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Electronic Supplementary Information

Solvent Effect on Photodeprotection of Anthraquinone Protected Carboxylic Acid Unravelled by Time-Resolved Spectroscopic Studies

Yan Guo,[a] Qingqing Song,[a] Tongyu Xu,[a] Jiani Ma,*[a] and David Lee Phillips[b]

[a]*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*

[b]*Department of Chemistry, The University of Hong Kong, Pokfulam Road, Hong Kong S.A.R., P. R. China*

Table of Contents

Graphi **Page**

Scheme S1. The synthetic route of the compound **1**. **S3**

Figure S1. The ^{1}H NMR spectra of **1** in $CDCl_3$. **S3**

Figure S2. Comparison of (a) ns-TA spectrum of **1** in ACN recorded at 400 ns to the (b) calculated triplet state species of **1** (the scale factor is 1.03 and the half-width is 800 cm^{-1}). **S4**

Figure S3. Ns-TA spectra of **1** in IPA recorded at later delay times. **S4**

Figure S4. (Left) Ns-TR^3 spectra of **1** in IPA. (Right) Comparison of (a) the 100 ns experimental Raman spectrum to (b) the calculated ketyl radical species of **1** (the scale factor is 0.968 and the half-width is 8cm^{-1}). **S4**

Figure S5. Comparison (a) ns-TA spectrum in MeOH recorded at 14 μs after photolysis of **1** with the (b) xylylene form of 2-ethyl-AQ (the scale factor is 0.93 and the half-width is 2000 cm^{-1}). **S5**

Figure S6. Reaction energy profiles found from (U)B3LYP/6-311G** computations for the intermolecular HAT processes that can occur after photolysis of **1** in MeOH and IPA via a triplet state surface are shown (the energy unit is kJ/mol). **S5**

Figure S7. Ns-TA results of **1** in (a-b) MeOH-ACN (v:v, 1:9), (c-d) MeOH-ACN (v:v, 1:1) and (e-f) MeOH-ACN (v:v, 9:1) under the irradiation of 355 nm. **S6**

Figure S8. Recordings at 250 nm of HPLC analysis of the (a) *p*-methoxybenzoic acid,(b) 2-ethyl-AQ, (c) compound **1** and (d) photoproduct of **1** in THF-H_2O upon 350 nm. **S7**

Figure S9. (Left) Ns-TR^3 spectra of **1** in THF-H_2O (v:v, 1:1). (Right) Comparison of the ns-TR^3 spectrum of **1** (a) in IPA at 100 ns with that (b) in THF-H_2O (v:v, 1:1). **S7**

Figure S10. (a) Ns-TA results of **1** in THF-H_2O (1:3) and (b) in THF-H_2O (4:1) obtained at various time delays upon the irradiation of 355 nm. **S8**

Figure S11. Reaction energy profile obtained from (U)B3LYP/6-311G** calculations for the photodeprotection reaction of **1** via ground state surface by assistance of two water molecules is shown (the energy unit is kJ/mol). **S8**

Figure S12. Recordings at 250 nm of HPLC analysis of the (a) *p*-methoxybenzoic acid,(b) 2-ethyl-AQ, (c) compound **1** and (d) photoproduct of **1** in MeOH-H_2O upon 350 nm. **S9**

Figure S13. Ns-TA spectra of **1** in MeOH-H_2O (v:v, 1:1) under the irradiation of 355 nm. **S9**

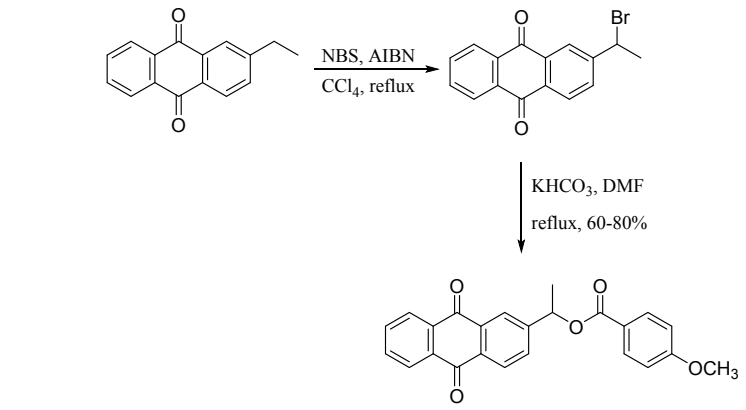
Figure S14. Ns-TA results of **1** in DMSO under the irradiation of 355 nm. **S9**

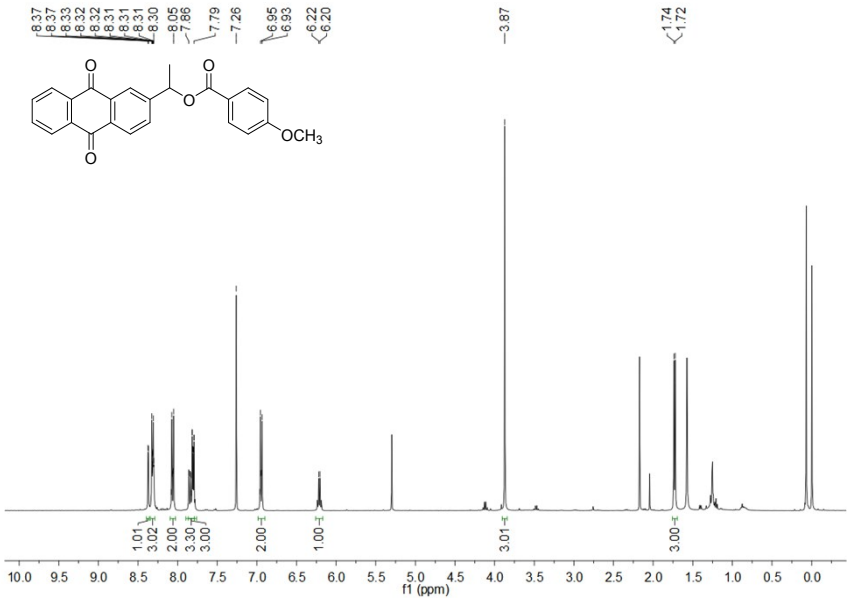
Figure S15. Fs-TA (a-b) and ns-TA (c-d) spectra of **1** in TFE under irradiation of 355 nm. **S10**

Figure S16. Comparison of the (a) ns-TA spectra of **1** recorded at 2 μs with (b) computed UV-vis spectrum of AQH^+ (the scale factor is 1.0 and the half-width is 1500 cm^{-1}). **S10**

Cartesian coordinates, total energies, and vibrational zero-point energies for the optimized geometry for the compounds and intermediates considered in this paper are given. **S11-S57**

Scheme S1. Synthetic route of compound **1**.





^{1}H NMR ($CDCl_3$) δ/ppm = 1.73 (d, 3H, $CHCH_3$), 3.87 (s, 3H, OCH_3), 6.21 (q, 1H, $CHCH_3$), 6.94–8.30 (m, 11H, H_{Ar})

Figure S1. The ^{1}H NMR spectra of **1** in $CDCl_3$.

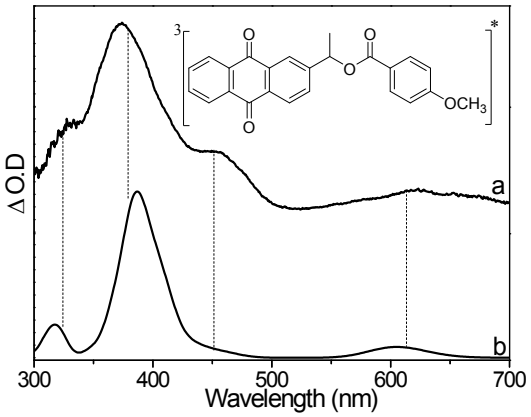


Figure S2. Comparison of (a) the ns-TA spectrum of **1** in ACN recorded at 400 ns to the (b) calculated triplet state species of **1** (the scale factor is 1.03 and the half-width is 800 cm^{-1}).

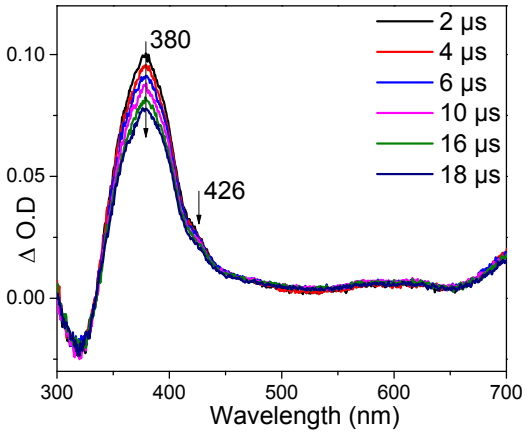
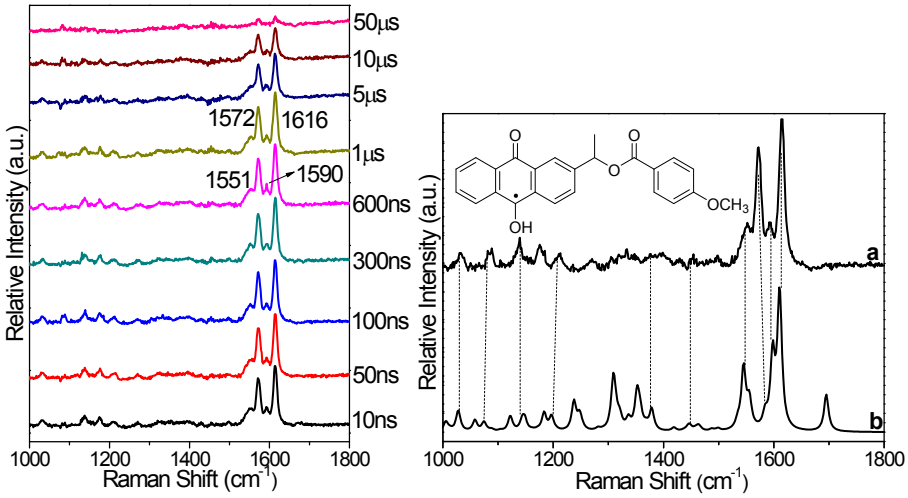


Figure S3. Ns-TA spectra of **1** in IPA recorded at later delay times.



