**Table S1.** Geometry of compound 6c obtained from DFT.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Number** | **Symbol** | **X** | **Y** | **Z** |
| 1 | C | -3.228 | -0.553 | -0.6 |
| 2 | H | -2.162 | -0.63 | -0.836 |
| 3 | H | -3.349 | 0.052 | 0.303 |
| 4 | H | -3.717 | -0.024 | -1.425 |
| 5 | C | -3.819 | -1.905 | -0.413 |
| 6 | C | -3.565 | -2.798 | 0.621 |
| 7 | S | -4.534 | -4.203 | 0.376 |
| 8 | C | -5.188 | -3.533 | -1.068 |
| 9 | N | -6.091 | -4.258 | -1.78 |
| 10 | H | -6.336 | -5.175 | -1.416 |
| 11 | N | -6.691 | -3.813 | -2.915 |
| 12 | C | -7.254 | -4.679 | -3.705 |
| 13 | H | -7.829 | -4.265 | -4.552 |
| 14 | C | -7.218 | -6.154 | -3.634 |
| 15 | C | -5.994 | -6.805 | -3.432 |
| 16 | H | -5.072 | -6.237 | -3.332 |
| 17 | C | -5.949 | -8.196 | -3.385 |
| 18 | H | -5.003 | -8.707 | -3.227 |
| 19 | C | -7.12 | -8.931 | -3.555 |
| 20 | H | -7.085 | -10.017 | -3.523 |
| 21 | C | -8.339 | -8.282 | -3.783 |
| 22 | H | -9.217 | -8.903 | -3.927 |
| 23 | C | -8.401 | -6.885 | -3.832 |
| 24 | O | -9.542 | -6.163 | -4.066 |
| 25 | C | -10.786 | -6.878 | -4.074 |
| 26 | H | -10.79 | -7.591 | -4.908 |
| 27 | H | -10.92 | -7.396 | -3.118 |
| 28 | C | -11.908 | -5.853 | -4.275 |
| 29 | H | -11.803 | -5.019 | -3.571 |
| 30 | O | -11.782 | -5.299 | -5.594 |
| 31 | H | -10.879 | -4.933 | -5.653 |
| 32 | C | -13.292 | -6.501 | -4.142 |
| 33 | H | -13.318 | -7.139 | -3.251 |
| 34 | H | -13.508 | -7.088 | -5.043 |
| 35 | O | -14.269 | -5.463 | -3.998 |
| 36 | C | -15.581 | -5.835 | -3.868 |
| 37 | C | -16.508 | -4.804 | -3.643 |
| 38 | C | -16.038 | -3.405 | -3.586 |
| 39 | H | -15.316 | -3.121 | -4.371 |
| 40 | N | -16.371 | -2.468 | -2.746 |
| 41 | N | -17.142 | -2.794 | -1.676 |
| 42 | H | -17.202 | -3.766 | -1.386 |
| 43 | C | -17.83 | -1.884 | -0.936 |
| 44 | S | -18.745 | -2.427 | 0.417 |
| 45 | N | -17.885 | -0.587 | -1.14 |
| 46 | C | -18.682 | 0.032 | -0.189 |
| 47 | C | -18.825 | 1.509 | -0.276 |
| 48 | H | -19.847 | 1.78 | -0.557 |
| 49 | H | -18.148 | 1.923 | -1.031 |
| 50 | H | -18.584 | 1.98 | 0.682 |
| 51 | C | -19.259 | -0.816 | 0.75 |
| 52 | N | -20.08 | -0.614 | 1.817 |
| 53 | N | -20.716 | 0.46 | 1.825 |
| 54 | C | -21.517 | 0.539 | 2.977 |
| 55 | C | -22.702 | -0.199 | 3.087 |
| 56 | H | -23.002 | -0.861 | 2.279 |
| 57 | C | -23.504 | -0.089 | 4.226 |
