -1.184238
H 3.994052 1.301324 -0.647343

Conformer **4A**

C -1.974313 -0.392170 -0.037086
C -0.699405 -1.214651 0.073322
C 0.360613 -0.338893 -0.585217
C -0.218527 1.102403 -0.397721
C 1.751208 -0.502749 -0.013999
C 0.232553 1.840231 0.855323
O -1.649028 0.899202 -0.346372
O 2.029178 -1.039651 1.026270
O -3.104304 -0.749783 0.107543
O 2.679111 0.063933 -0.821000
H -0.025905 1.711091 -1.281338
H -0.837887 -2.186790 -0.397908
H -0.472354 -1.388100 1.128638
H 0.413653 -0.538985 -1.657872

H 3.538616 -0.054092 -0.388353
H -0.354640 2.753080 0.967253
H 0.099206 1.232094 1.752993
H 1.286877 2.117075 0.777330

Conformer **4B**

C 1.830892 -0.259161 -0.051115
C 0.898119 -0.984146 0.911371
C -0.398035 -0.170034 0.880598
C 0.119907 1.236967 0.437979
C -1.393335 -0.749663 -0.107301
C -0.807160 2.107153 -0.388149
O 1.316097 0.975211 -0.326167
O -1.119663 -1.416535 -1.070879
O 2.862427 -0.644039 -0.511306
O -2.663665 -0.411787 0.216309
H 0.424382 1.775182 1.342504
H 1.356758 -0.972585 1.904082
H 0.783098 -2.019758 0.597587
H -0.889173 -0.088244 1.850155
H -3.236595 -0.788651 -0.469222
H -0.316247 3.054656 -0.616025
H -1.056474 1.618070 -1.332366
H -1.729646 2.311827 0.159335

Conformer **4C**

C 1.779691 -0.281402 -0.031353
C 0.849714 -0.944848 0.978800
C -0.435573 -0.108694 0.925782
C 0.111743 1.267863 0.433432
C -1.502793 -0.671571 0.005755
C -0.813396 2.128263 -0.404268

O 1.294727 0.956433 -0.335506
O -2.685672 -0.627841 0.221912
O 2.788274 -0.713969 -0.501189
O -0.979625 -1.215730 -1.117855
H 0.439540 1.826797 1.317045
H 1.320001 -0.879538 1.964554
H 0.725912 -1.998014 0.735114
H -0.915136 0.012832 1.896050
H -1.722137 -1.528753 -1.656422
H -0.316949 3.064357 -0.664680
H -1.082913 1.615732 -1.329794
H -1.726269 2.357780 0.150364

Conformer **4D**

C -1.932735 -0.479224 0.002472
C -0.591695 -1.177259 0.195186
C 0.380418 -0.256883 -0.545514
C -0.299673 1.132787 -0.419732
C 1.840104 -0.291840 -0.151896
C 0.045319 1.940271 0.823731
O -1.714563 0.805859 -0.401441
O 2.621604 0.609936 -0.315930
O -3.029343 -0.927299 0.157195
O 2.198379 -1.486377 0.369054
H -0.138258 1.734550 -1.313558
H -0.635372 -2.195419 -0.186586
H -0.376837 -1.237131 1.265470
H 0.368376 -0.530083 -1.608004
H 3.149857 -1.438424 0.549888
H -0.629488 2.795055 0.893492
H -0.069489 1.345306 1.734568

H 1.072172 2.302080 0.768227

Conformer **4E**

C -1.954549 -0.419180 -0.023674

C -0.654403 -1.206826 0.071576

C 0.362777 -0.304454 -0.624955

C -0.243909 1.119712 -0.406208

C 1.813428 -0.388480 -0.203555

C 0.210750 1.854908 0.847011

O -1.668343 0.879850 -0.335337

O -3.071670 -0.809021 0.137076

O 1.984844 -0.949956 1.015631

O 2.731081 0.023238 -0.865499

H -0.078934 1.742259 -1.285545

H -0.775578 -2.187064 -0.387587

H -0.416928 -1.361241 1.126361

H 0.356909 -0.496763 -1.700009

H 2.936737 -0.930951 1.198710

H -0.393524 2.754387 0.975671

H 0.101954 1.237103 1.741448

H 1.257507 2.155297 0.754804

Conformer **5A**

C -2.372134 -0.401693 -0.078794

C -1.096063 -1.214117 0.078633

C -0.020013 -0.335821 -0.550867

C -0.615008 1.101248 -0.391966

C 1.353819 -0.488759 0.069523

C -0.210963 1.851995 0.869492

C 3.650981 -0.019263 -0.236039

O -2.046029 0.889837 -0.385328

O 1.587437 -0.992469 1.138850
O -3.504232 -0.766262 0.030727
O 2.298229 0.041868 -0.732767
H -0.398394 1.705722 -1.273032
H -1.212765 -2.190677 -0.389529
H -0.901528 -1.378042 1.142002
H 0.069197 -0.542270 -1.619592
H -0.811176 2.759094 0.957388
H -0.363864 1.247836 1.766590
H 0.842256 2.140130 0.822011
H 4.262798 0.448472 -1.003538
H 3.735473 0.520789 0.707878
H 3.951043 -1.056371 -0.081919

Conformer **5B**

C 2.151930 -0.447400 -0.122936
C 1.210029 -1.009311 0.934684
C 0.027189 -0.037067 0.954947
C 0.684047 1.272988 0.414224
C -1.104291 -0.522662 0.064282
C -0.186927 2.221519 -0.386269
C -3.432225 -0.395181 -0.319182
O 1.779021 0.832418 -0.417572
O -0.977031 -1.243636 -0.892728
O 3.089428 -0.979071 -0.635906
O -2.288144 -0.027147 0.477791
H 1.120136 1.803055 1.268463
H 1.739783 -1.019049 1.891490
H 0.943272 -2.032715 0.678442
H -0.376957 0.142908 1.950916
H 0.398344 3.089497 -0.694377