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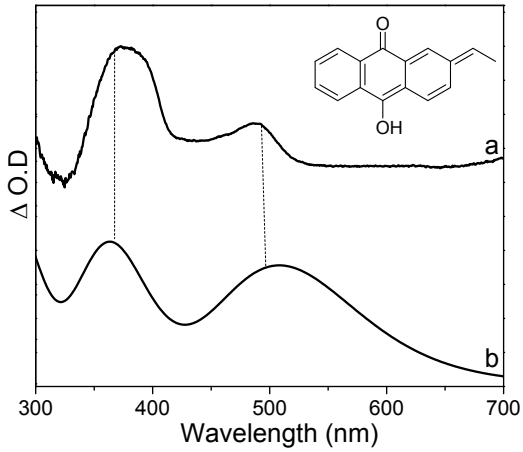

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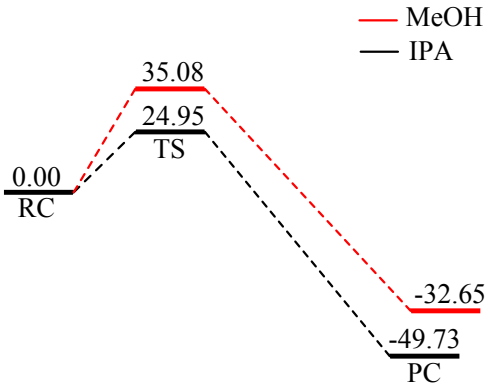

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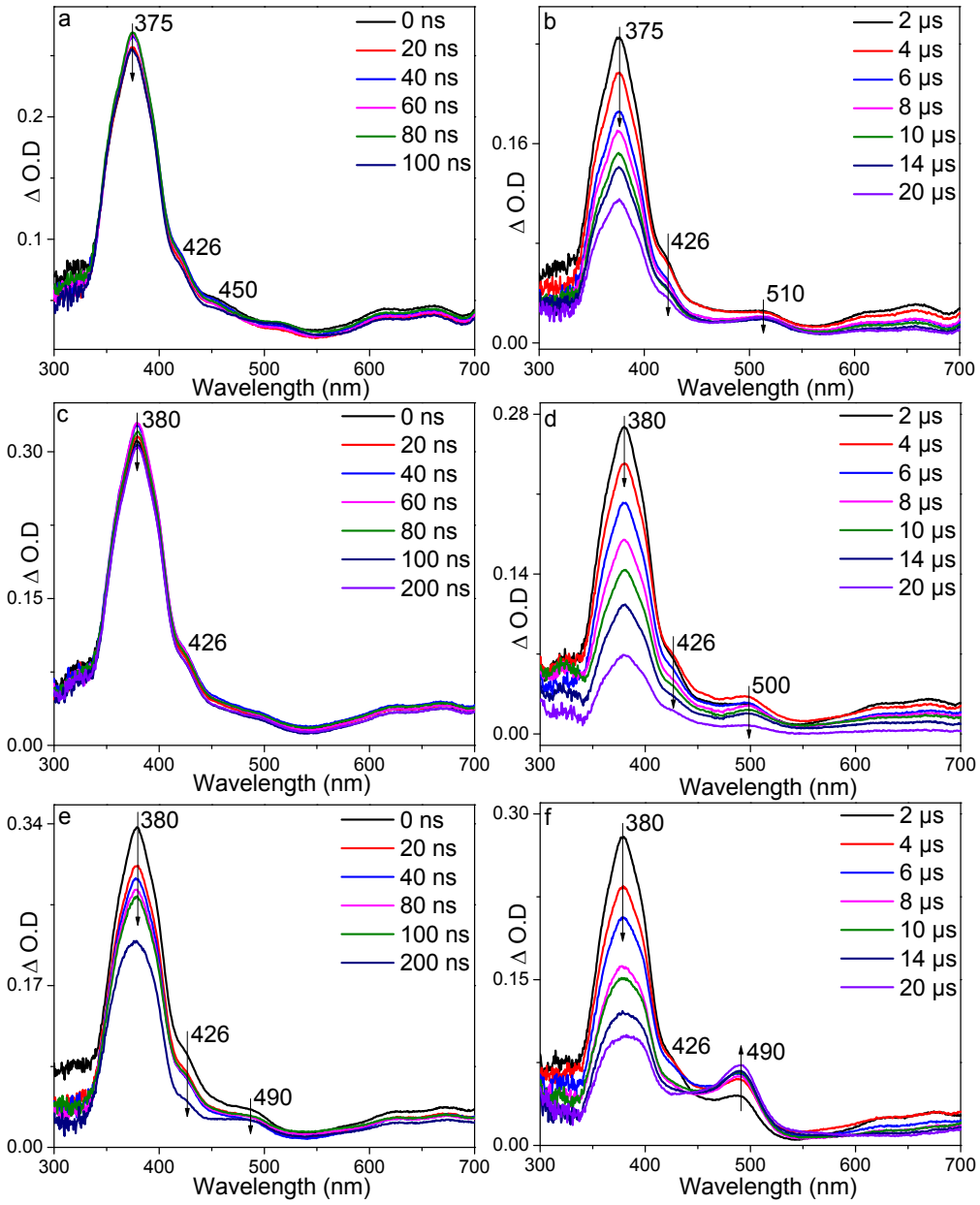

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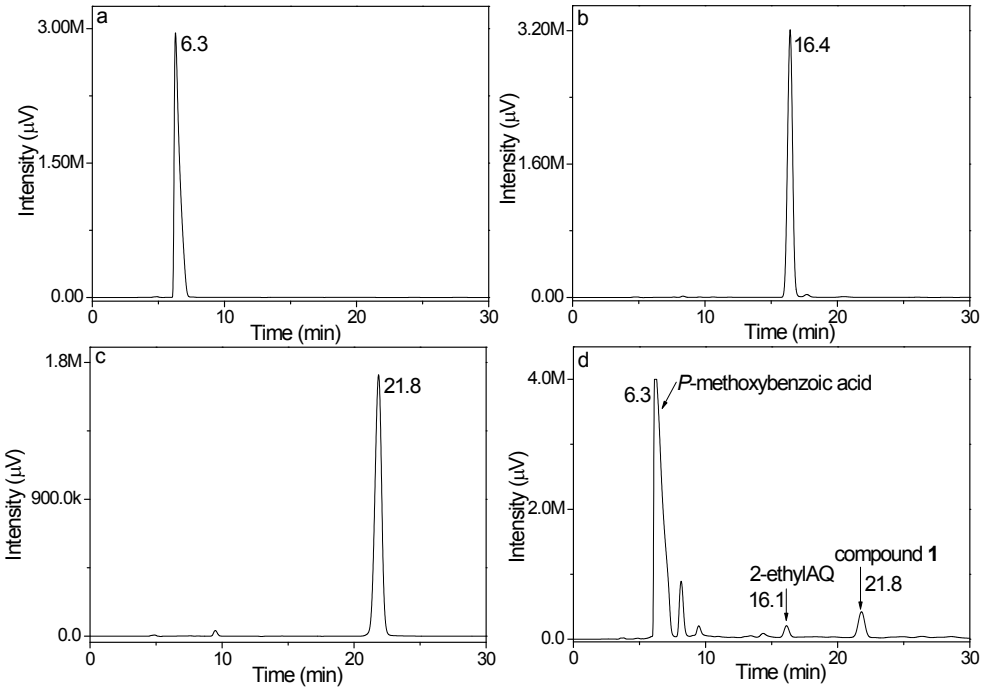
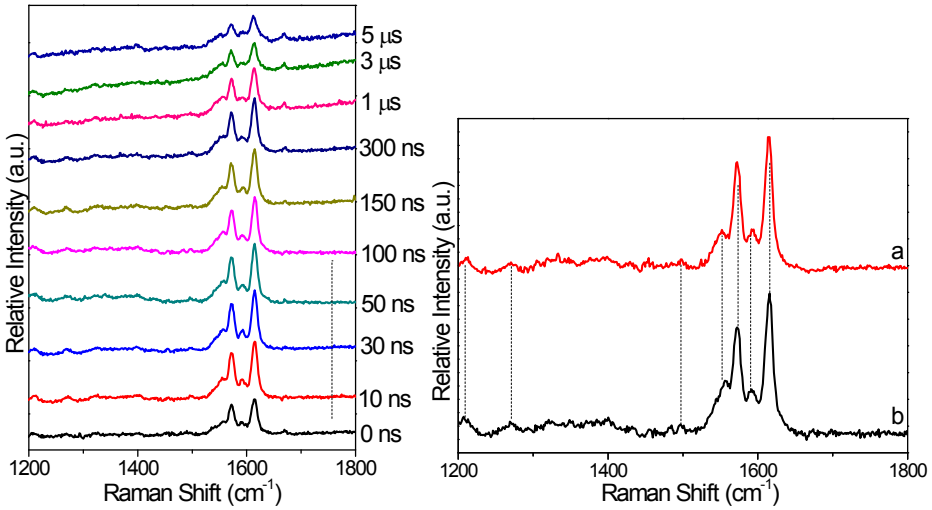


Figure S8. Recordings at 250 nm of HPLC analysis of the (a) *p*-methoxybenzoic acid, (b) 2-ethyl-AQ, (c) compound **1** and (d) photoproduct of **1** in THF-H_2O upon 350 nm.



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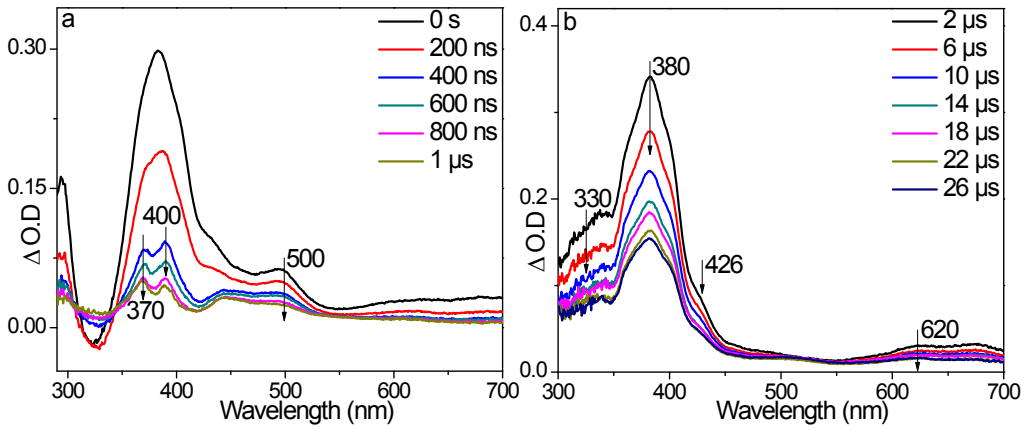
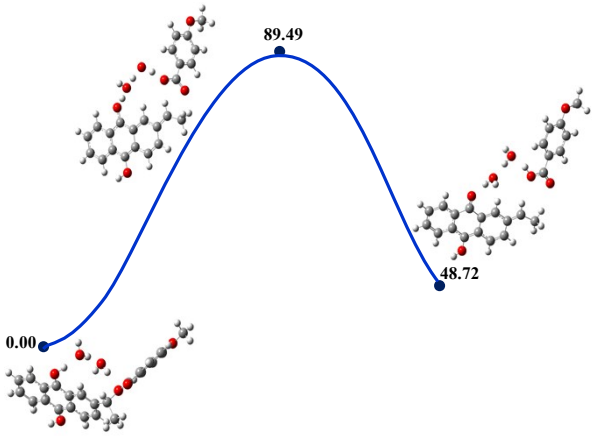


Figure S10. (a) Ns-TA results of **1** in THF-H_2O (1:3) and (b) in THF-H_2O (4:1) obtained at various time delays upon the irradiation of 355 nm.



