

# Supporting Information

## Unraveling the Photodeprotection Mechanism of Anthraquinon-2-ylmethoxycarbonyl Caged Alcohols Using Time-Resolved Spectroscopy

Yan Guo<sup>1</sup>, Qingqing Song<sup>1</sup>, Jialin Wang<sup>1</sup>, Jiani Ma<sup>\*1</sup>, Xiting Zhang<sup>2</sup> and David Lee Phillips<sup>\*2</sup>

- 1 Key Laboratory of Synthetic and Natural Functional Molecule Chemistry of Ministry of Education, College of Chemistry and Materials Science, Northwest University, Xi'an, P. R. China  
2 Department of Chemistry, The University of Hong Kong, Pokfulam Road, Hong Kong S.A.R., P. R. China

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S4

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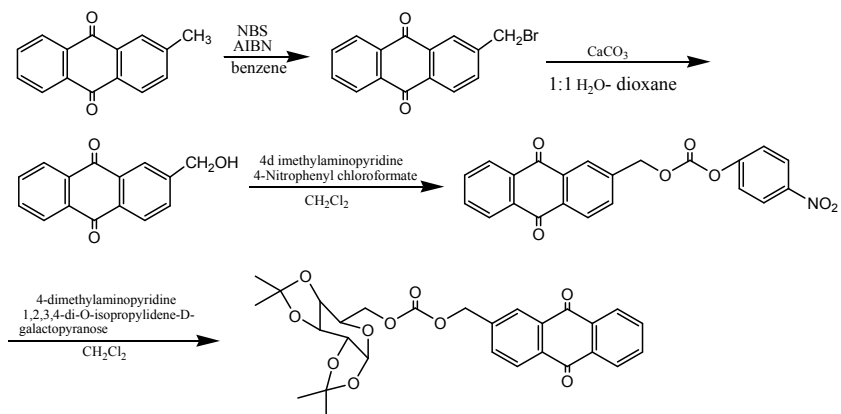
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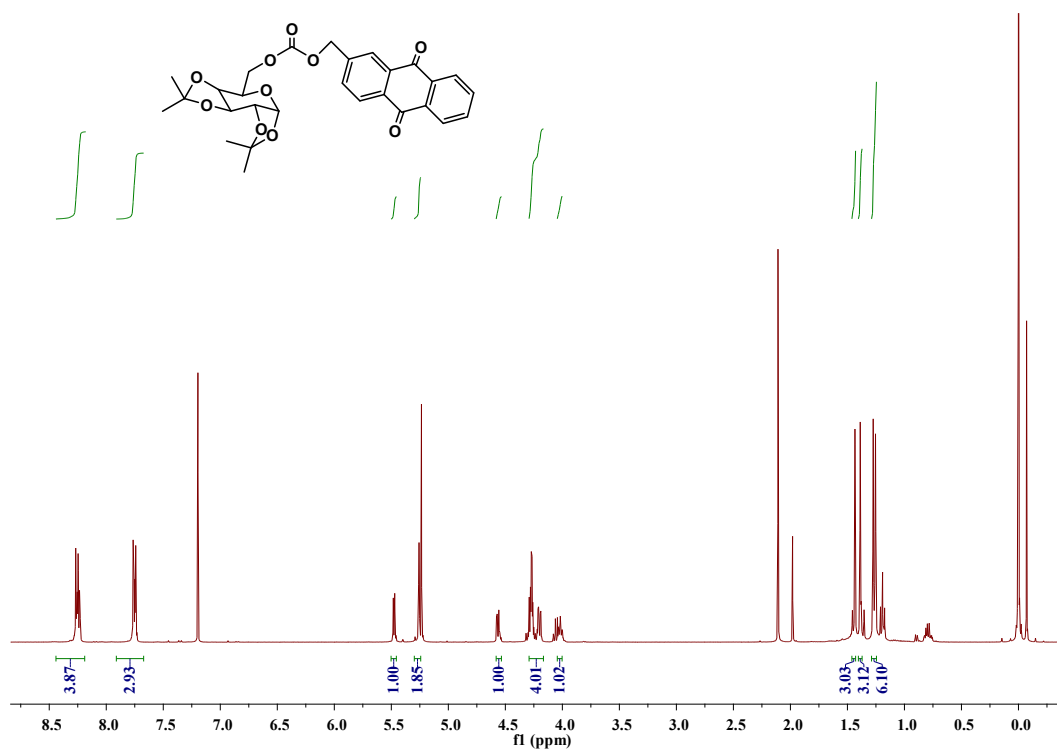
Cartesian coordinates for the optimized geometry for the compounds and intermediates considered in this paper are given.

S8-S34

S1



**Scheme S1.** The synthetic route of the compound **1**.<sup>[1]</sup>

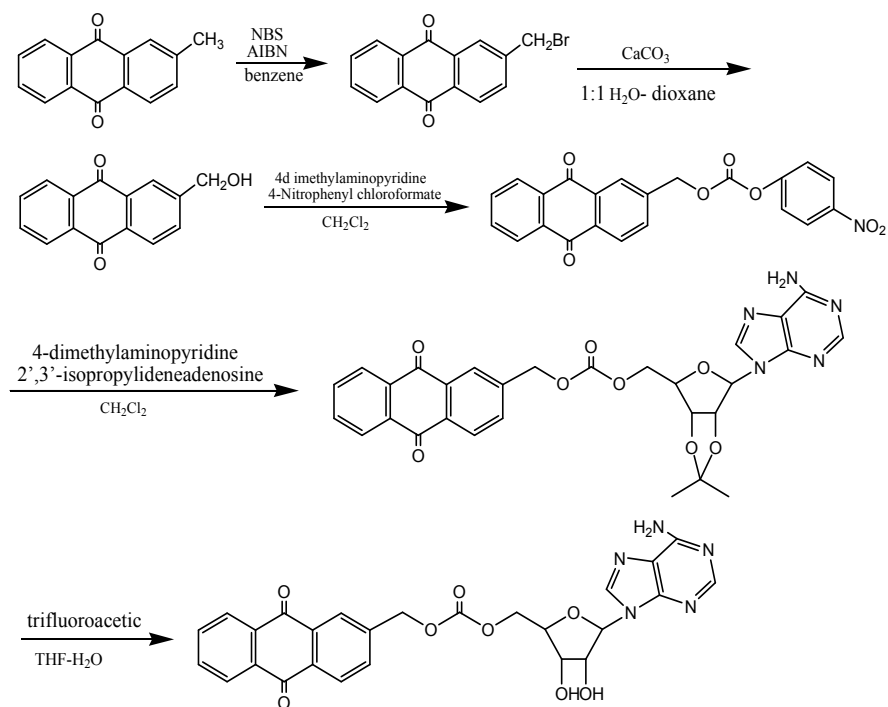


**Figure S1.** The <sup>1</sup>H NMR spectra of **1** in CDCl<sub>3</sub>.

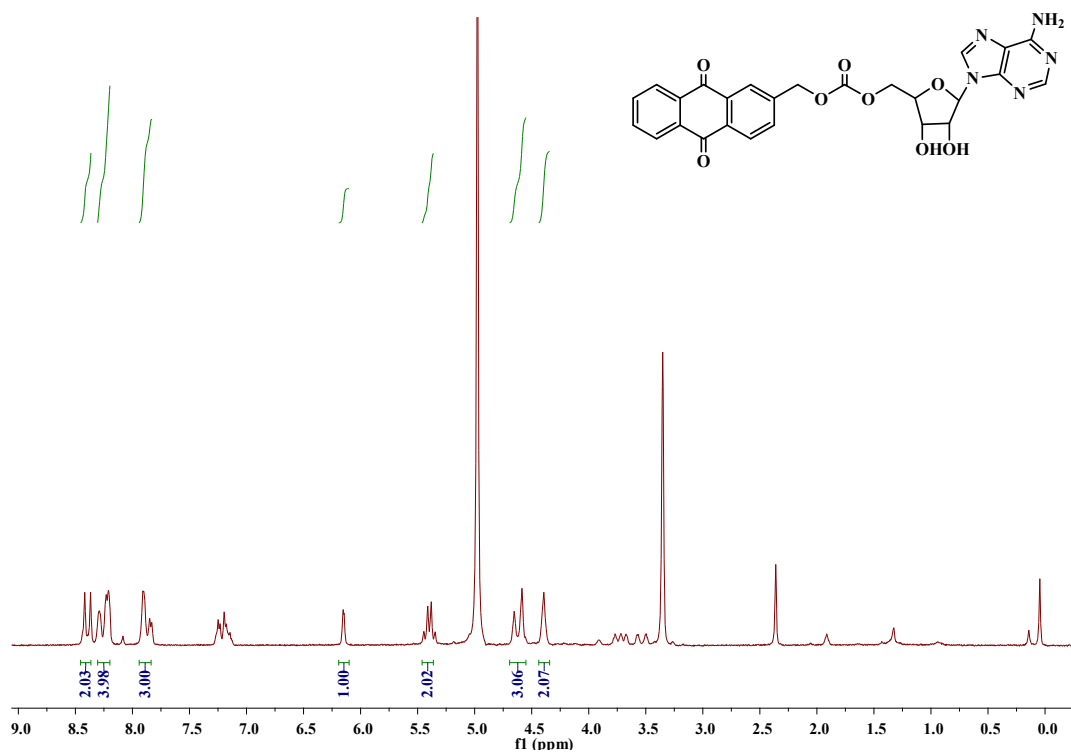
<sup>1</sup>H NMR (CDCl<sub>3</sub>) δ/ppm 8.30-8.25 (4H, m), 7.75-7.82 (3H, m), 5.25 (1H, d, J=5 Hz), 5.32 (2H, s), 4.63 (1H, dd, J=3 & 8 Hz), 4.36-4.32 (3H, m), 4.26 (1H, dd, J=2 & 8 Hz), 4.09 (1H, ddd, J=1.5, 5 & 8 Hz), 1.51 (3H, s), 1.46 (3H, s), 1.35 (3H, s), 1.33 (3H, s).

[1] T. Furuta, Y. Hirayama, M. Iwamura, *Org. Lett.*, **2001**, 3, 1809-1812.

S2



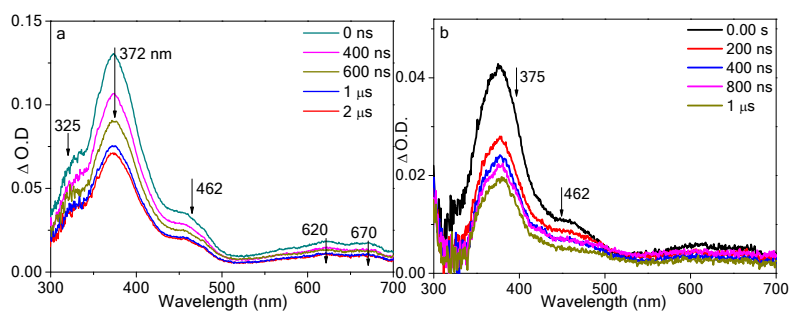
**Scheme S2.** The synthetic route of the compound **2**.



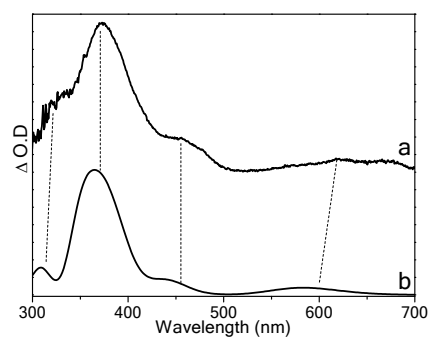
**Figure S2.** The <sup>1</sup>H NMR spectra of **2** in CD<sub>3</sub>OD.

<sup>1</sup>H NMR (CD<sub>3</sub>OD) δ/ppm 8.38-8.20 (5H, m), 7.90-7.80 (3H, m), 6.10 (1H, d, J=5 Hz), 5.38 (1H, d, J=13.5 Hz), 5.34 (1H, d, J=13.5 Hz), 4.61 (1H, m), 4.55-4.53 (2H, m), 4.37-4.32 (2H, m).

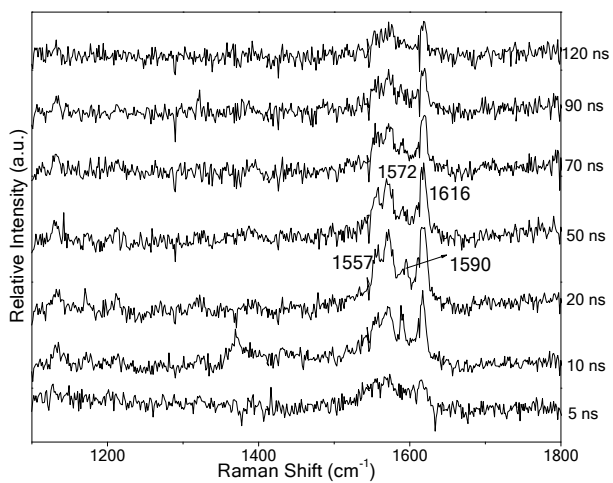
S3



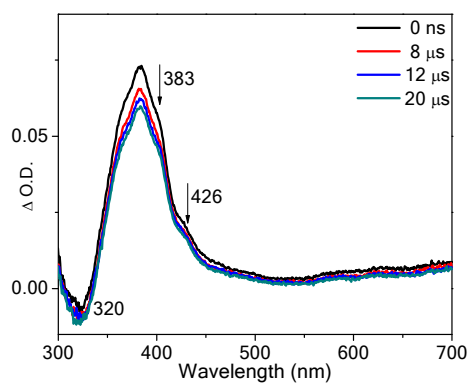
**Figure S3.** Ns-TA spectra of (a) **1** and (b) **2** in ACN obtained at different time delays displayed in different color spectra.