H -0.565711 1.730466 -1.285340
H -1.032373 2.563052 0.214799
H -4.286310 0.069657 0.167406
H -3.320847 -0.025037 -1.339212
H -3.544043 -1.479672 -0.343766

Conformer **5C**

C 1.840919 -0.710542 -0.028906
C 1.032502 -0.658251 1.262304
C 0.048981 0.499479 1.050225
C 0.831430 1.380638 0.028521
C -1.313145 0.070957 0.528239
C 0.018915 2.204421 -0.950697
C -2.455777 -1.414866 -0.918200
O 1.667826 0.459382 -0.707947
O -2.353555 0.594152 0.837651
O 2.543079 -1.590598 -0.427251
O -1.217007 -0.950596 -0.344815
H 1.499441 2.036017 0.598828
H 1.722761 -0.441288 2.083471
H 0.573284 -1.625434 1.454856
H -0.147612 1.073628 1.954916
H 0.684086 2.787093 -1.590074
H -0.586667 1.557086 -1.587992
H -0.642758 2.889168 -0.415136
H -2.177763 -2.221474 -1.591819
H -3.122598 -1.776585 -0.134636
H -2.947867 -0.607946 -1.462431

Conformer **5D**

C -0.780782 1.210133 -0.236618
C -2.240988 -0.588605 0.028613

C -0.859828 -1.196397 -0.175706
C -0.052930 -0.055265 -0.792509
C 1.444542 -0.013202 -0.562657
C -0.246441 1.762064 1.077843
C 3.248001 -0.755121 0.770466
O -2.147790 0.771671 -0.055150
O -3.275792 -1.148678 0.234239
O 2.200582 0.650813 -1.226919
O 1.835687 -0.772796 0.478693
H -0.806931 1.997761 -0.989608
H -0.930629 -2.086683 -0.799303
H -0.465107 -1.501901 0.795584
H -0.183431 -0.052617 -1.877101
H -0.923172 2.534426 1.447148
H -0.165049 0.983642 1.840141
H 0.738818 2.211147 0.929602
H 3.378243 -1.430643 1.612399
H 3.817109 -1.098841 -0.093769
H 3.569201 0.253992 1.031408

Conformer **5E**

C -2.196750 -0.729129 0.020799
C -0.745407 -1.192011 0.049641
C -0.006050 -0.049661 -0.647351
C -0.903250 1.179478 -0.334619
C 1.464095 0.154392 -0.344497
C -0.595565 1.921266 0.958686
C 3.452193 -0.872789 0.411550
O -2.235216 0.607064 -0.253725
O 2.064164 1.178598 -0.558799
O -3.185090 -1.377366 0.196988

O 2.035793 -0.958135 0.151029
H -0.922170 1.877827 -1.170611
H -0.647332 -2.161392 -0.435342
H -0.435398 -1.314278 1.090662
H -0.053427 -0.215797 -1.730346
H -1.395747 2.634781 1.162577
H -0.529941 1.236406 1.809317
H 0.346842 2.462626 0.869638
H 3.735702 -1.851678 0.790201
H 3.992937 -0.641128 -0.506752
H 3.655723 -0.097941 1.151461

Conformer **6A**

C 3.036582 1.590995 -0.074317
C 3.464241 0.236020 -0.088001
C 2.540850 -0.782930 0.002759
C 1.155630 -0.485364 0.110940
C 0.723467 0.874927 0.125078
C 1.707584 1.896519 0.028783
C 0.169865 -1.501494 0.203184
C -1.163687 -1.191290 0.309015
C -1.599821 0.159279 0.329243
C -0.659517 1.161352 0.232099
C 5.327424 -1.253202 -0.219100
C -3.080954 0.491983 0.482717
C -3.641773 0.062497 1.847863
C -3.862454 -0.165854 -0.646497
O 4.812021 0.070348 -0.195325
O -4.332181 -1.276079 -0.621874
O -3.957913 0.640188 -1.729126

H 3.794411 2.361447 -0.148320
H 2.845052 -1.821430 -0.006507
H 1.390247 2.934014 0.037764
H 0.484100 -2.540067 0.186159
H -1.899499 -1.985496 0.364327
H -0.973967 2.200785 0.238176
H 6.407512 -1.150986 -0.309302
H 5.089430 -1.791788 0.705004
H 4.942920 -1.816652 -1.076624
H -3.192152 1.571674 0.361968
H -4.686994 0.364899 1.952642
H -3.063592 0.526208 2.649499
H -3.594317 -1.020773 1.964073
H -4.423180 0.131876 -2.410863

Conformer **6B**

C 2.684626 -1.687573 0.160320
C 3.351909 -0.446082 -0.025540
C 2.629824 0.724806 -0.098934
C 1.212745 0.699117 0.011398
C 0.539699 -0.546399 0.199419
C 1.322717 -1.732317 0.268385
C 0.428606 1.877430 -0.061307
C -0.940740 1.824477 0.046477
C -1.614937 0.593796 0.238630
C -0.870730 -0.566190 0.309367
C 5.455827 0.649935 -0.304803
C -3.134232 0.577873 0.398584
C -3.567700 0.239984 1.834054
C -3.735652 -0.410241 -0.589520
O 4.707458 -0.542769 -0.117624