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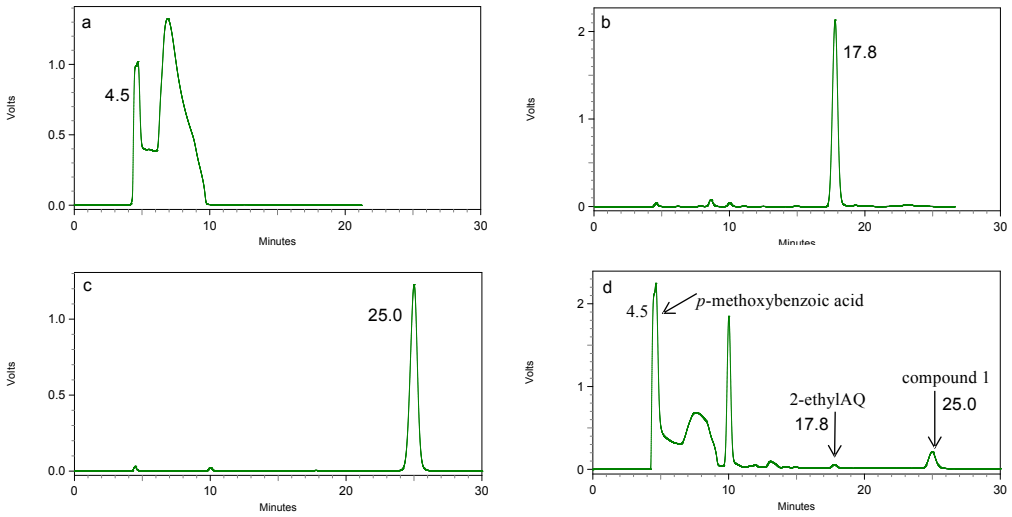

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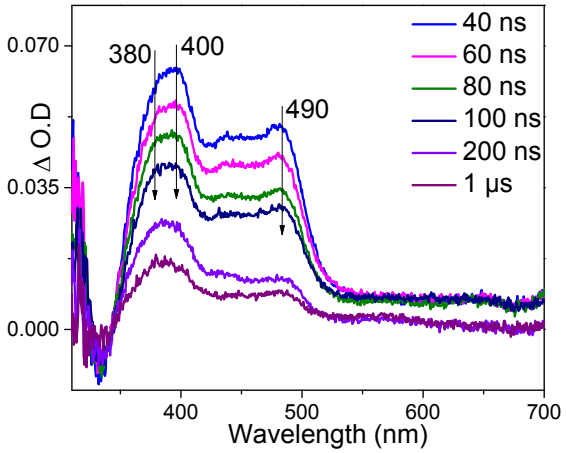


Figure S13. Ns-TA spectra of **1** in MeOH-H_2O (v:v, 1:1) under the irradiation of 355 nm.

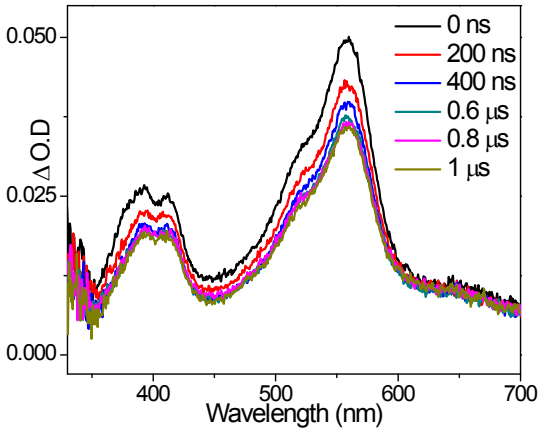


Figure S14. Ns-TA results of **1** in DMSO under the irradiation of 355 nm

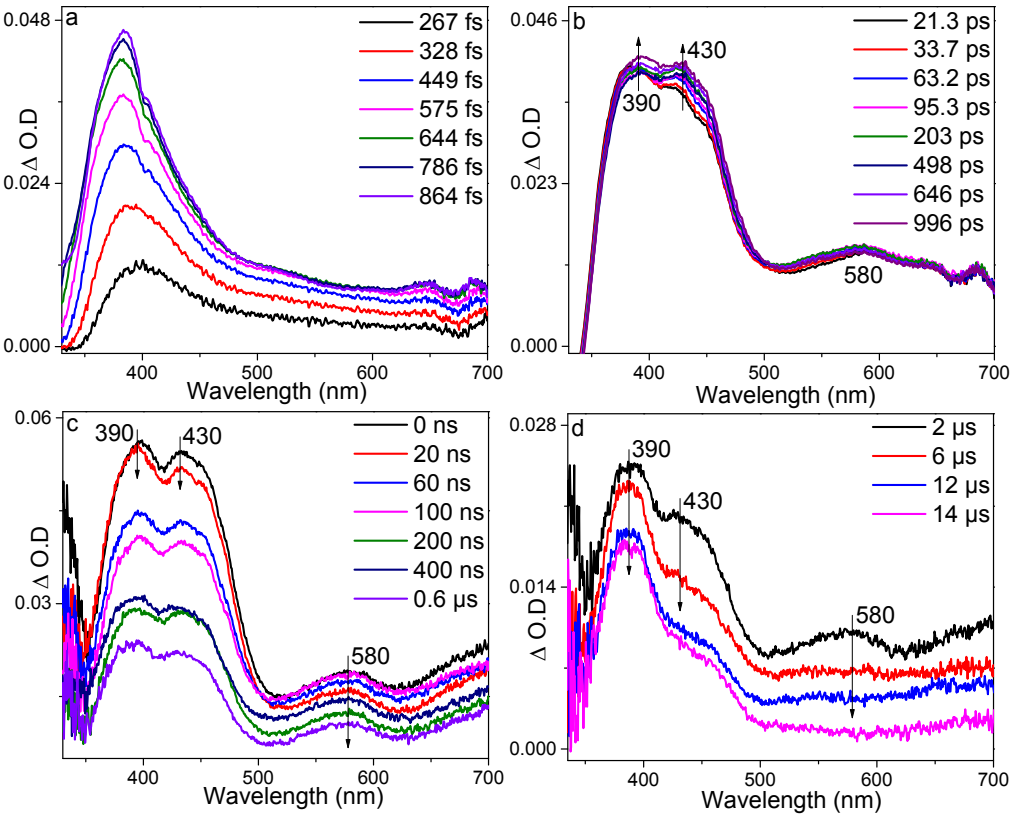


Figure S15. Fs-TA (a-b) and ns-TA (c-d) spectra of **1** in TFE under irradiation of 355 nm.

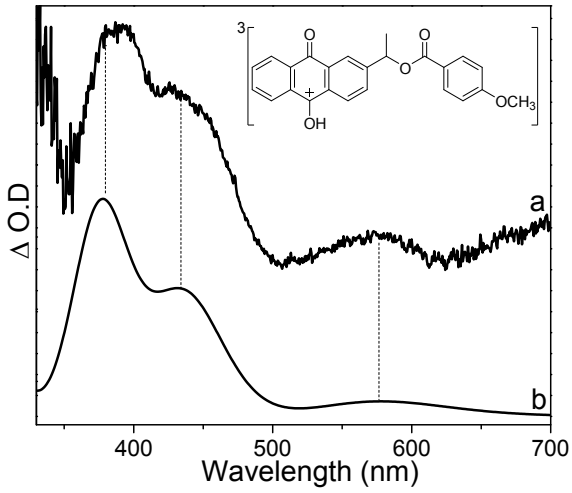
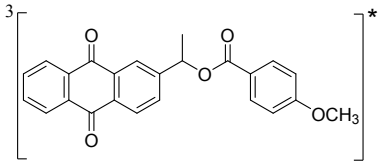


Figure S16. Comparison of the (a) ns-TA spectra of 1 recorded at 2 μs with (b)computed UV-vis spectrum of AQH^+ (the scale factor is 1.0 and the half-width is 1500 cm^{-1}).

Cartesian coordinates, total energies, and vibrational zero-point energies for the optimized geometry for the compounds and intermediates considered in this paper are given.

Triplet state of compound **1**:



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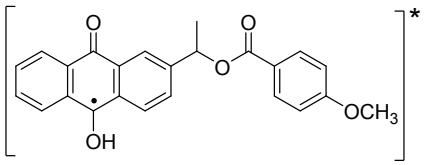
Sum of electronic and zero-point Energies= -1301.417311

Sum of electronic and thermal Free Energies= -1301.475286

Ketyl radical species of compound **1**



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47	1	0	7.336205	-3.105657	-1.512396
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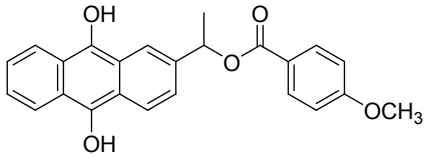
Sum of electronic and zero-point Energies= -1302.078941

Sum of electronic and thermal Free Energies= -1302.136733

Ground state of dihydroxy anthraquinone of compound **1**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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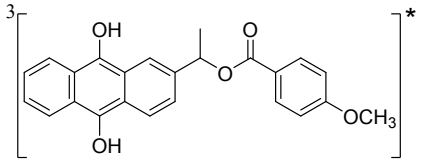
21	1	0	-5.997472	1.188657	-1.921472
22	8	0	-3.627357	2.072556	-1.359283
23	8	0	-3.351288	-2.558375	1.716551
24	6	0	0.874999	2.330703	1.08634
25	6	0	0.814417	3.57758	0.212424
26	8	0	2.153729	1.628063	0.940232
27	1	0	-0.035221	4.19633	0.511443
28	1	0	1.72503	4.162412	0.359211
29	1	0	0.724183	3.327661	-0.842854
30	6	0	2.467998	1.060038	-0.249294
31	8	0	1.770302	1.123332	-1.23484
32	6	0	3.776661	0.355593	-0.196405
33	6	0	4.568897	0.29704	0.960547

34	6	0	4.230099	-0.274162	-1.356629
35	6	0	5.778388	-0.373722	0.949991
36	1	0	4.226832	0.782971	1.864466
37	6	0	5.443871	-0.951882	-1.380045
38	1	0	3.61231	-0.225179	-2.244814
39	6	0	6.226269	-1.004106	-0.220274
40	1	0	6.402091	-0.428905	1.833776
41	1	0	5.767371	-1.430723	-2.294099
42	1	0	0.94246	2.651148	2.130147
43	8	0	7.425301	-1.635219	-0.126486
44	6	0	7.941902	-2.296844	-1.275012
45	1	0	8.105095	-1.596337	-2.100924
46	1	0	8.896555	-2.719874	-0.967543
47	1	0	7.278048	-3.1029	-1.605368
48	1	0	-4.17529	1.94939	-2.140112
49	1	0	-4.22389	-2.913789	1.909153

Sum of electronic and zero-point Energies= -1302.676419

Sum of electronic and thermal Free Energies= -1302.733015

Triplet state of dihydroxy anthraquinone of compound **1**



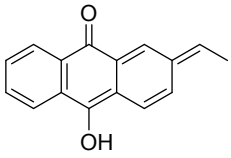
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.271018	1.565688	-0.461042
2	6	0	-5.993597	2.058947	-0.13964
3	6	0	-4.895962	1.198947	-0.053307
4	6	0	-5.076439	-0.199962	-0.311554
5	6	0	-6.362949	-0.666719	-0.605345
6	6	0	-7.456685	0.214861	-0.68577
7	6	0	-3.583791	1.666778	0.286213
8	6	0	-3.922929	-1.051798	-0.269888
9	6	0	-2.62559	-0.594214	0.131214
10	6	0	-2.458415	0.795465	0.444003
11	6	0	-1.198052	1.23171	0.86525
12	1	0	-1.036371	2.26512	1.15692
13	6	0	-0.106219	0.347922	0.951531
14	6	0	-0.25847	-0.986485	0.621967
15	6	0	-1.528664	-1.451727	0.213847
16	1	0	-8.108389	2.250854	-0.52386
17	1	0	-5.846891	3.114152	0.04695
18	1	0	-6.548891	-1.72597	-0.755084
19	1	0	-8.440476	-0.174736	-0.919481
20	1	0	0.859006	0.720498	1.269304
21	1	0	-1.66247	-2.492392	-0.053722
22	8	0	-4.01328	-2.369096	-0.589986
23	1	0	-4.852403	-2.536387	-1.032703
24	8	0	-3.464931	3.006826	0.477854
25	1	0	-2.532013	3.245458	0.507212
26	6	0	0.876524	-1.98441	0.735693
27	8	0	2.161315	-1.314767	0.665562
28	6	0	2.758636	-1.228186	-0.552021
29	8	0	2.28681	-1.694141	-1.562379
30	6	0	4.054682	-0.506505	-0.488437
31	6	0	4.589802	-0.009928	0.701517
32	6	0	4.769592	-0.324013	-1.682348

