*Article*

# Non-Linear Quantitative Structure–Activity Relationships Modelling, Mechanistic Study and In-Silico Design of Flavonoids as Potent Antioxidants

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**Contents:**

**Ref S1.** Gaussian 16, Revision B.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2016.

**Equations describing the parameters of the HAT and SPLET mechanisms of antioxidant activity.** The enthalpies (bond dissociation enthalpy – BDE, electron transfer enthalpy – ETE, and proton affinity – PA) were defined as follows ($n$ = number of hydroxyl groups, $1 \leq k \leq n$):

$$BDE_k = H(Ar(OH)_{n-k}(O^{\bullet})_k) + H(H^{\bullet}) - H(Ar(OH)_{n-k+1}(O^{\bullet})_{k-1}) \quad (1)$$

$$ETE_k = H(Ar(OH)_{n-k}(O^{\bullet})_k) + H(e^{-}) - H([Ar(OH)_{n-k}(O^{\bullet})_{k-1}O:]^{-}) \quad (2)$$

$$PA_k = H([Ar(OH)_{n-k}(O^{\bullet})_{k-1}O:)]^{-} + H(H^{+}) - H(Ar(OH)_{n-k+1}) \quad (3)$$

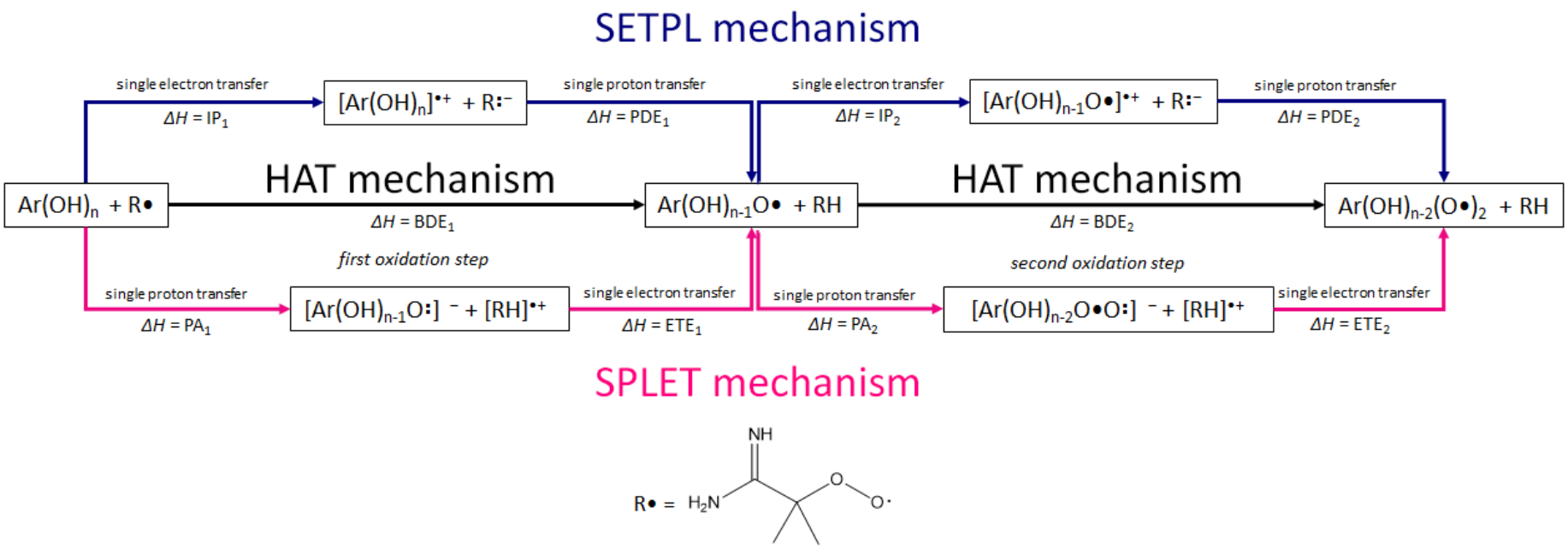


**Figure S1.** Schematic representation of three prominent antioxidant activity mechanisms of the ORAC assay. HAT stands for the hydrogen atom transfer, SPLET for the sequential proton-loss electron transfer, while SETPL stands for single electron transfer followed by proton loss mechanism.

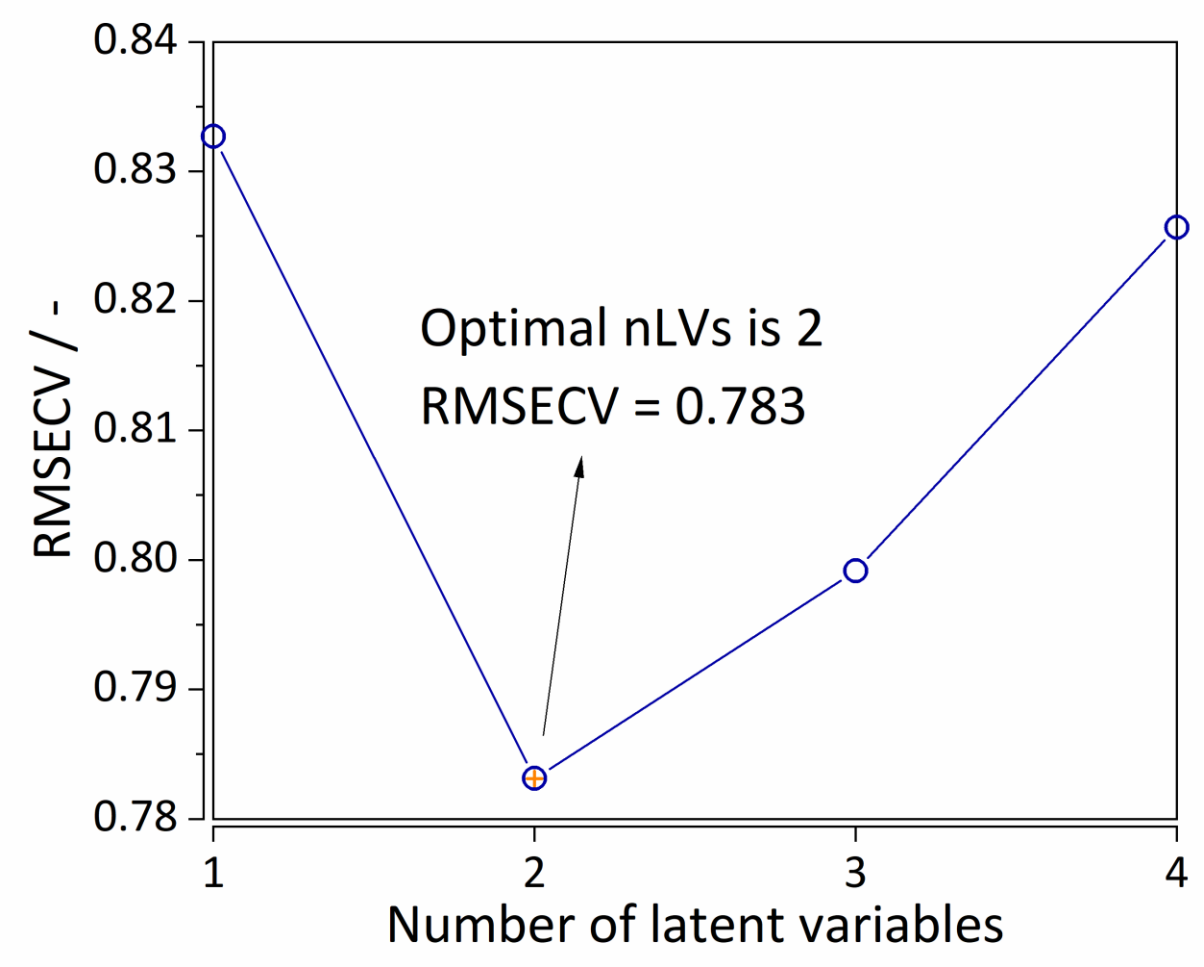


**Figure S2.** Optimization of the number of partial least squares latent variables. The optimal number (two) is denoted with an orange cross.

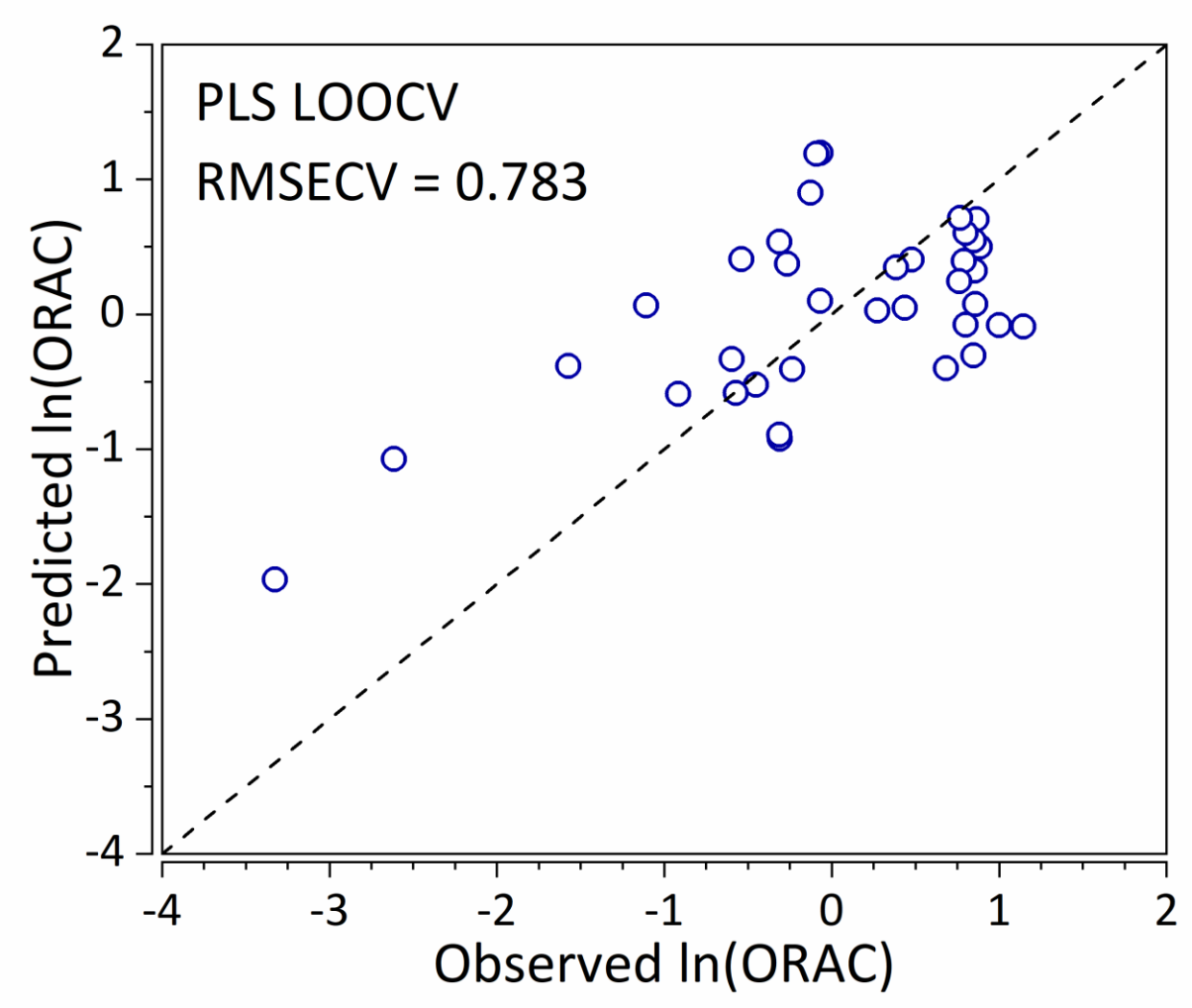


**Figure S3.** Predictive ability of the cross-validated (using leave-one-out cross-validation) PLS-based quantitative structure–activity relationships (QSAR) model.

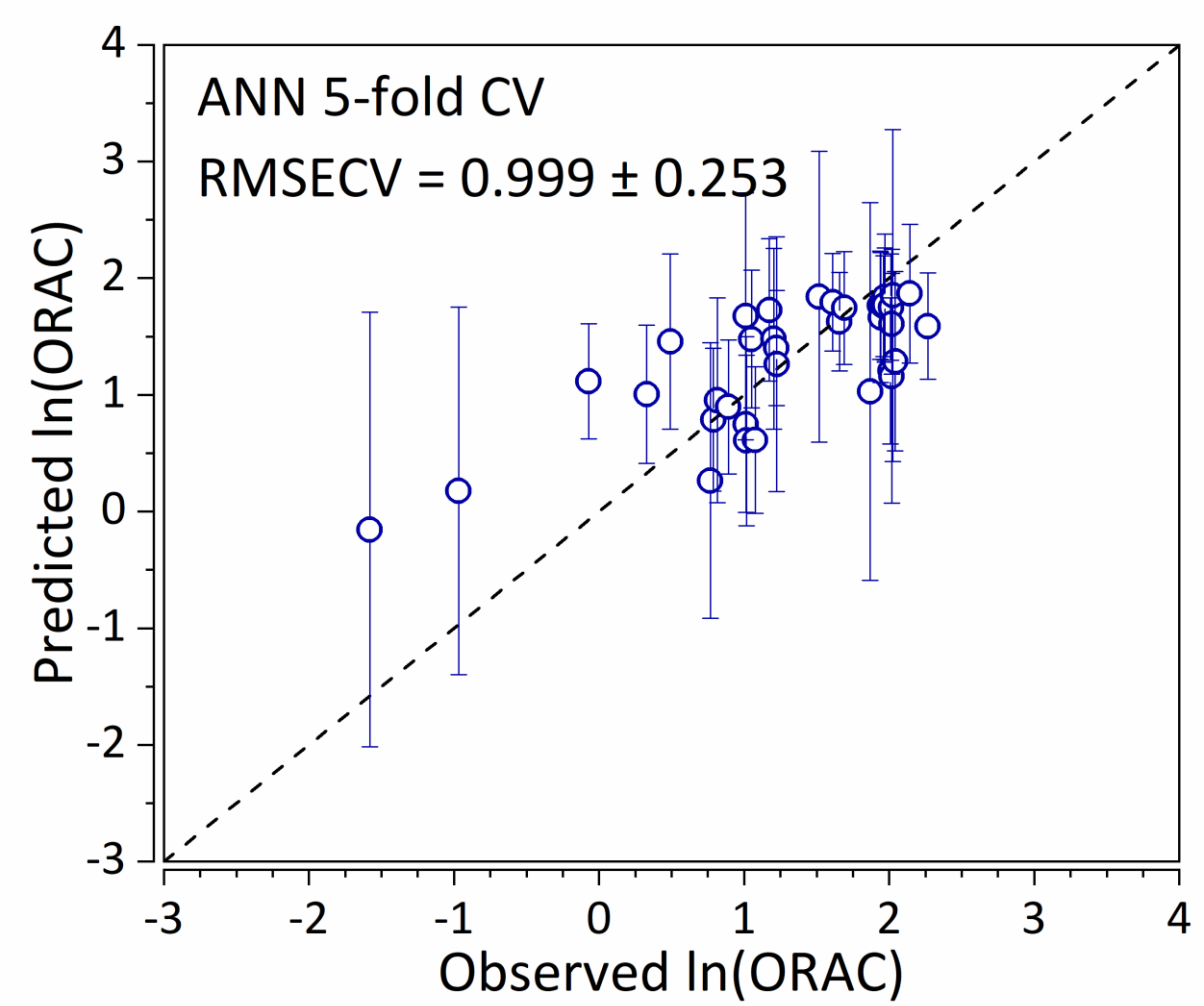


**Figure S4.** Predictive ability of the cross-validated (using five-fold cross-validation) artificial neural network (ANN)-based QSAR model.

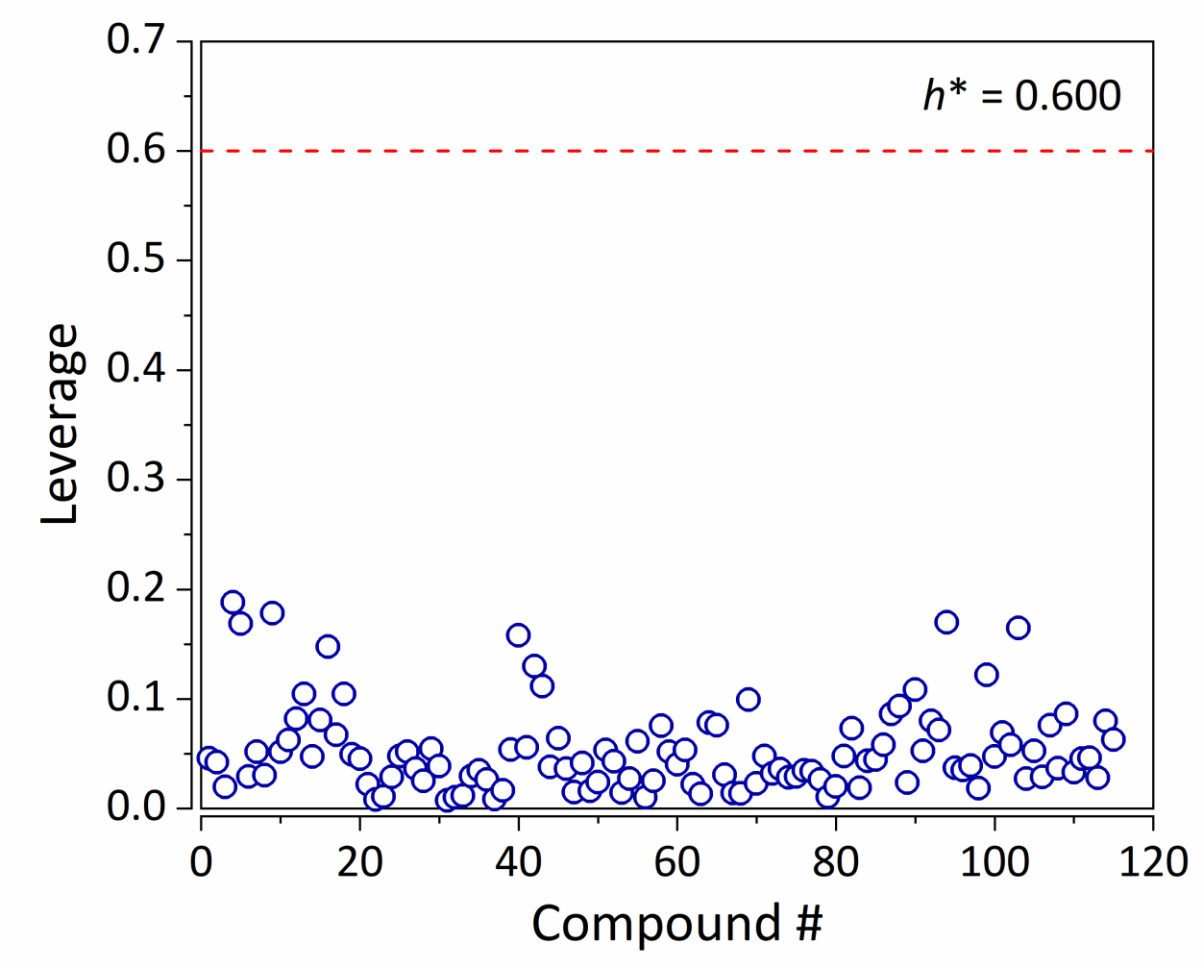


**Figure S5.** Leverage values of the 115 flavonoids designed using a combinatorial approach.

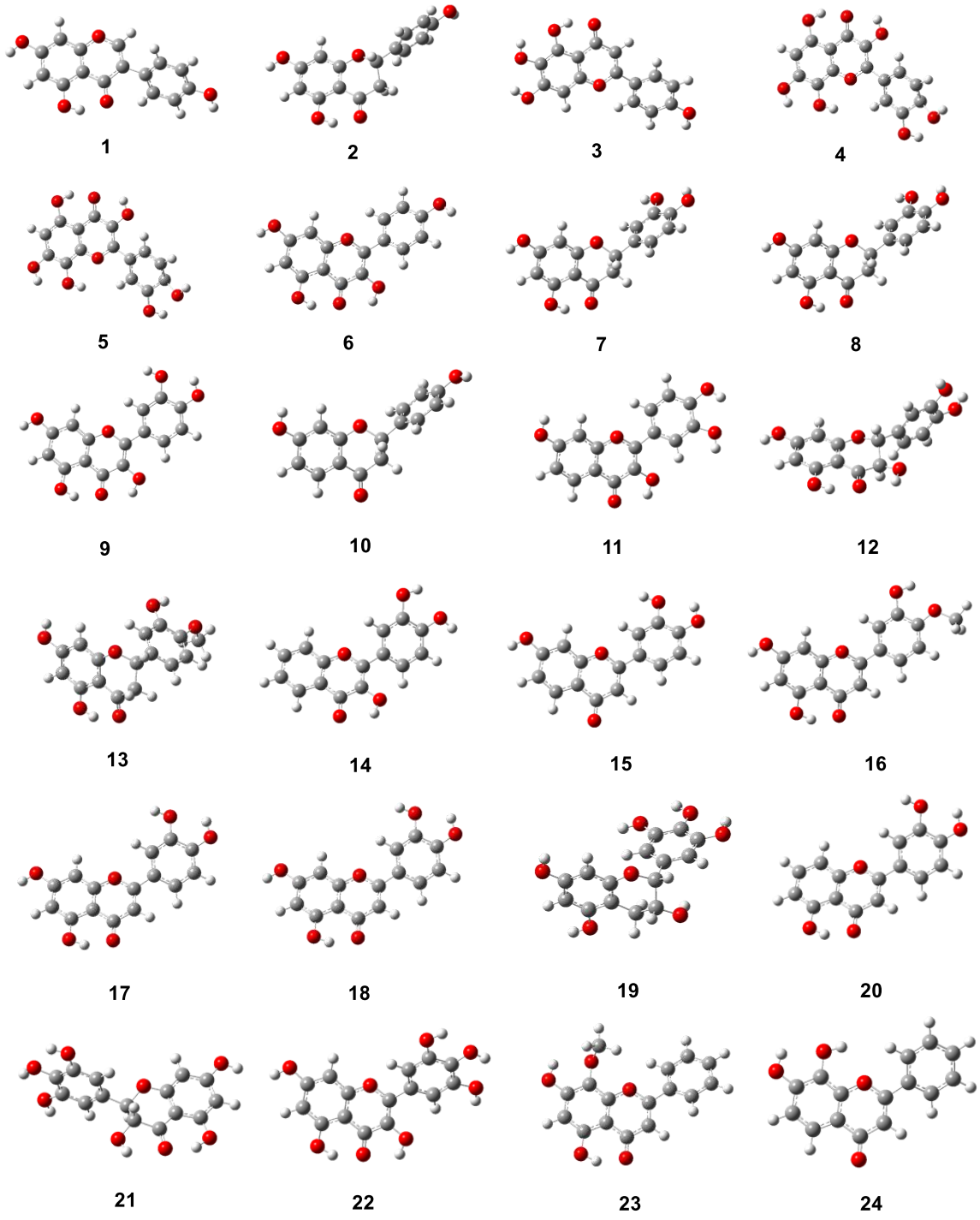


**Figure S6.** Optimized geometries (ωB97XD/6-311+G**) of 36 flavonoids.

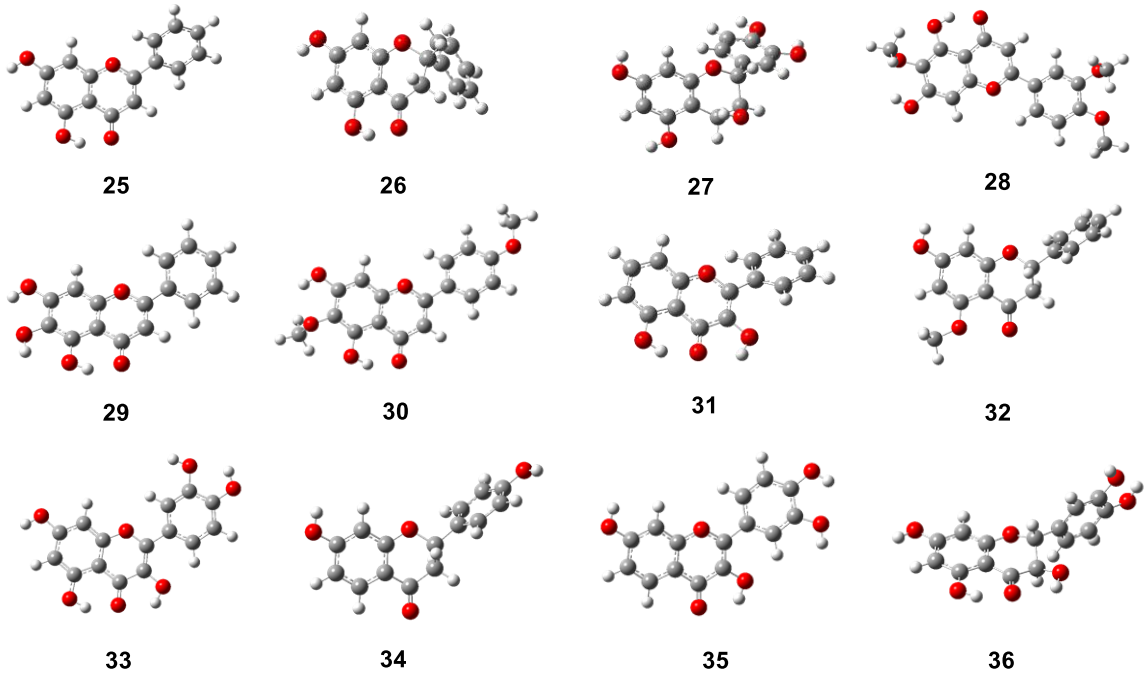


**Figure S6.** (cont.)

**Table S1.** List of 115 flavonoids designed using a combinatorial approach and calculated quantum mechanical parameters of the two considered antioxidant mechanisms.

| # | R1 | R2 | R3 | R4 | R5 | R6 | R7 | R8 | R1' | R2' | R3' | R4' | R5' | R6' | *n*(OH) | ETE(1) | PA(1) | $BDE_{min}(1)$ | HE | ln(ORAC) | ORAC |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | H | H | H | H | H | H | H | OH | H | H | OH | OH | H | H | 3 | 86.059 | 32.448 | 81.032 | -19.988 | 2.454 | 11.637 |
| 2 | H | H | H | H | H | H | OH | OH | H | OH | H | H | H | H | 3 | 85.372 | 31.407 | 79.303 | -18.638 | 2.451 | 11.603 |
| 3 | H | H | H | H | H | OH | H | H | H | OH | H | OH | H | H | 3 | 87.056 | 37.591 | 87.171 | -22.490 | 2.439 | 11.467 |
| 4 | H | H | H | H | H | H | H | H | H | H | OH | OH | OH | H | 3 | 83.880 | 30.484 | 76.888 | -18.857 | 2.386 | 10.865 |
| 5 | H | H | H | H | H | H | H | OH | H | OH | OH | H | H | H | 3 | 85.465 | 32.135 | 80.124 | -18.622 | 2.378 | 10.787 |
| 6 | H | H | H | H | H | H | OH | OH | H | H | OH | H | H | H | 3 | 84.458 | 32.382 | 79.364 | -19.773 | 2.281 | 9.784 |
| 7 | H | H | H | H | H | OH | OH | H | H | OH | H | H | H | H | 3 | 86.983 | 33.352 | 82.858 | -18.691 | 2.259 | 9.574 |
| 8 | H | H | H | H | H | OH | H | OH | H | OH | H | H | H | H | 3 | 88.851 | 32.785 | 84.160 | -20.605 | 2.219 | 9.202 |
| 9 | H | H | H | H | H | H | OH | OH | H | H | H | OH | H | H | 3 | 84.210 | 32.455 | 79.188 | -20.236 | 2.204 | 9.057 |
| 10 | H | H | H | H | H | OH | H | H | H | OH | OH | H | H | H | 3 | 85.096 | 33.237 | 80.857 | -19.449 | 2.154 | 8.619 |
| 11 | H | H | H | H | H | OH | H | H | H | H | OH | H | OH | H | 3 | 86.784 | 37.637 | 86.945 | -24.768 | 2.144 | 8.530 |
| 12 | H | H | H | H | H | H | OH | H | H | H | OH | H | OH | H | 3 | 87.599 | 37.512 | 87.636 | -24.208 | 2.092 | 8.099 |
| 13 | H | H | H | H | H | H | OH | H | H | H | OH | OH | H | H | 3 | 85.448 | 32.717 | 80.689 | -21.691 | 2.089 | 8.076 |
| 14 | H | H | H | H | OH | H | H | OH | H | H | H | OH | H | H | 3 | 78.758 | 37.392 | 78.674 | -17.839 | 2.060 | 7.848 |
| 15 | H | H | H | H | H | H | OH | H | H | OH | OH | H | H | H | 3 | 84.837 | 33.450 | 80.811 | -19.010 | 2.057 | 7.820 |
| 16 | H | H | H | H | OH | H | H | OH | H | H | OH | H | H | H | 3 | 79.216 | 37.143 | 78.884 | -17.262 | 2.056 | 7.813 |
| 17 | H | H | H | H | H | H | H | H | H | OH | H | H | OH | OH | 3 | 77.230 | 35.919 | 75.673 | -18.741 | 2.037 | 7.667 |
| 18 | H | H | H | H | H | OH | OH | H | H | H | OH | H | H | H | 3 | 86.409 | 33.587 | 82.520 | -20.876 | 2.020 | 7.539 |
| 19 | H | H | H | H | H | H | H | OH | H | OH | H | OH | H | H | 3 | 88.479 | 33.642 | 84.644 | -20.532 | 2.006 | 7.430 |
| 20 | H | H | H | H | H | OH | H | H | H | H | OH | OH | H | H | 3 | 85.763 | 32.702 | 80.989 | -22.326 | 1.980 | 7.239 |
| 21 | H | H | H | H | H | OH | OH | H | H | H | H | OH | H | H | 3 | 86.091 | 33.680 | 82.295 | -21.060 | 1.950 | 7.031 |
| 22 | H | H | H | H | OH | H | H | OH | H | OH | H | H | H | H | 3 | 79.951 | 36.234 | 78.709 | -15.724 | 1.938 | 6.944 |
| 23 | H | H | H | H | H | H | H | H | H | OH | H | H | OH | H | 2 | 80.370 | 38.289 | 81.183 | -16.872 | 1.914 | 6.783 |
| 24 | H | H | H | H | H | H | H | H | H | H | OH | H | OH | H | 2 | 87.660 | 37.605 | 87.789 | -19.166 | 1.914 | 6.780 |

*QM parameters (ETE(1), PA(1), BDEmin(1), and HE) are expressed in kcal $mol^{-1}$. The index one refers to the first oxidation step.
**All the abbreviations explained in the main text.

**Table S1.** (cont.)

| # | R1 | R2 | R3 | R4 | R5 | R6 | R7 | R8 | R1' | R2' | R3' | R4' | R5' | R6' | *n*(OH) | ETE(1) | PA(1) | $BDE_{min}(1)$ | HE | ln(ORAC) | ORAC |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 26 | H | H | H | H | H | H | OH | H | H | H | H | OH | H | H | 2 | 88.671 | 35.611 | 86.806 | -19.013 | 1.911 | 6.761 |
| 27 | H | H | H | H | H | OH | H | H | H | H | H | OH | H | H | 2 | 86.377 | 37.862 | 86.763 | -19.780 | 1.906 | 6.727 |
| 28 | H | H | H | H | H | OH | OH | OH | H | H | H | H | H | H | 3 | 88.302 | 28.686 | 79.513 | -17.657 | 1.899 | 6.681 |
| 29 | H | H | H | H | OH | H | H | H | H | OH | H | H | OH | H | 3 | 80.680 | 38.167 | 81.371 | -16.482 | 1.897 | 6.664 |
| 30 | H | H | OH | H | H | H | H | OH | H | H | H | OH | H | H | 3 | 80.969 | 37.585 | 81.078 | -16.021 | 1.890 | 6.621 |
| 31 | H | H | OH | H | H | OH | H | H | H | H | H | OH | H | H | 3 | 80.200 | 38.392 | 81.116 | -18.337 | 1.888 | 6.605 |
| 32 | H | H | H | H | H | H | H | OH | H | OH | H | H | OH | H | 3 | 80.701 | 37.656 | 80.881 | -20.615 | 1.879 | 6.544 |
| 33 | H | H | H | H | H | OH | H | H | H | OH | H | H | OH | H | 3 | 80.246 | 38.321 | 81.091 | -22.349 | 1.860 | 6.424 |
| 34 | H | H | H | H | H | OH | H | H | H | H | OH | H | H | H | 2 | 86.689 | 37.724 | 86.937 | -19.404 | 1.857 | 6.403 |
| 35 | H | H | H | H | H | H | OH | H | H | OH | H | H | OH | H | 3 | 80.130 | 38.400 | 81.054 | -21.940 | 1.841 | 6.303 |
| 36 | H | H | H | H | OH | OH | H | OH | H | H | H | H | H | H | 3 | 78.695 | 36.270 | 77.489 | -14.056 | 1.832 | 6.245 |
| 37 | H | H | OH | H | H | H | OH | H | H | H | H | H | OH | H | 3 | 82.200 | 37.501 | 82.225 | -18.144 | 1.812 | 6.120 |
| 38 | H | H | H | H | H | OH | H | OH | H | H | H | H | H | H | 2 | 87.926 | 34.028 | 84.478 | -17.375 | 1.803 | 6.070 |
| 39 | H | H | H | H | H | H | H | H | H | OH | OH | H | OH | H | 3 | 78.485 | 34.605 | 75.614 | -18.595 | 1.802 | 6.062 |
| 40 | H | H | H | H | OH | H | H | H | H | H | OH | H | OH | H | 3 | 87.892 | 37.438 | 87.854 | -18.694 | 1.798 | 6.037 |
| 41 | H | H | H | H | H | H | H | H | H | OH | H | OH | OH | H | 3 | 79.469 | 35.415 | 77.408 | -19.433 | 1.797 | 6.029 |
| 42 | H | H | OH | H | H | OH | H | H | H | H | H | H | OH | H | 3 | 82.441 | 37.598 | 82.562 | -18.524 | 1.785 | 5.962 |
| 43 | H | H | H | OH | H | H | OH | OH | H | H | H | H | H | H | 3 | 78.133 | 33.916 | 74.573 | -14.781 | 1.767 | 5.856 |
| 44 | H | H | H | H | OH | H | OH | H | H | H | H | OH | H | H | 3 | 89.428 | 35.301 | 87.253 | -18.055 | 1.758 | 5.801 |
| 45 | H | H | H | H | H | H | OH | H | H | OH | H | H | H | OH | 3 | 88.074 | 35.484 | 86.082 | -21.229 | 1.753 | 5.771 |
| 46 | H | H | OH | H | H | H | H | H | H | H | OH | H | OH | H | 3 | 83.177 | 37.158 | 82.859 | -18.335 | 1.748 | 5.744 |
| 47 | H | H | H | H | H | H | OH | H | H | H | OH | H | H | H | 2 | 87.055 | 38.328 | 87.908 | -18.833 | 1.726 | 5.619 |
| 48 | H | H | OH | H | H | OH | H | OH | H | H | H | H | H | H | 3 | 82.607 | 37.332 | 82.463 | -16.338 | 1.723 | 5.599 |
| 49 | H | H | OH | H | H | OH | OH | H | H | H | H | H | H | H | 3 | 81.359 | 38.176 | 82.059 | -14.926 | 1.712 | 5.541 |
| 26 | H | H | H | H | H | H | OH | H | H | H | H | OH | H | H | 2 | 88.671 | 35.611 | 86.806 | -19.013 | 1.911 | 6.761 |

*QM parameters (ETE(1), PA(1), BDEmin(1), and HE) are expressed in kcal $mol^{-1}$. The index one refers to the first oxidation step.
**All the abbreviations explained in the main text.

**Table S1.** (cont.)

| # | R1 | R2 | R3 | R4 | R5 | R6 | R7 | R8 | R1' | R2' | R3' | R4' | R5' | R6' | *n*(OH) | ETE(1) | PA(1) | $BDE_{min}(1)$ | HE | ln(ORAC) | ORAC |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 50 | H | H | H | H | H | H | H | H | H | H | OH | OH | H | H | 2 | 85.782 | 32.494 | 80.800 | -16.511 | 1.710 | 5.531 |
| 51 | H | H | H | H | H | H | H | H | H | OH | H | OH | H | OH | 3 | 89.872 | 35.342 | 87.737 | -20.666 | 1.694 | 5.441 |
| 52 | H | H | OH | H | H | H | H | H | H | H | H | H | H | OH | 2 | 91.104 | 29.154 | 82.782 | -13.667 | 1.640 | 5.155 |
| 53 | H | H | OH | H | H | OH | H | H | H | H | H | H | H | OH | 3 | 88.902 | 29.919 | 81.344 | -15.598 | 1.631 | 5.107 |
| 54 | H | H | H | H | H | OH | H | H | H | OH | H | H | H | OH | 3 | 88.145 | 35.486 | 86.155 | -21.685 | 1.623 | 5.068 |
| 55 | H | H | OH | H | H | H | H | H | H | H | OH | H | H | OH | 3 | 89.102 | 29.987 | 81.613 | -15.214 | 1.622 | 5.062 |
| 56 | H | H | H | H | OH | H | H | H | H | H | OH | OH | H | H | 3 | 86.385 | 32.008 | 80.916 | -15.993 | 1.598 | 4.943 |
| 57 | H | H | H | H | H | H | H | H | H | OH | OH | OH | H | H | 3 | 82.008 | 33.355 | 77.887 | -16.316 | 1.578 | 4.845 |
| 58 | H | H | H | H | H | H | H | OH | H | OH | H | H | H | OH | 3 | 88.218 | 35.098 | 85.839 | -21.599 | 1.568 | 4.796 |
| 59 | H | H | OH | H | H | H | OH | H | H | H | H | H | H | OH | 3 | 88.514 | 29.945 | 80.983 | -15.199 | 1.561 | 4.766 |
| 60 | H | H | OH | H | H | H | H | H | H | H | H | H | OH | OH | 3 | 90.509 | 28.816 | 81.849 | -12.070 | 1.553 | 4.724 |
| 61 | H | H | OH | H | H | H | H | OH | H | H | H | H | H | OH | 3 | 89.648 | 29.363 | 81.535 | -12.955 | 1.535 | 4.642 |
| 62 | H | H | H | H | OH | H | OH | H | H | H | OH | H | H | H | 3 | 87.322 | 38.247 | 88.093 | -18.012 | 1.535 | 4.640 |
| 63 | H | H | H | H | H | H | H | OH | H | H | H | OH | H | H | 2 | 87.450 | 35.206 | 85.180 | -17.504 | 1.532 | 4.629 |
| 64 | H | H | OH | H | H | H | H | OH | H | H | H | H | OH | H | 3 | 83.671 | 36.524 | 82.719 | -16.041 | 1.497 | 4.467 |
| 65 | H | H | OH | H | OH | H | H | H | H | H | H | H | H | OH | 3 | 89.875 | 28.582 | 80.982 | -10.372 | 1.405 | 4.077 |
| 66 | H | H | H | H | OH | OH | H | H | H | H | H | OH | H | H | 3 | 83.755 | 36.793 | 83.071 | -15.515 | 1.401 | 4.058 |
| 67 | H | H | H | H | H | H | H | OH | H | H | OH | H | OH | H | 3 | 87.717 | 35.136 | 85.377 | -22.299 | 1.399 | 4.049 |
| 68 | H | H | OH | H | H | H | H | H | H | H | H | OH | H | OH | 3 | 87.212 | 29.891 | 79.627 | -15.129 | 1.396 | 4.040 |
| 69 | H | H | OH | H | H | H | H | H | H | H | H | H | H | OH | 2 | 89.155 | 29.678 | 81.357 | -9.953 | 1.390 | 4.014 |
| 70 | H | H | H | H | H | OH | H | OH | H | H | OH | H | H | H | 3 | 87.980 | 34.116 | 84.620 | -22.341 | 1.374 | 3.949 |
| 71 | H | H | H | H | OH | H | H | OH | H | H | H | H | H | H | 2 | 78.908 | 37.225 | 78.657 | -12.375 | 1.361 | 3.899 |
| 72 | H | H | H | H | H | H | H | OH | H | H | OH | H | H | H | 2 | 87.670 | 35.172 | 85.365 | -17.018 | 1.355 | 3.877 |
| 73 | H | H | OH | H | H | OH | H | H | H | H | H | H | H | H | 2 | 81.779 | 38.073 | 82.377 | -13.477 | 1.313 | 3.716 |
| 74 | H | H | H | H | H | H | H | H | H | OH | H | OH | H | H | 2 | 90.735 | 35.359 | 88.618 | -16.904 | 1.302 | 3.678 |

*QM parameters (ETE(1), PA(1), BDEmin(1), and HE) are expressed in kcal $mol^{-1}$. The index one refers to the first oxidation step.
**All the abbreviations explained in the main text.

**Table S1.** (cont.)

| # | R1 | R2 | R3 | R4 | R5 | R6 | R7 | R8 | R1' | R2' | R3' | R4' | R5' | R6' | *n*(OH) | ETE(1) | PA(1) | $BDE_{min}(1)$ | HE | ln(ORAC) | ORAC |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 75 | H | H | H | H | H | OH | H | H | H | OH | H | H | H | H | 2 | 87.362 | 37.396 | 87.281 | -17.180 | 1.301 | 3.674 |
| 76 | H | H | OH | H | H | H | H | H | H | H | H | OH | OH | H | 3 | 84.029 | 33.177 | 79.730 | -15.632 | 1.277 | 3.586 |
| 77 | H | H | H | H | H | OH | H | OH | H | H | H | OH | H | H | 3 | 87.751 | 34.080 | 84.355 | -22.744 | 1.266 | 3.548 |
| 78 | H | H | OH | H | H | H | H | H | H | H | H | OH | H | H | 2 | 80.484 | 38.050 | 81.057 | -12.540 | 1.222 | 3.393 |
| 79 | H | H | H | H | H | OH | OH | H | H | H | H | H | H | H | 2 | 86.402 | 33.495 | 82.421 | -15.692 | 1.210 | 3.354 |
| 80 | H | H | H | H | OH | OH | H | H | H | H | OH | H | H | H | 3 | 84.125 | 36.495 | 83.144 | -15.054 | 1.178 | 3.249 |
| 81 | H | H | OH | H | H | H | OH | H | H | H | H | H | H | H | 2 | 81.511 | 37.894 | 81.928 | -12.924 | 1.169 | 3.220 |
| 82 | H | H | H | H | OH | H | OH | H | H | H | H | H | H | H | 2 | 96.432 | 33.747 | 92.703 | -12.982 | 1.168 | 3.217 |
| 83 | H | H | H | H | H | H | OH | OH | H | H | H | H | H | H | 2 | 84.518 | 32.200 | 79.243 | -14.804 | 1.131 | 3.098 |
| 84 | H | H | H | H | H | H | OH | H | H | OH | H | OH | H | H | 3 | 90.495 | 35.349 | 88.368 | -21.989 | 1.104 | 3.016 |
| 85 | H | H | OH | H | OH | H | H | OH | H | H | H | H | H | H | 3 | 78.670 | 37.046 | 78.239 | -11.573 | 1.095 | 2.989 |
| 86 | H | H | H | H | H | H | H | OH | H | OH | H | H | H | H | 2 | 88.676 | 33.799 | 84.998 | -15.445 | 1.094 | 2.986 |
| 87 | H | H | H | H | H | H | OH | H | H | OH | H | H | H | H | 2 | 88.243 | 36.744 | 87.510 | -16.767 | 1.090 | 2.976 |
| 88 | H | H | OH | H | H | OH | H | H | H | H | H | OH | H | H | 3 | 81.349 | 36.778 | 80.651 | -12.777 | 1.064 | 2.898 |
| 89 | H | H | H | H | H | H | OH | H | H | H | H | H | H | H | 1 | 94.781 | 34.135 | 91.440 | -13.838 | 1.043 | 2.837 |
| 90 | H | H | H | H | H | H | H | H | H | OH | H | H | H | OH | 2 | 87.988 | 35.149 | 85.661 | -16.085 | 0.929 | 2.531 |
| 91 | H | H | H | H | OH | H | H | H | H | OH | H | OH | H | H | 3 | 90.130 | 36.181 | 88.835 | -16.457 | 0.915 | 2.497 |
| 92 | H | H | OH | H | H | H | OH | OH | H | H | H | H | H | H | 3 | 83.899 | 32.343 | 78.766 | -13.698 | 0.890 | 2.435 |
| 93 | H | H | OH | H | H | H | H | H | H | H | H | H | OH | H | 2 | 82.899 | 37.260 | 82.683 | -12.977 | 0.869 | 2.386 |
| 94 | H | H | H | H | OH | OH | OH | H | H | H | H | H | H | H | 3 | 81.332 | 37.052 | 80.908 | -12.087 | 0.859 | 2.361 |
| 95 | H | H | H | H | H | H | H | H | H | OH | OH | H | H | H | 2 | 85.128 | 33.115 | 80.767 | -13.871 | 0.754 | 2.125 |
| 96 | H | H | OH | H | OH | H | OH | H | H | H | H | H | H | H | 3 | 82.513 | 36.478 | 81.515 | -12.572 | 0.754 | 2.125 |
| 97 | H | H | H | H | OH | H | H | H | H | OH | OH | H | H | H | 3 | 85.434 | 32.874 | 80.832 | -13.430 | 0.749 | 2.114 |

*QM parameters (ETE(1), PA(1), BDEmin(1), and HE) are expressed in kcal $mol^{-1}$. The index one refers to the first oxidation step.
**All the abbreviations explained in the main text.

**Table S1.** (cont.)

| # | R1 | R2 | R3 | R4 | R5 | R6 | R7 | R8 | R1' | R2' | R3' | R4' | R5' | R6' | *n*(OH) | ETE(1) | PA(1) | $BDE_{min}(1)$ | HE | ln(ORAC) | ORAC |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 98 | H | H | H | H | OH | H | H | H | H | OH | H | H | H | OH | 3 | 88.379 | 35.349 | 86.251 | -15.618 | 0.639 | 1.895 |
| 99 | H | H | H | H | OH | H | H | H | H | H | H | H | H | H | 1 | 83.029 | 36.288 | 81.841 | -7.764 | 0.633 | 1.884 |
| 100 | H | H | OH | H | OH | H | H | H | H | OH | H | H | H | H | 3 | 88.592 | 36.584 | 87.700 | -15.873 | 0.631 | 1.880 |
| 101 | H | H | OH | H | H | OH | H | H | H | H | H | H | OH | H | 3 | 83.693 | 35.979 | 82.196 | -13.036 | 0.596 | 1.814 |
| 102 | H | H | OH | H | OH | OH | H | H | H | H | H | OH | H | H | 4 | 79.917 | 38.405 | 80.846 | -10.250 | 0.491 | 1.634 |
| 103 | H | H | OH | H | OH | OH | H | H | H | H | H | H | H | H | 3 | 79.694 | 38.341 | 80.559 | -10.013 | 0.451 | 1.570 |
| 104 | H | H | H | H | H | OH | H | H | H | H | H | H | H | H | 1 | 86.589 | 37.717 | 86.830 | -14.319 | 0.447 | 1.564 |
| 105 | H | H | H | H | OH | OH | H | H | H | OH | H | H | H | H | 3 | 84.863 | 36.042 | 83.429 | -13.042 | 0.367 | 1.444 |
| 106 | H | H | H | H | H | H | H | H | H | H | H | H | OH | H | 1 | 82.546 | 37.345 | 82.415 | -7.713 | 0.362 | 1.436 |
| 107 | H | H | OH | H | H | H | H | OH | H | H | H | H | H | H | 2 | 83.105 | 36.984 | 82.613 | -11.073 | 0.357 | 1.429 |
| 108 | H | H | H | H | H | H | H | H | H | H | OH | H | H | H | 1 | 87.243 | 38.215 | 87.982 | -13.668 | 0.075 | 1.078 |
| 109 | H | H | H | H | H | H | H | OH | H | H | H | H | H | H | 1 | 87.713 | 35.091 | 85.328 | -12.124 | -0.032 | 0.969 |
| 110 | H | H | H | H | H | H | H | H | H | H | H | OH | H | H | 1 | 89.163 | 35.855 | 87.542 | -14.168 | -0.129 | 0.879 |
| 111 | H | H | H | H | OH | H | H | H | H | H | OH | H | H | H | 2 | 87.482 | 38.131 | 88.137 | -13.228 | -0.142 | 0.868 |
| 112 | H | H | H | H | OH | H | H | H | H | H | H | OH | H | H | 2 | 89.832 | 35.557 | 87.913 | -13.711 | -0.213 | 0.808 |
| 113 | H | H | H | H | OH | H | H | H | H | OH | H | H | H | H | 2 | 88.813 | 36.373 | 87.710 | -11.199 | -0.459 | 0.632 |
| 114 | H | H | H | H | H | H | H | H | H | OH | H | H | H | H | 1 | 88.469 | 36.738 | 87.731 | -11.707 | -0.499 | 0.607 |
| 115 | H | H | H | H | H | H | H | H | H | H | H | H | H | OH | 1 | 89.792 | 40.096 | 92.412 | -8.368 | -1.233 | 0.291 |

*QM parameters (ETE(1), PA(1), BDEmin(1), and HE) are expressed in kcal $mol^{-1}$. The index one refers to the first oxidation step.
**All the abbreviations explained in the main text.