O -3.920773 -1.584195 -0.385244
O -4.030099 0.176665 -1.772864
H 3.290201 -2.584235 0.211926
H 3.117981 1.680124 -0.241049
H 0.821086 -2.683760 0.409708
H 0.924819 2.831359 -0.207661
H -1.520424 2.739649 -0.016506
H -1.368130 -1.521504 0.442534
H 6.499389 0.343192 -0.350307
H 5.183110 1.150408 -1.240686
H 5.317379 1.344283 0.531527
H -3.506797 1.567706 0.125744
H -4.653988 0.302581 1.940381
H -3.108987 0.939053 2.536191
H -3.260927 -0.772425 2.099065
H -4.359171 -0.525744 -2.354182

Conformer **6C**

C 3.041569 1.596854 -0.092313
C 3.472431 0.242810 -0.095410
C 2.551855 -0.777675 0.006948
C 1.166390 -0.482125 0.116340
C 0.731042 0.876853 0.119835
C 1.712197 1.900157 0.012037
C 0.182403 -1.498581 0.220947
C -1.151692 -1.190633 0.327586
C -1.592721 0.158904 0.336680
C -0.652125 1.160708 0.228824
C 5.338813 -1.242898 -0.220804
C -3.070158 0.509386 0.480388
C -3.676533 0.004888 1.803507

C -3.856575 0.031959 -0.734435
O 4.820225 0.079466 -0.205192
O -4.214267 0.729851 -1.647141
O -4.121865 -1.299934 -0.696514
H 3.797301 2.368385 -0.175706
H 2.858642 -1.815466 0.005753
H 1.392148 2.936805 0.012244
H 0.498736 -2.536711 0.213733
H -1.882322 -1.987730 0.390943
H -0.967923 2.199636 0.226941
H 6.418324 -1.138710 -0.315524
H 5.105396 -1.775121 0.708166
H 4.952752 -1.813694 -1.072755
H -3.155253 1.596677 0.441210
H -4.725767 0.299993 1.889765
H -3.128719 0.435459 2.644424
H -3.623863 -1.081669 1.878132
H -4.593582 -1.506554 -1.517333

Conformer **6D**

C 2.697766 -1.682086 0.137372
C 3.360821 -0.436722 -0.038150
C 2.635236 0.732928 -0.093094
C 1.218913 0.702246 0.025426
C 0.549874 -0.546939 0.202315
C 1.336710 -1.731387 0.253068
C 0.430986 1.878620 -0.028132
C -0.937343 1.819831 0.087890
C -1.609410 0.585569 0.269247
C -0.859782 -0.572511 0.320304
C 5.460026 0.667761 -0.319285

C -3.129075 0.577991 0.421525
C -3.585341 0.080073 1.805636
C -3.777757 -0.196145 -0.718415
O 4.715876 -0.528951 -0.139945
O -4.279295 0.297231 -1.694795
O -3.732425 -1.541208 -0.531405
H 3.305964 -2.577678 0.174918
H 3.119912 1.691173 -0.227043
H 0.838832 -2.686019 0.386697
H 0.922956 2.836027 -0.165458
H -1.519413 2.734180 0.039232
H -1.350326 -1.532087 0.440390
H 6.503959 0.364139 -0.375626
H 5.179285 1.177748 -1.247579
H 5.325833 1.352394 0.525677
H -3.479043 1.601898 0.278709
H -4.674185 0.120660 1.897617
H -3.151376 0.711802 2.583655
H -3.267391 -0.948091 1.980567
H -4.138000 -1.938099 -1.316840

Conformer **6E**

C -3.124381 -1.164864 0.042815
C -3.426360 0.213860 -0.088591
C -2.407289 1.146005 -0.081433
C -1.060996 0.746969 0.055988
C -0.750238 -0.643331 0.189538
C -1.816986 -1.572156 0.177580
C 0.014216 1.678067 0.063974
C 1.312072 1.259945 0.201628
C 1.627811 -0.120801 0.341022

C 0.605610 -1.040355 0.326953
C -5.783927 -0.208405 -0.241744
C 3.075152 -0.565101 0.528740
C 3.677567 -0.063531 1.850875
C 3.905271 -0.082665 -0.653302
O -4.693570 0.701748 -0.226447
O 4.474396 0.977751 -0.725882
O 3.918824 -0.985706 -1.661017
H -3.914200 -1.903822 0.037910
H -2.660668 2.194751 -0.184055
H -1.594067 -2.629405 0.277226
H -0.208224 2.734393 -0.044438
H 2.116922 1.986152 0.191140
H 0.827626 -2.098950 0.424237
H -6.676820 0.403396 -0.359935
H -5.715328 -0.908754 -1.081693
H -5.855830 -0.770313 0.696239
H 3.091925 -1.656882 0.506822
H 4.693633 -0.443574 1.985210
H 3.065951 -0.401705 2.689630
H 3.723736 1.025840 1.868750
H 4.423012 -0.583295 -2.384534

Conformer **6F**

C 2.856595 1.613300 0.289192
C 3.400619 0.307188 0.158938
C 2.575164 -0.763551 -0.108315
C 1.175441 -0.568257 -0.254471
C 0.626047 0.742417 -0.125399
C 1.511865 1.819943 0.150419
C 0.287252 -1.639972 -0.528216

C -1.060785 -1.422963 -0.668422
C -1.615128 -0.121478 -0.547212
C -0.770520 0.931616 -0.273212
C 5.379777 -1.029661 0.205531
C -3.127152 0.042192 -0.702798
C -3.592138 1.450304 -1.095374
C -3.795607 -0.455071 0.575507
O 4.751595 0.239366 0.319309
O -4.252504 -1.558612 0.733701
O -3.800093 0.480086 1.555328
H 3.539624 2.427259 0.499718
H 2.968519 -1.766463 -0.211027
H 1.105427 2.820844 0.251589
H 0.688696 -2.643040 -0.629434
H -1.723740 -2.257723 -0.869811
H -1.160621 1.937243 -0.167059
H 6.441716 -0.852192 0.366689
H 5.009144 -1.728770 0.963515
H 5.230706 -1.461842 -0.790304
H -3.453569 -0.664170 -1.469896
H -4.670978 1.459538 -1.268951
H -3.096610 1.765837 -2.016139
H -3.377990 2.179687 -0.314006
H -4.200894 0.061032 2.331408