33	6	0	5.811315	0.657693	0.712973
34	1	0	4.047761	-0.150306	1.627256
35	6	0	5.982125	0.337544	-1.68405
36	1	0	4.34961	-0.713022	-2.601488
37	6	0	6.513985	0.834973	-0.484381
38	1	0	6.202878	1.030592	1.649511
39	1	0	6.544969	0.48689	-2.597206
40	8	0	7.70957	1.469277	-0.590087
41	6	0	8.310519	1.999819	0.585183
42	1	0	7.677984	2.765131	1.047483
43	1	0	8.524901	1.212296	1.315486
44	1	0	9.244979	2.453365	0.259939
45	6	0	0.863395	-2.747667	2.058666
46	1	0	1.677823	-3.475287	2.08503
47	1	0	0.976764	-2.058172	2.898371
48	1	0	-0.084531	-3.277245	2.175807
49	1	0	0.81912	-2.678032	-0.105084

Sum of electronic and zero-point Energies= -1302.629249

Sum of electronic and thermal Free Energies= -1302.688153

Ground state of xylylene form of 2-ethyl-AQ

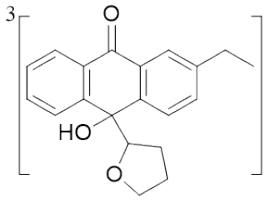


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.861054	1.19415	-0.018173
2	6	0	1.621008	1.730415	-0.041616
3	6	0	0.432782	0.906892	-0.027283
4	6	0	0.620846	-0.534627	-0.010773
5	6	0	1.874466	-1.061537	0.00717
6	6	0	3.07014	-0.24716	0.015665
7	6	0	-0.83009	1.437373	-0.027763
8	6	0	-0.547934	-1.454902	-0.043286
9	6	0	-1.887521	-0.810199	-0.030009
10	6	0	-2.016951	0.600365	0.006693
11	6	0	-3.311595	1.147321	0.088996
12	1	0	-3.452042	2.218481	0.185918
13	6	0	-4.432797	0.329656	0.091345
14	6	0	-4.296276	-1.059207	0.024583
15	6	0	-3.026709	-1.618153	-0.026364
16	1	0	3.721836	1.850937	-0.028398
17	1	0	1.489079	2.804452	-0.067917
18	1	0	1.970098	-2.142229	0.009328
19	1	0	-5.418866	0.775834	0.156026
20	1	0	-5.17426	-1.694308	0.026217
21	1	0	-2.880342	-2.691005	-0.057034
22	8	0	-0.423348	-2.672851	-0.069575
23	8	0	-0.965568	2.801078	-0.023794
24	6	0	4.290188	-0.857699	0.046201
25	6	0	5.63599	-0.212877	0.061369
26	1	0	6.199148	-0.519081	0.951489
27	1	0	6.229641	-0.539563	-0.801273
28	1	0	5.595568	0.87604	0.048393
29	1	0	4.292131	-1.944922	0.062345
30	1	0	-1.800271	3.040689	-0.438672

Sum of electronic and zero-point Energies= -767.318427

Sum of electronic and thermal Free Energies= -767.359990

Triplet state of coupling complex



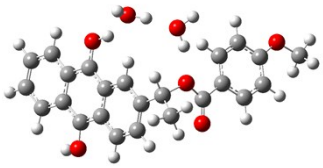
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.693058	-2.013056	0.894983
2	6	0	2.87101	-0.91635	1.160782
3	6	0	1.63536	-0.782479	0.538795
4	6	0	1.181294	-1.814412	-0.320805
5	6	0	2.032433	-2.904333	-0.612297
6	6	0	3.275979	-2.993946	-0.009187
7	6	0	0.796541	0.474089	0.694982
8	6	0	-0.176542	-1.760212	-0.805165
9	6	0	-1.153992	-0.905876	-0.171607
10	6	0	-0.691723	0.123636	0.683064
11	6	0	-1.625943	0.83383	1.423893
12	1	0	-1.281468	1.591106	2.116217
13	6	0	-2.992024	0.590152	1.286283
14	6	0	-3.46682	-0.382598	0.393039
15	6	0	-2.540107	-1.126644	-0.326022
16	1	0	4.654959	-2.098031	1.386924
17	1	0	3.182817	-0.145165	1.852906
18	1	0	1.68499	-3.686965	-1.27581
19	1	0	3.915014	-3.843473	-0.223029
20	1	0	-3.697844	1.163815	1.878012
21	1	0	-2.87597	-1.921213	-0.983299
22	6	0	-4.952098	-0.606928	0.210659
23	1	0	-5.457212	-0.492844	1.175303
24	1	0	-5.127091	-1.637794	-0.112127
25	6	0	-5.581273	0.358723	-0.808699
26	1	0	-6.653653	0.171146	-0.9135
27	1	0	-5.44784	1.398654	-0.498969
28	1	0	-5.118149	0.243742	-1.792254
29	8	0	-0.55817	-2.581334	-1.753333
30	8	0	1.17738	1.153823	1.878538
31	1	0	0.94129	2.079207	1.716636
32	6	0	1.075571	1.435389	-0.517852

33	8	0	0.501001	2.708064	-0.161927
34	6	0	2.539016	1.745491	-0.838104
35	1	0	0.564282	1.038923	-1.402535
36	6	0	1.289742	3.78369	-0.710985
37	6	0	2.427837	3.124759	-1.501708
38	1	0	2.995686	0.992254	-1.479919
39	1	0	3.117417	1.80531	0.087413
40	1	0	0.643704	4.410875	-1.330938
41	1	0	1.667708	4.391577	0.118139
42	1	0	2.151087	3.017366	-2.554269
43	1	0	3.354668	3.699524	-1.455408

Sum of electronic and zero-point Energies= -999.649987

Sum of electronic and thermal Free Energies= -999.699923

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



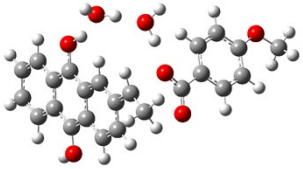
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.491031	-2.205795	-0.833922
2	6	0	5.767479	-1.198584	-1.496443
3	6	0	4.586488	-0.678396	-0.954066
4	6	0	4.137579	-1.161049	0.31748
5	6	0	4.87088	-2.164223	0.960065
6	6	0	6.039526	-2.686768	0.381638
7	6	0	3.793241	0.317093	-1.616996
8	6	0	2.948284	-0.599845	0.902938
9	6	0	2.213806	0.463281	0.270382
10	6	0	2.638952	0.913756	-1.024922
11	6	0	1.911969	1.919795	-1.67142
12	1	0	2.231399	2.246924	-2.651503
13	6	0	0.779512	2.496791	-1.074369
14	6	0	0.369004	2.090223	0.183805
15	6	0	1.101842	1.077116	0.84997
16	1	0	7.399947	-2.593678	-1.27865
17	1	0	6.165102	-0.817089	-2.432535
18	1	0	4.521653	-2.530885	1.915305
19	1	0	6.589195	-3.465119	0.898713
20	1	0	0.224333	3.250609	-1.616292
21	1	0	0.78194	0.780577	1.840208
22	6	0	-0.842601	2.648129	0.888936
23	8	0	-1.982665	1.67831	0.792461
24	6	0	-2.600089	1.473571	-0.405525
25	8	0	-2.421196	2.17474	-1.371909
26	6	0	-3.53027	0.313022	-0.391592
27	6	0	-3.513991	-0.691077	0.589139
28	6	0	-4.437562	0.201466	-1.44849
29	6	0	-4.388779	-1.760125	0.518052

30	1	0	-2.803263	-0.647062	1.402832
31	6	0	-5.328305	-0.862434	-1.526176
32	1	0	-4.431992	0.965473	-2.215821
33	6	0	-5.307899	-1.853306	-0.537055
34	1	0	-4.377138	-2.548652	1.260372
35	1	0	-6.022358	-0.914619	-2.35377
36	8	0	-6.124142	-2.936018	-0.511435
37	6	0	-7.068902	-3.108952	-1.562396
38	1	0	-6.57233	-3.204133	-2.533577
39	1	0	-7.596599	-4.033192	-1.334948
40	1	0	-7.78507	-2.281224	-1.595994
41	1	0	-0.6537	2.598919	1.963063
42	6	0	-1.268337	4.071398	0.555393
43	1	0	-2.173124	4.326267	1.112894
44	1	0	-0.473642	4.753654	0.868513
45	1	0	-1.465576	4.212784	-0.503422
46	8	0	2.60114	-1.126426	2.089251
47	8	0	4.124245	0.760973	-2.858438
48	1	0	4.793536	0.180826	-3.23681
49	1	0	1.751318	-0.820321	2.471008
50	8	0	0.526438	-0.536505	3.755027
51	1	0	-0.393689	-0.230385	3.630843
52	1	0	0.890778	0.042216	4.431934
53	8	0	-1.95321	0.640303	3.40613
54	1	0	-2.138874	0.993172	2.517525
55	1	0	-2.803859	0.4014	3.784854

Sum of electronic and zero-point Energies= -1455.510221

Sum of electronic and thermal Free Energies= -1455.574891

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



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.021608	-2.748938	0.324534
2	6	0	-5.330134	-1.9387	1.219815
3	6	0	-4.283316	-1.110564	0.791706
4	6	0	-3.936328	-1.085099	-0.593287
5	6	0	-4.643203	-1.919581	-1.481623
6	6	0	-5.667916	-2.737477	-1.026913
7	6	0	-3.527712	-0.276947	1.692158
8	6	0	-2.886076	-0.226778	-1.057589
9	6	0	-2.195167	0.661822	-0.159844
10	6	0	-2.517619	0.592135	1.242121
11	6	0	-1.795082	1.408084	2.152652
12	1	0	-2.018363	1.329353	3.207852
13	6	0	-0.816411	2.270761	1.7162
14	6	0	-0.518204	2.405917	0.340098
15	6	0	-1.230537	1.569939	-0.57881
16	1	0	-6.827601	-3.380537	0.677072
17	1	0	-5.637411	-1.959549	2.261835
18	1	0	-4.370096	-1.906627	-2.527558
19	1	0	-6.199528	-3.369707	-1.728852
20	1	0	-0.257559	2.847115	2.440612
21	1	0	-0.979852	1.647033	-1.627108
22	6	0	0.489504	3.278637	-0.139218
23	8	0	2.110989	1.973253	-0.466762
24	6	0	2.587137	1.39307	0.599868
25	8	0	2.387339	1.774386	1.750822
26	6	0	3.451084	0.176368	0.356348
27	6	0	3.511533	-0.489599	-0.875472
28	6	0	4.21206	-0.320618	1.414729
29	6	0	4.311165	-1.609054	-1.041524
30	1	0	2.915004	-0.135588	-1.706063
31	6	0	5.028724	-1.438154	1.261859
32	1	0	4.147122	0.18684	2.36926