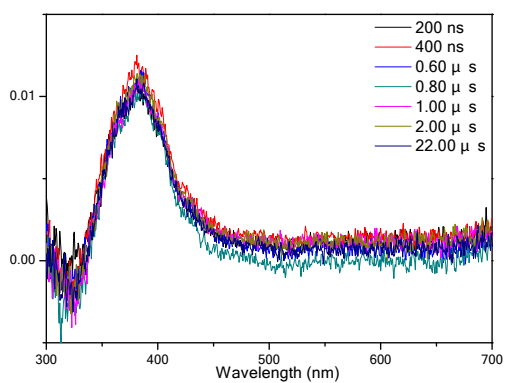
**Figure S4.** Comparison of (a) the ns-TA spectrum of **1** recorded at 400 ns in ACN to the calculated triplet state species of **1** (the scale factor is 1.0 and the half-width is  $1200\text{ cm}^{-1}$ ).



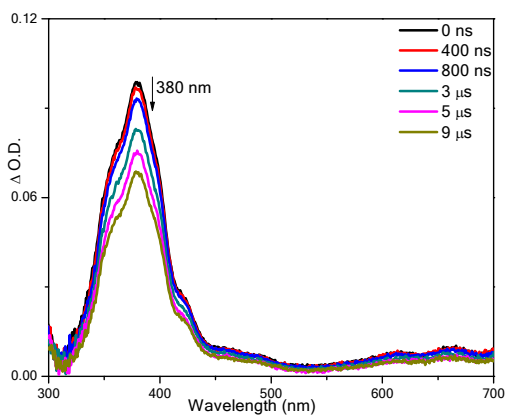
**Figure S5.** The ns-TR<sup>3</sup> spectra of **2** in ACN obtained at various time delays indicated next to the spectra.



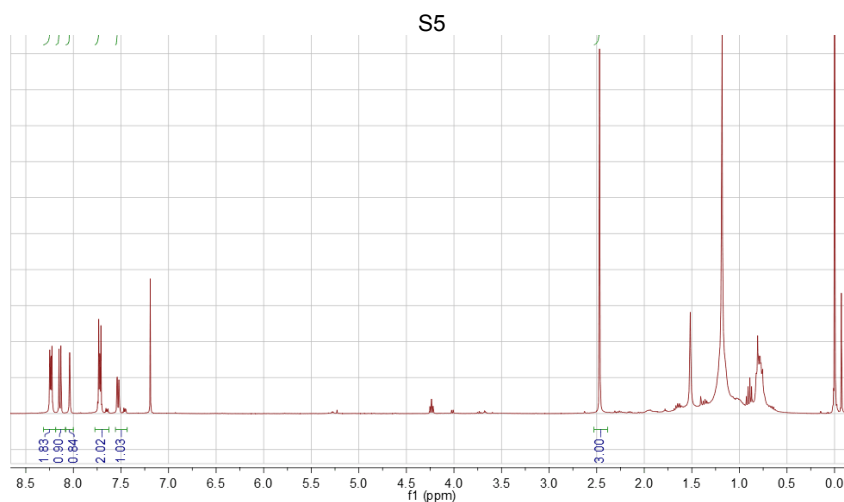
**Figure S6.** The ns-TA results of **1** in IPA under irradiation of 266 nm.



**Figure S7.** The ns-TA spectra of **2** in IPA under irradiation of 266 nm

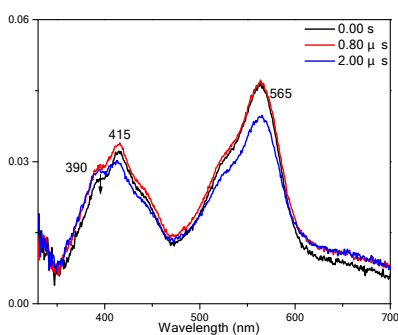


**Figure S8.** The ns-TA spectra of **2** in THF under irradiation of 266 nm.

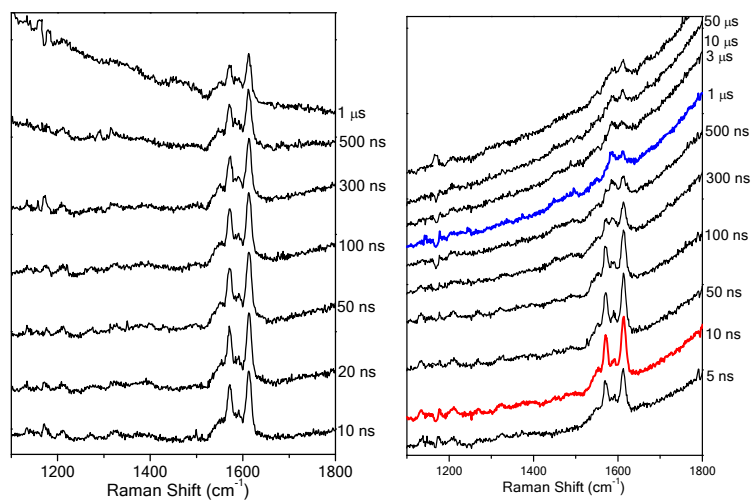


**Figure S9.** The  $^1\text{H}$  NMR spectrum of the photorelease product 2-methylAQ after photolysis experiments of **1** in THF- $\text{H}_2\text{O}$ .

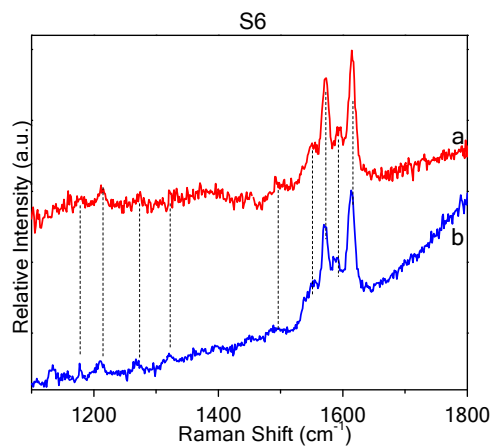
$^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta/\text{ppm}$  8.33–8.29 (m, 2H), 8.23 (1H, d,  $J=7.9$  Hz), 8.16 (1H, d,  $J=1.7$  Hz), 7.82–7.78 (m, 2H), 7.58 (1H, dd,  $J = 7.9, 1.8$  Hz), 2.51 (3H, s).



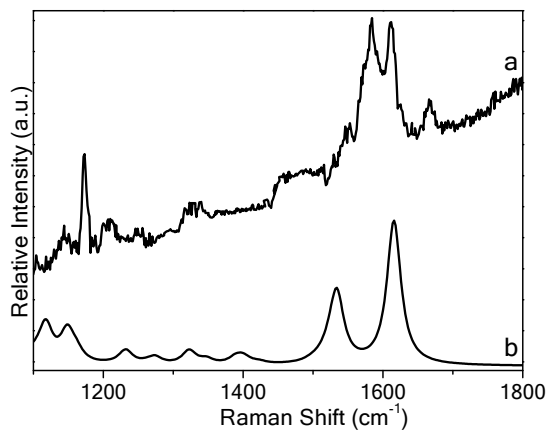
**Figure S10.** ns-TA results of **1** in DMSO under the irradiation of 266 nm.



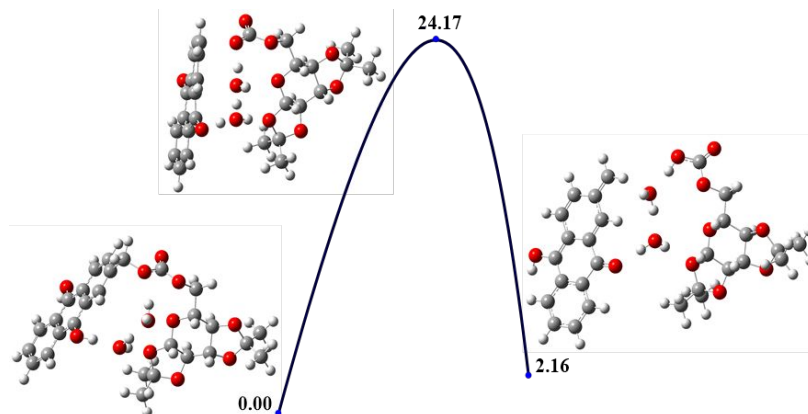
**Figure S11.** The ns-TR<sup>3</sup> results of **1** (left) in THF-H<sub>2</sub>O (1:1) and (right) in THF-KMOPS (1:1) solutions obtained at various time delays indicated next to the spectra.



**Figure S12.** The comparison of the ns-TR<sup>3</sup> spectrum of **1** (a) in IPA at 100 ns with that (b) in THF-H<sub>2</sub>O.



**Figure S13.** Comparison of the ns-TR<sup>3</sup> spectrum of **2** in THF-KMOPS at 10  $\mu$ s to the calculated Raman spectrum of the 2-methyl AQ (the scale factor is 0.975 and the half-width is 12 ).



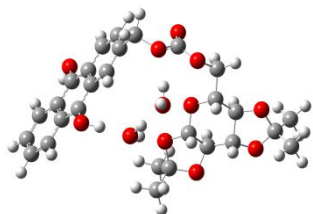


**Figure S14.** Reaction energy profile obtained from (U)B3LYP/6-311G\*\* calculations for the photodeprotection reaction of **1** via ground state surface accompanied by the decarboxylation with the assistance of two water molecules is shown.

S7

Cartesian coordinates for the optimized geometry for the compounds and intermediates considered in this paper are given.

The reaction complex of the photodeprotection process of compound **1** via ground surface:



| Center | Atomic | Atomic | Coordinates |           |           |
|--------|--------|--------|-------------|-----------|-----------|
| Number |        | Number | X           | Y         | Z         |
| 1      | C      | 6      | 0.937434    | -3.033945 | 0.172725  |
| 2      | O      | 8      | 2.375225    | -3.160966 | 0.052335  |
| 3      | C      | 6      | 2.829115    | -1.899958 | -0.402085 |
| 4      | C      | 6      | 1.918511    | -0.976087 | 0.412972  |
| 5      | O      | 8      | 0.666152    | -1.591236 | 0.26656   |
| 6      | C      | 6      | 4.214286    | -1.41131  | -0.075239 |
| 7      | C      | 6      | 4.234732    | 0.055327  | -0.527986 |
| 8      | C      | 6      | 3.232071    | 0.924127  | 0.233687  |
| 9      | O      | 8      | 1.928108    | 0.354291  | -0.02778  |
| 10     | O      | 8      | 5.341319    | -1.910618 | -0.770505 |
| 11     | C      | 6      | 6.32656     | -0.84827  | -0.746708 |
| 12     | O      | 8      | 5.606755    | 0.369132  | -0.3915   |
| 13     | C      | 6      | 3.187228    | 2.368637  | -0.2205   |
| 14     | O      | 8      | 2.239455    | 3.053399  | 0.619485  |
| 15     | C      | 6      | 1.094245    | 3.467948  | 0.04627   |
| 16     | O      | 8      | 0.202971    | 3.613727  | 1.04139   |
| 17     | C      | 6      | 7.366634    | -1.102307 | 0.333141  |
| 18     | C      | 6      | 6.912289    | -0.724975 | -2.143524 |
| 19     | C      | 6      | 0.236327    | -3.552832 | -1.071543 |
| 20     | C      | 6      | 0.508604    | -3.723102 | 1.454561  |
| 21     | O      | 8      | 0.909212    | 3.687567  | -1.117749 |
| 22     | C      | 6      | -1.136382   | 4.083557  | 0.659447  |
| 23     | C      | 6      | -1.995966   | 3.018281  | 0.035217  |
| 24     | C      | 6      | -2.515052   | 2.000812  | 0.796921  |
| 25     | C      | 6      | -3.376197   | 1.012851  | 0.238614  |
| 26     | C      | 6      | -3.746681   | 1.135363  | -1.148781 |