Conformer **6G**

C 2.827253 -1.246153 0.182420
C 3.361428 0.042135 -0.075490
C 2.515864 1.126496 -0.198493
C 1.118422 0.973983 -0.070281
C 0.573379 -0.323578 0.191226

C 1.468265 -1.413878 0.310168
C 0.217240 2.065658 -0.193506
C -1.135892 1.880661 -0.064910
C -1.683821 0.597433 0.199975
C -0.830277 -0.476765 0.320944
C 5.615648 -0.782062 -0.099421
C -3.193104 0.443483 0.381523
C -3.579686 0.160254 1.842126
C -3.702263 -0.661390 -0.531629
O 4.695540 0.293925 -0.215617
O -3.763634 -1.832773 -0.251333
O -4.070196 -0.184210 -1.743300
H 3.480492 -2.102657 0.280075
H 2.945378 2.101648 -0.396556
H 1.066592 -2.402265 0.507153
H 0.615622 3.054344 -0.395496
H -1.806273 2.727869 -0.167026
H -1.229338 -1.468003 0.510637
H 6.601527 -0.343603 -0.245522
H 5.573044 -1.246311 0.892189
H 5.445439 -1.545464 -0.866805
H -3.663488 1.372051 0.050679
H -4.665990 0.124630 1.960376
H -3.185165 0.944779 2.490960
H -3.173230 -0.798242 2.166826
H -4.333021 -0.951992 -2.273415

Conformer **6H**

C -3.129382 -1.172525 0.017624
C -3.435472 0.207456 -0.089162
C -2.419543 1.142730 -0.061463

C -1.072561 0.745194 0.072575
C -0.757699 -0.645965 0.181449
C -1.821172 -1.578074 0.149198
C 0.000459 1.678161 0.101448
C 1.299380 1.261661 0.234693
C 1.620880 -0.120448 0.349291
C 0.598814 -1.040882 0.316194
C -5.790870 -0.219843 -0.260778
C 3.063282 -0.584210 0.522919
C 3.720768 -0.023937 1.798336
C 3.879186 -0.281201 -0.728136
O -4.703770 0.693663 -0.221923
O 4.170011 -1.082827 -1.577233
O 4.256350 1.021509 -0.804653
H -3.916714 -1.913811 -0.004007
H -2.676140 2.192345 -0.145648
H -1.594857 -2.636207 0.229369
H -0.224686 2.735883 0.013420
H 2.098960 1.992291 0.238417
H 0.822777 -2.100484 0.395143
H -6.685314 0.391133 -0.371226
H -5.715531 -0.903023 -1.114130
H -5.865366 -0.800524 0.665476
H 3.053881 -1.674181 0.576243
H 4.741156 -0.400671 1.909119
H 3.144128 -0.332624 2.672886
H 3.763055 1.065464 1.780610
H 4.737503 1.116950 -1.640321

Conformer **7A**

C 0.736459 0.049942 0.331800
C 2.003130 -0.722738 0.010137
N -0.386943 -0.656794 -0.343356
N -1.513757 -0.245748 -0.056100
N -2.591844 0.047819 0.128848
O 0.807242 1.405625 -0.045597
H 0.551945 0.072185 1.409943
H 2.859586 -0.229373 0.472024
H 1.936674 -1.748406 0.377249
H 2.154292 -0.759926 -1.072790
H 1.049844 1.440351 -0.979019

Conformer **7B**

C 0.921350 0.113111 0.400654
C 1.249359 -1.225442 -0.237814
N -0.467326 0.174632 0.940461
N -1.369645 -0.004440 0.118351
N -2.280294 -0.142397 -0.541580
O 1.153230 1.111263 -0.567678
H 1.533359 0.275498 1.292216
H 2.292520 -1.231121 -0.557834
H 1.087710 -2.037209 0.472975
H 0.620833 -1.388042 -1.116879
H 1.036339 1.970199 -0.146712

Conformer **7C**

C 0.745165 0.051497 0.302300
C 1.206147 -1.342193 -0.082925
N -0.436176 0.482403 -0.515773
N -1.534037 0.133352 -0.087152
N -2.591885 -0.134337 0.226526
O 1.791053 0.937623 0.036385

H 0.450122 0.084640 1.362863
H 2.092467 -1.607605 0.497068
H 0.423391 -2.078260 0.112591
H 1.458091 -1.358355 -1.144329
H 1.474324 1.832851 0.199270

Conformer **7D**

C 0.903507 0.097738 0.433018
C 1.493319 -0.986373 -0.461880
N -0.457695 -0.298346 0.916869
N -1.372665 -0.148227 0.111613
N -2.287555 -0.026093 -0.550476
O 0.923727 1.366292 -0.170788
H 1.475726 0.197340 1.353700
H 2.514756 -0.720240 -0.742139
H 1.503027 -1.948718 0.051976
H 0.898315 -1.095996 -1.375540
H 0.662814 1.277741 -1.094560

Conformer **8A**

C 0.292807 0.487626 0.279486
C 1.725781 0.241031 -0.177124
C 2.248596 -1.160534 0.142305
N -0.583663 -0.446007 -0.480446
N -1.749801 -0.512570 -0.085956
N -2.840572 -0.650580 0.186028
O -0.110018 1.827605 0.116073
H 0.186262 0.292211 1.351576
H 2.346223 1.002794 0.303354
H 1.769688 0.421287 -1.258267
H 0.040058 2.069965 -0.805893

