

## Supporting Information for

### **New Methods for Labeling RGD Peptides with Bromine-76**

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**Table S1.** The optimized Cartesian coordinates of stationary points for the reaction **1** + **CH<sub>3</sub>COOBr** with the SCRF-B3LYP/6-31G\* method in water with the Gaussian 09 program package

**Table S2.** Frequencies of stationary points for the reactions of **1** + **CH<sub>3</sub>COOBr** with the SCRF-B3LYP/6-31G\* method in water with the Gaussian 09 program package

**Table S3.** The total energies of reactants, products, and transition states of the reaction **1** + **CH<sub>3</sub>COOBr** with the SCRF-B3LYP/6-31G\* method in water with the Gaussian 09 program package

**Table S4.** The relative energies of reactants, products, and transition states of the reaction **1** + **CH<sub>3</sub>COOBr** with the SCRF-B3LYP/6-31G\* method in water with the Gaussian 09 program package

**Table S1.** The optimized Cartesian coordinates of stationary points for the reaction **1** + **CH<sub>3</sub>COOBr** with the SCRF-B3LYP/6-31G\* method in water with the Gaussian 09 program package

| <b>1 (DMB-c(RGDyK))</b> |           |           |           | <b>2 (CH<sub>3</sub>COOBr)</b> |           |           |           |
|-------------------------|-----------|-----------|-----------|--------------------------------|-----------|-----------|-----------|
| N                       | 2.210586  | -1.232473 | -0.750431 | C                              | 1.403063  | 0.198600  | 0.000384  |
| C                       | 1.010937  | -0.852577 | -1.496203 | O                              | 1.232801  | 1.391850  | -0.000070 |
| C                       | 3.265868  | -1.859716 | -1.338246 | O                              | 0.402795  | -0.730915 | 0.000063  |
| O                       | 3.268227  | -2.250713 | -2.504452 | C                              | 2.728493  | -0.533009 | -0.000151 |
| C                       | -0.266815 | -1.231619 | -0.731790 | H                              | 2.807747  | -1.169651 | 0.885574  |
| C                       | -1.556891 | -0.979096 | -1.524245 | H                              | 2.805621  | -1.172854 | -0.883730 |
| C                       | -2.807611 | -1.442901 | -0.766953 | H                              | 3.531841  | 0.204319  | -0.002381 |
| C                       | -4.095305 | -1.210196 | -1.569369 | Br                             | -1.343409 | -0.032653 | -0.000023 |
| N                       | -5.291491 | -1.671819 | -0.875225 |                                |           |           |           |
| C                       | 1.154062  | 0.629135  | -1.910156 |                                |           |           |           |
| O                       | 1.686996  | 0.931814  | -2.984933 |                                |           |           |           |
| N                       | 0.734398  | 1.567696  | -1.026389 |                                |           |           |           |
| C                       | 0.878983  | 3.006264  | -1.280897 |                                |           |           |           |
| C                       | 2.312760  | 3.427690  | -0.884874 |                                |           |           |           |
| O                       | 2.569170  | 3.968026  | 0.199399  |                                |           |           |           |
| N                       | 3.262206  | 3.117115  | -1.797767 |                                |           |           |           |
| C                       | 4.682635  | 3.360140  | -1.562198 |                                |           |           |           |
| C                       | 5.332002  | 2.275740  | -0.686495 |                                |           |           |           |
| O                       | 6.202946  | 1.514733  | -1.121196 |                                |           |           |           |
| N                       | 4.852646  | 2.217291  | 0.580347  |                                |           |           |           |
| C                       | 5.241715  | 1.162432  | 1.515447  |                                |           |           |           |
| C                       | 4.934224  | 1.612801  | 2.944978  |                                |           |           |           |
| C                       | 5.275569  | 0.602417  | 4.020669  |                                |           |           |           |

|   |           |           |           |  |
|---|-----------|-----------|-----------|--|
| O | 4.747224  | 0.555987  | 5.111256  |  |
| O | 6.274007  | -0.228698 | 3.651933  |  |
| C | 4.477888  | -0.138243 | 1.166027  |  |
| O | 3.440012  | -0.452479 | 1.766217  |  |
| N | 5.020822  | -0.842983 | 0.150564  |  |
| C | -0.191630 | 3.796364  | -0.525865 |  |
| C | -0.235603 | 5.276549  | -0.925370 |  |
| C | -1.341825 | 6.033765  | -0.187321 |  |
| N | -1.345847 | 7.438177  | -0.579526 |  |
| C | -2.142766 | 8.346608  | 0.093087  |  |
| N | -2.120260 | 9.631794  | -0.457687 |  |
| N | -2.742028 | 8.012066  | 1.188746  |  |
| C | 4.498222  | -2.088355 | -0.431761 |  |
| C | 4.277319  | -3.193968 | 0.635027  |  |
| C | 3.948391  | -4.542114 | 0.029566  |  |
| C | 4.955536  | -5.360491 | -0.500204 |  |
| C | 4.662925  | -6.600121 | -1.067677 |  |
| C | 3.337220  | -7.047743 | -1.113325 |  |
| C | 2.316883  | -6.247978 | -0.587168 |  |
| C | 2.628058  | -5.011748 | -0.023965 |  |
| O | 2.981759  | -8.254062 | -1.652105 |  |
| C | -6.094751 | -0.858874 | -0.144848 |  |
| O | -5.928201 | 0.359496  | -0.053546 |  |
| C | -7.236183 | -1.567838 | 0.551284  |  |
| C | -7.059856 | -2.081648 | 1.846255  |  |
| C | -8.127767 | -2.686796 | 2.523160  |  |
| C | -9.368104 | -2.763839 | 1.890375  |  |

|   |           |           |           |  |
|---|-----------|-----------|-----------|--|
| C | -9.571550 | -2.257844 | 0.606785  |  |
| C | -8.496991 | -1.654249 | -0.061111 |  |
| O | -5.802431 | -1.946045 | 2.360310  |  |
| C | -5.547602 | -2.445964 | 3.671952  |  |
| O | -8.573019 | -1.125417 | -1.316809 |  |
| C | -9.820777 | -1.187545 | -2.005497 |  |
| H | 2.316850  | -0.929892 | 0.217935  |  |
| H | 1.053657  | -1.408777 | -2.434680 |  |
| H | -0.187966 | -2.298675 | -0.490452 |  |
| H | -0.312668 | -0.710931 | 0.235509  |  |
| H | -1.649430 | 0.089687  | -1.759248 |  |
| H | -1.496212 | -1.505684 | -2.487056 |  |
| H | -2.719300 | -2.511619 | -0.528487 |  |
| H | -2.886100 | -0.910631 | 0.189977  |  |
| H | -4.232945 | -0.144205 | -1.767525 |  |
| H | -4.038829 | -1.726538 | -2.534606 |  |
| H | -5.477919 | -2.665508 | -0.850216 |  |
| H | 0.369282  | 1.286469  | -0.125540 |  |
| H | 0.757880  | 3.142970  | -2.359645 |  |
| H | 2.983620  | 2.511823  | -2.568478 |  |
| H | 5.200366  | 3.369106  | -2.521270 |  |
| H | 4.791099  | 4.339249  | -1.086424 |  |
| H | 4.080105  | 2.840347  | 0.818549  |  |
| H | 6.313759  | 0.990574  | 1.395183  |  |
| H | 5.502948  | 2.526241  | 3.158271  |  |
| H | 3.873947  | 1.850510  | 3.058209  |  |
| H | 6.444413  | -0.832685 | 4.400849  |  |

|   |            |           |           |  |
|---|------------|-----------|-----------|--|
| H | 5.764187   | -0.372182 | -0.362205 |  |
| H | -1.160855  | 3.326776  | -0.733225 |  |
| H | -0.006245  | 3.709704  | 0.551433  |  |
| H | 0.727555   | 5.752120  | -0.708980 |  |
| H | -0.398422  | 5.355391  | -2.010046 |  |
| H | -2.317996  | 5.559011  | -0.376569 |  |
| H | -1.178640  | 5.991917  | 0.893398  |  |
| H | -1.258265  | 7.592759  | -1.577080 |  |
| H | -2.948824  | 10.177311 | -0.252573 |  |
| H | -1.878457  | 9.694264  | -1.440848 |  |
| H | -3.197499  | 8.832576  | 1.594043  |  |
| H | 5.274007   | -2.433041 | -1.117831 |  |
| H | 5.204516   | -3.255749 | 1.216943  |  |
| H | 3.488661   | -2.883109 | 1.323244  |  |
| H | 5.991308   | -5.029845 | -0.465062 |  |
| H | 5.460964   | -7.221462 | -1.468136 |  |
| H | 1.292155   | -6.605695 | -0.621399 |  |
| H | 1.826498   | -4.401676 | 0.385724  |  |
| H | 3.777179   | -8.706163 | -1.978037 |  |
| H | -8.003088  | -3.089013 | 3.520787  |  |
| H | -10.198732 | -3.231810 | 2.411436  |  |
| H | -10.547301 | -2.334036 | 0.143415  |  |
| H | -4.497601  | -2.228765 | 3.872282  |  |
| H | -5.713178  | -3.528300 | 3.725373  |  |
| H | -6.173343  | -1.943278 | 4.418491  |  |
| H | -9.648532  | -0.713341 | -2.972612 |  |
| H | -10.139913 | -2.224984 | -2.159118 |  |

|   |            |           |           |  |
|---|------------|-----------|-----------|--|
| H | -10.602473 | -0.641031 | -1.465171 |  |
|---|------------|-----------|-----------|--|