| 58 | H | -24.422 | -0.67 | 4.288 |
| 59 | C | -23.132 | 0.76 | 5.274 |
| 60 | C | -24.009 | 0.904 | 6.483 |
| 61 | H | -24.541 | -0.03 | 6.693 |
| 62 | H | -24.742 | 1.701 | 6.32 |
| 63 | H | -23.414 | 1.145 | 7.37 |
| 64 | C | -21.961 | 1.519 | 5.154 |
| 65 | H | -21.666 | 2.203 | 5.946 |
| 66 | C | -21.161 | 1.407 | 4.014 |
| 67 | H | -20.253 | 2 | 3.932 |
| 68 | C | -17.878 | -5.078 | -3.537 |
| 69 | H | -18.599 | -4.272 | -3.419 |
| 70 | C | -18.329 | -6.393 | -3.61 |
| 71 | H | -19.391 | -6.613 | -3.526 |
| 72 | C | -17.415 | -7.426 | -3.804 |
| 73 | H | -17.766 | -8.454 | -3.865 |
| 74 | C | -16.049 | -7.15 | -3.937 |
| 75 | H | -15.382 | -7.99 | -4.101 |
| 76 | N | -4.731 | -2.337 | -1.363 |
| 77 | N | -2.762 | -2.759 | 1.72 |
| 78 | N | -1.828 | -1.931 | 1.688 |
| 79 | C | -1.085 | -1.994 | 2.88 |
| 80 | C | -1.198 | -0.969 | 3.824 |
| 81 | H | -1.877 | -0.14 | 3.641 |
| 82 | C | -0.445 | -1.001 | 5.001 |
| 83 | H | -0.547 | -0.192 | 5.72 |
| 84 | C | 0.432 | -2.064 | 5.251 |
| 85 | C | 1.265 | -2.083 | 6.499 |
| 86 | H | 0.739 | -1.595 | 7.326 |
| 87 | H | 2.212 | -1.563 | 6.324 |
| 88 | H | 1.477 | -3.111 | 6.811 |
| 89 | C | 0.566 | -3.077 | 4.294 |
| 90 | H | 1.258 | -3.899 | 4.458 |
| 91 | C | -0.188 | -3.042 | 3.118 |
| 92 | H | -0.076 | -3.833 | 2.382 |

**Table S2.** Geometry of compound 6f obtained from DFT.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Number** | **Symbol** | **X** | **Y** | **Z** |
| 1 | C | -3.552 | -0.215 | -0.211 |
| 2 | H | -2.984 | 0.051 | 0.686 |
| 3 | H | -4.529 | 0.275 | -0.149 |
| 4 | H | -3.035 | 0.184 | -1.09 |
| 5 | C | -3.704 | -1.69 | -0.313 |
| 6 | C | -2.707 | -2.622 | -0.582 |
| 7 | S | -3.423 | -4.189 | -0.621 |
| 8 | C | -4.97 | -3.521 | -0.263 |
| 9 | N | -6.036 | -4.355 | -0.141 |
| 10 | H | -5.865 | -5.349 | -0.263 |
| 11 | N | -7.302 | -3.93 | 0.106 |
| 12 | C | -8.155 | -4.773 | 0.611 |
| 13 | H | -9.2 | -4.425 | 0.68 |
| 14 | C | -7.912 | -6.134 | 1.134 |
| 15 | C | -6.813 | -6.374 | 1.969 |
| 16 | H | -6.132 | -5.57 | 2.238 |
| 17 | C | -6.601 | -7.649 | 2.489 |
| 18 | H | -5.746 | -7.84 | 3.134 |
| 19 | C | -7.489 | -8.679 | 2.186 |
| 20 | H | -7.317 | -9.677 | 2.583 |
| 21 | C | -8.602 | -8.434 | 1.378 |
| 22 | H | -9.265 | -9.263 | 1.15 |
| 23 | C | -8.836 | -7.153 | 0.867 |