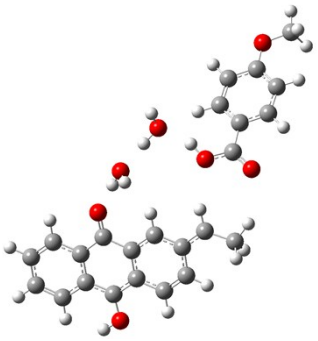
33	6	0	5.081546	-2.088831	0.025075
34	1	0	4.356497	-2.136615	-1.986889
35	1	0	5.609783	-1.791136	2.103473
36	8	0	5.841172	-3.190315	-0.240756
37	6	0	6.63952	-3.730234	0.801853
38	1	0	6.02696	-4.062268	1.647684
39	1	0	7.151225	-4.589184	0.370236
40	1	0	7.383173	-3.007353	1.155873
41	1	0	0.507842	3.414898	-1.214346
42	6	0	1.142417	4.3614	0.655911
43	1	0	2.041057	4.705281	0.14262
44	1	0	0.459479	5.217249	0.74793
45	1	0	1.431765	4.018109	1.646595
46	8	0	-2.628216	-0.299817	-2.360839
47	8	0	-3.769693	-0.291506	3.018041
48	1	0	-4.406436	-0.980826	3.23468
49	1	0	-1.82387	0.172308	-2.703415
50	8	0	-0.676343	0.795576	-3.759621
51	1	0	0.25792	1.00648	-3.516784
52	1	0	-0.972419	1.544157	-4.285959
53	8	0	1.751285	1.673644	-3.057262
54	1	0	1.975525	1.747841	-2.0915
55	1	0	2.585259	1.6156	-3.5301

Sum of electronic and zero-point Energies= -1455.495777

Sum of electronic and thermal Free Energies= -1455.560278

The imaginary frequency: -139.51

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



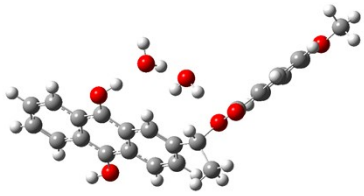
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.485302	-2.074309	-0.829894
2	6	0	7.082134	-0.768003	-0.983341
3	6	0	5.768102	-0.359031	-0.627538
4	6	0	4.869766	-1.340239	-0.101269
5	6	0	5.311214	-2.666223	0.043595
6	6	0	6.593185	-3.035702	-0.312305
7	6	0	5.311656	0.973441	-0.769612
8	6	0	3.502251	-0.996501	0.295503
9	6	0	3.07606	0.397876	0.118265
10	6	0	3.979452	1.360463	-0.403111
11	6	0	3.541141	2.69824	-0.555335
12	1	0	4.23007	3.43286	-0.950761
13	6	0	2.262625	3.063839	-0.210572
14	6	0	1.327686	2.118058	0.308953
15	6	0	1.774851	0.789822	0.459802
16	1	0	8.491847	-2.36407	-1.108199
17	1	0	7.799581	-0.057145	-1.384327
18	1	0	4.60761	-3.384757	0.444515
19	1	0	6.91672	-4.063219	-0.194877
20	1	0	1.956372	4.095217	-0.337761
21	1	0	1.094155	0.044539	0.850582
22	6	0	-0.002809	2.481734	0.661491
23	8	0	-2.603917	0.362297	1.293093
24	6	0	-3.671721	1.046754	0.853745
25	8	0	-3.684544	2.255452	0.944193
26	6	0	-4.816109	0.287058	0.258317
27	6	0	-4.733204	-1.04362	-0.181144
28	6	0	-6.021213	0.972688	0.085938
29	6	0	-5.829415	-1.664195	-0.75738

30	1	0	-3.811433	-1.60365	-0.083736
31	6	0	-7.130942	0.357232	-0.481024
32	1	0	-6.071892	2.006378	0.404189
33	6	0	-7.038251	-0.972754	-0.907733
34	1	0	-5.7747	-2.687516	-1.10824
35	1	0	-8.0503	0.916516	-0.590128
36	8	0	-8.053805	-1.673358	-1.478867
37	6	0	-9.304672	-1.025441	-1.672491
38	1	0	-9.208128	-0.157329	-2.333368
39	1	0	-9.951415	-1.764929	-2.141475
40	1	0	-9.74531	-0.71111	-0.720141
41	1	0	-0.649784	1.701325	1.046086
42	6	0	-0.583761	3.849973	0.538807
43	1	0	-0.130659	4.552807	1.253724
44	1	0	-0.428232	4.280506	-0.458706
45	1	0	-1.655674	3.814188	0.733625
46	8	0	2.746388	-1.871508	0.765194
47	8	0	6.093694	1.96033	-1.258272
48	1	0	6.961276	1.614746	-1.493377
49	1	0	1.210487	-2.088975	1.575066
50	8	0	0.393314	-2.139597	2.116754
51	1	0	-1.220936	-2.263615	1.545192
52	1	0	0.539188	-1.528378	2.844424
53	8	0	-2.188805	-2.270799	1.35688
54	1	0	-2.669004	-0.623673	1.288077
55	1	0	-2.578401	-2.850228	2.017814

Sum of electronic and zero-point Energies= -1455.531513

Sum of electronic and thermal Free Energies= -1455.600636

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



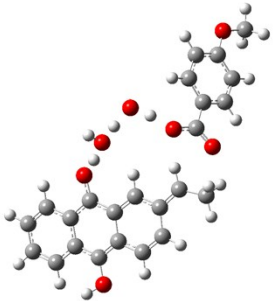
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.113078	-1.477913	0.797148
2	6	0	-6.275889	-0.592766	1.419129
3	6	0	-5.016229	-0.232634	0.849215
4	6	0	-4.636636	-0.850677	-0.397272
5	6	0	-5.534995	-1.773387	-1.009376
6	6	0	-6.740025	-2.074446	-0.436881
7	6	0	-4.131797	0.670229	1.466579
8	6	0	-3.392913	-0.552052	-0.988472
9	6	0	-2.535199	0.388151	-0.382645
10	6	0	-2.898358	0.982156	0.879348
11	6	0	-1.977298	1.882829	1.496394
12	1	0	-2.243959	2.30875	2.454689
13	6	0	-0.791838	2.204448	0.897974
14	6	0	-0.451098	1.674709	-0.38476
15	6	0	-1.312803	0.798242	-0.993432
16	1	0	-8.062886	-1.734654	1.252517
17	1	0	-6.579766	-0.180582	2.376618
18	1	0	-5.230303	-2.225756	-1.943612
19	1	0	-7.412412	-2.775791	-0.917535
20	1	0	-0.110462	2.88335	1.396529
21	1	0	-1.058745	0.392532	-1.964611
22	6	0	0.842655	2.041454	-1.071341
23	8	0	1.903252	1.240372	-0.414276
24	6	0	3.06578	1.071868	-1.112008
25	8	0	3.217024	1.476469	-2.240821
26	6	0	4.095115	0.338264	-0.33631
27	6	0	3.934296	-0.018848	1.012055
28	6	0	5.287418	0.006532	-0.984471
29	6	0	4.937273	-0.692163	1.684047
30	1	0	3.020835	0.238262	1.53104

31	6	0	6.301296	-0.672379	-0.320358
32	1	0	5.407934	0.290521	-2.022529
33	6	0	6.129013	-1.026843	1.023716
34	1	0	4.82863	-0.974953	2.723655
35	1	0	7.21143	-0.91763	-0.850022
36	8	0	7.048415	-1.688104	1.769278
37	6	0	8.282715	-2.061416	1.165624
38	1	0	8.842782	-1.183764	0.82643
39	1	0	8.848114	-2.571796	1.942951
40	1	0	8.125238	-2.743938	0.323994
41	1	0	0.810712	1.712927	-2.110342
42	6	0	1.208988	3.520014	-1.01497
43	1	0	2.113502	3.706564	-1.593325
44	1	0	0.395257	4.11126	-1.441791
45	1	0	1.372242	3.851888	0.01233
46	8	0	-3.082573	-1.167505	-2.157533
47	8	0	-4.415173	1.2725	2.667987
48	1	0	-5.358942	1.21313	2.840224
49	1	0	-2.131587	-1.426595	-2.187561
50	8	0	-0.504568	-2.004469	-2.222451
51	1	0	-0.030185	-1.916709	-1.367275
52	1	0	-0.35559	-2.9036	-2.52784
53	8	0	0.691722	-1.458737	0.206357
54	1	0	1.131393	-0.607311	0.053768
55	1	0	-0.056369	-1.230564	0.769765

Sum of electronic and zero-point Energies= -1455.567869

Sum of electronic and thermal Free Energies= -1455.631491

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



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.642658	-2.565477	1.183883
2	6	0	-6.398169	-1.211971	1.285484
3	6	0	-5.228097	-0.639174	0.733142
4	6	0	-4.28669	-1.50629	0.103118
5	6	0	-4.567575	-2.886575	0.006478
6	6	0	-5.727816	-3.412324	0.531238
7	6	0	-4.969983	0.767057	0.798875
8	6	0	-3.048559	-0.985553	-0.426036
9	6	0	-2.77399	0.423038	-0.246665
10	6	0	-3.784544	1.294338	0.342637
11	6	0	-3.491491	2.702819	0.451458
12	1	0	-4.263911	3.341515	0.858575
13	6	0	-2.295991	3.212635	0.081513
14	6	0	-1.25321	2.354259	-0.446782
15	6	0	-1.551697	0.969554	-0.601683
16	1	0	-7.543955	-2.980712	1.620676
17	1	0	-7.098806	-0.589147	1.82913
18	1	0	-3.839217	-3.51858	-0.483712
19	1	0	-5.930777	-4.473715	0.454807
20	1	0	-2.106474	4.273061	0.184932
21	1	0	-0.770521	0.343577	-1.010024
22	6	0	0.01518	2.769526	-0.803924
23	8	0	2.244339	0.604071	-1.190154
24	6	0	3.038655	1.088945	-0.292559
25	8	0	2.821437	2.135247	0.327545
26	6	0	4.311529	0.322588	0.000674
27	6	0	4.783184	-0.707252	-0.825916
28	6	0	5.070397	0.670974	1.118012

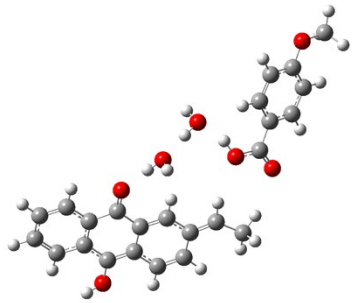
29	6	0	5.964136	-1.372715	-0.533209
30	1	0	4.2222	-0.983718	-1.709806
31	6	0	6.254106	0.007296	1.431377
32	1	0	4.712995	1.482895	1.739356
33	6	0	6.706571	-1.023231	0.601229
34	1	0	6.340389	-2.164158	-1.170744
35	1	0	6.811609	0.301787	2.310744
36	8	0	7.850662	-1.739773	0.807271
37	6	0	8.654955	-1.418371	1.931564
38	1	0	8.111407	-1.564546	2.872023
39	1	0	9.50209	-2.102008	1.897039
40	1	0	9.021385	-0.386646	1.883639
41	1	0	0.712922	2.009692	-1.159304
42	6	0	0.576644	4.130028	-0.703507
43	1	0	1.482729	4.043622	-0.090723
44	1	0	0.929731	4.451339	-1.6921
45	1	0	-0.097857	4.88341	-0.298514
46	8	0	-2.253255	-1.819131	-1.000203
47	8	0	-5.884402	1.615345	1.377632
48	1	0	-6.774934	1.310605	1.176
49	1	0	-1.4119	-1.538685	-1.74711
50	8	0	-0.533801	-1.33902	-2.592233
51	1	0	0.500232	-1.54676	-2.287921
52	1	0	-0.718909	-1.732366	-3.4493
53	8	0	1.768352	-1.67905	-1.895931
54	1	0	2.075028	-0.698966	-1.55887
55	1	0	1.898556	-2.287764	-1.162633