| TS1a |           |           |           | TS1a' |           |           |           |
|------|-----------|-----------|-----------|-------|-----------|-----------|-----------|
| N    | 3.388404  | -1.611810 | -0.739137 | N     | 3.548497  | -1.369705 | -0.729530 |
| C    | 2.300169  | -0.928030 | -1.437337 | C     | 2.542181  | -0.891025 | -1.676947 |
| C    | 4.197019  | -2.514937 | -1.358120 | C     | 4.625297  | -2.100207 | -1.131995 |
| O    | 4.024232  | -2.914837 | -2.508284 | O     | 4.782594  | -2.510727 | -2.280769 |
| C    | 1.016061  | -0.921905 | -0.594178 | C     | 1.111642  | -1.179359 | -1.195326 |
| C    | -0.194384 | -0.316657 | -1.318679 | C     | 0.046518  | -0.832011 | -2.244776 |
| C    | -1.487086 | -0.445678 | -0.503341 | C     | -1.376400 | -1.166085 | -1.779643 |
| C    | -2.695494 | 0.155860  | -1.233421 | C     | -2.415895 | -0.876765 | -2.870846 |
| N    | -3.945050 | -0.012743 | -0.495870 | N     | -3.780765 | -1.183772 | -2.452548 |
| C    | 2.822451  | 0.446165  | -1.914029 | C     | 2.854707  | 0.581583  | -2.021841 |
| O    | 3.363961  | 0.560896  | -3.020612 | O     | 3.531101  | 0.866063  | -3.018404 |
| N    | 2.720050  | 1.487197  | -1.051868 | N     | 2.405572  | 1.528138  | -1.161855 |
| C    | 3.239755  | 2.824169  | -1.365862 | C     | 2.668531  | 2.960753  | -1.352442 |
| C    | 4.755124  | 2.841813  | -1.058024 | C     | 4.078604  | 3.276959  | -0.800857 |
| O    | 5.212823  | 3.313382  | -0.008541 | O     | 4.253234  | 3.808174  | 0.304086  |
| N    | 5.528070  | 2.262395  | -2.005626 | N     | 5.097008  | 2.884231  | -1.600568 |
| C    | 6.971768  | 2.109240  | -1.851539 | C     | 6.496277  | 2.997566  | -1.198346 |
| C    | 7.349281  | 0.906392  | -0.971370 | C     | 6.929217  | 1.867763  | -0.248308 |
| O    | 7.949966  | -0.074816 | -1.422070 | O     | 7.763100  | 1.016760  | -0.574076 |
| N    | 6.950343  | 1.009495  | 0.320241  | N     | 6.303988  | 1.880446  | 0.955055  |
| C    | 7.092070  | -0.091545 | 1.272373  | C     | 6.465010  | 0.804686  | 1.931776  |
| C    | 7.003692  | 0.457906  | 2.697753  | C     | 6.026096  | 1.304988  | 3.309599  |
| C    | 7.116794  | -0.583021 | 3.792252  | C     | 6.129972  | 0.285533  | 4.425064  |
| O    | 6.656590  | -0.459540 | 4.907452  | O     | 5.473547  | 0.314871  | 5.444363  |

|   |           |           |           |   |           |           |           |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| O | 7.830372  | -1.663141 | 3.407554  | O | 7.071718  | -0.652009 | 4.184342  |
| C | 5.983285  | -1.140251 | 1.012191  | C | 5.622221  | -0.417158 | 1.490854  |
| O | 4.937413  | -1.143813 | 1.677322  | O | 4.477065  | -0.597125 | 1.929000  |
| N | 6.250720  | -1.989150 | -0.003105 | N | 6.231265  | -1.212004 | 0.584761  |
| C | 2.473298  | 3.892217  | -0.583404 | C | 1.577459  | 3.793496  | -0.676335 |
| C | 2.813301  | 5.321512  | -1.023887 | C | 1.649181  | 5.285787  | -1.023563 |
| C | 2.005387  | 6.361125  | -0.244137 | C | 0.538740  | 6.077164  | -0.328528 |
| N | 2.348585  | 7.708871  | -0.682337 | N | 0.620339  | 7.491255  | -0.674380 |
| C | 1.858997  | 8.806868  | 0.001973  | C | -0.150521 | 8.418715  | 0.003178  |
| N | 2.179084  | 10.030916 | -0.593547 | N | -0.055883 | 9.714782  | -0.513625 |
| N | 1.264075  | 8.661117  | 1.140534  | N | -0.790988 | 8.085636  | 1.075819  |
| C | 5.372460  | -3.054568 | -0.509964 | C | 5.668512  | -2.420483 | -0.036521 |
| C | 4.923834  | -4.033294 | 0.608044  | C | 5.163624  | -3.445612 | 1.013405  |
| C | 4.183470  | -5.241853 | 0.075266  | C | 4.764729  | -4.772310 | 0.402264  |
| C | 4.875552  | -6.318711 | -0.495966 | C | 5.731682  | -5.716281 | 0.029618  |
| C | 4.203303  | -7.433060 | -0.996574 | C | 5.374823  | -6.939576 | -0.536647 |
| C | 2.805998  | -7.489126 | -0.930845 | C | 4.023289  | -7.242785 | -0.740817 |
| C | 2.095740  | -6.426696 | -0.361459 | C | 3.041714  | -6.316300 | -0.372621 |
| C | 2.784477  | -5.320728 | 0.133382  | C | 3.417089  | -5.098394 | 0.191406  |
| O | 2.085568  | -8.553707 | -1.399041 | O | 3.604015  | -8.424869 | -1.287262 |
| C | -4.461197 | 0.936397  | 0.314118  | C | -4.683611 | -0.239182 | -2.110991 |
| O | -3.969601 | 2.049043  | 0.493110  | O | -4.481732 | 0.973200  | -2.147071 |
| C | -5.748131 | 0.529597  | 1.015971  | C | -6.032065 | -0.785610 | -1.667477 |
| C | -5.721586 | 0.213767  | 2.390444  | C | -6.279301 | -1.023816 | -0.321885 |
| C | -6.926163 | -0.059338 | 3.133426  | C | -7.630189 | -1.435889 | 0.148334  |
| C | -8.116830 | -0.039455 | 2.497949  | C | -8.635100 | -1.645890 | -0.913340 |
| C | -8.237709 | 0.232006  | 1.050167  | C | -8.376035 | -1.416018 | -2.218946 |

|   |           |           |           |   |           |           |           |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | -6.968840 | 0.607672  | 0.360618  | C | -7.064790 | -0.966279 | -2.608229 |
| O | -4.525901 | 0.184882  | 2.939743  | O | -5.259160 | -0.885286 | 0.494458  |
| C | -4.340448 | -0.099364 | 4.348209  | C | -5.303742 | -1.059591 | 1.939207  |
| O | -6.953399 | 0.989575  | -0.897057 | O | -6.740820 | -0.704693 | -3.859120 |
| C | -8.157156 | 1.371018  | -1.625298 | C | -7.694984 | -0.858388 | -4.937352 |
| H | 3.631492  | -1.328836 | 0.210316  | H | 3.529527  | -1.046447 | 0.237737  |
| H | 2.131099  | -1.493477 | -2.355882 | H | 2.727267  | -1.436676 | -2.604006 |
| H | 0.803765  | -1.966263 | -0.334724 | H | 1.061736  | -2.249231 | -0.959438 |
| H | 1.180627  | -0.406091 | 0.362852  | H | 0.897538  | -0.654460 | -0.253645 |
| H | -0.006630 | 0.741981  | -1.541469 | H | 0.102548  | 0.235888  | -2.495504 |
| H | -0.322881 | -0.820694 | -2.286836 | H | 0.266433  | -1.380983 | -3.171125 |
| H | -1.685096 | -1.504975 | -0.291611 | H | -1.433857 | -2.225544 | -1.495337 |
| H | -1.373066 | 0.056126  | 0.466347  | H | -1.626665 | -0.582992 | -0.883994 |
| H | -2.554953 | 1.228430  | -1.388723 | H | -2.400863 | 0.180521  | -3.145519 |
| H | -2.820350 | -0.312674 | -2.215541 | H | -2.193256 | -1.461371 | -3.770892 |
| H | -4.404185 | -0.913680 | -0.533747 | H | -4.044276 | -2.156394 | -2.358044 |
| H | 2.324450  | 1.344571  | -0.131458 | H | 1.915746  | 1.253486  | -0.319831 |
| H | 3.097963  | 2.968663  | -2.441132 | H | 2.666240  | 3.136616  | -2.432643 |
| H | 5.049703  | 1.738854  | -2.737154 | H | 4.858131  | 2.300361  | -2.401297 |
| H | 7.414405  | 1.954715  | -2.835385 | H | 7.121814  | 2.943804  | -2.089182 |
| H | 7.372834  | 3.030111  | -1.418043 | H | 6.641313  | 3.968541  | -0.715628 |
| H | 6.391536  | 1.824344  | 0.575590  | H | 5.571912  | 2.577555  | 1.095204  |
| H | 8.067752  | -0.553241 | 1.104425  | H | 7.520702  | 0.524659  | 1.949446  |
| H | 7.812487  | 1.183646  | 2.847704  | H | 6.648830  | 2.163820  | 3.588958  |
| H | 6.057672  | 0.981317  | 2.854895  | H | 4.987928  | 1.644648  | 3.286013  |
| H | 7.870632  | -2.273932 | 4.169138  | H | 7.086847  | -1.256111 | 4.952241  |
| H | 7.059518  | -1.749578 | -0.573912 | H | 7.082748  | -0.835788 | 0.172661  |



|   |           |           |           |   |           |           |           |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | 1.401877  | 3.706208  | -0.726202 | H | 0.607112  | 3.388427  | -0.988226 |
| H | 2.689488  | 3.774449  | 0.485246  | H | 1.654924  | 3.665129  | 0.410034  |
| H | 3.881721  | 5.514867  | -0.877230 | H | 2.620567  | 5.694749  | -0.724703 |
| H | 2.609514  | 5.429026  | -2.099043 | H | 1.565811  | 5.410477  | -2.112865 |
| H | 0.926875  | 6.163993  | -0.354355 | H | -0.445863 | 5.654891  | -0.587030 |
| H | 2.227564  | 6.292833  | 0.824619  | H | 0.637180  | 5.997642  | 0.757700  |
| H | 2.408938  | 7.816891  | -1.687998 | H | 0.748620  | 7.672496  | -1.662972 |
| H | 1.537003  | 10.778401 | -0.358358 | H | -0.859212 | 10.295278 | -0.303758 |
| H | 2.363408  | 10.010226 | -1.590864 | H | 0.199007  | 9.789066  | -1.492779 |
| H | 1.062771  | 9.579672  | 1.541201  | H | -1.219863 | 8.915750  | 1.490295  |
| H | 5.980200  | -3.614123 | -1.223156 | H | 6.496049  | -2.877000 | -0.582488 |
| H | 5.834329  | -4.347384 | 1.132032  | H | 5.981976  | -3.588306 | 1.729255  |
| H | 4.306825  | -3.497958 | 1.332591  | H | 4.326914  | -3.016221 | 1.567743  |
| H | 5.961922  | -6.293770 | -0.546866 | H | 6.785516  | -5.499237 | 0.190248  |
| H | 4.761062  | -8.259608 | -1.431083 | H | 6.142089  | -7.659364 | -0.813310 |
| H | 1.012494  | -6.481236 | -0.308584 | H | 1.995570  | -6.562761 | -0.527829 |
| H | 2.220652  | -4.504122 | 0.578097  | H | 2.644077  | -4.389351 | 0.478081  |
| H | 2.694525  | -9.217189 | -1.762798 | H | 4.377410  | -8.974265 | -1.495149 |
| H | -6.872366 | -0.285415 | 4.190064  | H | -7.599484 | -2.252003 | 0.874428  |
| H | -9.037606 | -0.249466 | 3.030755  | H | -9.612730 | -1.985771 | -0.590202 |
| H | -9.087693 | 0.867296  | 0.793170  | H | -9.145401 | -1.563572 | -2.965243 |
| H | -3.264091 | -0.049741 | 4.499061  | H | -4.464839 | -1.716351 | 2.173015  |
| H | -4.709058 | -1.099883 | 4.582730  | H | -6.244199 | -1.469154 | 2.312564  |
| H | -4.841847 | 0.657553  | 4.954665  | H | -5.136270 | -0.071581 | 2.372123  |
| H | -7.863031 | 1.320800  | -2.672819 | H | -7.146078 | -0.576434 | -5.833604 |
| H | -9.009693 | 0.714627  | -1.422735 | H | -8.021706 | -1.897952 | -5.006764 |
| H | -8.395873 | 2.403427  | -1.355679 | H | -8.544015 | -0.188040 | -4.788624 |