| 24 | O | -9.905 | -6.854 | 0.062 |
| 25 | C | -11.131 | -7.506 | 0.433 |
| 26 | H | -11.115 | -8.536 | 0.058 |
| 27 | H | -11.25 | -7.496 | 1.523 |
| 28 | C | -12.278 | -6.733 | -0.223 |
| 29 | H | -12.166 | -5.656 | -0.052 |
| 30 | O | -12.21 | -6.935 | -1.642 |
| 31 | H | -11.317 | -6.656 | -1.919 |
| 32 | C | -13.64 | -7.22 | 0.284 |
| 33 | H | -13.594 | -7.379 | 1.369 |
| 34 | H | -13.917 | -8.15 | -0.226 |
| 35 | O | -14.619 | -6.211 | -0.009 |
| 36 | C | -15.787 | -6.312 | 0.701 |
| 37 | C | -16.445 | -5.122 | 1.044 |
| 38 | C | -15.828 | -3.824 | 0.7 |
| 39 | H | -14.736 | -3.769 | 0.853 |
| 40 | N | -16.4 | -2.739 | 0.266 |
| 41 | N | -17.711 | -2.791 | -0.086 |
| 42 | H | -18.119 | -3.688 | -0.332 |
| 43 | C | -18.517 | -1.699 | -0.159 |
| 44 | S | -20.152 | -1.897 | -0.659 |
| 45 | N | -18.187 | -0.459 | 0.128 |
| 46 | C | -19.261 | 0.396 | -0.056 |
| 47 | C | -19.036 | 1.842 | 0.206 |
| 48 | H | -19.58 | 2.159 | 1.101 |
| 49 | H | -19.367 | 2.448 | -0.644 |
| 50 | H | -17.973 | 2.049 | 0.368 |
| 51 | C | -20.441 | -0.208 | -0.474 |
| 52 | N | -21.685 | 0.267 | -0.76 |
| 53 | N | -21.985 | 1.359 | -0.235 |
| 54 | C | -23.282 | 1.742 | -0.616 |
| 55 | C | -24.413 | 1.108 | -0.083 |
| 56 | H | -24.29 | 0.287 | 0.619 |
| 57 | C | -25.697 | 1.521 | -0.448 |
| 58 | H | -26.562 | 1.014 | -0.028 |
| 59 | C | -25.852 | 2.579 | -1.342 |
| 60 | Br | -27.588 | 3.142 | -1.836 |
| 61 | C | -24.738 | 3.229 | -1.871 |
| 62 | H | -24.853 | 4.058 | -2.564 |
| 63 | C | -23.456 | 2.811 | -1.503 |
| 64 | H | -22.586 | 3.319 | -1.912 |
| 65 | C | -17.629 | -5.155 | 1.792 |
| 66 | H | -18.105 | -4.235 | 2.123 |
| 67 | C | -18.193 | -6.379 | 2.146 |
| 68 | H | -19.114 | -6.409 | 2.723 |
| 69 | C | -17.571 | -7.566 | 1.764 |
| 70 | H | -18.016 | -8.522 | 2.031 |
| 71 | C | -16.373 | -7.534 | 1.045 |
| 72 | H | -15.925 | -8.479 | 0.752 |
| 73 | N | -4.973 | -2.214 | -0.125 |
| 74 | N | -1.371 | -2.519 | -0.821 |
| 75 | N | -0.818 | -1.488 | -0.385 |
| 76 | C | 0.551 | -1.497 | -0.706 |
| 77 | C | 1.04 | -0.618 | -1.679 |
| 78 | H | 0.354 | 0.047 | -2.198 |
| 79 | C | 2.402 | -0.589 | -1.991 |
| 80 | H | 2.763 | 0.098 | -2.752 |
| 81 | C | 3.28 | -1.438 | -1.32 |
| 82 | Br | 5.124 | -1.4 | -1.738 |
| 83 | C | 2.811 | -2.312 | -0.34 |
| 84 | H | 3.492 | -2.973 | 0.19 |
| 85 | C | 1.449 | -2.336 | -0.032 |