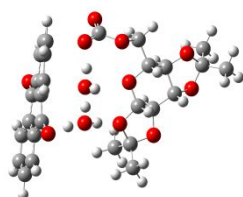
|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 27 | C | 6 | -3.162204 | 2.181764  | -1.922763 |
| 28 | C | 6 | -2.308673 | 3.084074  | -1.355119 |
| 29 | C | 6 | -4.669855 | 0.236127  | -1.700592 |
| 30 | C | 6 | -5.251808 | -0.773941 | -0.916649 |
| 31 | C | 6 | -4.826996 | -0.936114 | 0.452271  |
| 32 | C | 6 | -3.885961 | -0.05073  | 1.011907  |
| 33 | C | 6 | -6.251276 | -1.662277 | -1.421007 |
| 34 | C | 6 | -6.764194 | -2.667448 | -0.647872 |
| 35 | C | 6 | -6.313034 | -2.849674 | 0.687656  |
| S8 |   |   |           |           |           |
| 36 | C | 6 | -5.378825 | -2.004255 | 1.219856  |
| 37 | O | 8 | -3.528171 | -0.224213 | 2.311481  |
| 38 | O | 8 | -4.994833 | 0.40853   | -3.025663 |
| 39 | O | 8 | -0.890081 | -0.556401 | 2.470953  |
| 40 | O | 8 | 0.84029   | 1.529911  | 3.073931  |
| 41 | H | 1 | -1.011621 | 4.934778  | -0.009359 |
| 42 | H | 1 | -1.546175 | 4.424232  | 1.609289  |
| 43 | H | 1 | -2.288064 | 1.939566  | 1.854241  |
| 44 | H | 1 | -1.85666  | 3.862539  | -1.958151 |
| 45 | H | 1 | -3.415776 | 2.245744  | -2.972587 |
| 46 | H | 1 | -5.03697  | -2.114901 | 2.240401  |
| 47 | H | 1 | -6.6442   | -1.520572 | -2.422912 |
| 48 | H | 1 | -6.724196 | -3.654716 | 1.286147  |
| 49 | H | 1 | -7.528452 | -3.32281  | -1.050609 |
| 50 | H | 1 | 2.88092   | 2.455233  | -1.263416 |
| 51 | H | 1 | 4.160903  | 2.837447  | -0.075573 |
| 52 | H | 1 | 3.430424  | 0.895921  | 1.312649  |
| 53 | H | 1 | 3.942112  | 0.088815  | -1.587775 |
| 54 | H | 1 | 2.222964  | -0.996286 | 1.472465  |
| 55 | H | 1 | 4.37887   | -1.479294 | 1.009178  |
| 56 | H | 1 | 2.625533  | -1.771885 | -1.472236 |
| 57 | H | 1 | -2.54133  | -0.279117 | 2.397081  |
| 58 | H | 1 | -5.328707 | -0.4218   | -3.377651 |
| 59 | H | 1 | -0.300586 | 0.170815  | 2.749703  |
| 60 | H | 1 | -0.517161 | -0.878988 | 1.635479  |
| 61 | H | 1 | 0.860753  | 1.959865  | 3.933792  |
| 62 | H | 1 | 0.741643  | 2.244433  | 2.425735  |
| 63 | H | 1 | 6.12813   | -0.472444 | -2.858938 |
| 64 | H | 1 | 7.677146  | 0.053729  | -2.164593 |
| 65 | H | 1 | 7.361869  | -1.673652 | -2.443916 |
| 66 | H | 1 | 6.880812  | -1.248887 | 1.299115  |
| 67 | H | 1 | 7.94805   | -1.994149 | 0.091682  |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 68 | H | 1 | 8.041893  | -0.247622 | 0.411037  |
| 69 | H | 1 | 0.6229    | -3.058432 | -1.963835 |
| 70 | H | 1 | 0.3969    | -4.628677 | -1.164598 |
| 71 | H | 1 | -0.835658 | -3.356704 | -1.00667  |
| 72 | H | 1 | 0.801321  | -4.774437 | 1.419334  |
| 73 | H | 1 | 0.985413  | -3.253949 | 2.315512  |
| 74 | H | 1 | -0.573818 | -3.658643 | 1.577227  |

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# S9

The transition state of photodeprotection process of compound **1** via the ground surface:



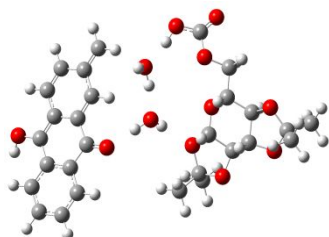
| Center | Atomic | Atomic | Coordinates |           |           |
|--------|--------|--------|-------------|-----------|-----------|
| Number |        | Number | X           | Y         | Z         |
| 1      | C      | 6      | 0.779618    | -2.883151 | 1.245663  |
| 2      | O      | 8      | 2.108934    | -3.117254 | 0.741795  |
| 3      | C      | 6      | 2.483246    | -1.922958 | 0.070543  |
| 4      | C      | 6      | 1.912339    | -0.881578 | 1.033183  |
| 5      | O      | 8      | 0.638899    | -1.414461 | 1.326553  |
| 6      | C      | 6      | 3.927005    | -1.516459 | -0.051459 |
| 7      | C      | 6      | 3.888032    | -0.080494 | -0.601036 |
| 8      | C      | 6      | 3.189453    | 0.91858   | 0.326003  |
| 9      | O      | 8      | 1.840661    | 0.402721  | 0.508809  |
| 10     | O      | 8      | 4.773388    | -2.136668 | -0.998802 |
| 11     | C      | 6      | 5.767192    | -1.13942  | -1.358681 |
| 12     | O      | 8      | 5.257681    | 0.135281  | -0.882441 |
| 13     | C      | 6      | 3.064987    | 2.321242  | -0.239819 |
| 14     | O      | 8      | 2.308093    | 3.093429  | 0.682084  |
| 15     | C      | 6      | 1.167436    | 3.733327  | 0.179157  |
| 16     | O      | 8      | 0.395648    | 4.0845    | 1.139602  |
| 17     | C      | 6      | 7.079976    | -1.411934 | -0.641803 |
| 18     | C      | 6      | 5.888294    | -1.130397 | -2.873962 |
| 19     | C      | 6      | -0.278735   | -3.394213 | 0.282177  |
| 20     | C      | 6      | 0.686541    | -3.479692 | 2.637244  |

|     |   |   |           |           |           |
|-----|---|---|-----------|-----------|-----------|
| 21  | O | 8 | 1.018589  | 3.894243  | -1.018243 |
| 22  | C | 6 | -1.773904 | 4.399539  | 0.422065  |
| 23  | C | 6 | -2.240967 | 3.273733  | -0.21914  |
| 24  | C | 6 | -2.706774 | 2.171918  | 0.546988  |
| 25  | C | 6 | -3.200281 | 1.023908  | -0.036161 |
| 26  | C | 6 | -3.344307 | 0.966738  | -1.483527 |
| 27  | C | 6 | -2.784737 | 2.049872  | -2.257326 |
| 28  | C | 6 | -2.235458 | 3.133402  | -1.661807 |
| 29  | C | 6 | -4.002829 | -0.09708  | -2.055055 |
| 30  | C | 6 | -4.567409 | -1.141384 | -1.251232 |
| 31  | C | 6 | -4.34151  | -1.164879 | 0.158074  |
| 32  | C | 6 | -3.576397 | -0.108681 | 0.79399   |
| 33  | C | 6 | -5.351265 | -2.177477 | -1.813782 |
| 34  | C | 6 | -5.854178 | -3.19567  | -1.029102 |
| 35  | C | 6 | -5.602519 | -3.228675 | 0.354502  |
| 36  | C | 6 | -4.85681  | -2.222042 | 0.933147  |
| S10 |   |   |           |           |           |
| 37  | O | 8 | -3.258764 | -0.192411 | 2.020961  |
| 38  | O | 8 | -4.167717 | -0.113257 | -3.424694 |
| 39  | O | 8 | -0.967488 | 0.234196  | 2.80128   |
| 40  | O | 8 | -0.171779 | 2.543963  | 3.044884  |
| 41  | H | 1 | -1.413685 | 5.25164   | -0.135603 |
| 42  | H | 1 | -1.901286 | 4.524278  | 1.486976  |
| 43  | H | 1 | -2.670518 | 2.239513  | 1.628037  |
| 44  | H | 1 | -1.785931 | 3.923649  | -2.249768 |
| 45  | H | 1 | -2.817947 | 1.965726  | -3.335524 |
| 46  | H | 1 | -4.659426 | -2.207194 | 1.997809  |
| 47  | H | 1 | -5.593733 | -2.153276 | -2.869793 |
| 48  | H | 1 | -6.004511 | -4.031801 | 0.960711  |
| 49  | H | 1 | -6.45934  | -3.971844 | -1.484623 |
| 50  | H | 1 | 2.568312  | 2.314572  | -1.21192  |
| 51  | H | 1 | 4.066086  | 2.748306  | -0.355744 |
| 52  | H | 1 | 3.688126  | 0.958102  | 1.303554  |
| 53  | H | 1 | 3.30899   | -0.091936 | -1.536148 |
| 54  | H | 1 | 2.521149  | -0.866274 | 1.95358   |
| 55  | H | 1 | 4.395013  | -1.533374 | 0.942905  |
| 56  | H | 1 | 1.983107  | -1.848593 | -0.901835 |
| 57  | H | 1 | -1.976196 | 0.141233  | 2.47759   |
| 58  | H | 1 | -4.077933 | -1.018339 | -3.740602 |
| 59  | H | 1 | -0.594034 | 1.235468  | 2.866654  |
| 60  | H | 1 | -0.395434 | -0.341274 | 2.245645  |
| 61  | H | 1 | 0.431838  | 2.696681  | 3.77694   |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 62 | H | 1 | 0.14303   | 3.137703  | 2.260172  |
| 63 | H | 1 | 4.933956  | -0.856304 | -3.32615  |
| 64 | H | 1 | 6.647763  | -0.411223 | -3.186608 |
| 65 | H | 1 | 6.168636  | -2.123163 | -3.232133 |
| 66 | H | 1 | 6.915914  | -1.472289 | 0.435251  |
| 67 | H | 1 | 7.50818   | -2.35467  | -0.987654 |
| 68 | H | 1 | 7.788764  | -0.605025 | -0.839362 |
| 69 | H | 1 | -0.139357 | -2.957205 | -0.70728  |
| 70 | H | 1 | -0.207505 | -4.480659 | 0.20255   |
| 71 | H | 1 | -1.276527 | -3.129531 | 0.63801   |
| 72 | H | 1 | 0.866327  | -4.555358 | 2.587258  |
| 73 | H | 1 | 1.437518  | -3.032173 | 3.289536  |
| 74 | H | 1 | -0.304751 | -3.306075 | 3.060207  |

# S11

The product complex of photodeprotection process of compound **1** via ground surface:

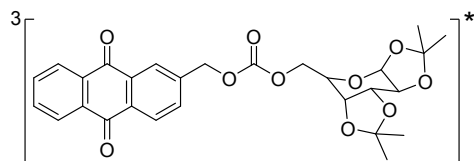


| Center | Atomic | Atomic | Coordinates |           |           |
|--------|--------|--------|-------------|-----------|-----------|
| Number |        | Number | X           | Y         | Z         |
| 1      | C      | 6      | -1.511909   | -2.80834  | 1.068917  |
| 2      | O      | 8      | -2.870198   | -3.101335 | 0.654108  |
| 3      | C      | 6      | -3.576707   | -1.876272 | 0.759568  |
| 4      | C      | 6      | -2.496353   | -0.90365  | 0.284321  |
| 5      | O      | 8      | -1.361108   | -1.354132 | 0.979203  |
| 6      | C      | 6      | -4.7389     | -1.56943  | -0.146599 |
| 7      | C      | 6      | -5.055502   | -0.085056 | 0.096389  |
| 8      | C      | 6      | -3.899446   | 0.845617  | -0.280969 |
| 9      | O      | 8      | -2.781758   | 0.436562  | 0.544369  |
| 10     | O      | 8      | -6.010353   | -2.146454 | 0.083755  |
| 11     | C      | 6      | -6.976513   | -1.204158 | -0.446964 |
| 12     | O      | 8      | -6.268105   | 0.056038  | -0.617452 |

|     |   |   |           |           |           |
|-----|---|---|-----------|-----------|-----------|
| 13  | C | 6 | -4.157256 | 2.308554  | -0.004439 |
| 14  | O | 8 | -2.992579 | 3.007513  | -0.455092 |
| 15  | C | 6 | -2.820829 | 4.273857  | 0.02214   |
| 16  | O | 8 | -1.628566 | 4.734733  | -0.318687 |
| 17  | C | 6 | -7.465076 | -1.650103 | -1.816329 |
| 18  | C | 6 | -8.088391 | -1.050218 | 0.578021  |
| 19  | C | 6 | -1.292864 | -3.207201 | 2.518887  |
| 20  | C | 6 | -0.565921 | -3.486775 | 0.093741  |
| 21  | O | 8 | -3.646316 | 4.874639  | 0.653362  |
| 22  | C | 6 | 2.909792  | 4.142619  | 0.3094    |
| 23  | C | 6 | 3.847625  | 3.160432  | 0.348603  |
| 24  | C | 6 | 3.516879  | 1.821524  | -0.087607 |
| 25  | C | 6 | 4.428108  | 0.807045  | -0.096559 |
| 26  | C | 6 | 5.79278   | 1.05143   | 0.351061  |
| 27  | C | 6 | 6.119382  | 2.380846  | 0.820709  |
| 28  | C | 6 | 5.20797   | 3.375913  | 0.819505  |
| 29  | C | 6 | 6.719292  | 0.043423  | 0.320403  |
| 30  | C | 6 | 6.39492   | -1.281369 | -0.172335 |
| 31  | C | 6 | 5.067878  | -1.58202  | -0.570987 |
| 32  | C | 6 | 4.014289  | -0.544935 | -0.540847 |
| 33  | C | 6 | 7.368194  | -2.292685 | -0.284538 |
| 34  | C | 6 | 7.031055  | -3.560426 | -0.734459 |
| 35  | C | 6 | 5.714594  | -3.856524 | -1.100612 |
| S12 |   |   |           |           |           |
| 36  | C | 6 | 4.74738   | -2.865812 | -1.025108 |
| 37  | O | 8 | 2.859518  | -0.816123 | -0.884811 |
| 38  | O | 8 | 7.99737   | 0.318433  | 0.730446  |
| 39  | O | 8 | 0.289525  | 0.274698  | -0.809296 |
| 40  | O | 8 | 0.122083  | 2.94358   | -1.294224 |
| 41  | H | 1 | 3.144055  | 5.149051  | 0.637851  |
| 42  | H | 1 | 1.909618  | 3.948686  | -0.061067 |
| 43  | H | 1 | 2.499489  | 1.626368  | -0.40278  |
| 44  | H | 1 | 5.475912  | 4.365865  | 1.172272  |
| 45  | H | 1 | 7.128318  | 2.555148  | 1.170798  |
| 46  | H | 1 | 3.723818  | -3.053569 | -1.324244 |
| 47  | H | 1 | 8.40627   | -2.083539 | -0.051648 |
| 48  | H | 1 | 5.456592  | -4.847816 | -1.453637 |
| 49  | H | 1 | 7.799629  | -4.321104 | -0.812385 |
| 50  | H | 1 | -4.31266  | 2.488913  | 1.061004  |
| 51  | H | 1 | -5.042935 | 2.642853  | -0.551284 |
| 52  | H | 1 | -3.635029 | 0.72146   | -1.339256 |
| 53  | H | 1 | -5.232497 | 0.053196  | 1.173336  |