H 3.279356 -1.276282 -0.200449
H 1.639359 -1.924531 -0.344101
H 2.234339 -1.350923 1.219822

Conformer **8B**

C 0.251679 0.066072 0.190935
C 1.496368 -0.686659 -0.266151
C 2.786261 -0.110019 0.318758
N -0.919295 -0.641450 -0.393003
N -2.019544 -0.263869 0.016986
N -3.079458 0.000031 0.316282
O 0.264128 1.432281 -0.159040
H 0.173350 0.061766 1.283105
H 1.522179 -0.660392 -1.362520
H 1.379973 -1.737589 0.013221
H 0.383447 1.489347 -1.115392
H 3.658500 -0.641750 -0.067915
H 2.800100 -0.196585 1.409302
H 2.891662 0.947617 0.069411

Conformer **8C**

C 0.237692 0.412700 0.519752
C 1.631298 -0.186899 0.699660
C 2.283485 -0.663480 -0.601226
N -0.649110 -0.670211 0.006518
N -1.847011 -0.385878 -0.048525
N -2.965482 -0.233977 -0.143886
O 0.212119 1.548722 -0.312931
H -0.148416 0.764606 1.480824
H 1.548394 -1.021142 1.402119
H 2.251641 0.578988 1.174148
H 0.589192 1.301825 -1.165649

H 3.257439 -1.113472 -0.397534
H 2.458450 0.164767 -1.295842
H 1.662719 -1.408811 -1.102488

Conformer **8D**

C 0.338537 0.491850 0.482095
C 1.073805 -0.785095 0.088193
C 2.558784 -0.551153 -0.197541
N -1.064803 0.237571 0.911655
N -1.806895 -0.255092 0.058005
N -2.586538 -0.690340 -0.639614
O 0.399550 1.380568 -0.611356
H 0.792293 0.931618 1.375799
H 0.580813 -1.199875 -0.797812
H 0.947034 -1.507797 0.899145
H 0.052773 2.233442 -0.327796
H 3.048437 -1.485042 -0.483322
H 3.075114 -0.162976 0.686002
H 2.688031 0.167505 -1.007973

Conformer **8E**

C 0.391185 0.763036 0.366697
C 1.311247 -0.007287 -0.574644
C 2.031608 -1.179805 0.092684
N -0.704934 -0.073380 0.936060
N -1.485589 -0.561662 0.114850
N -2.270284 -1.051984 -0.539124
O -0.113757 1.866793 -0.350087
H 0.939079 1.083010 1.258532
H 2.033658 0.712953 -0.968554
H 0.716532 -0.349509 -1.428537
H -0.619911 2.414729 0.259917

H 2.674729 -1.693765 -0.625100
H 1.324613 -1.908888 0.494544
H 2.662760 -0.839347 0.918977

Conformer **8F**

C 0.272340 0.398869 0.213222
C 1.073418 -0.721433 -0.439668
C 2.439958 -0.934537 0.216311
N -1.062219 0.569466 -0.447286
N -1.958797 -0.159936 -0.029013
N -2.853755 -0.782054 0.289098
O 0.979138 1.592805 0.052177
H 0.099000 0.176010 1.278807
H 1.186340 -0.464817 -1.496726
H 0.480037 -1.640252 -0.389094
H 0.447137 2.309749 0.413751
H 2.986300 -1.736446 -0.285695
H 2.337550 -1.211537 1.270249
H 3.039641 -0.024879 0.162520

Conformer **8G**

C 0.380900 0.586113 0.250387
C 1.682998 -0.110828 -0.116070
C 1.654072 -1.622775 0.104224
N -0.710273 0.115676 -0.659259
N -1.735082 -0.291665 -0.114776
N -2.722874 -0.688028 0.279973
O 0.586416 1.964292 0.082072
H 0.092251 0.350209 1.286180
H 2.471041 0.352975 0.484109
H 1.893431 0.125933 -1.162796
H -0.233257 2.427234 0.284596

H 2.617298 -2.067005 -0.155887
H 0.889839 -2.097551 -0.515380
H 1.447853 -1.873070 1.149791

Conformer **8H**

C -0.301959 -0.598998 0.416852
C -1.135566 0.642283 0.726571
C -1.864848 1.220545 -0.487587
N 0.764757 -0.322945 -0.602267
N 1.817171 0.130757 -0.158170
N 2.827991 0.544206 0.152001
O -1.146311 -1.578316 -0.111998
H 0.195151 -0.952815 1.333578
H -0.473116 1.391419 1.173572
H -1.854707 0.355897 1.501131
H -0.602199 -2.315943 -0.408149
H -2.449353 2.097351 -0.199189
H -2.542318 0.481530 -0.917224
H -1.158173 1.521982 -1.263700

Conformer **8I**

C 0.509620 -0.891117 -0.341906
C 1.570217 0.198688 -0.500058
C 1.331469 1.461273 0.332828
N -0.816912 -0.501804 -0.903805
N -1.539645 0.198968 -0.194811
N -2.308077 0.812557 0.369841
O 0.436464 -1.242288 1.020596
H 0.788048 -1.751397 -0.957911
H 1.632191 0.447334 -1.563258
H 2.525831 -0.255914 -0.219110
H -0.090000 -2.044842 1.101709

H	2.181596	2.140520	0.235266
H	1.212676	1.216339	1.389491
H	0.442547	2.005153	0.005287

Conformer **8J**

C	0.261331	0.061821	0.192596
C	1.507433	-0.682786	-0.255606
C	2.795041	-0.070144	0.295722
N	-0.913563	-0.713708	-0.308163
N	-2.015055	-0.279911	0.022291
N	-3.077512	0.040824	0.262636
O	0.307980	1.366930	-0.336367
H	0.201826	0.095779	1.290520
H	1.511959	-0.674247	-1.349685
H	1.405271	-1.725332	0.056917
H	-0.298578	1.932985	0.151204
H	3.667986	-0.614880	-0.070937
H	2.818237	-0.106489	1.389665
H	2.889539	0.972962	-0.010363