| 86 | H | 1.082 | -3.012 | 0.737 |

**Table S3.** Geometry of compound 9b obtained from DFT.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Number** | **Symbol** | **X** | **Y** | **Z** |
| 1 | O | 2.847 | 0.185 | -0.389 |
| 2 | C | 3.322 | -0.932 | -0.227 |
| 3 | C | 2.562 | -2.106 | -0.777 |
| 4 | S | 3.515 | -3.458 | -0.281 |
| 5 | C | 4.729 | -2.444 | 0.47 |
| 6 | N | 5.783 | -3.127 | 1.022 |
| 7 | H | 5.738 | -4.14 | 0.951 |
| 8 | N | 6.862 | -2.549 | 1.61 |
| 9 | C | 7.618 | -3.274 | 2.384 |
| 10 | H | 8.55 | -2.798 | 2.737 |
| 11 | C | 7.392 | -4.648 | 2.881 |
| 12 | C | 6.136 | -4.992 | 3.4 |
| 13 | H | 5.331 | -4.263 | 3.442 |
| 14 | C | 5.92 | -6.272 | 3.906 |
| 15 | H | 4.949 | -6.541 | 4.313 |
| 16 | C | 6.96 | -7.199 | 3.908 |
| 17 | H | 6.798 | -8.197 | 4.313 |
| 18 | C | 8.219 | -6.85 | 3.41 |
| 19 | H | 8.999 | -7.604 | 3.45 |
| 20 | C | 8.454 | -5.568 | 2.901 |
| 21 | O | 9.662 | -5.133 | 2.418 |
| 22 | C | 10.716 | -6.101 | 2.309 |
| 23 | H | 10.95 | -6.502 | 3.302 |
| 24 | H | 10.411 | -6.902 | 1.625 |
| 25 | C | 11.945 | -5.378 | 1.755 |
| 26 | H | 11.687 | -4.794 | 0.864 |
| 27 | O | 12.407 | -4.437 | 2.739 |
| 28 | H | 11.637 | -3.887 | 2.972 |
| 29 | C | 13.085 | -6.353 | 1.45 |
| 30 | H | 12.735 | -7.169 | 0.809 |
| 31 | H | 13.477 | -6.765 | 2.39 |
| 32 | O | 14.097 | -5.627 | 0.731 |
| 33 | C | 15.366 | -6.015 | 1.065 |
| 34 | C | 16.263 | -5.055 | 1.543 |
| 35 | C | 15.789 | -3.682 | 1.8 |
| 36 | H | 14.838 | -3.611 | 2.354 |
| 37 | N | 16.352 | -2.554 | 1.48 |
| 38 | N | 17.444 | -2.58 | 0.675 |
| 39 | H | 17.655 | -3.421 | 0.145 |
| 40 | C | 18.295 | -1.523 | 0.487 |
| 41 | S | 19.579 | -1.813 | -0.665 |
| 42 | C | 20.211 | -0.216 | -0.493 |
| 43 | N | 21.197 | 0.373 | -1.085 |
| 44 | N | 21.867 | -0.361 | -2.006 |
| 45 | H | 21.6 | -1.318 | -2.221 |
| 46 | C | 22.959 | 0.188 | -2.696 |
| 47 | C | 23.639 | -0.59 | -3.645 |
| 48 | H | 23.322 | -1.61 | -3.845 |
| 49 | C | 24.731 | -0.074 | -4.349 |
| 50 | H | 25.246 | -0.691 | -5.081 |
| 51 | C | 25.16 | 1.23 | -4.114 |
| 52 | H | 26.009 | 1.632 | -4.661 |
| 53 | C | 24.497 | 2.018 | -3.176 |
| 54 | H | 24.828 | 3.036 | -2.989 |
| 55 | C | 23.406 | 1.499 | -2.474 |
| 56 | H | 22.899 | 2.127 | -1.745 |
| 57 | N | 18.282 | -0.359 | 1.037 |
| 58 | C | 19.324 | 0.394 | 0.555 |