**Table S2.** Cartesian coordinates of optimized geometries (ωB97XD/6-311+G**) for the reactions of genistein/quercetin (ROH) with peroxyl radical derived from AAPH (PO•) as depicted in **Table 3** of the main text. Total energy (E) in Hartrees. $N_i$ is the number of imaginary frequencies.

| PO• (gas phase) E = -417.655794, $N_i$ = 0 | | | | PO• (aqueous phase) E = -417.672069, $N_i$ = 0 | | | |
|---|---|---|---|---|---|---|---|
| C | -0.290267 | 0.724586 | -0.860905 | C | -0.260301 | 0.702239 | -0.923418 |
| H | -1.244617 | 1.854299 | -2.059450 | H | -0.949697 | 1.793777 | -2.305185 |
| N | -1.234037 | 0.902399 | -1.697201 | N | -0.969667 | 0.825576 | -1.984143 |
| N | 0.613761 | 1.656958 | -0.415208 | N | 0.406689 | 1.702721 | -0.286959 |
| H | 0.682332 | 2.522230 | -0.925077 | H | 0.519736 | 2.584267 | -0.764545 |
| H | 1.462281 | 1.330873 | 0.018356 | H | 1.085955 | 1.483357 | 0.424518 |
| C | -0.218998 | -0.637345 | -0.165952 | C | -0.212699 | -0.652785 | -0.217193 |
| C | -0.550541 | -1.781076 | -1.105300 | C | -0.646934 | -1.810885 | -1.090354 |
| H | 0.126723 | -1.785657 | -1.961150 | H | -0.079633 | -1.839877 | -2.021475 |
| H | -1.566596 | -1.651842 | -1.475576 | H | -1.706287 | -1.711456 | -1.326213 |
| H | -0.467365 | -2.728207 | -0.570033 | H | -0.500450 | -2.744723 | -0.544599 |
| C | -1.087019 | -0.622674 | 1.085921 | C | -0.972020 | -0.595841 | 1.100369 |
| H | -0.803229 | 0.198768 | 1.747089 | H | -0.548162 | 0.152717 | 1.771917 |
| H | -0.983092 | -1.568330 | 1.619750 | H | -0.956479 | -1.570879 | 1.588535 |
| H | -2.127424 | -0.489387 | 0.786305 | H | -2.009766 | -0.329691 | 0.888982 |
| O | 1.199181 | -0.766692 | 0.247001 | O | 1.244499 | -0.825013 | 0.069197 |
| O | 1.446291 | -1.844735 | 0.924175 | O | 1.512600 | -1.849334 | 0.813312 |

| $PO^-$ (gas phase) E = -417.705167, $N_i$ = 0 | | | | $PO^-$ (aqueous phase) E = -417.833891, $N_i$ = 0 | | | |
|---|---|---|---|---|---|---|---|
| C | 0.116371 | 0.629058 | -0.948064 | C | 0.127969 | 0.640560 | -0.912234 |
| H | 1.753047 | 0.200819 | -1.686004 | H | 1.931491 | 0.369321 | -1.339764 |
| N | 1.099243 | 0.984738 | -1.674135 | N | 1.217054 | 1.087487 | -1.424084 |
| N | -0.969818 | 1.491340 | -0.795224 | N | -1.006158 | 1.400157 | -0.943840 |
| H | -0.742798 | 2.439487 | -1.057330 | H | -0.884692 | 2.379816 | -1.152723 |
| H | -1.451801 | 1.419722 | 0.087038 | H | -1.768285 | 1.175998 | -0.324425 |
| C | -0.014067 | -0.725391 | -0.244973 | C | -0.018802 | -0.740808 | -0.254506 |
| C | -1.172286 | -1.521593 | -0.869495 | C | -1.239198 | -1.481887 | -0.805950 |
| H | -1.032937 | -1.584541 | -1.952354 | H | -1.196893 | -1.535448 | -1.897037 |
| H | -2.146619 | -1.066667 | -0.663122 | H | -2.172001 | -0.994012 | -0.515618 |
| H | -1.113803 | -2.528333 | -0.450604 | H | -1.254925 | -2.496135 | -0.403817 |
| C | -0.238173 | -0.534430 | 1.267343 | C | -0.117691 | -0.552026 | 1.263780 |
| H | 0.466652 | 0.199741 | 1.670553 | H | 0.777205 | -0.052049 | 1.644006 |
| H | -0.020522 | -1.511773 | 1.707137 | H | -0.216574 | -1.521243 | 1.754414 |
| H | -1.262840 | -0.233838 | 1.519707 | H | -0.990662 | 0.050410 | 1.525797 |
| O | 1.201711 | -1.381430 | -0.458084 | O | 1.180127 | -1.423426 | -0.609116 |
| O | 1.171954 | -2.699095 | 0.166696 | O | 1.275347 | -2.728900 | 0.014204 |

**Table S2.** (cont.)

| POH (gas phase) E = -418.293640, $N_i$ = 0 | | | | POH (aqueous phase) E = -418.317993, $N_i$ = 0 | | | |
|---|---|---|---|---|---|---|---|
| C | 0.148481 | 0.680255 | -0.837826 | C | 0.154720 | 0.666881 | -0.868560 |
| H | 2.013180 | 0.571843 | -1.078539 | H | 1.775587 | 0.247098 | -1.740736 |
| N | 1.234843 | 1.205544 | -1.234523 | N | 1.099412 | 1.000975 | -1.669400 |
| N | -1.021367 | 1.414725 | -0.866313 | N | -0.848875 | 1.543265 | -0.583044 |
| H | -0.931714 | 2.281797 | -1.374688 | H | -0.931822 | 2.344188 | -1.191212 |
| H | -1.886118 | 0.925827 | -1.025298 | H | -1.708576 | 1.203850 | -0.181935 |
| C | 0.010302 | -0.707901 | -0.191422 | C | 0.044670 | -0.688117 | -0.155750 |
| C | -1.196146 | -1.487092 | -0.714515 | C | -1.023424 | -1.537757 | -0.841472 |
| H | -1.210515 | -1.504087 | -1.807045 | H | -0.779239 | -1.681358 | -1.896840 |
| H | -2.134544 | -1.064306 | -0.347633 | H | -1.997123 | -1.049433 | -0.770420 |
| H | -1.146053 | -2.512384 | -0.343572 | H | -1.101851 | -2.511372 | -0.354383 |
| C | -0.028256 | -0.551084 | 1.328852 | C | -0.209671 | -0.530313 | 1.339593 |
| H | 0.887160 | -0.069549 | 1.677135 | H | 0.532976 | 0.131871 | 1.790139 |
| H | -0.121348 | -1.526509 | 1.808201 | H | -0.155911 | -1.508152 | 1.820936 |
| H | -0.878770 | 0.070530 | 1.614469 | H | -1.204921 | -0.123995 | 1.527680 |
| O | 1.220352 | -1.366295 | -0.600605 | O | 1.356518 | -1.266471 | -0.360396 |
| O | 1.329788 | -2.611312 | 0.080758 | O | 1.407405 | -2.579512 | 0.168766 |
| H | 1.372408 | -3.219201 | -0.664242 | H | 1.251810 | -3.130850 | -0.609772 |

| $POH^{\bullet+}$ (gas phase) E = -417.978247, $N_i$ = 0 | | | | $POH^{\bullet+}$ (aqueous phase) E = -418.086010, $N_i$ = 0 | | | |
|---|---|---|---|---|---|---|---|
| C | 0.032953 | 0.594468 | -0.930532 | C | 0.050583 | 0.582294 | -0.948990 |
| H | 1.720413 | 0.355702 | -2.007566 | H | 1.952722 | 0.728783 | -1.515100 |
| N | 0.742598 | 0.652598 | -2.049360 | N | 0.995637 | 0.786420 | -1.880902 |
| N | -0.674059 | 1.616425 | -0.532732 | N | -0.839873 | 1.488641 | -0.708836 |
| H | -0.656788 | 2.493208 | -1.039106 | H | -0.800219 | 2.390471 | -1.172006 |
| H | -1.235582 | 1.561979 | 0.306042 | H | -1.581210 | 1.326524 | -0.036264 |
| C | -0.065806 | -0.762240 | -0.215840 | C | -0.038120 | -0.785068 | -0.266594 |
| C | -1.163919 | -1.574873 | -0.909334 | C | -1.236453 | -1.534818 | -0.840235 |
| H | -0.938917 | -1.712655 | -1.967535 | H | -1.137678 | -1.652713 | -1.920804 |
| H | -2.131363 | -1.078720 | -0.806476 | H | -2.157187 | -0.992358 | -0.618942 |
| H | -1.225244 | -2.551867 | -0.430551 | H | -1.296972 | -2.515975 | -0.369958 |
| C | -0.289665 | -0.620362 | 1.284033 | C | -0.095178 | -0.626064 | 1.247886 |
| H | 0.446772 | 0.039727 | 1.746366 | H | 0.736334 | -0.017272 | 1.607244 |
| H | -0.196137 | -1.612587 | 1.727301 | H | -0.038554 | -1.618533 | 1.698524 |
| H | -1.300853 | -0.273807 | 1.513704 | H | -1.039218 | -0.176244 | 1.559781 |
| O | 1.239419 | -1.275805 | -0.507360 | O | 1.207273 | -1.387482 | -0.671724 |
| O | 1.269086 | -2.640554 | -0.133332 | O | 1.235026 | -2.743727 | -0.280943 |
| H | 2.088779 | -2.679838 | 0.375470 | H | 1.744773 | -2.722079 | 0.541058 |

**Table S2.** (cont.)

| ROH (gas phase) E = -1104.12955, $N_i$ = 0 | | | | ROH (aqueous phase) E = -1104.16782, $N_i$ = 0 | | | |
|---|---|---|---|---|---|---|---|
| H | 0.137270 | 1.319117 | -3.031008 | H | 0.155010 | 1.313485 | -3.004989 |
| C | -0.495780 | 0.447916 | -2.939162 | C | -0.478530 | 0.440032 | -2.927245 |
| C | -2.132770 | -1.832971 | -2.719430 | C | -2.123276 | -1.830134 | -2.726425 |
| C | -0.608845 | -0.233774 | -1.739077 | C | -0.606976 | -0.242034 | -1.729043 |
| C | -1.215990 | -0.033157 | -4.025443 | C | -1.189587 | -0.037489 | -4.020212 |
| C | -2.030805 | -1.163055 | -3.928076 | C | -2.010379 | -1.168039 | -3.931831 |
| C | -1.409576 | -1.371136 | -1.588879 | C | -1.413414 | -1.377069 | -1.584453 |
| H | -2.590821 | -1.531970 | -4.780006 | H | -2.557020 | -1.522468 | -4.798061 |
| O | 0.105283 | 0.245928 | -0.694341 | O | 0.100182 | 0.234039 | -0.677104 |
| C | 0.056058 | -0.362288 | 0.521990 | C | 0.037478 | -0.359428 | 0.543800 |
| C | -0.726213 | -1.440255 | 0.766105 | C | -0.753177 | -1.437244 | 0.771634 |
| C | -1.512908 | -2.043033 | -0.309963 | C | -1.523001 | -2.029885 | -0.305100 |
| O | -2.217589 | -3.038725 | -0.130867 | O | -2.242143 | -3.033167 | -0.118016 |
| C | 0.894435 | 0.319522 | 1.522530 | C | 0.883188 | 0.322833 | 1.535789 |
| C | 2.468004 | 1.640153 | 3.419014 | C | 2.492507 | 1.646253 | 3.384915 |
| C | 1.717925 | -0.399872 | 2.387890 | C | 1.731809 | -0.399349 | 2.373588 |
| C | 0.875981 | 1.716835 | 1.602033 | C | 0.849306 | 1.719332 | 1.619911 |
| C | 1.653690 | 2.366680 | 2.538628 | C | 1.644664 | 2.376211 | 2.539657 |
| C | 2.496706 | 0.258433 | 3.332836 | C | 2.532117 | 0.264421 | 3.295083 |
| H | 1.785307 | -1.478607 | 2.302340 | H | 1.788758 | -1.478856 | 2.296747 |
| H | 0.249846 | 2.287170 | 0.923545 | H | 0.195911 | 2.296819 | 0.974845 |
| H | 3.146341 | -0.290883 | 4.002971 | H | 3.201426 | -0.285524 | 3.945980 |
| O | -0.862292 | -2.028310 | 1.975861 | O | -0.914815 | -2.041745 | 1.982621 |
| H | -0.462106 | -1.475312 | 2.653227 | H | -0.530359 | -1.508648 | 2.688072 |
| O | -1.089664 | 0.646879 | -5.187288 | O | -1.053783 | 0.643226 | -5.184093 |
| H | -1.617258 | 0.228563 | -5.870122 | H | -1.594256 | 0.244462 | -5.874901 |
| O | 1.702151 | 3.721436 | 2.698492 | O | 1.665937 | 3.732159 | 2.699015 |
| H | 1.146826 | 4.163483 | 2.054960 | H | 1.075837 | 4.156535 | 2.067612 |
| O | 3.225144 | 2.276422 | 4.336654 | O | 3.283308 | 2.278645 | 4.295339 |
| H | 3.089482 | 3.224975 | 4.246386 | H | 3.151459 | 3.231953 | 4.230211 |
| O | -2.914398 | -2.906317 | -2.634832 | O | -2.919103 | -2.914259 | -2.646065 |
| H | -2.863434 | -3.233845 | -1.706968 | H | -2.879078 | -3.235066 | -1.717282 |

**Table S2.** (cont.)

| RO• (gas phase) E = -1103.508461, $N_i$ = 0 | | | | RO• (aqueous phase) E = -1103.532714, $N_i$ = 0 | | | |
|---|---|---|---|---|---|---|---|
| H | -0.238901 | 1.634658 | -2.731142 | H | -0.228861 | 1.634860 | -2.707473 |
| C | -0.730969 | 0.672634 | -2.712300 | C | -0.725976 | 0.674145 | -2.702280 |
| C | -2.026270 | -1.833176 | -2.695640 | C | -2.023969 | -1.823360 | -2.702316 |
| C | -0.682866 | -0.138180 | -1.592973 | C | -0.683615 | -0.143921 | -1.587651 |
| C | -1.435877 | 0.208439 | -3.817735 | C | -1.428514 | 0.217845 | -3.811848 |
| C | -2.082338 | -1.032534 | -3.821355 | C | -2.078268 | -1.023172 | -3.823256 |
| C | -1.315239 | -1.388823 | -1.551021 | C | -1.317167 | -1.394137 | -1.549032 |
| H | -2.628448 | -1.382341 | -4.689926 | H | -2.618922 | -1.354001 | -4.702336 |
| O | 0.003194 | 0.321783 | -0.527229 | O | 0.002322 | 0.313463 | -0.519005 |
| C | 0.126848 | -0.380230 | 0.637411 | C | 0.123275 | -0.391689 | 0.643092 |
| C | -0.465790 | -1.607007 | 0.744523 | C | -0.471039 | -1.619434 | 0.747418 |
| C | -1.225416 | -2.175231 | -0.362471 | C | -1.229536 | -2.182841 | -0.362853 |
| O | -1.742819 | -3.295823 | -0.207557 | O | -1.753045 | -3.306941 | -0.218142 |
| C | 0.912887 | 0.331450 | 1.629627 | C | 0.908553 | 0.318664 | 1.635137 |
| C | 2.453587 | 1.732745 | 3.566588 | C | 2.451202 | 1.732197 | 3.561573 |
| C | 1.162842 | -0.232008 | 2.923706 | C | 1.163318 | -0.237333 | 2.931416 |
| C | 1.433846 | 1.595560 | 1.305368 | C | 1.428965 | 1.582656 | 1.309739 |
| C | 2.179653 | 2.281150 | 2.233992 | C | 2.175475 | 2.274563 | 2.232209 |
| C | 1.898750 | 0.433992 | 3.853005 | C | 1.899974 | 0.435923 | 3.853499 |
| H | 0.757178 | -1.203629 | 3.160438 | H | 0.764561 | -1.207535 | 3.182837 |
| H | 1.256701 | 2.037584 | 0.335341 | H | 1.252473 | 2.026066 | 0.339567 |
| H | 2.090328 | 0.012359 | 4.832176 | H | 2.091899 | 0.014483 | 4.833242 |
| O | -0.411093 | -2.382605 | 1.835937 | O | -0.408492 | -2.386635 | 1.847156 |
| H | -0.921465 | -3.178622 | 1.605447 | H | -0.911814 | -3.195014 | 1.648795 |
| O | -1.466864 | 1.018222 | -4.894978 | O | -1.458551 | 1.031397 | -4.891501 |
| H | -1.973683 | 0.613140 | -5.601387 | H | -1.966823 | 0.629028 | -5.604734 |
| O | 2.695977 | 3.477356 | 1.982819 | O | 2.680230 | 3.477975 | 1.944547 |
| O | 3.134334 | 2.412252 | 4.347639 | O | 3.135745 | 2.404692 | 4.360360 |
| H | 3.169187 | 3.732333 | 2.795087 | H | 3.168545 | 3.787709 | 2.724973 |
| O | -2.641632 | -3.014395 | -2.699156 | O | -2.648538 | -3.015778 | -2.713898 |
| H | -2.497819 | -3.439533 | -1.829515 | H | -2.505581 | -3.442352 | -1.844516 |

**Table S2.** (cont.)

| $ROH^{\bullet+}$ (gas phase) E = -1103.871343, $N_i$ = 0 | | | | $ROH^{\bullet+}$ (aqueous phase) E=-1103.964126, $N_i$ = 0 | | | |
|---|---|---|---|---|---|---|---|
| H | -0.366125 | 1.640515 | -2.746438 | H | -0.224834 | 1.581521 | -2.778673 |
| C | -0.819995 | 0.660105 | -2.718148 | C | -0.723635 | 0.622170 | -2.753599 |
| C | -2.030397 | -1.889926 | -2.716251 | C | -2.035203 | -1.868540 | -2.711205 |
| C | -0.741385 | -0.143308 | -1.614585 | C | -0.697856 | -0.164036 | -1.626260 |
| C | -1.519143 | 0.170645 | -3.837201 | C | -1.421265 | 0.140535 | -3.864731 |
| C | -2.118705 | -1.087146 | -3.842348 | C | -2.074230 | -1.094797 | -3.853358 |
| C | -1.329508 | -1.422361 | -1.568084 | C | -1.337248 | -1.413427 | -1.560709 |
| H | -2.655097 | -1.455990 | -4.708496 | H | -2.608314 | -1.445263 | -4.728513 |
| O | -0.057237 | 0.351416 | -0.537495 | O | -0.011064 | 0.326201 | -0.559119 |
| C | 0.106568 | -0.318017 | 0.617757 | C | 0.099258 | -0.323470 | 0.617641 |
| C | -0.455972 | -1.596004 | 0.724410 | C | -0.543187 | -1.556384 | 0.763398 |
| C | -1.210998 | -2.203481 | -0.394229 | C | -1.285105 | -2.164786 | -0.355471 |
| O | -1.666620 | -3.335046 | -0.197970 | O | -1.813425 | -3.270985 | -0.163391 |
| C | 0.852238 | 0.386685 | 1.603201 | C | 0.859466 | 0.376579 | 1.593783 |
| C | 2.323323 | 1.815099 | 3.503859 | C | 2.385466 | 1.778968 | 3.464611 |
| C | 1.124810 | -0.166964 | 2.887324 | C | 1.286183 | -0.245090 | 2.805790 |
| C | 1.340087 | 1.684949 | 1.294422 | C | 1.230231 | 1.720077 | 1.337886 |
| C | 2.058227 | 2.383692 | 2.220640 | C | 1.964816 | 2.414887 | 2.255836 |
| C | 1.845813 | 0.536730 | 3.814763 | C | 2.038590 | 0.445054 | 3.714633 |
| H | 0.763660 | -1.150921 | 3.141933 | H | 1.039227 | -1.275613 | 3.005828 |
| H | 1.139498 | 2.116239 | 0.322253 | H | 0.917740 | 2.216172 | 0.428416 |
| H | 2.060064 | 0.128168 | 4.793801 | H | 2.380427 | -0.018738 | 4.630873 |
| O | -0.370815 | -2.350455 | 1.787926 | O | -0.545656 | -2.231570 | 1.886804 |
| H | -0.855690 | -3.176886 | 1.566554 | H | -1.058399 | -3.050197 | 1.739345 |
| O | -1.567339 | 0.990885 | -4.886998 | O | -1.433998 | 0.931471 | -4.953706 |
| H | -2.056540 | 0.602177 | -5.617360 | H | -1.940580 | 0.524621 | -5.666336 |
| O | 2.579436 | 3.614796 | 2.068348 | O | 2.349849 | 3.697888 | 2.137506 |
| H | 2.399542 | 3.994301 | 1.204779 | H | 2.039047 | 4.082780 | 1.309700 |
| O | 3.014253 | 2.486436 | 4.396039 | O | 3.101670 | 2.438700 | 4.354217 |
| H | 3.277898 | 3.349136 | 4.045714 | H | 3.266626 | 3.347045 | 4.058967 |
| O | -2.602159 | -3.081713 | -2.729911 | O | -2.663355 | -3.053136 | -2.702971 |
| H | -2.461692 | -3.533759 | -1.878211 | H | -2.541242 | -3.468636 | -1.827193 |

**Table S2.** (cont.)

| RO (gas phase) E = -1103.613959, $N_i$ = 0 | | | | RO (aqueous phase) E = -1103.703205, $N_i$ = 0 | | | |
|---|---|---|---|---|---|---|---|
| H | -0.238810 | 1.635037 | -2.731468 | H | -0.229977 | 1.631432 | -2.706227 |
| C | -0.733593 | 0.673950 | -2.720236 | C | -0.728755 | 0.671384 | -2.705728 |
| C | -2.022628 | -1.828869 | -2.692284 | C | -2.026361 | -1.823291 | -2.708078 |
| C | -0.686152 | -0.143320 | -1.594461 | C | -0.690013 | -0.152922 | -1.591883 |
| C | -1.435527 | 0.211766 | -3.821068 | C | -1.429365 | 0.219467 | -3.816100 |
| C | -2.081273 | -1.028809 | -3.823447 | C | -2.079551 | -1.020796 | -3.829343 |
| C | -1.314954 | -1.385139 | -1.554901 | C | -1.322248 | -1.398316 | -1.555966 |
| H | -2.628211 | -1.380122 | -4.692120 | H | -2.620007 | -1.350671 | -4.709112 |
| O | -0.002979 | 0.311841 | -0.529657 | O | -0.005130 | 0.297959 | -0.517724 |
| C | 0.127463 | -0.384785 | 0.644517 | C | 0.113225 | -0.409389 | 0.641067 |
| C | -0.485787 | -1.628538 | 0.723558 | C | -0.487239 | -1.636418 | 0.730029 |
| C | -1.220855 | -2.176199 | -0.350366 | C | -1.232811 | -2.189921 | -0.361712 |
| O | -1.767054 | -3.314238 | -0.242451 | O | -1.770488 | -3.321910 | -0.240821 |
| C | 0.898955 | 0.313359 | 1.618827 | C | 0.899982 | 0.299332 | 1.638633 |
| C | 2.457253 | 1.743863 | 3.561521 | C | 2.456805 | 1.747114 | 3.556316 |
| C | 1.158248 | -0.223377 | 2.901967 | C | 1.161808 | -0.226175 | 2.913510 |
| C | 1.440541 | 1.602202 | 1.313180 | C | 1.431676 | 1.575019 | 1.326031 |
| C | 2.177005 | 2.273902 | 2.236727 | C | 2.174738 | 2.259224 | 2.249773 |
| C | 1.904753 | 0.459394 | 3.835730 | C | 1.916252 | 0.476123 | 3.841957 |
| H | 0.759980 | -1.194925 | 3.156175 | H | 0.774883 | -1.195075 | 3.191181 |
| H | 1.269583 | 2.054715 | 0.344979 | H | 1.259509 | 2.026205 | 0.356888 |
| H | 2.090883 | 0.028139 | 4.813762 | H | 2.102779 | 0.044865 | 4.820622 |
| O | -0.421558 | -2.406987 | 1.841266 | O | -0.416514 | -2.406919 | 1.853605 |
| H | -0.932241 | -3.195332 | 1.600586 | H | -0.919008 | -3.212265 | 1.653653 |
| O | -1.474722 | 1.021298 | -4.917597 | O | -1.458955 | 1.036412 | -4.898996 |
| H | -1.986093 | 0.591362 | -5.604064 | H | -1.967567 | 0.631847 | -5.610275 |
| O | 2.716969 | 3.498282 | 2.007091 | O | 2.696906 | 3.497543 | 1.960758 |
| O | 3.150288 | 2.447888 | 4.341484 | O | 3.167581 | 2.462027 | 4.365079 |
| H | 3.167733 | 3.681647 | 2.854532 | H | 3.169894 | 3.754251 | 2.770192 |
| O | -2.635700 | -3.017813 | -2.680733 | O | -2.652346 | -3.018598 | -2.719323 |
| H | -2.463693 | -3.408666 | -1.786330 | H | -2.501878 | -3.436014 | -1.843287 |

**Table S2.** (cont.)

| POH (gas phase) E = -418.293640, $N_i$ = 0 | | | | POH (aqueous phase) E = -418.317993, $N_i$ = 0 | | | |
|---|---|---|---|---|---|---|---|
| C | 0.148481 | 0.680255 | -0.837826 | C | 0.154720 | 0.666881 | -0.868560 |
| H | 2.013180 | 0.571843 | -1.078539 | H | 1.775587 | 0.247098 | -1.740736 |
| N | 1.234843 | 1.205544 | -1.234523 | N | 1.099412 | 1.000975 | -1.669400 |
| N | -1.021367 | 1.414725 | -0.866313 | N | -0.848875 | 1.543265 | -0.583044 |
| H | -0.931714 | 2.281797 | -1.374688 | H | -0.931822 | 2.344188 | -1.191212 |
| H | -1.886118 | 0.925827 | -1.025298 | H | -1.708576 | 1.203850 | -0.181935 |
| C | 0.010302 | -0.707901 | -0.191422 | C | 0.044670 | -0.688117 | -0.155750 |
| C | -1.196146 | -1.487092 | -0.714515 | C | -1.023424 | -1.537757 | -0.841472 |
| H | -1.210515 | -1.504087 | -1.807045 | H | -0.779239 | -1.681358 | -1.896840 |
| H | -2.134544 | -1.064306 | -0.347633 | H | -1.997123 | -1.049433 | -0.770420 |
| H | -1.146053 | -2.512384 | -0.343572 | H | -1.101851 | -2.511372 | -0.354383 |
| C | -0.028256 | -0.551084 | 1.328852 | C | -0.209671 | -0.530313 | 1.339593 |
| H | 0.887160 | -0.069549 | 1.677135 | H | 0.532976 | 0.131871 | 1.790139 |
| H | -0.121348 | -1.526509 | 1.808201 | H | -0.155911 | -1.508152 | 1.820936 |
| H | -0.878770 | 0.070530 | 1.614469 | H | -1.204921 | -0.123995 | 1.527680 |
| O | 1.220352 | -1.366295 | -0.600605 | O | 1.356518 | -1.266471 | -0.360396 |
| O | 1.329788 | -2.611312 | 0.080758 | O | 1.407405 | -2.579512 | 0.168766 |
| H | 1.372408 | -3.219201 | -0.664242 | H | 1.251810 | -3.130850 | -0.609772 |

| $POH^{\bullet+}$ (gas phase) E = -417.978247, $N_i$ = 0 | | | | $POH^{\bullet+}$ (aqueous phase) E = -418.086010, $N_i$ = 0 | | | |
|---|---|---|---|---|---|---|---|
| C | 0.032953 | 0.594468 | -0.930532 | C | 0.050583 | 0.582294 | -0.948990 |
| H | 1.720413 | 0.355702 | -2.007566 | H | 1.952722 | 0.728783 | -1.515100 |
| N | 0.742598 | 0.652598 | -2.049360 | N | 0.995637 | 0.786420 | -1.880902 |
| N | -0.674059 | 1.616425 | -0.532732 | N | -0.839873 | 1.488641 | -0.708836 |
| H | -0.656788 | 2.493208 | -1.039106 | H | -0.800219 | 2.390471 | -1.172006 |
| H | -1.235582 | 1.561979 | 0.306042 | H | -1.581210 | 1.326524 | -0.036264 |
| C | -0.065806 | -0.762240 | -0.215840 | C | -0.038120 | -0.785068 | -0.266594 |
| C | -1.163919 | -1.574873 | -0.909334 | C | -1.236453 | -1.534818 | -0.840235 |
| H | -0.938917 | -1.712655 | -1.967535 | H | -1.137678 | -1.652713 | -1.920804 |
| H | -2.131363 | -1.078720 | -0.806476 | H | -2.157187 | -0.992358 | -0.618942 |
| H | -1.225244 | -2.551867 | -0.430551 | H | -1.296972 | -2.515975 | -0.369958 |
| C | -0.289665 | -0.620362 | 1.284033 | C | -0.095178 | -0.626064 | 1.247886 |
| H | 0.446772 | 0.039727 | 1.746366 | H | 0.736334 | -0.017272 | 1.607244 |
| H | -0.196137 | -1.612587 | 1.727301 | H | -0.038554 | -1.618533 | 1.698524 |
| H | -1.300853 | -0.273807 | 1.513704 | H | -1.039218 | -0.176244 | 1.559781 |
| O | 1.239419 | -1.275805 | -0.507360 | O | 1.207273 | -1.387482 | -0.671724 |
| O | 1.269086 | -2.640554 | -0.133332 | O | 1.235026 | -2.743727 | -0.280943 |
| H | 2.088779 | -2.679838 | 0.375470 | H | 1.744773 | -2.722079 | 0.541058 |

**Table S2.** (cont.)

| ROH [quercetin] (gas phase) E = -1104.141590, $N_i$ = 0 | | | | ROH [quercetin] (aqueous phase) E = -1104.171173, $N_i$ = 0 | | | |
|---|---|---|---|---|---|---|---|
| C | 0.677212 | -0.215461 | 0.145641 | C | 0.645258 | -0.211182 | 0.159416 |
| O | -0.599041 | 0.181579 | -0.127662 | O | -0.643081 | 0.209765 | 0.048163 |
| C | 1.399374 | 2.117553 | -0.008199 | C | 1.420344 | 2.071922 | -0.218915 |
| C | -0.932536 | 1.470777 | -0.342088 | C | -0.959150 | 1.500382 | -0.202889 |
| C | 1.670156 | 0.709986 | 0.209404 | C | 1.669737 | 0.670026 | 0.027823 |
| C | 0.040901 | 2.474623 | -0.291288 | C | 0.046373 | 2.466137 | -0.331247 |
| C | -2.263177 | 1.746459 | -0.610356 | C | -2.305077 | 1.805426 | -0.319515 |
| C | -2.616125 | 3.071794 | -0.832569 | C | -2.646581 | 3.126809 | -0.576054 |
| H | -3.004546 | 0.960963 | -0.646533 | H | -3.060758 | 1.037904 | -0.218909 |
| C | -1.677253 | 4.107877 | -0.791739 | C | -1.679415 | 4.131580 | -0.708698 |
| H | -1.965019 | 5.138312 | -0.966863 | H | -1.971797 | 5.155973 | -0.908384 |
| C | -0.351722 | 3.816929 | -0.522557 | C | -0.345039 | 3.803954 | -0.590302 |
| O | 2.340797 | 2.930458 | 0.060031 | O | 2.385713 | 2.860538 | -0.339837 |
| C | 0.774441 | -1.665744 | 0.337780 | C | 0.739831 | -1.655827 | 0.395679 |
| C | 0.890414 | -4.445256 | 0.693556 | C | 0.863212 | -4.412061 | 0.828433 |
| C | -0.385853 | -2.449062 | 0.227329 | C | -0.285827 | -2.490832 | -0.069115 |
| C | 1.986163 | -2.300708 | 0.628454 | C | 1.816454 | -2.216877 | 1.085748 |
| C | 2.037005 | -3.676630 | 0.803419 | C | 1.872367 | -3.587379 | 1.299229 |
| C | -0.325153 | -3.814683 | 0.402769 | C | -0.224621 | -3.854247 | 0.145158 |
| H | -1.336204 | -1.979648 | 0.002877 | H | -1.134491 | -2.082662 | -0.605890 |
| H | 2.892834 | -1.722696 | 0.718925 | H | 2.606983 | -1.590025 | 1.473113 |
| H | 2.973658 | -4.171663 | 1.028593 | H | 2.701638 | -4.028949 | 1.839349 |
| O | 0.947800 | -5.782919 | 0.865008 | O | 0.939957 | -5.754893 | 1.041477 |
| H | 0.063455 | -6.145503 | 0.752194 | H | 0.174171 | -6.185823 | 0.643552 |
| O | -1.402483 | -4.653376 | 0.313723 | O | -1.179083 | -4.736429 | -0.278525 |
| H | -2.200032 | -4.162740 | 0.112271 | H | -1.902443 | -4.268923 | -0.708465 |
| O | -3.919364 | 3.315362 | -1.092109 | O | -3.967076 | 3.405439 | -0.694924 |
| H | -4.058350 | 4.254196 | -1.229996 | H | -4.099015 | 4.339435 | -0.891254 |
| O | 0.543215 | 4.803103 | -0.483494 | O | 0.585063 | 4.770403 | -0.724783 |
| H | 1.418562 | 4.409955 | -0.281450 | H | 1.465988 | 4.351678 | -0.622742 |
| O | 2.958319 | 0.411826 | 0.472885 | O | 2.970997 | 0.286410 | 0.093846 |
| H | 3.422551 | 1.264337 | 0.452045 | H | 3.499367 | 1.082328 | -0.070538 |

**Table S2.** (cont.)

| RO• [quercetin] (gas phase) E = -1103.508461, $N_i$ = 0 | | | | RO• [quercetin] (aqueous phase) E = -1103.532714, $N_i$ = 0 | | | |
|---|---|---|---|---|---|---|---|
| H | -0.238901 | 1.634658 | -2.731142 | H | -0.228861 | 1.634860 | -2.707473 |
| C | -0.730969 | 0.672634 | -2.712300 | C | -0.725976 | 0.674145 | -2.702280 |
| C | -2.026270 | -1.833176 | -2.695640 | C | -2.023969 | -1.823360 | -2.702316 |
| C | -0.682866 | -0.138180 | -1.592973 | C | -0.683615 | -0.143921 | -1.587651 |
| C | -1.435877 | 0.208439 | -3.817735 | C | -1.428514 | 0.217845 | -3.811848 |
| C | -2.082338 | -1.032534 | -3.821355 | C | -2.078268 | -1.023172 | -3.823256 |
| C | -1.315239 | -1.388823 | -1.551021 | C | -1.317167 | -1.394137 | -1.549032 |
| H | -2.628448 | -1.382341 | -4.689926 | H | -2.618922 | -1.354001 | -4.702336 |
| O | 0.003194 | 0.321783 | -0.527229 | O | 0.002322 | 0.313463 | -0.519005 |
| C | 0.126848 | -0.380230 | 0.637411 | C | 0.123275 | -0.391689 | 0.643092 |
| C | -0.465790 | -1.607007 | 0.744523 | C | -0.471039 | -1.619434 | 0.747418 |
| C | -1.225416 | -2.175231 | -0.362471 | C | -1.229536 | -2.182841 | -0.362853 |
| O | -1.742819 | -3.295823 | -0.207557 | O | -1.753045 | -3.306941 | -0.218142 |
| C | 0.912887 | 0.331450 | 1.629627 | C | 0.908553 | 0.318664 | 1.635137 |
| C | 2.453587 | 1.732745 | 3.566588 | C | 2.451202 | 1.732197 | 3.561573 |
| C | 1.162842 | -0.232008 | 2.923706 | C | 1.163318 | -0.237333 | 2.931416 |
| C | 1.433846 | 1.595560 | 1.305368 | C | 1.428965 | 1.582656 | 1.309739 |
| C | 2.179653 | 2.281150 | 2.233992 | C | 2.175475 | 2.274563 | 2.232209 |
| C | 1.898750 | 0.433992 | 3.853005 | C | 1.899974 | 0.435923 | 3.853499 |
| H | 0.757178 | -1.203629 | 3.160438 | H | 0.764561 | -1.207535 | 3.182837 |
| H | 1.256701 | 2.037584 | 0.335341 | H | 1.252473 | 2.026066 | 0.339567 |
| H | 2.090328 | 0.012359 | 4.832176 | H | 2.091899 | 0.014483 | 4.833242 |
| O | -0.411093 | -2.382605 | 1.835937 | O | -0.408492 | -2.386635 | 1.847156 |
| H | -0.921465 | -3.178622 | 1.605447 | H | -0.911814 | -3.195014 | 1.648795 |
| O | -1.466864 | 1.018222 | -4.894978 | O | -1.458551 | 1.031397 | -4.891501 |
| H | -1.973683 | 0.613140 | -5.601387 | H | -1.966823 | 0.629028 | -5.604734 |
| O | 2.695977 | 3.477356 | 1.982819 | O | 2.680230 | 3.477975 | 1.944547 |
| O | 3.134334 | 2.412252 | 4.347639 | O | 3.135745 | 2.404692 | 4.360360 |
| H | 3.169187 | 3.732333 | 2.795087 | H | 3.168545 | 3.787709 | 2.724973 |
| O | -2.641632 | -3.014395 | -2.699156 | O | -2.648538 | -3.015778 | -2.713898 |
| H | -2.497819 | -3.439533 | -1.829515 | H | -2.505581 | -3.442352 | -1.844516 |

**Table S2.** (cont.)

| $ROH^{\bullet+}$ [quercetin] (gas phase) E = -1103.871343, $N_i$ = 0 | | | | $ROH^{\bullet+}$ [quercetin] (aqueous phase) E= -1103.964126, $N_i$ = 0 | | | |
|---|---|---|---|---|---|---|---|
| H | -0.366125 | 1.640515 | -2.746438 | H | -0.224834 | 1.581521 | -2.778673 |
| C | -0.819995 | 0.660105 | -2.718148 | C | -0.723635 | 0.622170 | -2.753599 |
| C | -2.030397 | -1.889926 | -2.716251 | C | -2.035203 | -1.868540 | -2.711205 |
| C | -0.741385 | -0.143308 | -1.614585 | C | -0.697856 | -0.164036 | -1.626260 |
| C | -1.519143 | 0.170645 | -3.837201 | C | -1.421265 | 0.140535 | -3.864731 |
| C | -2.118705 | -1.087146 | -3.842348 | C | -2.074230 | -1.094797 | -3.853358 |
| C | -1.329508 | -1.422361 | -1.568084 | C | -1.337248 | -1.413427 | -1.560709 |
| H | -2.655097 | -1.455990 | -4.708496 | H | -2.608314 | -1.445263 | -4.728513 |
| O | -0.057237 | 0.351416 | -0.537495 | O | -0.011064 | 0.326201 | -0.559119 |
| C | 0.106568 | -0.318017 | 0.617757 | C | 0.099258 | -0.323470 | 0.617641 |
| C | -0.455972 | -1.596004 | 0.724410 | C | -0.543187 | -1.556384 | 0.763398 |
| C | -1.210998 | -2.203481 | -0.394229 | C | -1.285105 | -2.164786 | -0.355471 |
| O | -1.666620 | -3.335046 | -0.197970 | O | -1.813425 | -3.270985 | -0.163391 |
| C | 0.852238 | 0.386685 | 1.603201 | C | 0.859466 | 0.376579 | 1.593783 |
| C | 2.323323 | 1.815099 | 3.503859 | C | 2.385466 | 1.778968 | 3.464611 |
| C | 1.124810 | -0.166964 | 2.887324 | C | 1.286183 | -0.245090 | 2.805790 |
| C | 1.340087 | 1.684949 | 1.294422 | C | 1.230231 | 1.720077 | 1.337886 |
| C | 2.058227 | 2.383692 | 2.220640 | C | 1.964816 | 2.414887 | 2.255836 |
| C | 1.845813 | 0.536730 | 3.814763 | C | 2.038590 | 0.445054 | 3.714633 |
| H | 0.763660 | -1.150921 | 3.141933 | H | 1.039227 | -1.275613 | 3.005828 |
| H | 1.139498 | 2.116239 | 0.322253 | H | 0.917740 | 2.216172 | 0.428416 |
| H | 2.060064 | 0.128168 | 4.793801 | H | 2.380427 | -0.018738 | 4.630873 |
| O | -0.370815 | -2.350455 | 1.787926 | O | -0.545656 | -2.231570 | 1.886804 |
| H | -0.855690 | -3.176886 | 1.566554 | H | -1.058399 | -3.050197 | 1.739345 |
| O | -1.567339 | 0.990885 | -4.886998 | O | -1.433998 | 0.931471 | -4.953706 |
| H | -2.056540 | 0.602177 | -5.617360 | H | -1.940580 | 0.524621 | -5.666336 |
| O | 2.579436 | 3.614796 | 2.068348 | O | 2.349849 | 3.697888 | 2.137506 |
| H | 2.399542 | 3.994301 | 1.204779 | H | 2.039047 | 4.082780 | 1.309700 |
| O | 3.014253 | 2.486436 | 4.396039 | O | 3.101670 | 2.438700 | 4.354217 |
| H | 3.277898 | 3.349136 | 4.045714 | H | 3.266626 | 3.347045 | 4.058967 |
| O | -2.602159 | -3.081713 | -2.729911 | O | -2.663355 | -3.053136 | -2.702971 |
| H | -2.461692 | -3.533759 | -1.878211 | H | -2.541242 | -3.468636 | -1.827193 |

**Table S2.** (cont.)

| $RO^-$ [quercetin] (gas phase) E = -1103.613959, $N_i$ = 0 | | | | $RO^-$ [quercetin] (aqueous phase) E = -1103.703205, $N_i$ = 0 | | | |
|---|---|---|---|---|---|---|---|
| H | -0.238810 | 1.635037 | -2.731468 | H | -0.229977 | 1.631432 | -2.706227 |
| C | -0.733593 | 0.673950 | -2.720236 | C | -0.728755 | 0.671384 | -2.705728 |
| C | -2.022628 | -1.828869 | -2.692284 | C | -2.026361 | -1.823291 | -2.708078 |
| C | -0.686152 | -0.143320 | -1.594461 | C | -0.690013 | -0.152922 | -1.591883 |
| C | -1.435527 | 0.211766 | -3.821068 | C | -1.429365 | 0.219467 | -3.816100 |
| C | -2.081273 | -1.028809 | -3.823447 | C | -2.079551 | -1.020796 | -3.829343 |
| C | -1.314954 | -1.385139 | -1.554901 | C | -1.322248 | -1.398316 | -1.555966 |
| H | -2.628211 | -1.380122 | -4.692120 | H | -2.620007 | -1.350671 | -4.709112 |
| O | -0.002979 | 0.311841 | -0.529657 | O | -0.005130 | 0.297959 | -0.517724 |
| C | 0.127463 | -0.384785 | 0.644517 | C | 0.113225 | -0.409389 | 0.641067 |
| C | -0.485787 | -1.628538 | 0.723558 | C | -0.487239 | -1.636418 | 0.730029 |
| C | -1.220855 | -2.176199 | -0.350366 | C | -1.232811 | -2.189921 | -0.361712 |
| O | -1.767054 | -3.314238 | -0.242451 | O | -1.770488 | -3.321910 | -0.240821 |
| C | 0.898955 | 0.313359 | 1.618827 | C | 0.899982 | 0.299332 | 1.638633 |
| C | 2.457253 | 1.743863 | 3.561521 | C | 2.456805 | 1.747114 | 3.556316 |
| C | 1.158248 | -0.223377 | 2.901967 | C | 1.161808 | -0.226175 | 2.913510 |
| C | 1.440541 | 1.602202 | 1.313180 | C | 1.431676 | 1.575019 | 1.326031 |
| C | 2.177005 | 2.273902 | 2.236727 | C | 2.174738 | 2.259224 | 2.249773 |
| C | 1.904753 | 0.459394 | 3.835730 | C | 1.916252 | 0.476123 | 3.841957 |
| H | 0.759980 | -1.194925 | 3.156175 | H | 0.774883 | -1.195075 | 3.191181 |
| H | 1.269583 | 2.054715 | 0.344979 | H | 1.259509 | 2.026205 | 0.356888 |
| H | 2.090883 | 0.028139 | 4.813762 | H | 2.102779 | 0.044865 | 4.820622 |
| O | -0.421558 | -2.406987 | 1.841266 | O | -0.416514 | -2.406919 | 1.853605 |
| H | -0.932241 | -3.195332 | 1.600586 | H | -0.919008 | -3.212265 | 1.653653 |
| O | -1.474722 | 1.021298 | -4.917597 | O | -1.458955 | 1.036412 | -4.898996 |
| H | -1.986093 | 0.591362 | -5.604064 | H | -1.967567 | 0.631847 | -5.610275 |
| O | 2.716969 | 3.498282 | 2.007091 | O | 2.696906 | 3.497543 | 1.960758 |
| O | 3.150288 | 2.447888 | 4.341484 | O | 3.167581 | 2.462027 | 4.365079 |
| H | 3.167733 | 3.681647 | 2.854532 | H | 3.169894 | 3.754251 | 2.770192 |
| O | -2.635700 | -3.017813 | -2.680733 | O | -2.652346 | -3.018598 | -2.719323 |
| H | -2.463693 | -3.408666 | -1.786330 | H | -2.501878 | -3.436014 | -1.843287 |

**Table S2.** (cont.)

| ROH [genistein] (gas phase) E = -953.683910, $N_i$ = 0 | | | | ROH [genistein] (aqueous phase) E = -953.710691, $N_i$ = 0 | | | |
|---|---|---|---|---|---|---|---|
| H | 0.692452 | -4.428508 | -0.968010 | H | 0.778934 | -4.416083 | -0.941836 |
| C | 0.761648 | -3.484674 | -1.490014 | C | 0.814266 | -3.476835 | -1.477470 |
| C | 0.949317 | -1.029644 | -2.856473 | C | 0.901167 | -1.036531 | -2.866864 |
| C | 0.481579 | -2.290795 | -0.852126 | C | 0.500759 | -2.286571 | -0.847999 |
| C | 1.136716 | -3.428529 | -2.827814 | C | 1.174367 | -3.420888 | -2.818723 |
| C | 1.232821 | -2.217198 | -3.513684 | C | 1.220603 | -2.211950 | -3.518843 |
| C | 0.561749 | -1.047288 | -1.491182 | C | 0.532607 | -1.045375 | -1.496989 |
| H | 1.526466 | -2.179601 | -4.556717 | H | 1.501739 | -2.191332 | -4.565527 |
| C | 0.251589 | 0.179641 | -0.779991 | C | 0.184356 | 0.166356 | -0.786173 |
| C | -0.159704 | 0.008066 | 0.617192 | C | -0.172465 | -0.000666 | 0.616276 |
| C | -0.174102 | -1.239602 | 1.125332 | C | -0.163097 | -1.244334 | 1.137656 |
| H | -0.428557 | -1.457359 | 2.154774 | H | -0.404992 | -1.463848 | 2.169631 |
| O | 0.120330 | -2.364924 | 0.456241 | O | 0.147780 | -2.364249 | 0.465631 |
| O | 0.329096 | 1.287031 | -1.324988 | O | 0.181108 | 1.277743 | -1.353959 |
| C | -0.559925 | 1.159387 | 1.455759 | C | -0.564388 | 1.154118 | 1.457827 |
| C | -1.299159 | 3.300922 | 3.102592 | C | -1.287565 | 3.308086 | 3.088944 |
| C | -1.700941 | 1.090972 | 2.259264 | C | -1.741499 | 1.120129 | 2.208964 |
| C | 0.194662 | 2.333000 | 1.480081 | C | 0.242367 | 2.291756 | 1.537196 |
| C | -0.167198 | 3.393609 | 2.296428 | C | -0.111409 | 3.362916 | 2.344529 |
| C | -2.069981 | 2.143652 | 3.081386 | C | -2.103936 | 2.183727 | 3.023928 |
| H | -2.326739 | 0.205102 | 2.226358 | H | -2.390097 | 0.252463 | 2.150538 |
| H | 1.070825 | 2.421782 | 0.851004 | H | 1.165363 | 2.340285 | 0.971260 |
| H | 0.433769 | 4.298310 | 2.302990 | H | 0.523949 | 4.240733 | 2.402459 |
| H | -2.958650 | 2.089311 | 3.698197 | H | -3.019812 | 2.151902 | 3.602738 |
| O | -1.701724 | 4.309350 | 3.920162 | O | -1.684928 | 4.338198 | 3.897681 |
| H | -1.106574 | 5.055667 | 3.833182 | H | -1.045205 | 5.056254 | 3.849639 |
| O | 1.045276 | 0.117110 | -3.523834 | O | 0.945957 | 0.120622 | -3.553866 |
| H | 0.807777 | 0.839058 | -2.896410 | H | 0.678266 | 0.834755 | -2.930799 |
| O | 1.405151 | -4.606506 | -3.432530 | O | 1.478663 | -4.594827 | -3.422086 |
| H | 1.652030 | -4.457342 | -4.347167 | H | 1.717139 | -4.446555 | -4.343762 |

**Table S2.** (cont.)

| RO• [genistein] (gas phase) E = -953.0363578, $N_i$ = 0 | | | | RO• [genistein] (aqueous phase) E = -953.0633030, $N_i$ = 0 | | | |
|---|---|---|---|---|---|---|---|
| H | 0.585629 | -4.248582 | -0.840286 | H | 0.611737 | -4.239689 | -0.829365 |
| C | 0.687278 | -3.305023 | -1.357388 | C | 0.706617 | -3.297952 | -1.353107 |
| C | 0.958283 | -0.850547 | -2.712903 | C | 0.942822 | -0.849686 | -2.712682 |
| C | 0.404335 | -2.109257 | -0.730181 | C | 0.401643 | -2.104336 | -0.731968 |
| C | 1.110146 | -3.252585 | -2.683014 | C | 1.136472 | -3.242705 | -2.675509 |
| C | 1.246797 | -2.042057 | -3.361676 | C | 1.257170 | -2.030625 | -3.358720 |
| C | 0.524825 | -0.864647 | -1.361220 | C | 0.506579 | -0.858281 | -1.363097 |
| H | 1.575627 | -2.006636 | -4.394131 | H | 1.589453 | -2.010092 | -4.390238 |
| C | 0.210873 | 0.364271 | -0.658326 | C | 0.162292 | 0.357699 | -0.659148 |
| C | -0.247795 | 0.194810 | 0.728685 | C | -0.268046 | 0.185388 | 0.727267 |
| C | -0.307912 | -1.059923 | 1.228704 | C | -0.337709 | -1.071033 | 1.230124 |
| H | -0.597772 | -1.279883 | 2.248342 | H | -0.637141 | -1.295918 | 2.245829 |
| O | -0.006178 | -2.180172 | 0.567885 | O | -0.025322 | -2.182619 | 0.564354 |
| O | 0.311294 | 1.470273 | -1.198798 | O | 0.207621 | 1.470157 | -1.215833 |
| C | -0.629817 | 1.339069 | 1.569320 | C | -0.629267 | 1.326385 | 1.576346 |
| C | -1.320712 | 3.502189 | 3.289203 | C | -1.304591 | 3.505750 | 3.264807 |
| C | -1.725758 | 1.229585 | 2.460024 | C | -1.730538 | 1.233870 | 2.464845 |
| C | 0.103114 | 2.550959 | 1.525942 | C | 0.131762 | 2.523893 | 1.542890 |
| C | -0.216095 | 3.590922 | 2.351971 | C | -0.181181 | 3.574774 | 2.354321 |
| C | -2.068731 | 2.257650 | 3.291978 | C | -2.066480 | 2.274801 | 3.280978 |
| H | -2.320577 | 0.322050 | 2.457112 | H | -2.327590 | 0.328983 | 2.476026 |
| H | 0.925848 | 2.642409 | 0.829933 | H | 0.984850 | 2.591275 | 0.880881 |
| H | 0.345774 | 4.517562 | 2.338364 | H | 0.406794 | 4.485522 | 2.346022 |
| H | -2.913305 | 2.187746 | 3.967536 | H | -2.916530 | 2.213375 | 3.950930 |
| O | -1.616499 | 4.440086 | 4.045654 | O | -1.604440 | 4.469392 | 4.007710 |
| O | 1.093770 | 0.292601 | -3.377500 | O | 1.058604 | 0.307943 | -3.388194 |
| H | 0.843695 | 1.021095 | -2.765328 | H | 0.777986 | 1.028275 | -2.780344 |
| O | 1.380854 | -4.432929 | -3.277067 | O | 1.430532 | -4.420311 | -3.273161 |
| H | 1.663012 | -4.291037 | -4.182835 | H | 1.715900 | -4.274236 | -4.181965 |