|    |            |           |           |    |           |           |          |
|----|------------|-----------|-----------|----|-----------|-----------|----------|
| Br | -8.787558  | -1.536658 | 0.239754  | Br | -8.359671 | 0.073378  | 1.282366 |
| O  | -11.077333 | 0.337528  | -0.984343 | O  | -7.907611 | -1.902783 | 3.719986 |
| C  | -11.709678 | -0.721319 | -1.273336 | C  | -8.449822 | -1.027258 | 4.452279 |
| O  | -11.235279 | -1.862041 | -1.524631 | O  | -8.733080 | 0.170916  | 4.161008 |
| C  | -13.249701 | -0.575118 | -1.352550 | C  | -8.778297 | -1.472501 | 5.899011 |
| H  | -13.517712 | 0.012514  | -2.240233 | H  | -7.845338 | -1.569137 | 6.469382 |
| H  | -13.747662 | -1.547198 | -1.416777 | H  | -9.425237 | -0.754969 | 6.412286 |
| H  | -13.627340 | -0.027711 | -0.481202 | H  | -9.255638 | -2.458834 | 5.894702 |

| <b>TS1b</b> |           |           |           | <b>TS1b'</b> |           |           |           |
|-------------|-----------|-----------|-----------|--------------|-----------|-----------|-----------|
| N           | 2.120118  | 0.517496  | -0.827526 | N            | 1.271947  | 0.537076  | -0.162433 |
| C           | 0.850571  | 0.527878  | -1.555898 | C            | 0.160300  | 0.115958  | -1.016929 |
| C           | 3.305356  | 0.244633  | -1.433274 | C            | 2.562081  | 0.526488  | -0.592055 |
| O           | 3.415379  | -0.132785 | -2.598533 | O            | 2.929512  | 0.034915  | -1.658166 |
| C           | -0.241905 | -0.226554 | -0.783740 | C            | -0.811292 | -0.808131 | -0.267278 |
| C           | -1.554164 | -0.380026 | -1.565121 | C            | -1.900381 | -1.407195 | -1.168228 |
| C           | -2.600327 | -1.192684 | -0.791832 | C            | -2.810517 | -2.387497 | -0.417954 |
| C           | -3.897152 | -1.386203 | -1.589175 | C            | -3.865732 | -3.018254 | -1.336852 |
| N           | -4.890420 | -2.172025 | -0.867720 | N            | -4.730674 | -3.966293 | -0.645484 |
| C           | 0.545654  | 1.992092  | -1.945267 | C            | -0.445715 | 1.383980  | -1.660675 |
| O           | 0.988354  | 2.463006  | -3.000229 | O            | 0.009546  | 1.824639  | -2.723325 |
| N           | -0.156361 | 2.741780  | -1.060833 | N            | -1.436866 | 2.014387  | -0.985174 |
| C           | -0.435925 | 4.165365  | -1.286120 | C            | -2.048339 | 3.260166  | -1.464650 |
| C           | 0.805942  | 4.979061  | -0.854189 | C            | -1.142539 | 4.440531  | -1.043090 |
| O           | 0.882180  | 5.536442  | 0.248872  | O            | -1.380029 | 5.134850  | -0.045933 |
| N           | 1.811075  | 4.994559  | -1.760231 | N            | -0.052971 | 4.620646  | -1.825248 |
| C           | 3.089841  | 5.647619  | -1.497354 | C            | 0.960368  | 5.628905  | -1.530014 |

|   |           |           |           |   |           |           |           |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 4.032792  | 4.785242  | -0.642501 | C | 1.959131  | 5.167964  | -0.456244 |
| O | 5.098797  | 4.342530  | -1.084418 | O | 3.155967  | 4.988620  | -0.707259 |
| N | 3.585833  | 4.539103  | 0.613204  | N | 1.413694  | 4.957117  | 0.766500  |
| C | 4.279779  | 3.633610  | 1.528449  | C | 2.177546  | 4.396275  | 1.880821  |
| C | 3.832333  | 3.923395  | 2.962590  | C | 1.461706  | 4.715480  | 3.194823  |
| C | 4.463088  | 3.041842  | 4.020535  | C | 2.136613  | 4.174918  | 4.438453  |
| O | 3.962073  | 2.796365  | 5.097192  | O | 1.562781  | 3.921548  | 5.476209  |
| O | 5.680039  | 2.584912  | 3.654609  | O | 3.472024  | 4.043996  | 4.285909  |
| C | 3.969067  | 2.169557  | 1.133628  | C | 2.324183  | 2.867357  | 1.686617  |
| O | 3.098885  | 1.513946  | 1.723127  | O | 1.588463  | 2.068145  | 2.282763  |
| N | 4.692755  | 1.712786  | 0.087445  | N | 3.277672  | 2.509982  | 0.798715  |
| C | -1.701022 | 4.588289  | -0.537042 | C | -3.473221 | 3.396866  | -0.925226 |
| C | -2.162301 | 6.007706  | -0.890698 | C | -4.250246 | 4.555207  | -1.563204 |
| C | -3.468133 | 6.373313  | -0.181235 | C | -5.682164 | 4.636729  | -1.030023 |
| N | -3.871220 | 7.732442  | -0.522078 | N | -6.398707 | 5.743061  | -1.653830 |
| C | -4.926138 | 8.332111  | 0.141750  | C | -7.658772 | 6.093790  | -1.203521 |
| N | -5.265885 | 9.591333  | -0.362702 | N | -8.274113 | 7.090155  | -1.967825 |
| N | -5.438844 | 7.783823  | 1.194342  | N | -8.128025 | 5.594118  | -0.107264 |
| C | 4.568442  | 0.397528  | -0.550194 | C | 3.604826  | 1.145628  | 0.370458  |
| C | 4.728214  | -0.763031 | 0.468203  | C | 3.946404  | 0.221627  | 1.571698  |
| C | 4.767597  | -2.118866 | -0.199863 | C | 4.490414  | -1.119353 | 1.130007  |
| C | 5.927592  | -2.523456 | -0.934883 | C | 5.825692  | -1.314247 | 0.909974  |
| C | 6.032478  | -3.739384 | -1.588723 | C | 6.369744  | -2.593873 | 0.435030  |
| C | 4.952808  | -4.624439 | -1.555214 | C | 5.396190  | -3.691392 | 0.281943  |
| C | 3.745725  | -4.314325 | -0.766425 | C | 4.035194  | -3.473724 | 0.494741  |
| C | 3.719333  | -2.991241 | -0.126451 | C | 3.608210  | -2.222742 | 0.912261  |
| O | 4.908994  | -5.768388 | -2.210135 | O | 5.923279  | -4.856561 | -0.044201 |

|   |           |           |           |   |           |           |           |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | -5.985980 | -1.638722 | -0.271633 | C | -5.986214 | -3.671079 | -0.225636 |
| O | -6.272255 | -0.440199 | -0.318305 | O | -6.530685 | -2.581747 | -0.419382 |
| C | -6.848211 | -2.639944 | 0.466051  | C | -6.684572 | -4.798618 | 0.503340  |
| C | -6.746716 | -2.755774 | 1.862675  | C | -6.715222 | -4.813239 | 1.907726  |
| C | -7.581217 | -3.635192 | 2.565993  | C | -7.411313 | -5.818131 | 2.593533  |
| C | -8.518352 | -4.386171 | 1.856711  | C | -8.077399 | -6.797974 | 1.857707  |
| C | -8.643712 | -4.287006 | 0.471470  | C | -8.066603 | -6.804810 | 0.463269  |
| C | -7.802523 | -3.406345 | -0.223027 | C | -7.366812 | -5.795758 | -0.213058 |
| O | -5.790458 | -1.975424 | 2.444425  | O | -6.022708 | -3.807214 | 2.516481  |
| C | -5.622995 | -2.046572 | 3.859346  | C | -6.005314 | -3.760670 | 3.942216  |
| O | -7.834390 | -3.221924 | -1.575153 | O | -7.288712 | -5.695084 | -1.572046 |
| C | -8.776607 | -3.971177 | -2.340660 | C | -7.956695 | -6.674047 | -2.366202 |
| H | 2.140150  | 0.818330  | 0.146612  | H | 1.075787  | 0.957756  | 0.746023  |
| H | 1.044118  | 0.021341  | -2.503595 | H | 0.612282  | -0.429719 | -1.847585 |
| H | 0.162581  | -1.218785 | -0.549604 | H | -0.212115 | -1.617610 | 0.167023  |
| H | -0.435920 | 0.250980  | 0.187448  | H | -1.270947 | -0.288349 | 0.586043  |
| H | -1.966644 | 0.609054  | -1.805267 | H | -2.511346 | -0.605276 | -1.603626 |
| H | -1.343929 | -0.871718 | -2.525197 | H | -1.421135 | -1.925378 | -2.010769 |
| H | -2.184754 | -2.176649 | -0.534339 | H | -2.203027 | -3.183606 | 0.033795  |
| H | -2.838628 | -0.693031 | 0.156256  | H | -3.320808 | -1.872450 | 0.406470  |
| H | -4.359270 | -0.420969 | -1.810107 | H | -4.514241 | -2.246365 | -1.758671 |
| H | -3.683202 | -1.882929 | -2.543259 | H | -3.378153 | -3.539012 | -2.169478 |
| H | -4.725523 | -3.163015 | -0.751462 | H | -4.356580 | -4.876608 | -0.412968 |
| H | -0.444197 | 2.343118  | -0.176424 | H | -1.736750 | 1.664417  | -0.084397 |
| H | -0.577797 | 4.287329  | -2.364145 | H | -2.061815 | 3.199595  | -2.557069 |
| H | 1.734743  | 4.351110  | -2.546374 | H | 0.159971  | 3.885770  | -2.498116 |
| H | 3.586277  | 5.841481  | -2.447999 | H | 1.522687  | 5.838800  | -2.439754 |