| 59 | O | 19.581 | 1.532 | 0.929 |
| 60 | C | 17.572 | -5.419 | 1.871 |
| 61 | H | 18.26 | -4.695 | 2.301 |
| 62 | C | 17.993 | -6.736 | 1.679 |
| 63 | H | 19.011 | -7.023 | 1.934 |
| 64 | C | 17.108 | -7.687 | 1.168 |
| 65 | H | 17.438 | -8.713 | 1.017 |
| 66 | C | 15.796 | -7.327 | 0.855 |
| 67 | H | 15.122 | -8.073 | 0.444 |
| 68 | N | 4.504 | -1.176 | 0.428 |
| 69 | N | 1.463 | -2.046 | -1.451 |
| 70 | N | 0.944 | -3.23 | -1.857 |
| 71 | H | 1.402 | -4.113 | -1.646 |
| 72 | C | -0.254 | -3.269 | -2.588 |
| 73 | C | -0.962 | -2.109 | -2.932 |
| 74 | H | -0.584 | -1.135 | -2.632 |
| 75 | C | -2.153 | -2.181 | -3.661 |
| 76 | H | -2.686 | -1.27 | -3.918 |
| 77 | C | -2.654 | -3.419 | -4.056 |
| 78 | H | -3.579 | -3.476 | -4.623 |
| 79 | C | -1.965 | -4.583 | -3.724 |
| 80 | H | -2.354 | -5.55 | -4.031 |
| 81 | C | -0.774 | -4.507 | -2.995 |
| 82 | H | -0.254 | -5.429 | -2.747 |

**Table S4.** Geometry of compound 9d obtained from DFT.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Number** | **Symbol** | **X** | **Y** | **Z** |
| 1 | O | 3.299 | -0.407 | 0.982 |
| 2 | C | 3.943 | -1.413 | 0.714 |
| 3 | C | 3.729 | -2.051 | -0.629 |
| 4 | S | 4.75 | -3.443 | -0.57 |
| 5 | C | 5.346 | -3.052 | 1.03 |
| 6 | N | 6.275 | -3.93 | 1.525 |
| 7 | H | 6.505 | -4.717 | 0.923 |
| 8 | N | 6.91 | -3.799 | 2.718 |
| 9 | C | 7.503 | -4.838 | 3.232 |
| 10 | H | 8.108 | -4.653 | 4.136 |
| 11 | C | 7.464 | -6.247 | 2.784 |
| 12 | C | 6.233 | -6.829 | 2.456 |
| 13 | H | 5.309 | -6.259 | 2.527 |
| 14 | C | 6.178 | -8.166 | 2.069 |
| 15 | H | 5.223 | -8.622 | 1.817 |
| 16 | C | 7.347 | -8.922 | 2.025 |
| 17 | H | 7.306 | -9.97 | 1.735 |
| 18 | C | 8.573 | -8.347 | 2.375 |
| 19 | H | 9.45 | -8.987 | 2.343 |
| 20 | C | 8.647 | -7.006 | 2.767 |
| 21 | O | 9.801 | -6.372 | 3.151 |
| 22 | C | 11.037 | -7.073 | 2.945 |
| 23 | H | 11.049 | -7.979 | 3.562 |
| 24 | H | 11.144 | -7.321 | 1.883 |
| 25 | C | 12.178 | -6.146 | 3.382 |
| 26 | H | 12.059 | -5.148 | 2.946 |
| 27 | O | 12.107 | -5.986 | 4.808 |
| 28 | H | 11.203 | -5.678 | 5.008 |
| 29 | C | 13.548 | -6.737 | 3.024 |
| 30 | H | 13.532 | -7.11 | 1.993 |
| 31 | H | 13.792 | -7.544 | 3.725 |
| 32 | O | 14.535 | -5.699 | 3.122 |
| 33 | C | 15.838 | -6.032 | 2.856 |
| 34 | C | 16.78 | -4.99 | 2.897 |
| 35 | C | 16.341 | -3.624 | 3.254 |