**Table S2.** (cont.)

| $ROH^{\bullet+}$ [genistein] (gas phase) E = -953.4031426, $N_i$ = 0 | | | | $ROH^{\bullet+}$ [genistein] (aqueous phase) E= -953.497316924, $N_i$ = 0 | | | |
|---|---|---|---|---|---|---|---|
| H | 3.690503 | -2.434336 | -0.154428 | H | 3.685238 | -2.440190 | -0.046796 |
| C | 3.413415 | -1.391807 | -0.083323 | C | 3.415016 | -1.393298 | -0.016973 |
| C | 2.713189 | 1.334226 | 0.102008 | C | 2.706596 | 1.327185 | 0.044849 |
| C | 2.107271 | -0.991828 | -0.049949 | C | 2.099565 | -0.996398 | -0.024598 |
| C | 4.396475 | -0.386649 | -0.021999 | C | 4.385649 | -0.390826 | 0.025442 |
| C | 4.052593 | 0.956104 | 0.069534 | C | 4.041207 | 0.959494 | 0.058256 |
| C | 1.692907 | 0.345485 | 0.044115 | C | 1.688021 | 0.341394 | 0.009684 |
| H | 4.808121 | 1.731801 | 0.114028 | H | 4.809413 | 1.723590 | 0.085290 |
| C | 0.298822 | 0.701141 | 0.071908 | C | 0.285878 | 0.686836 | -0.016307 |
| C | -0.655608 | -0.441803 | -0.023706 | C | -0.650271 | -0.450584 | -0.043847 |
| C | -0.113287 | -1.710860 | -0.104525 | C | -0.122672 | -1.717069 | -0.089504 |
| H | -0.710105 | -2.614105 | -0.130851 | H | -0.721476 | -2.618790 | -0.102754 |
| O | 1.158356 | -1.992012 | -0.110922 | O | 1.160502 | -2.000955 | -0.075562 |
| O | -0.085353 | 1.868664 | 0.144495 | O | -0.096210 | 1.865678 | -0.050488 |
| C | -2.080366 | -0.279923 | -0.013177 | C | -2.081494 | -0.283839 | -0.013162 |
| C | -4.872871 | 0.015528 | 0.036802 | C | -4.859445 | 0.028212 | 0.041906 |
| C | -2.944286 | -1.287530 | -0.548826 | C | -2.940760 | -1.252076 | -0.620089 |
| C | -2.690979 | 0.890387 | 0.537903 | C | -2.679081 | 0.841311 | 0.634814 |
| C | -4.048817 | 1.029348 | 0.571741 | C | -4.031241 | 0.992950 | 0.671153 |
| C | -4.297551 | -1.147470 | -0.532872 | C | -4.291185 | -1.100611 | -0.605402 |
| H | -2.528791 | -2.165119 | -1.027428 | H | -2.515139 | -2.098490 | -1.143014 |
| H | -2.060584 | 1.668409 | 0.940966 | H | -2.049999 | 1.563929 | 1.132188 |
| H | -4.495736 | 1.914344 | 1.012045 | H | -4.490417 | 1.829800 | 1.184264 |
| H | -4.954553 | -1.895019 | -0.959088 | H | -4.949550 | -1.811853 | -1.087689 |
| O | -6.186662 | 0.085005 | 0.028303 | O | -6.167698 | 0.122178 | 0.030965 |
| H | -6.517203 | 0.900170 | 0.422319 | H | -6.483624 | 0.915349 | 0.487895 |
| O | 2.426776 | 2.621008 | 0.187042 | O | 2.401450 | 2.634229 | 0.065976 |
| H | 1.454309 | 2.728967 | 0.191802 | H | 1.424017 | 2.712049 | 0.025293 |
| O | 5.661274 | -0.811077 | -0.057903 | O | 5.673792 | -0.793265 | 0.029130 |
| H | 6.280818 | -0.078040 | -0.011448 | H | 6.265994 | -0.032933 | 0.053644 |

**Table S2.** (cont.)

| $RO^-$ [genistein] (gas phase) E= -953.1446378, $N_i$ = 0 | | | | $RO^-$ [genistein] (aqueous phase) E = -953.2426674, $N_i$ = 0 | | | |
|---|---|---|---|---|---|---|---|
| H | 4.576103 | 0.707523 | -1.105729 | H | 4.560679 | 0.853637 | -1.068290 |
| C | 3.636099 | 0.795901 | -1.636460 | C | 3.628966 | 0.885783 | -1.620594 |
| C | 1.190104 | 1.037555 | -3.011363 | C | 1.198391 | 0.952542 | -3.021115 |
| C | 2.459427 | 0.519408 | -1.012172 | C | 2.448216 | 0.563925 | -0.998354 |
| C | 3.652607 | 1.218405 | -3.024417 | C | 3.627292 | 1.262889 | -2.996400 |
| C | 2.355642 | 1.320530 | -3.663841 | C | 2.361614 | 1.280053 | -3.668528 |
| C | 1.185270 | 0.616310 | -1.635275 | C | 1.193985 | 0.581697 | -1.642995 |
| H | 2.324069 | 1.634264 | -4.700897 | H | 2.328659 | 1.559626 | -4.716075 |
| C | -0.012845 | 0.309040 | -0.941609 | C | -0.003119 | 0.232413 | -0.941975 |
| C | 0.158853 | -0.132383 | 0.460513 | C | 0.158913 | -0.121080 | 0.467480 |
| C | 1.403276 | -0.167194 | 0.971082 | C | 1.398738 | -0.107720 | 0.993382 |
| H | 1.612631 | -0.437067 | 2.000164 | H | 1.614748 | -0.348153 | 2.026706 |
| O | 2.526173 | 0.130907 | 0.313863 | O | 2.520581 | 0.207417 | 0.324421 |
| O | -1.156761 | 0.392441 | -1.451588 | O | -1.127588 | 0.217211 | -1.504073 |
| C | -0.993640 | -0.521153 | 1.301530 | C | -0.998344 | -0.510199 | 1.307581 |
| C | -3.145914 | -1.224372 | 2.965411 | C | -3.156716 | -1.224340 | 2.940075 |
| C | -0.926124 | -1.628895 | 2.151427 | C | -0.973967 | -1.690974 | 2.053457 |
| C | -2.182579 | 0.213530 | 1.288249 | C | -2.130417 | 0.304203 | 1.393586 |
| C | -3.245621 | -0.130709 | 2.110955 | C | -3.203441 | -0.044613 | 2.200938 |
| C | -1.980839 | -1.978206 | 2.984712 | C | -2.039134 | -2.048974 | 2.869166 |
| H | -0.034009 | -2.246536 | 2.146587 | H | -0.111743 | -2.346409 | 1.990516 |
| H | -2.274827 | 1.053411 | 0.612855 | H | -2.172377 | 1.230264 | 0.832017 |
| H | -4.160576 | 0.456092 | 2.082864 | H | -4.076169 | 0.597420 | 2.263320 |
| H | -1.918236 | -2.841958 | 3.636360 | H | -2.013401 | -2.967841 | 3.443656 |
| O | -4.169099 | -1.601879 | 3.794623 | O | -4.189356 | -1.616982 | 3.749461 |
| H | -4.915151 | -1.018675 | 3.650065 | H | -4.901764 | -0.970898 | 3.704406 |
| O | 0.008435 | 1.148386 | -3.656896 | O | 0.025244 | 0.983983 | -3.703841 |
| H | -0.687185 | 0.898129 | -3.008448 | H | -0.676273 | 0.710918 | -3.068112 |
| O | 4.714717 | 1.477198 | -3.622567 | O | 4.707786 | 1.574201 | -3.609817 |

**Table S2.** (cont.)

| POH (gas phase) E = -418.293640, $N_i$ = 0 | | | | POH (aqueous phase) E = -418.317993, $N_i$ = 0 | | | |
|---|---|---|---|---|---|---|---|
| C | 0.148481 | 0.680255 | -0.837826 | C | 0.154720 | 0.666881 | -0.868560 |
| H | 2.013180 | 0.571843 | -1.078539 | H | 1.775587 | 0.247098 | -1.740736 |
| N | 1.234843 | 1.205544 | -1.234523 | N | 1.099412 | 1.000975 | -1.669400 |
| N | -1.021367 | 1.414725 | -0.866313 | N | -0.848875 | 1.543265 | -0.583044 |
| H | -0.931714 | 2.281797 | -1.374688 | H | -0.931822 | 2.344188 | -1.191212 |
| H | -1.886118 | 0.925827 | -1.025298 | H | -1.708576 | 1.203850 | -0.181935 |
| C | 0.010302 | -0.707901 | -0.191422 | C | 0.044670 | -0.688117 | -0.155750 |
| C | -1.196146 | -1.487092 | -0.714515 | C | -1.023424 | -1.537757 | -0.841472 |
| H | -1.210515 | -1.504087 | -1.807045 | H | -0.779239 | -1.681358 | -1.896840 |
| H | -2.134544 | -1.064306 | -0.347633 | H | -1.997123 | -1.049433 | -0.770420 |
| H | -1.146053 | -2.512384 | -0.343572 | H | -1.101851 | -2.511372 | -0.354383 |
| C | -0.028256 | -0.551084 | 1.328852 | C | -0.209671 | -0.530313 | 1.339593 |
| H | 0.887160 | -0.069549 | 1.677135 | H | 0.532976 | 0.131871 | 1.790139 |
| H | -0.121348 | -1.526509 | 1.808201 | H | -0.155911 | -1.508152 | 1.820936 |
| H | -0.878770 | 0.070530 | 1.614469 | H | -1.204921 | -0.123995 | 1.527680 |
| O | 1.220352 | -1.366295 | -0.600605 | O | 1.356518 | -1.266471 | -0.360396 |
| O | 1.329788 | -2.611312 | 0.080758 | O | 1.407405 | -2.579512 | 0.168766 |
| H | 1.372408 | -3.219201 | -0.664242 | H | 1.251810 | -3.130850 | -0.609772 |

| $POH^{\bullet+}$ (gas phase) E = -417.978247, $N_i$ = 0 | | | | $POH^{\bullet+}$ (aqueous phase) E = -418.086010, $N_i$ = 0 | | | |
|---|---|---|---|---|---|---|---|
| C | 0.032953 | 0.594468 | -0.930532 | C | 0.050583 | 0.582294 | -0.948990 |
| H | 1.720413 | 0.355702 | -2.007566 | H | 1.952722 | 0.728783 | -1.515100 |
| N | 0.742598 | 0.652598 | -2.049360 | N | 0.995637 | 0.786420 | -1.880902 |
| N | -0.674059 | 1.616425 | -0.532732 | N | -0.839873 | 1.488641 | -0.708836 |
| H | -0.656788 | 2.493208 | -1.039106 | H | -0.800219 | 2.390471 | -1.172006 |
| H | -1.235582 | 1.561979 | 0.306042 | H | -1.581210 | 1.326524 | -0.036264 |
| C | -0.065806 | -0.762240 | -0.215840 | C | -0.038120 | -0.785068 | -0.266594 |
| C | -1.163919 | -1.574873 | -0.909334 | C | -1.236453 | -1.534818 | -0.840235 |
| H | -0.938917 | -1.712655 | -1.967535 | H | -1.137678 | -1.652713 | -1.920804 |
| H | -2.131363 | -1.078720 | -0.806476 | H | -2.157187 | -0.992358 | -0.618942 |
| H | -1.225244 | -2.551867 | -0.430551 | H | -1.296972 | -2.515975 | -0.369958 |
| C | -0.289665 | -0.620362 | 1.284033 | C | -0.095178 | -0.626064 | 1.247886 |
| H | 0.446772 | 0.039727 | 1.746366 | H | 0.736334 | -0.017272 | 1.607244 |
| H | -0.196137 | -1.612587 | 1.727301 | H | -0.038554 | -1.618533 | 1.698524 |
| H | -1.300853 | -0.273807 | 1.513704 | H | -1.039218 | -0.176244 | 1.559781 |
| O | 1.239419 | -1.275805 | -0.507360 | O | 1.207273 | -1.387482 | -0.671724 |
| O | 1.269086 | -2.640554 | -0.133332 | O | 1.235026 | -2.743727 | -0.280943 |
| H | 2.088779 | -2.679838 | 0.375470 | H | 1.744773 | -2.722079 | 0.541058 |

**Table S2.** (cont.)

| ROH (gas phase) E = -1104.12955, $N_i$ = 0 | | | | ROH (aqueous phase) E = -1104.16782, $N_i$ = 0 | | | |
|---|---|---|---|---|---|---|---|
| H | 0.137270 | 1.319117 | -3.031008 | H | 0.155010 | 1.313485 | -3.004989 |
| C | -0.495780 | 0.447916 | -2.939162 | C | -0.478530 | 0.440032 | -2.927245 |
| C | -2.132770 | -1.832971 | -2.719430 | C | -2.123276 | -1.830134 | -2.726425 |
| C | -0.608845 | -0.233774 | -1.739077 | C | -0.606976 | -0.242034 | -1.729043 |
| C | -1.215990 | -0.033157 | -4.025443 | C | -1.189587 | -0.037489 | -4.020212 |
| C | -2.030805 | -1.163055 | -3.928076 | C | -2.010379 | -1.168039 | -3.931831 |
| C | -1.409576 | -1.371136 | -1.588879 | C | -1.413414 | -1.377069 | -1.584453 |
| H | -2.590821 | -1.531970 | -4.780006 | H | -2.557020 | -1.522468 | -4.798061 |
| O | 0.105283 | 0.245928 | -0.694341 | O | 0.100182 | 0.234039 | -0.677104 |
| C | 0.056058 | -0.362288 | 0.521990 | C | 0.037478 | -0.359428 | 0.543800 |
| C | -0.726213 | -1.440255 | 0.766105 | C | -0.753177 | -1.437244 | 0.771634 |
| C | -1.512908 | -2.043033 | -0.309963 | C | -1.523001 | -2.029885 | -0.305100 |
| O | -2.217589 | -3.038725 | -0.130867 | O | -2.242143 | -3.033167 | -0.118016 |
| C | 0.894435 | 0.319522 | 1.522530 | C | 0.883188 | 0.322833 | 1.535789 |
| C | 2.468004 | 1.640153 | 3.419014 | C | 2.492507 | 1.646253 | 3.384915 |
| C | 1.717925 | -0.399872 | 2.387890 | C | 1.731809 | -0.399349 | 2.373588 |
| C | 0.875981 | 1.716835 | 1.602033 | C | 0.849306 | 1.719332 | 1.619911 |
| C | 1.653690 | 2.366680 | 2.538628 | C | 1.644664 | 2.376211 | 2.539657 |
| C | 2.496706 | 0.258433 | 3.332836 | C | 2.532117 | 0.264421 | 3.295083 |
| H | 1.785307 | -1.478607 | 2.302340 | H | 1.788758 | -1.478856 | 2.296747 |
| H | 0.249846 | 2.287170 | 0.923545 | H | 0.195911 | 2.296819 | 0.974845 |
| H | 3.146341 | -0.290883 | 4.002971 | H | 3.201426 | -0.285524 | 3.945980 |
| O | -0.862292 | -2.028310 | 1.975861 | O | -0.914815 | -2.041745 | 1.982621 |
| H | -0.462106 | -1.475312 | 2.653227 | H | -0.530359 | -1.508648 | 2.688072 |
| O | -1.089664 | 0.646879 | -5.187288 | O | -1.053783 | 0.643226 | -5.184093 |
| H | -1.617258 | 0.228563 | -5.870122 | H | -1.594256 | 0.244462 | -5.874901 |
| O | 1.702151 | 3.721436 | 2.698492 | O | 1.665937 | 3.732159 | 2.699015 |
| H | 1.146826 | 4.163483 | 2.054960 | H | 1.075837 | 4.156535 | 2.067612 |
| O | 3.225144 | 2.276422 | 4.336654 | O | 3.283308 | 2.278645 | 4.295339 |
| H | 3.089482 | 3.224975 | 4.246386 | H | 3.151459 | 3.231953 | 4.230211 |
| O | -2.914398 | -2.906317 | -2.634832 | O | -2.919103 | -2.914259 | -2.646065 |
| H | -2.863434 | -3.233845 | -1.706968 | H | -2.879078 | -3.235066 | -1.717282 |

**Table S2.** (cont.)

| RO• (gas phase) E = -1103.508461, $N_i$ = 0 | | | | RO• (aqueous phase) E = -1103.532714, $N_i$ = 0 | | | |
|---|---|---|---|---|---|---|---|
| H | -0.238901 | 1.634658 | -2.731142 | H | -0.228861 | 1.634860 | -2.707473 |
| C | -0.730969 | 0.672634 | -2.712300 | C | -0.725976 | 0.674145 | -2.702280 |
| C | -2.026270 | -1.833176 | -2.695640 | C | -2.023969 | -1.823360 | -2.702316 |
| C | -0.682866 | -0.138180 | -1.592973 | C | -0.683615 | -0.143921 | -1.587651 |
| C | -1.435877 | 0.208439 | -3.817735 | C | -1.428514 | 0.217845 | -3.811848 |
| C | -2.082338 | -1.032534 | -3.821355 | C | -2.078268 | -1.023172 | -3.823256 |
| C | -1.315239 | -1.388823 | -1.551021 | C | -1.317167 | -1.394137 | -1.549032 |
| H | -2.628448 | -1.382341 | -4.689926 | H | -2.618922 | -1.354001 | -4.702336 |
| O | 0.003194 | 0.321783 | -0.527229 | O | 0.002322 | 0.313463 | -0.519005 |
| C | 0.126848 | -0.380230 | 0.637411 | C | 0.123275 | -0.391689 | 0.643092 |
| C | -0.465790 | -1.607007 | 0.744523 | C | -0.471039 | -1.619434 | 0.747418 |
| C | -1.225416 | -2.175231 | -0.362471 | C | -1.229536 | -2.182841 | -0.362853 |
| O | -1.742819 | -3.295823 | -0.207557 | O | -1.753045 | -3.306941 | -0.218142 |
| C | 0.912887 | 0.331450 | 1.629627 | C | 0.908553 | 0.318664 | 1.635137 |
| C | 2.453587 | 1.732745 | 3.566588 | C | 2.451202 | 1.732197 | 3.561573 |
| C | 1.162842 | -0.232008 | 2.923706 | C | 1.163318 | -0.237333 | 2.931416 |
| C | 1.433846 | 1.595560 | 1.305368 | C | 1.428965 | 1.582656 | 1.309739 |
| C | 2.179653 | 2.281150 | 2.233992 | C | 2.175475 | 2.274563 | 2.232209 |
| C | 1.898750 | 0.433992 | 3.853005 | C | 1.899974 | 0.435923 | 3.853499 |
| H | 0.757178 | -1.203629 | 3.160438 | H | 0.764561 | -1.207535 | 3.182837 |
| H | 1.256701 | 2.037584 | 0.335341 | H | 1.252473 | 2.026066 | 0.339567 |
| H | 2.090328 | 0.012359 | 4.832176 | H | 2.091899 | 0.014483 | 4.833242 |
| O | -0.411093 | -2.382605 | 1.835937 | O | -0.408492 | -2.386635 | 1.847156 |
| H | -0.921465 | -3.178622 | 1.605447 | H | -0.911814 | -3.195014 | 1.648795 |
| O | -1.466864 | 1.018222 | -4.894978 | O | -1.458551 | 1.031397 | -4.891501 |
| H | -1.973683 | 0.613140 | -5.601387 | H | -1.966823 | 0.629028 | -5.604734 |
| O | 2.695977 | 3.477356 | 1.982819 | O | 2.680230 | 3.477975 | 1.944547 |
| O | 3.134334 | 2.412252 | 4.347639 | O | 3.135745 | 2.404692 | 4.360360 |
| H | 3.169187 | 3.732333 | 2.795087 | H | 3.168545 | 3.787709 | 2.724973 |
| O | -2.641632 | -3.014395 | -2.699156 | O | -2.648538 | -3.015778 | -2.713898 |
| H | -2.497819 | -3.439533 | -1.829515 | H | -2.505581 | -3.442352 | -1.844516 |

**Table S2.** (cont.)

| $ROH^{\bullet+}$ (gas phase) E = -1103.871343, $N_i$ = 0 | | | | $ROH^{\bullet+}$ (aqueous phase) E=-1103.964126, $N_i$ = 0 | | | |
|---|---|---|---|---|---|---|---|
| H | -0.366125 | 1.640515 | -2.746438 | H | -0.224834 | 1.581521 | -2.778673 |
| C | -0.819995 | 0.660105 | -2.718148 | C | -0.723635 | 0.622170 | -2.753599 |
| C | -2.030397 | -1.889926 | -2.716251 | C | -2.035203 | -1.868540 | -2.711205 |
| C | -0.741385 | -0.143308 | -1.614585 | C | -0.697856 | -0.164036 | -1.626260 |
| C | -1.519143 | 0.170645 | -3.837201 | C | -1.421265 | 0.140535 | -3.864731 |
| C | -2.118705 | -1.087146 | -3.842348 | C | -2.074230 | -1.094797 | -3.853358 |
| C | -1.329508 | -1.422361 | -1.568084 | C | -1.337248 | -1.413427 | -1.560709 |
| H | -2.655097 | -1.455990 | -4.708496 | H | -2.608314 | -1.445263 | -4.728513 |
| O | -0.057237 | 0.351416 | -0.537495 | O | -0.011064 | 0.326201 | -0.559119 |
| C | 0.106568 | -0.318017 | 0.617757 | C | 0.099258 | -0.323470 | 0.617641 |
| C | -0.455972 | -1.596004 | 0.724410 | C | -0.543187 | -1.556384 | 0.763398 |
| C | -1.210998 | -2.203481 | -0.394229 | C | -1.285105 | -2.164786 | -0.355471 |
| O | -1.666620 | -3.335046 | -0.197970 | O | -1.813425 | -3.270985 | -0.163391 |
| C | 0.852238 | 0.386685 | 1.603201 | C | 0.859466 | 0.376579 | 1.593783 |
| C | 2.323323 | 1.815099 | 3.503859 | C | 2.385466 | 1.778968 | 3.464611 |
| C | 1.124810 | -0.166964 | 2.887324 | C | 1.286183 | -0.245090 | 2.805790 |
| C | 1.340087 | 1.684949 | 1.294422 | C | 1.230231 | 1.720077 | 1.337886 |
| C | 2.058227 | 2.383692 | 2.220640 | C | 1.964816 | 2.414887 | 2.255836 |
| C | 1.845813 | 0.536730 | 3.814763 | C | 2.038590 | 0.445054 | 3.714633 |
| H | 0.763660 | -1.150921 | 3.141933 | H | 1.039227 | -1.275613 | 3.005828 |
| H | 1.139498 | 2.116239 | 0.322253 | H | 0.917740 | 2.216172 | 0.428416 |
| H | 2.060064 | 0.128168 | 4.793801 | H | 2.380427 | -0.018738 | 4.630873 |
| O | -0.370815 | -2.350455 | 1.787926 | O | -0.545656 | -2.231570 | 1.886804 |
| H | -0.855690 | -3.176886 | 1.566554 | H | -1.058399 | -3.050197 | 1.739345 |
| O | -1.567339 | 0.990885 | -4.886998 | O | -1.433998 | 0.931471 | -4.953706 |
| H | -2.056540 | 0.602177 | -5.617360 | H | -1.940580 | 0.524621 | -5.666336 |
| O | 2.579436 | 3.614796 | 2.068348 | O | 2.349849 | 3.697888 | 2.137506 |
| H | 2.399542 | 3.994301 | 1.204779 | H | 2.039047 | 4.082780 | 1.309700 |
| O | 3.014253 | 2.486436 | 4.396039 | O | 3.101670 | 2.438700 | 4.354217 |
| H | 3.277898 | 3.349136 | 4.045714 | H | 3.266626 | 3.347045 | 4.058967 |
| O | -2.602159 | -3.081713 | -2.729911 | O | -2.663355 | -3.053136 | -2.702971 |
| H | -2.461692 | -3.533759 | -1.878211 | H | -2.541242 | -3.468636 | -1.827193 |

**Table S2.** (cont.)

| RO (gas phase) E = -1103.613959, $N_i$ = 0 | | | | RO (aqueous phase) E = -1103.703205, $N_i$ = 0 | | | |
|---|---|---|---|---|---|---|---|
| H | -0.238810 | 1.635037 | -2.731468 | H | -0.229977 | 1.631432 | -2.706227 |
| C | -0.733593 | 0.673950 | -2.720236 | C | -0.728755 | 0.671384 | -2.705728 |
| C | -2.022628 | -1.828869 | -2.692284 | C | -2.026361 | -1.823291 | -2.708078 |
| C | -0.686152 | -0.143320 | -1.594461 | C | -0.690013 | -0.152922 | -1.591883 |
| C | -1.435527 | 0.211766 | -3.821068 | C | -1.429365 | 0.219467 | -3.816100 |
| C | -2.081273 | -1.028809 | -3.823447 | C | -2.079551 | -1.020796 | -3.829343 |
| C | -1.314954 | -1.385139 | -1.554901 | C | -1.322248 | -1.398316 | -1.555966 |
| H | -2.628211 | -1.380122 | -4.692120 | H | -2.620007 | -1.350671 | -4.709112 |
| O | -0.002979 | 0.311841 | -0.529657 | O | -0.005130 | 0.297959 | -0.517724 |
| C | 0.127463 | -0.384785 | 0.644517 | C | 0.113225 | -0.409389 | 0.641067 |
| C | -0.485787 | -1.628538 | 0.723558 | C | -0.487239 | -1.636418 | 0.730029 |
| C | -1.220855 | -2.176199 | -0.350366 | C | -1.232811 | -2.189921 | -0.361712 |
| O | -1.767054 | -3.314238 | -0.242451 | O | -1.770488 | -3.321910 | -0.240821 |
| C | 0.898955 | 0.313359 | 1.618827 | C | 0.899982 | 0.299332 | 1.638633 |
| C | 2.457253 | 1.743863 | 3.561521 | C | 2.456805 | 1.747114 | 3.556316 |
| C | 1.158248 | -0.223377 | 2.901967 | C | 1.161808 | -0.226175 | 2.913510 |
| C | 1.440541 | 1.602202 | 1.313180 | C | 1.431676 | 1.575019 | 1.326031 |
| C | 2.177005 | 2.273902 | 2.236727 | C | 2.174738 | 2.259224 | 2.249773 |
| C | 1.904753 | 0.459394 | 3.835730 | C | 1.916252 | 0.476123 | 3.841957 |
| H | 0.759980 | -1.194925 | 3.156175 | H | 0.774883 | -1.195075 | 3.191181 |
| H | 1.269583 | 2.054715 | 0.344979 | H | 1.259509 | 2.026205 | 0.356888 |
| H | 2.090883 | 0.028139 | 4.813762 | H | 2.102779 | 0.044865 | 4.820622 |
| O | -0.421558 | -2.406987 | 1.841266 | O | -0.416514 | -2.406919 | 1.853605 |
| H | -0.932241 | -3.195332 | 1.600586 | H | -0.919008 | -3.212265 | 1.653653 |
| O | -1.474722 | 1.021298 | -4.917597 | O | -1.458955 | 1.036412 | -4.898996 |
| H | -1.986093 | 0.591362 | -5.604064 | H | -1.967567 | 0.631847 | -5.610275 |
| O | 2.716969 | 3.498282 | 2.007091 | O | 2.696906 | 3.497543 | 1.960758 |
| O | 3.150288 | 2.447888 | 4.341484 | O | 3.167581 | 2.462027 | 4.365079 |
| H | 3.167733 | 3.681647 | 2.854532 | H | 3.169894 | 3.754251 | 2.770192 |
| O | -2.635700 | -3.017813 | -2.680733 | O | -2.652346 | -3.018598 | -2.719323 |
| H | -2.463693 | -3.408666 | -1.786330 | H | -2.501878 | -3.436014 | -1.843287 |

**Table S3.** Cartesian coordinates of optimized geometries (ωB97XD/6-311+G**) of 36 flavonoids involved in the QSAR modelling. Total energy (E) in Hartrees. $N_i$ is the number of imaginary frequencies.

| Genistein | | | | Naringenin | | | |
|---|---|---|---|---|---|---|---|
| $N_i$ = 0; E = -953.710691 | | | | $N_i$ = 0; E = -954.93386 | | | |
| C | 0.2866 | 0.6498 | 0.0806 | C | -0.6931 | 0.4042 | 0.4493 |
| O | -0.1046 | 1.8215 | 0.2585 | C | -0.2129 | 1.6599 | -0.2612 |
| C | 1.6954 | 0.3211 | 0.0353 | C | 1.273 | 1.8242 | -0.1183 |
| C | -0.6319 | -0.4697 | -0.0786 | C | 2.0415 | 0.6069 | -0.001 |
| C | 2.1126 | -1.0054 | -0.1355 | C | 3.4586 | 0.6211 | 0.0196 |
| C | 2.7048 | 1.3079 | 0.1756 | C | 4.1863 | -0.5569 | 0.0226 |
| C | -0.1165 | -1.705 | -0.2427 | C | 3.4992 | -1.7691 | -0.0045 |
| C | -2.1005 | -0.2775 | -0.0375 | C | 2.1057 | -1.8311 | -0.0181 |
| O | 1.1927 | -2.0015 | -0.269 | C | 1.3913 | -0.6492 | -0.01 |
| C | 3.4428 | -1.3798 | -0.1776 | O | 0.0427 | -0.7466 | -0.032 |
| O | 2.3746 | 2.6016 | 0.3498 | O | 1.7994 | 2.9455 | -0.1438 |
| C | 4.0413 | 0.9603 | 0.1356 | C | -2.1556 | 0.1207 | 0.2546 |
| C | -2.8978 | -1.0633 | 0.7979 | C | -3.0141 | 0.0798 | 1.3504 |
| C | -2.7231 | 0.6759 | -0.8467 | C | -4.3713 | -0.1656 | 1.1874 |
| C | 4.3981 | -0.3797 | -0.0406 | C | -4.8791 | -0.3846 | -0.0887 |
| C | -4.2774 | -0.9127 | 0.8231 | C | -4.0327 | -0.3547 | -1.1964 |
| C | -4.1006 | 0.8389 | -0.8271 | C | -2.6812 | -0.0978 | -1.019 |
| O | 5.697 | -0.7615 | -0.0837 | O | -6.2206 | -0.6281 | -0.2036 |
| C | -4.8787 | 0.0427 | 0.0103 | O | 4.1577 | -2.9512 | -0.0071 |
| O | -6.2404 | 0.1653 | 0.0711 | O | 4.1305 | 1.7871 | 0.0212 |
| H | -0.7198 | -2.5936 | -0.3769 | H | -0.4797 | 0.4924 | 1.5198 |
| H | 3.7257 | -2.4153 | -0.3122 | H | -0.4336 | 1.6001 | -1.3338 |
| H | 1.391 | 2.6475 | 0.3625 | H | -0.7193 | 2.5382 | 0.1414 |
| H | 4.8029 | 1.7241 | 0.243 | H | 5.2696 | -0.5299 | 0.0367 |
| H | -2.4333 | -1.7994 | 1.4454 | H | 1.5945 | -2.7849 | -0.019 |
| H | -2.1285 | 1.2927 | -1.5104 | H | -2.6194 | 0.2423 | 2.348 |
| H | -4.8903 | -1.5243 | 1.4752 | H | -5.0381 | -0.1944 | 2.0415 |
| H | -4.5754 | 1.5797 | -1.4623 | H | -4.4372 | -0.5286 | -2.1883 |
| H | 6.275 | 0.0029 | 0.0163 | H | -2.0305 | -0.0741 | -1.887 |
| H | -6.5325 | 0.861 | -0.527 | H | -6.4524 | -0.7674 | -1.1276 |
| | | | | H | 5.1095 | -2.8038 | 0.0164 |
| | | | | H | 3.466 | 2.5099 | -0.0252 |

**Table S3.** (cont.)

| Scutellarin | | | | 3,5,7,8,3',4'-Hexahydroxyflavone | | | |
|---|---|---|---|---|---|---|---|
| $N_i$ = 0; E = -1028.94282 | | | | $N_i$ = 0; E =-1179.08417 | | | |
| C | 0.4861 | 1.6956 | -0.0903 | C | 0.1421 | 1.8662 | 0.0645 |
| C | 1.0268 | 0.4542 | -0.0001 | C | -0.5111 | 0.6765 | -0.0304 |
| C | -0.9341 | 1.8871 | -0.0954 | C | 1.5909 | 1.9323 | 0.09 |
| O | -1.4676 | 3.0195 | -0.1683 | O | 2.1501 | 3.0519 | 0.1803 |
| C | -1.7298 | 0.6786 | -0.0257 | C | 2.2942 | 0.6838 | 0.0239 |
| C | -3.1404 | 0.7108 | -0.039 | C | 3.7086 | 0.599 | 0.06 |
| C | -3.8626 | -0.467 | 0.0213 | C | 4.3308 | -0.635 | 0.0041 |
| C | -3.1868 | -1.6927 | 0.0982 | C | 3.5558 | -1.7971 | -0.0912 |
| C | -1.8012 | -1.7535 | 0.1145 | C | 2.1612 | -1.7473 | -0.1172 |
| C | -1.0971 | -0.5645 | 0.0515 | C | 1.5501 | -0.5017 | -0.053 |
| O | 0.2634 | -0.6527 | 0.0741 | O | 0.2005 | -0.4863 | -0.0903 |
| C | 2.4618 | 0.1449 | 0.0123 | C | -1.9577 | 0.4356 | -0.0587 |
| C | 3.3998 | 1.1102 | 0.3959 | C | -2.8661 | 1.4327 | -0.4288 |
| C | 4.7529 | 0.8242 | 0.3911 | C | -4.2304 | 1.1636 | -0.455 |
| C | 5.1907 | -0.4399 | -0.0018 | C | -4.7059 | -0.0953 | -0.1158 |
| C | 4.2695 | -1.4147 | -0.3804 | C | -3.7983 | -1.1031 | 0.2501 |
| C | 2.9161 | -1.1214 | -0.3686 | C | -2.4408 | -0.8413 | 0.2775 |
| O | -3.8874 | -2.8493 | 0.1594 | O | 1.4648 | -2.9321 | -0.1522 |
| O | -5.229 | -0.5072 | 0.0143 | O | 4.4563 | 1.7198 | 0.1437 |
| O | -3.8204 | 1.8756 | -0.1105 | O | 4.187 | -2.9899 | -0.1548 |
| O | 6.5317 | -0.6729 | 0.0065 | O | -0.5048 | 3.0561 | 0.1587 |
| H | 1.1269 | 2.5621 | -0.1774 | H | 5.4115 | -0.7091 | 0.0246 |
| H | -1.2897 | -2.705 | 0.1747 | H | -2.5158 | 2.4163 | -0.7107 |
| H | 3.074 | 2.0919 | 0.7189 | H | -1.7581 | -1.6344 | 0.5635 |
| H | 5.4774 | 1.5697 | 0.6967 | H | 0.715 | -2.8491 | -0.7557 |
| H | 4.6168 | -2.3956 | -0.6867 | H | 3.835 | 2.4805 | 0.174 |
| H | 2.2092 | -1.8836 | -0.6718 | H | 3.5173 | -3.6824 | -0.2584 |
| H | -4.8333 | -2.6593 | 0.1356 | H | 0.1985 | 3.724 | 0.2391 |
| H | -5.5855 | 0.3849 | -0.0622 | O | -6.043 | -0.344 | -0.1447 |
| H | -3.1444 | 2.5924 | -0.1515 | H | -6.1891 | -1.2642 | 0.114 |
| H | 6.7124 | -1.5741 | -0.2819 | O | -4.3547 | -2.3104 | 0.565 |
| | | | | H | -3.6644 | -2.9456 | 0.7907 |
| | | | | H | -4.94 | 1.9302 | -0.7466 |

**Table S3.** (cont.)

| Epicatechin | | | | Kaempferol | | | |
|---|---|---|---|---|---|---|---|
| $N_i$ = 0; E = -1031.09796 | | | | $N_i$ = 0; E = -1028.94154 | | | |
| O | -0.7521 | 0.3034 | -1.7342 | O | 1.8105 | 2.8523 | -0.1725 |
| C | 0.3915 | 1.0369 | -1.2833 | C | 1.3166 | 1.7046 | -0.0832 |
| C | -1.7673 | 0.05 | -0.849 | C | 2.0938 | 0.5022 | -0.0083 |
| C | 1.4416 | 0.1347 | -0.6657 | C | -0.1187 | 1.5436 | -0.0731 |
| C | -0.0565 | 2.187 | -0.3571 | C | 1.4422 | -0.735 | 0.0699 |
| C | -1.8353 | 0.6506 | 0.4083 | C | 3.5113 | 0.5086 | -0.0221 |
| C | -2.7346 | -0.8507 | -1.2985 | O | -0.8609 | 2.6767 | -0.1856 |
| C | 2.7776 | 0.5543 | -0.6978 | C | -0.6853 | 0.3138 | 0.0168 |
| C | 1.1324 | -1.0726 | -0.0447 | O | 0.0915 | -0.7998 | 0.0913 |
| C | -0.7918 | 1.6389 | 0.8551 | C | 2.129 | -1.936 | 0.1333 |
| O | 1.0284 | 3.0225 | -0.0043 | O | 4.1849 | 1.6739 | -0.098 |
| C | -2.9154 | 0.2954 | 1.2273 | C | 4.2163 | -0.6751 | 0.0411 |
| C | -3.7977 | -1.1614 | -0.4586 | C | -2.1165 | -0.0048 | 0.014 |
| C | 3.781 | -0.2027 | -0.1087 | C | 3.5166 | -1.8862 | 0.1166 |
| C | 2.138 | -1.8392 | 0.5432 | C | -2.5566 | -1.2132 | -0.5416 |
| C | -3.8983 | -0.597 | 0.8132 | C | -3.0618 | 0.864 | 0.5676 |
| O | -2.9543 | 0.8742 | 2.4618 | O | 4.173 | -3.0697 | 0.1766 |
| O | -4.7812 | -2.0327 | -0.8297 | C | -3.9005 | -1.5402 | -0.5555 |
| C | 3.4594 | -1.4142 | 0.522 | C | -4.4095 | 0.5399 | 0.5625 |
| O | 4.4898 | -2.118 | 1.0801 | C | -4.8305 | -0.662 | -0.0019 |
| H | 0.8058 | 1.4842 | -2.1903 | O | -6.1423 | -1.0294 | -0.036 |
| H | -0.7381 | 2.813 | -0.9414 | H | -0.2299 | 3.4071 | -0.2775 |
| H | -2.644 | -1.2969 | -2.283 | H | 1.5997 | -2.8776 | 0.192 |
| H | 3.047 | 1.4831 | -1.1943 | H | 3.5239 | 2.3974 | -0.1445 |
| H | 0.1122 | -1.4374 | -0.0127 | H | 5.3002 | -0.6646 | 0.0286 |
| H | -0.0685 | 1.1625 | 1.5316 | H | -1.8413 | -1.9008 | -0.9762 |
| H | -1.252 | 2.4633 | 1.4062 | H | -2.7479 | 1.794 | 1.0225 |
| H | 1.6058 | 2.5225 | 0.5867 | H | 5.1254 | -2.9272 | 0.1495 |
| H | -4.7288 | -0.8533 | 1.4626 | H | -4.2397 | -2.4715 | -0.9935 |
| H | -3.7403 | 0.5694 | 2.9311 | H | -5.1364 | 1.2147 | 1.0017 |
| H | -4.6009 | -2.3543 | -1.7212 | H | -6.6866 | -0.3489 | 0.3742 |
| H | 4.1383 | -2.9255 | 1.4743 | | | | |
| O | 5.098 | 0.1622 | -0.1141 | | | | |
| H | 5.1905 | 0.998 | -0.587 | | | | |
| H | 1.8974 | -2.7826 | 1.0253 | | | | |

**Table S3.** (cont.)

| Eriodictyol | | | | Apigenin | | | |
|---|---|---|---|---|---|---|---|
| $N_i$ = 0; E = -1030.16395 | | | | $N_i$ = 0; E = -953.71779 | | | |
| C | 3.7126 | 1.7945 | -0.0232 | O | 1.8051 | 2.9807 | -0.1619 |
| C | 4.4184 | 0.5954 | 0.0553 | C | 1.2633 | 1.8522 | -0.0928 |
| C | 3.71 | -0.594 | 0.0795 | C | 2.0455 | 0.6365 | -0.0226 |
| C | 2.2939 | -0.6048 | 0.0185 | C | -0.161 | 1.6784 | -0.0935 |
| C | 1.6252 | 0.6377 | -0.0775 | C | 1.3981 | -0.6018 | 0.0511 |
| C | 2.3198 | 1.8313 | -0.0939 | C | 3.4609 | 0.6381 | -0.0324 |
| C | 1.5394 | -1.8284 | 0.1567 | C | -0.7151 | 0.4449 | -0.0055 |
| C | 0.0454 | -1.6856 | 0.2058 | O | 0.0388 | -0.6721 | 0.0701 |
| C | -0.4139 | -0.4765 | -0.594 | C | 2.0794 | -1.8032 | 0.1129 |
| O | 0.276 | 0.7109 | -0.1356 | O | 4.1359 | 1.8022 | -0.1033 |
| C | -1.8894 | -0.2086 | -0.4941 | C | 4.1675 | -0.5484 | 0.0289 |
| C | -2.686 | -0.2355 | -1.632 | C | -2.1523 | 0.1471 | 0.0042 |
| C | -4.0552 | 0.0014 | -1.5404 | C | 3.4691 | -1.757 | 0.0997 |
| C | -4.6309 | 0.2749 | -0.3115 | C | -2.6161 | -1.1185 | -0.3733 |
| C | -3.8316 | 0.3061 | 0.8384 | C | -3.0825 | 1.12 | 0.382 |
| C | -2.4731 | 0.0625 | 0.7456 | O | 4.1212 | -2.9436 | 0.1587 |
| O | -5.9745 | 0.5148 | -0.2352 | C | -3.9701 | -1.4019 | -0.3849 |
| O | -4.4789 | 0.5835 | 2.0116 | C | -4.4391 | 0.8435 | 0.3776 |
| O | 2.081 | -2.9367 | 0.2723 | C | -4.8848 | -0.4204 | -0.0078 |
| O | 4.3976 | -1.7463 | 0.1772 | O | -6.2048 | -0.7517 | -0.0308 |
| O | 4.3511 | 2.9875 | -0.0458 | H | -0.7904 | 2.5531 | -0.182 |
| H | 5.5008 | 0.5875 | 0.106 | H | 1.5476 | -2.7436 | 0.1687 |
| H | 1.7949 | 2.7742 | -0.174 | H | 3.4621 | 2.5209 | -0.1426 |
| H | -0.423 | -2.5925 | -0.1789 | H | 5.2514 | -0.5368 | 0.0197 |
| H | -0.2357 | -1.5772 | 1.2603 | H | -1.9137 | -1.8862 | -0.6729 |
| H | -0.143 | -0.6157 | -1.6458 | H | -2.751 | 2.1012 | 0.7008 |
| H | -2.2411 | -0.4416 | -2.5993 | H | 5.0741 | -2.804 | 0.1345 |
| H | -4.6844 | -0.018 | -2.4228 | H | -4.329 | -2.3791 | -0.6853 |
| H | -1.8715 | 0.0917 | 1.649 | H | -5.155 | 1.5998 | 0.6807 |
| H | -6.2126 | 0.6974 | 0.6813 | H | -6.7424 | -0.0055 | 0.2551 |
| H | -3.8575 | 0.5803 | 2.7473 | | | | |
| H | 3.7407 | -2.4764 | 0.2219 | | | | |
| H | 5.305 | 2.859 | 0.0001 | | | | |

**Table S3.** (cont.)

| Quercetin | | | | Liquiritigenin | | | |
|---|---|---|---|---|---|---|---|
| $N_i$ = 0; E = -1104.17117 | | | | $N_i$ = 0; E = -879.69586 | | | |
| C | 0.6453 | -0.2112 | 0.1594 | C | -0.4742 | 0.4842 | 0.4414 |
| O | -0.6431 | 0.2098 | 0.0482 | C | -0.068 | 1.761 | -0.2791 |
| C | 1.4203 | 2.0719 | -0.2189 | C | 1.404 | 2.0355 | -0.1163 |
| C | -0.9592 | 1.5004 | -0.2029 | O | 1.8498 | 3.1779 | -0.1299 |
| C | 1.6697 | 0.6700 | 0.0278 | C | 2.2516 | 0.8487 | -0.001 |
| C | 0.0464 | 2.4661 | -0.3312 | C | 3.6525 | 0.946 | 0.0273 |
| C | -2.3051 | 1.8054 | -0.3195 | C | 4.4515 | -0.1724 | 0.0336 |
| C | -2.6466 | 3.1268 | -0.5761 | C | 3.846 | -1.438 | 0.0069 |
| H | -3.0608 | 1.0379 | -0.2189 | C | 2.4653 | -1.5733 | -0.0098 |
| C | -1.6794 | 4.1316 | -0.7087 | C | 1.6714 | -0.4313 | -0.0069 |
| H | -1.9718 | 5.1560 | -0.9084 | O | 0.3316 | -0.6247 | -0.024 |
| C | -0.3450 | 3.8040 | -0.5903 | C | -1.9171 | 0.1143 | 0.2435 |
| O | 2.3857 | 2.8605 | -0.3398 | C | -2.7809 | 0.0537 | 1.3321 |
| C | 0.7398 | -1.6558 | 0.3957 | C | -4.1252 | -0.2595 | 1.1635 |
| C | 0.8632 | -4.4121 | 0.8284 | C | -4.6114 | -0.5248 | -0.1123 |
| C | -0.2858 | -2.4908 | -0.0691 | C | -3.7563 | -0.4806 | -1.2127 |
| C | 1.8165 | -2.2169 | 1.0857 | C | -2.4213 | -0.1574 | -1.0302 |
| C | 1.8724 | -3.5874 | 1.2992 | O | 4.667 | -2.5165 | 0.0093 |
| C | -0.2246 | -3.8542 | 0.1452 | O | -5.9234 | -0.8358 | -0.3461 |
| H | -1.1345 | -2.0827 | -0.6059 | H | -0.2719 | 0.5953 | 1.5124 |
| H | 2.6070 | -1.5900 | 1.4731 | H | -0.2642 | 1.6665 | -1.3544 |
| H | 2.7016 | -4.0289 | 1.8393 | H | -0.6454 | 2.6063 | 0.0979 |
| O | 0.9400 | -5.7549 | 1.0415 | H | 4.1027 | 1.932 | 0.0301 |
| H | 0.1742 | -6.1858 | 0.6436 | H | 5.5317 | -0.0973 | 0.0513 |
| O | -1.1791 | -4.7364 | -0.2785 | H | 2.0019 | -2.5532 | -0.0121 |
| H | -1.9024 | -4.2689 | -0.7085 | H | -2.4046 | 0.2553 | 2.3297 |
| O | -3.9671 | 3.4054 | -0.6949 | H | -4.7935 | -0.2998 | 2.0174 |
| H | -4.0990 | 4.3394 | -0.8913 | H | -4.1474 | -0.6932 | -2.2011 |
| O | 0.5851 | 4.7704 | -0.7248 | H | -1.7639 | -0.1193 | -1.8927 |
| H | 1.4660 | 4.3517 | -0.6227 | H | 4.1501 | -3.3298 | -0.0098 |
| O | 2.9710 | 0.2864 | 0.0938 | H | -6.4211 | -0.8077 | 0.4778 |
| H | 3.4994 | 1.0823 | -0.0705 | | | | |

**Table S3.** (cont.)

| Fisetin | | | | Taxifolin | | | |
|---|---|---|---|---|---|---|---|
| $N_i$ = 0; E = -1028.93476 | | | | $N_i$ = 0; E = -1105.38614 | | | |
| O | -5.0532 | -2.509 | -0.288 | C | 2.3585 | 0.4811 | -0.0106 |
| C | -4.1971 | -1.4629 | -0.1863 | C | 1.7196 | -0.7792 | -0.0477 |
| C | -2.8251 | -1.6326 | -0.183 | C | 2.4412 | -1.9536 | -0.0051 |
| C | -4.7714 | -0.1809 | -0.0829 | C | 3.8319 | -1.8766 | 0.0908 |
| C | -2.0206 | -0.5016 | -0.0702 | C | 4.5053 | -0.6578 | 0.1602 |
| C | -3.959 | 0.9181 | 0.0257 | C | 3.7695 | 0.5133 | 0.1124 |
| C | -2.5578 | 0.7822 | 0.0347 | C | 1.5827 | 1.6815 | -0.1619 |
| O | -0.6851 | -0.7138 | -0.0737 | C | 0.1115 | 1.4906 | -0.4733 |
| C | -1.6603 | 1.9091 | 0.1572 | C | -0.403 | 0.261 | 0.2728 |
| C | 0.1978 | 0.3123 | 0.0483 | O | 0.3722 | -0.8828 | -0.1408 |
| O | -2.0167 | 3.0934 | 0.2748 | C | -1.8494 | -0.042 | 0.0035 |
| C | -0.2457 | 1.59 | 0.161 | C | -2.2913 | -0.3428 | -1.2826 |
| C | 1.5891 | -0.1542 | 0.0759 | C | -3.6334 | -0.6124 | -1.5164 |
| O | 0.6054 | 2.6376 | 0.3199 | C | -4.545 | -0.5737 | -0.471 |
| C | 1.879 | -1.4303 | 0.5662 | C | -4.1062 | -0.2691 | 0.8199 |
| C | 2.6338 | 0.6534 | -0.3898 | C | -2.7641 | -0.009 | 1.0532 |
| C | 3.1881 | -1.8876 | 0.6032 | O | -5.0657 | -0.253 | 1.7958 |
| C | 3.9366 | 0.1909 | -0.3552 | O | -5.8629 | -0.8372 | -0.7206 |
| C | 4.2214 | -1.0842 | 0.1462 | O | -0.6429 | 2.6206 | -0.1097 |
| O | 5.0114 | 0.9115 | -0.7965 | O | 2.0457 | 2.8236 | -0.081 |
| O | 5.5016 | -1.5483 | 0.1885 | O | 4.4287 | 1.6848 | 0.1699 |
| H | -4.5658 | -3.3385 | -0.3446 | O | 4.4996 | -3.0507 | 0.1311 |
| H | -2.3753 | -2.6152 | -0.2626 | H | 1.9403 | -2.9124 | -0.028 |
| H | -5.8502 | -0.0848 | -0.0898 | H | 5.5846 | -0.6218 | 0.2493 |
| H | -4.3879 | 1.9096 | 0.108 | H | 0.0458 | 1.3018 | -1.5558 |
| H | 0.0431 | 3.4225 | 0.4155 | H | -0.2462 | 0.4082 | 1.3471 |
| H | 1.0839 | -2.0676 | 0.9309 | H | -1.5901 | -0.3722 | -2.1092 |
| H | 2.4414 | 1.6391 | -0.7944 | H | -3.9885 | -0.8516 | -2.5123 |
| H | 3.4205 | -2.8727 | 0.9907 | H | -2.4389 | 0.221 | 2.0632 |
| H | 4.7322 | 1.7808 | -1.1009 | H | -4.6772 | -0.0168 | 2.6445 |
| H | 6.0974 | -0.8737 | -0.159 | H | -6.3631 | -0.765 | 0.1007 |
| | | | | H | -0.0515 | 3.3833 | -0.1504 |
| | | | | H | 3.7726 | 2.409 | 0.1222 |
| | | | | H | 5.4475 | -2.8946 | 0.206 |