|   |           |           |           |   |           |           |           |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | 2.893908  | 6.598617  | -0.993567 | H | 0.453849  | 6.541405  | -1.202356 |
| H | 2.659692  | 4.890067  | 0.859769  | H | 0.403679  | 5.069725  | 0.857893  |
| H | 5.352618  | 3.810721  | 1.423019  | H | 3.170085  | 4.852852  | 1.868589  |
| H | 4.084275  | 4.962770  | 3.206757  | H | 1.394169  | 5.804896  | 3.303707  |
| H | 2.749835  | 3.814331  | 3.062031  | H | 0.443247  | 4.320277  | 3.188150  |
| H | 6.024457  | 2.044717  | 4.392380  | H | 3.832391  | 3.711758  | 5.131143  |
| H | 5.238446  | 2.415202  | -0.410430 | H | 3.685675  | 3.271799  | 0.258025  |
| H | -2.490876 | 3.868899  | -0.784976 | H | -3.994732 | 2.451434  | -1.117687 |
| H | -1.517792 | 4.518430  | 0.541884  | H | -3.430738 | 3.535533  | 0.161682  |
| H | -1.388857 | 6.732402  | -0.613232 | H | -3.739363 | 5.504124  | -1.364974 |
| H | -2.302396 | 6.084855  | -1.978642 | H | -4.271369 | 4.420740  | -2.654350 |
| H | -4.253725 | 5.643498  | -0.434987 | H | -6.201870 | 3.678542  | -1.191451 |
| H | -3.339153 | 6.328161  | 0.904023  | H | -5.677498 | 4.811140  | 0.049786  |
| H | -3.796862 | 7.954840  | -1.507826 | H | -6.259914 | 5.817601  | -2.654702 |
| H | -6.224436 | 9.860433  | -0.175206 | H | -9.285318 | 7.083443  | -1.905871 |
| H | -5.021600 | 9.767000  | -1.331480 | H | -7.970246 | 7.167664  | -2.932617 |
| H | -6.132618 | 8.412810  | 1.603903  | H | -9.020882 | 6.038752  | 0.115980  |
| H | 5.392833  | 0.344476  | -1.263774 | H | 4.503635  | 1.239991  | -0.241266 |
| H | 5.662756  | -0.589192 | 1.013818  | H | 4.696915  | 0.742547  | 2.174078  |
| H | 3.916565  | -0.727731 | 1.196074  | H | 3.062451  | 0.088575  | 2.198786  |
| H | 6.777053  | -1.846952 | -0.978066 | H | 6.542799  | -0.513844 | 1.062784  |
| H | 6.932414  | -3.996097 | -2.138534 | H | 7.335731  | -2.902709 | 0.855008  |
| H | 2.807128  | -4.647127 | -1.228257 | H | 3.324024  | -4.282277 | 0.357842  |
| H | 2.820885  | -2.744488 | 0.429688  | H | 2.545971  | -2.077847 | 1.088373  |
| H | 5.738920  | -5.936380 | -2.696130 | H | 5.236797  | -5.541509 | -0.157354 |
| H | -7.508382 | -3.737333 | 3.641596  | H | -7.438165 | -5.842334 | 3.675895  |
| H | -9.167975 | -5.068095 | 2.398409  | H | -8.618687 | -7.578200 | 2.385636  |

|    |           |           |           |    |           |           |           |
|----|-----------|-----------|-----------|----|-----------|-----------|-----------|
| H  | -9.382843 | -4.883204 | -0.049171 | H  | -8.594694 | -7.579756 | -0.078202 |
| H  | -4.819559 | -1.348173 | 4.097336  | H  | -5.406671 | -2.886685 | 4.202326  |
| H  | -5.335304 | -3.055646 | 4.177049  | H  | -5.541856 | -4.659854 | 4.364770  |
| H  | -6.536498 | -1.744499 | 4.384788  | H  | -7.016440 | -3.644984 | 4.349616  |
| H  | -8.621253 | -3.670074 | -3.377539 | H  | -7.760702 | -6.397258 | -3.402986 |
| H  | -8.601921 | -5.049028 | -2.243360 | H  | -7.562056 | -7.679050 | -2.176109 |
| H  | -9.806196 | -3.739766 | -2.043510 | H  | -9.037683 | -6.665443 | -2.184270 |
| Br | 3.787263  | -5.646944 | 0.777936  | Br | 7.002056  | -2.196978 | -1.464304 |
| O  | 1.183511  | -6.274093 | -0.771778 | O  | 9.513014  | -3.147527 | 0.074174  |
| C  | 0.963696  | -7.173192 | 0.080542  | C  | 10.149446 | -3.009639 | -1.003729 |
| O  | 1.676169  | -7.525335 | 1.069409  | O  | 9.723861  | -2.638918 | -2.138514 |
| C  | -0.336158 | -8.000420 | -0.094874 | C  | 11.660222 | -3.354120 | -0.941512 |
| H  | -0.081570 | -9.000644 | -0.466890 | H  | 11.777520 | -4.423554 | -0.728835 |
| H  | -0.843992 | -8.130506 | 0.866427  | H  | 12.174831 | -3.118752 | -1.876590 |
| H  | -1.012383 | -7.522527 | -0.808954 | H  | 12.129934 | -2.805788 | -0.117358 |

| <b>3a</b> |           |           |           | <b>3a'</b> |           |           |           |
|-----------|-----------|-----------|-----------|------------|-----------|-----------|-----------|
| N         | 2.978673  | -1.355291 | -0.731924 | N          | 2.891871  | -1.331767 | -0.734493 |
| C         | 1.805886  | -0.895411 | -1.475666 | C          | 1.792560  | -0.851234 | -1.571400 |
| C         | 3.990052  | -2.048787 | -1.322526 | C          | 3.952054  | -2.014477 | -1.247454 |
| O         | 3.963079  | -2.441617 | -2.487791 | O          | 4.023457  | -2.392732 | -2.415624 |
| C         | 0.508240  | -1.174122 | -0.702068 | C          | 0.428117  | -1.137081 | -0.925744 |
| C         | -0.763610 | -0.851582 | -1.498634 | C          | -0.760445 | -0.779052 | -1.828707 |
| C         | -2.042191 | -1.181115 | -0.717807 | C          | -2.112971 | -1.112046 | -1.186149 |
| C         | -3.309720 | -0.902181 | -1.536588 | C          | -3.287243 | -0.771089 | -2.112773 |
| N         | -4.535103 | -1.218212 | -0.810936 | N          | -4.586093 | -1.092003 | -1.530658 |
| C         | 2.053790  | 0.569470  | -1.901832 | C          | 2.082529  | 0.620724  | -1.944401 |

|   |           |           |           |   |           |           |           |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| O | 2.617467  | 0.824544  | -2.973324 | O | 2.747030  | 0.892959  | -2.951947 |
| N | 1.689489  | 1.542987  | -1.031669 | N | 1.637223  | 1.580443  | -1.096719 |
| C | 1.935682  | 2.966431  | -1.294640 | C | 1.904029  | 3.007480  | -1.316174 |
| C | 3.393283  | 3.290679  | -0.893774 | C | 3.317790  | 3.326732  | -0.777694 |
| O | 3.681402  | 3.817026  | 0.189433  | O | 3.502938  | 3.831649  | 0.337722  |
| N | 4.322803  | 2.913539  | -1.801936 | N | 4.329026  | 2.971198  | -1.603702 |
| C | 5.755491  | 3.062284  | -1.563344 | C | 5.732305  | 3.116508  | -1.228140 |
| C | 6.329554  | 1.941348  | -0.681213 | C | 6.223820  | 1.976150  | -0.321358 |
| O | 7.151485  | 1.124351  | -1.109901 | O | 7.083359  | 1.168346  | -0.689592 |
| N | 5.842539  | 1.918373  | 0.583732  | N | 5.621637  | 1.925531  | 0.892052  |
| C | 6.158755  | 0.844474  | 1.524859  | C | 5.852685  | 0.832603  | 1.836271  |
| C | 5.873892  | 1.320180  | 2.951005  | C | 5.433905  | 1.279068  | 3.238599  |
| C | 6.139334  | 0.292171  | 4.031352  | C | 5.604406  | 0.233018  | 4.320655  |
| O | 5.594402  | 0.277453  | 5.114669  | O | 4.962949  | 0.198384  | 5.349238  |
| O | 7.092682  | -0.596086 | 3.676445  | O | 6.589865  | -0.646713 | 4.039725  |
| C | 5.315027  | -0.406414 | 1.177677  | C | 5.049530  | -0.413389 | 1.388095  |
| O | 4.262248  | -0.657176 | 1.781870  | O | 3.949842  | -0.682680 | 1.892555  |
| N | 5.810222  | -1.142012 | 0.159859  | N | 5.634751  | -1.123314 | 0.400156  |
| C | 0.919611  | 3.832866  | -0.548064 | C | 0.821645  | 3.861786  | -0.653697 |
| C | 0.984735  | 5.313127  | -0.945042 | C | 0.918826  | 5.348192  | -1.019841 |
| C | -0.063417 | 6.144818  | -0.202373 | C | -0.203982 | 6.162842  | -0.373838 |
| N | 0.021339  | 7.545705  | -0.597844 | N | -0.078858 | 7.573282  | -0.722609 |
| C | -0.706626 | 8.505680  | 0.081483  | C | -0.903264 | 8.511216  | -0.127414 |
| N | -0.612029 | 9.784568  | -0.476425 | N | -0.743438 | 9.804796  | -0.633991 |
| N | -1.308914 | 8.214598  | 1.187938  | N | -1.651567 | 8.187114  | 0.875867  |
| C | 5.210601  | -2.352237 | -0.422094 | C | 5.096492  | -2.325368 | -0.254316 |
| C | 4.930040  | -3.446014 | 0.642963  | C | 4.740763  | -3.443196 | 0.762210  |