Conformer **8K**

C	0.256980	0.419650	0.525936
C	1.660579	-0.149165	0.672015
C	2.254446	-0.669194	-0.639079
N	-0.642991	-0.701648	0.107854
N	-1.827515	-0.407248	-0.028344
N	-2.938674	-0.235472	-0.189729
O	0.290966	1.465997	-0.416242
H	-0.105338	0.789932	1.495189
H	1.618964	-0.948566	1.417430
H	2.286543	0.648381	1.082721
H	-0.513740	1.988705	-0.342512

H 3.265506 -1.048905 -0.473578
H 2.304673 0.125836 -1.384679
H 1.647899 -1.480532 -1.046333

Conformer **9A**

C 1.901915 -0.626592 0.293068
C 1.127807 0.633871 -0.105375
C -0.342212 0.623255 0.294539
C 3.375078 -0.570753 -0.120447
N -1.000901 -0.481870 -0.455657
N -2.150801 -0.747930 -0.099347
N -3.208422 -1.074839 0.140285
H -0.453558 0.447111 1.369362
O -0.980465 1.858547 0.065341
H 1.577478 1.518037 0.357547
H 1.181635 0.774453 -1.192880
H -0.837951 2.096547 -0.858936
H 1.420964 -1.498229 -0.159653
H 1.832433 -0.762168 1.379163
H 3.903769 -1.478870 0.179998
H 3.477425 -0.471257 -1.205380
H 3.886875 0.279796 0.340378

Conformer **9B**

C 2.231760 0.229375 0.397996
C 1.008938 -0.474524 -0.197297
C -0.311879 0.167583 0.209938
C 3.553419 -0.391776 -0.061506
N -1.396588 -0.669826 -0.370398
N -2.536733 -0.385539 0.004351
N -3.623384 -0.213927 0.273562

O -0.425618 1.516361 -0.186952
H -0.414315 0.191388 1.299758
H 1.063329 -0.473925 -1.294006
H 0.986457 -1.525522 0.107840
H -0.287190 1.554122 -1.141652
H 2.171316 0.192715 1.492219
H 2.202466 1.288981 0.128011
H 4.408048 0.126189 0.380967
H 3.618892 -1.446010 0.224517
H 3.659453 -0.337724 -1.149431

Conformer **9C**

C 1.873884 -0.222972 -0.474517
C 1.093625 0.230699 0.764932
C -0.370899 0.578551 0.506268
C 3.319086 -0.610078 -0.147508
N -1.052303 -0.668114 0.053382
N -2.277976 -0.588975 -0.048167
N -3.402454 -0.629919 -0.178931
O -0.552316 1.635666 -0.407551
H -0.843803 0.926898 1.429127
H 1.122325 -0.556191 1.525581
H 1.565428 1.118892 1.197678
H -0.109610 1.397557 -1.230597
H 1.887237 0.582671 -1.219640
H 1.357030 -1.070603 -0.933948
H 3.858258 -0.920057 -1.046164
H 3.864598 0.228430 0.296043
H 3.352017 -1.441067 0.563294

Conformer **9D**

C 2.135741 0.255965 0.017049

C 0.733528 -0.308372 0.270476
C -0.328005 0.772900 0.438682
C 3.187877 -0.841354 -0.164004
N -1.650041 0.222585 0.850187
N -2.173428 -0.565377 0.058217
N -2.759231 -1.286490 -0.590495
O -0.413631 1.488165 -0.774207
H -0.069457 1.434796 1.271008
H 0.435034 -0.951934 -0.565518
H 0.731057 -0.926907 1.173615
H -0.988783 2.248708 -0.636522
H 2.421364 0.901085 0.857009
H 2.104230 0.895414 -0.868696
H 4.178024 -0.413477 -0.340783
H 3.255113 -1.480239 0.722091
H 2.946517 -1.482632 -1.017129

Conformer **9E**

C -2.385666 0.221888 0.328663
C -1.010244 -0.096385 0.929837
C 0.153734 0.091951 -0.038531
C -2.834960 -0.747464 -0.770202
N 1.390206 -0.262882 0.710330
N 2.413398 -0.341151 0.026054
N 3.413073 -0.438371 -0.497398
O 0.225457 1.393036 -0.578432
H 0.060945 -0.562783 -0.909310
H -0.821436 0.545259 1.799417
H -0.983197 -1.127160 1.297876
H 0.251606 2.016680 0.158089
H -2.375476 1.242352 -0.066165

H -3.120380 0.210762 1.140173
H -3.847631 -0.511062 -1.106603
H -2.184168 -0.700224 -1.647419
H -2.837842 -1.781217 -0.410109

Conformer **9F**

C -2.062916 -0.378760 0.611233
C -1.188864 0.866691 0.408843
C 0.160204 0.620053 -0.258257
C -2.541200 -1.032745 -0.689916
N 0.930777 -0.299141 0.624912
N 1.979148 -0.734573 0.144146
N 2.959661 -1.190501 -0.192965
O 0.863975 1.815253 -0.507535
H 0.043602 0.159597 -1.243080
H -1.715075 1.605642 -0.204074
H -0.991449 1.334321 1.381600
H 0.913680 2.306379 0.321712
H -2.934717 -0.086460 1.205580
H -1.509261 -1.106509 1.211518
H -3.213766 -1.868197 -0.479495
H -3.084918 -0.319416 -1.317442
H -1.710342 -1.429304 -1.280104