**Table S3.** (cont.)

| Hesperetin | | | | 3,3',4'-Trihydroxyflavone | | | |
|---|---|---|---|---|---|---|---|
| $N_i$ = 0; E = -1069.45336 | | | | $N_i$ = 0; E = -953.46443 | | | |
| O | -1.8939 | -2.8917 | 0.5853 | C | -0.8325 | 1.5388 | -0.1318 |
| C | -1.6412 | -1.9675 | -0.1993 | C | -0.0944 | 0.4077 | 0.0351 |
| C | -2.0347 | -0.6002 | 0.0558 | C | -2.2824 | 1.508 | -0.1671 |
| C | -0.9453 | -2.2212 | -1.5068 | O | -2.9092 | 2.5689 | -0.3303 |
| C | -1.7513 | 0.4079 | -0.8929 | C | -2.8913 | 0.1965 | -0.0212 |
| C | -2.7693 | -0.2365 | 1.2119 | C | -4.2844 | 0.0062 | -0.0403 |
| C | -0.1646 | -1.0011 | -1.9634 | C | -4.8129 | -1.2605 | 0.0908 |
| O | -1.0624 | 0.1344 | -2.0263 | C | -3.9571 | -2.3655 | 0.2422 |
| C | -2.1855 | 1.7072 | -0.7173 | C | -2.5852 | -2.2046 | 0.2633 |
| O | -3.0679 | -1.1561 | 2.1491 | C | -2.0605 | -0.9161 | 0.1305 |
| C | -3.2059 | 1.0626 | 1.4027 | O | -0.7099 | -0.8003 | 0.1636 |
| C | 1.0435 | -0.6379 | -1.1173 | C | 1.3685 | 0.2951 | 0.0783 |
| C | -2.9148 | 2.0179 | 0.432 | C | 2.1742 | 1.3564 | 0.5014 |
| C | 1.6923 | 0.5725 | -1.3903 | C | 3.5573 | 1.2144 | 0.5417 |
| C | 1.5303 | -1.4462 | -0.1002 | C | 4.1521 | 0.0192 | 0.162 |
| O | -3.3622 | 3.2749 | 0.6592 | C | 3.3475 | -1.0525 | -0.2587 |
| C | 2.7916 | 0.961 | -0.6539 | C | 1.9717 | -0.917 | -0.2969 |
| C | 2.6461 | -1.0614 | 0.6476 | O | 4.0177 | -2.1883 | -0.6162 |
| O | 3.4088 | 2.148 | -0.9349 | O | 5.5066 | -0.1048 | 0.2026 |
| C | 3.2775 | 0.1407 | 0.3786 | O | -0.2702 | 2.7637 | -0.3017 |
| O | 4.364 | 0.6353 | 1.0312 | H | -4.9248 | 0.8734 | -0.1601 |
| C | 4.9026 | -0.1283 | 2.1061 | H | -5.8868 | -1.4083 | 0.0767 |
| H | -0.3139 | -3.1065 | -1.4349 | H | -4.3765 | -3.3607 | 0.3445 |
| H | -1.7263 | -2.4323 | -2.2457 | H | -1.9102 | -3.0449 | 0.3794 |
| H | 0.1459 | -1.1351 | -2.9992 | H | 1.7282 | 2.2912 | 0.814 |
| H | -1.9497 | 2.4668 | -1.4528 | H | 1.3695 | -1.7567 | -0.6281 |
| H | -2.7123 | -2.0173 | 1.8396 | H | -1.0267 | 3.3652 | -0.4234 |
| H | -3.7681 | 1.3293 | 2.2885 | H | 3.3926 | -2.8671 | -0.8982 |
| H | 1.3368 | 1.2252 | -2.18 | H | 5.7425 | -0.9928 | -0.0986 |
| H | 1.0622 | -2.3934 | 0.1372 | H | 4.1887 | 2.0312 | 0.8743 |
| H | -3.1099 | 3.8564 | -0.0667 | | | | |
| H | 3.0054 | -1.7082 | 1.4374 | | | | |
| H | 4.1543 | 2.2572 | -0.3316 | | | | |
| H | 5.7443 | 0.4465 | 2.4877 | | | | |
| H | 4.1595 | -0.2621 | 2.897 | | | | |
| H | 5.2524 | -1.1025 | 1.7537 | | | | |

**Table S3.** (cont.)

| Luteolin | | | | Morin | | | |
|---|---|---|---|---|---|---|---|
| $N_i$ = 0; E = -1028.94743 | | | | $N_i$ = 0; E = -1103.88849 | | | |
| O | -4.1377 | 3.0981 | -0.2216 | C | 4.3367 | -0.6114 | -0.1366 |
| C | -3.5766 | 1.8669 | -0.1406 | C | 3.6448 | -1.8206 | -0.3056 |
| C | -4.362 | 0.7153 | -0.0368 | C | 2.2531 | -1.8775 | -0.3286 |
| C | -3.7453 | -0.5185 | 0.0517 | C | 1.556 | -0.6883 | -0.1761 |
| O | -4.5049 | -1.6264 | 0.1563 | C | 2.2024 | 0.5454 | -0.0018 |
| C | -2.3338 | -0.623 | 0.0339 | C | 3.6221 | 0.5625 | 0.0154 |
| C | -1.6432 | -1.8906 | 0.1393 | O | 0.2039 | -0.7591 | -0.209 |
| O | -2.2656 | -2.9736 | 0.245 | C | -0.574 | 0.35 | -0.0399 |
| C | -0.2097 | -1.8228 | 0.129 | C | -0.0137 | 1.5714 | 0.1429 |
| C | 0.4335 | -0.6379 | -0.0042 | C | 1.4246 | 1.7386 | 0.1628 |
| O | -0.2364 | 0.5293 | -0.1074 | C | -2.0145 | 0.0742 | -0.1014 |
| C | -1.597 | 0.5612 | -0.0768 | C | -2.8439 | 0.846 | -0.922 |
| C | -2.1874 | 1.8082 | -0.1656 | C | -4.2082 | 0.619 | -1.0036 |
| C | 1.8897 | -0.4503 | -0.0451 | C | -4.7677 | -0.41 | -0.2414 |
| C | 2.7384 | -1.5098 | -0.3705 | C | -3.9691 | -1.195 | 0.5874 |
| C | 4.1121 | -1.3216 | -0.4008 | C | -2.6012 | -0.9528 | 0.6624 |
| C | 4.6544 | -0.0785 | -0.1092 | O | -6.0971 | -0.6924 | -0.2645 |
| O | 6.0037 | 0.0883 | -0.1474 | O | 1.9123 | 2.8827 | 0.3359 |
| C | 3.8074 | 0.9891 | 0.2137 | O | -0.7623 | 2.6901 | 0.3327 |
| O | 4.4218 | 2.1787 | 0.4862 | O | 4.2807 | 1.7242 | 0.1812 |
| C | 2.4382 | 0.8052 | 0.2432 | O | 4.3047 | -2.9917 | -0.4548 |
| H | -5.098 | 3.0347 | -0.1758 | H | 5.4212 | -0.5923 | -0.1219 |
| H | -5.4437 | 0.7838 | -0.0214 | H | 1.7311 | -2.8167 | -0.4601 |
| H | -3.8867 | -2.3917 | 0.2124 | H | -4.8366 | 1.2232 | -1.6498 |
| H | 0.3518 | -2.7396 | 0.2407 | H | -4.4195 | -1.9837 | 1.1817 |
| H | -1.5875 | 2.7048 | -0.2476 | H | -6.5477 | -0.0755 | -0.8546 |
| H | 2.3366 | -2.4832 | -0.6226 | H | -0.1224 | 3.4099 | 0.4644 |
| H | 4.7772 | -2.1363 | -0.6614 | H | 3.601 | 2.431 | 0.2777 |
| H | 6.2187 | 1.0057 | 0.0603 | H | 5.2579 | -2.8428 | -0.4124 |
| H | 3.7683 | 2.8648 | 0.6571 | O | -1.7976 | -1.6752 | 1.4845 |
| H | 1.8027 | 1.6444 | 0.5013 | H | -2.325 | -2.3297 | 1.9593 |
| | | | | H | -2.4008 | 1.6386 | -1.5154 |

**Table S3.** (cont.)

| Epigallocatechin | | | | 5,3',4'-Trihydroxyflavone | | | |
|---|---|---|---|---|---|---|---|
| $N_i$ = 0; E = -1106.59312 | | | | $N_i$ = 0; E = -953.71227 | | | |
| O | 0.7627 | 3.1915 | 0.4934 | C | 0.15 | -0.4605 | -0.0111 |
| C | -0.28 | 2.3793 | -0.0155 | C | -0.5884 | -1.5833 | 0.171 |
| C | 0.2371 | 1.4216 | -1.1063 | C | -2.0201 | -1.5325 | 0.1882 |
| C | -1.009 | 1.6177 | 1.0767 | O | -2.7308 | -2.55 | 0.3465 |
| O | -0.8639 | 0.7083 | -1.6834 | C | -2.6084 | -0.2118 | 0.0239 |
| C | 1.3392 | 0.4913 | -0.6428 | C | -4.0061 | 0.0016 | 0.0327 |
| C | -1.9877 | 0.6553 | 0.4615 | C | -4.5155 | 1.2809 | -0.1261 |
| C | -1.8674 | 0.2559 | -0.8674 | C | -3.6427 | 2.3542 | -0.2904 |
| C | 2.6575 | 0.9268 | -0.7557 | C | -2.2673 | 2.1831 | -0.3004 |
| C | 1.0716 | -0.7591 | -0.0867 | C | -1.773 | 0.8966 | -0.1421 |
| C | -3.0473 | 0.1104 | 1.1942 | O | -0.4176 | 0.751 | -0.1641 |
| C | -2.7635 | -0.6296 | -1.4639 | C | 1.6165 | -0.4028 | -0.0574 |
| C | 3.6997 | 0.1252 | -0.3075 | C | 2.2772 | 0.7855 | 0.2763 |
| C | 2.1186 | -1.5573 | 0.3531 | C | 3.6577 | 0.8428 | 0.25 |
| O | -3.1443 | 0.497 | 2.5011 | C | 4.4015 | -0.2837 | -0.1247 |
| C | -3.9567 | -0.7777 | 0.6359 | C | 3.747 | -1.4584 | -0.4646 |
| C | -3.8026 | -1.1378 | -0.6996 | C | 2.3619 | -1.5221 | -0.4301 |
| O | 4.985 | 0.5733 | -0.436 | O | 5.7604 | -0.2416 | -0.1631 |
| C | 3.4373 | -1.1216 | 0.2508 | O | 4.3812 | 1.9543 | 0.5774 |
| O | 1.9457 | -2.7974 | 0.9035 | O | -4.8552 | -1.0348 | 0.197 |
| O | -4.7144 | -2.0186 | -1.2157 | H | -0.1006 | -2.536 | 0.3243 |
| O | 4.4997 | -1.8772 | 0.6672 | H | -5.5883 | 1.4297 | -0.1191 |
| H | 1.3856 | 2.6315 | 0.9697 | H | -4.0513 | 3.3505 | -0.4135 |
| H | -0.9751 | 3.0655 | -0.505 | H | -1.5847 | 3.0132 | -0.4279 |
| H | 0.6251 | 2.0299 | -1.9241 | H | 1.7209 | 1.6672 | 0.5734 |
| H | -0.2781 | 1.0805 | 1.6952 | H | 4.3343 | -2.3189 | -0.7626 |
| H | -1.5241 | 2.3257 | 1.729 | H | 1.8688 | -2.4424 | -0.7172 |
| H | 2.89 | 1.8856 | -1.2052 | H | 6.062 | 0.6389 | 0.0907 |
| H | 0.0603 | -1.138 | 0.0071 | H | 3.7964 | 2.6745 | 0.8348 |
| H | -2.6344 | -0.9178 | -2.5008 | H | -4.3044 | -1.8445 | 0.2949 |
| H | -3.9195 | 0.0927 | 2.9036 | | | | |
| H | -4.7691 | -1.1857 | 1.2267 | | | | |
| H | 5.5955 | -0.108 | -0.1313 | | | | |
| H | 1.0115 | -3.0302 | 0.9126 | | | | |
| H | -4.5019 | -2.2065 | -2.1358 | | | | |
| H | 4.1876 | -2.7423 | 0.9557 | | | | |

**Table S3.** (cont.)

| Ampelopsin | | | | Myricetin | | | |
|---|---|---|---|---|---|---|---|
| $N_i$ = 0; E = -1180.61604 | | | | $N_i$ = 0; E = -1179.40046 | | | |
| C | 0.3165 | 1.4881 | -0.47 | C | 1.8283 | -1.7172 | -0.2251 |
| C | 1.8054 | 1.6742 | -0.2563 | O | 2.3459 | -2.8437 | -0.4009 |
| C | 2.5683 | 0.4758 | -0.041 | C | 2.5788 | -0.5096 | -0.0456 |
| C | 1.9084 | -0.7686 | 0.0761 | C | 0.3884 | -1.5881 | -0.2125 |
| O | 0.5562 | -0.8522 | 0.0661 | C | 1.9012 | 0.7041 | 0.1246 |
| C | -0.178 | 0.3402 | 0.4081 | C | 3.9964 | -0.487 | -0.0414 |
| C | 3.9845 | 0.489 | -0.0095 | O | -0.3251 | -2.7253 | -0.4162 |
| C | 4.7029 | -0.6881 | 0.1036 | C | -0.203 | -0.3807 | -0.0303 |
| C | 4.0079 | -1.8935 | 0.1928 | O | 0.5494 | 0.7395 | 0.1354 |
| C | 2.6126 | -1.949 | 0.188 | C | 2.5621 | 1.9092 | 0.2954 |
| O | 4.6578 | -3.0732 | 0.3043 | O | 4.6951 | -1.6283 | -0.2028 |
| O | 4.6629 | 1.6466 | -0.1065 | C | 4.6755 | 0.7009 | 0.1284 |
| O | 2.2914 | 2.8085 | -0.3083 | C | -1.6423 | -0.0913 | -0.013 |
| O | -0.4004 | 2.6597 | -0.1682 | C | 3.9507 | 1.8884 | 0.2939 |
| C | -1.6418 | 0.0462 | 0.2352 | C | -2.09 | 1.1551 | -0.4575 |
| C | -2.1346 | -0.3562 | -1.0038 | C | -2.5568 | -1.0369 | 0.4575 |
| C | -3.4897 | -0.6066 | -1.1545 | O | 4.5814 | 3.0754 | 0.4618 |
| C | -4.3609 | -0.4487 | -0.0773 | C | -3.4444 | 1.4455 | -0.4403 |
| C | -3.8603 | -0.0454 | 1.1564 | C | -3.9085 | -0.7313 | 0.4748 |
| C | -2.5015 | 0.1998 | 1.3173 | O | -3.8682 | 2.6645 | -0.8862 |
| O | -3.9648 | -1.0041 | -2.3726 | C | -4.3632 | 0.5064 | 0.025 |
| O | -5.6868 | -0.704 | -0.2898 | O | -4.87 | -1.5899 | 0.9262 |
| O | -4.7794 | 0.0801 | 2.1603 | O | -5.6814 | 0.852 | 0.0209 |
| H | 0.1901 | 1.207 | -1.5269 | H | 0.3244 | -3.4323 | -0.5516 |
| H | 0.0313 | 0.5808 | 1.4562 | H | 2.0127 | 2.832 | 0.4252 |
| H | 5.7862 | -0.6674 | 0.1196 | H | 4.0503 | -2.3584 | -0.3166 |
| H | 2.0961 | -2.895 | 0.284 | H | 5.7593 | 0.7118 | 0.131 |
| H | 5.6115 | -2.9345 | 0.3019 | H | -1.3992 | 1.9021 | -0.8264 |
| H | 4.014 | 2.3749 | -0.188 | H | -2.2315 | -1.9999 | 0.8285 |
| H | 0.1912 | 3.4061 | -0.3278 | H | 5.5374 | 2.9582 | 0.4334 |
| H | -1.4787 | -0.4801 | -1.8579 | H | -4.8277 | 2.7196 | -0.8079 |
| H | -2.1267 | 0.5114 | 2.2866 | H | -4.4678 | -2.4167 | 1.2119 |
| H | -4.9192 | -1.131 | -2.3186 | H | -6.2133 | 0.1249 | 0.3643 |
| H | -6.1783 | -0.5789 | 0.53 | | | | |
| H | -4.3489 | 0.3722 | 2.9701 | | | | |

**Table S3.** (cont.)

| Wogonin | | | | 7,8-Dihydroxyflavone | | | |
|---|---|---|---|---|---|---|---|
| $N_i$ = 0; E = -992.99634 | | | | $N_i$ = 0; E = -878.47167 | | | |
| C | 3.7176 | 0.1102 | -0.095 | O | 0.1045 | -0.4228 | 0.0472 |
| C | 2.9104 | 1.2297 | -0.0409 | O | -1.074 | 3.4631 | -0.1687 |
| C | 1.5011 | 1.1022 | -0.0335 | C | -1.2209 | -0.1282 | 0.0227 |
| C | 0.9536 | -0.1845 | -0.0819 | C | -1.7012 | 1.1787 | -0.0419 |
| C | 1.748 | -1.3219 | -0.1272 | C | -0.7317 | 2.2734 | -0.1066 |
| C | 3.1335 | -1.1561 | -0.1355 | C | 0.6541 | 1.8669 | -0.1053 |
| C | 0.6125 | 2.244 | 0.0116 | C | 1.0181 | 0.5671 | -0.0209 |
| C | -0.794 | 1.9439 | -0.0047 | C | -3.088 | 1.3776 | -0.0498 |
| C | -1.2354 | 0.666 | -0.0405 | C | -2.075 | -1.2279 | 0.0722 |
| O | -0.3863 | -0.3814 | -0.0812 | C | -3.4456 | -1.0016 | 0.0643 |
| O | 1.0479 | 3.4165 | 0.0527 | C | -3.948 | 0.303 | 0.0041 |
| O | 3.4815 | 2.4516 | 0.0019 | C | 2.3975 | 0.0494 | -0.0053 |
| O | 3.943 | -2.2355 | -0.1871 | O | -4.3219 | -2.0372 | 0.1139 |
| O | 1.2205 | -2.5851 | -0.2135 | O | -1.6296 | -2.5127 | 0.1325 |
| C | 0.7502 | -3.1127 | 1.0386 | C | 3.4614 | 0.869 | 0.3834 |
| C | -2.6444 | 0.2378 | -0.0547 | C | 4.7579 | 0.3736 | 0.3841 |
| C | -3.6464 | 1.077 | 0.4416 | C | 5.0062 | -0.941 | 0.0007 |
| C | -4.9727 | 0.6698 | 0.4131 | C | 3.9504 | -1.7621 | -0.3808 |
| C | -5.3123 | -0.5754 | -0.1075 | C | 2.6509 | -1.2732 | -0.3819 |
| C | -4.318 | -1.4163 | -0.5964 | H | 1.4123 | 2.6337 | -0.1873 |
| C | -2.9888 | -1.0164 | -0.568 | H | -3.4758 | 2.3873 | -0.1007 |
| H | 4.7958 | 0.2095 | -0.1039 | H | -5.0221 | 0.4438 | -0.0014 |
| H | -1.4976 | 2.7646 | -0.0021 | H | -3.8438 | -2.8748 | 0.1425 |
| H | 2.7493 | 3.1091 | 0.0329 | H | -0.6668 | -2.5361 | 0.0763 |
| H | 3.4002 | -3.0344 | -0.2342 | H | 3.2811 | 1.8883 | 0.7037 |
| H | 0.4097 | -4.1267 | 0.8343 | H | 5.5757 | 1.0144 | 0.6926 |
| H | 1.5637 | -3.1331 | 1.7685 | H | 6.02 | -1.3251 | 0.0037 |
| H | -0.0802 | -2.5137 | 1.4199 | H | 4.1375 | -2.787 | -0.6798 |
| H | -3.394 | 2.0407 | 0.8681 | H | 1.8337 | -1.9166 | -0.6843 |
| H | -5.7422 | 1.3242 | 0.806 | | | | |
| H | -6.3493 | -0.8907 | -0.1281 | | | | |
| H | -4.5769 | -2.3872 | -1.003 | | | | |
| H | -2.2197 | -1.6736 | -0.9546 | | | | |

**Table S3.** (cont.)

| Chrysin | | | | Pinocembrin | | | |
|---|---|---|---|---|---|---|---|
| $N_i$ = 0; E = -878.48325 | | | | $N_i$ = 0; E = -879.69920 | | | |
| C | -0.8076 | 1.8407 | -0.1086 | C | 0.2185 | 1.9405 | 0.3212 |
| O | -1.3001 | 2.9896 | -0.186 | O | 0.308 | 2.9623 | -0.3719 |
| C | -1.6374 | 0.6583 | -0.0314 | C | 1.065 | 0.7854 | 0.12 |
| C | 0.6109 | 1.6079 | -0.1027 | C | -0.7513 | 1.8467 | 1.4644 |
| C | -1.0414 | -0.6056 | 0.0525 | C | 0.9282 | -0.3492 | 0.9533 |
| C | -3.0521 | 0.7179 | -0.0401 | C | 2.1007 | 0.7777 | -0.8453 |
| C | 1.1097 | 0.3543 | -0.0076 | C | -1.2037 | 0.4087 | 1.6643 |
| O | 0.3141 | -0.7321 | 0.0715 | O | -0.0421 | -0.4141 | 1.8982 |
| C | -1.7712 | -1.777 | 0.1269 | C | 1.7833 | -1.427 | 0.8538 |
| O | -3.6792 | 1.9074 | -0.12 | O | 2.2799 | 1.8282 | -1.6674 |
| C | -3.8065 | -0.438 | 0.0324 | C | 2.9635 | -0.3 | -0.9599 |
| C | 2.5398 | 0.0019 | 0.0047 | C | -2.0287 | -0.1768 | 0.525 |
| C | -3.1577 | -1.6733 | 0.1154 | C | 2.7996 | -1.3852 | -0.1024 |
| C | 2.9574 | -1.253 | -0.4481 | C | -2.7817 | 0.6288 | -0.3282 |
| C | 3.4889 | 0.9207 | 0.4612 | C | -2.0644 | -1.562 | 0.3478 |
| O | -3.8584 | -2.8302 | 0.19 | O | 3.6147 | -2.4635 | -0.1669 |
| C | 4.3078 | -1.5757 | -0.4559 | C | -3.5526 | 0.0618 | -1.3395 |
| C | 4.8369 | 0.5902 | 0.4554 | C | -2.8305 | -2.1272 | -0.6636 |
| C | 5.2496 | -0.6565 | -0.0051 | C | -3.5784 | -1.3163 | -1.5124 |
| H | 1.2787 | 2.4536 | -0.1916 | H | -0.2191 | 2.1716 | 2.3654 |
| H | -1.2788 | -2.7379 | 0.1924 | H | -1.5865 | 2.5292 | 1.3144 |
| H | -2.978 | 2.5984 | -0.1648 | H | -1.7687 | 0.3318 | 2.5932 |
| H | -4.889 | -0.3821 | 0.024 | H | 1.6588 | -2.2918 | 1.4923 |
| H | 2.2289 | -1.97 | -0.8061 | H | 1.607 | 2.5038 | -1.4341 |
| H | 3.1755 | 1.8867 | 0.8391 | H | 3.7538 | -0.2899 | -1.7013 |
| H | -4.8041 | -2.6483 | 0.1756 | H | -2.7787 | 1.7065 | -0.2176 |
| H | 4.6246 | -2.5475 | -0.8166 | H | -1.484 | -2.2027 | 1.0014 |
| H | 5.5656 | 1.3055 | 0.8187 | H | 4.2776 | -2.3414 | -0.8556 |
| H | 6.3032 | -0.9121 | -0.0089 | H | -4.1301 | 0.7044 | -1.9946 |
| | | | | H | -2.8431 | -3.2042 | -0.789 |
| | | | | H | -4.1755 | -1.7569 | -2.3029 |

**Table S3.** (cont.)

| Catechin | | | | Eupatilin | | | |
|---|---|---|---|---|---|---|---|
| $N_i$ = 0; E = -1031.09808 | | | | $N_i$ = 0; E = -1222.03662 | | | |
| O | -0.8696 | 3.2095 | -0.6197 | C | 4.4539 | 0.4367 | -0.0462 |
| C | -0.0194 | 2.2182 | -0.0626 | C | 3.8 | 1.6644 | 0.1412 |
| C | 0.4177 | 1.2178 | -1.1423 | C | 2.4159 | 1.7588 | 0.1394 |
| C | -0.6776 | 1.4741 | 1.0937 | C | 1.6939 | 0.5949 | -0.0549 |
| O | -0.7148 | 0.5047 | -1.6498 | C | 2.2994 | -0.6492 | -0.255 |
| C | 1.5101 | 0.2816 | -0.6633 | C | 3.7125 | -0.7148 | -0.255 |
| C | -1.6963 | 0.4971 | 0.5661 | O | 0.3374 | 0.7106 | -0.0378 |
| C | -1.6614 | 0.0657 | -0.7603 | C | -0.4531 | -0.3632 | -0.2374 |
| C | 1.3129 | -1.0847 | -0.5003 | C | 0.0592 | -1.5991 | -0.456 |
| C | 2.7661 | 0.8258 | -0.3688 | C | 1.4759 | -1.8216 | -0.468 |
| C | -2.7233 | -0.013 | 1.3729 | O | 4.5295 | 2.7847 | 0.3263 |
| C | -2.6027 | -0.8218 | -1.2842 | O | 5.8275 | 0.4307 | -0.0662 |
| C | 2.3522 | -1.8945 | -0.039 | C | 6.4272 | -0.0271 | 1.1577 |
| C | 3.8024 | 0.0249 | 0.0865 | O | 4.3513 | -1.8796 | -0.4574 |
| O | -2.7402 | 0.4107 | 2.6693 | O | 1.9813 | -2.9525 | -0.6595 |
| C | -3.6763 | -0.9015 | 0.8875 | C | -1.8796 | -0.0172 | -0.1996 |
| C | -3.607 | -1.296 | -0.4491 | C | -2.2953 | 1.301 | -0.3794 |
| C | 3.5944 | -1.3534 | 0.2582 | C | -3.6437 | 1.633 | -0.3664 |
| O | -4.5617 | -2.1671 | -0.889 | C | -4.6055 | 0.6464 | -0.1634 |
| H | -1.7116 | 2.7943 | -0.8421 | C | -4.1879 | -0.6839 | 0.0289 |
| H | 0.8658 | 2.751 | 0.2911 | C | -2.8484 | -1.0067 | 0.0103 |
| H | 0.7811 | 1.788 | -2.0015 | O | -5.1297 | -1.6711 | 0.2067 |
| H | 0.0932 | 0.9541 | 1.6745 | C | -5.5512 | -1.819 | 1.5674 |
| H | -1.1475 | 2.1998 | 1.7626 | O | -5.9369 | 0.8619 | -0.1379 |
| H | 2.9498 | 1.8894 | -0.5042 | C | -6.4055 | 2.1983 | -0.3081 |
| H | -2.5389 | -1.1289 | -2.3226 | H | 1.919 | 2.7084 | 0.2868 |
| H | -3.5016 | 0.0262 | 3.1203 | H | -0.5971 | -2.4379 | -0.6413 |
| H | -4.4615 | -1.2836 | 1.5314 | H | 5.4671 | 2.5562 | 0.2605 |
| H | -4.4138 | -2.3562 | -1.8236 | H | 6.1141 | 0.6069 | 1.9917 |
| H | 0.3571 | -1.5389 | -0.7341 | H | 6.153 | -1.0657 | 1.3551 |
| H | 2.2 | -2.9626 | 0.0892 | H | 7.5044 | 0.0502 | 1.0183 |
| O | 5.0481 | 0.5053 | 0.3793 | H | 3.6526 | -2.5649 | -0.5806 |
| O | 4.6541 | -2.0901 | 0.7099 | H | -1.5665 | 2.0836 | -0.546 |
| H | 4.3844 | -3.014 | 0.7773 | H | -3.9347 | 2.6635 | -0.5198 |
| H | 5.0639 | 1.4555 | 0.2119 | H | -2.5747 | -2.0417 | 0.1782 |
| | | | | H | -6.3088 | -2.6017 | 1.5753 |
| | | | | H | -4.7058 | -2.1175 | 2.1948 |
| | | | | H | -5.9812 | -0.8874 | 1.9456 |
| | | | | H | -7.4901 | 2.1399 | -0.2428 |
| | | | | H | -6.0238 | 2.8478 | 0.484 |
| | | | | H | -6.1171 | 2.5907 | -1.2867 |

**Table S3.** (cont.)

| Baicalein | | | | Pectolinarigenin | | | |
|---|---|---|---|---|---|---|---|
| $N_i$ = 0; E = -953.70820 | | | | $N_i$ = 0; E = -1107.52139 | | | |
| C | -0.7443 | -0.585 | 0.0453 | C | 0.9422 | 0.6233 | -0.0505 |
| C | -1.3259 | 0.6832 | -0.0359 | C | 0.3422 | 1.8349 | 0.0538 |
| C | -2.7342 | 0.7724 | -0.043 | C | -1.0856 | 1.9594 | 0.0325 |
| C | -3.5033 | -0.3742 | 0.0298 | O | -1.6694 | 3.0661 | 0.1157 |
| C | -2.8783 | -1.6263 | 0.1107 | C | -1.8241 | 0.7185 | -0.0774 |
| C | -1.4962 | -1.7438 | 0.1186 | C | -3.2381 | 0.6871 | -0.0974 |
| O | 0.6118 | -0.7283 | 0.0639 | C | -3.8968 | -0.5275 | -0.1937 |
| C | 1.4157 | 0.3486 | -0.0111 | C | -3.1585 | -1.7174 | -0.2891 |
| C | 0.9293 | 1.6092 | -0.1048 | C | -1.7711 | -1.7153 | -0.2775 |
| C | -0.4842 | 1.8586 | -0.1122 | C | -1.1323 | -0.4931 | -0.1679 |
| C | 2.8436 | -0.0143 | 0.0042 | O | 0.2292 | -0.516 | -0.1628 |
| C | 3.2529 | -1.2738 | -0.4435 | C | 2.3891 | 0.3775 | -0.0412 |
| C | 4.6009 | -1.6067 | -0.4471 | C | 2.8914 | -0.8858 | 0.2729 |
| C | 5.5487 | -0.6929 | 0.0024 | C | 4.2581 | -1.129 | 0.3062 |
| C | 5.1443 | 0.5584 | 0.4577 | C | 5.1464 | -0.0947 | 0.0131 |
| C | 3.7988 | 0.8988 | 0.4595 | C | 4.655 | 1.1742 | -0.3125 |
| O | -0.9692 | 3.011 | -0.1887 | C | 3.2954 | 1.4052 | -0.3381 |
| O | -3.3687 | 1.9619 | -0.1188 | O | -5.2667 | -0.61 | -0.253 |
| O | -4.87 | -0.3559 | 0.0286 | C | -5.914 | -0.502 | 1.0259 |
| O | -3.6258 | -2.7518 | 0.1851 | O | 6.4948 | -0.2264 | 0.0142 |
| H | -1.0238 | -2.715 | 0.1831 | C | 7.0482 | -1.5015 | 0.3304 |
| H | 1.607 | 2.4474 | -0.1907 | O | -3.8092 | -2.8947 | -0.4001 |
| H | 2.5199 | -1.9866 | -0.8006 | O | -3.9565 | 1.8207 | -0.0274 |
| H | 4.9112 | -2.582 | -0.8037 | H | 0.936 | 2.7307 | 0.1707 |
| H | 6.6003 | -0.9564 | 0.0018 | H | -1.209 | -2.6366 | -0.3531 |
| H | 5.8775 | 1.2696 | 0.8199 | H | 2.2123 | -1.6957 | 0.5083 |
| H | 3.4924 | 1.8686 | 0.8334 | H | 4.6125 | -2.1185 | 0.5616 |
| H | -2.6671 | 2.6524 | -0.1642 | H | 5.3554 | 1.9661 | -0.5502 |
| H | -5.1858 | 0.5543 | 0 | H | 2.9387 | 2.3917 | -0.6093 |
| H | -4.5631 | -2.5217 | 0.1762 | H | -6.981 | -0.6146 | 0.8398 |
| | | | | H | -5.5672 | -1.2965 | 1.6924 |
| | | | | H | -5.7175 | 0.474 | 1.4752 |
| | | | | H | 8.1277 | -1.3789 | 0.2673 |
| | | | | H | 6.773 | -1.8064 | 1.3436 |
| | | | | H | 6.7227 | -2.2577 | -0.389 |
| | | | | H | -4.7599 | -2.7179 | -0.4321 |
| | | | | H | -3.3069 | 2.5601 | 0.0433 |

**Table S3.** (cont.)

| 3,5-Dihydroxyflavone | | | | Alpinetin | | | |
|---|---|---|---|---|---|---|---|
| $N_i$ = 0; E = -878.47189 | | | | $N_i$ = 0; E = -918.98149 | | | |
| C | -0.1532 | 1.3062 | -0.0909 | C | 1.362 | -0.3214 | 0.403 |
| C | -0.7951 | 0.1154 | 0.0205 | O | 0.6483 | 0.8555 | -0.0225 |
| C | 1.2891 | 1.3756 | -0.1005 | C | -0.7025 | 0.78 | -0.0047 |
| O | 1.856 | 2.4833 | -0.213 | C | -2.7452 | 2.0076 | 0.0399 |
| C | 1.9909 | 0.1218 | 0.0064 | C | -1.359 | 2.002 | 0.0165 |
| C | 3.4055 | 0.0428 | 0.003 | O | -3.4545 | 3.1607 | 0.0633 |
| C | 4.0284 | -1.1878 | 0.1011 | C | -3.4842 | 0.8244 | 0.0608 |
| C | 3.2555 | -2.3463 | 0.2 | C | -2.8204 | -0.391 | 0.0343 |
| C | 1.8725 | -2.3072 | 0.2043 | O | -3.4776 | -1.5624 | 0.055 |
| C | 1.2566 | -1.0648 | 0.1063 | C | -4.9035 | -1.5515 | 0.0983 |
| O | -0.097 | -1.0424 | 0.1175 | C | -1.3966 | -0.4519 | -0.0234 |
| C | -2.2489 | -0.1051 | 0.0176 | C | -0.6391 | -1.6884 | -0.2125 |
| C | -3.1208 | 0.813 | 0.6099 | O | -1.1302 | -2.8107 | -0.2934 |
| C | -4.4895 | 0.5766 | 0.6013 | C | 2.8325 | -0.0661 | 0.2101 |
| C | -5 | -0.5694 | 0.0009 | C | 0.8526 | -1.5175 | -0.3752 |
| C | -4.1349 | -1.4879 | -0.5865 | C | 3.3271 | 0.3348 | -1.0318 |
| C | -2.7657 | -1.2622 | -0.5755 | C | 3.7166 | -0.2627 | 1.2674 |
| O | 4.1548 | 1.1621 | -0.094 | C | 5.0831 | -0.0667 | 1.0877 |
| O | -0.8248 | 2.4776 | -0.2269 | C | 5.5709 | 0.3379 | -0.1495 |
| H | 5.1102 | -1.2378 | 0.0986 | C | 4.6893 | 0.5414 | -1.2087 |
| H | 3.7559 | -3.3048 | 0.2753 | H | 1.1515 | -0.4606 | 1.4691 |
| H | 1.2711 | -3.2036 | 0.28 | H | -0.7903 | 2.9239 | 0.0319 |
| H | -2.7311 | 1.7007 | 1.0906 | H | -2.8599 | 3.9183 | 0.0446 |
| H | -5.1581 | 1.2897 | 1.0698 | H | -4.5618 | 0.8889 | 0.0989 |
| H | -6.0692 | -0.7487 | -0.0068 | H | -5.2004 | -2.5983 | 0.1068 |
| H | -4.5273 | -2.3826 | -1.0559 | H | -5.2626 | -1.0605 | 1.0062 |
| H | -2.0959 | -1.9786 | -1.0357 | H | -5.3174 | -1.0598 | -0.7856 |
| H | 3.5457 | 1.9262 | -0.1617 | H | 1.3537 | -2.4285 | -0.0459 |
| H | -0.1542 | 3.1696 | -0.332 | H | 1.0559 | -1.3816 | -1.4445 |
| | | | | H | 2.6444 | 0.4886 | -1.861 |
| | | | | H | 3.335 | -0.5709 | 2.2355 |
| | | | | H | 5.764 | -0.2244 | 1.9167 |
| | | | | H | 6.6344 | 0.4963 | -0.2899 |
| | | | | H | 5.0653 | 0.8584 | -2.1751 |

**Table S3.** (cont.)

| Galangin | | | | Genkwanin | | | |
|---|---|---|---|---|---|---|---|
| $N_i$ = 0; E = -953.70715 | | | | $N_i$ = 0; E = -993.00741 | | | |
| O | -1.2853 | 2.8737 | -0.189 | C | -1.9203 | -1.4677 | 0.0739 |
| C | -0.862 | 1.6997 | -0.0974 | C | -3.3056 | -1.2973 | 0.0666 |
| C | -1.707 | 0.5448 | -0.0199 | C | -3.885 | -0.0259 | 0.0081 |
| C | 0.5641 | 1.4539 | -0.0792 | C | -3.0633 | 1.0881 | -0.0427 |
| C | -1.1299 | -0.7292 | 0.0636 | C | -1.6572 | 0.9565 | -0.0359 |
| C | -3.1223 | 0.6349 | -0.0295 | C | -1.1289 | -0.3395 | 0.023 |
| O | 1.3736 | 2.5386 | -0.1855 | C | -0.7657 | 2.0948 | -0.0919 |
| C | 1.0527 | 0.1934 | 0.0121 | C | 0.6361 | 1.7889 | -0.0911 |
| O | 0.2147 | -0.8747 | 0.0809 | C | 1.0728 | 0.5082 | -0.0153 |
| C | -1.8864 | -1.8865 | 0.139 | O | 0.2195 | -0.5359 | 0.0426 |
| O | -3.7269 | 1.8366 | -0.1108 | C | 2.4775 | 0.0816 | 0.0018 |
| C | -3.8957 | -0.5045 | 0.0447 | C | 3.4873 | 0.9633 | 0.3998 |
| C | 2.468 | -0.2056 | 0.0153 | C | 4.8135 | 0.5668 | 0.4025 |
| C | -3.2684 | -1.7539 | 0.1296 | C | 5.1492 | -0.7262 | 0.0039 |
| C | 2.8489 | -1.3897 | -0.6249 | C | 4.1548 | -1.6188 | -0.3913 |
| C | 3.4356 | 0.5706 | 0.6594 | C | 2.831 | -1.2159 | -0.3869 |
| O | -3.9951 | -2.8936 | 0.208 | O | 6.4368 | -1.1669 | -0.0126 |
| C | 4.1802 | -1.7819 | -0.6309 | O | -1.2002 | 3.2694 | -0.1485 |
| C | 4.7651 | 0.168 | 0.6553 | O | -3.6285 | 2.3101 | -0.0996 |
| C | 5.1413 | -1.0043 | 0.0083 | O | -4.0282 | -2.4359 | 0.1198 |
| H | 0.7907 | 3.309 | -0.2658 | C | -5.4526 | -2.3459 | 0.1204 |
| H | -1.414 | -2.8574 | 0.2054 | H | -1.4817 | -2.4555 | 0.1212 |
| H | -3.0264 | 2.5209 | -0.1614 | H | -4.9564 | 0.1179 | 0.0024 |
| H | -4.9769 | -0.4294 | 0.0364 | H | 1.3441 | 2.6024 | -0.1671 |
| H | 2.1038 | -1.9965 | -1.1255 | H | 3.2435 | 1.9658 | 0.7306 |
| H | 3.1494 | 1.477 | 1.177 | H | 5.5915 | 1.2522 | 0.721 |
| H | -4.9363 | -2.6891 | 0.2002 | H | 4.428 | -2.6209 | -0.7001 |
| H | 4.4675 | -2.6963 | -1.1373 | H | 2.0662 | -1.9147 | -0.7019 |
| H | 5.5081 | 0.7714 | 1.1642 | H | 7.0297 | -0.4649 | 0.2768 |
| H | 6.1805 | -1.3134 | 0.0044 | H | -2.8913 | 2.964 | -0.1307 |
| | | | | H | -5.8103 | -3.3721 | 0.1715 |
| | | | | H | -5.8068 | -1.7897 | 0.992 |
| | | | | H | -5.8137 | -1.8768 | -0.7983 |

**Table S3.** (cont.)

| Primuletin | | | | Tectochrysin | | | |
|---|---|---|---|---|---|---|---|
| $N_i$ = 0; E = -803.24804 | | | | $_i$ = 0; E = -917.77285 | | | |
| C | 1.2395 | -1.528 | -0.1224 | C | 0.7754 | -0.3607 | 0.0291 |
| O | 1.8567 | -2.611 | -0.2197 | C | 1.2318 | 0.9624 | -0.0395 |
| C | 1.9391 | -0.2574 | -0.0127 | C | 0.2803 | 2.05 | -0.0983 |
| C | -0.1931 | -1.4513 | -0.1248 | C | -1.105 | 1.6667 | -0.093 |
| C | 1.2024 | 0.9264 | 0.0906 | C | -1.467 | 0.3659 | -0.0102 |
| C | 3.3506 | -0.1671 | -0.0129 | O | -0.5601 | -0.6308 | 0.0532 |
| C | -0.8293 | -0.2617 | -0.0064 | C | 1.6274 | -1.4435 | 0.0844 |
| O | -0.1605 | 0.9012 | 0.1019 | C | 3.0013 | -1.1977 | 0.0712 |
| C | 1.8065 | 2.1711 | 0.1932 | C | 3.5102 | 0.1032 | 0.0032 |
| O | 4.107 | -1.2805 | -0.1114 | C | 2.6292 | 1.1704 | -0.0518 |
| C | 3.9685 | 1.0692 | 0.0893 | C | -2.8517 | -0.1378 | 0.0067 |
| C | -2.29 | -0.0729 | 0.0028 | O | 0.6473 | 3.2458 | -0.16 |
| C | 3.1915 | 2.2211 | 0.1905 | O | 3.785 | -2.2942 | 0.1299 |
| C | -3.1332 | -1.1035 | 0.4277 | C | -3.8969 | 0.6779 | 0.4502 |
| C | -2.842 | 1.1394 | -0.4212 | C | -5.2005 | 0.2017 | 0.4491 |
| C | -4.5095 | -0.9242 | 0.4196 | C | -5.4742 | -1.0893 | 0.0077 |
| C | -4.2197 | 1.3105 | -0.4315 | C | -4.4368 | -1.9065 | -0.4293 |
| C | -5.0557 | 0.2808 | -0.0119 | C | -3.13 | -1.4372 | -0.4275 |
| H | -0.7621 | -2.3633 | -0.2401 | O | 3.127 | 2.4206 | -0.1178 |
| H | 1.1986 | 3.0629 | 0.2715 | C | 5.2026 | -2.1264 | 0.1282 |
| H | 3.4895 | -2.0436 | -0.1751 | H | -1.8579 | 2.4385 | -0.1722 |
| H | 5.0503 | 1.1234 | 0.0887 | H | 1.2432 | -2.4533 | 0.1393 |
| H | 3.6849 | 3.1829 | 0.2697 | H | 4.5722 | 0.305 | -0.0075 |
| H | -2.7172 | -2.0389 | 0.7832 | H | -3.6949 | 1.678 | 0.8151 |
| H | -2.1958 | 1.942 | -0.7547 | H | -6.0036 | 0.8387 | 0.8012 |
| H | -5.1562 | -1.7255 | 0.758 | H | -6.4935 | -1.4586 | 0.0085 |
| H | -4.6406 | 2.2502 | -0.7699 | H | -4.6443 | -2.9128 | -0.7744 |
| H | -6.1311 | 0.4182 | -0.0173 | H | -2.3273 | -2.0758 | -0.7747 |
| | | | | H | 2.3565 | 3.0342 | -0.1471 |
| | | | | H | 5.6157 | -3.1312 | 0.186 |
| | | | | H | 5.5365 | -1.6445 | -0.7941 |
| | | | | H | 5.5263 | -1.5457 | 0.9956 |

**Table S4.** Cartesian coordinates of optimized geometries (ωB97XD/6-311+G**) of 115 combinatorially-designed flavonoids. Total energy (E) in Hartrees. $N_i$ is the number of imaginary frequencies.

| Compound 1 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -803.241795704 | | |
| C | 4.6749 | -0.1022 | -0.1472 |
| C | 3.8715 | -1.1475 | 0.2724 |
| C | 2.4844 | -1.0067 | 0.3097 |
| O | 1.7894 | -2.0886 | 0.7582 |
| C | 1.8945 | 0.214 | -0.0702 |
| C | 2.7317 | 1.2537 | -0.5011 |
| C | 4.1057 | 1.1076 | -0.5418 |
| C | 0.4441 | 0.4508 | -0.0112 |
| C | -0.144 | 1.6465 | 0.2248 |
| C | -1.5771 | 1.7947 | 0.2464 |
| O | -2.1336 | 2.8832 | 0.4401 |
| C | -2.3342 | 0.5525 | 0.0399 |
| C | -3.7357 | 0.514 | 0.0602 |
| C | -4.4039 | -0.6781 | -0.1266 |
| C | -3.6821 | -1.8607 | -0.3367 |
| C | -2.3012 | -1.85 | -0.3616 |
| C | -1.644 | -0.6379 | -0.1729 |
| O | -0.2786 | -0.6723 | -0.2161 |
| H | 5.7506 | -0.2343 | -0.1741 |
| H | 4.3004 | -2.0948 | 0.578 |
| H | 0.8428 | -1.9663 | 0.6153 |
| H | 2.2843 | 2.1862 | -0.824 |
| H | 4.7282 | 1.9246 | -0.8851 |
| H | 0.468 | 2.5167 | 0.418 |
| H | -4.2791 | 1.4366 | 0.2269 |
| H | -5.4868 | -0.703 | -0.1104 |
| H | -4.2095 | -2.7961 | -0.4825 |
| H | -1.7235 | -2.7518 | -0.5238 |

| Compound 2 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -803.243888406 | | |
| C | 4.4767 | 0.1655 | 0.1754 |
| C | 3.6921 | -0.9153 | -0.2172 |
| O | 4.235 | -2.1181 | -0.5749 |
| C | 2.3075 | -0.8038 | -0.2601 |
| C | 1.7016 | 0.4052 | 0.0812 |
| C | 2.4824 | 1.4937 | 0.4795 |
| C | 3.8633 | 1.3628 | 0.5233 |
| C | 0.2332 | 0.526 | 0.0145 |
| C | -0.4464 | 1.677 | -0.1989 |
| C | -1.8857 | 1.7066 | -0.2463 |
| O | -2.5283 | 2.7487 | -0.4342 |
| C | -2.5371 | 0.4026 | -0.0686 |
| C | -3.931 | 0.2484 | -0.0981 |
| C | -4.4995 | -0.9969 | 0.0663 |
| C | -3.6826 | -2.1189 | 0.2641 |
| C | -2.3081 | -1.9943 | 0.2976 |
| C | -1.7487 | -0.7294 | 0.1299 |
| O | -0.3874 | -0.657 | 0.1775 |
| H | 5.5565 | 0.0648 | 0.2091 |
| H | 5.1954 | -2.0712 | -0.5267 |
| H | 1.7171 | -1.6558 | -0.5734 |
| H | 2.0192 | 2.4277 | 0.772 |
| H | 4.473 | 2.2014 | 0.8386 |
| H | 0.0945 | 2.6005 | -0.3547 |
| H | -4.5481 | 1.1255 | -0.2531 |
| H | -5.5764 | -1.1115 | 0.0429 |
| H | -4.1314 | -3.097 | 0.3933 |
| H | -1.6597 | -2.8483 | 0.4505 |

**Table S4.** (cont.)

| Compound 3 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -803.245724740 | | |
| C | -4.3668 | -0.3052 | -0.0043 |
| O | -5.7023 | -0.5689 | -0.0361 |
| C | -3.8623 | 0.9338 | 0.3884 |
| C | -2.4942 | 1.1471 | 0.393 |
| C | -1.6108 | 0.1337 | 0.0099 |
| C | -2.1327 | -1.109 | -0.3672 |
| C | -3.4988 | -1.3288 | -0.3798 |
| C | -0.1616 | 0.3697 | -0.0102 |
| C | 0.4376 | 1.5799 | -0.137 |
| C | 1.8681 | 1.7198 | -0.1418 |
| O | 2.4362 | 2.8177 | -0.2398 |
| C | 2.6142 | 0.4588 | -0.0347 |
| C | 4.0158 | 0.4116 | -0.0432 |
| C | 4.6748 | -0.7955 | 0.0592 |
| C | 3.9424 | -1.9852 | 0.1715 |
| C | 2.5616 | -1.9662 | 0.1804 |
| C | 1.9106 | -0.7388 | 0.0759 |
| O | 0.547 | -0.7709 | 0.0969 |
| H | -6.2024 | 0.211 | 0.2278 |
| H | -4.5417 | 1.7222 | 0.6937 |
| H | -2.1168 | 2.1101 | 0.716 |
| H | -1.4668 | -1.9079 | -0.6689 |
| H | -3.9027 | -2.2874 | -0.6833 |
| H | -0.1677 | 2.4686 | -0.253 |
| H | 4.5665 | 1.3407 | -0.1313 |
| H | 5.7577 | -0.827 | 0.0529 |
| H | 4.462 | -2.9329 | 0.252 |
| H | 1.9778 | -2.8745 | 0.265 |

| Compound 4 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -803.236101342 | | |
| C | -4.6956 | -0.7834 | 0.0063 |
| C | -4.255 | 0.3853 | 0.6185 |
| C | -2.9031 | 0.7047 | 0.6277 |
| C | -1.9778 | -0.1516 | 0.0243 |
| C | -2.424 | -1.3325 | -0.579 |
| C | -3.7769 | -1.6415 | -0.5907 |
| C | -0.5402 | 0.1599 | 0.0219 |
| C | 0.0239 | 1.3882 | -0.1001 |
| C | 1.4612 | 1.5642 | -0.1276 |
| O | 1.9359 | 2.7026 | -0.2534 |
| C | 2.2464 | 0.3475 | -0.0168 |
| C | 3.6522 | 0.3543 | -0.0282 |
| C | 4.3513 | -0.8261 | 0.079 |
| C | 3.6599 | -2.0431 | 0.1986 |
| C | 2.2818 | -2.0767 | 0.2096 |
| C | 1.5824 | -0.8734 | 0.1003 |
| O | 0.2302 | -0.9509 | 0.1205 |
| H | -5.752 | -1.0269 | -0.0028 |
| H | -4.9652 | 1.0515 | 1.0947 |
| H | -2.5674 | 1.6098 | 1.1171 |
| H | -1.7124 | -2.002 | -1.0472 |
| H | -4.1146 | -2.5537 | -1.0691 |
| O | -0.7241 | 2.5134 | -0.2353 |
| H | 5.4345 | -0.8206 | 0.0713 |
| H | 4.2147 | -2.9703 | 0.2825 |
| H | 1.7321 | -3.0055 | 0.2997 |
| H | 4.1679 | 1.3026 | -0.122 |
| H | -0.0916 | 3.2415 | -0.3407 |