|   |           |           |           |   |           |           |           |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 4.517127  | -4.769519 | 0.034534  | C | 4.379670  | -4.754602 | 0.097364  |
| C | 5.471564  | -5.648576 | -0.495633 | C | 5.374121  | -5.617552 | -0.383463 |
| C | 5.102484  | -6.865479 | -1.067958 | C | 5.053418  | -6.823646 | -1.005545 |
| C | 3.751167  | -7.227785 | -1.118555 | C | 3.711271  | -7.191534 | -1.157698 |
| C | 2.782385  | -6.366661 | -0.591737 | C | 2.702827  | -6.346695 | -0.681401 |
| C | 3.169802  | -5.154577 | -0.023341 | C | 3.042171  | -5.145067 | -0.062251 |
| O | 3.321061  | -8.407068 | -1.662702 | O | 3.327529  | -8.361156 | -1.754804 |
| C | -5.337220 | -0.282758 | -0.250119 | C | -5.472707 | -0.155801 | -1.111449 |
| O | -5.157312 | 0.932773  | -0.359024 | O | -5.264721 | 1.057068  | -1.154311 |
| C | -6.511718 | -0.843100 | 0.525427  | C | -6.778399 | -0.713904 | -0.580028 |
| C | -6.339368 | -1.324638 | 1.838130  | C | -6.977300 | -0.821064 | 0.800332  |
| C | -7.443539 | -1.787095 | 2.563960  | C | -8.222591 | -1.248805 | 1.285319  |
| C | -8.709807 | -1.775777 | 1.977674  | C | -9.250560 | -1.566952 | 0.406032  |
| C | -8.880969 | -1.303147 | 0.681722  | C | -9.059117 | -1.463012 | -0.972209 |
| C | -7.785373 | -0.825345 | -0.052565 | C | -7.824934 | -1.028936 | -1.469077 |
| O | -5.064458 | -1.295346 | 2.312400  | O | -5.962988 | -0.453437 | 1.648623  |
| C | -4.820877 | -1.760044 | 3.641567  | C | -5.168550 | -1.539917 | 2.159491  |
| O | -7.922539 | -0.405106 | -1.351287 | O | -7.536246 | -0.880530 | -2.790009 |
| C | -8.315320 | 0.974273  | -1.502023 | C | -8.553183 | -1.180340 | -3.747544 |
| H | 3.105998  | -1.061455 | 0.236564  | H | 2.936462  | -1.051048 | 0.245184  |
| H | 1.803670  | -1.460514 | -2.409889 | H | 1.872424  | -1.397390 | -2.513481 |
| H | 0.515877  | -2.238971 | -0.439531 | H | 0.403236  | -2.208326 | -0.691992 |
| H | 0.500090  | -0.632504 | 0.254843  | H | 0.337620  | -0.620160 | 0.040509  |
| H | -0.773146 | 0.210564  | -1.777392 | H | -0.732823 | 0.290308  | -2.077109 |
| H | -0.751236 | -1.420309 | -2.438860 | H | -0.663432 | -1.321469 | -2.779544 |
| H | -2.029717 | -2.238217 | -0.418850 | H | -2.148919 | -2.180003 | -0.931102 |
| H | -2.079563 | -0.591517 | 0.207402  | H | -2.228998 | -0.557435 | -0.245832 |



|   |           |           |           |   |           |           |           |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | -3.368108 | 0.154719  | -1.806894 | H | -3.299463 | 0.298206  | -2.336764 |
| H | -3.296680 | -1.485763 | -2.464637 | H | -3.187995 | -1.311923 | -3.061693 |
| H | -4.745061 | -2.191348 | -0.630295 | H | -4.860832 | -2.064221 | -1.479249 |
| H | 1.291507  | 1.295457  | -0.134934 | H | 1.145830  | 1.321694  | -0.250745 |
| H | 1.829524  | 3.105617  | -2.374737 | H | 1.897314  | 3.162491  | -2.399289 |
| H | 4.006462  | 2.322053  | -2.568806 | H | 4.088887  | 2.392336  | -2.406938 |
| H | 6.274887  | 3.031951  | -2.521139 | H | 6.339835  | 3.108855  | -2.132910 |
| H | 5.928060  | 4.034304  | -1.091863 | H | 5.855992  | 4.077595  | -0.720388 |
| H | 5.112079  | 2.591691  | 0.817441  | H | 4.871092  | 2.593411  | 1.071419  |
| H | 7.218111  | 0.603526  | 1.410786  | H | 6.918942  | 0.595567  | 1.816413  |
| H | 6.502658  | 2.193348  | 3.164432  | H | 6.034010  | 2.151374  | 3.525554  |
| H | 4.831606  | 1.630018  | 3.056773  | H | 4.384148  | 1.581195  | 3.252754  |
| H | 7.217553  | -1.207978 | 4.427915  | H | 6.646966  | -1.271001 | 4.789205  |
| H | 6.581841  | -0.718548 | -0.352807 | H | 6.444438  | -0.685114 | -0.035687 |
| H | -0.079793 | 3.435493  | -0.762627 | H | -0.152783 | 3.466770  | -0.965773 |
| H | 1.090117  | 3.733100  | 0.530599  | H | 0.892170  | 3.745687  | 0.434458  |
| H | 1.980229  | 5.715941  | -0.727923 | H | 1.885200  | 5.750838  | -0.696530 |
| H | 0.827231  | 5.406210  | -2.029362 | H | 0.871238  | 5.457950  | -2.112923 |
| H | -1.070021 | 5.734550  | -0.383317 | H | -1.184937 | 5.759254  | -0.671790 |
| H | 0.104824  | 6.095114  | 0.877192  | H | -0.151982 | 6.083647  | 0.715966  |
| H | 0.107834  | 7.692336  | -1.596615 | H | 0.137604  | 7.743470  | -1.697652 |
| H | -1.399455 | 10.383002 | -0.257201 | H | -1.558093 | 10.394079 | -0.510154 |
| H | -0.387464 | 9.827857  | -1.464751 | H | -0.383333 | 9.875856  | -1.579697 |
| H | -1.706099 | 9.063974  | 1.594997  | H | -2.111218 | 9.022634  | 1.243810  |
| H | 5.960553  | -2.741237 | -1.113110 | H | 5.904793  | -2.693198 | -0.888815 |
| H | 5.855407  | -3.565757 | 1.218642  | H | 5.620715  | -3.573222 | 1.403223  |
| H | 4.165989  | -3.090249 | 1.337275  | H | 3.925540  | -3.103647 | 1.404547  |

|    |            |           |           |    |            |           |           |
|----|------------|-----------|-----------|----|------------|-----------|-----------|
| H  | 6.526194   | -5.384335 | -0.457498 | H  | 6.421873   | -5.349359 | -0.266174 |
| H  | 5.860746   | -7.534616 | -1.468749 | H  | 5.842157   | -7.480171 | -1.366246 |
| H  | 1.737093   | -6.658561 | -0.629331 | H  | 1.664602   | -6.643098 | -0.797365 |
| H  | 2.407132   | -4.497025 | 0.387144  | H  | 2.248650   | -4.500381 | 0.308196  |
| H  | 4.086940   | -8.907465 | -1.988780 | H  | 4.117357   | -8.850465 | -2.037770 |
| H  | -9.564046  | -2.142884 | 2.536215  | H  | -10.209843 | -1.893319 | 0.792623  |
| H  | -3.749405  | -1.638906 | 3.803758  | H  | -9.875476  | -1.711810 | -1.638740 |
| H  | -5.090329  | -2.817085 | 3.747444  | H  | -4.422352  | -1.084086 | 2.812479  |
| H  | -5.372658  | -1.163479 | 4.376939  | H  | -4.668522  | -2.068762 | 1.340961  |
| H  | -8.389221  | 1.147689  | -2.577284 | H  | -5.783611  | -2.237790 | 2.736018  |
| H  | -9.289188  | 1.153169  | -1.034734 | H  | -8.104503  | -0.988950 | -4.722731 |
| H  | -7.555164  | 1.629994  | -1.067844 | H  | -8.859059  | -2.230820 | -3.684666 |
| H  | -7.333313  | -2.159952 | 3.574735  | H  | -9.427274  | -0.533299 | -3.612724 |
| Br | -10.616922 | -1.333011 | -0.119192 | Br | -8.522793  | -1.359095 | 3.170217  |

| <b>3b</b> |           |           |           | <b>3b'</b> |           |           |           |
|-----------|-----------|-----------|-----------|------------|-----------|-----------|-----------|
| N         | 2.343387  | -0.406804 | -0.685800 | N          | 1.984744  | -0.011709 | -0.415541 |
| C         | 1.100171  | -0.289400 | -1.448456 | C          | 0.778457  | -0.195469 | -1.222502 |
| C         | 3.510903  | -0.805512 | -1.260125 | C          | 3.233481  | -0.193394 | -0.924337 |
| O         | 3.601351  | -1.218927 | -2.414956 | O          | 3.457487  | -0.624220 | -2.054220 |
| C         | -0.086884 | -0.905701 | -0.692699 | C          | -0.295268 | -0.979500 | -0.452672 |
| C         | -1.385533 | -0.928182 | -1.511299 | C          | -1.524016 | -1.330672 | -1.302933 |
| C         | -2.558858 | -1.544918 | -0.740048 | C          | -2.571203 | -2.133722 | -0.520897 |
| C         | -3.847546 | -1.576230 | -1.574129 | C          | -3.771758 | -2.526774 | -1.393028 |
| N         | -4.990047 | -2.119265 | -0.848469 | N          | -4.784332 | -3.278904 | -0.662169 |
| C         | 0.945136  | 1.185154  | -1.885746 | C          | 0.359319  | 1.183862  | -1.780252 |

|   |           |           |           |   |           |           |           |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| O | 1.435572  | 1.579255  | -2.951189 | O | 0.809548  | 1.586881  | -2.859787 |
| N | 0.311568  | 2.025984  | -1.032193 | N | -0.461291 | 1.945785  | -1.015456 |
| C | 0.150844  | 3.457786  | -1.313974 | C | -0.865806 | 3.300023  | -1.412159 |
| C | 1.453240  | 4.183190  | -0.903580 | C | 0.256757  | 4.280882  | -1.002005 |
| O | 1.569983  | 4.775131  | 0.177644  | O | 0.203950  | 4.952211  | 0.037055  |
| N | 2.461141  | 4.077635  | -1.800376 | N | 1.315824  | 4.306839  | -1.844019 |
| C | 3.792696  | 4.619833  | -1.547829 | C | 2.507006  | 5.107886  | -1.578003 |
| C | 4.646479  | 3.702447  | -0.657211 | C | 3.465127  | 4.436060  | -0.580905 |
| O | 5.665375  | 3.142760  | -1.076044 | O | 4.595410  | 4.058917  | -0.909267 |
| N | 4.175665  | 3.549232  | 0.604893  | N | 2.958175  | 4.278441  | 0.666316  |
| C | 4.776939  | 2.614436  | 1.555264  | C | 3.666636  | 3.542577  | 1.713461  |
| C | 4.368203  | 3.005803  | 2.976809  | C | 3.097021  | 3.933731  | 3.078655  |
| C | 4.908027  | 2.105216  | 4.068411  | C | 3.729549  | 3.229125  | 4.260840  |
| O | 4.386327  | 1.950711  | 5.152180  | O | 3.177828  | 3.041446  | 5.324439  |
| O | 6.072840  | 1.515365  | 3.723073  | O | 5.007861  | 2.864825  | 4.021786  |
| C | 4.317016  | 1.174717  | 1.220535  | C | 3.517932  | 2.021376  | 1.462910  |
| O | 3.373149  | 0.646117  | 1.825203  | O | 2.664074  | 1.352512  | 2.062317  |
| N | 5.002180  | 0.596003  | 0.210504  | N | 4.358345  | 1.531962  | 0.525883  |
| C | -1.078710 | 4.011339  | -0.591682 | C | -2.216329 | 3.664799  | -0.792615 |
| C | -1.437380 | 5.438134  | -1.025401 | C | -2.796119 | 4.970124  | -1.351575 |
| C | -2.691219 | 5.948670  | -0.312164 | C | -4.168678 | 5.284274  | -0.751949 |
| N | -3.016919 | 7.299840  | -0.753574 | N | -4.697248 | 6.525984  | -1.304920 |
| C | -3.998547 | 8.025269  | -0.102844 | C | -5.847004 | 7.085925  | -0.776832 |
| N | -4.283123 | 9.254894  | -0.705111 | N | -6.306816 | 8.202578  | -1.482304 |
| N | -4.493091 | 7.607632  | 1.016218  | N | -6.344061 | 6.645083  | 0.332358  |
| C | 4.765706  | -0.738971 | -0.357687 | C | 4.405991  | 0.150930  | 0.024667  |
| C | 4.803473  | -1.852088 | 0.724126  | C | 4.592864  | -0.887103 | 1.162641  |