Conformer **9G**

C 1.821850 -0.166510 0.496928
C 0.796704 0.555207 -0.382866
C -0.470503 0.975139 0.353416
C 3.080992 -0.567179 -0.276667
N -1.233864 -0.174371 0.920473
N -1.636059 -1.004392 0.101169
N -2.065292 -1.823341 -0.553824

O -1.252590 1.724034 -0.549832
H -0.219612 1.560836 1.243172
H 1.234234 1.465237 -0.805135
H 0.508010 -0.073487 -1.233441
H -2.010784 2.075359 -0.069881
H 1.362980 -1.055277 0.940994
H 2.099659 0.483297 1.335305
H 3.798480 -1.075310 0.372562
H 2.839717 -1.245846 -1.100337
H 3.580283 0.307713 -0.704177

Conformer **9H**

C 2.311981 -0.660336 0.372521
C 0.954824 -0.934387 -0.294545
C -0.199813 -0.069095 0.201224
C 3.000625 0.648750 -0.031386
N -1.439160 -0.626451 -0.411179
N -2.492415 -0.134150 -0.000511
N -3.517040 0.245869 0.297291
O -0.062569 1.306942 -0.077642
H -0.281362 -0.122692 1.291894
H 1.030857 -0.816314 -1.383667
H 0.667705 -1.975684 -0.122372
H 0.107247 1.401325 -1.023051
H 2.973605 -1.497350 0.126102
H 2.188266 -0.689553 1.461880
H 3.987547 0.723976 0.432989
H 3.144915 0.694731 -1.116242
H 2.416385 1.519555 0.267520

Conformer **9I**

C -2.041186 -0.558348 0.612934

C -0.611566 -0.767034 0.092330
C 0.081103 0.513124 -0.366851
C -3.036474 -0.069820 -0.445132
N 1.430266 0.253003 -0.943622
N 2.250046 -0.266321 -0.181841
N 3.092024 -0.724944 0.422157
O 0.142074 1.390746 0.736058
H -0.453074 0.968246 -1.204703
H 0.001495 -1.211453 0.884139
H -0.611707 -1.467151 -0.749403
H 0.472434 2.241367 0.427088
H -2.011458 0.146808 1.447578
H -2.392173 -1.511890 1.021070
H -4.046668 -0.015061 -0.031317
H -2.785586 0.928921 -0.813459
H -3.067470 -0.745452 -1.306005

Conformer **9J**

C -1.721884 -0.782904 0.478537
C -0.736752 0.331213 0.856991
C 0.123855 0.856269 -0.288797
C -2.817949 -0.354593 -0.503658
N 0.942000 -0.204273 -0.945123
N 1.750145 -0.785237 -0.216221
N 2.534149 -1.377708 0.347877
O 0.929927 1.885477 0.241046
H -0.495468 1.225787 -1.109706
H -1.276882 1.191221 1.265691
H -0.060225 -0.013386 1.646835
H 1.402182 2.302018 -0.488295
H -2.188661 -1.143274 1.400822

H -1.171355 -1.632790 0.062873
H -3.532748 -1.165417 -0.665578
H -3.375174 0.507878 -0.124104
H -2.408753 -0.085235 -1.481074

Conformer **9K**

C 2.219939 -0.043401 0.467489
C 1.223504 0.972948 -0.119378
C -0.242226 0.779914 0.257639
C 2.310795 -1.382931 -0.271855
N -0.740768 -0.472358 -0.373253
N -1.866965 -0.826139 -0.014803
N -2.889372 -1.243561 0.235762
O -1.038926 1.886251 -0.105474
H -0.351687 0.704424 1.344505
H 1.481509 1.976541 0.230685
H 1.299130 0.985891 -1.214396
H -0.915714 2.039595 -1.050286
H 1.973466 -0.216419 1.522311
H 3.209690 0.424753 0.468440
H 3.063483 -2.027074 0.191182
H 1.357408 -1.911780 -0.270009
H 2.601786 -1.230722 -1.315962

Conformer **9L**

C 2.092697 -0.048378 0.410945
C 0.754877 -0.260145 -0.307225
C -0.358401 0.636392 0.219710
C 3.203932 -0.944464 -0.142551
N -1.651160 0.376925 -0.494325
N -2.325301 -0.550012 -0.050570
N -3.022265 -1.381026 0.285528

O -0.003013 1.965455 -0.022677
H -0.522057 0.454935 1.294477
H 0.858046 -0.057071 -1.377808
H 0.435246 -1.303349 -0.203319
H -0.733211 2.528543 0.255983
H 1.964779 -0.243996 1.482737
H 2.379011 1.002406 0.319500
H 4.146601 -0.775216 0.384206
H 2.951160 -2.004391 -0.039330
H 3.376979 -0.747145 -1.204740

Conformer **9M**

C -2.149092 -0.670582 -0.376344
C -0.618887 -0.819008 -0.304942
C 0.171754 0.425317 -0.700053
C -2.790696 0.093323 0.786932
N 1.626885 0.143743 -0.864764
N 2.215527 -0.247067 0.146748
N 2.866715 -0.597456 1.005304
O -0.050847 1.436171 0.258758
H -0.125769 0.757101 -1.699788
H -0.315324 -1.114761 0.706233
H -0.301699 -1.617183 -0.982314
H 0.368577 2.245115 -0.055633
H -2.577223 -1.677736 -0.417768
H -2.417943 -0.194510 -1.327594
H -3.878470 0.119476 0.676809
H -2.565418 -0.393066 1.741150
H -2.422321 1.117362 0.844261