|       |   |   |           |           |           |
|-------|---|---|-----------|-----------|-----------|
| 54    | H | 1 | -2.339319 | -1.030534 | -0.799745 |
| 55    | H | 1 | -4.4358   | -1.728788 | -1.190992 |
| 56    | H | 1 | -3.840805 | -1.663699 | 1.802461  |
| 57    | H | 1 | 1.179265  | -0.108047 | -0.923791 |
| 58    | H | 1 | 8.401944  | -0.480651 | 1.082871  |
| 59    | H | 1 | 0.080812  | 1.985279  | -1.061142 |
| 60    | H | 1 | -0.068346 | -0.144208 | -0.013151 |
| 61    | H | 1 | 0.242926  | 2.966507  | -2.248195 |
| 62    | H | 1 | -1.065917 | 4.018649  | -0.71294  |
| 63    | H | 1 | -7.685388 | -0.660038 | 1.513842  |
| 64    | H | 1 | -8.851038 | -0.363175 | 0.206397  |
| 65    | H | 1 | -8.54904  | -2.020065 | 0.777255  |
| 66    | H | 1 | -6.618359 | -1.808777 | -2.485987 |
| 67    | H | 1 | -8.026325 | -2.582435 | -1.729355 |
| 68    | H | 1 | -8.111326 | -0.884423 | -2.250639 |
| 69    | H | 1 | -2.029291 | -2.722818 | 3.161465  |
| 70    | H | 1 | -1.388372 | -4.289649 | 2.623766  |
| 71    | H | 1 | -0.296108 | -2.904243 | 2.846298  |
| 72    | H | 1 | -0.734052 | -4.565633 | 0.106085  |
| 73    | H | 1 | -0.73974  | -3.118275 | -0.917954 |
| 74    | H | 1 | 0.470776  | -3.283406 | 0.369138  |
| ----- |   |   |           |           |           |

Triplet state of compound 1:



| Center Number | Atomic | Atomic Number | Coordinates |           |           |
|---------------|--------|---------------|-------------|-----------|-----------|
|               |        |               | X           | Y         | Z         |
| 1             | C      | 6             | -3.731163   | -0.597387 | -0.868146 |
| 2             | C      | 6             | -4.993416   | -0.234906 | -0.375563 |
| 3             | C      | 6             | -5.088585   | 0.323606  | 0.91982   |
| 4             | C      | 6             | -3.911656   | 0.498786  | 1.689328  |
| 5             | C      | 6             | -2.687714   | 0.138784  | 1.17501   |
| 6             | C      | 6             | -6.182206   | -0.452301 | -1.223177 |
| 7             | C      | 6             | -6.378873   | 0.699941  | 1.433716  |
| 8             | C      | 6             | -7.576235   | 0.517303  | 0.651582  |
| 9             | C      | 6             | -7.478479   | -0.046374 | -0.643278 |
| 10            | C      | 6             | -8.647875   | -0.222603 | -1.397319 |
| 11            | H      | 1             | -8.540769   | -0.656092 | -2.384455 |
| 12            | C      | 6             | -9.882403   | 0.145385  | -0.892821 |
| 13            | C      | 6             | -9.975899   | 0.705308  | 0.393355  |
| 14            | C      | 6             | -8.843538   | 0.890625  | 1.158887  |
| 15            | H      | 1             | -3.69678    | -1.02818  | -1.862768 |
| 16            | H      | 1             | -3.985848   | 0.919849  | 2.685093  |
| 17            | H      | 1             | -1.793262   | 0.267527  | 1.773236  |
| 18            | H      | 1             | -10.776901  | 0.002703  | -1.487651 |
| 19            | H      | 1             | -10.943133  | 0.994013  | 0.788766  |
| 20            | H      | 1             | -8.912837   | 1.321412  | 2.150783  |
| 21            | C      | 6             | -2.580571   | -0.41263  | -0.120777 |
| 22            | C      | 6             | -1.233686   | -0.76056  | -0.688974 |
| 23            | H      | 1             | -1.333407   | -1.273442 | -1.646461 |
| 24            | H      | 1             | -0.621803   | 0.13251   | -0.838842 |
| 25            | O      | 8             | -0.55903    | -1.628269 | 0.261842  |
| 26            | C      | 6             | 0.717275    | -1.979774 | 0.057303  |
| 27            | O      | 8             | 1.337354    | -2.645046 | 0.839953  |
| 28            | O      | 8             | 1.185207    | -1.499774 | -1.113103 |
| 29            | C      | 6             | 2.571066    | -1.76038  | -1.407969 |
| 30            | H      | 1             | 2.806669    | -2.804037 | -1.1949   |
| 31            | C      | 6             | 3.510208    | -0.867013 | -0.619912 |
| 32            | C      | 6             | 4.994168    | -1.239126 | -0.948153 |
| 33            | H      | 1             | 3.360667    | -1.050608 | 0.448463  |



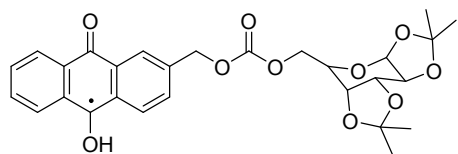
|    |   |   |          |           |           |
|----|---|---|----------|-----------|-----------|
| 34 | C | 6 | 6.030844 | -0.170281 | -0.512373 |
| 35 | H | 1 | 5.099117 | -1.490355 | -2.007838 |
| 36 | C | 6 | 4.054602 | 1.308014  | -0.163452 |
| 37 | C | 6 | 5.441921 | 1.195249  | -0.749742 |
| 38 | H | 1 | 6.967305 | -0.303316 | -1.068151 |
| 39 | H | 1 | 4.024498 | 0.998149  | 0.891478  |

# S14

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 40 | H | 1 | 5.32079   | 1.285569  | -1.841379 |
| 41 | O | 8 | 3.175673  | 0.500197  | -0.910298 |
| 42 | O | 8 | 3.787355  | 2.677888  | -0.287881 |
| 43 | O | 8 | 6.091226  | 2.333889  | -0.227567 |
| 44 | C | 6 | 5.197377  | 4.280913  | -1.404136 |
| 45 | H | 1 | 6.137865  | 4.833611  | -1.357184 |
| 46 | H | 1 | 5.172093  | 3.700548  | -2.327831 |
| 47 | H | 1 | 4.367432  | 4.990249  | -1.422323 |
| 48 | C | 6 | 5.069159  | 3.362636  | -0.197748 |
| 49 | C | 6 | 5.178654  | 4.086154  | 1.133483  |
| 50 | H | 1 | 4.417787  | 4.866042  | 1.202036  |
| 51 | H | 1 | 5.040843  | 3.380097  | 1.953286  |
| 52 | H | 1 | 6.166233  | 4.542448  | 1.229403  |
| 53 | O | 8 | 6.212404  | -0.493461 | 0.857781  |
| 54 | O | 8 | 5.380484  | -2.36881  | -0.177397 |
| 55 | C | 6 | 6.176177  | -1.922051 | 0.952655  |
| 56 | C | 6 | 5.499871  | -2.304646 | 2.258378  |
| 57 | H | 1 | 6.079196  | -1.925602 | 3.102919  |
| 58 | H | 1 | 4.493422  | -1.888989 | 2.304112  |
| 59 | H | 1 | 5.429877  | -3.390927 | 2.336658  |
| 60 | C | 6 | 7.574518  | -2.517781 | 0.813364  |
| 61 | H | 1 | 8.045195  | -2.185849 | -0.113637 |
| 62 | H | 1 | 7.513598  | -3.607658 | 0.793627  |
| 63 | H | 1 | 8.199496  | -2.211397 | 1.65471   |
| 64 | O | 8 | -6.097213 | -0.941672 | -2.349624 |
| 65 | O | 8 | -6.468428 | 1.208834  | 2.628077  |
| 66 | H | 1 | 2.661132  | -1.557823 | -2.475468 |

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Ketyl radical species of compound 1



| Center<br>Number | Atomic | Atomic<br>Number | X         | Coordinates<br>Y | Z         |
|------------------|--------|------------------|-----------|------------------|-----------|
| 1                | C      | 6                | 2.710689  | -0.542318        | 0.149141  |
| 2                | C      | 6                | 3.757003  | -0.587228        | -0.758683 |
| 3                | C      | 6                | 5.067095  | -0.275811        | -0.376525 |
| 4                | C      | 6                | 5.337646  | 0.080479         | 0.970788  |
| 5                | C      | 6                | 4.263368  | 0.108703         | 1.894344  |
| 6                | C      | 6                | 2.982032  | -0.192742        | 1.488745  |
| 7                | C      | 6                | 6.143712  | -0.335217        | -1.383352 |
| 8                | C      | 6                | 6.669643  | 0.393821         | 1.364204  |
| 9                | C      | 6                | 7.755388  | 0.366215         | 0.439279  |
| 10               | C      | 6                | 7.504611  | 0.004875         | -0.916478 |
| 11               | C      | 6                | 8.561707  | -0.02951         | -1.8332   |
| 12               | H      | 1                | 8.327262  | -0.310283        | -2.852669 |
| 13               | C      | 6                | 9.853286  | 0.284585         | -1.446139 |
| 14               | C      | 6                | 10.111175 | 0.645279         | -0.113589 |
| 15               | C      | 6                | 9.086255  | 0.686075         | 0.809667  |
| 16               | H      | 1                | 3.594041  | -0.865157        | -1.793924 |
| 17               | H      | 1                | 4.463552  | 0.370781         | 2.92461   |
| 18               | H      | 1                | 2.170779  | -0.179652        | 2.206383  |
| 19               | H      | 1                | 10.662813 | 0.254278         | -2.165728 |
| 20               | H      | 1                | 11.120143 | 0.894786         | 0.194305  |
| 21               | H      | 1                | 9.331414  | 0.975051         | 1.827821  |
| 22               | O      | 8                | 5.922757  | -0.649206        | -2.553916 |
| 23               | C      | 6                | 1.304154  | -0.814585        | -0.308761 |
| 24               | H      | 1                | 1.300466  | -1.350995        | -1.258584 |
| 25               | H      | 1                | 0.742434  | 0.114558         | -0.440844 |
| 26               | O      | 8                | 0.641109  | -1.611842        | 0.706547  |
| 27               | C      | 6                | -0.652087 | -1.928289        | 0.572238  |
| 28               | O      | 8                | -1.262751 | -2.528516        | 1.412661  |

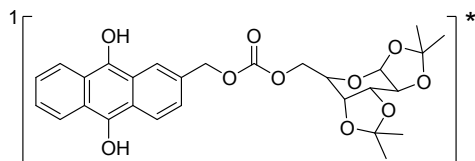
|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 29 | O | 8 | -1.153215 | -1.49542  | -0.60441  |
| 30 | C | 6 | -2.548957 | -1.76151  | -0.840327 |
| 31 | H | 1 | -2.793867 | -2.774785 | -0.520131 |
| 32 | H | 1 | -2.668419 | -1.66175  | -1.918849 |
| 33 | C | 6 | -3.451108 | -0.780526 | -0.118438 |
| 34 | C | 6 | -4.931965 | -1.027271 | -0.427047 |
| 35 | H | 1 | -3.268382 | -0.839833 | 0.960857  |
| 36 | C | 6 | -4.000674 | 1.471991  | 0.030095  |
| 37 | C | 6 | -5.864659 | -0.010644 | 0.241724  |
| 38 | H | 1 | -5.044601 | -0.920661 | -1.516827 |
| 39 | C | 6 | -5.477205 | 1.311679  | -0.358456 |
| 40 | H | 1 | -3.896775 | 1.349421  | 1.122889  |
| 41 | H | 1 | -5.693192 | 0.013447  | 1.326742  |
| 42 | H | 1 | -5.568544 | 1.270548  | -1.450995 |