|   |           |           |           |   |           |           |           |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 4.689503  | -3.244645 | 0.142044  | C | 4.798666  | -2.295719 | 0.646133  |
| C | 5.791825  | -3.888585 | -0.436216 | C | 6.014335  | -2.674689 | 0.058148  |
| C | 5.677221  | -5.162089 | -0.987425 | C | 6.197328  | -3.963484 | -0.430384 |
| C | 4.449237  | -5.836904 | -0.979297 | C | 5.177872  | -4.923152 | -0.347717 |
| C | 3.348586  | -5.195949 | -0.396580 | C | 3.965909  | -4.548788 | 0.244629  |
| C | 3.465385  | -3.924043 | 0.156205  | C | 3.782917  | -3.255330 | 0.730895  |
| O | 4.284682  | -7.080644 | -1.504812 | O | 5.409889  | -6.170051 | -0.839477 |
| C | -5.836756 | -1.349335 | -0.120922 | C | -5.932190 | -2.729584 | -0.192608 |
| O | -5.753593 | -0.120198 | -0.062857 | O | -6.233792 | -1.544604 | -0.354249 |
| C | -6.915625 | -2.115440 | 0.613175  | C | -6.830211 | -3.690072 | 0.555913  |
| C | -6.676553 | -2.603872 | 1.907882  | C | -6.866417 | -3.663309 | 1.960560  |
| C | -7.692492 | -3.254048 | 2.622056  | C | -7.739183 | -4.503232 | 2.665924  |
| C | -8.944774 | -3.401460 | 2.026335  | C | -8.576339 | -5.358715 | 1.949901  |
| C | -9.210141 | -2.922683 | 0.743564  | C | -8.565034 | -5.401850 | 0.556176  |
| C | -8.187242 | -2.273685 | 0.038298  | C | -7.686696 | -4.559525 | -0.140123 |
| O | -5.414011 | -2.396780 | 2.384208  | O | -5.997960 | -2.791835 | 2.550141  |
| C | -5.097027 | -2.863692 | 3.694444  | C | -5.970316 | -2.718628 | 3.974633  |
| O | -8.325222 | -1.765880 | -1.220665 | O | -7.592640 | -4.508198 | -1.501119 |
| C | -9.588372 | -1.895116 | -1.870818 | C | -8.437624 | -5.360236 | -2.272734 |
| H | 2.376550  | -0.069693 | 0.276295  | H | 1.904350  | 0.366923  | 0.527848  |
| H | 1.267119  | -0.838288 | -2.377483 | H | 1.088926  | -0.766101 | -2.100158 |
| H | 0.198215  | -1.930876 | -0.426854 | H | 0.178616  | -1.901229 | -0.093852 |
| H | -0.254145 | -0.386322 | 0.262184  | H | -0.604779 | -0.433945 | 0.450451  |
| H | -1.652911 | 0.092898  | -1.814773 | H | -1.987236 | -0.412633 | -1.688608 |
| H | -1.214926 | -1.493306 | -2.438320 | H | -1.198526 | -1.907368 | -2.180000 |
| H | -2.305012 | -2.566332 | -0.425969 | H | -2.110995 | -3.042218 | -0.108843 |
| H | -2.747721 | -0.968635 | 0.174792  | H | -2.932094 | -1.546390 | 0.333499  |

|   |           |           |           |   |           |           |           |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | -4.117310 | -0.563737 | -1.886879 | H | -4.262959 | -1.633851 | -1.788058 |
| H | -3.702318 | -2.178741 | -2.477428 | H | -3.438342 | -3.131801 | -2.244323 |
| H | -5.093001 | -3.123553 | -0.790719 | H | -4.613328 | -4.256965 | -0.470121 |
| H | -0.026230 | 1.683580  | -0.142040 | H | -0.751158 | 1.619244  | -0.102582 |
| H | 0.024487  | 3.548598  | -2.397051 | H | -0.942648 | 3.290825  | -2.503499 |
| H | 2.333555  | 3.414538  | -2.563376 | H | 1.351631  | 3.589316  | -2.566021 |
| H | 4.310352  | 4.736499  | -2.499841 | H | 3.047803  | 5.253033  | -2.512978 |
| H | 3.682516  | 5.600701  | -1.076174 | H | 2.189997  | 6.081140  | -1.191816 |
| H | 3.284286  | 3.991317  | 0.831491  | H | 1.988170  | 4.556624  | 0.818205  |
| H | 5.861613  | 2.677826  | 1.442079  | H | 4.723557  | 3.812586  | 1.652591  |
| H | 4.728151  | 4.021970  | 3.179353  | H | 3.237488  | 5.012058  | 3.223647  |
| H | 3.280785  | 3.014158  | 3.080459  | H | 2.024445  | 3.731300  | 3.124452  |
| H | 6.361696  | 0.971189  | 4.481456  | H | 5.346719  | 2.436524  | 4.832015  |
| H | 5.624695  | 1.213441  | -0.307903 | H | 4.878194  | 2.230258  | -0.003843 |
| H | -1.919164 | 3.338543  | -0.801100 | H | -2.908210 | 2.837214  | -0.990478 |
| H | -0.898330 | 3.987695  | 0.489659  | H | -2.101482 | 3.746892  | 0.294887  |
| H | -0.603441 | 6.116424  | -0.812739 | H | -2.115116 | 5.802899  | -1.142866 |
| H | -1.599813 | 5.456861  | -2.112718 | H | -2.882729 | 4.889597  | -2.444920 |
| H | -3.531613 | 5.256072  | -0.480858 | H | -4.858259 | 4.441935  | -0.922616 |
| H | -2.527623 | 5.984308  | 0.768560  | H | -4.091893 | 5.410505  | 0.331780  |
| H | -2.973596 | 7.431831  | -1.757289 | H | -4.596148 | 6.610245  | -2.309709 |
| H | -5.211723 | 9.603421  | -0.498903 | H | -7.298287 | 8.376578  | -1.365548 |
| H | -4.080116 | 9.326368  | -1.696407 | H | -6.042507 | 8.254792  | -2.460503 |
| H | -5.126195 | 8.314833  | 1.395518  | H | -7.127514 | 7.238079  | 0.614752  |
| H | 5.594302  | -0.910385 | -1.046940 | H | 5.286150  | 0.109493  | -0.619487 |
| H | 5.754879  | -1.741342 | 1.256937  | H | 5.462915  | -0.563529 | 1.746184  |
| H | 4.006941  | -1.677800 | 1.450054  | H | 3.729834  | -0.855105 | 1.830515  |

|    |            |           |           |    |           |           |           |
|----|------------|-----------|-----------|----|-----------|-----------|-----------|
| H  | 6.759018   | -3.392601 | -0.453390 | H  | 6.830882  | -1.962690 | -0.018653 |
| H  | 6.545509   | -5.647815 | -1.426417 | H  | 3.165039  | -5.280202 | 0.324371  |
| H  | 2.591075   | -3.460870 | 0.602175  | H  | 2.831699  | -2.993258 | 1.187188  |
| H  | 5.130234   | -7.384533 | -1.874817 | H  | 4.616771  | -6.715974 | -0.707578 |
| H  | -7.519236  | -3.636285 | 3.620336  | H  | -7.771161 | -4.495886 | 3.748393  |
| H  | -9.735418  | -3.904165 | 2.576470  | H  | -9.255441 | -6.010171 | 2.493111  |
| H  | -10.193520 | -3.054478 | 0.309663  | H  | -9.229333 | -6.076223 | 0.029993  |
| H  | -4.053785  | -2.592055 | 3.860770  | H  | -5.215764 | -1.969092 | 4.217296  |
| H  | -5.207034  | -3.951941 | 3.767321  | H  | -5.685800 | -3.679955 | 4.418149  |
| H  | -5.725248  | -2.381214 | 4.452208  | H  | -6.940177 | -2.403453 | 4.376918  |
| H  | -9.467480  | -1.424900 | -2.847643 | H  | -8.197101 | -5.149162 | -3.315657 |
| H  | -9.862494  | -2.948152 | -2.004071 | H  | -8.240105 | -6.417186 | -2.059240 |
| H  | -10.378831 | -1.379489 | -1.313169 | H  | -9.496547 | -5.142555 | -2.090874 |
| Br | 1.654392   | -6.085244 | -0.356043 | Br | 7.871828  | -4.443096 | -1.226130 |

| <b>CH<sub>3</sub>COOH</b> |           |           |           |
|---------------------------|-----------|-----------|-----------|
| H                         | 1.729193  | -0.814625 | 0.000386  |
| O                         | 0.779703  | -1.042909 | -0.000027 |
| C                         | 0.091812  | 0.122115  | -0.000170 |
| O                         | 0.643165  | 1.204694  | 0.000027  |
| C                         | -1.396176 | -0.111851 | -0.000065 |
| H                         | -1.683538 | -0.687119 | 0.886047  |
| H                         | -1.919782 | 0.844201  | -0.006029 |
| H                         | -1.682634 | -0.698324 | -0.878996 |