**Table S4.** (cont.)

| Compound 5 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -803.248088959 | | |
| C | -5.0557 | 0.2799 | -0.0044 |
| C | -4.5072 | -0.9231 | 0.4298 |
| C | -3.1309 | -1.102 | 0.4331 |
| C | -2.2899 | -0.0731 | -0.0001 |
| C | -2.8439 | 1.1369 | -0.4281 |
| C | -4.2218 | 1.3076 | -0.4331 |
| C | -0.8292 | -0.2612 | -0.0123 |
| C | -0.193 | -1.4507 | -0.1315 |
| C | 1.2396 | -1.5276 | -0.1276 |
| O | 1.8572 | -2.6105 | -0.2241 |
| C | 1.939 | -0.2569 | -0.0154 |
| C | 3.3506 | -0.1669 | -0.0101 |
| O | 4.1067 | -1.281 | -0.1039 |
| C | 3.9684 | 1.0691 | 0.0951 |
| C | 3.1913 | 2.2211 | 0.1949 |
| C | 1.8063 | 2.1715 | 0.1928 |
| C | 1.2023 | 0.9271 | 0.0866 |
| O | -0.1607 | 0.902 | 0.0948 |
| H | -6.1311 | 0.4173 | -0.0055 |
| H | -5.1523 | -1.7228 | 0.7748 |
| H | -2.7129 | -2.0354 | 0.7916 |
| H | -2.1994 | 1.9377 | -0.769 |
| H | -4.6443 | 2.2457 | -0.7741 |
| H | -0.7627 | -2.3624 | -0.2458 |
| H | 5.0502 | 1.1234 | 0.0989 |
| H | 3.6849 | 3.1825 | 0.2771 |
| H | 1.1987 | 3.0636 | 0.2698 |
| H | 3.4884 | -2.0433 | -0.1702 |

| Compound 6 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -803.242690040 | | |
| C | -5.1121 | -0.5967 | 0.0131 |
| C | -4.1908 | -1.5424 | -0.4255 |
| C | -2.834 | -1.247 | -0.4273 |
| C | -2.3895 | 0.0063 | 0.0036 |
| C | -3.3179 | 0.9516 | 0.448 |
| C | -4.6725 | 0.6487 | 0.4516 |
| C | -0.9515 | 0.3285 | -0.0181 |
| C | -0.433 | 1.5739 | -0.1501 |
| C | 0.9862 | 1.8056 | -0.1621 |
| O | 1.4834 | 2.9357 | -0.268 |
| C | 1.8113 | 0.5942 | -0.0491 |
| C | 3.2099 | 0.6483 | -0.0591 |
| C | 3.9445 | -0.5142 | 0.0549 |
| C | 3.2951 | -1.7525 | 0.1781 |
| C | 1.9183 | -1.8189 | 0.187 |
| C | 1.1829 | -0.6421 | 0.0719 |
| O | -0.178 | -0.7637 | 0.0935 |
| H | -6.1707 | -0.8306 | 0.0165 |
| H | -4.5288 | -2.513 | -0.7698 |
| H | -2.1213 | -1.9838 | -0.7769 |
| H | -2.983 | 1.917 | 0.8091 |
| H | -5.3856 | 1.3842 | 0.8055 |
| H | -1.0961 | 2.4207 | -0.2645 |
| O | 5.3075 | -0.4154 | 0.0429 |
| H | 3.8835 | -2.6595 | 0.2649 |
| H | 1.4034 | -2.7669 | 0.2815 |
| H | 3.7093 | 1.6049 | -0.1546 |
| H | 5.7051 | -1.2868 | 0.139 |

**Table S4.** (cont.)

| Compound 7 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -803.245832575 | | |
| C | 4.9635 | -0.8984 | 0.0063 |
| C | 4.6466 | 0.3845 | 0.4428 |
| C | 3.3274 | 0.8161 | 0.4444 |
| C | 2.3097 | -0.0359 | 0.0059 |
| C | 2.6315 | -1.327 | -0.4232 |
| C | 3.9535 | -1.7517 | -0.4257 |
| C | 0.9083 | 0.4211 | -0.0133 |
| C | 0.5019 | 1.7066 | -0.1192 |
| C | -0.897 | 2.0594 | -0.1325 |
| O | -1.2868 | 3.2345 | -0.213 |
| C | -1.8176 | 0.9268 | -0.0559 |
| C | -3.2128 | 1.0783 | -0.0763 |
| C | -4.0458 | -0.0123 | 0.0019 |
| C | -3.4938 | -1.301 | 0.1044 |
| O | -4.2777 | -2.4046 | 0.1881 |
| C | -2.1224 | -1.4878 | 0.1238 |
| C | -1.3052 | -0.368 | 0.0419 |
| O | 0.0361 | -0.6043 | 0.0727 |
| H | 5.9946 | -1.233 | 0.0069 |
| H | 5.428 | 1.0497 | 0.7914 |
| H | 3.0912 | 1.8103 | 0.805 |
| H | 1.8504 | -1.9938 | -0.767 |
| H | 4.1942 | -2.7518 | -0.7676 |
| H | 1.2342 | 2.4969 | -0.2133 |
| H | -3.6296 | 2.0752 | -0.1547 |
| H | -5.1235 | 0.1067 | -0.0141 |
| H | -5.2068 | -2.1508 | 0.176 |
| H | -1.6923 | -2.4781 | 0.2032 |

| Compound 8 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -803.240618920 | | |
| C | 4.8247 | -0.5244 | 0.0156 |
| C | 4.422 | 0.747 | -0.382 |
| C | 3.0754 | 1.0822 | -0.3897 |
| C | 2.1169 | 0.1439 | 0.0036 |
| C | 2.5247 | -1.1356 | 0.3933 |
| C | 3.8738 | -1.4636 | 0.4014 |
| C | 0.6873 | 0.498 | 0.0151 |
| C | 0.1815 | 1.7502 | 0.1122 |
| C | -1.2378 | 2 | 0.1141 |
| O | -1.7156 | 3.1397 | 0.1836 |
| C | -2.0843 | 0.7998 | 0.0393 |
| C | -3.4841 | 0.8563 | 0.0525 |
| C | -4.2155 | -0.3117 | -0.0194 |
| C | -3.5771 | -1.5538 | -0.1026 |
| C | -2.1983 | -1.63 | -0.1136 |
| O | -1.5845 | -2.841 | -0.1889 |
| C | -1.4607 | -0.4403 | -0.0437 |
| O | -0.1089 | -0.5844 | -0.0678 |
| H | 5.8774 | -0.7833 | 0.0207 |
| H | 5.158 | 1.4785 | -0.6947 |
| H | 2.7723 | 2.069 | -0.7188 |
| H | 1.7894 | -1.8692 | 0.7006 |
| H | 4.1825 | -2.455 | 0.7123 |
| H | 0.8515 | 2.5943 | 0.203 |
| H | -3.9727 | 1.8201 | 0.1197 |
| H | -5.2982 | -0.2759 | -0.0104 |
| H | -4.1517 | -2.4712 | -0.1561 |
| H | -0.6267 | -2.7287 | -0.1671 |

**Table S4.** (cont.)

| Compound 9 | | | | Compound 10 | | | |
|---|---|---|---|---|---|---|---|
| $N_i = 0$ | E = -878.471944424 | | | $N_i = 0$ | E = -878.467411519 | | |
| C | 5.0001 | -0.5691 | -0.0043 | C | 5.0161 | -0.925 | 0.0235 |
| C | 4.491 | 0.5755 | 0.6001 | C | 4.6115 | 0.246 | 0.656 |
| C | 3.1221 | 0.8116 | 0.6124 | C | 3.2724 | 0.6157 | 0.656 |
| C | 2.249 | -0.1057 | 0.0208 | C | 2.3243 | -0.1921 | 0.0224 |
| C | 2.7644 | -1.2626 | -0.5741 | C | 2.7336 | -1.3746 | -0.6029 |
| C | 4.1337 | -1.4876 | -0.5896 | C | 4.0741 | -1.7341 | -0.6049 |
| C | 0.7953 | 0.1156 | 0.0235 | C | 0.8985 | 0.1707 | 0.0145 |
| C | 0.1535 | 1.3065 | -0.088 | C | 0.3822 | 1.4213 | -0.1077 |
| C | -1.2888 | 1.3753 | -0.1041 | C | -1.0444 | 1.6559 | -0.1364 |
| O | -1.8554 | 2.4827 | -0.221 | O | -1.4753 | 2.8123 | -0.2607 |
| C | -1.991 | 0.1217 | 0.0035 | C | -1.879 | 0.4706 | -0.0282 |
| C | -3.4057 | 0.043 | 0.0012 | C | -3.2802 | 0.5452 | -0.0414 |
| C | -4.0286 | -1.1874 | 0.1018 | C | -4.0259 | -0.6074 | 0.0667 |
| C | -3.2558 | -2.3458 | 0.2029 | C | -3.389 | -1.8559 | 0.1862 |
| C | -1.8728 | -2.3069 | 0.2063 | C | -2.0157 | -1.9418 | 0.1973 |
| C | -1.2569 | -1.0647 | 0.1053 | C | -1.2618 | -0.7726 | 0.0888 |
| O | 0.0968 | -1.0423 | 0.1161 | O | 0.0886 | -0.9074 | 0.1108 |
| H | 6.0694 | -0.7478 | -0.0159 | H | 6.0626 | -1.2082 | 0.0225 |
| H | 5.1608 | 1.288 | 1.0678 | H | 5.3398 | 0.8739 | 1.1562 |
| H | 2.7333 | 1.6986 | 1.0953 | H | 2.9637 | 1.5216 | 1.1614 |
| H | 2.0936 | -1.9792 | -1.0326 | H | 2.0032 | -2.0055 | -1.0954 |
| H | 4.5247 | -2.3817 | -1.0613 | H | 4.384 | -2.6473 | -1.1 |
| O | 0.8251 | 2.4786 | -0.2185 | O | 1.1782 | 2.5146 | -0.2416 |
| H | -5.1105 | -1.2376 | 0.1004 | O | -5.3879 | -0.4977 | 0.0536 |
| H | -3.7565 | -3.3038 | 0.2808 | H | -3.9895 | -2.7555 | 0.2683 |
| H | -1.2718 | -3.2035 | 0.2831 | H | -1.5134 | -2.8968 | 0.2888 |
| O | -4.155 | 1.1625 | -0.0944 | H | -3.7667 | 1.5085 | -0.1347 |
| H | 0.1546 | 3.1718 | -0.3166 | H | 0.5784 | 3.2695 | -0.3485 |
| H | -3.546 | 1.9262 | -0.1643 | H | -5.7926 | -1.3664 | 0.1451 |

**Table S4.** (cont.)

| Compound 11 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -878.470877296 | | |
| C | 4.8366 | -1.2613 | 0.0111 |
| C | 4.5578 | -0.0483 | 0.6317 |
| C | 3.2629 | 0.4546 | 0.6386 |
| C | 2.2311 | -0.2592 | 0.0224 |
| C | 2.5143 | -1.4844 | -0.5914 |
| C | 3.8114 | -1.9782 | -0.5989 |
| C | 0.8503 | 0.2478 | 0.0182 |
| C | 0.4586 | 1.5413 | -0.0831 |
| C | -0.9448 | 1.9111 | -0.1161 |
| O | -1.2552 | 3.108 | -0.2255 |
| C | -1.8827 | 0.8135 | -0.0348 |
| C | -3.2767 | 0.9996 | -0.0583 |
| C | -4.1306 | -0.0715 | 0.0159 |
| C | -3.605 | -1.3749 | 0.1159 |
| C | -2.2401 | -1.5935 | 0.1385 |
| C | -1.3941 | -0.492 | 0.0622 |
| O | -0.0666 | -0.752 | 0.094 |
| H | 5.8492 | -1.6487 | 0.0053 |
| H | 5.35 | 0.5087 | 1.1187 |
| H | 3.0536 | 1.3923 | 1.1365 |
| H | 1.7205 | -2.0443 | -1.0714 |
| H | 4.0223 | -2.9243 | -1.0843 |
| O | 1.3526 | 2.5571 | -0.1988 |
| H | -5.2057 | 0.0689 | -0.0014 |
| O | -4.4143 | -2.4595 | 0.1934 |
| H | -1.8332 | -2.5937 | 0.2156 |
| H | -3.6694 | 2.0063 | -0.1361 |
| H | 0.8256 | 3.3659 | -0.2958 |
| H | -5.338 | -2.1867 | 0.1756 |

| Compound 12 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -878.465443388 | | |
| C | 4.7409 | -0.8651 | 0.0106 |
| C | 3.7668 | -1.6734 | 0.5893 |
| C | 2.4361 | -1.28 | 0.5765 |
| C | 2.0678 | -0.0638 | -0.0097 |
| C | 3.0484 | 0.7424 | -0.5951 |
| C | 4.3775 | 0.3386 | -0.584 |
| C | 0.6522 | 0.3323 | -0.011 |
| C | 0.1497 | 1.59 | 0.0837 |
| C | -1.278 | 1.8432 | 0.1045 |
| O | -1.6886 | 3.008 | 0.2005 |
| C | -2.134 | 0.6705 | 0.0252 |
| C | -3.5361 | 0.7483 | 0.0393 |
| C | -4.2792 | -0.4087 | -0.0363 |
| C | -3.6546 | -1.6608 | -0.123 |
| C | -2.2793 | -1.7569 | -0.1337 |
| C | -1.5225 | -0.5762 | -0.0609 |
| O | -0.1812 | -0.7335 | -0.0846 |
| H | 5.7798 | -1.1747 | 0.0203 |
| H | 4.0438 | -2.6127 | 1.0539 |
| H | 1.6819 | -1.9122 | 1.03 |
| H | 2.774 | 1.6739 | -1.0722 |
| H | 5.1304 | 0.9666 | -1.0462 |
| O | 0.9537 | 2.6777 | 0.1924 |
| H | -5.3614 | -0.3608 | -0.0277 |
| O | -1.68 | -2.9745 | -0.2122 |
| H | -4.0112 | 1.7187 | 0.1095 |
| H | 0.3605 | 3.441 | 0.2766 |
| H | -4.2421 | -2.5698 | -0.1794 |
| H | -0.7209 | -2.8738 | -0.1868 |

**Table S4.** (cont.)

| Compound 13 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -878.468497178 | | |
| C | 4.4701 | -1.1865 | -0.1012 |
| C | 4.1434 | 0.0256 | 0.4812 |
| C | 2.8251 | 0.4816 | 0.4863 |
| C | 1.8146 | -0.301 | -0.0998 |
| C | 2.1708 | -1.5247 | -0.6882 |
| C | 3.4807 | -1.9669 | -0.6973 |
| C | 0.389 | 0.0628 | -0.085 |
| C | -0.1518 | 1.2883 | -0.2891 |
| C | -1.5783 | 1.5222 | -0.2581 |
| O | -2.0175 | 2.6675 | -0.427 |
| C | -2.3934 | 0.3381 | -0.0439 |
| C | -3.7976 | 0.3864 | -0.0148 |
| C | -4.5262 | -0.7647 | 0.1806 |
| C | -3.866 | -1.9922 | 0.3522 |
| C | -2.4894 | -2.0659 | 0.328 |
| C | -1.7601 | -0.8928 | 0.1289 |
| O | -0.4088 | -1.012 | 0.1218 |
| H | 5.5009 | -1.5221 | -0.0949 |
| H | 4.9016 | 0.6441 | 0.9471 |
| O | 2.5915 | 1.66 | 1.1331 |
| H | 1.3956 | -2.1273 | -1.1461 |
| H | 3.7307 | -2.912 | -1.1639 |
| O | 0.6422 | 2.3661 | -0.5454 |
| H | -5.6085 | -0.7274 | 0.2026 |
| H | -4.2888 | 1.3425 | -0.151 |
| H | 0.0601 | 3.1413 | -0.5921 |
| H | -4.4434 | -2.8963 | 0.5061 |
| H | -1.964 | -3.0037 | 0.4599 |
| H | 1.8722 | 2.1459 | 0.6928 |

| Compound 14 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -878.468776164 | | |
| C | 4.3163 | -1.116 | -0.2125 |
| C | 3.9672 | 0.1093 | 0.3477 |
| C | 2.6362 | 0.5061 | 0.4116 |
| C | 1.6417 | -0.332 | -0.0921 |
| C | 1.9842 | -1.5693 | -0.6487 |
| C | 3.3178 | -1.9469 | -0.7068 |
| C | 0.2262 | 0.0678 | -0.0448 |
| C | -0.2703 | 1.3229 | -0.1879 |
| C | -1.6963 | 1.5811 | -0.1734 |
| O | -2.1089 | 2.7403 | -0.3223 |
| C | -2.5455 | 0.4158 | 0.001 |
| C | -3.9483 | 0.5033 | 0.0302 |
| C | -4.7096 | -0.6311 | 0.1944 |
| C | -4.0849 | -1.8816 | 0.3339 |
| C | -2.7113 | -1.994 | 0.3079 |
| C | -1.9483 | -0.8369 | 0.1394 |
| O | -0.6029 | -0.9915 | 0.1218 |
| H | 5.3591 | -1.4118 | -0.2587 |
| O | 4.8992 | 0.9717 | 0.857 |
| H | 1.216 | -2.2219 | -1.0432 |
| H | 3.588 | -2.9005 | -1.1457 |
| O | 0.5344 | 2.3968 | -0.3911 |
| H | -5.7904 | -0.5634 | 0.217 |
| H | -4.4123 | 1.4763 | -0.0792 |
| H | -0.0582 | 3.1561 | -0.5071 |
| H | -4.6885 | -2.7723 | 0.4634 |
| H | -2.2128 | -2.9496 | 0.4141 |
| H | 2.3917 | 1.4583 | 0.8632 |
| H | 5.7813 | 0.6001 | 0.754 |

**Table S4.** (cont.)

| Compound 15 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -878.470418532 | | |
| C | 4.3539 | -0.5043 | 0.0036 |
| C | 3.4759 | -1.4329 | -0.5531 |
| C | 2.1152 | -1.184 | -0.5379 |
| C | 1.6069 | -0.0044 | 0.0209 |
| C | 2.4999 | 0.9133 | 0.5816 |
| C | 3.8639 | 0.6669 | 0.5768 |
| C | 0.1598 | 0.235 | 0.0178 |
| C | -0.4697 | 1.4339 | -0.0975 |
| C | -1.9115 | 1.5367 | -0.1214 |
| O | -2.4465 | 2.6495 | -0.2453 |
| C | -2.635 | 0.2813 | -0.0126 |
| C | -4.0391 | 0.2174 | -0.0183 |
| C | -4.6774 | -0.9977 | 0.0835 |
| C | -3.9252 | -2.179 | 0.1911 |
| C | -2.547 | -2.1427 | 0.1964 |
| C | -1.9099 | -0.9049 | 0.0937 |
| O | -0.5552 | -0.9132 | 0.1106 |
| O | 5.6851 | -0.7938 | -0.0367 |
| H | 2.1319 | 1.8208 | 1.0414 |
| H | 4.5507 | 1.3798 | 1.0204 |
| O | 0.222 | 2.597 | -0.2291 |
| H | -5.7595 | -1.0467 | 0.0808 |
| H | -4.6023 | 1.1392 | -0.1027 |
| H | -0.4451 | 3.2938 | -0.3311 |
| H | -4.4322 | -3.1334 | 0.2709 |
| H | -1.951 | -3.0434 | 0.277 |
| H | 1.44 | -1.9092 | -0.9758 |
| H | 3.8682 | -2.3407 | -0.9961 |
| H | 6.1915 | -0.0839 | 0.3723 |

| Compound 16 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -878.476247490 | | |
| C | 5.3749 | -0.4183 | 0.0099 |
| C | 4.5087 | -1.4124 | -0.4339 |
| C | 3.1375 | -1.1941 | -0.4357 |
| C | 2.6232 | 0.0304 | 0.0003 |
| C | 3.4964 | 1.0253 | 0.4485 |
| C | 4.8658 | 0.7989 | 0.4523 |
| C | 1.1699 | 0.2702 | -0.0175 |
| C | 0.5814 | 1.4863 | -0.1371 |
| C | -0.8447 | 1.6222 | -0.1377 |
| O | -1.4237 | 2.7261 | -0.2355 |
| C | -1.5941 | 0.3786 | -0.0273 |
| C | -3.0004 | 0.3599 | -0.0224 |
| O | -3.732 | 1.4934 | -0.1095 |
| C | -3.6753 | -0.8521 | 0.0786 |
| C | -2.9569 | -2.0391 | 0.1773 |
| C | -1.571 | -2.0447 | 0.177 |
| C | -0.906 | -0.8337 | 0.0737 |
| O | 0.46 | -0.8649 | 0.0849 |
| H | 6.4449 | -0.5929 | 0.0139 |
| H | 4.9009 | -2.3612 | -0.7814 |
| H | 2.4678 | -1.9685 | -0.7891 |
| H | 3.1078 | 1.9692 | 0.8127 |
| H | 5.536 | 1.5722 | 0.8094 |
| H | 1.1897 | 2.3732 | -0.2481 |
| O | -5.042 | -0.8986 | 0.0866 |
| H | -3.5049 | -2.9709 | 0.2557 |
| H | -1.0111 | -2.9675 | 0.2544 |
| H | -3.0933 | 2.2392 | -0.1764 |
| H | -5.3934 | -0.0048 | 0.0002 |

**Table S4.** (cont.)

| Compound 17 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -878.483254598 | | |
| C | -5.2499 | -0.653 | -0.0027 |
| C | -4.3135 | -1.5597 | -0.489 |
| C | -2.9625 | -1.2395 | -0.4822 |
| C | -2.5398 | 0.001 | 0.0041 |
| C | -3.483 | 0.9073 | 0.496 |
| C | -4.8316 | 0.5787 | 0.4918 |
| C | -1.1096 | 0.3523 | -0.0101 |
| C | -0.6117 | 1.6057 | -0.1087 |
| C | 0.8067 | 1.8391 | -0.1163 |
| O | 1.2983 | 2.9879 | -0.1978 |
| C | 1.637 | 0.6573 | -0.0352 |
| C | 3.0517 | 0.7178 | -0.0426 |
| O | 3.6781 | 1.9076 | -0.1256 |
| C | 3.8068 | -0.4372 | 0.0355 |
| C | 3.1588 | -1.6725 | 0.1238 |
| C | 1.7724 | -1.7772 | 0.1348 |
| C | 1.0417 | -0.6067 | 0.0533 |
| O | -0.314 | -0.7342 | 0.0713 |
| H | -6.3038 | -0.9068 | -0.0056 |
| H | -4.6352 | -2.5194 | -0.8767 |
| H | -2.2379 | -1.9459 | -0.8683 |
| H | -3.164 | 1.8608 | 0.9002 |
| H | -5.5564 | 1.2834 | 0.8828 |
| H | -1.2802 | 2.4507 | -0.2005 |
| O | 3.8606 | -2.8285 | 0.2022 |
| H | 1.2806 | -2.7382 | 0.2043 |
| H | 2.9768 | 2.5982 | -0.171 |
| H | 4.8893 | -0.3806 | 0.0276 |
| H | 4.8061 | -2.6451 | 0.1916 |

| Compound 18 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -878.474239485 | | |
| C | 5.1073 | 0.2298 | 0.0134 |
| C | 4.2409 | 1.2332 | 0.4355 |
| C | 2.8692 | 1.0188 | 0.4311 |
| C | 2.3546 | -0.211 | 0.0098 |
| C | 3.2279 | -1.2148 | -0.4183 |
| C | 4.5977 | -0.9923 | -0.415 |
| C | 0.9014 | -0.4442 | 0.0209 |
| C | 0.2932 | -1.6506 | 0.1123 |
| C | -1.1385 | -1.7682 | 0.1046 |
| O | -1.7233 | -2.869 | 0.1709 |
| C | -1.8788 | -0.5157 | 0.0245 |
| C | -3.2879 | -0.4601 | 0.0205 |
| O | -4.0294 | -1.5946 | 0.0819 |
| C | -3.9229 | 0.768 | -0.0521 |
| C | -3.1772 | 1.9429 | -0.1208 |
| C | -1.794 | 1.9194 | -0.1197 |
| C | -1.1613 | 0.6805 | -0.0461 |
| O | 0.1981 | 0.7009 | -0.0568 |
| H | 6.1778 | 0.4011 | 0.0148 |
| H | 4.6334 | 2.186 | 0.7711 |
| H | 2.1995 | 1.8015 | 0.766 |
| H | 2.8398 | -2.1628 | -0.772 |
| H | 5.2682 | -1.7727 | -0.7556 |
| H | 0.8853 | -2.5506 | 0.2025 |
| O | -1.0907 | 3.0897 | -0.1875 |
| H | -3.4004 | -2.3461 | 0.1241 |
| H | -5.0052 | 0.808 | -0.0559 |
| H | -3.6808 | 2.901 | -0.1779 |
| H | -0.1446 | 2.9049 | -0.1891 |

**Table S4.** (cont.)

| Compound 19 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -878.478627286 | | |
| C | -4.9448 | -0.1132 | -0.122 |
| C | -4.207 | 0.9774 | 0.3025 |
| C | -2.8134 | 0.9263 | 0.3258 |
| C | -2.15 | -0.2503 | -0.0725 |
| C | -2.9224 | -1.338 | -0.5071 |
| C | -4.3029 | -1.2797 | -0.5353 |
| C | -0.6879 | -0.3936 | -0.0288 |
| C | -0.0193 | -1.5513 | 0.1833 |
| C | 1.4159 | -1.5881 | 0.1931 |
| O | 2.0593 | -2.6436 | 0.3735 |
| C | 2.0854 | -0.3107 | 0 |
| C | 3.4933 | -0.1823 | 0.0133 |
| O | 4.2774 | -1.2637 | 0.2018 |
| C | 4.0794 | 1.0615 | -0.1651 |
| C | 3.275 | 2.1823 | -0.3542 |
| C | 1.8912 | 2.0949 | -0.3707 |
| C | 1.3229 | 0.8439 | -0.193 |
| O | -0.0409 | 0.7763 | -0.2223 |
| H | -6.027 | -0.0511 | -0.1378 |
| H | -4.6935 | 1.8913 | 0.6229 |
| O | -2.1862 | 2.0453 | 0.7816 |
| H | -2.4195 | -2.237 | -0.8432 |
| H | -4.8748 | -2.1314 | -0.8821 |
| H | -0.5624 | -2.4674 | 0.3685 |
| H | 3.6798 | -2.0367 | 0.3141 |
| H | 5.1592 | 1.1451 | -0.1539 |
| H | 3.7442 | 3.1495 | -0.4925 |
| H | 1.2594 | 2.9612 | -0.5177 |
| H | -1.2349 | 1.9877 | 0.6289 |

| Compound 20 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -878.480741177 | | |
| C | -4.7521 | -0.3158 | 0.1513 |
| C | -4.0189 | 0.8016 | -0.2392 |
| C | -2.6304 | 0.7583 | -0.2712 |
| C | -1.9687 | -0.417 | 0.084 |
| C | -2.6972 | -1.5405 | 0.4838 |
| C | -4.0833 | -1.4785 | 0.5137 |
| C | -0.4963 | -0.4658 | 0.0322 |
| C | 0.2418 | -1.5842 | -0.1606 |
| C | 1.6756 | -1.5272 | -0.1909 |
| O | 2.3867 | -2.5411 | -0.3585 |
| C | 2.2582 | -0.2048 | -0.0273 |
| C | 3.6549 | 0.0153 | -0.0505 |
| O | 4.5081 | -1.0155 | -0.2261 |
| C | 4.1595 | 1.2967 | 0.1052 |
| C | 3.2835 | 2.3653 | 0.283 |
| C | 1.9092 | 2.1875 | 0.3091 |
| C | 1.4191 | 0.8994 | 0.1519 |
| O | 0.0647 | 0.7475 | 0.1871 |
| H | -5.8359 | -0.2683 | 0.175 |
| O | -4.6169 | 1.9754 | -0.6044 |
| H | -2.1902 | -2.4474 | 0.7889 |
| H | -4.6533 | -2.3443 | 0.8298 |
| H | -0.244 | -2.5383 | -0.3112 |
| H | 3.9632 | -1.829 | -0.3208 |
| H | 5.2314 | 1.4509 | 0.0861 |
| H | 3.6886 | 3.3634 | 0.4036 |
| H | 1.2243 | 3.0139 | 0.4471 |
| H | -2.0801 | 1.6365 | -0.5849 |
| H | -5.5742 | 1.8892 | -0.5462 |

**Table S4.** (cont.)

| Compound 21 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -878.482737034 | | |
| C | -4.6637 | 0.178 | 0.0111 |
| C | -3.845 | 1.2417 | 0.3859 |
| C | -2.4703 | 1.0867 | 0.3706 |
| C | -1.8911 | -0.13 | -0.0083 |
| C | -2.726 | -1.1848 | -0.3894 |
| C | -4.1023 | -1.0362 | -0.3825 |
| C | -0.4331 | -0.2949 | 0.0057 |
| C | 0.2273 | -1.4748 | 0.1187 |
| C | 1.6585 | -1.5267 | 0.1145 |
| O | 2.2968 | -2.5996 | 0.2044 |
| C | 2.3377 | -0.2434 | 0.013 |
| C | 3.7471 | -0.1294 | 0.0123 |
| O | 4.5213 | -1.2318 | 0.1005 |
| C | 4.3443 | 1.1178 | -0.0823 |
| C | 3.548 | 2.2571 | -0.1754 |
| C | 2.1639 | 2.1835 | -0.1766 |
| C | 1.5811 | 0.928 | -0.0814 |
| O | 0.2187 | 0.8794 | -0.093 |
| O | -6.0098 | 0.3767 | 0.0432 |
| H | -2.3048 | -2.129 | -0.7138 |
| H | -4.745 | -1.8553 | -0.6866 |
| H | -0.324 | -2.398 | 0.2295 |
| H | 3.9137 | -2.0038 | 0.1596 |
| H | 5.425 | 1.1903 | -0.083 |
| H | 4.0251 | 3.2274 | -0.2496 |
| H | 1.5413 | 3.0658 | -0.2483 |
| H | -1.8422 | 1.9161 | 0.6707 |
| H | -4.2935 | 2.1799 | 0.6901 |
| H | -6.4698 | -0.4262 | -0.225 |

| Compound 22 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -878.475045845 | | |
| C | 5.3071 | -0.8686 | 0.0111 |
| C | 4.9778 | 0.4135 | 0.4404 |
| C | 3.6545 | 0.8325 | 0.4389 |
| C | 2.6451 | -0.0311 | 0.004 |
| C | 2.9795 | -1.3211 | -0.4184 |
| C | 4.3055 | -1.7336 | -0.4172 |
| C | 1.2392 | 0.4126 | -0.0167 |
| C | 0.8215 | 1.6961 | -0.1209 |
| C | -0.578 | 2.0392 | -0.1329 |
| O | -0.9788 | 3.2115 | -0.2124 |
| C | -1.4905 | 0.9001 | -0.0552 |
| C | -2.8871 | 1.0561 | -0.0708 |
| C | -3.7076 | -0.0399 | 0.0081 |
| C | -3.1514 | -1.3367 | 0.1046 |
| C | -1.7846 | -1.5106 | 0.119 |
| C | -0.9678 | -0.3864 | 0.038 |
| O | 0.376 | -0.6168 | 0.0664 |
| H | 6.3413 | -1.1937 | 0.0143 |
| H | 5.7526 | 1.088 | 0.786 |
| H | 3.4092 | 1.8263 | 0.7943 |
| H | 2.2051 | -1.997 | -0.7596 |
| H | 4.5559 | -2.7333 | -0.7533 |
| H | 1.5476 | 2.4923 | -0.2132 |
| O | -5.0709 | 0.0068 | 0.0035 |
| O | -3.9592 | -2.42 | 0.1854 |
| H | -1.3547 | -2.5013 | 0.1952 |
| H | -3.3145 | 2.0498 | -0.1436 |
| H | -5.3769 | 0.9189 | -0.0321 |
| H | -4.8812 | -2.1338 | 0.1765 |

**Table S4.** (cont.)

| Compound 23 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -878.472305433 | | |
| C | -5.1642 | -0.576 | -0.0106 |
| C | -4.2031 | -1.5015 | -0.4042 |
| C | -2.8582 | -1.1568 | -0.399 |
| C | -2.4647 | 0.1256 | -0.0042 |
| C | -3.4333 | 1.0501 | 0.3966 |
| C | -4.7759 | 0.6983 | 0.3916 |
| C | -1.039 | 0.4962 | -0.017 |
| C | -0.5489 | 1.7563 | -0.1134 |
| C | 0.8648 | 2.0269 | -0.1177 |
| O | 1.3285 | 3.1727 | -0.1881 |
| C | 1.7298 | 0.8379 | -0.0436 |
| C | 3.1249 | 0.9279 | -0.0565 |
| C | 3.8748 | -0.23 | 0.0189 |
| C | 3.2591 | -1.4857 | 0.1018 |
| C | 1.883 | -1.5812 | 0.1113 |
| C | 1.1206 | -0.4073 | 0.0399 |
| O | -0.2307 | -0.5732 | 0.0643 |
| H | -6.2136 | -0.8479 | -0.0135 |
| H | -4.5005 | -2.4952 | -0.7188 |
| H | -2.1148 | -1.8797 | -0.7126 |
| H | -3.1414 | 2.0389 | 0.7297 |
| H | -5.5197 | 1.4192 | 0.7104 |
| H | -1.2307 | 2.5911 | -0.2026 |
| O | 5.2351 | -0.1109 | 0.0083 |
| O | 1.2988 | -2.8039 | 0.1873 |
| H | 3.6073 | 1.8946 | -0.123 |
| H | 5.6473 | -0.9787 | 0.0714 |
| H | 3.8558 | -2.3897 | 0.1556 |
| H | 0.3386 | -2.7138 | 0.1651 |

| Compound 24 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -878.473365707 | | |
| C | 5.0262 | -0.22 | -0.1545 |
| C | 4.4943 | 1.0046 | -0.5553 |
| C | 3.1255 | 1.1938 | -0.5139 |
| C | 2.2571 | 0.183 | -0.0764 |
| C | 2.8093 | -1.0534 | 0.3095 |
| C | 4.1912 | -1.2377 | 0.2717 |
| C | 0.8147 | 0.4644 | -0.0142 |
| C | 0.2659 | 1.6801 | 0.2231 |
| C | -1.1595 | 1.8765 | 0.2538 |
| O | -1.6805 | 2.9822 | 0.4501 |
| C | -1.9598 | 0.659 | 0.0532 |
| C | -3.3583 | 0.6796 | 0.0847 |
| C | -4.0677 | -0.4903 | -0.0994 |
| C | -3.3929 | -1.7013 | -0.3163 |
| C | -2.0147 | -1.7345 | -0.3489 |
| C | -1.3082 | -0.5505 | -0.1635 |
| O | 0.0572 | -0.6327 | -0.2146 |
| H | 6.0973 | -0.3853 | -0.1813 |
| H | 5.1417 | 1.7998 | -0.9039 |
| H | 2.707 | 2.1382 | -0.841 |
| O | 2.0808 | -2.1104 | 0.7643 |
| H | 4.591 | -2.1959 | 0.5823 |
| H | 0.9074 | 2.5299 | 0.4113 |
| O | -5.4317 | -0.4253 | -0.0606 |
| H | -3.8773 | 1.6151 | 0.2552 |
| H | -5.8095 | -1.2993 | -0.2024 |
| H | -3.9621 | -2.6133 | -0.4599 |
| H | -1.4786 | -2.6605 | -0.5163 |
| H | 1.1385 | -1.959 | 0.6206 |

**Table S4.** (cont.)

| Compound 25 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -878.475412727 | | |
| C | 4.8451 | 0.006 | 0.1608 |
| C | 4.2926 | 1.2361 | 0.4967 |
| C | 2.9194 | 1.4337 | 0.4615 |
| C | 2.0831 | 0.3795 | 0.084 |
| C | 2.6275 | -0.8614 | -0.2458 |
| C | 4.0052 | -1.0398 | -0.2115 |
| C | 0.6213 | 0.5681 | 0.0239 |
| C | -0.0051 | 1.751 | -0.1876 |
| C | -1.4396 | 1.8503 | -0.2353 |
| O | -2.0341 | 2.9222 | -0.4163 |
| C | -2.1535 | 0.5766 | -0.0668 |
| C | -3.5507 | 0.5003 | -0.1093 |
| C | -4.177 | -0.7192 | 0.0466 |
| C | -3.4202 | -1.8834 | 0.2495 |
| C | -2.0441 | -1.8213 | 0.2935 |
| C | -1.4174 | -0.5881 | 0.1325 |
| O | -0.0524 | -0.5818 | 0.1869 |
| H | 5.9189 | -0.1472 | 0.1877 |
| H | 4.9446 | 2.0486 | 0.7957 |
| H | 2.5049 | 2.3933 | 0.7441 |
| O | 4.4843 | -2.2725 | -0.5582 |
| H | 0.5795 | 2.6474 | -0.3429 |
| O | -5.542 | -0.756 | -0.0064 |
| H | -4.1327 | 1.4002 | -0.2674 |
| H | -5.8496 | -1.6597 | 0.1189 |
| H | -3.9265 | -2.8351 | 0.3721 |
| H | -1.447 | -2.7113 | 0.4492 |
| H | 1.9948 | -1.688 | -0.5439 |
| H | 5.446 | -2.2724 | -0.5189 |

| Compound 26 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -878.477203098 | | |
| C | -4.7283 | -0.3981 | -0.0024 |
| C | -4.2625 | 0.8591 | -0.3857 |
| C | -2.9016 | 1.116 | -0.3832 |
| C | -1.9877 | 0.1299 | -0.0009 |
| C | -2.4714 | -1.129 | 0.3736 |
| C | -3.8294 | -1.3927 | 0.3786 |
| C | -0.5454 | 0.4065 | 0.0166 |
| C | 0.0199 | 1.6352 | 0.1378 |
| C | 1.444 | 1.8177 | 0.1419 |
| O | 1.982 | 2.9313 | 0.2355 |
| C | 2.2282 | 0.5779 | 0.0394 |
| C | 3.6277 | 0.5838 | 0.0494 |
| C | 4.3212 | -0.6052 | -0.0497 |
| C | 3.6299 | -1.8214 | -0.1598 |
| C | 2.2513 | -1.84 | -0.169 |
| C | 1.5575 | -0.637 | -0.0675 |
| O | 0.1933 | -0.7112 | -0.0879 |
| O | -6.0533 | -0.7112 | 0.0151 |
| H | -4.9655 | 1.626 | -0.6923 |
| H | -2.5535 | 2.0918 | -0.701 |
| H | -0.6112 | 2.5064 | 0.2495 |
| O | 5.6872 | -0.5554 | -0.0355 |
| H | 4.1599 | 1.5236 | 0.1347 |
| H | 6.0509 | -1.4429 | -0.1172 |
| H | 4.1874 | -2.7487 | -0.2356 |
| H | 1.7036 | -2.7706 | -0.2519 |
| H | -1.7813 | -1.9066 | 0.6766 |
| H | -4.204 | -2.3646 | 0.6775 |
| H | -6.58 | 0.0418 | -0.2734 |

**Table S4.** (cont.)

| Compound 27 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -878.471656674 | | |
| C | 5.0069 | -0.942 | -0.0048 |
| C | 4.7622 | 0.3801 | 0.354 |
| C | 3.4657 | 0.8751 | 0.3581 |
| C | 2.3977 | 0.048 | -0.0026 |
| C | 2.6476 | -1.2822 | -0.3544 |
| C | 3.9472 | -1.7712 | -0.3567 |
| C | 1.0183 | 0.5661 | -0.0163 |
| C | 0.6546 | 1.8662 | -0.0996 |
| C | -0.731 | 2.2738 | -0.0991 |
| O | -1.0725 | 3.4639 | -0.1576 |
| C | -1.701 | 1.1794 | -0.0385 |
| C | -3.0877 | 1.3789 | -0.0495 |
| C | -3.9483 | 0.3046 | -0.0006 |
| C | -3.4466 | -1.0003 | 0.058 |
| O | -4.3233 | -2.0359 | 0.1023 |
| C | -2.0761 | -1.2271 | 0.0693 |
| C | -1.2213 | -0.1278 | 0.025 |
| O | 0.1039 | -0.4232 | 0.0529 |
| H | 6.021 | -1.3255 | -0.0056 |
| H | 5.5832 | 1.0275 | 0.6395 |
| H | 3.2898 | 1.9008 | 0.6596 |
| H | 1.8277 | -1.9318 | -0.6353 |
| H | 4.1314 | -2.8021 | -0.6361 |
| H | 1.4128 | 2.6327 | -0.1819 |
| H | -3.4752 | 2.3888 | -0.0988 |
| H | -5.0223 | 0.4461 | -0.0083 |
| H | -3.8456 | -2.8736 | 0.1335 |
| O | -1.6311 | -2.5122 | 0.1275 |
| H | -0.6679 | -2.5348 | 0.0788 |

| Compound 28 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -878.476559801 | | |
| C | -4.9107 | -0.5252 | -0.1894 |
| C | -3.9947 | -1.4425 | 0.2948 |
| C | -2.6372 | -1.1284 | 0.3491 |
| C | -2.1935 | 0.1372 | -0.0795 |
| C | -3.1416 | 1.0439 | -0.5753 |
| C | -4.486 | 0.7262 | -0.6327 |
| C | -0.7843 | 0.5527 | -0.0064 |
| C | -0.3467 | 1.8154 | 0.1946 |
| C | 1.0616 | 2.1329 | 0.2322 |
| O | 1.4763 | 3.2894 | 0.3957 |
| C | 1.9588 | 0.9881 | 0.0797 |
| C | 3.3566 | 1.1066 | 0.1128 |
| C | 4.1654 | 0.004 | -0.0322 |
| C | 3.5856 | -1.2633 | -0.2134 |
| O | 4.3446 | -2.3759 | -0.3648 |
| C | 2.2099 | -1.4181 | -0.2476 |
| C | 1.4216 | -0.286 | -0.1021 |
| O | 0.0725 | -0.4844 | -0.161 |
| H | -5.9611 | -0.7904 | -0.2281 |
| H | -4.3109 | -2.4203 | 0.6391 |
| O | -1.8229 | -2.0924 | 0.8622 |
| H | -2.8044 | 2.0089 | -0.9352 |
| H | -5.1967 | 1.4421 | -1.0269 |
| H | -1.0603 | 2.6137 | 0.346 |
| H | 3.7947 | 2.0873 | 0.2543 |
| H | 5.2454 | 0.0983 | -0.0098 |
| H | 5.279 | -2.1435 | -0.3371 |
| H | 1.7561 | -2.3908 | -0.3895 |
| H | -0.8964 | -1.8599 | 0.7236 |

**Table S4.** (cont.)

| Compound 29 | | | |
|---|---|---|---|
| $N_i$ = 0 | E = -878.478733555 | | |
| C | -4.7477 | -0.1953 | 0.178 |
| C | -3.838 | -1.1736 | -0.2132 |
| C | -2.4773 | -0.8956 | -0.2589 |
| C | -2.0207 | 0.3772 | 0.0831 |
| C | -2.9272 | 1.3631 | 0.4827 |
| C | -4.2823 | 1.0671 | 0.5259 |
| C | -0.5778 | 0.6745 | 0.0153 |
| C | -0.0393 | 1.9021 | -0.1605 |
| C | 1.389 | 2.1005 | -0.213 |
| O | 1.9006 | 3.2211 | -0.3576 |
| C | 2.1841 | 0.8804 | -0.0926 |
| C | 3.5867 | 0.8806 | -0.1387 |
| C | 4.3008 | -0.2884 | -0.0226 |
| C | 3.6161 | -1.5053 | 0.143 |
| O | 4.2764 | -2.6843 | 0.2606 |
| C | 2.2331 | -1.5423 | 0.1927 |
| C | 1.5384 | -0.346 | 0.0726 |
| O | 0.1804 | -0.4344 | 0.1338 |
| H | -5.8073 | -0.4263 | 0.2123 |
| O | -4.2328 | -2.4337 | -0.5672 |
| H | -2.5793 | 2.3457 | 0.7759 |
| H | -4.9884 | 1.8262 | 0.8418 |
| H | -0.6858 | 2.761 | -0.2786 |
| H | 4.1038 | 1.8239 | -0.2685 |
| H | 5.3846 | -0.2862 | -0.0584 |
| H | 5.2276 | -2.5398 | 0.2137 |
| H | 1.7012 | -2.4765 | 0.3208 |
| H | -1.7891 | -1.6705 | -0.5723 |
| H | -5.191 | -2.5027 | -0.5052 |

| Compound 30 | | | |
|---|---|---|---|
| $N_i$ = 0 | E = -878.480009032 | | |
| C | -4.6125 | -0.5882 | 0 |
| C | -4.2653 | 0.7623 | 0 |
| C | -2.931 | 1.1289 | 0 |
| C | -1.9186 | 0.1624 | 0 |
| C | -2.2878 | -1.1886 | 0 |
| C | -3.6196 | -1.5646 | 0 |
| C | -0.4987 | 0.5466 | 0 |
| C | -0.0076 | 1.8104 | 0 |
| C | 1.4073 | 2.0766 | 0 |
| O | 1.8684 | 3.23 | 0 |
| C | 2.2608 | 0.8905 | 0 |
| C | 3.6623 | 0.9583 | 0 |
| C | 4.4278 | -0.184 | 0 |
| C | 3.7972 | -1.4402 | 0 |
| O | 4.5107 | -2.5939 | 0 |
| C | 2.4168 | -1.5438 | 0 |
| C | 1.6699 | -0.3732 | 0 |
| O | 0.3176 | -0.5282 | 0 |
| O | -5.9087 | -1.0033 | 0 |
| H | -1.5276 | -1.9588 | 0 |
| H | -3.8988 | -2.6116 | 0 |
| H | -0.6783 | 2.6579 | 0 |
| H | 4.1381 | 1.9317 | 0 |
| H | 5.511 | -0.1303 | 0 |
| H | 5.4536 | -2.3979 | 0 |
| H | 1.9266 | -2.5091 | 0 |
| H | -2.6924 | 2.185 | 0 |
| H | -5.0428 | 1.5188 | 0 |
| H | -6.4997 | -0.2425 | 0 |

**Table S4.** (cont.)

| Compound 31 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -878.470935916 | | |
| C | -4.7621 | -0.1549 | -0.184 |
| C | -3.9301 | -1.1163 | 0.3624 |
| C | -2.5528 | -0.9089 | 0.4246 |
| C | -2.0028 | 0.2896 | -0.0651 |
| C | -2.8669 | 1.2451 | -0.6189 |
| C | -4.2321 | 1.0345 | -0.6812 |
| C | -0.5656 | 0.5943 | 0.0032 |
| C | -0.0391 | 1.8234 | 0.2038 |
| C | 1.3849 | 2.0465 | 0.2341 |
| O | 1.8806 | 3.1673 | 0.3988 |
| C | 2.2127 | 0.8412 | 0.0699 |
| C | 3.6119 | 0.8821 | 0.0967 |
| C | 4.3325 | -0.2842 | -0.0621 |
| C | 3.6811 | -1.5059 | -0.2522 |
| C | 2.3007 | -1.5683 | -0.2821 |
| O | 1.6906 | -2.7682 | -0.4709 |
| C | 1.5752 | -0.3811 | -0.1146 |
| O | 0.2161 | -0.4974 | -0.1595 |
| H | -5.83 | -0.3364 | -0.2259 |
| H | -4.3293 | -2.0446 | 0.754 |
| O | -1.8278 | -1.9031 | 1.0081 |
| H | -2.4461 | 2.1595 | -1.0204 |
| H | -4.8778 | 1.785 | -1.1202 |
| H | -0.6973 | 2.667 | 0.3607 |
| H | 4.1081 | 1.8334 | 0.2425 |
| H | 5.4155 | -0.2613 | -0.0432 |
| H | 4.2454 | -2.422 | -0.3819 |
| H | 0.734 | -2.6621 | -0.514 |
| H | -0.8834 | -1.7304 | 0.9288 |

| Compound 32 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -878.473366613 | | |
| C | -4.5684 | 0.16 | 0.1701 |
| C | -3.7381 | -0.8743 | -0.2535 |
| C | -2.3599 | -0.7011 | -0.2944 |
| C | -1.8074 | 0.5245 | 0.0771 |
| C | -2.6336 | 1.5676 | 0.5036 |
| C | -4.0071 | 1.374 | 0.547 |
| C | -0.3468 | 0.7089 | 0.011 |
| C | 0.2927 | 1.8889 | -0.1624 |
| C | 1.7311 | 1.9746 | -0.2141 |
| O | 2.3312 | 3.0465 | -0.3632 |
| C | 2.4385 | 0.6914 | -0.0883 |
| C | 3.8352 | 0.5875 | -0.1286 |
| C | 4.4314 | -0.651 | -0.0066 |
| C | 3.6592 | -1.8065 | 0.1551 |
| C | 2.2814 | -1.7245 | 0.1957 |
| O | 1.5367 | -2.8509 | 0.354 |
| C | 1.6815 | -0.464 | 0.0719 |
| O | 0.3229 | -0.4527 | 0.1279 |
| H | -5.6426 | 0.0108 | 0.2028 |
| O | -4.2272 | -2.0892 | -0.6453 |
| H | -2.2109 | 2.5136 | 0.8181 |
| H | -4.6524 | 2.1764 | 0.8852 |
| H | -0.2822 | 2.7971 | -0.2813 |
| H | 4.427 | 1.4854 | -0.2552 |
| H | 5.5108 | -0.7395 | -0.0357 |
| H | 4.1279 | -2.7789 | 0.2516 |
| H | 0.5979 | -2.6292 | 0.3617 |
| H | -1.7334 | -1.5182 | -0.6305 |
| H | -5.189 | -2.0833 | -0.6054 |