Sum of electronic and zero-point Energies= -1455.532988

Sum of electronic and thermal Free Energies= -1455.597421

The imaginary frequency: -752.61

The product complex of water-assisted photodeprotection process of compound **1** via the ground surface:



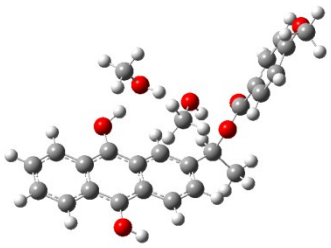
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.518327	-2.100567	0.913538
2	6	0	-7.121187	-0.774788	0.973083
3	6	0	-5.837438	-0.381761	0.541905
4	6	0	-4.947457	-1.389094	0.084811
5	6	0	-5.36897	-2.723998	0.033237
6	6	0	-6.645142	-3.08408	0.433776
7	6	0	-5.41299	0.999769	0.566362
8	6	0	-3.568248	-1.055063	-0.316016
9	6	0	-3.176929	0.364693	-0.213729
10	6	0	-4.141268	1.369397	0.215054
11	6	0	-3.700989	2.746115	0.25391
12	1	0	-4.421731	3.492989	0.560236
13	6	0	-2.439031	3.101406	-0.071548
14	6	0	-1.456364	2.112361	-0.486232
15	6	0	-1.905937	0.74546	-0.545114
16	1	0	-8.510696	-2.3763	1.252606
17	1	0	-7.803242	-0.042904	1.390635
18	1	0	-4.660508	-3.461262	-0.323257
19	1	0	-6.961434	-4.119445	0.389332
20	1	0	-2.149304	4.14373	-0.028769
21	1	0	-1.200031	-0.008799	-0.874945
22	6	0	-0.157781	2.389653	-0.819804
23	8	0	2.534992	0.431346	-0.632516
24	6	0	3.628112	1.109427	-0.249851
25	8	0	3.571115	2.314368	-0.123874
26	6	0	4.893352	0.349096	-0.006242
27	6	0	5.102913	-0.977778	-0.41443
28	6	0	5.942578	1.028877	0.618017

29	6	0	6.319087	-1.600345	-0.187447
30	1	0	4.319125	-1.536084	-0.91068
31	6	0	7.164679	0.412367	0.857964
32	1	0	5.782451	2.058907	0.910784
33	6	0	7.358959	-0.913446	0.452499
34	1	0	6.494632	-2.621455	-0.503231
35	1	0	7.951634	0.967111	1.350549
36	8	0	8.509723	-1.614123	0.629547
37	6	0	9.612371	-0.969075	1.255108
38	1	0	9.369193	-0.660204	2.277428
39	1	0	10.41048	-1.708786	1.282957
40	1	0	9.945199	-0.098214	0.680322
41	1	0	0.474277	1.55287	-1.102296
42	6	0	0.524496	3.709824	-0.818694
43	1	0	1.503411	3.607021	-0.338913
44	1	0	0.737257	4.018124	-1.851783
45	1	0	-0.046938	4.504531	-0.338555
46	8	0	-2.798386	-1.945744	-0.706166
47	8	0	-6.286911	1.972118	0.991786
48	1	0	-7.179683	1.738137	0.718042
49	1	0	-1.190741	-2.177231	-1.32228
50	8	0	-0.311548	-2.267543	-1.749532
51	1	0	1.250296	-2.267019	-1.038055
52	1	0	-0.454815	-2.097446	-2.684163
53	8	0	2.134422	-2.202016	-0.609071
54	1	0	2.565947	-0.553807	-0.544284
55	1	0	2.057037	-2.672388	0.225986

Sum of electronic and zero-point Energies= -1455.559198

Sum of electronic and thermal Free Energies= -1455.627062

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



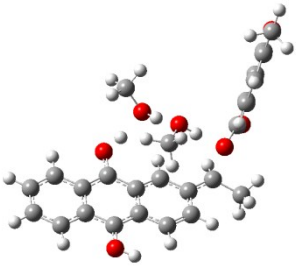
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.972853	-1.462598	0.622075
2	6	0	6.174882	-0.506578	1.278744
3	6	0	4.930333	-0.135721	0.757651
4	6	0	4.471097	-0.738262	-0.458191
5	6	0	5.276248	-1.694679	-1.089849
6	6	0	6.525347	-2.052612	-0.551208
7	6	0	4.082249	0.825743	1.410121
8	6	0	3.187976	-0.357142	-0.981894
9	6	0	2.377757	0.65654	-0.362846
10	6	0	2.805224	1.214994	0.893699
11	6	0	1.956283	2.122852	1.544265
12	1	0	2.213283	2.522793	2.520328
13	6	0	0.745122	2.538882	0.95943
14	6	0	0.365497	2.065931	-0.287193
15	6	0	1.189636	1.115633	-0.938663
16	1	0	7.935777	-1.735454	1.043031
17	1	0	6.521356	-0.053813	2.200415
18	1	0	4.923601	-2.157586	-2.004061
19	1	0	7.13442	-2.793881	-1.05997
20	1	0	0.890177	0.744521	-1.912276
21	8	0	2.773306	-0.974677	-2.110168
22	8	0	4.581332	1.356023	2.556485
23	1	0	4.041239	2.100585	2.861526
24	1	0	0.120506	3.244442	1.496178
25	8	0	-1.969783	1.590648	-0.427684
26	6	0	-3.051122	1.364962	-1.21391
27	8	0	-3.151652	1.816302	-2.347021
28	6	0	-4.06521	0.517402	-0.559306
29	6	0	-5.149281	0.055677	-1.326772

30	6	0	-3.989531	0.164056	0.794861
31	6	0	-6.121705	-0.747081	-0.758571
32	1	0	-5.212291	0.330521	-2.373978
33	6	0	-4.964206	-0.637886	1.379047
34	1	0	-3.169245	0.525992	1.402886
35	6	0	-6.034627	-1.100708	0.599599
36	1	0	-6.959433	-1.115299	-1.341417
37	1	0	-4.886207	-0.892724	2.428037
38	8	0	-7.034282	-1.889692	1.066198
39	6	0	-7.000037	-2.290467	2.440916
40	1	0	-7.883606	-2.912242	2.58831
41	1	0	-6.099813	-2.874687	2.658709
42	1	0	-7.047717	-1.422162	3.106355
43	1	0	1.792993	-1.210892	-2.056442
44	6	0	0.762412	-3.268168	-1.396002
45	1	0	1.260819	-3.783612	-2.220842
46	1	0	1.451289	-3.222758	-0.543171
47	1	0	-0.125766	-3.840946	-1.106197
48	8	0	0.39573	-1.960939	-1.852639
49	1	0	-0.132276	-1.543767	-1.123502
50	6	0	-0.273245	-1.141058	1.439793
51	1	0	-0.144232	-2.201736	1.66761
52	1	0	-0.804986	-0.665437	2.271735
53	1	0	0.711952	-0.676554	1.333545
54	8	0	-1.035309	-1.05674	0.230507
55	1	0	-1.237911	-0.118499	0.06473
56	6	0	-0.916845	2.489796	-0.954858
57	1	0	-0.851	2.292292	-2.026046
58	6	0	-1.348954	3.925776	-0.712182
59	1	0	-2.265609	4.141266	-1.266418
60	1	0	-1.533591	4.111223	0.349098
61	1	0	-0.567372	4.609322	-1.056137

Sum of electronic and zero-point Energies= -1533.874635

Sum of electronic and thermal Free Energies= -1533.942339

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



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.782929	-1.908066	0.649623
2	6	0	6.129727	-0.820435	1.236026
3	6	0	4.919828	-0.349822	0.71228
4	6	0	4.345067	-0.985019	-0.429739
5	6	0	5.014378	-2.085808	-0.997979
6	6	0	6.220804	-2.536397	-0.464119
7	6	0	4.215033	0.760135	1.309414
8	6	0	3.098774	-0.510232	-0.951117
9	6	0	2.442035	0.648959	-0.403486
10	6	0	3.001647	1.257951	0.779475
11	6	0	2.311146	2.35545	1.358416
12	1	0	2.680749	2.831296	2.260301
13	6	0	1.147481	2.852184	0.800228
14	6	0	0.615048	2.311358	-0.386797
15	6	0	1.296555	1.19659	-0.975117
16	1	0	7.721243	-2.261728	1.064225
17	1	0	6.55637	-0.335018	2.105976
18	1	0	4.578567	-2.579523	-1.858316
19	1	0	6.723009	-3.384344	-0.920089
20	1	0	0.897753	0.778659	-1.891089
21	8	0	2.586708	-1.1663	-2.003441
22	8	0	4.80803	1.284238	2.394723
23	1	0	4.318626	2.04041	2.754121
24	1	0	0.651521	3.684333	1.287383
25	8	0	-1.964278	1.631398	-0.241342
26	6	0	-3.017427	1.440951	-0.996076
27	8	0	-3.179716	1.951866	-2.115587
28	6	0	-4.052965	0.530962	-0.411647

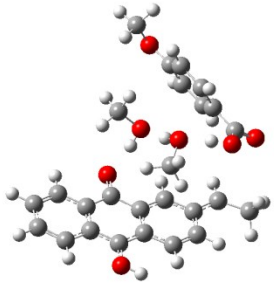
29	6	0	-5.105963	0.07458	-1.221083
30	6	0	-4.007217	0.12269	0.926219
31	6	0	-6.074196	-0.775632	-0.71182
32	1	0	-5.150537	0.391717	-2.257301
33	6	0	-4.977758	-0.724912	1.455813
34	1	0	-3.207453	0.477143	1.566265
35	6	0	-6.015197	-1.181498	0.631738
36	1	0	-6.886857	-1.139944	-1.332165
37	1	0	-4.919779	-1.019197	2.496125
38	8	0	-7.010074	-2.015576	1.040681
39	6	0	-7.000926	-2.462961	2.399528
40	1	0	-7.871205	-3.112164	2.503184
41	1	0	-6.092042	-3.031986	2.623264
42	1	0	-7.08848	-1.621027	3.094792
43	1	0	1.569356	-1.212998	-1.989876
44	6	0	0.003168	-3.02706	-1.87341
45	1	0	0.219042	-3.437684	-2.863195
46	1	0	0.738135	-3.421541	-1.160496
47	1	0	-0.9978	-3.349378	-1.566864
48	8	0	0.065859	-1.598269	-1.961405
49	1	0	-0.307242	-1.243047	-1.105337
50	6	0	-0.070225	-0.869933	1.448438
51	1	0	0.738384	-1.571632	1.224189
52	1	0	-0.593761	-1.215357	2.348879
53	1	0	0.364669	0.11294	1.648543
54	8	0	-0.966597	-0.830257	0.334797
55	1	0	-1.293027	0.091364	0.215172
56	6	0	-0.588793	2.809232	-0.97599
57	1	0	-0.773885	2.484654	-1.994604
58	6	0	-1.183707	4.133498	-0.614574
59	1	0	-2.16991	4.240588	-1.069282
60	1	0	-1.276995	4.269246	0.465409
61	1	0	-0.543387	4.9368	-1.002098