**Table S2.** Frequencies of stationary points for the reactions of **1** + **CH<sub>3</sub>COOBr** with the SCRF-B3LYP/6-31G\* method in water with the Gaussian 09 program package

| Species                    | Frequencies (cm <sup>-1</sup> )  |
|----------------------------|--|
| <b>1</b>                   | 5 8 9 14 16 20 22 24 30 33 35 37 43 45 51 55 63 63 72 72 78 84 84<br>94 100 101 103 108 115 118 119 120 132 135 141 161 170 175 180<br>186 190 195 200 206 216 222 240 247 253 259 280 283 285 290<br>293 306 309 311 314 328 329 336 351 353 369 370 377 386 400<br>415 422 427 428 444 460 467 475 480 500 505 507 524 525 543<br>555 560 572 585 587 595 599 602 611 615 625 631 636 639 648<br>656 667 668 678 687 699 712 726 727 733 741 749 760 762 769<br>775 778 780 783 790 791 797 814 826 840 849 852 853 865 874<br>877 905 915 926 927 951 959 962 965 965 978 985 1004 1012 1020<br>1032 1034 1036 1045 1050 1059 1064 1064 1066 1073 1087 1097<br>1103 1115 1118 1120 1127 1130 1135 1146 1151 1158 1175 1177<br>1181 1182 1182 1193 1193 1205 1206 1209 1211 1217 1220 1221<br>1234 1240 1264 1269 1274 1277 1288 1289 1292 1296 1299 1301<br>1305 1310 1321 1327 1337 1337 1341 1344 1348 1350 1353 1358<br>1359 1369 1373 1374 1381 1381 1382 1387 1394 1402 1404 1408<br>1418 1423 1428 1442 1473 1480 1481 1484 1496 1496 1502 1509<br>1513 1513 1516 1518 1519 1521 1522 1528 1533 1533 1542 1551<br>1562 1565 1572 1579 1580 1590 1600 1642 1643 1646 1671 1683<br>1697 1712 1718 1720 1729 1733 1749 1824 2999 3029 3031 3033<br>3039 3044 3044 3055 3059 3066 3066 3076 3077 3086 3089 3096<br>3098 3105 3109 3110 3113 3118 3125 3132 3133 3144 3146 3169<br>3169 3173 3177 3187 3192 3199 3212 3240 3243 3458 3463 3466<br>3500 3504 3545 3580 3613 3618 3644 3676 3739 |
| <b>CH<sub>3</sub>COOBr</b> | 14 143 196 323 556 599 714 899 994 1072 1194 1409 1486 1487<br>1830 3083 3154 3189   |
| <b>TS1a</b>                | -45i 5 6 9 12 14 18 19 23 25 26 29 31 36 39 40 45 46 49 53 55 58 63<br>71 72 75 79 83 86 89 98 101 106 111 114 119 121 125 131 133 135<br>140 145 154 161 166 170 173 182 186 191 198 205 215 218 223 234<br>240 247 258 280 281 290 293 302 308 312 318 327 329 333 347 350<br>353 364 378 379 384 400 415 422 427 438 444 447 456 463 472 480<br>489 500 507 508 520 543 553 559 572 586 594 595 598 610 610 613<br>616 630 631 633 637 647 655 658 666 668 685 689 693 711 715 725<br>727 743 748 760 768 774 775 778 780 790 791 795 814 822 825 840<br>850 852 865 874 877 887 895 904 914 925 950 957 962 965 978 984<br>997 1000 1003 1007 1018 1021 1024 1032 1035 1038 1048 1052<br>1053 1060 1064 1065 1074 1087 1090 1098 1104 1115 1116 1119<br>1127 1131 1135 1138 1151 1158 1164 1173 1178 1182 1192 1195<br>1205 1207 1208 1211 1217 1218 1230 1233 1242 1264 1268 1274<br>1275 1288 1290 1295 1299 1301 1304 1311 1321 1322 1335 1337  |

|              |  |
|--------------|--|
|              | <p>1340 1343 1348 1350 1352 1359 1364 1367 1369 1373 1374 1379<br/> 1381 1383 1387 1395 1395 1402 1405 1407 1417 1424 1428 1432<br/> 1442 1464 1473 1482 1484 1488 1489 1497 1502 1503 1511 1511<br/> 1514 1517 1518 1520 1520 1522 1531 1535 1544 1549 1557 1562<br/> 1567 1571 1575 1579 1580 1594 1600 1641 1646 1671 1679 1685<br/> 1698 1712 1718 1720 1733 1746 1750 1824 2998 3028 3032 3033<br/> 3039 3041 3049 3055 3061 3066 3073 3077 3079 3087 3090 3090<br/> 3096 3099 3102 3105 3115 3118 3124 3128 3130 3132 3138 3143<br/> 3144 3149 3175 3177 3179 3187 3192 3195 3212 3214 3239 3264<br/> 3461 3465 3466 3499 3502 3546 3581 3612 3612 3644 3677 3737</p>  |
| <b>TS1a'</b> | <p>-47i 1 7 9 11 13 18 20 24 25 26 28 30 33 39 42 45 49 50 52 57 60 60<br/> 62 66 74 77 81 83 92 92 98 103 105 112 113 119 120 123 129 135<br/> 139 141 151 164 169 172 174 182 189 191 192 203 215 216 222<br/> 239 247 248 259 278 281 287 292 302 307 311 324 327 328 335<br/> 351 351 358 361 379 381 383 398 415 423 426 431 441 448 450<br/> 461 468 478 487 500 504 509 528 542 552 558 570 585 592 594<br/> 602 609 610 613 616 627 633 636 637 642 655 663 666 671 684<br/> 693 702 708 713 725 728 744 749 761 768 770 773 778 780 789<br/> 791 795 814 821 825 839 850 851 865 874 877 885 893 904 914<br/> 925 948 956 958 965 978 983 996 1002 1004 1009 1018 1023 1024<br/> 1032 1034 1035 1048 1053 1053 1060 1064 1066 1072 1086 1098<br/> 1100 1102 1117 1119 1121 1126 1132 1134 1139 1151 1154 1173<br/> 1176 1179 1181 1190 1196 1197 1204 1207 1210 1211 1216 1232<br/> 1233 1243 1264 1268 1274 1275 1286 1290 1292 1298 1301 1301<br/> 1311 1322 1326 1336 1339 1341 1344 1347 1348 1353 1359 1361<br/> 1367 1367 1369 1375 1380 1381 1381 1388 1391 1396 1401 1403<br/> 1408 1417 1424 1429 1435 1442 1465 1472 1482 1484 1490 1491<br/> 1499 1503 1505 1508 1513 1514 1517 1519 1519 1521 1522 1530<br/> 1532 1541 1544 1549 1562 1565 1572 1578 1579 1583 1584 1596<br/> 1630 1645 1671 1677 1683 1698 1712 1718 1720 1735 1745 1748<br/> 1824 2996 3030 3032 3035 3041 3041 3054 3059 3065 3067 3077<br/> 3079 3080 3086 3088 3090 3096 3098 3105 3105 3117 3119 3120<br/> 3123 3132 3133 3140 3143 3147 3174 3176 3177 3178 3186 3188<br/> 3192 3212 3212 3241 3264 3460 3464 3465 3491 3510 3544 3578<br/> 3604 3609 3643 3676 3738</p> |
| <b>TS1b</b>  | <p>-61i 2 5 7 10 12 15 15 18 21 24 26 30 31 35 41 44 48 52 54 60 62 64<br/> 69 71 76 80 82 86 93 94 98 100 102 105 110 115 118 122 127 134<br/> 141 149 152 158 167 170 180 181 190 196 198 203 211 224 237 247<br/> 249 252 278 281 283 286 294 301 305 310 314 320 324 331 335 347<br/> 352 369 376 384 388 409 427 435 443 448 461 467 469 476 488<br/> 498 507 511 519 524 542 547 558 572 583 587 591 594 598 600<br/> 609 610 619 625 629 633 634 638 638 650 668 674 682 695 699<br/> 712 727 733 735 741 750 761 761 769 773 779 779 784 788 791<br/> 798 811 822 849 851 852 853 873 877 889 902 908 925 926 928<br/> 961 965 966 977 984 999 1004 1011 1015 1020 1021 1034 1036</p>  |



|              |   |
|--------------|---|
|              | <p>1046 1051 1054 1059 1061 1064 1064 1074 1079 1087 1097 1104<br/> 1106 1115 1118 1120 1127 1131 1145 1151 1156 1174 1177 1181<br/> 1182 1182 1189 1193 1195 1205 1209 1215 1215 1219 1221 1226<br/> 1241 1265 1269 1275 1276 1287 1288 1290 1296 1300 1305 1309<br/> 1323 1327 1334 1338 1341 1343 1347 1349 1349 1352 1357 1357<br/> 1360 1368 1374 1374 1375 1381 1382 1389 1394 1404 1404 1410<br/> 1418 1424 1425 1429 1441 1455 1474 1480 1481 1487 1496 1498<br/> 1502 1502 1510 1511 1513 1515 1520 1520 1521 1524 1528 1529<br/> 1533 1534 1543 1555 1565 1572 1580 1583 1585 1594 1599 1611<br/> 1641 1643 1669 1687 1699 1712 1718 1721 1729 1732 1750 1824<br/> 2997 3030 3031 3033 3039 3043 3043 3046 3055 3057 3062 3063<br/> 3076 3077 3077 3087 3089 3096 3099 3105 3108 3109 3114 3114<br/> 3116 3122 3129 3136 3140 3143 3158 3168 3168 3175 3199 3211<br/> 3226 3229 3240 3243 3460 3464 3473 3487 3504 3544 3579 3613<br/> 3617 3644 3676 3683</p>  |
| <b>TS1b'</b> | <p>-56i 5 7 8 11 12 15 17 19 24 26 30 33 36 37 39 43 48 53 58 63 65 66<br/> 72 76 77 79 83 87 92 95 101 101 102 107 111 117 118 123 133 134<br/> 140 151 159 162 165 168 179 181 188 196 198 202 209 221 234<br/> 247 250 251 276 281 283 285 292 296 305 310 314 321 328 332<br/> 338 351 352 369 377 385 391 409 426 439 444 451 461 463 467<br/> 476 487 498 504 508 513 524 543 553 560 573 582 587 588 593<br/> 597 601 611 614 616 625 628 629 633 637 638 651 667 672 676<br/> 684 691 712 728 731 734 741 749 761 762 769 772 778 780 783<br/> 790 792 797 813 827 849 851 851 854 872 877 890 905 911 920<br/> 926 927 960 965 966 977 984 997 1004 1013 1014 1021 1023 1035<br/> 1037 1046 1049 1055 1059 1064 1065 1067 1072 1083 1087 1093<br/> 1103 1104 1114 1118 1120 1127 1131 1146 1150 1157 1174 1178<br/> 1182 1183 1183 1189 1193 1196 1206 1209 1211 1216 1219 1220<br/> 1224 1242 1262 1270 1274 1276 1288 1288 1292 1295 1300 1304<br/> 1310 1322 1327 1334 1339 1343 1344 1349 1350 1351 1352 1357<br/> 1357 1359 1371 1374 1375 1376 1380 1381 1389 1394 1403 1406<br/> 1408 1418 1424 1424 1428 1444 1451 1475 1480 1484 1488 1496<br/> 1496 1501 1504 1510 1513 1513 1516 1519 1520 1521 1525 1528<br/> 1530 1532 1533 1544 1552 1565 1571 1578 1582 1584 1587 1599<br/> 1608 1641 1643 1666 1683 1699 1712 1718 1721 1729 1732 1746<br/> 1824 2998 3026 3030 3032 3038 3043 3043 3048 3055 3059 3060<br/> 3064 3077 3078 3086 3089 3090 3095 3100 3105 3108 3109 3114<br/> 3114 3115 3125 3131 3135 3143 3146 3151 3168 3168 3174 3199<br/> 3214 3225 3227 3238 3241 3462 3464 3465 3485 3500 3544 3579<br/> 3615 3619 3643 3676 3683</p> |
| <b>3a</b>    | <p>2 5 9 12 14 17 18 25 28 31 35 37 43 47 51 55 59 66 72 73 78 80 87<br/> 93 100 105 110 111 113 115 120 122 127 133 137 141 154 161 172<br/> 175 176 183 184 191 202 215 223 231 239 242 246 256 257 267<br/> 282 285 290 295 309 312 326 329 331 339 349 353 355 364 375<br/> 378 395 401 416 423 428 445 448 461 471 476 489 500 502 508</p>   |