**Table S4.** (cont.)

| Compound 33 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -878.475166208 | | |
| C | -4.4576 | -0.303 | -0.0127 |
| C | -4.0164 | 0.9711 | 0.3437 |
| C | -2.6605 | 1.2513 | 0.3466 |
| C | -1.7264 | 0.2721 | -0.0046 |
| C | -2.1857 | -1.0037 | -0.3533 |
| C | -3.5387 | -1.2908 | -0.3623 |
| C | -0.2892 | 0.5693 | -0.0152 |
| C | 0.2744 | 1.7998 | -0.1044 |
| C | 1.701 | 1.987 | -0.1034 |
| O | 2.2301 | 3.1055 | -0.1672 |
| C | 2.4963 | 0.7512 | -0.0346 |
| C | 3.8971 | 0.747 | -0.0456 |
| C | 4.5772 | -0.4523 | 0.0186 |
| C | 3.8853 | -1.6659 | 0.0936 |
| C | 2.5044 | -1.6818 | 0.1039 |
| O | 1.8381 | -2.8653 | 0.1736 |
| C | 1.8196 | -0.4608 | 0.0393 |
| O | 0.4629 | -0.546 | 0.0608 |
| O | -5.7763 | -0.6388 | -0.0325 |
| H | -1.4805 | -1.7777 | -0.6302 |
| H | -3.8938 | -2.2762 | -0.6398 |
| H | -0.3557 | 2.6745 | -0.1914 |
| H | 4.4269 | 1.6896 | -0.1053 |
| H | 5.6606 | -0.4637 | 0.0108 |
| H | 4.4195 | -2.6076 | 0.1431 |
| H | 0.8862 | -2.7098 | 0.1714 |
| H | -2.3338 | 2.2408 | 0.6431 |
| H | -4.7352 | 1.733 | 0.6249 |
| H | -6.3174 | 0.1106 | 0.238 |

| Compound 34 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -878.471785150 | | |
| C | -4.382 | 0.4438 | 0.2728 |
| C | -3.6732 | -0.6721 | -0.1321 |
| C | -2.274 | -0.6417 | -0.2045 |
| O | -1.7026 | -1.7971 | -0.648 |
| C | -1.5877 | 0.5348 | 0.1256 |
| C | -2.3215 | 1.6551 | 0.543 |
| C | -3.7014 | 1.6098 | 0.614 |
| C | -0.1225 | 0.6287 | 0.0315 |
| C | 0.5732 | 1.7487 | -0.2687 |
| C | 2.0142 | 1.7532 | -0.3193 |
| O | 2.6697 | 2.772 | -0.571 |
| C | 2.6497 | 0.4522 | -0.0691 |
| C | 4.0398 | 0.2725 | -0.1123 |
| C | 4.5902 | -0.9717 | 0.1145 |
| C | 3.7595 | -2.0662 | 0.3896 |
| C | 2.3876 | -1.916 | 0.4401 |
| C | 1.8502 | -0.653 | 0.2106 |
| O | 0.4896 | -0.5497 | 0.2796 |
| H | -5.4632 | 0.3885 | 0.3259 |
| O | -4.3483 | -1.8117 | -0.465 |
| H | -0.7542 | -1.7987 | -0.4675 |
| H | -1.7948 | 2.5572 | 0.8289 |
| H | -4.2557 | 2.4795 | 0.9448 |
| H | 0.0445 | 2.6658 | -0.4894 |
| H | 4.6687 | 1.1277 | -0.3294 |
| H | 5.6646 | -1.1061 | 0.0794 |
| H | 4.1943 | -3.0433 | 0.5651 |
| H | 1.7261 | -2.7472 | 0.6519 |
| H | -3.711 | -2.5009 | -0.6885 |

**Table S4.** (cont.)

| Compound 35 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -878.476712717 | | |
| C | 4.3068 | -0.0455 | -0.0777 |
| C | 3.5055 | -1.1211 | 0.2718 |
| C | 2.1214 | -0.9905 | 0.2791 |
| O | 1.4328 | -2.1002 | 0.6559 |
| C | 1.5188 | 0.2416 | -0.0556 |
| C | 2.3633 | 1.3014 | -0.4193 |
| C | 3.7362 | 1.1784 | -0.4368 |
| C | 0.0717 | 0.4681 | -0.0092 |
| C | -0.5338 | 1.6628 | 0.2029 |
| C | -1.9657 | 1.7978 | 0.2113 |
| O | -2.5354 | 2.8853 | 0.3793 |
| C | -2.712 | 0.5448 | 0.0283 |
| C | -4.1128 | 0.4922 | 0.0487 |
| C | -4.7687 | -0.7108 | -0.1124 |
| C | -4.0347 | -1.8901 | -0.2959 |
| C | -2.6538 | -1.8654 | -0.3206 |
| C | -2.0099 | -0.6425 | -0.1582 |
| O | -0.6442 | -0.6629 | -0.2005 |
| O | 5.6525 | -0.238 | -0.0648 |
| H | 0.487 | -1.9745 | 0.5064 |
| H | 1.9234 | 2.2469 | -0.7124 |
| H | 4.3657 | 2.0109 | -0.7293 |
| H | 0.0652 | 2.5433 | 0.3897 |
| H | -4.6659 | 1.4123 | 0.1956 |
| H | -5.8513 | -0.7465 | -0.0957 |
| H | -4.5522 | -2.8341 | -0.4208 |
| H | -2.0662 | -2.7644 | -0.4616 |
| H | 3.9506 | -2.0711 | 0.5419 |
| H | 6.1046 | 0.5761 | -0.3115 |

| Compound 36 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -878.471699745 | | |
| C | -4.3355 | -0.6227 | 0.0414 |
| C | -3.4221 | -1.6067 | 0.3745 |
| C | -2.0529 | -1.3524 | 0.3655 |
| O | -1.246 | -2.3934 | 0.7355 |
| C | -1.5946 | -0.0672 | 0.026 |
| C | -2.5296 | 0.9166 | -0.3232 |
| C | -3.8849 | 0.6463 | -0.3162 |
| C | -0.1703 | 0.3029 | 0.0538 |
| C | 0.3125 | 1.5354 | 0.3331 |
| C | 1.727 | 1.812 | 0.3323 |
| O | 2.1877 | 2.9354 | 0.5711 |
| C | 2.5871 | 0.6557 | 0.0461 |
| C | 3.9863 | 0.7444 | 0.033 |
| C | 4.7542 | -0.3722 | -0.2236 |
| C | 4.1367 | -1.6053 | -0.4728 |
| C | 2.7602 | -1.7193 | -0.4681 |
| C | 2.0016 | -0.5816 | -0.2087 |
| O | 0.6443 | -0.7381 | -0.2234 |
| H | -0.3274 | -2.1997 | 0.5133 |
| H | -2.1925 | 1.9024 | -0.6203 |
| O | -4.7414 | 1.6568 | -0.6757 |
| H | -0.37 | 2.3369 | 0.5799 |
| H | 4.4488 | 1.7043 | 0.2297 |
| H | 5.8349 | -0.2988 | -0.2322 |
| H | 4.7423 | -2.4814 | -0.6728 |
| H | 2.2619 | -2.6619 | -0.6589 |
| H | -3.7624 | -2.5983 | 0.6487 |
| H | -5.3983 | -0.8407 | 0.0476 |
| H | -5.6486 | 1.3363 | -0.6521 |

**Table S4.** (cont.)

| Compound 37 | | | |
|---|---|---|---|
| $N_i$ = 0 | E = -878.471241770 | | |
| C | 4.5025 | -0.5545 | -0.0392 |
| C | 3.6258 | -1.495 | 0.4773 |
| C | 2.2621 | -1.2245 | 0.4965 |
| O | 1.4676 | -2.1887 | 1.0414 |
| C | 1.7616 | 0.0018 | 0.0155 |
| C | 2.6787 | 0.9287 | -0.514 |
| C | 4.0409 | 0.6533 | -0.5419 |
| C | 0.325 | 0.3143 | 0.0795 |
| C | -0.2188 | 1.4753 | 0.5027 |
| C | -1.6472 | 1.6721 | 0.5449 |
| O | -2.1626 | 2.7322 | 0.9215 |
| C | -2.4471 | 0.5136 | 0.1266 |
| C | -3.8496 | 0.5271 | 0.1311 |
| C | -4.5594 | -0.5899 | -0.2563 |
| C | -3.88 | -1.7484 | -0.657 |
| C | -2.4997 | -1.7884 | -0.6694 |
| C | -1.7987 | -0.6517 | -0.2761 |
| O | -0.4354 | -0.7358 | -0.3127 |
| H | 0.5385 | -2.0329 | 0.8354 |
| O | 2.1895 | 2.0926 | -1.0153 |
| H | 0.4283 | 2.2789 | 0.8246 |
| H | -4.3605 | 1.4293 | 0.446 |
| H | -5.6426 | -0.575 | -0.2509 |
| H | -4.4404 | -2.6251 | -0.96 |
| H | -1.9545 | -2.6733 | -0.9742 |
| H | 3.9777 | -2.4428 | 0.8653 |
| H | 5.5651 | -0.768 | -0.058 |
| H | 4.7236 | 1.3843 | -0.9605 |
| H | 2.9141 | 2.6194 | -1.3687 |

| Compound 38 | | | |
|---|---|---|---|
| $N_i$ = 0 | E = -878.475193551 | | |
| C | 4.1157 | 0.1607 | -0.1023 |
| C | 3.3189 | -0.9491 | 0.2038 |
| O | 3.8867 | -2.1592 | 0.4862 |
| C | 1.9429 | -0.8261 | 0.2271 |
| C | 1.3399 | 0.4063 | -0.0499 |
| C | 2.1394 | 1.5058 | -0.3662 |
| C | 3.5207 | 1.3804 | -0.3908 |
| C | -0.1243 | 0.5308 | -0.0023 |
| C | -0.8123 | 1.6861 | 0.1739 |
| C | -2.2497 | 1.7151 | 0.1979 |
| O | -2.8976 | 2.7616 | 0.3478 |
| C | -2.8989 | 0.4061 | 0.0474 |
| C | -4.2926 | 0.2507 | 0.0644 |
| C | -4.8576 | -1.0001 | -0.0697 |
| C | -4.0372 | -2.1261 | -0.2237 |
| C | -2.6623 | -1.9999 | -0.2446 |
| C | -2.1068 | -0.7296 | -0.1083 |
| O | -0.7454 | -0.6558 | -0.1428 |
| O | 5.4609 | -0.0489 | -0.0999 |
| H | 4.8464 | -2.081 | 0.4301 |
| H | 1.3483 | -1.6959 | 0.477 |
| H | 1.6955 | 2.4618 | -0.6135 |
| H | 4.1478 | 2.229 | -0.6422 |
| H | -0.2786 | 2.6157 | 0.3163 |
| H | -4.9127 | 1.131 | 0.1853 |
| H | -5.9347 | -1.1156 | -0.0558 |
| H | -4.4829 | -3.1085 | -0.3283 |
| H | -2.0111 | -2.8572 | -0.363 |
| H | 5.9311 | 0.7729 | -0.2777 |

**Table S4.** (cont.)

| Compound 39 | | | |
|---|---|---|---|
| $N_i$ = 0 | E = -878.476571497 | | |
| C | 4.178 | 0.352 | -0.0156 |
| C | 3.2867 | 1.3751 | 0.2889 |
| O | 3.7187 | 2.6342 | 0.5916 |
| C | 1.9147 | 1.1528 | 0.3 |
| C | 1.4348 | -0.1236 | 0.0104 |
| C | 2.3105 | -1.1629 | -0.3013 |
| C | 3.6773 | -0.9122 | -0.311 |
| C | -0.019 | -0.3758 | 0.0466 |
| C | -0.597 | -1.5724 | 0.3014 |
| C | -2.029 | -1.7299 | 0.3214 |
| O | -2.5803 | -2.8172 | 0.5389 |
| C | -2.7892 | -0.4981 | 0.076 |
| C | -4.1916 | -0.4685 | 0.0774 |
| C | -4.8653 | 0.7118 | -0.1546 |
| C | -4.1477 | 1.8922 | -0.3935 |
| C | -2.7672 | 1.8902 | -0.4006 |
| C | -2.1008 | 0.6897 | -0.1639 |
| O | -0.738 | 0.7373 | -0.1867 |
| H | 4.6806 | 2.6654 | 0.5721 |
| H | 1.2441 | 1.9651 | 0.5474 |
| H | 1.952 | -2.1523 | -0.5551 |
| O | 4.5018 | -1.9532 | -0.6279 |
| H | 0.0214 | -2.4339 | 0.5132 |
| H | -4.731 | -1.3895 | 0.2647 |
| H | -5.9484 | 0.73 | -0.1527 |
| H | -4.6792 | 2.8189 | -0.5761 |
| H | -2.1948 | 2.791 | -0.5847 |
| H | 5.2477 | 0.5377 | -0.0279 |
| H | 5.4195 | -1.6623 | -0.6188 |

| Compound 40 | | | |
|---|---|---|---|
| $N_i$ = 0 | E = -953.699757227 | | |
| C | 5.288 | -0.7373 | 0.0084 |
| C | 4.3881 | -1.6111 | -0.5946 |
| C | 3.0293 | -1.3291 | -0.5849 |
| C | 2.5589 | -0.1596 | 0.0222 |
| C | 3.4653 | 0.7128 | 0.6314 |
| C | 4.8231 | 0.4198 | 0.6246 |
| C | 1.1155 | 0.1224 | 0.0199 |
| C | 0.5294 | 1.3434 | -0.0929 |
| C | -0.9053 | 1.4817 | -0.112 |
| O | -1.4232 | 2.6131 | -0.2277 |
| C | -1.6654 | 0.261 | -0.0074 |
| C | -3.0748 | 0.2633 | -0.0116 |
| C | -3.7621 | -0.9382 | 0.0835 |
| C | -3.0557 | -2.1359 | 0.1843 |
| C | -1.6726 | -2.1619 | 0.1915 |
| C | -0.9881 | -0.9578 | 0.0941 |
| O | 0.3683 | -1.0011 | 0.1092 |
| O | 1.2572 | 2.4829 | -0.2219 |
| O | -3.7905 | 1.408 | -0.1011 |
| O | -5.1294 | -0.976 | 0.0837 |
| H | 6.3491 | -0.9599 | 0.001 |
| H | 4.7449 | -2.5143 | -1.076 |
| H | 2.332 | -2.0106 | -1.0573 |
| H | 3.1105 | 1.6091 | 1.1232 |
| H | 5.5188 | 1.0977 | 1.1056 |
| H | -3.617 | -3.0602 | 0.2576 |
| H | -1.1258 | -3.0923 | 0.2698 |
| H | 0.6194 | 3.2058 | -0.3235 |
| H | -3.1553 | 2.1506 | -0.1713 |
| H | -5.4767 | -0.081 | -0.0059 |

**Table S4.** (cont.)

| Compound 41 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.707189124 | | |
| C | -5.1419 | -1.0033 | 0.0032 |
| C | -4.1807 | -1.7787 | -0.6386 |
| C | -2.849 | -1.3874 | -0.6295 |
| C | -2.468 | -0.2068 | 0.0169 |
| C | -3.4354 | 0.5671 | 0.6638 |
| C | -4.7653 | 0.1658 | 0.6559 |
| C | -1.0526 | 0.1919 | 0.0158 |
| C | -0.5648 | 1.4525 | -0.0755 |
| C | 0.861 | 1.6993 | -0.0968 |
| O | 1.2825 | 2.8737 | -0.1904 |
| C | 1.707 | 0.545 | -0.0206 |
| C | 3.1222 | 0.6356 | -0.0335 |
| C | 3.8962 | -0.5033 | 0.0415 |
| C | 3.2698 | -1.7528 | 0.1316 |
| C | 1.8878 | -1.8859 | 0.1449 |
| C | 1.1306 | -0.7292 | 0.0667 |
| O | -0.214 | -0.8759 | 0.0854 |
| O | -1.3749 | 2.5369 | -0.1799 |
| O | 3.7268 | 1.8372 | -0.1186 |
| O | 3.9974 | -2.892 | 0.2088 |
| H | -6.1812 | -1.3116 | -0.003 |
| H | -4.4684 | -2.6903 | -1.1496 |
| H | -2.104 | -1.9922 | -1.1327 |
| H | -3.149 | 1.4705 | 1.1864 |
| H | -5.5085 | 0.7673 | 1.1667 |
| H | 4.9774 | -0.4279 | 0.0294 |
| H | 1.416 | -2.8568 | 0.2149 |
| H | -0.7919 | 3.3071 | -0.2635 |
| H | 3.0269 | 2.5221 | -0.1658 |
| H | 4.9384 | -2.6863 | 0.2003 |

| Compound 42 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.698139027 | | |
| C | 5.0418 | 0.551 | 0.0197 |
| C | 4.5777 | -0.6164 | -0.5771 |
| C | 3.2188 | -0.9042 | -0.5911 |
| C | 2.3102 | -0.0159 | -0.0083 |
| C | 2.7802 | 1.1643 | 0.5791 |
| C | 4.1399 | 1.4407 | 0.5958 |
| C | 0.8665 | -0.2898 | -0.0128 |
| C | 0.2594 | -1.5011 | 0.0747 |
| C | -1.182 | -1.6189 | 0.0877 |
| O | -1.7082 | -2.7466 | 0.1766 |
| C | -1.9313 | -0.3888 | 0.0098 |
| C | -3.3437 | -0.3528 | 0.0144 |
| C | -3.9905 | 0.8655 | -0.0562 |
| C | -3.2559 | 2.0509 | -0.1299 |
| C | -1.8748 | 2.0458 | -0.1353 |
| C | -1.2234 | 0.8132 | -0.0646 |
| O | 0.1267 | 0.8439 | -0.0797 |
| O | 0.9647 | -2.655 | 0.1784 |
| O | -4.0701 | -1.4976 | 0.0815 |
| O | -1.1842 | 3.2231 | -0.2064 |
| H | 6.1036 | 0.7694 | 0.0327 |
| H | 5.2749 | -1.3068 | -1.0376 |
| H | 2.8657 | -1.8086 | -1.0688 |
| H | 2.0822 | 1.8594 | 1.0302 |
| H | 4.4959 | 2.3523 | 1.0618 |
| H | -5.0732 | 0.8954 | -0.0539 |
| H | -3.772 | 3.0025 | -0.1846 |
| H | 0.3136 | -3.3687 | 0.2618 |
| H | -3.4433 | -2.246 | 0.1284 |
| H | -0.2362 | 3.0485 | -0.2068 |

**Table S4.** (cont.)

| Compound 43 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.704142476 | | |
| C | 4.7926 | -0.9768 | -0.1208 |
| C | 3.8504 | -1.8173 | -0.7117 |
| C | 2.5156 | -1.4584 | -0.6939 |
| C | 2.087 | -0.2596 | -0.1019 |
| C | 3.0502 | 0.5849 | 0.4782 |
| C | 4.3944 | 0.2119 | 0.4651 |
| C | 0.6415 | 0.0127 | -0.0771 |
| C | 0.0211 | 1.2022 | -0.2677 |
| C | -1.4149 | 1.3258 | -0.2267 |
| O | -1.9486 | 2.4421 | -0.388 |
| C | -2.146 | 0.1023 | -0.0167 |
| C | -3.5613 | 0.0648 | 0.021 |
| C | -4.2144 | -1.1399 | 0.2084 |
| C | -3.4704 | -2.311 | 0.3597 |
| C | -2.0865 | -2.3114 | 0.3298 |
| C | -1.4404 | -1.0961 | 0.1411 |
| O | -0.0848 | -1.1132 | 0.1247 |
| O | 0.7353 | 2.3339 | -0.5227 |
| O | -4.2824 | 1.1968 | -0.1258 |
| O | 2.7488 | 1.7461 | 1.1276 |
| H | 5.8424 | -1.2471 | -0.1212 |
| H | 4.1565 | -2.7442 | -1.1812 |
| H | 1.7768 | -2.1087 | -1.1467 |
| H | 5.1153 | 0.8766 | 0.9267 |
| H | -5.2968 | -1.1598 | 0.2349 |
| H | -3.9939 | -3.2488 | 0.5053 |
| H | -1.5085 | -3.2184 | 0.4482 |
| H | 0.108 | 3.0731 | -0.5527 |
| H | -3.657 | 1.939 | -0.2541 |
| H | 1.9982 | 2.1883 | 0.6937 |

| Compound 44 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.704664175 | | |
| C | -4.6371 | -0.9405 | -0.2167 |
| C | -3.6932 | -1.8248 | -0.7245 |
| C | -2.3392 | -1.5281 | -0.6691 |
| C | -1.9223 | -0.3187 | -0.1026 |
| C | -2.862 | 0.5735 | 0.4136 |
| C | -4.2142 | 0.2559 | 0.3551 |
| C | -0.4857 | -0.0056 | -0.0542 |
| C | 0.0851 | 1.2178 | -0.1917 |
| C | 1.5208 | 1.3758 | -0.1623 |
| O | 2.0205 | 2.5121 | -0.3022 |
| C | 2.2941 | 0.1739 | 0.0152 |
| C | 3.7102 | 0.1846 | 0.0601 |
| C | 4.4037 | -1.0004 | 0.2248 |
| C | 3.7001 | -2.2003 | 0.3462 |
| C | 2.3178 | -2.2481 | 0.3076 |
| C | 1.6304 | -1.0514 | 0.1414 |
| O | 0.2786 | -1.1129 | 0.1103 |
| O | -0.6481 | 2.3411 | -0.3934 |
| O | 4.3915 | 1.3447 | -0.0556 |
| O | -5.0932 | 1.1625 | 0.8809 |
| H | -5.6962 | -1.1726 | -0.2598 |
| H | -4.0224 | -2.7557 | -1.1715 |
| H | -1.6123 | -2.2215 | -1.0722 |
| H | -2.5579 | 1.5044 | 0.8738 |
| H | 5.4861 | -0.9832 | 0.2576 |
| H | 4.2554 | -3.1223 | 0.4742 |
| H | 1.7709 | -3.1771 | 0.4015 |
| H | -0.0131 | 3.0659 | -0.5001 |
| H | 3.7395 | 2.0663 | -0.172 |
| H | -5.9943 | 0.8353 | 0.7903 |

**Table S4.** (cont.)

| Compound 45 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.706366441 | | |
| C | -4.6447 | -0.3762 | -0.0035 |
| C | -4.1044 | 0.7697 | 0.5756 |
| C | -2.731 | 0.956 | 0.5824 |
| C | -1.8793 | 0.0018 | 0.0183 |
| C | -2.4383 | -1.1512 | -0.5478 |
| C | -3.8084 | -1.3396 | -0.5652 |
| C | -0.4234 | 0.1745 | 0.0205 |
| C | 0.2607 | 1.3438 | -0.0885 |
| C | 1.7017 | 1.3655 | -0.0979 |
| O | 2.3077 | 2.4538 | -0.2108 |
| C | 2.3629 | 0.0886 | 0.0068 |
| C | 3.7738 | -0.0368 | 0.0038 |
| C | 4.356 | -1.2874 | 0.1004 |
| C | 3.5456 | -2.4202 | 0.1972 |
| C | 2.1645 | -2.3354 | 0.1996 |
| C | 1.5903 | -1.073 | 0.1031 |
| O | 0.2378 | -1.0053 | 0.1141 |
| O | -0.374 | 2.5378 | -0.2236 |
| O | 4.5589 | 1.0584 | -0.0898 |
| O | -5.9869 | -0.6068 | -0.0443 |
| H | -4.7598 | 1.5098 | 1.0224 |
| H | -2.3239 | 1.8441 | 1.0473 |
| H | -1.7949 | -1.903 | -0.9886 |
| H | -4.2399 | -2.227 | -1.0129 |
| H | 5.4357 | -1.3729 | 0.0989 |
| H | 4.0141 | -3.3946 | 0.2726 |
| H | 1.5342 | -3.2119 | 0.273 |
| H | 0.318 | 3.2092 | -0.321 |
| H | 3.9732 | 1.8407 | -0.1587 |
| H | -6.46 | 0.1202 | 0.3742 |

| Compound 46 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.700078213 | | |
| C | 5.1674 | -1.2334 | 0.0203 |
| C | 4.1519 | -1.9567 | -0.5984 |
| C | 2.8505 | -1.4739 | -0.5968 |
| C | 2.5533 | -0.2537 | 0.0202 |
| C | 3.5754 | 0.4667 | 0.6449 |
| C | 4.8746 | -0.0251 | 0.6437 |
| C | 1.1678 | 0.2409 | 0.0125 |
| C | 0.7656 | 1.5326 | -0.0884 |
| C | -0.6379 | 1.8933 | -0.1192 |
| O | -0.9582 | 3.0891 | -0.227 |
| C | -1.5688 | 0.7905 | -0.0364 |
| C | -2.9643 | 0.9816 | -0.0552 |
| C | -3.8062 | -0.095 | 0.0208 |
| C | -3.2767 | -1.4068 | 0.1155 |
| C | -1.9162 | -1.6132 | 0.1321 |
| C | -1.0705 | -0.5074 | 0.0561 |
| O | 0.2594 | -0.7627 | 0.0855 |
| O | 1.6534 | 2.5546 | -0.2035 |
| O | -5.168 | -0.0236 | 0.0148 |
| O | -4.1104 | -2.4692 | 0.1919 |
| H | 6.1832 | -1.6122 | 0.0191 |
| H | 4.3737 | -2.8991 | -1.0861 |
| H | 2.0644 | -2.0385 | -1.0836 |
| H | 3.3551 | 1.4007 | 1.145 |
| H | 5.6593 | 0.537 | 1.1371 |
| H | -3.3681 | 1.9851 | -0.1281 |
| H | -1.5098 | -2.6139 | 0.2064 |
| H | 1.1207 | 3.3598 | -0.2994 |
| H | -5.4592 | 0.8937 | -0.0159 |
| H | -5.0252 | -2.1605 | 0.1804 |

**Table S4.** (cont.)

| Compound 47 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.697011491 | | |
| C | 5.0543 | -0.938 | 0.004 |
| C | 4.7103 | 0.2692 | -0.5949 |
| C | 3.3887 | 0.6969 | -0.6028 |
| C | 2.396 | -0.0886 | -0.0098 |
| C | 2.7447 | -1.3082 | 0.5813 |
| C | 4.0681 | -1.7257 | 0.5906 |
| C | 0.987 | 0.3311 | -0.0094 |
| C | 0.5065 | 1.599 | 0.0849 |
| C | -0.9138 | 1.8798 | 0.1085 |
| O | -1.3043 | 3.0519 | 0.2057 |
| C | -1.7937 | 0.723 | 0.0302 |
| C | -3.1903 | 0.8411 | 0.0454 |
| C | -3.9571 | -0.3021 | -0.032 |
| C | -3.3611 | -1.5702 | -0.1181 |
| C | -1.9894 | -1.6926 | -0.1285 |
| C | -1.2027 | -0.5313 | -0.056 |
| O | 0.1369 | -0.7171 | -0.0815 |
| O | 1.3334 | 2.6705 | 0.1932 |
| O | -5.3157 | -0.1654 | -0.0207 |
| O | -1.4265 | -2.9243 | -0.207 |
| H | 6.0875 | -1.2664 | 0.0109 |
| H | 5.4726 | 0.881 | -1.0634 |
| H | 3.1292 | 1.631 | -1.0833 |
| H | 1.9808 | -1.9241 | 1.0411 |
| H | 4.3299 | -2.6677 | 1.0588 |
| H | -3.6542 | 1.8166 | 0.1151 |
| H | -3.9746 | -2.4628 | -0.1735 |
| H | 0.757 | 3.4461 | 0.2797 |
| H | -5.7384 | -1.0282 | -0.0827 |
| H | -0.4649 | -2.8514 | -0.1814 |

| Compound 48 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.699831399 | | |
| C | 4.773 | -1.3035 | -0.0733 |
| C | 3.767 | -2.0472 | -0.6882 |
| C | 2.4721 | -1.5624 | -0.6933 |
| C | 2.148 | -0.3324 | -0.1 |
| C | 3.1753 | 0.413 | 0.5049 |
| C | 4.478 | -0.0854 | 0.5137 |
| C | 0.7342 | 0.0761 | -0.0972 |
| C | 0.2355 | 1.321 | -0.3011 |
| C | -1.1799 | 1.6054 | -0.2779 |
| O | -1.58 | 2.7659 | -0.444 |
| C | -2.0387 | 0.4493 | -0.0729 |
| C | -3.437 | 0.5582 | -0.0514 |
| C | -4.206 | -0.569 | 0.1373 |
| C | -3.5949 | -1.8242 | 0.3057 |
| C | -2.224 | -1.9432 | 0.2866 |
| C | -1.4467 | -0.8005 | 0.0967 |
| O | -0.0983 | -0.9699 | 0.0978 |
| O | 1.0715 | 2.3706 | -0.5456 |
| O | -5.5646 | -0.4281 | 0.1547 |
| O | 2.9706 | 1.5937 | 1.1571 |
| H | 5.7923 | -1.6723 | -0.0558 |
| H | 3.9926 | -2.9965 | -1.1585 |
| H | 1.6839 | -2.1362 | -1.166 |
| H | 5.2497 | 0.5046 | 0.9942 |
| H | -3.9031 | 1.5269 | -0.1847 |
| H | -4.2133 | -2.7032 | 0.4525 |
| H | -1.7419 | -2.9039 | 0.4175 |
| H | 0.521 | 3.1684 | -0.5909 |
| H | -5.9854 | -1.2842 | 0.2853 |
| H | 2.2757 | 2.1065 | 0.7079 |

**Table S4.** (cont.)

| Compound 49 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.700074784 | | |
| C | -4.6472 | -1.1755 | -0.1968 |
| C | -3.6432 | -1.9688 | -0.7394 |
| C | -2.3167 | -1.5646 | -0.6967 |
| C | -1.9887 | -0.3388 | -0.1076 |
| C | -2.9885 | 0.4621 | 0.4434 |
| C | -4.3117 | 0.0382 | 0.3962 |
| C | -0.5799 | 0.0861 | -0.0702 |
| C | -0.1095 | 1.3523 | -0.2142 |
| C | 1.3083 | 1.6422 | -0.2048 |
| O | 1.6978 | 2.8098 | -0.3556 |
| C | 2.1844 | 0.495 | -0.0308 |
| C | 3.5816 | 0.6244 | -0.0022 |
| C | 4.3665 | -0.495 | 0.1637 |
| C | 3.7741 | -1.763 | 0.3019 |
| C | 2.4057 | -1.9026 | 0.2738 |
| C | 1.6117 | -0.7673 | 0.1062 |
| O | 0.2679 | -0.9546 | 0.0901 |
| O | -0.9424 | 2.4068 | -0.4129 |
| O | 5.7233 | -0.3352 | 0.1909 |
| O | -5.2512 | 0.8596 | 0.9567 |
| H | -5.6846 | -1.4916 | -0.2294 |
| H | -3.9033 | -2.9133 | -1.2031 |
| H | -1.5428 | -2.1875 | -1.1269 |
| H | -2.7526 | 1.4039 | 0.9212 |
| H | 4.0335 | 1.6029 | -0.1098 |
| H | 4.4058 | -2.6352 | 0.4318 |
| H | 1.9378 | -2.8734 | 0.3803 |
| H | -0.3708 | 3.1813 | -0.5316 |
| H | 6.155 | -1.1884 | 0.3049 |
| H | -6.1243 | 0.4626 | 0.8735 |

| Compound 50 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.701694282 | | |
| C | -4.683 | -0.6328 | 0.0089 |
| C | -3.7691 | -1.526 | -0.5478 |
| C | -2.4198 | -1.2213 | -0.5369 |
| C | -1.9589 | -0.0204 | 0.0176 |
| C | -2.8878 | 0.8631 | 0.575 |
| C | -4.2407 | 0.5612 | 0.5738 |
| C | -0.5217 | 0.274 | 0.0151 |
| C | 0.0612 | 1.498 | -0.0985 |
| C | 1.4952 | 1.6603 | -0.1223 |
| O | 1.9854 | 2.7951 | -0.2405 |
| C | 2.2707 | 0.4349 | -0.0205 |
| C | 3.6736 | 0.4396 | -0.034 |
| C | 4.3601 | -0.7503 | 0.0632 |
| C | 3.6619 | -1.9661 | 0.1733 |
| C | 2.2856 | -1.9829 | 0.1848 |
| C | 1.5918 | -0.7763 | 0.0863 |
| O | 0.2363 | -0.8422 | 0.1078 |
| O | -0.6765 | 2.6336 | -0.2279 |
| O | 5.7261 | -0.711 | 0.0472 |
| O | -6.0009 | -0.9788 | -0.0236 |
| H | -4.1247 | -2.4508 | -0.9866 |
| H | -1.7168 | -1.9199 | -0.9742 |
| H | -2.5567 | 1.7873 | 1.0295 |
| H | -4.9551 | 1.2476 | 1.0155 |
| H | 4.2075 | 1.3783 | -0.1198 |
| H | 4.2176 | -2.8947 | 0.2474 |
| H | 1.7359 | -2.9122 | 0.2673 |
| H | -0.0355 | 3.3548 | -0.3287 |
| H | 6.0827 | -1.6016 | 0.1266 |
| H | -6.5339 | -0.2918 | 0.3905 |

**Table S4.** (cont.)

| Compound 51 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.696628343 | | |
| C | -4.8583 | -1.3446 | 0.002 |
| C | -3.7848 | -2.0269 | -0.5628 |
| C | -2.5174 | -1.4617 | -0.5565 |
| C | -2.3123 | -0.1986 | 0.011 |
| C | -3.3924 | 0.4797 | 0.5836 |
| C | -4.6572 | -0.0947 | 0.5776 |
| C | -0.9613 | 0.3805 | 0.0077 |
| C | -0.6258 | 1.6919 | -0.0749 |
| C | 0.7605 | 2.129 | -0.0991 |
| O | 1.0116 | 3.3399 | -0.1902 |
| C | 1.756 | 1.08 | -0.0312 |
| C | 3.1383 | 1.3272 | -0.0438 |
| C | 4.0286 | 0.2816 | 0.0121 |
| C | 3.5661 | -1.0408 | 0.0773 |
| C | 2.206 | -1.3126 | 0.0846 |
| C | 1.3134 | -0.2408 | 0.0365 |
| O | 0.0055 | -0.5719 | 0.0652 |
| O | -1.5627 | 2.6686 | -0.1754 |
| O | 4.4785 | -2.0437 | 0.1354 |
| O | 1.7992 | -2.6101 | 0.1466 |
| H | -5.8477 | -1.7879 | -0.0037 |
| H | -3.9344 | -3.0021 | -1.0116 |
| H | -1.6861 | -1.9968 | -0.9998 |
| H | -3.2443 | 1.4459 | 1.0473 |
| H | -5.4869 | 0.4361 | 1.0302 |
| H | 3.4915 | 2.3493 | -0.0974 |
| H | 5.098 | 0.4545 | 0.0067 |
| H | -1.0719 | 3.5021 | -0.253 |
| H | 4.0315 | -2.8972 | 0.1871 |
| H | 0.8369 | -2.6617 | 0.0964 |

| Compound 52 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.703406058 | | |
| C | -4.5621 | -1.6255 | -0.0869 |
| C | -3.4935 | -2.2481 | -0.7297 |
| C | -2.254 | -1.6352 | -0.7344 |
| C | -2.0489 | -0.3932 | -0.1135 |
| C | -3.1393 | 0.2295 | 0.5189 |
| C | -4.3852 | -0.3979 | 0.5271 |
| C | -0.685 | 0.1583 | -0.1104 |
| C | -0.3162 | 1.4488 | -0.2811 |
| C | 1.0701 | 1.8712 | -0.2499 |
| O | 1.3466 | 3.0726 | -0.3811 |
| C | 2.0329 | 0.8048 | -0.0824 |
| C | 3.4208 | 1.0304 | -0.061 |
| C | 4.3002 | -0.0125 | 0.0843 |
| C | 3.8071 | -1.3259 | 0.212 |
| C | 2.4484 | -1.5826 | 0.1957 |
| C | 1.5765 | -0.5097 | 0.0487 |
| O | 0.2546 | -0.8086 | 0.051 |
| O | -1.2504 | 2.418 | -0.4962 |
| O | 4.6418 | -2.3838 | 0.3555 |
| O | -3.0465 | 1.4082 | 1.2003 |
| H | -5.5383 | -2.0966 | -0.0694 |
| H | -3.6274 | -3.2041 | -1.2211 |
| H | -1.4172 | -2.1153 | -1.2274 |
| H | -5.2067 | 0.0993 | 1.0296 |
| H | 3.7874 | 2.0447 | -0.1632 |
| H | 5.3711 | 0.1576 | 0.1005 |
| H | 2.0664 | -2.5906 | 0.2958 |
| H | -0.7805 | 3.2669 | -0.5182 |
| H | 5.5589 | -2.0885 | 0.352 |
| H | -2.4126 | 2.0011 | 0.7595 |

**Table S4.** (cont.)

| Compound 53 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.703612755 | | |
| C | 4.4682 | -1.4364 | -0.2105 |
| C | 3.3898 | -2.1437 | -0.7284 |
| C | 2.1059 | -1.6207 | -0.6785 |
| C | 1.8955 | -0.3612 | -0.1058 |
| C | 2.9712 | 0.3531 | 0.4219 |
| C | 4.2503 | -0.1888 | 0.3663 |
| C | 0.5324 | 0.1916 | -0.0638 |
| C | 0.176 | 1.495 | -0.1717 |
| C | -1.2176 | 1.905 | -0.161 |
| O | -1.4975 | 3.1084 | -0.2779 |
| C | -2.1836 | 0.8375 | -0.0307 |
| C | -3.5716 | 1.065 | -0.011 |
| C | -4.4534 | 0.0209 | 0.1062 |
| C | -3.963 | -1.2963 | 0.2069 |
| C | -2.6052 | -1.5553 | 0.1896 |
| C | -1.7305 | -0.4803 | 0.0696 |
| O | -0.411 | -0.7783 | 0.0612 |
| O | 1.0927 | 2.4826 | -0.3343 |
| O | -4.8009 | -2.3556 | 0.3245 |
| O | 5.2665 | 0.5526 | 0.9046 |
| H | 5.4722 | -1.846 | -0.2492 |
| H | 3.5575 | -3.1154 | -1.1785 |
| H | 1.2745 | -2.1788 | -1.0896 |
| H | 2.8284 | 1.3183 | 0.8889 |
| H | -3.9363 | 2.0822 | -0.09 |
| H | -5.5241 | 0.1925 | 0.1217 |
| H | -2.2254 | -2.566 | 0.2671 |
| H | 0.5865 | 3.3047 | -0.4305 |
| H | -5.7172 | -2.0579 | 0.3245 |
| H | 6.0993 | 0.0775 | 0.8167 |

| Compound 54 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.705068250 | | |
| C | -4.5536 | -0.8237 | 0.0019 |
| C | -3.582 | -1.6285 | -0.5899 |
| C | -2.258 | -1.2271 | -0.5736 |
| C | -1.8814 | -0.0168 | 0.022 |
| C | -2.8672 | 0.7759 | 0.6165 |
| C | -4.1949 | 0.3769 | 0.61 |
| C | -0.4701 | 0.384 | 0.0184 |
| C | 0.0211 | 1.6445 | -0.082 |
| C | 1.4457 | 1.9069 | -0.1139 |
| O | 1.8476 | 3.0777 | -0.2199 |
| C | 2.2994 | 0.7419 | -0.0365 |
| C | 3.7031 | 0.8225 | -0.0633 |
| C | 4.4745 | -0.3098 | 0.0117 |
| C | 3.8521 | -1.5689 | 0.117 |
| C | 2.4747 | -1.6845 | 0.1424 |
| C | 1.714 | -0.5227 | 0.063 |
| O | 0.3704 | -0.6815 | 0.0947 |
| O | -0.7941 | 2.7274 | -0.1927 |
| O | 4.5785 | -2.711 | 0.1954 |
| O | -5.845 | -1.2586 | -0.0389 |
| H | -3.8728 | -2.5601 | -1.061 |
| H | -1.5094 | -1.8562 | -1.0398 |
| H | -2.6001 | 1.7047 | 1.1034 |
| H | -4.9554 | 0.9921 | 1.0792 |
| H | 4.1698 | 1.7968 | -0.145 |
| H | 5.557 | -0.2501 | -0.0101 |
| H | 1.9941 | -2.6512 | 0.2222 |
| H | -0.205 | 3.4924 | -0.2878 |
| H | 5.5192 | -2.5054 | 0.1757 |
| H | -6.4209 | -0.6178 | 0.3918 |

**Table S4.** (cont.)

| Compound 55 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.697822379 | | |
| C | 4.4911 | -1.2931 | -0.1333 |
| C | 4.2455 | -0.0719 | 0.4693 |
| C | 2.9606 | 0.4708 | 0.4831 |
| C | 1.9018 | -0.232 | -0.1188 |
| C | 2.1753 | -1.468 | -0.7261 |
| C | 3.4525 | -1.9968 | -0.7411 |
| C | 0.5051 | 0.2265 | -0.1008 |
| C | 0.0402 | 1.4882 | -0.2716 |
| C | -1.37 | 1.8131 | -0.23 |
| O | -1.7332 | 2.9886 | -0.3587 |
| C | -2.2667 | 0.6794 | -0.0577 |
| C | -3.664 | 0.8119 | -0.0314 |
| C | -4.4477 | -0.3109 | 0.1198 |
| C | -3.8688 | -1.5811 | 0.2434 |
| C | -2.4981 | -1.7311 | 0.2177 |
| C | -1.7003 | -0.5855 | 0.0698 |
| O | -0.3643 | -0.797 | 0.0697 |
| O | 0.903 | 2.5178 | -0.4981 |
| O | -1.9444 | -2.9667 | 0.3341 |
| O | 2.8046 | 1.6479 | 1.1537 |
| H | 5.4974 | -1.6962 | -0.1333 |
| H | 5.043 | 0.486 | 0.9462 |
| H | 1.3618 | -2.0105 | -1.1932 |
| H | 3.6395 | -2.9493 | -1.2219 |
| H | -4.1037 | 1.796 | -0.1333 |
| H | -5.527 | -0.2206 | 0.1418 |
| H | -4.4882 | -2.4631 | 0.3582 |
| H | 0.3787 | 3.334 | -0.5177 |
| H | -0.9838 | -2.9079 | 0.266 |
| H | 2.1169 | 2.1893 | 0.7274 |

| Compound 56 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.698175129 | | |
| C | 4.3651 | -1.1852 | 0.2298 |
| C | 4.0916 | 0.0582 | -0.3326 |
| C | 2.7879 | 0.5373 | -0.3934 |
| C | 1.7444 | -0.237 | 0.1133 |
| C | 2.0105 | -1.4929 | 0.671 |
| C | 3.3182 | -1.9522 | 0.7271 |
| C | 0.3558 | 0.2446 | 0.0627 |
| C | -0.0764 | 1.5275 | 0.167 |
| C | -1.4885 | 1.8616 | 0.1465 |
| O | -1.8361 | 3.0448 | 0.2592 |
| C | -2.4065 | 0.7414 | 0.0109 |
| C | -3.8018 | 0.8987 | -0.0201 |
| C | -4.6054 | -0.2127 | -0.1454 |
| C | -4.0497 | -1.4965 | -0.2377 |
| C | -2.6824 | -1.6707 | -0.2054 |
| C | -1.8638 | -0.5362 | -0.0825 |
| O | -0.5338 | -0.7688 | -0.0669 |
| O | 0.7844 | 2.5621 | 0.3339 |
| O | -2.1508 | -2.9189 | -0.2905 |
| O | 5.0736 | 0.8582 | -0.8495 |
| H | 5.3876 | -1.5453 | 0.2736 |
| H | 2.6022 | 1.5006 | -0.8487 |
| H | 1.2037 | -2.0976 | 1.0651 |
| H | 3.5296 | -2.9206 | 1.1657 |
| H | -4.2239 | 1.8929 | 0.055 |
| H | -5.6828 | -0.1033 | -0.172 |
| H | -4.6853 | -2.3692 | -0.3329 |
| H | 0.2364 | 3.357 | 0.4283 |
| H | -1.1892 | -2.8749 | -0.2276 |
| H | 5.9294 | 0.4253 | -0.7643 |

**Table S4.** (cont.)

| Compound 57 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.699808922 | | |
| C | 4.4288 | -0.522 | 0.0084 |
| C | 4.001 | 0.6834 | -0.5433 |
| C | 2.6512 | 0.9983 | -0.5483 |
| C | 1.7108 | 0.1165 | -0.007 |
| C | 2.1573 | -1.0963 | 0.5344 |
| C | 3.5034 | -1.4136 | 0.5485 |
| C | 0.2776 | 0.4229 | -0.0083 |
| C | -0.3073 | 1.6469 | 0.0811 |
| C | -1.7453 | 1.8093 | 0.099 |
| O | -2.2308 | 2.9465 | 0.1926 |
| C | -2.5268 | 0.585 | 0.0216 |
| C | -3.9309 | 0.5748 | 0.0317 |
| C | -4.5998 | -0.6273 | -0.0389 |
| C | -3.8972 | -1.8378 | -0.1181 |
| C | -2.5183 | -1.847 | -0.1265 |
| C | -1.8378 | -0.6208 | -0.0566 |
| O | -0.489 | -0.6927 | -0.0777 |
| O | 0.4266 | 2.7853 | 0.1863 |
| O | -1.8435 | -3.0249 | -0.1997 |
| O | 5.7429 | -0.8803 | 0.0436 |
| H | 4.7243 | 1.3687 | -0.9722 |
| H | 2.3319 | 1.9312 | -0.9931 |
| H | 1.4458 | -1.795 | 0.9579 |
| H | 3.8479 | -2.3476 | 0.9767 |
| H | -4.4656 | 1.5143 | 0.0949 |
| H | -5.6829 | -0.6477 | -0.0332 |
| H | -4.4263 | -2.7821 | -0.1723 |
| H | -0.2155 | 3.508 | 0.2699 |
| H | -0.8927 | -2.8628 | -0.1956 |
| H | 6.2842 | -0.193 | -0.3592 |

| Compound 58 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.699565001 | | |
| C | 4.1406 | -1.3696 | -0.2878 |
| C | 3.8482 | -0.1493 | 0.2936 |
| C | 2.5304 | 0.326 | 0.3379 |
| C | 1.4992 | -0.443 | -0.2114 |
| C | 1.8081 | -1.6795 | -0.7989 |
| C | 3.1137 | -2.1332 | -0.8378 |
| C | 0.0914 | -0.0214 | -0.1632 |
| C | -0.3946 | 1.2238 | -0.3823 |
| C | -1.8071 | 1.5273 | -0.3103 |
| O | -2.1985 | 2.6859 | -0.5007 |
| C | -2.6675 | 0.391 | -0.026 |
| C | -4.065 | 0.5107 | 0.0611 |
| C | -4.8403 | -0.5964 | 0.3203 |
| C | -4.2346 | -1.8507 | 0.4986 |
| C | -2.8657 | -1.9942 | 0.4194 |
| C | -2.0887 | -0.8652 | 0.1565 |
| O | -0.7459 | -1.0529 | 0.0962 |
| O | 0.4423 | 2.2544 | -0.6904 |
| O | 2.3581 | 1.5116 | 0.9939 |
| O | 4.8514 | 0.597 | 0.8404 |
| H | 5.1688 | -1.7116 | -0.3095 |
| H | 1.0109 | -2.2726 | -1.2292 |
| H | 3.3418 | -3.0863 | -1.2995 |
| H | -4.514 | 1.4865 | -0.0811 |
| H | -5.9174 | -0.5038 | 0.387 |
| H | -4.8487 | -2.72 | 0.703 |
| H | -2.3817 | -2.9534 | 0.5563 |
| H | -0.1021 | 3.0559 | -0.7473 |
| H | 1.7061 | 2.0587 | 0.5185 |
| H | 4.4691 | 1.4211 | 1.169 |

**Table S4.** (cont.)

| Compound 59 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.703022402 | | |
| C | -4.2051 | -0.779 | -0.0613 |
| C | -3.7945 | 0.4277 | 0.4833 |
| C | -2.4498 | 0.7837 | 0.4686 |
| C | -1.4913 | -0.0822 | -0.0947 |
| C | -1.9443 | -1.2935 | -0.6405 |
| C | -3.2769 | -1.6489 | -0.637 |
| C | -0.0452 | 0.1698 | -0.0856 |
| C | 0.5964 | 1.3487 | -0.2838 |
| C | 2.0347 | 1.4671 | -0.2476 |
| O | 2.5666 | 2.5743 | -0.4125 |
| C | 2.7534 | 0.2215 | -0.0381 |
| C | 4.1567 | 0.1572 | -0.0081 |
| C | 4.7905 | -1.0505 | 0.1774 |
| C | 4.034 | -2.2227 | 0.3364 |
| C | 2.6558 | -2.1855 | 0.3109 |
| C | 2.0234 | -0.9559 | 0.1234 |
| O | 0.667 | -0.9653 | 0.1175 |
| O | -0.1047 | 2.4903 | -0.5447 |
| O | -2.1387 | 1.9611 | 1.0779 |
| O | -5.5337 | -1.0699 | -0.0141 |
| H | -4.5165 | 1.1029 | 0.9264 |
| H | -1.222 | -1.9697 | -1.0813 |
| H | -3.6041 | -2.5867 | -1.0714 |
| H | 4.7232 | 1.072 | -0.1356 |
| H | 5.8723 | -1.1002 | 0.2005 |
| H | 4.5371 | -3.1716 | 0.4815 |
| H | 2.0566 | -3.0794 | 0.4325 |
| H | 0.5399 | 3.2154 | -0.5776 |
| H | -1.371 | 2.3721 | 0.6408 |
| H | -5.6954 | -1.9243 | -0.4283 |

| Compound 60 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.698926826 | | |
| C | 4.3377 | -0.4533 | 0.1774 |
| C | 3.8305 | 0.7429 | 0.6535 |
| C | 2.4686 | 1.0262 | 0.588 |
| C | 1.5973 | 0.0776 | 0.0295 |
| C | 2.1207 | -1.1288 | -0.4555 |
| C | 3.4764 | -1.3919 | -0.3864 |
| C | 0.1377 | 0.2571 | -0.031 |
| C | -0.5361 | 1.3859 | -0.358 |
| C | -1.9816 | 1.4447 | -0.3816 |
| O | -2.5497 | 2.5092 | -0.6581 |
| C | -2.6552 | 0.1919 | -0.0852 |
| C | -4.0554 | 0.0705 | -0.0937 |
| C | -4.6469 | -1.1414 | 0.1808 |
| C | -3.8505 | -2.2616 | 0.469 |
| C | -2.4752 | -2.1683 | 0.4845 |
| C | -1.8855 | -0.9345 | 0.2065 |
| O | -0.5304 | -0.8879 | 0.2441 |
| O | 0.1322 | 2.5263 | -0.6885 |
| O | 2.0525 | 2.2046 | 1.151 |
| O | 3.9231 | -2.589 | -0.886 |
| H | 5.4012 | -0.6597 | 0.2376 |
| H | 4.4914 | 1.4795 | 1.0949 |
| H | 1.4585 | -1.8662 | -0.8927 |
| H | -4.6531 | 0.9451 | -0.3212 |
| H | -5.726 | -1.2351 | 0.174 |
| H | -4.3207 | -3.2144 | 0.6825 |
| H | -1.8455 | -3.0212 | 0.706 |
| H | -0.5344 | 3.2221 | -0.8049 |
| H | 1.3332 | 2.587 | 0.6198 |
| H | 4.8784 | -2.6444 | -0.7839 |