| 36 | H | 15.641 | -3.567 | 4.105 |
| 37 | N | 16.681 | -2.489 | 2.714 |
| 38 | N | 17.419 | -2.5 | 1.574 |
| 39 | H | 17.458 | -3.347 | 1.015 |
| 40 | C | 18.111 | -1.424 | 1.081 |
| 41 | S | 18.924 | -1.707 | -0.444 |
| 42 | C | 19.521 | -0.089 | -0.529 |
| 43 | N | 20.224 | 0.51 | -1.432 |
| 44 | N | 20.567 | -0.229 | -2.515 |
| 45 | H | 20.279 | -1.2 | -2.61 |
| 46 | C | 21.336 | 0.337 | -3.543 |
| 47 | C | 21.684 | -0.444 | -4.656 |
| 48 | H | 21.359 | -1.479 | -4.721 |
| 49 | C | 22.45 | 0.089 | -5.698 |
| 50 | H | 22.707 | -0.535 | -6.55 |
| 51 | C | 22.877 | 1.413 | -5.636 |
| 52 | Cl | 23.819 | 2.07 | -6.917 |
| 53 | C | 22.544 | 2.207 | -4.542 |
| 54 | H | 22.873 | 3.241 | -4.486 |
| 55 | C | 21.778 | 1.668 | -3.503 |
| 56 | H | 21.524 | 2.298 | -2.654 |
| 57 | N | 18.248 | -0.243 | 1.577 |
| 58 | C | 19.025 | 0.526 | 0.748 |
| 59 | O | 19.341 | 1.685 | 0.989 |
| 60 | C | 18.141 | -5.244 | 2.682 |
| 61 | H | 18.878 | -4.449 | 2.776 |
| 62 | C | 18.568 | -6.535 | 2.382 |
| 63 | H | 19.624 | -6.737 | 2.218 |
| 64 | C | 17.64 | -7.571 | 2.313 |
| 65 | H | 17.97 | -8.584 | 2.089 |
| 66 | C | 16.283 | -7.323 | 2.55 |
| 67 | H | 15.604 | -8.169 | 2.498 |
| 68 | N | 4.848 | -1.994 | 1.568 |
| 69 | N | 2.951 | -1.608 | -1.559 |
| 70 | N | 2.905 | -2.336 | -2.702 |
| 71 | H | 3.459 | -3.18 | -2.818 |
| 72 | C | 2.08 | -1.935 | -3.764 |
| 73 | C | 1.279 | -0.784 | -3.698 |
| 74 | H | 1.287 | -0.169 | -2.801 |
| 75 | C | 0.466 | -0.408 | -4.772 |
| 76 | H | -0.144 | 0.488 | -4.695 |
| 77 | C | 0.446 | -1.184 | -5.926 |
| 78 | Cl | -0.553 | -0.726 | -7.25 |
| 79 | C | 1.231 | -2.331 | -6.015 |
| 80 | H | 1.219 | -2.941 | -6.915 |
| 81 | C | 2.043 | -2.702 | -4.938 |
| 82 | H | 2.65 | -3.6 | -5.025 |

**Table S5.** Geometry of compound 12c obtained from DFT.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Tag** | **Symbol** | **X** | **Y** | **Z** |
| 1 | O | 0.266 | 0.252 | -1.004 |
| 2 | H | -0.444 | 0.922 | -1.014 |
| 3 | C | 1.354 | 0.828 | -0.275 |
| 4 | H | 1.027 | 0.949 | 0.765 |
| 5 | C | 1.689 | 2.204 | -0.862 |
| 6 | H | 1.857 | 2.112 | -1.941 |
| 7 | H | 2.575 | 2.621 | -0.368 |
| 8 | O | 0.55 | 3.053 | -0.641 |
| 9 | C | 0.78 | 4.399 | -0.784 |
| 10 | C | -0.016 | 5.276 | -0.029 |
| 11 | C | -1.004 | 4.722 | 0.919 |
| 12 | H | -0.667 | 3.83 | 1.476 |