|                   |   |
|-------------------|---|
|                   | <p>514 544 555 561 566 573 583 587 594 601 606 610 616 632 638<br/> 649 650 655 669 670 679 684 688 693 710 726 728 735 749 760<br/> 764 768 774 780 782 791 792 800 807 815 825 825 841 850 865<br/> 865 874 878 906 916 927 935 950 961 964 965 966 978 985 1004<br/> 1015 1021 1032 1034 1035 1037 1048 1050 1060 1065 1066 1074<br/> 1087 1097 1103 1118 1120 1121 1127 1130 1136 1145 1151 1157<br/> 1176 1181 1182 1183 1190 1191 1192 1206 1209 1210 1215 1216<br/> 1219 1234 1241 1259 1265 1270 1275 1276 1287 1291 1294 1299<br/> 1301 1304 1310 1317 1322 1332 1335 1338 1341 1341 1347 1349</p> <p>1354 1358 1369 1370 1373 1382 1382 1383 1388 1394 1403 1404</p> <p>1406 1419 1424 1432 1442 1444 1473 1483 1483 1484 1499 1503</p> <p>1503 1511 1511 1514 1514 1519 1521 1522 1525 1526 1534 1543</p> <p>1552 1563 1572 1574 1579 1583 1586 1603 1622 1629 1646 1671</p> <p>1686 1698 1712 1718 1720 1726 1733 1748 1824 2997 3030 3031</p> <p>3033 3040 3047 3055 3058 3060 3065 3066 3076 3078 3086 3090</p> <p>3096 3098 3105 3115 3115 3118 3122 3130 3138 3139 3143 3144</p> <p>3167 3174 3174 3176 3187 3192 3211 3224 3245 3459 3463 3467</p> <p>3500 3501 3545 3581 3613 3615 3645 3675 3738</p>   |
| <p><b>3a'</b></p> | <p>5 7 8 11 15 20 21 27 30 33 35 38 43 48 53 54 60 65 69 74 79 81 84<br/> 92 98 103 105 113 115 118 120 122 125 131 138 140 149 160 167<br/> 169 173 175 184 191 196 214 220 227 236 240 244 251 260 276<br/> 282 288 291 296 308 312 323 329 330 336 350 351 353 369 379<br/> 381 392 399 415 423 426 437 445 460 467 477 485 500 501 510<br/> 522 543 554 560 568 573 586 592 594 599 601 611 617 632 638<br/> 649 650 656 668 670 679 687 690 697 712 726 727 736 750 762<br/> 769 769 774 781 782 791 793 798 806 815 825 826 841 851 865<br/> 865 875 878 906 916 927 935 949 959 963 965 965 979 985 1004<br/> 1014 1021 1032 1034 1036 1038 1048 1051 1060 1065 1065 1074<br/> 1087 1097 1103 1117 1120 1123 1127 1130 1135 1144 1151 1157<br/> 1177 1179 1182 1182 1189 1190 1193 1205 1208 1210 1213 1217<br/> 1218 1233 1242 1258 1263 1268 1275 1277 1289 1292 1295 1299<br/> 1301 1304 1311 1317 1323 1332 1335 1339 1340 1344 1348 1348<br/> 1352 1359 1367 1370 1374 1378 1381 1381 1389 1395 1402 1405<br/> 1406 1417 1425 1428 1444 1445 1474 1482 1483 1484 1499 1504<br/> 1505 1510 1511 1513 1514 1520 1521 1522 1522 1526 1533 1544<br/> 1554 1562 1568 1573 1578 1584 1590 1599 1623 1629 1646 1671<br/> 1686 1698 1712 1717 1720 1733 1736 1749 1824 3001 3028 3032<br/> 3032 3039 3048 3055 3055 3057 3062 3065 3076 3077 3087 3089<br/> 3096 3099 3105 3114 3115 3117 3123 3129 3130 3138 3142 3143</p> |

|            |   |
|------------|---|
|            | 3168 3174 3175 3176 3187 3192 3212 3224 3245 3460 3464 3468<br>3499 3504 3544 3579 3612 3615 3643 3675 3737   |
| <b>3b</b>  | 4 5 8 9 10 11 16 20 25 26 30 34 41 44 52 52 57 62 65 72 80 80 84 94<br>96 99 104 108 115 118 119 122 129 134 139 150 161 167 176 177<br>186 188 195 197 198 208 221 224 241 247 251 259 266 282 282<br>283 290 297 305 308 314 328 330 336 351 352 357 369 370 379 384<br>400 415 427 445 456 462 466 470 478 492 494 506 509 511 521<br>546 557 572 583 586 595 598 598 610 613 620 625 632 636 639<br>644 666 672 685 689 695 699 711 727 732 741 741 749 760 763<br>768 776 777 782 783 790 793 797 816 832 850 852 854 870 878<br>890 908 912 925 927 930 957 962 965 966 980 986 1004 1013 1021<br>1035 1037 1044 1050 1057 1059 1064 1065 1069 1074 1087 1098<br>1102 1114 1118 1120 1127 1131 1146 1151 1157 1162 1174 1177<br>1181 1181 1182 1193 1195 1206 1208 1211 1217 1219 1220 1234<br>1242 1264 1269 1274 1277 1286 1288 1292 1295 1301 1306 1309<br>1311 1321 1327 1330 1335 1340 1343 1347 1350 1352 1354 1358<br>1360 1370 1374 1376 1381 1381 1389 1394 1399 1405 1407 1419<br>1424 1429 1443 1456 1475 1480 1485 1493 1496 1502 1509 1512<br>1513 1516 1519 1520 1521 1523 1528 1533 1533 1543 1552 1554<br>1562 1572 1582 1584 1588 1597 1625 1642 1643 1663 1684 1698<br>1712 1718 1721 1728 1733 1749 1824 2997 3027 3031 3032 3041<br>3043 3044 3055 3060 3071 3071 3077 3079 3086 3089 3095 3099<br>3105 3109 3109 3115 3118 3124 3129 3130 3145 3145 3168 3169<br>3174 3187 3199 3202 3216 3239 3242 3463 3465 3470 3499 3502<br>3544 3578 3615 3620 3643 3675 3738 |
| <b>3b'</b> | 4 8 9 10 14 17 18 23 26 30 34 35 41 44 49 54 58 66 70 73 79 82 84<br>95 100 102 105 106 111 113 117 121 126 134 138 151 162 167 174<br>180 184 192 198 202 202 205 220 225 241 249 258 262 266 281<br>284 288 290 296 305 311 316 326 331 336 350 350 356 368 369<br>378 385 400 414 426 445 453 460 470 471 478 484 492 508 509<br>511 522 547 557 571 583 587 595 598 605 609 611 613 625 632<br>638 640 653 660 676 683 687 696 700 716 729 734 739 740 749<br>762 762 771 778 779 782 785 791 794 796 816 830 851 852 854<br>871 878 895 907 913 926 927 930 954 962 966 966 980 986 1004<br>1014 1021 1035 1037 1045 1050 1056 1058 1064 1064 1069 1074<br>1089 1098 1105 1115 1118 1121 1127 1130 1145 1151 1157 1162<br>1174 1178 1183 1183 1183 1193 1197 1206 1209 1210 1216 1220<br>1222 1232 1241 1262 1269 1274 1276 1287 1288 1292 1296 1299<br>1304 1310 1313 1320 1327 1331 1337 1340 1343 1347 1350 1353<br>1357 1358 1360 1372 1374 1374 1381 1383 1389 1394 1403 1406<br>1408 1417 1424 1429 1443 1457 1474 1480 1485 1496 1497 1503<br>1508 1513 1514 1515 1520 1520 1521 1523 1528 1532 1533 1542<br>1549 1551 1564 1573 1581 1583 1589 1598 1622 1641 1642 1662<br>1686 1698 1712 1718 1720 1727 1732 1749 1824 2999 3028 3031<br>3032 3039 3043 3044 3056 3059 3063 3067 3075 3078 3086 3089  |

|                           |  |
|---------------------------|--|
|                           | 3097 3099 3107 3109 3109 3114 3116 3123 3130 3134 3144 3146<br>3168 3168 3176 3185 3198 3201 3204 3239 3242 3461 3464 3471<br>3494 3508 3542 3578 3612 3618 3640 3676 3734 |
| <b>CH<sub>3</sub>COOH</b> | 57 425 548 579 667 870 1010 1077 1213 1361 1430 1488 1493 1819<br>3075 3138 3187 3680  |

**Table S3.** The total energies of reactants, products, and transition states of the reaction **1** + **CH<sub>3</sub>COOBr** with the SCRF-B3LYP/6-31G\* method in water with the Gaussian 09 program package

| Compounds                  | energies (a.u.) |              | G            |
|----------------------------|-----------------|--------------|--------------|
|                            | without ZPE     | with ZPE     |              |
| <b>DMB-c(RGDyK)</b>        | -2721.71351702  | -2720.845194 | -2720.949058 |
| <b>CH<sub>3</sub>COOBr</b> | -2800.14063916  | -2800.089741 | -2800.122224 |
| <b>TS1a</b>                | -5521.83439160  | -5520.914709 | -5521.031054 |
| <b>TS1a'</b>               | -5521.83319022  | -5520.913758 | -5521.031850 |
| <b>TS1b</b>                | -5521.81959218  | -5520.900239 | -5521.018987 |
| <b>TS1b'</b>               | -5521.81906325  | -5520.899680 | -5521.016331 |
| <b>3a</b>                  | -5292.81372854  | -5291.955668 | -5292.063148 |
| <b>3a'</b>                 | -5292.81228815  | -5291.954324 | -5292.060596 |
| <b>3b</b>                  | -5292.81741075  | -5291.959249 | -5292.068211 |
| <b>3b'</b>                 | -5292.81706676  | -5291.958760 | -5292.065833 |
| <b>CH<sub>3</sub>COOH</b>  | -229.088412444  | -229.026635  | -229.054015  |

**Table S4.** The relative energies of reactants, products, and transition states of the reaction **1** + **CH<sub>3</sub>COOBr** with the SCRF-B3LYP/6-31G\* method in water with the Gaussian 09 program package

| Compounds                  | energies (kcal/mol) |          | G    |
|----------------------------|---------------------|----------|------|
|                            | without ZPE         | with ZPE |      |
| <b>DMB-c(RGDyK)</b>        | 0.0                 | 0.0      | 0.0  |
| <b>CH<sub>3</sub>COOBr</b> |                     |          |      |
| <b>TS1a</b>                | 12.4                | 12.7     | 25.2 |
| <b>TS1a'</b>               | 13.2                | 13.3     | 24.7 |
| <b>TS1b</b>                | 21.7                | 21.8     | 32.8 |
| <b>TS1b'</b>               | 22.0                | 22.1     | 34.5 |