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|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 43 | O | 8 | -3.150049 | 0.550155  | -0.601499 |
| 44 | O | 8 | -3.738275 | 2.796603  | -0.332223 |
| 45 | O | 8 | -6.003074 | 2.523255  | 0.146066  |
| 46 | C | 6 | -4.87225  | 4.413084  | 1.098493  |
| 47 | H | 1 | -4.586261 | 3.820897  | 1.968836  |
| 48 | H | 1 | -4.1206   | 5.187265  | 0.933186  |
| 49 | H | 1 | -5.834341 | 4.888199  | 1.301567  |
| 50 | C | 6 | -4.984876 | 3.52169   | -0.126242 |
| 51 | C | 6 | -5.302409 | 4.281478  | -1.405249 |
| 52 | H | 1 | -6.221619 | 4.857137  | -1.279975 |
| 53 | H | 1 | -4.48436  | 4.963126  | -1.646994 |
| 54 | H | 1 | -5.429284 | 3.588667  | -2.238351 |
| 55 | O | 8 | -7.124515 | -0.593331 | -0.038759 |
| 56 | O | 8 | -5.494523 | -2.251448 | 0.000116  |
| 57 | C | 6 | -7.419444 | -2.537614 | 1.41389   |
| 58 | H | 1 | -8.499973 | -2.405272 | 1.49707   |
| 59 | H | 1 | -7.180672 | -3.597924 | 1.519585  |
| 60 | H | 1 | -6.933215 | -1.992746 | 2.224476  |
| 61 | C | 6 | -6.93248  | -2.025237 | 0.067363  |
| 62 | C | 6 | -7.623113 | -2.67633  | -1.119731 |
| 63 | H | 1 | -8.685949 | -2.425551 | -1.116502 |
| 64 | H | 1 | -7.18585  | -2.315933 | -2.05217  |
| 65 | H | 1 | -7.513243 | -3.761419 | -1.07119  |
| 66 | O | 8 | 6.843049  | 0.721317  | 2.667886  |
| 67 | H | 1 | 7.772912  | 0.890511  | 2.849149  |

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S17

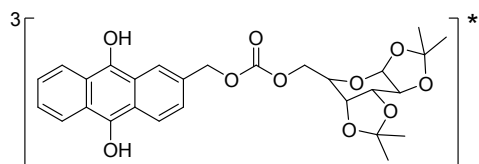
Singlet state of dihydroxy anthraquinone of compound **1**

| Center<br>Number | Atomic | Atomic<br>Number | Coordinates |           |           |
|------------------|--------|------------------|-------------|-----------|-----------|
|                  |        |                  | X           | Y         | Z         |
| 1                | C      | 6                | 2.663951    | -0.286249 | 0.05308   |
| 2                | C      | 6                | 3.742901    | -0.673321 | -0.694537 |
| 3                | C      | 6                | 5.07683     | -0.280135 | -0.367916 |
| 4                | C      | 6                | 5.285084    | 0.483881  | 0.840199  |
| 5                | C      | 6                | 4.132126    | 0.890021  | 1.581613  |
| 6                | C      | 6                | 2.871418    | 0.52942   | 1.205428  |
| 7                | C      | 6                | 6.177938    | -0.617969 | -1.168278 |
| 8                | C      | 6                | 6.591914    | 0.802144  | 1.236558  |
| 9                | C      | 6                | 7.697274    | 0.434221  | 0.449378  |
| 10               | C      | 6                | 7.484811    | -0.270325 | -0.785577 |
| 11               | C      | 6                | 8.615463    | -0.60738  | -1.586862 |
| 12               | H      | 1                | 8.445765    | -1.130536 | -2.518367 |
| 13               | C      | 6                | 9.880641    | -0.277772 | -1.18422  |
| 14               | C      | 6                | 10.091747   | 0.40603   | 0.043455  |
| 15               | C      | 6                | 9.032289    | 0.752742  | 0.836561  |
| 16               | H      | 1                | 3.573811    | -1.32545  | -1.546034 |
| 17               | H      | 1                | 4.250301    | 1.526817  | 2.452274  |
| 18               | H      | 1                | 2.015411    | 0.848631  | 1.787942  |

|     |   |   |           |           |           |
|-----|---|---|-----------|-----------|-----------|
| 19  | H | 1 | 10.731318 | -0.539792 | -1.803254 |
| 20  | H | 1 | 11.101573 | 0.654188  | 0.350328  |
| 21  | H | 1 | 9.184014  | 1.275705  | 1.771251  |
| 22  | O | 8 | 6.039547  | -1.318282 | -2.341383 |
| 23  | O | 8 | 6.856538  | 1.501229  | 2.387142  |
| 24  | C | 6 | 1.271939  | -0.682557 | -0.342071 |
| 25  | H | 1 | 1.279586  | -1.329702 | -1.22021  |
| 26  | H | 1 | 0.654528  | 0.191789  | -0.563712 |
| 27  | O | 8 | 0.671587  | -1.392295 | 0.778737  |
| 28  | C | 6 | -0.606763 | -1.780676 | 0.714617  |
| 29  | O | 8 | -1.175941 | -2.298766 | 1.635105  |
| 30  | O | 8 | -1.147741 | -1.522172 | -0.496351 |
| 31  | C | 6 | -2.539116 | -1.854077 | -0.659754 |
| 32  | H | 1 | -2.7448   | -2.830731 | -0.220218 |
| 33  | H | 1 | -2.688432 | -1.882237 | -1.738861 |
| 34  | C | 6 | -3.452697 | -0.821906 | -0.028378 |
| 35  | C | 6 | -4.931541 | -1.117382 | -0.30057  |
| 36  | H | 1 | -3.261383 | -0.773743 | 1.049936  |
| 37  | C | 6 | -4.033773 | 1.426008  | -0.092082 |
| S18 |   |   |           |           |           |
| 38  | C | 6 | -5.876572 | -0.052987 | 0.269698  |
| 39  | H | 1 | -5.052077 | -1.120748 | -1.39472  |
| 40  | C | 6 | -5.508976 | 1.210616  | -0.457054 |
| 41  | H | 1 | -3.924288 | 1.406006  | 1.00668   |
| 42  | H | 1 | -5.70293  | 0.079665  | 1.346364  |
| 43  | H | 1 | -5.603893 | 1.064186  | -1.540218 |
| 44  | O | 8 | -3.173335 | 0.460298  | -0.63941  |
| 45  | O | 8 | -3.789489 | 2.714365  | -0.576822 |
| 46  | O | 8 | -6.049467 | 2.457694  | -0.067681 |
| 47  | C | 6 | -4.944046 | 4.445953  | 0.694278  |
| 48  | H | 1 | -4.652208 | 3.943582  | 1.617526  |
| 49  | H | 1 | -4.200867 | 5.208841  | 0.454898  |
| 50  | H | 1 | -5.911471 | 4.927692  | 0.850832  |
| 51  | C | 6 | -5.046033 | 3.439141  | -0.438321 |
| 52  | C | 6 | -5.376454 | 4.066426  | -1.784117 |
| 53  | H | 1 | -6.302236 | 4.640616  | -1.712024 |
| 54  | H | 1 | -4.567574 | 4.730771  | -2.09506  |
| 55  | H | 1 | -5.497288 | 3.29353   | -2.544564 |
| 56  | O | 8 | -7.128359 | -0.678411 | 0.052372  |
| 57  | O | 8 | -5.473928 | -2.300842 | 0.249424  |
| 58  | C | 6 | -7.392589 | -2.474463 | 1.690023  |
| 59  | H | 1 | -8.475229 | -2.353406 | 1.761877  |

|       |   |   |           |           |           |
|-------|---|---|-----------|-----------|-----------|
| 60    | H | 1 | -7.135121 | -3.514569 | 1.900421  |
| 61    | H | 1 | -6.915784 | -1.843049 | 2.441233  |
| 62    | C | 6 | -6.915158 | -2.090294 | 0.298292  |
| 63    | C | 6 | -7.597479 | -2.864616 | -0.817501 |
| 64    | H | 1 | -8.662985 | -2.626454 | -0.839153 |
| 65    | H | 1 | -7.16327  | -2.594602 | -1.781437 |
| 66    | H | 1 | -7.475947 | -3.938156 | -0.660819 |
| 67    | H | 1 | 5.163559  | -1.161376 | -2.705929 |
| 68    | H | 1 | 6.131863  | 1.383042  | 3.008309  |
| ----- |   |   |           |           |           |

Triplet state of dihydroxy anthraquinone of compound 1



| Center<br>Number | Atomic | Atomic<br>Number | X         | Coordinate<br>Y | Z         |
|------------------|--------|------------------|-----------|-----------------|-----------|
| 1                | C      | 6                | 2.663513  | -1.11471        | -0.0672   |
| 2                | C      | 6                | 3.568893  | -0.293096       | -0.787123 |
| 3                | C      | 6                | 4.895631  | -0.127819       | -0.380717 |
| 4                | C      | 6                | 5.363407  | -0.85127        | 0.77317   |
| 5                | C      | 6                | 4.459361  | -1.678718       | 1.448828  |
| 6                | C      | 6                | 3.113569  | -1.797956       | 1.040675  |
| 7                | C      | 6                | 5.817536  | 0.725189        | -1.066631 |
| 8                | C      | 6                | 6.729787  | -0.696592       | 1.161411  |
| 9                | C      | 6                | 7.673986  | 0.087679        | 0.415982  |
| 10               | C      | 6                | 7.207698  | 0.814234        | -0.722505 |
| 11               | C      | 6                | 8.10737   | 1.601747        | -1.446692 |
| 12               | H      | 1                | 7.747592  | 2.15735         | -2.302394 |
| 13               | C      | 6                | 9.45611   | 1.675487        | -1.068483 |
| 14               | C      | 6                | 9.908437  | 0.970641        | 0.035784  |
| 15               | C      | 6                | 9.01996   | 0.180609        | 0.78052   |
| 16               | H      | 1                | 3.209219  | 0.18426         | -1.694681 |
| 17               | H      | 1                | 4.777152  | -2.274677       | 2.298903  |
| 18               | H      | 1                | 2.437557  | -2.438359       | 1.590171  |
| 19               | H      | 1                | 10.139813 | 2.289022        | -1.643752 |
| 20               | H      | 1                | 10.949396 | 1.027936        | 0.332426  |
| 21               | H      | 1                | 9.367351  | -0.362445       | 1.649234  |
| 22               | O      | 8                | 5.413823  | 1.489264        | -2.115011 |
| 23               | O      | 8                | 7.221869  | -1.319704       | 2.262688  |
| 24               | C      | 6                | 1.246947  | -1.197839       | -0.568484 |
| 25               | H      | 1                | 1.223952  | -1.53507        | -1.609831 |
| 26               | H      | 1                | 0.758734  | -0.219542       | -0.527335 |
| 27               | O      | 8                | 0.508332  | -2.129188       | 0.24758   |
| 28               | C      | 6                | -0.804915 | -2.300263       | 0.060586  |
| 29               | O      | 8                | -1.466386 | -3.026211       | 0.749497  |
| 30               | O      | 8                | -1.262648 | -1.569063       | -0.977957 |
| 31               | C      | 6                | -2.678378 | -1.642961       | -1.23437  |
| 32               | H      | 1                | -3.020681 | -2.673955       | -1.139987 |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 33 | H | 1 | -2.789871 | -1.294942 | -2.260939 |
| 34 | C | 6 | -3.474729 | -0.764329 | -0.290494 |
| 35 | C | 6 | -4.974482 | -0.787816 | -0.60477  |
| 36 | H | 1 | -3.294574 | -1.080922 | 0.743584  |

S20

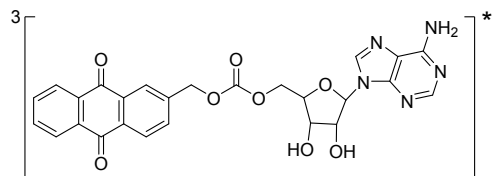
|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 37 | C | 6 | -3.787164 | 1.43949   | 0.372497  |
| 38 | C | 6 | -5.793864 | 0.139759  | 0.300327  |
| 39 | H | 1 | -5.082257 | -0.427907 | -1.639457 |
| 40 | C | 6 | -5.274431 | 1.518372  | 0.001636  |
| 41 | H | 1 | -3.688403 | 1.064582  | 1.406583  |
| 42 | H | 1 | -5.616382 | -0.099041 | 1.358047  |
| 43 | H | 1 | -5.376236 | 1.735116  | -1.069107 |
| 44 | O | 8 | -3.040358 | 0.603924  | -0.474064 |
| 45 | O | 8 | -3.392094 | 2.779223  | 0.307154  |
| 46 | O | 8 | -5.669566 | 2.629843  | 0.780817  |
| 47 | C | 6 | -4.341573 | 4.128836  | 2.102929  |
| 48 | H | 1 | -4.111025 | 3.327611  | 2.806398  |
| 49 | H | 1 | -3.515658 | 4.842562  | 2.094615  |
| 50 | H | 1 | -5.248029 | 4.636797  | 2.438888  |
| 51 | C | 6 | -4.555173 | 3.558045  | 0.711623  |
| 52 | C | 6 | -4.801493 | 4.618338  | -0.350877 |
| 53 | H | 1 | -5.653398 | 5.24019   | -0.068825 |
| 54 | H | 1 | -3.917896 | 5.250808  | -0.45818  |
| 55 | H | 1 | -5.008338 | 4.150582  | -1.314556 |
| 56 | O | 8 | -7.108151 | -0.23668  | -0.068774 |
| 57 | O | 8 | -5.657196 | -2.014785 | -0.445486 |
| 58 | C | 6 | -7.590198 | -2.415836 | 0.929537  |
| 59 | H | 1 | -8.651348 | -2.201793 | 1.071452  |
| 60 | H | 1 | -7.458221 | -3.491235 | 0.793494  |
| 61 | H | 1 | -7.046041 | -2.112854 | 1.825391  |
| 62 | C | 6 | -7.064079 | -1.66821  | -0.285808 |
| 63 | C | 6 | -7.827214 | -1.968176 | -1.56541  |
| 64 | H | 1 | -8.856855 | -1.61539  | -1.476934 |
| 65 | H | 1 | -7.358977 | -1.459397 | -2.409506 |
| 66 | H | 1 | -7.834439 | -3.042876 | -1.757148 |
| 67 | H | 1 | 4.452194  | 1.550851  | -2.116699 |
| 68 | H | 1 | 6.497599  | -1.697257 | 2.772953  |