| 13 | N | -2.203 | 5.143 | 1.202 |
| 14 | N | -2.739 | 6.148 | 0.466 |
| 15 | H | -2.355 | 6.362 | -0.451 |
| 16 | C | -3.798 | 6.911 | 0.844 |
| 17 | N | -4.268 | 7.888 | 0.095 |
| 18 | C | -5.349 | 8.502 | 0.706 |
| 19 | C | -6.029 | 9.615 | 0.054 |
| 20 | C | -5.378 | 10.308 | -0.98 |
| 21 | H | -4.375 | 10.016 | -1.287 |
| 22 | C | -5.997 | 11.379 | -1.631 |
| 23 | H | -5.47 | 11.898 | -2.426 |
| 24 | C | -7.28 | 11.764 | -1.253 |
| 25 | Br | -8.124 | 13.21 | -2.13 |
| 26 | C | -7.948 | 11.088 | -0.234 |
| 27 | H | -8.952 | 11.38 | 0.061 |
| 28 | C | -7.325 | 10.017 | 0.416 |
| 29 | H | -7.88 | 9.502 | 1.195 |
| 30 | C | -5.686 | 7.993 | 1.941 |
| 31 | H | -6.462 | 8.295 | 2.628 |
| 32 | S | -4.635 | 6.7 | 2.342 |
| 33 | C | 0.191 | 6.659 | -0.099 |
| 34 | H | -0.366 | 7.341 | 0.538 |
| 35 | C | 1.144 | 7.177 | -0.975 |
| 36 | H | 1.3 | 8.251 | -1.036 |
| 37 | C | 1.9 | 6.315 | -1.766 |
| 38 | H | 2.638 | 6.719 | -2.454 |
| 39 | C | 1.722 | 4.932 | -1.67 |
| 40 | H | 2.326 | 4.295 | -2.309 |
| 41 | C | 2.534 | -0.141 | -0.34 |
| 42 | H | 2.838 | -0.284 | -1.385 |
| 43 | H | 2.212 | -1.109 | 0.064 |
| 44 | O | 3.614 | 0.385 | 0.427 |
| 45 | C | 4.751 | -0.371 | 0.526 |
| 46 | C | 4.923 | -1.64 | -0.035 |
| 47 | H | 4.141 | -2.127 | -0.609 |
| 48 | C | 6.127 | -2.331 | 0.135 |
| 49 | H | 6.249 | -3.319 | -0.303 |
| 50 | C | 7.168 | -1.767 | 0.87 |
| 51 | H | 8.095 | -2.317 | 1.01 |
| 52 | C | 7.013 | -0.504 | 1.433 |
| 53 | H | 7.818 | -0.08 | 2.029 |
| 54 | C | 5.815 | 0.196 | 1.243 |
| 55 | C | 5.64 | 1.525 | 1.86 |
| 56 | H | 4.7 | 1.658 | 2.425 |
| 57 | N | 6.441 | 2.549 | 1.828 |
| 58 | N | 7.546 | 2.487 | 1.044 |
| 59 | H | 7.637 | 1.756 | 0.344 |
| 60 | C | 8.583 | 3.361 | 1.096 |
| 61 | N | 9.646 | 3.238 | 0.328 |
| 62 | C | 10.553 | 4.256 | 0.577 |
| 63 | C | 11.811 | 4.32 | -0.157 |
| 64 | C | 12.554 | 5.505 | -0.266 |
| 65 | H | 12.21 | 6.432 | 0.187 |
| 66 | C | 13.756 | 5.531 | -0.981 |
| 67 | H | 14.314 | 6.461 | -1.054 |
| 68 | C | 14.223 | 4.371 | -1.595 |
| 69 | Br | 15.847 | 4.408 | -2.562 |
| 70 | C | 13.498 | 3.186 | -1.504 |
| 71 | H | 13.853 | 2.277 | -1.982 |
| 72 | C | 12.298 | 3.164 | -0.79 |
| 73 | H | 11.741 | 2.23 | -0.727 |
| 74 | C | 10.174 | 5.147 | 1.557 |
| 75 | H | 10.696 | 6.006 | 1.953 |
| 76 | S | 8.635 | 4.713 | 2.172 |