Sum of electronic and zero-point Energies= -1533.860122

Sum of electronic and thermal Free Energies= -1533.929323

The imaginary frequency: -343.71

The product complex of methanol-assisted photodeprotection process of compound **1** via the triplet surface:



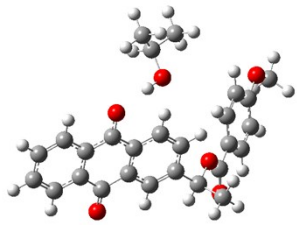
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.683286	-2.732849	0.256283
2	6	0	5.53073	-1.381904	0.491325
3	6	0	4.352427	-0.709258	0.076153
4	6	0	3.327429	-1.445396	-0.593265
5	6	0	3.512536	-2.82388	-0.816984
6	6	0	4.667915	-3.460556	-0.401383
7	6	0	4.167364	0.676976	0.317938
8	6	0	2.104038	-0.79798	-1.033658
9	6	0	1.94744	0.627157	-0.766186
10	6	0	2.966032	1.354294	-0.084964
11	6	0	2.745905	2.727923	0.190485
12	1	0	3.488745	3.316585	0.721107
13	6	0	1.583804	3.3549	-0.194986
14	6	0	0.556783	2.652572	-0.898259
15	6	0	0.774283	1.28788	-1.166476
16	1	0	6.587506	-3.239018	0.579262
17	1	0	6.308244	-0.822111	0.997794
18	1	0	2.725817	-3.371519	-1.323533
19	1	0	4.796104	-4.523522	-0.580631
20	1	0	0.015413	0.725695	-1.698513
21	8	0	1.190891	-1.458709	-1.618995
22	8	0	5.170356	1.308759	0.94426
23	1	0	4.998356	2.257222	1.046801
24	1	0	1.449523	4.40459	0.041094
25	8	0	-2.340891	2.353595	1.43442
26	6	0	-3.240367	2.140217	0.471939
27	8	0	-3.710389	3.086869	-0.154192
28	6	0	-3.641011	0.734071	0.207133

29	6	0	-3.907379	0.334324	-1.112212
30	6	0	-3.781824	-0.197062	1.242238
31	6	0	-4.246021	-0.979057	-1.39264
32	1	0	-3.820917	1.057384	-1.916725
33	6	0	-4.162289	-1.510136	0.978256
34	1	0	-3.599418	0.104029	2.267768
35	6	0	-4.36531	-1.911251	-0.348554
36	1	0	-4.419547	-1.310385	-2.411221
37	1	0	-4.277609	-2.207845	1.79765
38	8	0	-4.681033	-3.179663	-0.72429
39	6	0	-4.784457	-4.179029	0.294379
40	1	0	-5.015634	-5.108997	-0.226426
41	1	0	-3.840053	-4.289136	0.8377
42	1	0	-5.59041	-3.945359	0.998251
43	1	0	-0.274426	-1.339726	-0.769248
44	6	0	-0.869335	-2.67681	0.53398
45	1	0	-1.274501	-3.468691	-0.108578
46	1	0	0.17532	-2.913188	0.769378
47	1	0	-1.440245	-2.65121	1.464488
48	8	0	-0.988771	-1.396674	-0.090023
49	1	0	-0.886246	-0.266999	1.13414
50	6	0	0.420146	0.608976	2.358172
51	1	0	1.109764	-0.212509	2.139605
52	1	0	0.426932	0.795294	3.436231
53	1	0	0.763789	1.511928	1.844054
54	8	0	-0.91481	0.262098	1.977219
55	1	0	-1.826957	1.510214	1.680306
56	6	0	-0.644367	3.294849	-1.308841
57	1	0	-1.373357	2.683624	-1.832461
58	6	0	-0.98976	4.713383	-1.01121
59	1	0	-1.876036	5.02439	-1.568522
60	1	0	-1.210412	4.853772	0.057532
61	1	0	-0.170558	5.401176	-1.256451

Sum of electronic and zero-point Energies= -1533.892019

Sum of electronic and thermal Free Energies= -1533.960109

The reaction complex for ketyl formation in HAT process between IPA and para position of the compound **1** via the triplet surface:



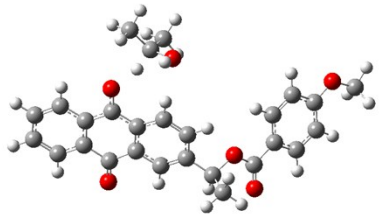
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.934366	-0.837072	-1.522483
2	6	0	-5.9555	-0.015213	-1.00439
3	6	0	-4.702402	-0.553294	-0.624961
4	6	0	-4.462271	-1.937597	-0.78512
5	6	0	-5.476581	-2.749565	-1.314733
6	6	0	-6.69839	-2.214265	-1.680083
7	6	0	-3.666369	0.292289	-0.079533
8	6	0	-3.172448	-2.553517	-0.415523
9	6	0	-2.15325	-1.642523	0.139846
10	6	0	-2.390566	-0.257755	0.306415
11	6	0	-1.367248	0.561622	0.84387
12	1	0	-1.543903	1.622857	0.974683
13	6	0	-0.160834	0.006488	1.209532
14	6	0	0.087709	-1.374042	1.050066
15	6	0	-0.910232	-2.17224	0.516323
16	1	0	-7.891294	-0.415858	-1.809471
17	1	0	-6.133399	1.046729	-0.883544
18	1	0	-5.25919	-3.80534	-1.424608
19	1	0	-7.472446	-2.853818	-2.087734
20	1	0	0.614901	0.642904	1.618721
21	1	0	-0.764236	-3.236812	0.368873
22	8	0	-2.962347	-3.758404	-0.559595
23	8	0	-3.902245	1.567278	0.037317
24	6	0	1.399352	-1.983884	1.486411
25	1	0	1.50962	-2.977659	1.050975
26	8	0	2.460958	-1.145025	0.945515
27	6	0	3.643613	-1.749336	0.672632
28	8	0	3.853926	-2.922603	0.884836
29	6	0	4.63432	-0.810972	0.089485
30	6	0	4.341064	0.532577	-0.191291

31	6	0	5.911062	-1.297693	-0.197225
32	6	0	5.302721	1.360326	-0.740609
33	1	0	3.352613	0.917974	0.01974
34	6	0	6.886721	-0.475039	-0.748288
35	1	0	6.128336	-2.336499	0.018452
36	6	0	6.584304	0.864261	-1.022889
37	1	0	5.093258	2.398789	-0.965755
38	1	0	7.866824	-0.88066	-0.958726
39	8	0	7.454998	1.756799	-1.558985
40	6	0	8.774133	1.32409	-1.87184
41	1	0	8.76565	0.523936	-2.619418
42	1	0	9.280893	2.195519	-2.282246
43	1	0	9.305692	0.983437	-0.97704
44	6	0	1.546029	-2.075685	3.005115
45	1	0	2.49782	-2.544109	3.260034
46	1	0	1.500846	-1.082712	3.458924
47	1	0	0.737333	-2.681367	3.421049
48	6	0	-1.30803	5.451762	0.302219
49	1	0	-1.163763	5.9001	1.288938
50	1	0	-1.253113	6.241739	-0.450901
51	1	0	-0.49348	4.746771	0.123607
52	6	0	-2.652271	4.741406	0.240213
53	1	0	-2.767472	4.274067	-0.747539
54	6	0	-3.832355	5.681802	0.483473
55	1	0	-3.866361	6.469219	-0.274933
56	1	0	-4.780759	5.137509	0.441785
57	1	0	-3.748122	6.148286	1.46863
58	8	0	-2.616187	3.709259	1.238871
59	1	0	-3.436546	3.204998	1.18405

Sum of electronic and zero-point Energies= -1495.740652

Sum of electronic and thermal Free Energies= -1495.812093

The transition state for ketyl formation in HAT process between IPA and para position of the compound **1** via the triplet surface:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.999308	-0.408559	-1.407265
2	6	0	-5.99442	0.340342	-0.830389
3	6	0	-4.745688	-0.251495	-0.519979
4	6	0	-4.542845	-1.623609	-0.819095
5	6	0	-5.578552	-2.358261	-1.414291
6	6	0	-6.795822	-1.767825	-1.702496
7	6	0	-3.68245	0.522442	0.077911
8	6	0	-3.257042	-2.289757	-0.546079
9	6	0	-2.214125	-1.462141	0.088267
10	6	0	-2.430823	-0.092498	0.409462
11	6	0	-1.391031	0.606282	1.077011
12	1	0	-1.529553	1.634042	1.380033
13	6	0	-0.19899	-0.015137	1.376824
14	6	0	0.029408	-1.363983	1.030181
15	6	0	-0.985055	-2.061462	0.39682
16	1	0	-7.950792	0.057575	-1.638239
17	1	0	-6.147435	1.389038	-0.611273
18	1	0	-5.38284	-3.399793	-1.638906
19	1	0	-7.589062	-2.348816	-2.158644
20	1	0	0.577953	0.545079	1.8841
21	1	0	-0.863545	-3.102965	0.120584
22	8	0	-3.066331	-3.476218	-0.823862
23	8	0	-3.973469	1.789589	0.31475
24	6	0	1.328009	-2.05012	1.38128
25	1	0	1.403231	-2.996522	0.845245
26	8	0	2.407907	-1.189228	0.908435
27	6	0	3.563328	-1.794693	0.544265
28	8	0	3.742655	-2.989676	0.622297
29	6	0	4.572219	-0.827759	0.042047
30	6	0	4.321052	0.548211	-0.071231

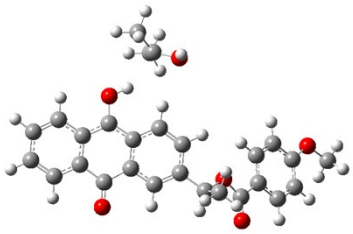
31	6	0	5.821781	-1.319569	-0.339418
32	6	0	5.296861	1.402443	-0.551196
33	1	0	3.353628	0.937842	0.215798
34	6	0	6.811122	-0.470885	-0.822927
35	1	0	6.006685	-2.38313	-0.252774
36	6	0	6.550582	0.900413	-0.930843
37	1	0	5.119734	2.466676	-0.646511
38	1	0	7.769294	-0.881352	-1.110727
39	8	0	7.438379	1.820144	-1.388644
40	6	0	8.72916	1.381577	-1.796527
41	1	0	8.666143	0.673806	-2.6298
42	1	0	9.255513	2.276661	-2.122898
43	1	0	9.276139	0.921626	-0.966669
44	6	0	1.500398	-2.299372	2.879217
45	1	0	2.444182	-2.813845	3.066925
46	1	0	1.489108	-1.356968	3.432146
47	1	0	0.683787	-2.924667	3.248008
48	6	0	-1.450113	4.031443	-0.679797
49	1	0	-0.978465	5.018801	-0.714387
50	1	0	-2.007947	3.873594	-1.604137
51	1	0	-0.664428	3.277609	-0.611274
52	6	0	-2.374038	3.946935	0.51967
53	1	0	-2.882662	2.894452	0.47961
54	6	0	-3.543942	4.921715	0.519641
55	1	0	-4.155442	4.78611	-0.373582
56	1	0	-4.187409	4.761878	1.389943
57	1	0	-3.172511	5.951342	0.542354
58	8	0	-1.597865	4.014108	1.687202
59	1	0	-2.181574	4.124121	2.447259