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S21

Triplet state of compound 2:



| Center Number | Atomic | Atomic Number | X         | Y         | Z         |
|---------------|--------|---------------|-----------|-----------|-----------|
| 1             | C      | 6             | 10.775584 | -0.194735 | 1.435651  |
| 2             | C      | 6             | 9.640854  | -0.940653 | 1.171267  |
| 3             | C      | 6             | 8.491838  | -0.340908 | 0.635231  |
| 4             | C      | 6             | 8.506487  | 1.048529  | 0.364256  |
| 5             | C      | 6             | 9.671813  | 1.8032    | 0.638982  |
| 6             | C      | 6             | 10.786459 | 1.185121  | 1.166361  |
| 7             | C      | 6             | 7.303175  | -1.176376 | 0.370576  |
| 8             | C      | 6             | 7.329813  | 1.672199  | -0.187944 |
| 9             | C      | 6             | 6.145485  | 0.906499  | -0.473882 |
| 10            | C      | 6             | 6.13352   | -0.48125  | -0.202722 |
| 11            | C      | 6             | 4.973994  | -1.218799 | -0.481449 |
| 12            | H      | 1             | 4.999175  | -2.278653 | -0.252782 |
| 13            | C      | 6             | 3.847901  | -0.622522 | -1.023995 |
| 14            | C      | 6             | 3.868516  | 0.764612  | -1.2873   |
| 15            | C      | 6             | 4.988338  | 1.517242  | -1.016925 |
| 16            | H      | 1             | 11.655595 | -0.672509 | 1.849905  |
| 17            | H      | 1             | 9.599141  | -2.005352 | 1.367394  |
| 18            | H      | 1             | 9.677795  | 2.866384  | 0.42963   |
| 19            | H      | 1             | 11.675754 | 1.769633  | 1.373144  |
| 20            | H      | 1             | 2.984211  | 1.240248  | -1.694002 |
| 21            | H      | 1             | 4.995041  | 2.581837  | -1.219399 |
| 22            | C      | 6             | 2.642167  | -1.451003 | -1.370454 |
| 23            | H      | 1             | 2.568963  | -1.621262 | -2.448797 |
| 24            | H      | 1             | 2.678178  | -2.426373 | -0.881925 |
| 25            | O      | 8             | 1.459328  | -0.738132 | -0.938584 |
| 26            | C      | 6             | 0.296107  | -1.307118 | -1.290054 |
| 27            | O      | 8             | -0.692338 | -0.523966 | -0.841653 |
| 28            | O      | 8             | 0.1674    | -2.335381 | -1.901228 |
| 29            | C      | 6             | -2.028449 | -1.007884 | -1.09887  |
| 30            | H      | 1             | -2.145297 | -2.012661 | -0.698075 |

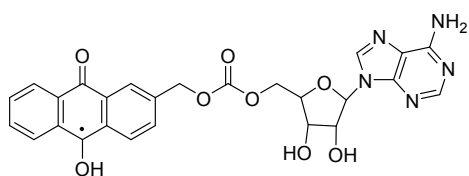
|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 31 | H | 1 | -2.21786  | -1.020587 | -2.173504 |
| 32 | C | 6 | -2.961617 | -0.028911 | -0.411526 |
| 33 | O | 8 | -4.310096 | -0.37311  | -0.787559 |
| 34 | C | 6 | -2.936972 | -0.052441 | 1.12336   |
| 35 | H | 1 | -2.745246 | 0.988957  | -0.75046  |
| 36 | C | 6 | -5.160317 | -0.334727 | 0.350079  |
| 37 | C | 6 | -4.363039 | 0.410828  | 1.447521  |
| 38 | H | 1 | -2.185858 | 0.630462  | 1.527651  |
| 39 | H | 1 | -5.40945  | -1.343608 | 0.687708  |
| 40 | H | 1 | -4.684627 | 0.103283  | 2.448966  |
| 41 | O | 8 | -2.738053 | -1.391952 | 1.556604  |

# S22

|    |   |   |            |           |           |
|----|---|---|------------|-----------|-----------|
| 42 | H | 1 | -2.573613  | -1.387157 | 2.504063  |
| 43 | O | 8 | -4.395842  | 1.817634  | 1.287408  |
| 44 | O | 8 | 7.288198   | -2.383498 | 0.611286  |
| 45 | O | 8 | 7.336487   | 2.952136  | -0.423599 |
| 46 | H | 1 | -5.294373  | 2.127363  | 1.444286  |
| 47 | C | 6 | -7.668018  | -0.094044 | 0.406753  |
| 48 | C | 6 | -6.612453  | 1.388747  | -0.849427 |
| 49 | C | 6 | -8.549876  | 0.797146  | -0.20517  |
| 50 | H | 1 | -5.780879  | 1.868744  | -1.339122 |
| 51 | C | 6 | -9.917215  | 0.596994  | 0.070289  |
| 52 | C | 6 | -9.307431  | -1.189344 | 1.396376  |
| 53 | H | 1 | -9.65117   | -1.992027 | 2.041787  |
| 54 | N | 7 | -10.271329 | -0.415586 | 0.878256  |
| 55 | N | 7 | -7.98667   | -1.102003 | 1.223353  |
| 56 | N | 7 | -10.881723 | 1.399679  | -0.4356   |
| 57 | H | 1 | -11.842448 | 1.13035   | -0.304138 |
| 58 | H | 1 | -10.642958 | 2.071184  | -1.145684 |
| 59 | N | 7 | -7.871871  | 1.713594  | -0.988742 |
| 60 | N | 7 | -6.41137   | 0.302812  | -0.010117 |

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S23

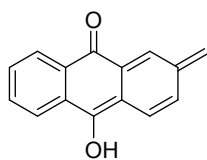
Ketyl radical species of compound **2**

| Center<br>Number | Atomic | Atomic<br>Number | X         | Y         | Z         |
|------------------|--------|------------------|-----------|-----------|-----------|
| 1                | C      | 6                | 3.954506  | -0.245042 | -1.872434 |
| 2                | C      | 6                | 5.061036  | 0.573427  | -1.898982 |
| 3                | C      | 6                | 6.058806  | 0.466467  | -0.897592 |
| 4                | C      | 6                | 5.890998  | -0.497925 | 0.13014   |
| 5                | C      | 6                | 4.750857  | -1.311174 | 0.135765  |
| 6                | C      | 6                | 3.783496  | -1.203574 | -0.850167 |
| 7                | C      | 6                | 7.212893  | 1.300186  | -0.902232 |
| 8                | C      | 6                | 6.893589  | -0.657022 | 1.200745  |
| 9                | C      | 6                | 8.067653  | 0.240065  | 1.145688  |
| 10               | C      | 6                | 8.216644  | 1.204567  | 0.107326  |
| 11               | C      | 6                | 9.3662    | 2.034167  | 0.12543   |
| 12               | H      | 1                | 9.524805  | 2.790026  | -0.638583 |
| 13               | C      | 6                | 10.317243 | 1.90995   | 1.117897  |
| 14               | C      | 6                | 10.162205 | 0.953685  | 2.13444   |
| 15               | C      | 6                | 9.046696  | 0.133582  | 2.140136  |
| 16               | H      | 1                | 3.194904  | -0.147401 | -2.639745 |
| 17               | H      | 1                | 5.181997  | 1.306599  | -2.685153 |
| 18               | H      | 1                | 4.654755  | -2.028323 | 0.942869  |
| 19               | H      | 1                | 11.187417 | 2.556279  | 1.110539  |
| 20               | H      | 1                | 10.912834 | 0.861386  | 2.910377  |
| 21               | H      | 1                | 8.895652  | -0.612398 | 2.910722  |
| 22               | O      | 8                | 1.393486  | -1.277551 | -0.883473 |
| 23               | C      | 6                | 2.584433  | -2.107966 | -0.848706 |
| 24               | H      | 1                | 2.559347  | -2.735849 | 0.042975  |

|     |   |   |            |           |           |
|-----|---|---|------------|-----------|-----------|
| 25  | H | 1 | 2.56939    | -2.763668 | -1.72392  |
| 26  | H | 1 | 0.237628   | -1.950442 | -0.938807 |
| 27  | O | 8 | 0.10842    | -3.146445 | -0.954768 |
| 28  | O | 8 | -0.757531  | -1.050446 | -0.975025 |
| 29  | C | 6 | -2.091631  | -1.602252 | -0.994959 |
| 30  | H | 1 | -2.22295   | -2.232895 | -1.875514 |
| 31  | H | 1 | -2.262215  | -2.19782  | -0.097665 |
| 32  | C | 6 | -3.03437   | -0.405992 | -1.057978 |
| 33  | O | 8 | -4.373071  | -0.890919 | -1.275463 |
| 34  | C | 6 | -3.091254  | 0.424548  | 0.232622  |
| 35  | H | 1 | -2.762659  | 0.220046  | -1.912741 |
| 36  | C | 6 | -5.1489    | -0.782349 | -0.101028 |
| 37  | C | 6 | -4.224565  | -0.239579 | 1.017943  |
| 38  | H | 1 | -2.153805  | 0.380544  | 0.792842  |
| 39  | H | 1 | -5.54036   | -1.76388  | 0.17945   |
| 40  | H | 1 | -4.73895   | 0.492304  | 1.643168  |
| 41  | O | 8 | -3.501928  | 1.764108  | -0.018653 |
| 42  | H | 1 | -2.787895  | 2.218323  | -0.476791 |
| S24 |   |   |            |           |           |
| 43  | O | 8 | -3.674619  | -1.300749 | 1.783327  |
| 44  | H | 1 | -4.376964  | -1.657105 | 2.338548  |
| 45  | C | 6 | -7.387044  | 0.172858  | 0.484917  |
| 46  | C | 6 | -6.556508  | 0.935337  | -1.409942 |
| 47  | C | 6 | -8.244714  | 1.086667  | -0.127659 |
| 48  | H | 1 | -5.850634  | 1.0425    | -2.216489 |
| 49  | C | 6 | -9.44649   | 1.351411  | 0.5573    |
| 50  | C | 6 | -8.753387  | -0.12387  | 2.192442  |
| 51  | H | 7 | -8.992844  | -0.596033 | 3.140641  |
| 52  | N | 7 | -6.300431  | 0.0813    | -0.354234 |
| 53  | N | 7 | -7.708013  | 1.552281  | -1.313613 |
| 54  | N | 7 | -9.675697  | 0.728382  | 1.726372  |
| 55  | N | 7 | -7.582274  | -0.463642 | 1.646871  |
| 56  | N | 7 | -10.382068 | 2.200169  | 0.075562  |
| 57  | H | 1 | -11.177978 | 2.418168  | 0.650718  |
| 58  | H | 1 | -10.185697 | 2.743894  | -0.74725  |
| 59  | O | 8 | 7.298514   | 2.190279  | -1.920521 |
| 60  | O | 8 | 6.761383   | -1.492516 | 2.0958    |
| 61  | H | 1 | 8.117883   | 2.691409  | -1.859328 |

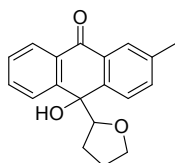
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The transient species IM1:



| Center<br>Number | Atomic | Atomic<br>Number | Coordinate |           |           |
|------------------|--------|------------------|------------|-----------|-----------|
|                  |        |                  | X          | Y         | Z         |
| 1                | C      | 6                | 3.917175   | -0.998066 | -0.013783 |
| 2                | C      | 6                | 2.658157   | -1.582    | 0.030753  |
| 3                | C      | 6                | 1.50457    | -0.795792 | 0.030683  |
| 4                | C      | 6                | 1.60623    | 0.616155  | -0.003545 |
| 5                | C      | 6                | 2.88927    | 1.18846   | -0.078916 |
| 6                | C      | 6                | 4.026845   | 0.392627  | -0.07751  |
| 7                | C      | 6                | 0.176506   | -1.46549  | 0.037516  |
| 8                | C      | 6                | 0.400452   | 1.429674  | 0.026048  |
| 9                | C      | 6                | -0.85278   | 0.876608  | 0.018723  |
| 10               | C      | 6                | -1.012959  | -0.568258 | 0.001077  |
| 11               | C      | 6                | -2.25365   | -1.12282  | -0.021036 |
| 12               | H      | 1                | -2.330562  | -2.204638 | -0.023013 |
| 13               | C      | 6                | -3.462179  | -0.324565 | -0.033352 |
| 14               | C      | 6                | -3.281987  | 1.120688  | -0.000187 |
| 15               | C      | 6                | -2.054724  | 1.68225   | 0.027618  |
| 16               | H      | 1                | 4.807285   | -1.615951 | -0.012437 |
| 17               | H      | 1                | 2.532824   | -2.657528 | 0.059242  |
| 18               | H      | 1                | 3.011714   | 2.262248  | -0.172352 |
| 19               | H      | 1                | 5.004109   | 0.858293  | -0.136589 |
| 20               | H      | 1                | -4.169042  | 1.74493   | 0.004506  |
| 21               | H      | 1                | -1.941407  | 2.758303  | 0.053054  |
| 22               | O      | 8                | 0.075207   | -2.684213 | 0.061491  |
| 23               | O      | 8                | 0.50883    | 2.793064  | 0.026543  |
| 24               | H      | 1                | 1.352361   | 3.049639  | 0.412142  |
| 25               | C      | 6                | -4.68621   | -0.909526 | -0.065762 |
| 26               | H      | 1                | -4.793414  | -1.987199 | -0.085288 |
| 27               | H      | 1                | -5.594456  | -0.318575 | -0.073495 |