**Table S4.** (cont.)

| Compound 61 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.698263633 | | |
| C | -4.463 | -0.8139 | 0.1396 |
| C | -3.573 | -1.6788 | -0.4785 |
| C | -2.2252 | -1.3504 | -0.5409 |
| C | -1.747 | -0.1384 | 0.0044 |
| C | -2.6816 | 0.7237 | 0.6152 |
| C | -4.0268 | 0.3827 | 0.6868 |
| C | -0.3123 | 0.1769 | -0.0396 |
| C | 0.2545 | 1.3598 | -0.3708 |
| C | 1.6894 | 1.5623 | -0.3636 |
| O | 2.1518 | 2.6742 | -0.6429 |
| C | 2.4796 | 0.387 | -0.0363 |
| C | 3.8842 | 0.4063 | -0.0193 |
| C | 4.5883 | -0.7385 | 0.2785 |
| C | 3.9033 | -1.9297 | 0.5657 |
| C | 2.5248 | -1.9744 | 0.5566 |
| C | 1.8232 | -0.8081 | 0.2553 |
| O | 0.4662 | -0.8937 | 0.2708 |
| O | -0.5162 | 2.4277 | -0.7129 |
| O | -1.4197 | -2.2438 | -1.1827 |
| O | -2.3126 | 1.8945 | 1.2144 |
| H | -5.5135 | -1.0758 | 0.192 |
| H | -3.9039 | -2.613 | -0.9152 |
| H | -4.7134 | 1.0673 | 1.169 |
| H | 4.3958 | 1.3339 | -0.247 |
| H | 5.6713 | -0.7237 | 0.2909 |
| H | 4.4621 | -2.8285 | 0.799 |
| H | 1.9786 | -2.8831 | 0.7774 |
| H | 0.0847 | 3.1785 | -0.8454 |
| H | -0.4904 | -2.0732 | -0.9917 |
| H | -1.6383 | 2.3466 | 0.6795 |

| Compound 62 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.699845708 | | |
| C | 4.0398 | -0.8026 | -0.1369 |
| C | 3.6192 | 0.4324 | 0.3689 |
| C | 2.2734 | 0.7459 | 0.4029 |
| C | 1.3249 | -0.1692 | -0.0671 |
| C | 1.7503 | -1.405 | -0.5611 |
| C | 3.1022 | -1.7155 | -0.5974 |
| C | -0.1084 | 0.1473 | -0.0415 |
| C | -0.679 | 1.3717 | -0.1893 |
| C | -2.1144 | 1.5487 | -0.1758 |
| O | -2.5933 | 2.6838 | -0.3233 |
| C | -2.8977 | 0.3374 | -0.0049 |
| C | -4.303 | 0.3452 | 0.0206 |
| C | -4.9993 | -0.8315 | 0.1776 |
| C | -4.305 | -2.0451 | 0.3126 |
| C | -2.9269 | -2.0791 | 0.2901 |
| C | -2.2307 | -0.8797 | 0.1303 |
| O | -0.8785 | -0.9568 | 0.1193 |
| O | 0.0627 | 2.4926 | -0.3899 |
| O | 4.5248 | 1.3421 | 0.8391 |
| O | 5.3839 | -1.026 | -0.1366 |
| H | 1.9768 | 1.7024 | 0.812 |
| H | 1.0303 | -2.1238 | -0.9306 |
| H | 3.44 | -2.6692 | -0.9887 |
| H | -4.8208 | 1.291 | -0.0865 |
| H | -6.0823 | -0.8254 | 0.1973 |
| H | -4.8572 | -2.9695 | 0.4357 |
| H | -2.3754 | -3.0055 | 0.3921 |
| H | -0.5756 | 3.2148 | -0.5009 |
| H | 5.4148 | 0.9829 | 0.747 |
| H | 5.5806 | -1.8877 | -0.5185 |

**Table S4.** (cont.)

| Compound 63 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.701525563 | | |
| C | -4.174 | -0.5267 | 0.0504 |
| C | -3.6828 | 0.6961 | 0.4934 |
| C | -2.3207 | 0.9739 | 0.475 |
| C | -1.4399 | 0.0011 | 0.0035 |
| C | -1.9122 | -1.2362 | -0.4386 |
| C | -3.2787 | -1.4844 | -0.4142 |
| C | 0.0107 | 0.2546 | -0.0211 |
| C | 0.6258 | 1.4375 | -0.2737 |
| C | 2.0711 | 1.5506 | -0.2947 |
| O | 2.5941 | 2.6469 | -0.5406 |
| C | 2.8028 | 0.3245 | -0.032 |
| C | 4.2078 | 0.2738 | -0.0169 |
| C | 4.8549 | -0.9152 | 0.2298 |
| C | 4.1112 | -2.0836 | 0.4652 |
| C | 2.7332 | -2.06 | 0.4561 |
| C | 2.0865 | -0.8482 | 0.2064 |
| O | 0.7327 | -0.868 | 0.2135 |
| O | -0.0696 | 2.5689 | -0.5505 |
| O | -4.5146 | 1.6697 | 0.9688 |
| O | -3.7057 | -2.7012 | -0.8643 |
| H | -5.2404 | -0.731 | 0.0663 |
| H | -1.9675 | 1.9276 | 0.8414 |
| H | -1.2366 | -1.9964 | -0.8086 |
| H | 4.7644 | 1.1847 | -0.2023 |
| H | 5.9373 | -0.9541 | 0.2424 |
| H | 4.6255 | -3.018 | 0.6581 |
| H | 2.1438 | -2.9504 | 0.6373 |
| H | 0.5948 | 3.2547 | -0.7218 |
| H | -5.4265 | 1.3617 | 0.9431 |
| H | -4.665 | -2.7541 | -0.8028 |

| Compound 64 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.708225588 | | |
| C | -5.5491 | -0.69 | 0.0028 |
| C | -4.6049 | -1.5965 | -0.4686 |
| C | -3.2564 | -1.2659 | -0.4648 |
| C | -2.8436 | -0.0154 | 0.004 |
| C | -3.7947 | 0.8904 | 0.4815 |
| C | -5.1408 | 0.5518 | 0.4798 |
| C | -1.4157 | 0.3467 | -0.0122 |
| C | -0.9301 | 1.6072 | -0.1093 |
| C | 0.4833 | 1.8574 | -0.1172 |
| O | 0.9673 | 3.0099 | -0.1967 |
| C | 1.3256 | 0.6826 | -0.0376 |
| C | 2.7339 | 0.7725 | -0.0443 |
| C | 3.5036 | -0.3736 | 0.0302 |
| C | 2.8793 | -1.6257 | 0.1164 |
| C | 1.4973 | -1.7438 | 0.126 |
| C | 0.7446 | -0.5859 | 0.0474 |
| O | -0.6117 | -0.7301 | 0.0658 |
| O | 3.3682 | 1.9621 | -0.1206 |
| O | 4.8702 | -0.3546 | 0.0275 |
| H | -6.6011 | -0.9517 | 0.0019 |
| H | -4.9187 | -2.5643 | -0.8426 |
| H | -2.5259 | -1.9725 | -0.8393 |
| H | -3.4844 | 1.8522 | 0.8725 |
| H | -5.8713 | 1.2568 | 0.8593 |
| O | 3.6275 | -2.7508 | 0.1921 |
| H | 1.0255 | -2.715 | 0.1946 |
| H | 2.6668 | 2.6526 | -0.166 |
| H | 5.1857 | 0.5551 | -0.0154 |
| H | -1.6082 | 2.4447 | -0.1987 |
| H | 4.5647 | -2.5203 | 0.1842 |

**Table S4.** (cont.)

| Compound 65 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.702726759 | | |
| C | 5.4116 | 0.3412 | 0.0068 |
| C | 4.9339 | -0.897 | -0.4119 |
| C | 3.5702 | -1.1548 | -0.413 |
| C | 2.6712 | -0.1708 | 0.0076 |
| C | 3.1539 | 1.0752 | 0.419 |
| C | 4.5195 | 1.3252 | 0.4211 |
| C | 1.2243 | -0.4419 | 0.0211 |
| C | 0.6517 | -1.668 | 0.1128 |
| C | -0.7734 | -1.8304 | 0.1075 |
| O | -1.3297 | -2.9459 | 0.1743 |
| C | -1.5512 | -0.5991 | 0.0288 |
| C | -2.9535 | -0.6011 | 0.0264 |
| C | -3.6342 | 0.6092 | -0.042 |
| C | -2.9348 | 1.8103 | -0.1089 |
| C | -1.551 | 1.8293 | -0.1096 |
| C | -0.8698 | 0.6173 | -0.0406 |
| O | 0.4911 | 0.6806 | -0.0545 |
| O | -3.6814 | -1.7469 | 0.0837 |
| O | -4.9991 | 0.6495 | -0.0476 |
| H | 6.4773 | 0.5399 | 0.0068 |
| H | 5.6243 | -1.6625 | -0.7464 |
| H | 3.207 | -2.1154 | -0.7588 |
| H | 2.4639 | 1.8428 | 0.7477 |
| H | 4.8875 | 2.2905 | 0.749 |
| O | -0.8971 | 3.0252 | -0.176 |
| H | -3.0399 | -2.488 | 0.1263 |
| H | -5.3453 | -0.2487 | 0.0095 |
| H | 1.272 | -2.5491 | 0.2013 |
| H | -3.4833 | 2.7436 | -0.1612 |
| H | 0.0557 | 2.8783 | -0.1644 |

| Compound 66 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.706886532 | | |
| C | -5.2642 | -0.0328 | -0.1515 |
| C | -4.4906 | -1.0897 | 0.2941 |
| C | -3.1002 | -0.986 | 0.3311 |
| C | -2.4774 | 0.2099 | -0.0746 |
| C | -3.2851 | 1.2629 | -0.5294 |
| C | -4.6621 | 1.1524 | -0.5713 |
| C | -1.0216 | 0.4069 | -0.0216 |
| C | -0.401 | 1.5932 | 0.1903 |
| C | 1.0296 | 1.6905 | 0.2095 |
| O | 1.6336 | 2.7685 | 0.3925 |
| C | 1.7506 | 0.4392 | 0.019 |
| C | 3.1553 | 0.3828 | 0.0342 |
| C | 3.8006 | -0.8371 | -0.1456 |
| C | 3.0541 | -1.9955 | -0.3312 |
| C | 1.6681 | -1.9649 | -0.3458 |
| C | 1.0367 | -0.7459 | -0.1724 |
| O | -0.3315 | -0.7361 | -0.205 |
| O | 3.9157 | 1.4844 | 0.2206 |
| O | 5.1649 | -0.9189 | -0.142 |
| H | -6.343 | -0.1364 | -0.1786 |
| H | -4.9458 | -2.0176 | 0.6202 |
| O | -2.4359 | -2.0756 | 0.8053 |
| H | -2.8119 | 2.1757 | -0.8713 |
| H | -5.2618 | 1.9777 | -0.9347 |
| H | 3.2975 | 2.2411 | 0.3325 |
| H | 5.5392 | -0.0383 | -0.0218 |
| H | -0.9845 | 2.4857 | 0.3677 |
| H | 3.5789 | -2.934 | -0.4673 |
| H | 1.0847 | -2.8647 | -0.4913 |
| H | -1.4857 | -1.9829 | 0.6639 |

c

**Table S4.** (cont.)

| Compound 67 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.709029716 | | |
| C | -5.0874 | 0.1497 | 0.1579 |
| C | -4.3011 | -0.9255 | -0.2474 |
| C | -2.9161 | -0.8162 | -0.2736 |
| C | -2.3116 | 0.3852 | 0.0956 |
| C | -3.0935 | 1.4687 | 0.5048 |
| C | -4.4749 | 1.3392 | 0.5334 |
| C | -0.8429 | 0.5023 | 0.0432 |
| C | -0.1594 | 1.6565 | -0.155 |
| C | 1.2735 | 1.6705 | -0.1958 |
| O | 1.9388 | 2.7139 | -0.3722 |
| C | 1.9191 | 0.3759 | -0.0324 |
| C | 3.3179 | 0.2358 | -0.0677 |
| C | 3.8913 | -1.0215 | 0.0903 |
| C | 3.0795 | -2.1349 | 0.28 |
| C | 1.6988 | -2.0216 | 0.3147 |
| C | 1.1354 | -0.7659 | 0.1568 |
| O | -0.2275 | -0.6804 | 0.1999 |
| O | 4.1409 | 1.2921 | -0.255 |
| O | 5.2485 | -1.1842 | 0.0605 |
| H | -6.1677 | 0.0514 | 0.1786 |
| O | -4.8407 | -2.1199 | -0.636 |
| H | -2.631 | 2.3967 | 0.817 |
| H | -5.0862 | 2.1733 | 0.8577 |
| H | 3.5673 | 2.0856 | -0.3506 |
| H | 5.6701 | -0.3258 | -0.0638 |
| H | -0.6934 | 2.5844 | -0.3053 |
| H | 3.5493 | -3.1041 | 0.4016 |
| H | 1.0658 | -2.8869 | 0.4619 |
| H | -2.324 | -1.6631 | -0.5974 |
| H | -5.8018 | -2.0717 | -0.6062 |

| Compound 68 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.710917861 | | |
| C | -4.9924 | -0.2571 | 0.0152 |
| C | -4.1497 | -1.2903 | -0.3918 |
| C | -2.7785 | -1.0952 | -0.396 |
| C | -2.2294 | 0.1305 | -0.0072 |
| C | -3.0894 | 1.1573 | 0.3988 |
| C | -4.4593 | 0.9687 | 0.4122 |
| C | -0.776 | 0.334 | -0.0267 |
| C | -0.1509 | 1.5356 | -0.1365 |
| C | 1.2759 | 1.6332 | -0.1298 |
| O | 1.8867 | 2.7224 | -0.2162 |
| C | 1.9929 | 0.3693 | -0.0269 |
| C | 3.3977 | 0.3128 | -0.0178 |
| C | 4.0403 | -0.917 | 0.0776 |
| C | 3.2908 | -2.0853 | 0.1645 |
| C | 1.905 | -2.0539 | 0.1575 |
| C | 1.2727 | -0.8247 | 0.0613 |
| O | -0.0935 | -0.8195 | 0.0679 |
| O | 4.16 | 1.4272 | -0.0944 |
| O | 5.4054 | -0.9979 | 0.0906 |
| O | -6.3463 | -0.3924 | 0.0492 |
| H | -2.6889 | 2.1085 | 0.7291 |
| H | -5.124 | 1.76 | 0.7377 |
| H | 3.5402 | 2.1896 | -0.156 |
| H | 5.778 | -0.1113 | 0.0196 |
| H | -0.7324 | 2.4406 | -0.244 |
| H | 3.8135 | -3.0318 | 0.2393 |
| H | 1.3207 | -2.9622 | 0.2253 |
| H | -2.1323 | -1.9023 | -0.7181 |
| H | -4.5707 | -2.2401 | -0.7033 |
| H | -6.6003 | -1.2777 | -0.2325 |

**Table S4.** (cont.)

| Compound 69 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.706244557 | | |
| C | 5.2882 | -0.6334 | 0.0227 |
| C | 4.3121 | -1.5378 | 0.4279 |
| C | 2.9726 | -1.1723 | 0.4147 |
| C | 2.6004 | 0.1102 | 0.0004 |
| C | 3.5839 | 1.0134 | -0.4126 |
| C | 4.9207 | 0.6408 | -0.3994 |
| C | 1.1819 | 0.505 | 0.007 |
| C | 0.7113 | 1.7703 | 0.0875 |
| C | -0.7018 | 2.0444 | 0.0867 |
| O | -1.1586 | 3.207 | 0.146 |
| C | -1.5695 | 0.8863 | 0.0265 |
| C | -2.9777 | 0.979 | 0.038 |
| C | -3.7512 | -0.165 | -0.0111 |
| C | -3.139 | -1.4161 | -0.0714 |
| C | -1.7512 | -1.5446 | -0.088 |
| C | -0.9924 | -0.3875 | -0.0393 |
| O | 0.3553 | -0.5592 | -0.0628 |
| O | -3.5871 | 2.1862 | 0.0995 |
| H | 3.3083 | 2.0014 | -0.7617 |
| H | 5.6762 | 1.3451 | -0.7275 |
| H | -2.8764 | 2.8637 | 0.1297 |
| H | 1.3987 | 2.601 | 0.1687 |
| O | -3.9293 | -2.5155 | -0.1108 |
| O | -1.2184 | -2.8019 | -0.1525 |
| H | 2.2175 | -1.8787 | 0.7374 |
| H | 4.5933 | -2.5312 | 0.7577 |
| H | -4.832 | -0.0979 | 0 |
| H | 6.3332 | -0.9218 | 0.0316 |
| H | -3.3855 | -3.3126 | -0.1337 |
| H | -0.2574 | -2.7582 | -0.0947 |

| Compound 70 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.713980135 | | |
| C | 5.1697 | -0.2662 | -0.1615 |
| C | 4.6511 | 0.9426 | -0.6229 |
| C | 3.2855 | 1.1531 | -0.5804 |
| C | 2.4079 | 0.1787 | -0.0825 |
| C | 2.946 | -1.0437 | 0.3631 |
| C | 4.325 | -1.2483 | 0.3249 |
| C | 0.9713 | 0.4853 | -0.0245 |
| C | 0.4388 | 1.7142 | 0.1571 |
| C | -0.9862 | 1.9086 | 0.1806 |
| O | -1.5058 | 3.0368 | 0.3325 |
| C | -1.7888 | 0.7134 | 0.0343 |
| C | -3.2041 | 0.737 | 0.0586 |
| C | -3.9299 | -0.4323 | -0.073 |
| C | -3.253 | -1.6451 | -0.2277 |
| C | -1.8635 | -1.7128 | -0.2573 |
| C | -1.1659 | -0.5285 | -0.1263 |
| O | 0.195 | -0.6145 | -0.1704 |
| O | -3.8598 | 1.9033 | 0.211 |
| O | 2.2076 | -2.0656 | 0.8779 |
| H | 4.7146 | -2.1943 | 0.6825 |
| H | -3.1766 | 2.6087 | 0.2893 |
| H | 1.0834 | 2.5696 | 0.3037 |
| O | -3.9242 | -2.8138 | -0.3581 |
| H | 2.8762 | 2.084 | -0.9547 |
| H | 5.3063 | 1.7083 | -1.0197 |
| H | -5.0134 | -0.4042 | -0.0537 |
| H | 6.2382 | -0.4477 | -0.1881 |
| H | -4.8747 | -2.6609 | -0.3238 |
| H | -1.3465 | -2.6551 | -0.3803 |
| H | 1.2668 | -1.9141 | 0.7264 |

**Table S4.** (cont.)

| Compound 71 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.716078346 | | |
| C | 4.9973 | -0.0026 | 0.1841 |
| C | 4.4482 | -1.2144 | 0.5852 |
| C | 3.0767 | -1.4224 | 0.546 |
| C | 2.24 | -0.3964 | 0.0986 |
| C | 2.7803 | 0.8265 | -0.2983 |
| C | 4.1567 | 1.0144 | -0.2603 |
| C | 0.7815 | -0.5999 | 0.0366 |
| C | 0.165 | -1.7913 | -0.1316 |
| C | -1.2693 | -1.8815 | -0.1794 |
| O | -1.8698 | -2.9703 | -0.3275 |
| C | -1.98 | -0.6272 | -0.0569 |
| C | -3.393 | -0.5447 | -0.0967 |
| C | -4.0316 | 0.6751 | 0.0212 |
| C | -3.2675 | 1.8354 | 0.1775 |
| C | -1.8779 | 1.7991 | 0.2213 |
| C | -1.265 | 0.5659 | 0.1013 |
| O | 0.096 | 0.5558 | 0.1521 |
| O | -4.1321 | -1.6606 | -0.25 |
| O | 4.6343 | 2.2262 | -0.6752 |
| H | -3.5012 | -2.4141 | -0.3179 |
| H | 0.7492 | -2.6933 | -0.2495 |
| O | -3.8501 | 3.0533 | 0.2933 |
| H | 2.663 | -2.3658 | 0.8799 |
| H | 5.1014 | -2.0032 | 0.9398 |
| H | -5.1138 | 0.7265 | -0.0107 |
| H | 6.0698 | 0.1585 | 0.2141 |
| H | -4.8092 | 2.9763 | 0.2434 |
| H | -1.2947 | 2.7021 | 0.3425 |
| H | 2.1456 | 1.6295 | -0.6517 |
| H | 5.5956 | 2.2334 | -0.6241 |

| Compound 72 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.717513680 | | |
| C | -4.8899 | -0.4066 | 0 |
| C | -3.9594 | -1.4431 | 0 |
| C | -2.6057 | -1.1506 | 0 |
| C | -2.1547 | 0.1739 | 0 |
| C | -3.1062 | 1.2025 | 0 |
| C | -4.4591 | 0.9197 | 0 |
| C | -0.715 | 0.469 | 0 |
| C | -0.1452 | 1.6998 | 0 |
| C | 1.2803 | 1.8592 | 0 |
| O | 1.832 | 2.9853 | 0 |
| C | 2.0527 | 0.6358 | 0 |
| C | 3.4678 | 0.6244 | 0 |
| C | 4.1623 | -0.5709 | 0 |
| C | 3.4516 | -1.7745 | 0 |
| C | 2.0615 | -1.8075 | 0 |
| C | 1.3927 | -0.5974 | 0 |
| O | 0.0336 | -0.6542 | 0 |
| O | 4.1548 | 1.7838 | 0 |
| H | 3.4889 | 2.5105 | 0 |
| H | -0.7561 | 2.591 | 0 |
| O | 4.0923 | -2.9689 | 0 |
| H | -1.8953 | -1.967 | 0 |
| H | -4.2987 | -2.4733 | 0 |
| H | 5.2463 | -0.5703 | 0 |
| O | -6.2316 | -0.6325 | 0 |
| H | 5.0466 | -2.8372 | 0 |
| H | 1.5195 | -2.7438 | 0 |
| H | -2.8002 | 2.2411 | 0 |
| H | -5.1905 | 1.7192 | 0 |
| H | -6.4107 | -1.5791 | 0 |

**Table S4.** (cont.)

| Compound 73 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.704692897 | | |
| C | -5.0151 | -0.138 | 0.1172 |
| C | -4.409 | -1.3224 | 0.5344 |
| C | -3.0316 | -1.4248 | 0.5008 |
| C | -2.2254 | -0.3655 | 0.056 |
| C | -2.8527 | 0.8305 | -0.3451 |
| C | -4.2443 | 0.9253 | -0.3163 |
| C | -0.7695 | -0.5582 | 0.0111 |
| C | -0.135 | -1.7432 | -0.1532 |
| C | 1.2983 | -1.828 | -0.1579 |
| O | 1.9055 | -2.9103 | -0.2911 |
| C | 2.0146 | -0.5662 | -0.0158 |
| C | 3.4232 | -0.485 | -0.0282 |
| C | 4.0371 | 0.749 | 0.095 |
| C | 3.2709 | 1.9061 | 0.2234 |
| C | 1.8873 | 1.8581 | 0.2335 |
| C | 1.2775 | 0.6113 | 0.1182 |
| O | -0.0837 | 0.5962 | 0.1508 |
| O | 4.1832 | -1.6008 | -0.1586 |
| H | 3.5656 | -2.3589 | -0.2401 |
| H | -0.7051 | -2.6499 | -0.2984 |
| H | -2.5572 | -2.3373 | 0.8414 |
| H | -5.0063 | -2.1531 | 0.8895 |
| H | 5.1184 | 0.8094 | 0.0877 |
| O | 1.0769 | 2.9503 | 0.3449 |
| O | -2.1953 | 1.9295 | -0.8047 |
| H | -4.702 | 1.8534 | -0.6382 |
| H | -6.0946 | -0.0404 | 0.138 |
| H | 3.7619 | 2.8691 | 0.3154 |
| H | 1.6137 | 3.7483 | 0.39 |
| H | -1.2451 | 1.8473 | -0.654 |

| Compound 74 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.706978362 | | |
| C | 4.816 | -0.3762 | -0.1374 |
| C | 4.1825 | -1.5527 | -0.5192 |
| C | 2.7989 | -1.6565 | -0.4952 |
| C | 2.0367 | -0.5606 | -0.0822 |
| C | 2.6622 | 0.6285 | 0.2924 |
| C | 4.0489 | 0.7127 | 0.2683 |
| C | 0.5671 | -0.6495 | -0.0333 |
| C | -0.1515 | -1.7864 | 0.1206 |
| C | -1.588 | -1.7617 | 0.1567 |
| O | -2.2749 | -2.795 | 0.2897 |
| C | -2.2048 | -0.4467 | 0.0428 |
| C | -3.6009 | -0.2517 | 0.0789 |
| C | -4.1145 | 1.0294 | -0.0286 |
| C | -3.2605 | 2.1217 | -0.168 |
| C | -1.887 | 1.9611 | -0.2031 |
| C | -1.3768 | 0.6695 | -0.0962 |
| O | -0.023 | 0.555 | -0.1435 |
| O | -4.4476 | -1.3023 | 0.2188 |
| H | -3.8946 | -2.1097 | 0.2848 |
| H | 0.3522 | -2.736 | 0.2361 |
| H | 2.3203 | -2.5741 | -0.8135 |
| H | 4.7789 | -2.3968 | -0.8452 |
| H | -5.1873 | 1.1762 | -0.002 |
| O | -1.0729 | 3.0507 | -0.3393 |
| O | 4.6094 | 1.8966 | 0.6587 |
| H | 5.898 | -0.2977 | -0.1552 |
| H | -3.6694 | 3.1221 | -0.2514 |
| H | -0.1504 | 2.7706 | -0.345 |
| H | 2.0851 | 1.4858 | 0.6164 |
| H | 5.5694 | 1.8342 | 0.6211 |

**Table S4.** (cont.)

| Compound 75 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.708908455 | | |
| C | 4.7343 | 0.1256 | -0.0214 |
| C | 4.2156 | -1.1209 | 0.3275 |
| C | 2.8453 | -1.3146 | 0.3392 |
| C | 1.9727 | -0.2733 | 0.0077 |
| C | 2.5093 | 0.9764 | -0.3253 |
| C | 3.8779 | 1.1768 | -0.3441 |
| C | 0.5212 | -0.4827 | -0.0024 |
| C | -0.1152 | -1.6785 | -0.0836 |
| C | -1.5462 | -1.7671 | -0.0797 |
| O | -2.155 | -2.8571 | -0.1372 |
| C | -2.2637 | -0.4995 | -0.0176 |
| C | -3.671 | -0.4152 | -0.0268 |
| C | -4.2816 | 0.8262 | 0.0272 |
| C | -3.5129 | 1.9867 | 0.09 |
| C | -2.1305 | 1.9344 | 0.1 |
| C | -1.523 | 0.682 | 0.045 |
| O | -0.1639 | 0.6751 | 0.0638 |
| O | -4.4343 | -1.5357 | -0.0837 |
| H | -3.8181 | -2.2988 | -0.1124 |
| H | 0.4553 | -2.5932 | -0.1633 |
| H | 2.4599 | -2.2857 | 0.6259 |
| H | 4.8867 | -1.931 | 0.5914 |
| H | -5.363 | 0.8881 | 0.0209 |
| O | -1.4023 | 3.0902 | 0.16 |
| O | 6.0723 | 0.3696 | -0.0584 |
| H | -3.9971 | 2.9555 | 0.1324 |
| H | -0.4608 | 2.8834 | 0.1714 |
| H | 1.8525 | 1.7976 | -0.5846 |
| H | 4.2929 | 2.1411 | -0.6122 |
| H | 6.563 | -0.4307 | 0.1587 |

| Compound 76 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.708578284 | | |
| C | -4.636 | -0.5949 | 0.2502 |
| C | -3.9804 | 0.5501 | -0.1628 |
| C | -2.5806 | 0.5916 | -0.2162 |
| C | -1.8392 | -0.5432 | 0.1392 |
| C | -2.5196 | -1.6945 | 0.5635 |
| C | -3.9005 | -1.719 | 0.6177 |
| C | -0.3713 | -0.5648 | 0.061 |
| C | 0.3822 | -1.6528 | -0.2172 |
| C | 1.816 | -1.5706 | -0.2543 |
| O | 2.5388 | -2.5605 | -0.4918 |
| C | 2.3827 | -0.2515 | -0.0169 |
| C | 3.7749 | -0.0072 | -0.0512 |
| C | 4.2614 | 1.2724 | 0.1691 |
| C | 3.3729 | 2.3139 | 0.4238 |
| C | 2.0016 | 2.1117 | 0.4654 |
| C | 1.5332 | 0.8268 | 0.244 |
| O | 0.1803 | 0.6456 | 0.2964 |
| O | -2.0656 | 1.7689 | -0.6698 |
| O | -4.7068 | 1.6484 | -0.5239 |
| H | -5.7192 | -0.5953 | 0.2884 |
| H | -1.9509 | -2.5645 | 0.8679 |
| H | -4.414 | -2.6113 | 0.9543 |
| O | 4.6412 | -1.011 | -0.2992 |
| H | 5.3301 | 1.4455 | 0.1401 |
| H | 3.7647 | 3.3101 | 0.5932 |
| H | 1.3052 | 2.9163 | 0.6625 |
| H | -1.1212 | 1.8255 | -0.4779 |
| H | -4.1 | 2.363 | -0.7531 |
| H | -0.0914 | -2.6011 | -0.4297 |
| H | 4.1096 | -1.8277 | -0.4306 |

**Table S4.** (cont.)

| Compound 77 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.713639254 | | |
| C | 4.5806 | -0.0939 | -0.0707 |
| C | 3.8345 | 1.0131 | 0.3025 |
| C | 2.4457 | 0.9531 | 0.3043 |
| C | 1.7825 | -0.2388 | -0.06 |
| C | 2.5722 | -1.3332 | -0.4442 |
| C | 3.9494 | -1.2797 | -0.4566 |
| C | 0.3266 | -0.3897 | -0.0241 |
| C | -0.3432 | -1.5525 | 0.1733 |
| C | -1.7756 | -1.5942 | 0.1745 |
| O | -2.4187 | -2.654 | 0.3395 |
| C | -2.4505 | -0.3167 | -0.0046 |
| C | -3.8585 | -0.1932 | 0.0075 |
| C | -4.4487 | 1.0511 | -0.1548 |
| C | -3.6476 | 2.1773 | -0.3261 |
| C | -2.2634 | 2.0943 | -0.3408 |
| C | -1.6918 | 0.8425 | -0.1796 |
| O | -0.3278 | 0.7787 | -0.2086 |
| O | 1.8128 | 2.0858 | 0.7083 |
| O | 5.9338 | 0.0298 | -0.0513 |
| H | 4.3269 | 1.9325 | 0.5952 |
| H | 2.0853 | -2.2485 | -0.7584 |
| H | 4.5372 | -2.1363 | -0.7658 |
| O | -4.6388 | -1.2805 | 0.1785 |
| H | -5.5288 | 1.1309 | -0.1448 |
| H | -4.1197 | 3.1448 | -0.4521 |
| H | -1.6341 | 2.9647 | -0.474 |
| H | 0.8624 | 2.0135 | 0.5535 |
| H | 6.3453 | -0.7963 | -0.3273 |
| H | 0.1996 | -2.4691 | 0.3565 |
| H | -4.0368 | -2.0519 | 0.2816 |

| Compound 78 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.708629162 | | |
| C | 4.6338 | 0.433 | -0.0595 |
| C | 3.7857 | 1.4762 | -0.383 |
| C | 2.4024 | 1.3136 | -0.365 |
| C | 1.8619 | 0.0611 | -0.0243 |
| C | 2.7326 | -0.9839 | 0.3156 |
| C | 4.1024 | -0.8045 | 0.2985 |
| C | 0.4172 | -0.2144 | -0.0392 |
| C | -0.1479 | -1.4184 | -0.2883 |
| C | -1.5737 | -1.5868 | -0.2679 |
| O | -2.1228 | -2.6885 | -0.4787 |
| C | -2.3516 | -0.3857 | -0.0047 |
| C | -3.7654 | -0.3881 | 0.0178 |
| C | -4.458 | 0.7897 | 0.254 |
| C | -3.7545 | 1.9724 | 0.4678 |
| C | -2.3683 | 2.0118 | 0.4557 |
| C | -1.6927 | 0.8255 | 0.2196 |
| O | -0.3281 | 0.881 | 0.2212 |
| O | 1.6656 | 2.4065 | -0.7282 |
| O | 4.8928 | -1.8705 | 0.6478 |
| H | 5.7089 | 0.5785 | -0.0731 |
| H | 4.1889 | 2.4438 | -0.6575 |
| H | 2.3343 | -1.9461 | 0.6135 |
| O | -4.4513 | -1.5307 | -0.1914 |
| H | -5.5409 | 0.7745 | 0.2677 |
| H | -4.3064 | 2.8872 | 0.6501 |
| H | -1.8155 | 2.9271 | 0.6231 |
| H | 0.7361 | 2.2714 | -0.5084 |
| H | 5.8196 | -1.6153 | 0.6029 |
| H | 0.4713 | -2.272 | -0.5257 |
| H | -3.789 | -2.242 | -0.3426 |

**Table S4.** (cont.)

| Compound 79 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.708057197 | | |
| C | -4.7913 | -0.342 | -0.0153 |
| C | -4.2606 | 0.827 | 0.5102 |
| C | -2.8834 | 1.0131 | 0.5091 |
| C | -2.0187 | 0.034 | -0.0159 |
| C | -2.5902 | -1.1521 | -0.5201 |
| C | -3.9689 | -1.3321 | -0.5282 |
| C | -0.5652 | 0.2539 | -0.0518 |
| C | 0.0603 | 1.3898 | -0.4286 |
| C | 1.4947 | 1.4783 | -0.4417 |
| O | 2.0988 | 2.518 | -0.7786 |
| C | 2.2085 | 0.2722 | -0.0528 |
| C | 3.6208 | 0.2008 | -0.0346 |
| C | 4.252 | -0.9776 | 0.3325 |
| C | 3.4885 | -2.0893 | 0.6799 |
| C | 2.1024 | -2.0566 | 0.672 |
| C | 1.4872 | -0.8702 | 0.3044 |
| O | 0.1216 | -0.8553 | 0.3128 |
| O | -2.3307 | 2.1369 | 1.0339 |
| O | -1.8513 | -2.1604 | -1.0618 |
| H | -5.8656 | -0.486 | -0.0169 |
| H | -4.9006 | 1.596 | 0.9282 |
| H | -4.3748 | -2.2504 | -0.9339 |
| H | 5.3343 | -1.0187 | 0.3427 |
| H | 3.9932 | -3.0052 | 0.9649 |
| H | 1.504 | -2.917 | 0.9417 |
| H | -3.028 | 2.7039 | 1.3801 |
| H | -0.9181 | -2.0664 | -0.8371 |
| O | 4.3644 | 1.2739 | -0.3746 |
| H | 3.7386 | 1.997 | -0.6053 |
| H | -0.5213 | 2.2478 | -0.7334 |

| Compound 80 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.712046115 | | |
| C | 4.3989 | -0.266 | -0.0713 |
| C | 3.6431 | 0.8867 | 0.1748 |
| C | 2.2634 | 0.819 | 0.1838 |
| C | 1.6145 | -0.3995 | -0.0488 |
| C | 2.3741 | -1.5433 | -0.302 |
| C | 3.759 | -1.4735 | -0.3122 |
| C | 0.1466 | -0.4628 | -0.0198 |
| C | -0.5953 | -1.5909 | 0.1141 |
| C | -2.0265 | -1.54 | 0.1257 |
| O | -2.7382 | -2.5631 | 0.2384 |
| C | -2.6143 | -0.2141 | 0.0121 |
| C | -4.0118 | -0.0005 | 0.0286 |
| C | -4.5197 | 1.285 | -0.0746 |
| C | -3.6455 | 2.3635 | -0.1924 |
| C | -2.2702 | 2.1914 | -0.21 |
| C | -1.7773 | 0.8989 | -0.1061 |
| O | -0.4225 | 0.7523 | -0.1311 |
| O | 4.2553 | 2.0843 | 0.4128 |
| O | 5.7504 | -0.109 | -0.0584 |
| H | 1.7012 | 1.7219 | 0.3858 |
| H | 1.8983 | -2.4932 | -0.5095 |
| H | 4.3541 | -2.3572 | -0.5152 |
| H | -5.5923 | 1.4348 | -0.0611 |
| H | -4.0526 | 3.3648 | -0.2722 |
| H | -1.5871 | 3.0258 | -0.3016 |
| H | 5.2116 | 1.9661 | 0.3715 |
| H | 6.1916 | -0.952 | -0.209 |
| H | -0.114 | -2.5517 | 0.2291 |
| O | -4.8616 | -1.0427 | 0.1458 |
| H | -4.3112 | -1.8562 | 0.211 |

**Table S4.** (cont.)

| Compound 81 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.713391332 | | |
| C | -4.4711 | 0.2109 | -0.0137 |
| C | -3.6315 | 1.2743 | -0.3266 |
| C | -2.2497 | 1.1243 | -0.3173 |
| C | -1.7081 | -0.1198 | 0.0026 |
| C | -2.5312 | -1.198 | 0.3249 |
| C | -3.9093 | -1.0192 | 0.3141 |
| C | -0.2435 | -0.2958 | -0.0172 |
| C | 0.3999 | -1.4614 | -0.259 |
| C | 1.8342 | -1.5256 | -0.2682 |
| O | 2.4592 | -2.5869 | -0.4802 |
| C | 2.5229 | -0.2672 | -0.0307 |
| C | 3.9335 | -0.1638 | -0.0312 |
| C | 4.5411 | 1.0607 | 0.1973 |
| C | 3.7546 | 2.1879 | 0.4247 |
| C | 2.3702 | 2.125 | 0.4306 |
| C | 1.7766 | 0.8926 | 0.2009 |
| O | 0.4142 | 0.8541 | 0.2154 |
| O | -4.1247 | 2.5031 | -0.6583 |
| O | -4.6825 | -2.0951 | 0.6422 |
| H | -5.5493 | 0.3383 | -0.0206 |
| H | -1.6193 | 1.9652 | -0.5744 |
| H | -2.1238 | -2.1618 | 0.6024 |
| O | 4.6989 | -1.2522 | -0.2559 |
| H | 5.6222 | 1.1254 | 0.1947 |
| H | 4.2401 | 3.1407 | 0.6016 |
| H | 1.7549 | 2.9975 | 0.607 |
| H | -5.0871 | 2.4864 | -0.6465 |
| H | -5.6146 | -1.8555 | 0.6116 |
| H | -0.1627 | -2.3599 | -0.4711 |
| H | 4.0875 | -2.0098 | -0.3959 |

| Compound 82 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.700442243 | | |
| C | -5.3376 | -0.8724 | -0.0103 |
| C | -4.2929 | -1.7231 | -0.3559 |
| C | -2.984 | -1.2597 | -0.3506 |
| C | -2.7091 | 0.0663 | -0.0016 |
| C | -3.762 | 0.9151 | 0.3528 |
| C | -5.068 | 0.4457 | 0.3456 |
| C | -1.3195 | 0.557 | -0.0129 |
| C | -0.9309 | 1.8515 | -0.0952 |
| C | 0.4596 | 2.2347 | -0.0946 |
| O | 0.8247 | 3.4184 | -0.1505 |
| C | 1.4115 | 1.1228 | -0.037 |
| C | 2.7992 | 1.3141 | -0.0527 |
| C | 3.6408 | 0.2271 | -0.0038 |
| C | 3.1179 | -1.0779 | 0.0593 |
| C | 1.7495 | -1.2826 | 0.0731 |
| C | 0.9061 | -0.1709 | 0.0278 |
| O | -0.4248 | -0.446 | 0.0565 |
| H | -3.5672 | 1.9382 | 0.6516 |
| H | -5.8771 | 1.1101 | 0.6261 |
| H | -1.6748 | 2.6321 | -0.1766 |
| O | 4.009 | -2.1001 | 0.1037 |
| O | 1.2926 | -2.5613 | 0.1326 |
| H | -2.176 | -1.9261 | -0.6268 |
| H | -4.4962 | -2.7511 | -0.633 |
| O | 4.9913 | 0.4135 | -0.0189 |
| H | -6.3589 | -1.2359 | -0.0137 |
| H | 3.5513 | -2.949 | 0.1291 |
| H | 0.3289 | -2.5725 | 0.0868 |
| H | 3.2098 | 2.3144 | -0.1049 |
| H | 5.4354 | -0.4422 | 0.0097 |

**Table S4.** (cont.)

| Compound 83 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.705746910 | | |
| C | 5.2389 | -0.4972 | -0.181 |
| C | 4.3286 | -1.4245 | 0.2946 |
| C | 2.9682 | -1.1222 | 0.3441 |
| C | 2.5156 | 0.1413 | -0.0811 |
| C | 3.4581 | 1.0583 | -0.5684 |
| C | 4.8055 | 0.7524 | -0.6207 |
| C | 1.1025 | 0.5447 | -0.011 |
| C | 0.6551 | 1.8051 | 0.1916 |
| C | -0.7533 | 2.114 | 0.2294 |
| O | -1.1778 | 3.2676 | 0.395 |
| C | -1.6433 | 0.9638 | 0.0753 |
| C | -3.0423 | 1.0874 | 0.1127 |
| C | -3.8395 | -0.0198 | -0.0304 |
| C | -3.2571 | -1.2954 | -0.2131 |
| C | -1.8864 | -1.4377 | -0.2516 |
| C | -1.0973 | -0.3018 | -0.1074 |
| O | 0.2539 | -0.4951 | -0.1679 |
| H | 3.1146 | 2.0221 | -0.9254 |
| H | 5.5119 | 1.4763 | -1.0082 |
| H | 1.3632 | 2.6079 | 0.3451 |
| O | -4.041 | -2.3891 | -0.3545 |
| O | 2.1596 | -2.0953 | 0.8491 |
| H | 4.6515 | -2.4011 | 0.6361 |
| O | -5.2028 | -0.0024 | -0.0112 |
| H | 6.2918 | -0.7531 | -0.2158 |
| H | -4.9694 | -2.1276 | -0.3111 |
| H | -3.4897 | 2.0647 | 0.2548 |
| H | -5.5269 | 0.8938 | 0.1261 |
| H | -1.434 | -2.411 | -0.3937 |
| H | 1.2318 | -1.8685 | 0.7097 |

| Compound 84 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.707895384 | | |
| C | 5.0772 | -0.2291 | 0.1709 |
| C | 4.156 | -1.2009 | -0.2094 |
| C | 2.7984 | -0.9084 | -0.2554 |
| C | 2.3556 | 0.3717 | 0.0775 |
| C | 3.2735 | 1.3511 | 0.4666 |
| C | 4.6257 | 1.0411 | 0.509 |
| C | 0.9147 | 0.6808 | 0.0135 |
| C | 0.383 | 1.9137 | -0.1562 |
| C | -1.0424 | 2.1235 | -0.2039 |
| O | -1.548 | 3.2485 | -0.3439 |
| C | -1.8473 | 0.9097 | -0.084 |
| C | -3.2524 | 0.9341 | -0.1238 |
| C | -3.9678 | -0.2306 | -0.0072 |
| C | -3.2944 | -1.4646 | 0.1498 |
| C | -1.9181 | -1.5088 | 0.1917 |
| C | -1.2091 | -0.317 | 0.0732 |
| O | 0.1492 | -0.4195 | 0.1293 |
| H | 2.9372 | 2.3399 | 0.7525 |
| H | 5.3404 | 1.7954 | 0.8167 |
| H | 1.035 | 2.7688 | -0.2723 |
| O | -3.9982 | -2.6154 | 0.262 |
| O | -5.3288 | -0.3158 | -0.0291 |
| H | 6.1343 | -0.471 | 0.2052 |
| H | -4.9425 | -2.4204 | 0.2154 |
| H | -3.7684 | 1.8798 | -0.2462 |
| H | -5.7228 | 0.5561 | -0.1354 |
| H | -1.3988 | -2.4508 | 0.3137 |
| H | 2.1016 | -1.6789 | -0.5604 |
| O | 4.5355 | -2.4687 | -0.5524 |
| H | 5.4927 | -2.5491 | -0.4898 |

**Table S4.** (cont.)

| Compound 85 | | | |
|---|---|---|---|
| $N_i$ = 0 | E = -953.709097155 | | |
| C | 4.9558 | -0.5686 | 0 |
| C | 3.967 | -1.5493 | 0 |
| C | 2.6321 | -1.1786 | 0 |
| C | 2.2582 | 0.1695 | 0 |
| C | 3.2681 | 1.1405 | 0 |
| C | 4.6027 | 0.7801 | 0 |
| C | 0.8367 | 0.5486 | 0 |
| C | 0.3432 | 1.8129 | 0 |
| C | -1.07 | 2.0788 | 0 |
| O | -1.5341 | 3.2318 | 0 |
| C | -1.9229 | 0.8923 | 0 |
| C | -3.3254 | 0.9741 | 0 |
| C | -4.0855 | -0.1676 | 0 |
| C | -3.4601 | -1.4358 | 0 |
| C | -2.0856 | -1.5361 | 0 |
| C | -1.331 | -0.3664 | 0 |
| O | 0.0227 | -0.5243 | 0 |
| H | 3.0244 | 2.1954 | 0 |
| H | 5.3789 | 1.5362 | 0 |
| H | 1.0129 | 2.6611 | 0 |
| O | -4.2071 | -2.5655 | 0 |
| O | -5.4494 | -0.192 | 0 |
| H | -5.1435 | -2.3314 | 0 |
| H | -3.8047 | 1.9466 | 0 |
| H | -5.8002 | 0.7046 | 0 |
| H | -1.6026 | -2.505 | 0 |
| H | 1.8757 | -1.9525 | 0 |
| H | 4.2454 | -2.5977 | 0 |
| O | 6.2821 | -0.8743 | 0 |
| H | 6.4015 | -1.8303 | 0 |

| Compound 86 | | | |
|---|---|---|---|
| $N_i$ = 0 | E = -953.702703229 | | |
| C | -5.0909 | -0.2081 | -0.1907 |
| C | -4.2469 | -1.157 | 0.3595 |
| C | -2.8729 | -0.9302 | 0.4244 |
| C | -2.3386 | 0.2749 | -0.0666 |
| C | -3.2143 | 1.2177 | -0.6234 |
| C | -4.5764 | 0.9879 | -0.6884 |
| C | -0.905 | 0.5962 | 0.0023 |
| C | -0.3926 | 1.8328 | 0.2034 |
| C | 1.0268 | 2.0746 | 0.2382 |
| O | 1.5095 | 3.2008 | 0.4056 |
| C | 1.8718 | 0.879 | 0.0753 |
| C | 3.2666 | 0.9499 | 0.1058 |
| C | 4.0037 | -0.208 | -0.0543 |
| C | 3.3723 | -1.4428 | -0.2451 |
| C | 1.9943 | -1.5209 | -0.2756 |
| C | 1.2466 | -0.3473 | -0.1101 |
| O | -0.1122 | -0.4837 | -0.1587 |
| H | -2.805 | 2.1374 | -1.0247 |
| H | -5.2317 | 1.7288 | -1.1297 |
| H | -1.0615 | 2.6682 | 0.3586 |
| O | 5.3643 | -0.1064 | -0.0209 |
| H | 3.7588 | 1.9028 | 0.2522 |
| H | 5.7685 | -0.9712 | -0.1465 |
| H | -4.6341 | -2.09 | 0.7518 |
| H | 3.957 | -2.347 | -0.3743 |
| O | 1.408 | -2.7298 | -0.4644 |
| H | 0.4491 | -2.6407 | -0.5001 |
| O | -2.1346 | -1.9124 | 1.0117 |
| H | -1.1926 | -1.7253 | 0.9345 |
| H | -6.1561 | -0.4044 | -0.2349 |

**Table S4.** (cont.)

| Compound 87 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.705070422 | | |
| C | -4.9124 | 0.0417 | 0.1444 |
| C | -4.0422 | -0.9732 | -0.2444 |
| C | -2.6706 | -0.7536 | -0.2763 |
| C | -2.1638 | 0.498 | 0.0737 |
| C | -3.0301 | 1.521 | 0.4683 |
| C | -4.3969 | 1.2822 | 0.5 |
| C | -0.7093 | 0.7298 | 0.0185 |
| C | -0.1067 | 1.9316 | -0.1491 |
| C | 1.3263 | 2.0667 | -0.1939 |
| O | 1.8928 | 3.1587 | -0.3313 |
| C | 2.0775 | 0.8062 | -0.0765 |
| C | 3.4744 | 0.7629 | -0.1216 |
| C | 4.1127 | -0.4569 | -0.0069 |
| C | 3.3842 | -1.643 | 0.1514 |
| C | 2.006 | -1.607 | 0.1954 |
| C | 1.3564 | -0.3703 | 0.0789 |
| O | -0.0035 | -0.4063 | 0.1373 |
| H | -2.6437 | 2.4876 | 0.7665 |
| H | -5.0727 | 2.0698 | 0.8121 |
| H | -0.7103 | 2.8208 | -0.2688 |
| O | 5.4771 | -0.4737 | -0.0562 |
| H | 4.0426 | 1.6761 | -0.2452 |
| H | 5.7991 | -1.3757 | 0.0415 |
| O | -4.4858 | -2.2135 | -0.6099 |
| H | 3.896 | -2.595 | 0.2404 |
| O | 1.311 | -2.7621 | 0.3493 |
| H | 0.3634 | -2.5809 | 0.3522 |
| H | -5.9812 | -0.144 | 0.1685 |
| H | -2.0132 | -1.5565 | -0.5864 |
| H | -5.4469 | -2.2428 | -0.5645 |

| Compound 88 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.706915900 | | |
| C | 4.8004 | -0.3612 | -0.0102 |
| C | 4.3795 | 0.9216 | 0.3387 |
| C | 3.0283 | 1.2234 | 0.3403 |
| C | 2.0783 | 0.2575 | -0.005 |
| C | 2.5174 | -1.0274 | -0.3463 |
| C | 3.8657 | -1.3364 | -0.3534 |
| C | 0.6457 | 0.578 | -0.0162 |
| C | 0.1042 | 1.8201 | -0.1049 |
| C | -1.3165 | 2.0364 | -0.1035 |
| O | -1.8252 | 3.1646 | -0.1667 |
| C | -2.1373 | 0.8157 | -0.0349 |
| C | -3.5347 | 0.8529 | -0.0462 |
| C | -4.2402 | -0.3334 | 0.0179 |
| C | -3.5777 | -1.5657 | 0.0907 |
| C | -2.1987 | -1.6083 | 0.0996 |
| C | -1.4817 | -0.4058 | 0.0378 |
| O | -0.125 | -0.5207 | 0.0593 |
| H | 1.8001 | -1.7918 | -0.6186 |
| H | 4.2047 | -2.3292 | -0.6247 |
| H | 0.7507 | 2.6828 | -0.1918 |
| O | -5.6042 | -0.2651 | 0.0061 |
| H | -4.0533 | 1.8013 | -0.1049 |
| H | -5.9834 | -1.1484 | 0.0575 |
| H | -4.1403 | -2.4917 | 0.1365 |
| O | -1.5669 | -2.8079 | 0.1651 |
| H | -0.611 | -2.6784 | 0.1504 |
| O | 6.1139 | -0.7171 | -0.0281 |
| H | 2.7182 | 2.22 | 0.6311 |
| H | 5.1106 | 1.6737 | 0.6149 |
| H | 6.6657 | 0.0263 | 0.2376 |