Conformer **9N**

C 1.688648 -0.682519 0.223672

C 1.085705 0.695442 -0.058284
C -0.398972 0.800547 0.254748
C 3.187499 -0.742248 -0.083926
N -1.166540 -0.100393 -0.661225
N -1.968710 -0.864151 -0.126638
N -2.733697 -1.609005 0.259053
O -0.774375 2.136934 0.042685
H -0.601258 0.491445 1.291550
H 1.592315 1.462828 0.535756
H 1.216968 0.964776 -1.111046
H -1.717137 2.226002 0.217528
H 1.162871 -1.434601 -0.372929
H 1.522827 -0.947006 1.275489
H 3.594263 -1.735395 0.122732
H 3.382918 -0.514996 -1.136142
H 3.746581 -0.021019 0.519982

Conformer **90**

C 1.740326 -0.229934 -0.454606
C 0.820526 0.036532 0.741554
C -0.430664 0.845043 0.409193
C 2.986005 -1.029861 -0.064683
N -1.294860 0.159017 -0.608857
N -2.081499 -0.672499 -0.161422
N -2.845198 -1.451891 0.152205
O -0.036521 2.071841 -0.131053
H -1.035502 0.986112 1.318586
H 0.503616 -0.908959 1.197455
H 1.363090 0.591561 1.515396
H -0.825776 2.534417 -0.432770
H 2.031570 0.727180 -0.894090

H 1.179619 -0.766755 -1.225790
H 3.627455 -1.206723 -0.931887
H 3.581727 -0.499056 0.684652
H 2.720111 -2.005558 0.354639

Conformer **9P**

C 2.236051 0.253795 0.380246
C 1.016436 -0.475769 -0.189312
C -0.302689 0.161767 0.209927
C 3.558321 -0.375664 -0.066180
N -1.389956 -0.732487 -0.292404
N -2.533340 -0.397010 0.009082
N -3.625507 -0.172254 0.224016
O -0.364526 1.450684 -0.356583
H -0.392104 0.220618 1.304633
H 1.053639 -0.487062 -1.283715
H 1.001284 -1.518480 0.141861
H -1.035032 1.969590 0.098767
H 2.182761 0.250520 1.476222
H 2.198162 1.301618 0.070679
H 4.413155 0.160084 0.354458
H 3.630763 -1.420182 0.252540
H 3.656482 -0.354692 -1.155717

Conformer **9Q**

C 1.447527 0.476663 0.243446
C 0.967795 -0.751119 -0.540211
C -0.493225 -1.143923 -0.322375
C 2.951249 0.714777 0.075012
N -1.458419 -0.149580 -0.877087
N -1.698731 0.839983 -0.185175
N -2.026499 1.774346 0.367404

O -0.689602 -1.376240 1.053673
H -0.711238 -2.041360 -0.909009
H 1.113895 -0.595008 -1.613758
H 1.569523 -1.622404 -0.257426
H -1.545868 -1.801158 1.172580
H 1.209358 0.342265 1.301806
H 0.906265 1.367445 -0.090436
H 3.275067 1.597514 0.632150
H 3.530461 -0.139213 0.439385
H 3.214828 0.870201 -0.975900

Conformer **9R**

C -1.964951 -0.773094 -0.337201
C -1.137321 0.251127 -1.131118
C 0.226764 0.642686 -0.558056
C -2.387399 -0.354029 1.077396
N 0.954931 -0.613654 -0.222903
N 2.139038 -0.466984 0.085477
N 3.230951 -0.450879 0.386347
O 0.169063 1.528336 0.537823
H 0.796847 1.189659 -1.315133
H -0.965007 -0.152353 -2.134157
H -1.700669 1.181934 -1.256207
H -0.398480 1.141288 1.212836
H -1.407961 -1.712353 -0.284344
H -2.866557 -0.980870 -0.922779
H -3.112145 -1.061732 1.488056
H -1.541818 -0.348033 1.773852
H -2.853709 0.636251 1.086713

Conformer **9S**

C 2.218198 -0.054636 0.137570

C 1.212602 -0.685033 -0.841641
C -0.234701 -0.820872 -0.361580
C 2.108609 1.462774 0.327312
N -0.850761 0.535599 -0.294908
N -2.066350 0.545603 -0.088760
N -3.176050 0.675356 0.097615
O -0.365305 -1.513906 0.857579
H -0.798220 -1.422785 -1.080903
H 1.206366 -0.125548 -1.782496
H 1.544483 -1.701449 -1.074532
H 0.161549 -1.054199 1.521801
H 3.221323 -0.293273 -0.230487
H 2.151739 -0.560729 1.109794
H 2.899378 1.824172 0.990672
H 2.213944 1.981530 -0.630108
H 1.145748 1.754225 0.748032

TABLE II: Additional calculations to check basis set convergence. B3LYP specific rotation in OR-units. n is the number of basis set functions. See text for further details.

Molecule	Basis Set					
	aVDZ	aVTZ	aVQZ	daVDZ	daVTZ	ORP
1A	100.4	97.4	97.4	101.4	97.9	100.4
1B	170.8	171.5	171.5	174.6	171.9	173.0
1C	25.7	27.3	27.4	26.5	27.4	26.6
1D	-227.0	-226.0	-226.0	-229.2	-226.2	-226.7
1E	-77.9	-77.3	-77.3	-78.5	-77.5	-77.5
n	279	598	1088	392	814	392
2A	83.5	81.5	81.8	82.8	82.2	83.0
n	347	759	1398	489	1036	489
3A	-112.1	-112.7		-111.7		-109.6
n	654	1403		919		919
4A	-47.8	-47.5	-47.0	-48.5	-46.7	-47.1
n	302	644	1168	424	876	424
5A	-3.2	-2.3	-2.0	-2.9	-1.9	-3.0
n	343	736	1340	482	1002	482
6A	215.7	212.7		214.5		213.8