The transient species **IM2**:

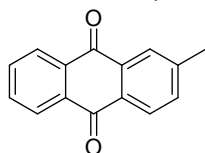


| Center | Atomic | Atomic | Coordinates |           |           |
|--------|--------|--------|-------------|-----------|-----------|
| Number | C      | Number | X           | Y         | Z         |
| 1      | C      | 6      | 3.24547     | 2.245065  | 0.944139  |
| 2      | C      | 6      | 2.496297    | 1.092585  | 1.186268  |
| 3      | C      | 6      | 1.290431    | 0.871117  | 0.534754  |
| 4      | C      | 6      | 0.795053    | 1.867709  | -0.341754 |
| 5      | C      | 6      | 1.568673    | 3.019373  | -0.606272 |
| 6      | C      | 6      | 2.784074    | 3.198353  | 0.032926  |
| 7      | C      | 6      | 0.531153    | -0.451585 | 0.665834  |
| 8      | C      | 6      | -0.535236   | 1.709456  | -0.881792 |
| 9      | C      | 6      | -1.466668   | 0.781681  | -0.288114 |
| 10     | C      | 6      | -0.965134   | -0.209296 | 0.589742  |
| 11     | H      | 6      | -1.871795   | -0.981503 | 1.307105  |
| 12     | C      | 1      | -1.484992   | -1.70256  | 2.015442  |
| 13     | C      | 6      | -3.244976   | -0.839023 | 1.118108  |
| 14     | C      | 6      | -3.75505    | 0.089979  | 0.195188  |
| 15     | H      | 6      | -2.86064    | 0.893209  | -0.497558 |
| 16     | H      | 1      | 4.18762     | 2.393318  | 1.458778  |
| 17     | H      | 1      | 2.857593    | 0.350735  | 1.886238  |
| 18     | H      | 1      | 1.183535    | 3.775636  | -1.279695 |
| 19     | H      | 1      | 3.365917    | 4.092569  | -0.160762 |
| 20     | H      | 1      | -3.929354   | -1.457523 | 1.689506  |
| 21     | C      | 1      | -3.229635   | 1.65155   | -1.178632 |
| 22     | H      | 6      | -5.244687   | 0.226559  | -0.008713 |
| 23     | H      | 1      | -5.681628   | -0.714216 | -0.358079 |
| 24     | H      | 1      | -5.748552   | 0.489299  | 0.926445  |
| 25     | O      | 1      | -5.478143   | 0.998385  | -0.744298 |
| 26     | O      | 8      | -0.940013   | 2.49938   | -1.846459 |
| 27     | H      | 8      | 0.839691    | -1.128648 | 1.872164  |
| 28     | C      | 1      | 1.664911    | -1.600331 | 1.686113  |
| 29     | O      | 6      | 0.966889    | -1.378405 | -0.526126 |
| 30     | C      | 8      | 2.311319    | -1.805458 | -0.234077 |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 31 | H | 6 | 0.181861  | -2.677291 | -0.717799 |
| 32 | C | 1 | 0.96289   | -0.786947 | -1.449086 |
| 33 | C | 6 | 2.533537  | -3.136646 | -0.742109 |
| 34 | H | 6 | 1.220556  | -3.570656 | -1.409528 |
| 35 | H | 1 | -0.725634 | -2.535982 | -1.304499 |
| 36 | H | 1 | -0.097552 | -3.088104 | 0.255785  |
| 37 | H | 1 | 3.377758  | -3.111653 | -1.436364 |
| 38 | H | 1 | 2.79894   | -3.784953 | 0.099754  |
| 39 | H | 1 | 1.247616  | -3.358943 | -2.482075 |
| 40 | C | 1 | 1.021888  | -4.636554 | -1.283389 |

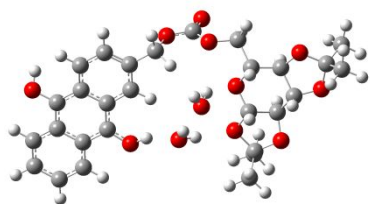
S27

The transient species **IM3**:



| Centre Number | Atomic | Atomic Number | X         | Y         | Z         |
|---------------|--------|---------------|-----------|-----------|-----------|
| 1             | C      | 6             | -3.393321 | -0.250922 | -0.000043 |
| 2             | C      | 6             | -2.253347 | -1.051905 | -0.000043 |
| 3             | C      | 6             | -0.973422 | -0.491122 | -0.000017 |
| 4             | C      | 6             | -0.821748 | 0.904498  | -0.000003 |
| 5             | C      | 6             | -1.962122 | 1.714153  | -0.000021 |
| 6             | C      | 6             | -3.22541  | 1.143768  | -0.000047 |
| 7             | C      | 6             | 0.211483  | -1.398566 | -0.000022 |
| 8             | C      | 6             | 0.524022  | 1.541987  | 0.000003  |
| 9             | C      | 6             | 1.710765  | 0.635553  | 0.000003  |
| 10            | C      | 6             | 1.561918  | -0.762152 | 0.000001  |
| 11            | C      | 6             | 2.695565  | -1.579684 | 0.000012  |
| 12            | H      | 1             | 2.554121  | -2.653278 | 0.000011  |
| 13            | C      | 6             | 3.964476  | -1.014044 | 0.000022  |
| 14            | C      | 6             | 4.112409  | 0.375415  | 0.000021  |
| 15            | C      | 6             | 2.991096  | 1.195733  | 0.000013  |
| 16            | H      | 1             | -2.333339 | -2.132659 | -0.000079 |
| 17            | H      | 1             | -1.829052 | 2.788944  | -0.000035 |
| 18            | H      | 1             | -4.101147 | 1.785085  | -0.000087 |
| 19            | H      | 1             | 4.840677  | -1.6524   | 0.000032  |
| 20            | H      | 1             | 5.103467  | 0.81474   | 0.000026  |
| 21            | H      | 1             | 3.078875  | 2.27506   | 0.000014  |
| 22            | O      | 8             | 0.083205  | -2.611305 | -0.000042 |
| 23            | O      | 8             | 0.654138  | 2.754941  | 0.000011  |
| 24            | C      | 6             | -4.774959 | -0.855043 | 0.000092  |
| 25            | H      | 1             | -4.733011 | -1.945079 | -0.001603 |
| 26            | H      | 1             | -5.342608 | -0.536372 | -0.879489 |
| 27            | H      | 1             | -5.341153 | -0.539143 | 0.88163   |

The reaction complex of the photodeprotection process of compound **1** via the triplet surface:



| Center<br>Number | Atomic | Atomic<br>Number | X         | Y         | Z         |
|------------------|--------|------------------|-----------|-----------|-----------|
| 1                | O      | 8                | -1.569694 | 2.709694  | -0.005345 |
| 2                | C      | 6                | -0.781479 | 3.005659  | 1.07767   |
| 3                | O      | 8                | -1.193513 | 3.154463  | 2.193071  |
| 4                | C      | 6                | 1.031468  | 2.958677  | -0.589398 |
| 5                | H      | 1                | 0.980497  | 3.935242  | -1.075094 |
| 6                | H      | 1                | 0.402231  | 2.253506  | -1.125389 |
| 7                | C      | 6                | 2.437769  | 2.457494  | -0.497295 |
| 8                | C      | 6                | 2.675622  | 1.071946  | -0.302999 |
| 9                | C      | 6                | 3.508619  | 3.323865  | -0.584381 |
| 10               | C      | 6                | 3.972482  | 0.558923  | -0.190951 |
| 11               | H      | 1                | 1.827565  | 0.402114  | -0.2476   |
| 12               | C      | 6                | 4.824268  | 2.840011  | -0.457146 |
| 13               | H      | 1                | 3.342374  | 4.38323   | -0.747537 |
| 14               | C      | 6                | 5.081173  | 1.480191  | -0.224471 |
| 15               | C      | 6                | 4.253361  | -0.842054 | -0.045292 |
| 16               | H      | 1                | 5.639958  | 3.54662   | -0.571606 |
| 17               | C      | 6                | 6.397997  | 0.977128  | -0.006457 |
| 18               | C      | 6                | 5.59519   | -1.338408 | 0.141986  |
| 19               | C      | 6                | 6.685411  | -0.418145 | 0.163074  |
| 20               | C      | 6                | 5.859275  | -2.702031 | 0.30703   |

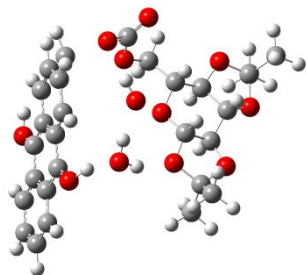


|     |   |   |           |           |           |
|-----|---|---|-----------|-----------|-----------|
| 21  | C | 6 | 7.987213  | -0.892959 | 0.350457  |
| 22  | H | 1 | 5.031143  | -3.397166 | 0.292295  |
| 23  | C | 6 | 7.170955  | -3.160166 | 0.491926  |
| 24  | C | 6 | 8.228912  | -2.263677 | 0.514631  |
| 25  | H | 1 | 8.805994  | -0.185954 | 0.36652   |
| 26  | H | 1 | 7.352457  | -4.221608 | 0.618738  |
| 27  | H | 1 | 9.243853  | -2.616121 | 0.658448  |
| 28  | O | 8 | 3.299078  | -1.783245 | -0.047754 |
| 29  | O | 8 | 7.464181  | 1.816791  | 0.064281  |
| 30  | C | 6 | -2.955162 | 2.451299  | 0.297069  |
| 31  | H | 1 | -3.079766 | 2.453566  | 1.378949  |
| 32  | H | 1 | -3.561301 | 3.246154  | -0.141673 |
| 33  | C | 6 | -3.365518 | 1.111469  | -0.290886 |
| 34  | C | 6 | -4.727337 | 0.645661  | 0.228306  |
| 35  | H | 1 | -3.363659 | 1.144844  | -1.388245 |
| 36  | C | 6 | -2.76744  | -1.155675 | -0.258122 |
| S29 |   |   |           |           |           |
| 37  | C | 6 | -5.117368 | -0.767051 | -0.228083 |
| 38  | H | 1 | -4.654973 | 0.633347  | 1.325755  |
| 39  | C | 6 | -4.066519 | -1.65944  | 0.374309  |
| 40  | H | 1 | -2.863643 | -1.153543 | -1.354941 |
| 41  | H | 1 | -5.082741 | -0.846884 | -1.323345 |
| 42  | H | 1 | -4.032825 | -1.525306 | 1.462105  |
| 43  | H | 1 | 2.41941   | -1.524368 | -0.40624  |
| 44  | H | 1 | 7.151405  | 2.720464  | 0.183569  |
| 45  | O | 8 | 0.797092  | -1.661042 | -1.016514 |
| 46  | H | 1 | 0.426432  | -1.04902  | -1.673121 |
| 47  | H | 1 | 0.039325  | -1.899868 | -0.461704 |
| 48  | O | 8 | -0.803706 | 0.290917  | -2.278836 |
| 49  | H | 1 | -0.633185 | 1.058837  | -2.83205  |
| 50  | H | 1 | -1.089276 | 0.635885  | -1.419374 |
| 51  | O | 8 | 0.504521  | 3.121929  | 0.770227  |
| 52  | O | 8 | -2.38601  | 0.135423  | 0.155816  |
| 53  | O | 8 | -5.853991 | 1.393938  | -0.177545 |
| 54  | O | 8 | -6.45646  | -0.816647 | 0.223293  |
| 55  | O | 8 | -3.988402 | -3.030223 | 0.030247  |
| 56  | O | 8 | -1.843632 | -2.132142 | 0.141289  |
| 57  | C | 6 | -7.000419 | 0.510613  | 0.011701  |
| 58  | C | 6 | -7.833711 | 0.555262  | -1.258949 |
| 59  | C | 6 | -7.767823 | 0.90458   | 1.262175  |
| 60  | H | 1 | -7.099796 | 0.923656  | 2.124596  |
| 61  | H | 1 | -8.212747 | 1.893323  | 1.135551  |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 62 | H | 1 | -8.561109 | 0.179573  | 1.455177  |
| 63 | H | 1 | -8.716899 | -0.076747 | -1.14928  |
| 64 | H | 1 | -8.152546 | 1.579742  | -1.461916 |
| 65 | H | 1 | -7.249189 | 0.199602  | -2.108888 |
| 66 | C | 6 | -2.596438 | -3.395559 | 0.189691  |
| 67 | C | 6 | -2.349136 | -4.030104 | 1.547685  |
| 68 | C | 6 | -2.197806 | -4.270988 | -0.983426 |
| 69 | H | 1 | -1.28342  | -4.223794 | 1.685098  |
| 70 | H | 1 | -2.684503 | -3.368691 | 2.34752   |
| 71 | H | 1 | -2.892565 | -4.974227 | 1.61675   |
| 72 | H | 1 | -2.797576 | -5.183298 | -0.984298 |
| 73 | H | 1 | -2.366006 | -3.742604 | -1.922631 |
| 74 | H | 1 | -1.141983 | -4.538465 | -0.913112 |