**Table S4.** (cont.)

| Compound 89 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.703338902 | | |
| C | -4.7497 | 0.2939 | 0.247 |
| C | -3.9874 | -0.7972 | -0.1261 |
| C | -2.59 | -0.7063 | -0.1873 |
| C | -1.9594 | 0.5067 | 0.122 |
| C | -2.7479 | 1.6008 | 0.5097 |
| C | -4.1247 | 1.4959 | 0.5692 |
| C | -0.4994 | 0.6681 | 0.0348 |
| C | 0.1436 | 1.8248 | -0.2517 |
| C | 1.5807 | 1.903 | -0.2973 |
| O | 2.1874 | 2.9563 | -0.5308 |
| C | 2.2808 | 0.6304 | -0.0667 |
| C | 3.6754 | 0.5312 | -0.122 |
| C | 4.2859 | -0.69 | 0.0822 |
| C | 3.5153 | -1.832 | 0.3474 |
| C | 2.1407 | -1.7469 | 0.4072 |
| C | 1.534 | -0.5127 | 0.1987 |
| O | 0.1679 | -0.4784 | 0.2731 |
| O | -1.9657 | -1.8469 | -0.5953 |
| O | -4.6069 | -1.9741 | -0.4365 |
| H | -5.8278 | 0.1911 | 0.2919 |
| H | -2.2662 | 2.5317 | 0.7818 |
| H | -4.7199 | 2.3471 | 0.8763 |
| H | 4.0092 | -2.7851 | 0.5051 |
| H | 1.531 | -2.6185 | 0.6114 |
| H | -1.0191 | -1.8002 | -0.4107 |
| H | -3.9365 | -2.6388 | -0.6362 |
| H | -0.4276 | 2.7175 | -0.4657 |
| H | 4.2688 | 1.4132 | -0.3301 |
| O | 5.6488 | -0.748 | 0.0133 |
| H | 5.948 | -1.6475 | 0.182 |

| Compound 90 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.708248305 | | |
| C | -4.6619 | -0.1303 | -0.0785 |
| C | -3.832 | -1.1851 | 0.2676 |
| C | -2.4517 | -1.0183 | 0.2724 |
| C | -1.882 | 0.2296 | -0.0612 |
| C | -2.7547 | 1.2672 | -0.4221 |
| C | -4.124 | 1.1083 | -0.4373 |
| C | -0.4413 | 0.4946 | -0.0139 |
| C | 0.1298 | 1.7081 | 0.1966 |
| C | 1.555 | 1.8863 | 0.2128 |
| O | 2.0936 | 2.99 | 0.3799 |
| C | 2.3403 | 0.6543 | 0.0386 |
| C | 3.7387 | 0.6558 | 0.0704 |
| C | 4.4312 | -0.5286 | -0.0851 |
| C | 3.7396 | -1.7345 | -0.2732 |
| C | 2.3608 | -1.7485 | -0.3063 |
| C | 1.672 | -0.5504 | -0.1494 |
| O | 0.3055 | -0.6137 | -0.1987 |
| O | -1.7337 | -2.1107 | 0.6449 |
| O | -6.0022 | -0.3577 | -0.0623 |
| H | -4.2516 | -2.1467 | 0.5374 |
| H | -2.3407 | 2.2246 | -0.7142 |
| H | -4.7754 | 1.9247 | -0.7272 |
| H | 4.2959 | -2.6578 | -0.3929 |
| H | 1.8111 | -2.6705 | -0.4509 |
| H | -0.7915 | -1.9582 | 0.4974 |
| H | -6.476 | 0.4456 | -0.3039 |
| H | -0.496 | 2.5712 | 0.3768 |
| H | 4.2713 | 1.5874 | 0.2192 |
| O | 5.7962 | -0.4836 | -0.046 |
| H | 6.1593 | -1.3663 | -0.1719 |

**Table S4.** (cont.)

| Compound 91 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.703240724 | | |
| C | 4.6831 | -0.6622 | 0.0257 |
| C | 3.7599 | -1.6337 | 0.3682 |
| C | 2.394 | -1.3627 | 0.3656 |
| C | 1.9494 | -0.0733 | 0.0241 |
| C | 2.894 | 0.8978 | -0.3345 |
| C | 4.246 | 0.6104 | -0.3352 |
| C | 0.529 | 0.3122 | 0.0591 |
| C | 0.0613 | 1.5513 | 0.3413 |
| C | -1.3481 | 1.8459 | 0.3518 |
| O | -1.795 | 2.9742 | 0.5946 |
| C | -2.2258 | 0.6992 | 0.0726 |
| C | -3.6202 | 0.8153 | 0.0764 |
| C | -4.4033 | -0.2941 | -0.1721 |
| C | -3.8077 | -1.5382 | -0.43 |
| C | -2.4349 | -1.6651 | -0.4382 |
| C | -1.6539 | -0.5419 | -0.1862 |
| O | -0.297 | -0.7172 | -0.2121 |
| O | 1.5763 | -2.3924 | 0.7437 |
| O | 5.1134 | 1.6076 | -0.7057 |
| H | 5.7431 | -0.8934 | 0.0268 |
| H | 4.0896 | -2.6283 | 0.6446 |
| H | 2.5671 | 1.8864 | -0.6334 |
| H | -4.4343 | -2.4021 | -0.6245 |
| H | -1.959 | -2.618 | -0.6353 |
| H | 0.6592 | -2.1882 | 0.5247 |
| H | 6.0159 | 1.2734 | -0.69 |
| H | 0.7553 | 2.3446 | 0.5828 |
| H | -4.0787 | 1.7758 | 0.2783 |
| O | -5.7605 | -0.1385 | -0.1567 |
| H | -6.1932 | -0.9838 | -0.3162 |

| Compound 92 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.702802856 | | |
| C | -4.8326 | -0.6428 | -0.064 |
| C | -4.3951 | 0.5708 | -0.5748 |
| C | -3.0399 | 0.878 | -0.5378 |
| C | -2.1064 | -0.0222 | 0.0087 |
| C | -2.582 | -1.2547 | 0.4979 |
| C | -3.9389 | -1.5577 | 0.4691 |
| C | -0.6779 | 0.3247 | 0.0832 |
| C | -0.1685 | 1.5002 | 0.5136 |
| C | 1.2514 | 1.7375 | 0.5696 |
| O | 1.7356 | 2.8107 | 0.9511 |
| C | 2.088 | 0.6009 | 0.1583 |
| C | 3.486 | 0.6643 | 0.1825 |
| C | 4.2304 | -0.4341 | -0.1969 |
| C | 3.5929 | -1.6149 | -0.6082 |
| C | 2.2167 | -1.6896 | -0.6365 |
| C | 1.4731 | -0.5781 | -0.2514 |
| O | 0.1109 | -0.7021 | -0.3029 |
| O | -2.5714 | 2.0477 | -1.0461 |
| O | -1.7695 | -2.194 | 1.0592 |
| H | -5.8897 | -0.881 | -0.0894 |
| H | -5.0911 | 1.2819 | -1.0055 |
| H | -4.2722 | -2.5094 | 0.8639 |
| H | 4.1904 | -2.4711 | -0.9029 |
| H | 1.7091 | -2.5932 | -0.9505 |
| H | -3.303 | 2.5565 | -1.411 |
| H | -0.8418 | -2.0116 | 0.8703 |
| H | -0.8405 | 2.2849 | 0.831 |
| H | 3.9771 | 1.5751 | 0.503 |
| O | 5.5924 | -0.3332 | -0.1542 |
| H | 5.9941 | -1.1582 | -0.4457 |

**Table S4.** (cont.)

| Compound 93 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.706652797 | | |
| C | 4.4831 | 0.0484 | -0.0914 |
| C | 3.6395 | -1.031 | 0.1981 |
| C | 2.2696 | -0.8529 | 0.2112 |
| C | 1.7184 | 0.4043 | -0.0612 |
| C | 2.5638 | 1.4731 | -0.3635 |
| C | 3.9393 | 1.2926 | -0.378 |
| C | 0.2598 | 0.5858 | -0.0174 |
| C | -0.382 | 1.7684 | 0.1629 |
| C | -1.8152 | 1.8575 | 0.1906 |
| O | -2.4214 | 2.9295 | 0.3372 |
| C | -2.519 | 0.5745 | 0.0487 |
| C | -3.9156 | 0.4875 | 0.0857 |
| C | -4.5309 | -0.741 | -0.0421 |
| C | -3.7636 | -1.9034 | -0.2115 |
| C | -2.3875 | -1.8304 | -0.2492 |
| C | -1.7722 | -0.5883 | -0.1161 |
| O | -0.407 | -0.5714 | -0.162 |
| O | 4.154 | -2.2659 | 0.4759 |
| O | 5.8189 | -0.2144 | -0.0755 |
| H | 1.639 | -1.7 | 0.4501 |
| H | 2.1604 | 2.4481 | -0.6062 |
| H | 4.6018 | 2.1175 | -0.6169 |
| H | -4.2608 | -2.8624 | -0.3121 |
| H | -1.7822 | -2.7192 | -0.3774 |
| H | 5.1163 | -2.2296 | 0.4235 |
| H | 6.3238 | 0.5887 | -0.2419 |
| H | 0.1903 | 2.6745 | 0.3063 |
| H | -4.5057 | 1.3864 | 0.2173 |
| O | -5.8962 | -0.7874 | 0.0055 |
| H | -6.1956 | -1.6971 | -0.092 |

| Compound 94 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.708043980 | | |
| C | -4.5301 | -0.4365 | -0.0239 |
| C | -3.6116 | -1.4351 | 0.2818 |
| C | -2.2463 | -1.1748 | 0.2969 |
| C | -1.8007 | 0.1143 | 0.0088 |
| C | -2.7039 | 1.1295 | -0.3036 |
| C | -4.0634 | 0.8413 | -0.3167 |
| C | -0.354 | 0.4055 | 0.0479 |
| C | 0.1898 | 1.6204 | 0.2997 |
| C | 1.6146 | 1.8203 | 0.3264 |
| O | 2.1353 | 2.9234 | 0.5418 |
| C | 2.4129 | 0.609 | 0.091 |
| C | 3.8122 | 0.6323 | 0.1053 |
| C | 4.5216 | -0.5302 | -0.1167 |
| C | 3.846 | -1.7367 | -0.3576 |
| C | 2.4681 | -1.7724 | -0.3736 |
| C | 1.758 | -0.596 | -0.147 |
| O | 0.3951 | -0.6854 | -0.1772 |
| O | -4.0082 | -2.7065 | 0.5813 |
| O | -4.9153 | 1.8598 | -0.6339 |
| H | -5.5942 | -0.6516 | -0.0393 |
| H | -1.5542 | -1.9685 | 0.5451 |
| H | -2.3721 | 2.1287 | -0.5554 |
| H | 4.4155 | -2.643 | -0.5331 |
| H | 1.9334 | -2.6958 | -0.5587 |
| H | -4.9685 | -2.7675 | 0.5534 |
| H | -5.8244 | 1.5431 | -0.6289 |
| H | -0.4541 | 2.465 | 0.5034 |
| H | 4.3311 | 1.5647 | 0.2923 |
| O | 5.8863 | -0.4645 | -0.092 |
| H | 6.2628 | -1.3362 | -0.2508 |

**Table S4.** (cont.)

| Compound 95 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.702073130 | | |
| C | 4.9865 | -0.5827 | 0.1612 |
| C | 4.0303 | -1.457 | -0.3239 |
| C | 2.6863 | -1.0873 | -0.3684 |
| C | 2.2978 | 0.1942 | 0.0684 |
| C | 3.2862 | 1.0558 | 0.5669 |
| C | 4.6162 | 0.6818 | 0.6162 |
| C | 0.9082 | 0.6723 | 0.0024 |
| C | 0.5229 | 1.9572 | -0.167 |
| C | -0.8698 | 2.3371 | -0.1965 |
| O | -1.2321 | 3.5143 | -0.329 |
| C | -1.8226 | 1.2309 | -0.0769 |
| C | -3.21 | 1.4145 | -0.1129 |
| C | -4.0591 | 0.3348 | -0.0049 |
| C | -3.5411 | -0.9564 | 0.1396 |
| C | -2.1674 | -1.1699 | 0.1773 |
| C | -1.3275 | -0.0642 | 0.0695 |
| O | 0.0069 | -0.3287 | 0.1292 |
| H | 2.9931 | 2.0314 | 0.9363 |
| H | 5.3574 | 1.3646 | 1.0128 |
| H | 1.268 | 2.7297 | -0.2986 |
| H | -3.6082 | 2.4148 | -0.2272 |
| H | 4.3032 | -2.4453 | -0.6755 |
| O | -1.613 | -2.4021 | 0.3162 |
| H | -2.3119 | -3.0636 | 0.3804 |
| O | 1.8322 | -2.0167 | -0.8792 |
| H | 0.9156 | -1.7526 | -0.7312 |
| H | 6.0249 | -0.8923 | 0.1928 |
| H | -5.1352 | 0.4664 | -0.0306 |
| O | -4.3163 | -2.0654 | 0.2506 |
| H | -5.2495 | -1.828 | 0.2326 |

| Compound 96 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.704569509 | | |
| C | -4.8205 | -0.2071 | 0.1297 |
| C | -3.8619 | -1.1604 | -0.2026 |
| C | -2.5137 | -0.8251 | -0.2338 |
| C | -2.1177 | 0.4786 | 0.0656 |
| C | -3.0739 | 1.4392 | 0.4075 |
| C | -4.4157 | 1.0869 | 0.4351 |
| C | -0.6868 | 0.83 | 0.0149 |
| C | -0.179 | 2.0754 | -0.1235 |
| C | 1.2443 | 2.3195 | -0.1608 |
| O | 1.7189 | 3.4592 | -0.2668 |
| C | 2.0829 | 1.1234 | -0.0766 |
| C | 3.4825 | 1.1624 | -0.1234 |
| C | 4.2162 | -0.0007 | -0.0501 |
| C | 3.5704 | -1.236 | 0.0709 |
| C | 2.1837 | -1.304 | 0.1233 |
| C | 1.4584 | -0.1166 | 0.0485 |
| O | 0.1084 | -0.2555 | 0.1081 |
| H | -2.7775 | 2.4477 | 0.6663 |
| H | -5.1597 | 1.8274 | 0.7043 |
| H | -0.8461 | 2.9211 | -0.2204 |
| H | 3.98 | 2.1191 | -0.2218 |
| O | -4.1904 | -2.4509 | -0.5114 |
| O | 1.6006 | -2.528 | 0.2429 |
| H | 0.6402 | -2.4464 | 0.2134 |
| H | -5.87 | -0.4813 | 0.152 |
| H | -1.7878 | -1.5832 | -0.5006 |
| H | -5.1449 | -2.5663 | -0.466 |
| H | 5.2988 | 0.0154 | -0.0883 |
| O | 4.3246 | -2.3632 | 0.1298 |
| H | 3.7548 | -3.1393 | 0.191 |

**Table S4.** (cont.)

| Compound 97 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.706295835 | | |
| C | -4.685 | -0.5752 | -0.009 |
| C | -3.6751 | -1.4838 | -0.3191 |
| C | -2.3548 | -1.0695 | -0.3118 |
| C | -2.0192 | 0.2541 | -0.002 |
| C | -3.0447 | 1.1513 | 0.3123 |
| C | -4.3678 | 0.7446 | 0.309 |
| C | -0.6158 | 0.6859 | -0.0138 |
| C | -0.1687 | 1.9626 | -0.0906 |
| C | 1.2368 | 2.2828 | -0.0864 |
| O | 1.6541 | 3.4502 | -0.1346 |
| C | 2.1385 | 1.1304 | -0.0349 |
| C | 3.5345 | 1.245 | -0.0503 |
| C | 4.3283 | 0.12 | -0.007 |
| C | 3.7478 | -1.1514 | 0.0513 |
| C | 2.3658 | -1.2941 | 0.0672 |
| C | 1.5793 | -0.1448 | 0.0247 |
| O | 0.2379 | -0.3576 | 0.0514 |
| H | -2.8182 | 2.1763 | 0.5803 |
| H | -5.1577 | 1.4439 | 0.5605 |
| H | -0.876 | 2.7767 | -0.1695 |
| H | 3.9827 | 2.2295 | -0.0986 |
| O | 1.8463 | -2.551 | 0.1234 |
| H | 0.8833 | -2.516 | 0.0894 |
| O | -5.9687 | -1.027 | -0.026 |
| H | -1.5776 | -1.7824 | -0.5583 |
| H | -3.9331 | -2.507 | -0.565 |
| H | -6.5725 | -0.3158 | 0.2137 |
| H | 5.4089 | 0.1951 | -0.0193 |
| O | 4.5593 | -2.2396 | 0.0877 |
| H | 4.0308 | -3.0465 | 0.1127 |

| Compound 98 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.706600899 | | |
| C | -4.6739 | 0.0883 | 0.2994 |
| C | -3.846 | -0.9335 | -0.1263 |
| C | -2.4596 | -0.7437 | -0.2111 |
| C | -1.9075 | 0.4986 | 0.1304 |
| C | -2.7616 | 1.5208 | 0.5719 |
| C | -4.1263 | 1.319 | 0.6525 |
| C | -0.4649 | 0.7681 | 0.0245 |
| C | 0.09 | 1.9746 | -0.2237 |
| C | 1.5219 | 2.1519 | -0.2836 |
| O | 2.0457 | 3.2567 | -0.4859 |
| C | 2.3046 | 0.9303 | -0.1038 |
| C | 3.7062 | 0.9109 | -0.1603 |
| C | 4.4066 | -0.2612 | 0.0012 |
| C | 3.7096 | -1.4617 | 0.2234 |
| C | 2.3259 | -1.4789 | 0.2863 |
| C | 1.6489 | -0.2795 | 0.1223 |
| O | 0.2878 | -0.3426 | 0.2051 |
| O | -1.7683 | -1.8243 | -0.6717 |
| O | -4.3896 | -2.1392 | -0.4668 |
| H | -5.7411 | -0.0911 | 0.3612 |
| H | -2.3389 | 2.4722 | 0.8695 |
| H | -4.7721 | 2.1155 | 1.0012 |
| H | 1.7819 | -2.3987 | 0.4603 |
| H | -0.8232 | -1.7211 | -0.503 |
| H | -3.679 | -2.7501 | -0.6965 |
| H | -0.5443 | 2.8338 | -0.3925 |
| H | 4.2338 | 1.8409 | -0.3361 |
| H | 5.49 | -0.2735 | -0.0422 |
| O | 4.3549 | -2.6428 | 0.3862 |
| H | 5.3079 | -2.5157 | 0.3237 |

**Table S4.** (cont.)

| Compound 99 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.711448908 | | |
| C | 4.5645 | -0.3219 | -0.122 |
| C | 3.6705 | -1.2843 | 0.322 |
| C | 2.3082 | -1.0116 | 0.3575 |
| C | 1.8223 | 0.2504 | -0.0461 |
| C | 2.756 | 1.1953 | -0.4951 |
| C | 4.1093 | 0.9317 | -0.5387 |
| C | 0.4043 | 0.6179 | 0.0087 |
| C | -0.0828 | 1.8677 | 0.1907 |
| C | -1.4992 | 2.1354 | 0.2102 |
| O | -1.9585 | 3.2787 | 0.3551 |
| C | -2.3556 | 0.958 | 0.0657 |
| C | -3.7565 | 1.0278 | 0.0896 |
| C | -4.5257 | -0.104 | -0.0474 |
| C | -3.9008 | -1.3515 | -0.2123 |
| C | -2.5202 | -1.4586 | -0.2364 |
| C | -1.773 | -0.298 | -0.0976 |
| O | -0.4173 | -0.449 | -0.1437 |
| O | 1.5224 | -2.0163 | 0.8299 |
| O | 5.8816 | -0.6595 | -0.1395 |
| H | 4.0263 | -2.2564 | 0.6412 |
| H | 2.4028 | 2.1608 | -0.8371 |
| H | 4.8092 | 1.6756 | -0.901 |
| O | -4.6199 | -2.4917 | -0.3569 |
| H | -2.0321 | -2.4164 | -0.3648 |
| H | 0.5904 | -1.808 | 0.6888 |
| H | 6.4095 | 0.073 | -0.4747 |
| H | 0.5996 | 2.6925 | 0.3432 |
| H | -4.2289 | 1.9943 | 0.2185 |
| H | -5.6085 | -0.0474 | -0.0307 |
| H | -5.5618 | -2.291 | -0.3361 |

| Compound 100 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.706461603 | | |
| C | 4.5515 | -0.9046 | 0.0056 |
| C | 3.566 | -1.7671 | -0.441 |
| C | 2.2296 | -1.3783 | -0.4725 |
| C | 1.8798 | -0.0835 | -0.0534 |
| C | 2.8849 | 0.7767 | 0.4067 |
| C | 4.2077 | 0.3752 | 0.435 |
| C | 0.4971 | 0.4196 | -0.1012 |
| C | 0.1361 | 1.6976 | -0.3479 |
| C | -1.2501 | 2.1054 | -0.3536 |
| O | -1.5952 | 3.2769 | -0.5629 |
| C | -2.2114 | 1.0313 | -0.1095 |
| C | -3.5989 | 1.2407 | -0.0967 |
| C | -4.4708 | 0.2018 | 0.1287 |
| C | -3.9675 | -1.0922 | 0.3484 |
| C | -2.6041 | -1.3356 | 0.34 |
| C | -1.7506 | -0.2663 | 0.1126 |
| O | -0.416 | -0.5525 | 0.1288 |
| O | 1.3438 | -2.2994 | -0.9621 |
| O | 5.1373 | 1.2706 | 0.9025 |
| H | 5.5874 | -1.226 | 0.0297 |
| H | 3.8233 | -2.7653 | -0.7755 |
| H | 2.6276 | 1.7673 | 0.7621 |
| O | -4.7878 | -2.1469 | 0.5785 |
| H | -2.2085 | -2.3291 | 0.5089 |
| H | 0.4379 | -2.0234 | -0.7799 |
| H | 6.0142 | 0.8752 | 0.8738 |
| H | 0.8946 | 2.4393 | -0.5576 |
| H | -3.9772 | 2.2416 | -0.2673 |
| H | -5.5425 | 0.3664 | 0.1411 |
| H | -5.7079 | -1.8612 | 0.5778 |

**Table S4.** (cont.)

| Compound 101 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.705974250 | | |
| C | -4.6914 | -0.9381 | 0.0798 |
| C | -4.3487 | 0.2712 | 0.6676 |
| C | -3.0288 | 0.7044 | 0.6182 |
| C | -2.035 | -0.0661 | -0.0122 |
| C | -2.4126 | -1.3004 | -0.5757 |
| C | -3.7352 | -1.7275 | -0.5393 |
| C | -0.6463 | 0.4143 | -0.0967 |
| C | -0.2539 | 1.6525 | -0.4583 |
| C | 1.1433 | 2.0167 | -0.5232 |
| O | 1.5169 | 3.1539 | -0.8435 |
| C | 2.0776 | 0.9403 | -0.2005 |
| C | 3.4704 | 1.109 | -0.234 |
| C | 4.3184 | 0.0677 | 0.0598 |
| C | 3.7842 | -1.1872 | 0.4008 |
| C | 2.4148 | -1.3896 | 0.4433 |
| C | 1.5849 | -0.3192 | 0.1423 |
| O | 0.2436 | -0.5647 | 0.2073 |
| O | -2.6555 | 1.8767 | 1.1952 |
| O | -1.532 | -2.1189 | -1.2187 |
| H | -5.7214 | -1.274 | 0.1137 |
| H | -5.0917 | 0.8829 | 1.1674 |
| H | -3.993 | -2.6759 | -0.9941 |
| O | 4.5807 | -2.2428 | 0.6998 |
| H | 1.997 | -2.3533 | 0.7053 |
| H | -3.424 | 2.2918 | 1.6006 |
| H | -0.6217 | -1.8778 | -1.0105 |
| H | -0.9992 | 2.3931 | -0.7113 |
| H | 3.8718 | 2.0798 | -0.4992 |
| H | 5.3945 | 0.1997 | 0.0331 |
| H | 5.5079 | -1.9874 | 0.6433 |

| Compound 102 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.709944028 | | |
| C | -4.3935 | -0.0827 | 0.1256 |
| C | -3.4949 | -1.0931 | -0.2386 |
| C | -2.1385 | -0.8331 | -0.2696 |
| C | -1.657 | 0.44 | 0.055 |
| C | -2.5562 | 1.4415 | 0.4234 |
| C | -3.9183 | 1.1783 | 0.4581 |
| C | -0.2132 | 0.7107 | -0.0002 |
| C | 0.3547 | 1.929 | -0.163 |
| C | 1.7849 | 2.0988 | -0.1969 |
| O | 2.3226 | 3.2102 | -0.3269 |
| C | 2.5553 | 0.862 | -0.0796 |
| C | 3.9576 | 0.8344 | -0.1147 |
| C | 4.6472 | -0.3499 | -0.0036 |
| C | 3.9377 | -1.5542 | 0.1454 |
| C | 2.5536 | -1.5637 | 0.1834 |
| C | 1.8841 | -0.3525 | 0.0686 |
| O | 0.5239 | -0.4135 | 0.1178 |
| O | -3.942 | -2.3413 | -0.5687 |
| O | -5.7098 | -0.4302 | 0.1313 |
| H | -1.4638 | -1.6287 | -0.56 |
| H | -2.2027 | 2.4258 | 0.7042 |
| H | -4.6225 | 1.9491 | 0.7515 |
| O | 4.5735 | -2.7478 | 0.2567 |
| H | 2.0018 | -2.4881 | 0.2978 |
| H | -4.9038 | -2.3628 | -0.5035 |
| H | -6.2585 | 0.3136 | 0.4014 |
| H | -0.2721 | 2.8018 | -0.2852 |
| H | 4.4947 | 1.7682 | -0.2318 |
| H | 5.7311 | -0.3685 | -0.031 |
| H | 5.5279 | -2.6233 | 0.2145 |

**Table S4.** (cont.)

| Compound 103 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.711369518 | | |
| C | -4.4151 | -0.6301 | 0.0306 |
| C | -4.0433 | 0.6712 | 0.3533 |
| C | -2.7103 | 1.0634 | 0.33 |
| C | -1.7364 | 0.1292 | -0.0212 |
| C | -2.0867 | -1.1828 | -0.3377 |
| C | -3.4277 | -1.5484 | -0.3105 |
| C | -0.317 | 0.5323 | -0.0662 |
| C | 0.1345 | 1.7896 | -0.2702 |
| C | 1.5463 | 2.0901 | -0.3009 |
| O | 1.9777 | 3.2396 | -0.4755 |
| C | 2.4244 | 0.936 | -0.1206 |
| C | 3.8243 | 1.0377 | -0.1302 |
| C | 4.6173 | -0.0708 | 0.0476 |
| C | 4.0182 | -1.3278 | 0.2401 |
| C | 2.641 | -1.4659 | 0.253 |
| C | 1.8652 | -0.3283 | 0.0725 |
| O | 0.5161 | -0.514 | 0.1047 |
| O | -4.9659 | 1.6108 | 0.7132 |
| O | -3.7287 | -2.8403 | -0.6333 |
| H | -5.4589 | -0.9275 | 0.0526 |
| H | -2.4521 | 2.0775 | 0.6066 |
| H | -1.3398 | -1.9148 | -0.6146 |
| O | 4.7619 | -2.4467 | 0.4234 |
| H | 2.1752 | -2.4316 | 0.4032 |
| H | -5.8469 | 1.2226 | 0.7203 |
| H | -4.6795 | -2.9832 | -0.5823 |
| H | -0.5694 | 2.5952 | -0.4287 |
| H | 4.2757 | 2.0113 | -0.2793 |
| H | 5.6987 | 0.0099 | 0.043 |
| H | 5.6994 | -2.2262 | 0.4013 |

| Compound 104 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.699972499 | | |
| C | 4.4464 | 0.3827 | -0.4839 |
| C | 3.753 | -0.5923 | 0.2113 |
| C | 2.3661 | -0.4969 | 0.3818 |
| C | 1.6815 | 0.5931 | -0.1603 |
| C | 2.3932 | 1.5774 | -0.8573 |
| C | 3.7634 | 1.4727 | -1.0178 |
| C | 0.2239 | 0.7358 | -0.0072 |
| C | -0.4042 | 1.8894 | 0.3145 |
| C | -1.8421 | 1.9761 | 0.3889 |
| O | -2.4359 | 3.0282 | 0.656 |
| C | -2.5553 | 0.7152 | 0.1362 |
| C | -3.9514 | 0.6099 | 0.1945 |
| C | -4.5552 | -0.6074 | -0.0452 |
| C | -3.7909 | -1.7411 | -0.3419 |
| C | -2.4141 | -1.658 | -0.4024 |
| C | -1.8063 | -0.4174 | -0.1656 |
| O | -0.4501 | -0.4018 | -0.2571 |
| O | 1.702 | -1.4424 | 1.0981 |
| O | 4.3398 | -1.688 | 0.78 |
| H | 5.5203 | 0.2849 | -0.6034 |
| H | 1.8537 | 2.4137 | -1.285 |
| H | 4.3071 | 2.2328 | -1.5651 |
| O | -1.6779 | -2.7646 | -0.6896 |
| H | 2.3403 | -2.0752 | 1.4495 |
| H | 5.2951 | -1.6541 | 0.6653 |
| H | 0.1846 | 2.7727 | 0.5232 |
| H | -4.5373 | 1.4896 | 0.4297 |
| H | -5.634 | -0.6964 | -0.0026 |
| H | -4.2653 | -2.6981 | -0.5256 |
| H | -0.7365 | -2.5555 | -0.6586 |

**Table S4.** (cont.)

| Compound 105 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.705730650 | | |
| C | -4.4125 | -0.0625 | -0.119 |
| C | -3.5897 | -1.052 | 0.3975 |
| C | -2.2133 | -0.8651 | 0.4382 |
| C | -1.6413 | 0.333 | -0.036 |
| C | -2.5044 | 1.3078 | -0.5566 |
| C | -3.8713 | 1.1297 | -0.6059 |
| C | -0.2041 | 0.6157 | 0.0193 |
| C | 0.3457 | 1.8391 | 0.206 |
| C | 1.7706 | 2.041 | 0.2213 |
| O | 2.2864 | 3.1557 | 0.3738 |
| C | 2.5803 | 0.8226 | 0.0597 |
| C | 3.9798 | 0.8448 | 0.0744 |
| C | 4.6836 | -0.3321 | -0.0828 |
| C | 4.0138 | -1.5453 | -0.2616 |
| C | 2.6323 | -1.5892 | -0.2804 |
| C | 1.924 | -0.3918 | -0.1105 |
| O | 0.5628 | -0.4883 | -0.14 |
| O | -1.5009 | -1.8834 | 0.9899 |
| O | -5.7493 | -0.309 | -0.134 |
| H | -4.0128 | -1.9747 | 0.7754 |
| H | -2.0822 | 2.2249 | -0.95 |
| H | -4.5174 | 1.8936 | -1.0228 |
| H | -0.555 | -1.722 | 0.9042 |
| H | -6.2194 | 0.4428 | -0.51 |
| H | -0.2976 | 2.6935 | 0.3662 |
| H | 4.4897 | 1.7904 | 0.2096 |
| H | 5.7669 | -0.3239 | -0.0728 |
| H | 4.5642 | -2.4697 | -0.3928 |
| O | 2.0071 | -2.7831 | -0.4603 |
| H | 1.0533 | -2.6649 | -0.5234 |

| Compound 106 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.700772588 | | |
| C | -4.4243 | -0.6622 | 0.0322 |
| C | -3.4879 | -1.5583 | 0.5165 |
| C | -2.1342 | -1.2356 | 0.5488 |
| C | -1.7167 | 0.0224 | 0.0852 |
| C | -2.6729 | 0.9202 | -0.4062 |
| C | -4.0143 | 0.5858 | -0.4316 |
| C | -0.3097 | 0.4528 | 0.1151 |
| C | 0.1167 | 1.7107 | 0.3643 |
| C | 1.5175 | 2.0558 | 0.3523 |
| O | 1.9224 | 3.2037 | 0.5675 |
| C | 2.4362 | 0.9389 | 0.081 |
| C | 3.8269 | 1.0985 | 0.0514 |
| C | 4.6348 | 0.0077 | -0.1984 |
| C | 4.0807 | -1.2554 | -0.425 |
| C | 2.7106 | -1.4338 | -0.403 |
| C | 1.8967 | -0.3229 | -0.1447 |
| O | 0.5527 | -0.5565 | -0.1395 |
| O | -1.3016 | -2.181 | 1.0823 |
| O | -4.8963 | 1.5119 | -0.9297 |
| H | -5.475 | -0.9313 | 0.0102 |
| H | -3.799 | -2.5292 | 0.8839 |
| H | -2.3612 | 1.8851 | -0.7881 |
| H | -0.3794 | -1.929 | 0.9664 |
| H | -5.7919 | 1.1614 | -0.8923 |
| H | -0.6049 | 2.4834 | 0.5918 |
| H | 4.2483 | 2.0804 | 0.2266 |
| H | 5.7116 | 0.1232 | -0.2222 |
| H | 4.7136 | -2.1125 | -0.6237 |
| O | 2.1914 | -2.6703 | -0.626 |
| H | 1.228 | -2.6416 | -0.6174 |

**Table S4.** (cont.)

| Compound 107 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.701177418 | | |
| C | -4.5716 | -0.5536 | -0.0581 |
| C | -4.0742 | 0.4234 | -0.9085 |
| C | -2.7227 | 0.7528 | -0.8507 |
| C | -1.8697 | 0.1071 | 0.0518 |
| C | -2.3994 | -0.876 | 0.8977 |
| C | -3.7487 | -1.2093 | 0.8478 |
| C | -0.4382 | 0.4531 | 0.1303 |
| C | 0.051 | 1.6494 | 0.5148 |
| C | 1.4709 | 1.9067 | 0.5721 |
| O | 1.938 | 2.9982 | 0.9177 |
| C | 2.3241 | 0.7684 | 0.2012 |
| C | 3.7238 | 0.8367 | 0.2189 |
| C | 4.4663 | -0.2704 | -0.1362 |
| C | 3.8399 | -1.4626 | -0.5158 |
| C | 2.4622 | -1.5503 | -0.5388 |
| C | 1.712 | -0.423 | -0.1758 |
| O | 0.3609 | -0.5746 | -0.224 |
| O | -2.1776 | 1.6929 | -1.6685 |
| O | -1.5377 | -1.4622 | 1.7726 |
| H | -5.624 | -0.8095 | -0.1018 |
| H | -4.7186 | 0.9294 | -1.6187 |
| H | -4.1396 | -1.9688 | 1.5156 |
| H | -2.8584 | 2.059 | -2.243 |
| H | -2.0092 | -2.0885 | 2.3319 |
| H | -0.6381 | 2.436 | 0.7918 |
| H | 4.2028 | 1.7618 | 0.5141 |
| H | 5.5487 | -0.2252 | -0.1246 |
| H | 4.4234 | -2.332 | -0.7957 |
| O | 1.8611 | -2.7122 | -0.9093 |
| H | 0.902 | -2.6128 | -0.882 |

| Compound 108 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.704594122 | | |
| C | -4.2221 | 0.1743 | -0.0864 |
| C | -3.3769 | -0.8997 | 0.2187 |
| C | -2.0077 | -0.7181 | 0.2341 |
| C | -1.4594 | 0.5377 | -0.0517 |
| C | -2.3059 | 1.6011 | -0.3692 |
| C | -3.6807 | 1.4166 | -0.3861 |
| C | -0.0027 | 0.7215 | -0.0074 |
| C | 0.6498 | 1.9015 | 0.1344 |
| C | 2.0869 | 1.9801 | 0.1619 |
| O | 2.6962 | 3.0527 | 0.2754 |
| C | 2.7876 | 0.6906 | 0.0609 |
| C | 4.1837 | 0.5781 | 0.0939 |
| C | 4.7706 | -0.6677 | 0.0018 |
| C | 3.9897 | -1.8219 | -0.123 |
| C | 2.6121 | -1.7307 | -0.1563 |
| C | 2.0222 | -0.4631 | -0.0629 |
| O | 0.6637 | -0.4442 | -0.1092 |
| O | -3.889 | -2.1324 | 0.5092 |
| O | -5.5568 | -0.0919 | -0.0717 |
| H | -1.3752 | -1.5612 | 0.4837 |
| H | -1.9038 | 2.5743 | -0.6215 |
| H | -4.3447 | 2.2368 | -0.6366 |
| H | -4.8513 | -2.099 | 0.455 |
| H | -6.0638 | 0.7072 | -0.251 |
| H | 0.086 | 2.8177 | 0.2431 |
| H | 4.7827 | 1.4749 | 0.1915 |
| H | 5.8495 | -0.7629 | 0.0263 |
| H | 4.4509 | -2.7999 | -0.195 |
| O | 1.8567 | -2.8549 | -0.2767 |
| H | 0.9202 | -2.6234 | -0.2888 |

**Table S4.** (cont.)

| Compound 109 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.705967192 | | |
| C | 4.2722 | 0.3898 | -0.0054 |
| C | 3.8429 | -0.9019 | 0.2842 |
| C | 2.4921 | -1.2279 | 0.2792 |
| C | 1.5589 | -0.2371 | -0.0235 |
| C | 1.9671 | 1.065 | -0.31 |
| C | 3.3245 | 1.3638 | -0.3009 |
| C | 0.1206 | -0.5644 | -0.0506 |
| C | -0.4088 | -1.7955 | -0.2361 |
| C | -1.834 | -2.0166 | -0.2491 |
| O | -2.3338 | -3.1384 | -0.3987 |
| C | -2.6559 | -0.8085 | -0.0845 |
| C | -4.0567 | -0.8357 | -0.096 |
| C | -4.7636 | 0.339 | 0.0609 |
| C | -4.0997 | 1.5592 | 0.2285 |
| C | -2.7196 | 1.6066 | 0.2405 |
| C | -2.0073 | 0.4096 | 0.0844 |
| O | -0.6531 | 0.5238 | 0.1165 |
| O | 4.7255 | -1.897 | 0.5899 |
| O | 3.6813 | 2.6479 | -0.595 |
| H | 5.3299 | 0.6346 | 0.0038 |
| H | 2.1913 | -2.2374 | 0.5285 |
| H | 1.2526 | 1.8415 | -0.5493 |
| H | 5.6247 | -1.5529 | 0.5823 |
| H | 4.6391 | 2.7398 | -0.5689 |
| H | 0.2437 | -2.6435 | -0.3933 |
| H | -4.5645 | -1.7827 | -0.2293 |
| H | -5.8469 | 0.3261 | 0.0542 |
| H | -4.6553 | 2.4817 | 0.3499 |
| O | -2.0805 | 2.7955 | 0.4028 |
| H | -1.1253 | 2.6659 | 0.367 |

| Compound 110 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.703205638 | | |
| C | 4.0566 | 0.3904 | -0.183 |
| C | 3.3247 | -0.7397 | 0.1626 |
| C | 1.9323 | -0.6948 | 0.2093 |
| C | 1.2562 | 0.5046 | -0.0785 |
| C | 2.0199 | 1.6265 | -0.4314 |
| C | 3.3982 | 1.5792 | -0.4843 |
| C | -0.204 | 0.6175 | -0.0067 |
| C | -0.8976 | 1.7515 | 0.2562 |
| C | -2.3366 | 1.7723 | 0.2766 |
| O | -2.9877 | 2.8039 | 0.4914 |
| C | -2.9833 | 0.4724 | 0.0471 |
| C | -4.3754 | 0.3073 | 0.0713 |
| C | -4.9346 | -0.9375 | -0.1305 |
| C | -4.1108 | -2.0474 | -0.3605 |
| C | -2.7366 | -1.9116 | -0.3912 |
| C | -2.191 | -0.6478 | -0.1881 |
| O | -0.8288 | -0.5586 | -0.2388 |
| O | 1.3499 | -1.8673 | 0.5816 |
| O | 4.015 | -1.8829 | 0.4506 |
| H | 1.5172 | 2.5501 | -0.6893 |
| H | 3.977 | 2.4489 | -0.7692 |
| H | 0.4018 | -1.8451 | 0.3979 |
| H | 3.3908 | -2.6023 | 0.6038 |
| H | -0.3675 | 2.6688 | 0.4721 |
| H | -4.9994 | 1.1741 | 0.2542 |
| H | -6.0107 | -1.0603 | -0.1102 |
| H | -4.5525 | -3.0247 | -0.5163 |
| H | -2.0796 | -2.7545 | -0.568 |
| O | 5.4138 | 0.346 | -0.2433 |
| H | 5.7188 | -0.5416 | -0.0202 |

**Table S4.** (cont.)

| Compound 111 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.702145144 | | |
| C | 4.1386 | -0.0979 | 0.098 |
| C | 3.3147 | -1.1623 | -0.2183 |
| C | 1.9231 | -1.013 | -0.2622 |
| C | 1.3641 | 0.2389 | 0.014 |
| C | 2.2008 | 1.3126 | 0.3479 |
| C | 3.5724 | 1.1414 | 0.3847 |
| C | -0.0882 | 0.4712 | -0.053 |
| C | -0.6764 | 1.6384 | -0.3989 |
| C | -2.1108 | 1.7848 | -0.4197 |
| O | -2.6684 | 2.8498 | -0.7122 |
| C | -2.8644 | 0.5698 | -0.0821 |
| C | -4.2661 | 0.5306 | -0.0807 |
| C | -4.9311 | -0.636 | 0.2337 |
| C | -4.2065 | -1.7921 | 0.553 |
| C | -2.8254 | -1.7804 | 0.5593 |
| C | -2.171 | -0.5941 | 0.2408 |
| O | -0.8054 | -0.6257 | 0.2704 |
| O | 1.2366 | -2.1383 | -0.6311 |
| O | 3.88 | -2.3717 | -0.4934 |
| H | 1.7789 | 2.2776 | 0.5981 |
| H | 0.309 | -2.0652 | -0.3757 |
| H | 3.1789 | -3.0154 | -0.6538 |
| H | -0.0654 | 2.4857 | -0.6781 |
| H | -4.8124 | 1.4319 | -0.332 |
| H | -6.0141 | -0.6614 | 0.2336 |
| H | -4.732 | -2.7074 | 0.7991 |
| H | -2.245 | -2.6616 | 0.8041 |
| H | 5.2132 | -0.2416 | 0.1307 |
| O | 4.3415 | 2.2247 | 0.7219 |
| H | 5.2712 | 1.976 | 0.7311 |

| Compound 112 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.698597308 | | |
| C | -4.1681 | -0.9213 | 0.121 |
| C | -3.7907 | 0.3299 | -0.328 |
| C | -2.4432 | 0.6934 | -0.3316 |
| C | -1.4634 | -0.2002 | 0.1228 |
| C | -1.8687 | -1.4777 | 0.56 |
| C | -3.2103 | -1.8258 | 0.5615 |
| C | -0.0489 | 0.2057 | 0.1547 |
| C | 0.4278 | 1.3829 | 0.6116 |
| C | 1.8406 | 1.6756 | 0.6183 |
| O | 2.2955 | 2.7515 | 1.0258 |
| C | 2.701 | 0.5939 | 0.1218 |
| C | 4.0986 | 0.7046 | 0.0787 |
| C | 4.8679 | -0.3419 | -0.3846 |
| C | 4.2544 | -1.5267 | -0.8135 |
| C | 2.8806 | -1.662 | -0.7807 |
| C | 2.1189 | -0.5948 | -0.3127 |
| O | 0.7642 | -0.7718 | -0.3089 |
| O | -2.0801 | 1.9155 | -0.7975 |
| O | -4.6633 | 1.2802 | -0.796 |
| H | -2.8716 | 2.3756 | -1.1037 |
| H | -5.562 | 0.9358 | -0.7927 |
| H | -0.2615 | 2.124 | 0.9911 |
| H | 4.5587 | 1.6255 | 0.4168 |
| H | 5.9469 | -0.251 | -0.4166 |
| H | 4.8613 | -2.3482 | -1.1758 |
| H | 2.3856 | -2.5683 | -1.1074 |
| H | -5.218 | -1.1939 | 0.1183 |
| H | -3.4994 | -2.8092 | 0.9108 |
| O | -0.995 | -2.4127 | 1.0479 |
| H | -0.0894 | -2.206 | 0.7912 |

**Table S4.** (cont.)

| Compound 113 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.703666852 | | |
| C | 4.0217 | -0.4359 | 0.032 |
| C | 3.1431 | -1.4635 | 0.3189 |
| C | 1.767 | -1.248 | 0.3071 |
| C | 1.2601 | 0.0297 | 0.0129 |
| C | 2.1746 | 1.0545 | -0.2901 |
| C | 3.5315 | 0.8399 | -0.2847 |
| C | -0.1697 | 0.3523 | 0.0427 |
| C | -0.6978 | 1.5753 | 0.2948 |
| C | -2.118 | 1.8036 | 0.2922 |
| O | -2.6178 | 2.9176 | 0.5026 |
| C | -2.9417 | 0.6119 | 0.0429 |
| C | -4.343 | 0.652 | 0.0391 |
| C | -5.0738 | -0.4964 | -0.185 |
| C | -4.4159 | -1.7129 | -0.4098 |
| C | -3.0362 | -1.7793 | -0.4119 |
| C | -2.316 | -0.6102 | -0.1853 |
| O | -0.9543 | -0.7197 | -0.2068 |
| O | 1.0044 | -2.3325 | 0.6299 |
| H | 0.0745 | -2.1512 | 0.4464 |
| H | -0.0447 | 2.406 | 0.5237 |
| H | -4.8368 | 1.5999 | 0.2174 |
| H | -6.1565 | -0.4604 | -0.1869 |
| H | -4.992 | -2.6139 | -0.5852 |
| H | -2.5068 | -2.7085 | -0.5846 |
| H | 3.5221 | -2.4513 | 0.5559 |
| H | 1.8138 | 2.0412 | -0.5542 |
| O | 5.3719 | -0.5794 | 0.021 |
| H | 5.6235 | -1.4827 | 0.242 |
| O | 4.3828 | 1.8688 | -0.5953 |
| H | 5.2905 | 1.5451 | -0.5819 |

| Compound 114 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.705948370 | | |
| C | 4.1831 | -0.3495 | -0.0244 |
| C | 3.3341 | -1.3437 | 0.4439 |
| C | 1.9648 | -1.1182 | 0.4522 |
| C | 1.416 | 0.1072 | 0.0172 |
| C | 2.3153 | 1.0824 | -0.4615 |
| C | 3.6832 | 0.8633 | -0.4849 |
| C | -0.026 | 0.3667 | 0.0794 |
| C | -0.6198 | 1.518 | 0.4688 |
| C | -2.0526 | 1.6615 | 0.501 |
| O | -2.6103 | 2.7119 | 0.8469 |
| C | -2.809 | 0.4632 | 0.1139 |
| C | -4.2108 | 0.4262 | 0.1097 |
| C | -4.8773 | -0.7273 | -0.2471 |
| C | -4.1539 | -1.8724 | -0.6063 |
| C | -2.7728 | -1.8627 | -0.609 |
| C | -2.1163 | -0.6892 | -0.2484 |
| O | -0.7509 | -0.7221 | -0.2795 |
| O | 1.2064 | -2.1348 | 0.9441 |
| H | 0.2759 | -2.0029 | 0.7244 |
| H | -0.0076 | 2.3546 | 0.7727 |
| H | -4.7561 | 1.3188 | 0.3926 |
| H | -5.9604 | -0.751 | -0.2498 |
| H | -4.6803 | -2.7775 | -0.8861 |
| H | -2.1941 | -2.7361 | -0.8838 |
| H | 3.7225 | -2.2922 | 0.7951 |
| O | 1.8007 | 2.2475 | -0.9274 |
| O | 5.5311 | -0.5165 | -0.0649 |
| H | 5.7693 | -1.3882 | 0.2685 |
| H | 4.3536 | 1.6246 | -0.8666 |
| H | 2.5146 | 2.809 | -1.2479 |

**Table S4.** (cont.)

| Compound 115 | | | |
|---|---|---|---|
| $N_i = 0$ | E = -953.704588977 | | |
| C | 3.8605 | -0.2279 | -0.0118 |
| C | 2.9917 | -1.283 | 0.2627 |
| C | 1.6213 | -1.081 | 0.2787 |
| C | 1.1102 | 0.1939 | 0.0232 |
| C | 1.9733 | 1.2535 | -0.2587 |
| C | 3.3421 | 1.0385 | -0.2755 |
| C | -0.344 | 0.4138 | 0.0567 |
| C | -0.9557 | 1.6013 | 0.2855 |
| C | -2.389 | 1.7253 | 0.2886 |
| O | -2.9693 | 2.8039 | 0.4789 |
| C | -3.1195 | 0.4713 | 0.0629 |
| C | -4.5205 | 0.4083 | 0.0534 |
| C | -5.1643 | -0.793 | -0.1561 |
| C | -4.4172 | -1.9613 | -0.3598 |
| C | -3.0369 | -1.9263 | -0.3557 |
| C | -2.4014 | -0.7048 | -0.1439 |
| O | -1.0378 | -0.7199 | -0.1578 |
| H | -0.3619 | 2.4823 | 0.4872 |
| H | -5.0834 | 1.3202 | 0.2143 |
| H | -6.2467 | -0.8368 | -0.1632 |
| H | -4.925 | -2.9047 | -0.5239 |
| H | -2.4417 | -2.8174 | -0.513 |
| O | 5.2125 | -0.3836 | -0.042 |
| H | 5.4362 | -1.3057 | 0.1312 |
| H | 0.9666 | -1.9142 | 0.5028 |
| H | 1.6022 | 2.2442 | -0.4893 |
| O | 3.5872 | -2.4868 | 0.5068 |
| H | 2.922 | -3.1669 | 0.6551 |
| O | 4.1749 | 2.081 | -0.5643 |
| H | 5.0882 | 1.7712 | -0.5757 |