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S30

The transition state of photodeprotection process of compound **1** via the triplet surface:

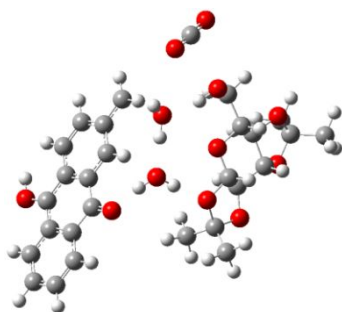
| Center | Atomic | Atomic | Coordinates |           |           |
|--------|--------|--------|-------------|-----------|-----------|
| Number |        | Number | X           | Y         | Z         |
| 1      | O      | 8      | -0.76115    | 2.683878  | -0.111294 |
| 2      | C      | 6      | -1.287674   | 3.610686  | -1.005272 |
| 3      | O      | 8      | -2.421734   | 4.02087   | -0.894764 |
| 4      | C      | 6      | 1.46237     | 3.965878  | -1.731619 |
| 5      | H      | 1      | 1.418419    | 5.006427  | -1.442629 |
| 6      | H      | 1      | 1.572678    | 3.792655  | -2.793118 |
| 7      | C      | 6      | 2.083728    | 3.059022  | -0.832918 |
| 8      | C      | 6      | 2.491205    | 1.73742   | -1.21056  |
| 9      | C      | 6      | 2.332343    | 3.466561  | 0.493721  |
| 10     | C      | 6      | 3.152416    | 0.889806  | -0.32302  |
| 11     | H      | 1      | 2.307769    | 1.409175  | -2.223804 |
| 12     | C      | 6      | 2.994942    | 2.653113  | 1.383776  |
| 13     | H      | 1      | 2.009332    | 4.452232  | 0.809977  |
| 14     | C      | 6      | 3.442448    | 1.355534  | 1.011228  |
| 15     | C      | 6      | 3.59755     | -0.433149 | -0.689596 |
| 16     | H      | 1      | 3.186094    | 3.047074  | 2.377797  |
| 17     | C      | 6      | 4.187883    | 0.542822  | 1.891569  |
| 18     | C      | 6      | 4.414408    | -1.215369 | 0.195313  |
| 19     | C      | 6      | 4.712258    | -0.737887 | 1.503394  |
| 20     | C      | 6      | 4.915165    | -2.472618 | -0.189736 |
| 21     | C      | 6      | 5.489281    | -1.513344 | 2.373131  |
| 22     | H      | 1      | 4.684512    | -2.838023 | -1.180925 |
| 23     | C      | 6      | 5.691015    | -3.223967 | 0.685133  |
| 24     | C      | 6      | 5.981262    | -2.750748 | 1.96681   |
| 25     | H      | 1      | 5.70197     | -1.137285 | 3.365102  |
| 26     | H      | 1      | 6.072303    | -4.187683 | 0.366475  |
| 27     | H      | 1      | 6.584876    | -3.341852 | 2.64497   |
| 28     | O      | 8      | 3.357225    | -0.966051 | -1.882746 |

|     |   |   |           |           |           |
|-----|---|---|-----------|-----------|-----------|
| 29  | O | 8 | 4.479369  | 0.92481   | 3.150891  |
| 30  | C | 6 | -1.682783 | 2.096152  | 0.807551  |
| 31  | H | 1 | -1.084358 | 1.754347  | 1.65378   |
| 32  | H | 1 | -2.425808 | 2.825575  | 1.132974  |
| 33  | C | 6 | -2.39364  | 0.920722  | 0.159011  |
| 34  | C | 6 | -3.30729  | 0.134576  | 1.099825  |
| S31 |   |   |           |           |           |
| 35  | H | 1 | -2.950046 | 1.275176  | -0.716382 |
| 36  | C | 6 | -1.968296 | -1.127329 | -0.889656 |
| 37  | C | 6 | -3.958441 | -1.084506 | 0.429377  |
| 38  | H | 1 | -2.675232 | -0.229483 | 1.924294  |
| 39  | C | 6 | -2.80709  | -1.980177 | 0.0647    |
| 40  | H | 1 | -2.591908 | -0.768784 | -1.723363 |
| 41  | H | 1 | -4.491941 | -0.780879 | -0.481786 |
| 42  | H | 1 | -2.220363 | -2.220296 | 0.959534  |
| 43  | H | 1 | 2.461699  | -0.768817 | -2.308967 |
| 44  | H | 1 | 4.087889  | 1.783881  | 3.342149  |
| 45  | O | 8 | 1.070574  | -0.913841 | -3.039385 |
| 46  | H | 1 | 0.557355  | -0.094553 | -3.207015 |
| 47  | H | 1 | 0.462807  | -1.44898  | -2.504207 |
| 48  | O | 8 | -0.585838 | 1.192333  | -2.808674 |
| 49  | H | 1 | -0.533973 | 2.159372  | -2.883329 |
| 50  | H | 1 | -0.568695 | 1.044102  | -1.849928 |
| 51  | O | 8 | -0.445201 | 3.896932  | -1.948881 |
| 52  | O | 8 | -1.363006 | -0.022437 | -0.273208 |
| 53  | O | 8 | -4.438361 | 0.805178  | 1.615969  |
| 54  | O | 8 | -4.879782 | -1.470468 | 1.43075   |
| 55  | O | 8 | -2.998881 | -3.134025 | -0.734927 |
| 56  | O | 8 | -1.029991 | -2.063569 | -1.364245 |
| 57  | C | 6 | -5.374974 | -0.236741 | 2.010562  |
| 58  | C | 6 | -6.736174 | 0.120653  | 1.434851  |
| 59  | C | 6 | -5.374288 | -0.401103 | 3.52161   |
| 60  | H | 1 | -4.360486 | -0.589547 | 3.878505  |
| 61  | H | 1 | -5.756535 | 0.503359  | 3.998694  |
| 62  | H | 1 | -6.004003 | -1.246871 | 3.805608  |
| 63  | H | 1 | -7.476011 | -0.62646  | 1.728807  |
| 64  | H | 1 | -7.052074 | 1.099538  | 1.801371  |
| 65  | H | 1 | -6.687658 | 0.160991  | 0.345656  |
| 66  | C | 6 | -1.740917 | -3.348278 | -1.415331 |
| 67  | C | 6 | -0.893415 | -4.376174 | -0.683096 |
| 68  | C | 6 | -2.039337 | -3.711628 | -2.85836  |
| 69  | H | 1 | 0.08482   | -4.468528 | -1.159603 |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 70 | H | 1 | -0.744181 | -4.078915 | 0.355795  |
| 71 | H | 1 | -1.391442 | -5.347323 | -0.705354 |
| 72 | H | 1 | -2.6272   | -4.631079 | -2.893917 |
| 73 | H | 1 | -2.610304 | -2.914854 | -3.336613 |
| 74 | H | 1 | -1.109832 | -3.862141 | -3.410813 |

# S32

The product complex of photodeprotection process of compound 1 via the triplet surface:



| Center | Atomic | Atomic | Coordinates |           |           |
|--------|--------|--------|-------------|-----------|-----------|
| Number |        | Number | X           | Y         | Z         |
| 1      | H      | 8      | -3.571859   | 2.499166  | -1.308384 |
| 2      | H      | 6      | -3.634321   | 5.248827  | -1.279454 |
| 3      | H      | 8      | -4.483042   | 5.297786  | -0.49064  |
| 4      | H      | 6      | 0.456011    | 3.273481  | 1.229346  |
| 5      | H      | 1      | 0.141942    | 3.958313  | 2.007833  |
| 6      | H      | 1      | -0.165615   | 3.150065  | 0.349562  |
| 7      | H      | 6      | 1.690355    | 2.582361  | 1.34135   |
| 8      | H      | 6      | 2.119942    | 1.672018  | 0.359287  |
| 9      | H      | 6      | 2.553904    | 2.796746  | 2.456668  |
| 10     | H      | 6      | 3.357492    | 1.014782  | 0.444944  |
| 11     | H      | 1      | 1.481304    | 1.463271  | -0.488557 |
| 12     | H      | 6      | 3.763254    | 2.155285  | 2.559137  |
| 13     | H      | 1      | 2.245317    | 3.487132  | 3.234199  |
| 14     | H      | 6      | 4.206103    | 1.253195  | 1.558545  |
| 15     | H      | 6      | 3.76399     | 0.087227  | -0.62247  |
| 16     | H      | 1      | 4.372012    | 2.366087  | 3.434322  |
| 17     | H      | 6      | 5.47663     | 0.580323  | 1.642127  |
| 18     | H      | 6      | 5.069641    | -0.561347 | -0.48732  |
| 19     | H      | 6      | 5.911405    | -0.313137 | 0.637957  |
| 20     | H      | 6      | 5.510676    | -1.44311  | -1.48798  |
| 21     | H      | 6      | 7.16901     | -0.968959 | 0.71909   |

|     |   |   |           |           |           |
|-----|---|---|-----------|-----------|-----------|
| 22  | H | 1 | 4.85706   | -1.608872 | -2.334961 |
| 23  | H | 6 | 6.738178  | -2.069326 | -1.390312 |
| 24  | H | 6 | 7.570048  | -1.829193 | -0.276875 |
| 25  | H | 1 | 7.803839  | -0.778749 | 1.574254  |
| 26  | H | 1 | 7.065312  | -2.746401 | -2.170979 |
| 27  | H | 1 | 8.531878  | -2.324178 | -0.206677 |
| 28  | H | 8 | 3.032498  | -0.146021 | -1.604227 |
| 29  | H | 8 | 6.313099  | 0.775689  | 2.684895  |
| 30  | H | 6 | -3.782363 | 1.70109   | -0.168403 |
| 31  | H | 1 | -3.068066 | 1.935736  | 0.634334  |
| 32  | H | 1 | -4.789646 | 1.903359  | 0.205245  |
| 33  | H | 6 | -3.683409 | 0.215653  | -0.485864 |
| 34  | H | 6 | -3.916232 | -0.70608  | 0.713768  |
| S33 |   |   |           |           |           |
| 35  | H | 1 | -4.371935 | -0.022034 | -1.306979 |
| 36  | H | 6 | -2.161271 | -1.390958 | -1.215596 |
| 37  | H | 6 | -3.70676  | -2.196681 | 0.407246  |
| 38  | H | 1 | -3.179536 | -0.415962 | 1.477802  |
| 39  | H | 6 | -2.259622 | -2.301495 | 0.01289   |
| 40  | H | 1 | -2.921758 | -1.687309 | -1.95787  |
| 41  | H | 1 | -4.341289 | -2.509966 | -0.433329 |
| 42  | H | 1 | -1.623602 | -1.908376 | 0.814953  |
| 43  | H | 1 | 1.470519  | 0.481774  | -2.434614 |
| 44  | H | 1 | 5.933408  | 1.401221  | 3.310419  |
| 45  | H | 8 | 0.555504  | 0.639523  | -2.727402 |
| 46  | H | 1 | -0.366388 | 2.009588  | -2.183739 |
| 47  | H | 1 | 0.079111  | -0.157168 | -2.448149 |
| 48  | H | 8 | -0.900358 | 2.745431  | -1.800747 |
| 49  | H | 1 | -0.794741 | 3.503537  | -2.383399 |
| 50  | H | 1 | -2.618929 | 2.459736  | -1.542314 |
| 51  | H | 8 | -2.780364 | 5.275768  | -2.067378 |
| 52  | H | 8 | -2.317836 | -0.036359 | -0.919355 |
| 53  | H | 8 | -5.214029 | -0.725128 | 1.280514  |
| 54  | H | 8 | -4.173771 | -2.778888 | 1.610616  |
| 55  | H | 8 | -1.717442 | -3.500145 | -0.514468 |
| 56  | H | 8 | -0.879493 | -1.690064 | -1.707461 |
| 57  | H | 6 | -5.295608 | -1.963247 | 2.036434  |
| 58  | H | 6 | -6.612544 | -2.637199 | 1.682873  |
| 59  | H | 6 | -5.131667 | -1.688566 | 3.523104  |
| 60  | H | 1 | -4.205698 | -1.140228 | 3.703139  |
| 61  | H | 1 | -5.971808 | -1.0971   | 3.892379  |
| 62  | H | 1 | -5.089167 | -2.630441 | 4.074206  |

|    |   |   |           |           |           |
|----|---|---|-----------|-----------|-----------|
| 63 | H | 1 | -6.725232 | -3.563321 | 2.249916  |
| 64 | H | 1 | -7.447349 | -1.972653 | 1.915577  |
| 65 | H | 1 | -6.64263  | -2.869731 | 0.617227  |
| 66 | H | 6 | -0.603355 | -3.081667 | -1.334905 |
| 67 | H | 6 | 0.702226  | -3.10375  | -0.554344 |
| 68 | H | 6 | -0.58652  | -3.948033 | -2.58022  |
| 69 | H | 1 | 1.499214  | -2.645978 | -1.143702 |
| 70 | H | 1 | 0.602441  | -2.540818 | 0.374818  |
| 71 | H | 1 | 0.975859  | -4.133362 | -0.314974 |
| 72 | H | 1 | -0.467767 | -4.996245 | -2.298172 |
| 73 | H | 1 | -1.524076 | -3.836128 | -3.126055 |
| 74 | H | 1 | 0.241618  | -3.65831  | -3.229569 |

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