Sum of electronic and zero-point Energies= -1495.735254

Sum of electronic and thermal Free Energies= -1495.802598

The imaginary frequency: -112.50

The product complex for ketyl formation in HAT process between IPA and para position of the compound **1** via the triplet surface:



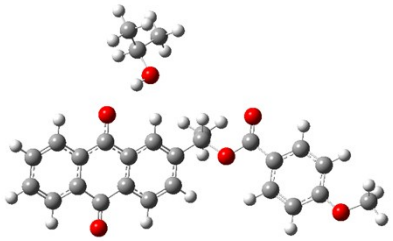
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.002012	-0.543671	-1.493838
2	6	0	-5.990365	0.245872	-0.985868
3	6	0	-4.750855	-0.328181	-0.611837
4	6	0	-4.570158	-1.728724	-0.771594
5	6	0	-5.613222	-2.507122	-1.290107
6	6	0	-6.818223	-1.928457	-1.648895
7	6	0	-3.690286	0.472109	-0.087154
8	6	0	-3.299076	-2.380265	-0.403972
9	6	0	-2.241512	-1.503254	0.139113
10	6	0	-2.442741	-0.10184	0.298265
11	6	0	-1.373907	0.663384	0.8335
12	1	0	-1.470056	1.732618	0.982111
13	6	0	-0.181123	0.070266	1.185759
14	6	0	0.019736	-1.315875	1.020254
15	6	0	-1.014896	-2.075315	0.497107
16	1	0	-7.945951	-0.090447	-1.775861
17	1	0	-6.130359	1.31181	-0.867402
18	1	0	-5.438678	-3.570515	-1.398497
19	1	0	-7.618565	-2.540024	-2.049358
20	1	0	0.619836	0.681742	1.584031
21	1	0	-0.906069	-3.143509	0.345771
22	8	0	-3.125964	-3.593098	-0.539736
23	8	0	-3.956637	1.792867	0.023159
24	6	0	1.314356	-1.971	1.440241
25	1	0	1.396874	-2.95692	0.981517
26	8	0	2.399824	-1.149075	0.918156
27	6	0	3.567024	-1.776477	0.635673
28	8	0	3.749651	-2.958298	0.825061
29	6	0	4.581787	-0.85079	0.072341
30	6	0	4.321117	0.504553	-0.182138

31	6	0	5.846976	-1.361982	-0.222421
32	6	0	5.303224	1.320165	-0.713362
33	1	0	3.34131	0.908459	0.034424
34	6	0	6.843027	-0.551841	-0.755663
35	1	0	6.038897	-2.409882	-0.027635
36	6	0	6.573098	0.799456	-1.003605
37	1	0	5.118771	2.367552	-0.918227
38	1	0	7.813569	-0.976294	-0.97315
39	8	0	7.466071	1.681867	-1.520329
40	6	0	8.774616	1.223787	-1.840808
41	1	0	8.747911	0.439078	-2.604181
42	1	0	9.302808	2.090696	-2.233472
43	1	0	9.296936	0.852616	-0.952687
44	6	0	1.461238	-2.102105	2.956074
45	1	0	2.400902	-2.600377	3.199377
46	1	0	1.441576	-1.118557	3.432036
47	1	0	0.637398	-2.696013	3.359016
48	6	0	-1.861504	4.427841	-0.827035
49	1	0	-1.448029	5.428016	-1.034111
50	1	0	-2.708571	4.27091	-1.49737
51	1	0	-1.083714	3.699755	-1.068939
52	6	0	-2.28191	4.303952	0.600915
53	1	0	-3.195076	2.31915	0.328635
54	6	0	-3.475089	5.044926	1.119467
55	1	0	-4.331382	4.919645	0.454419
56	1	0	-3.77287	4.68848	2.112062
57	1	0	-3.271311	6.125297	1.203871
58	8	0	-1.199255	4.190692	1.450823
59	1	0	-1.501601	4.250598	2.364075

Sum of electronic and zero-point Energies= -1495.760680

Sum of electronic and thermal Free Energies= -1495.831021

The reaction complex for ketyl formation in HAT process between IPA and meta position of the compound **1** via the triplet surface:



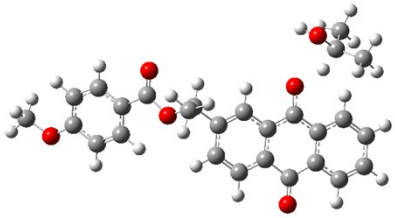
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.831957	-2.612005	-1.009634
2	6	0	5.663409	-3.112189	-0.464139
3	6	0	4.567188	-2.273639	-0.213152
4	6	0	4.667792	-0.897797	-0.524937
5	6	0	5.868706	-0.395907	-1.081633
6	6	0	6.93047	-1.243804	-1.318247
7	6	0	3.34188	-2.852811	0.373322
8	6	0	3.546016	-0.024684	-0.270748
9	6	0	2.326522	-0.535624	0.307034
10	6	0	2.232097	-1.913014	0.617118
11	6	0	1.03757	-2.400204	1.169212
12	1	0	0.990364	-3.459712	1.391288
13	6	0	-0.028532	-1.559257	1.419077
14	6	0	0.060794	-0.184286	1.113624
15	6	0	1.224383	0.316155	0.559954
16	1	0	7.670386	-3.272157	-1.198404
17	1	0	5.553017	-4.160106	-0.211802
18	1	0	5.94268	0.659375	-1.315772
19	1	0	7.846247	-0.849937	-1.744561
20	1	0	-0.944205	-1.954036	1.841997
21	1	0	1.296588	1.367895	0.305962
22	8	0	3.663188	1.237685	-0.569519
23	8	0	3.254427	-4.051412	0.642679
24	6	0	-1.082302	0.755865	1.426226
25	1	0	-0.957075	1.689414	0.876432
26	8	0	-2.300684	0.119224	0.947029
27	6	0	-3.329552	0.936335	0.611732
28	8	0	-3.282232	2.141263	0.720829
29	6	0	-4.504182	0.184609	0.105062

30	6	0	-4.502044	-1.207686	-0.072652
31	6	0	-5.657574	0.904404	-0.212481
32	6	0	-5.625756	-1.855097	-0.552129
33	1	0	-3.610753	-1.773817	0.162279
34	6	0	-6.794369	0.264562	-0.692621
35	1	0	-5.64996	1.97881	-0.07673
36	6	0	-6.782398	-1.124999	-0.864459
37	1	0	-5.640805	-2.928148	-0.697874
38	1	0	-7.673621	0.848453	-0.927545
39	8	0	-7.830974	-1.853692	-1.324143
40	6	0	-9.038829	-1.180461	-1.660481
41	1	0	-8.883205	-0.459915	-2.470382
42	1	0	-9.725287	-1.955974	-1.995124
43	1	0	-9.466001	-0.668106	-0.791963
44	6	0	-1.212172	1.055655	2.919902
45	1	0	-2.03166	1.755187	3.089875
46	1	0	-1.398232	0.137969	3.483054
47	1	0	-0.287386	1.504453	3.290413
48	6	0	1.624707	5.26603	0.564047
49	1	0	0.812169	5.627449	-0.0717
50	1	0	2.112791	6.12602	1.029294
51	1	0	1.191706	4.6468	1.352212
52	6	0	2.620582	4.463815	-0.260218
53	1	0	3.41696	4.090317	0.398606
54	6	0	3.253368	5.280386	-1.386951
55	1	0	3.801851	6.137119	-0.985165
56	1	0	3.958535	4.672987	-1.962698
57	1	0	2.481287	5.647485	-2.068263
58	8	0	1.9007	3.341267	-0.794965
59	1	0	2.519829	2.791388	-1.289682

Sum of electronic and zero-point Energies= -1495.740399

Sum of electronic and thermal Free Energies= -1495.810956

The transition state for ketyl formation in HAT process between IPA and meta position of the compound **1** via the triplet surface:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.168974	-2.796765	-1.099344
2	6	0	5.028193	-3.208812	-0.434808
3	6	0	3.98817	-2.311561	-0.154263
4	6	0	4.113947	-0.94666	-0.541304
5	6	0	5.277397	-0.554592	-1.248477
6	6	0	6.281786	-1.460444	-1.52017
7	6	0	2.771107	-2.823924	0.504358
8	6	0	3.054967	-0.023821	-0.245592
9	6	0	1.835161	-0.484563	0.367651
10	6	0	1.688506	-1.849763	0.722478
11	6	0	0.494132	-2.271635	1.325524
12	1	0	0.414884	-3.318493	1.592783
13	6	0	-0.534755	-1.383888	1.571512
14	6	0	-0.397827	-0.020854	1.228137
15	6	0	0.771317	0.411909	0.63413
16	1	0	6.964586	-3.502015	-1.30945
17	1	0	4.893962	-4.236098	-0.118549
18	1	0	5.362828	0.46107	-1.607869
19	1	0	7.158839	-1.139789	-2.071679
20	1	0	-1.454166	-1.730491	2.02801
21	1	0	0.891652	1.454717	0.367601
22	8	0	3.107798	1.261294	-0.541152
23	8	0	2.663254	-4.005276	0.842972
24	6	0	-1.49423	0.97137	1.54289
25	1	0	-1.303872	1.911686	1.024543
26	8	0	-2.735506	0.422231	1.0119
27	6	0	-3.680964	1.308168	0.616578
28	8	0	-3.545656	2.508868	0.704825
29	6	0	-4.887142	0.638222	0.070452
30	6	0	-4.984452	-0.753866	-0.080524

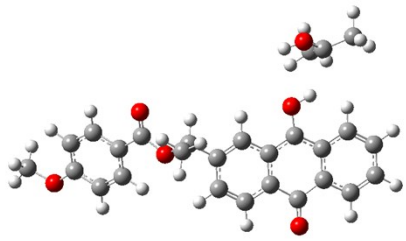
31	6	0	-5.966271	1.436472	-0.313276
32	6	0	-6.13197	-1.324261	-0.599819
33	1	0	-4.150964	-1.380594	0.207011
34	6	0	-7.126236	0.87454	-0.833895
35	1	0	-5.882462	2.509927	-0.196826
36	6	0	-7.213416	-0.515336	-0.97984
37	1	0	-6.222797	-2.396048	-0.726065
38	1	0	-7.946421	1.518539	-1.119991
39	8	0	-8.292781	-1.171652	-1.476446
40	6	0	-9.426255	-0.414962	-1.885533
41	1	0	-9.173544	0.277422	-2.695506
42	1	0	-10.151915	-1.141842	-2.245686
43	1	0	-9.857597	0.143569	-1.048036
44	6	0	-1.658	1.240114	3.038089
45	1	0	-2.442593	1.980807	3.200828
46	1	0	-1.915386	0.321638	3.570564
47	1	0	-0.722871	1.625921	3.451252
48	6	0	6.360848	2.76525	0.274911
49	1	0	6.961858	3.679389	0.322832
50	1	0	6.945543	1.987522	-0.218078
51	1	0	6.140932	2.446221	1.294679
52	6	0	5.074305	3.038352	-0.478338
53	1	0	4.454187	2.04157	-0.529683
54	6	0	5.231594	3.488526	-1.927441
55	1	0	5.813656	2.765422	-2.502332
56	1	0	4.256748	3.594832	-2.411392
57	1	0	5.74519	4.454727	-1.959719
58	8	0	4.289853	3.907554	0.281738
59	1	0	3.490718	4.122949	-0.21445

Sum of electronic and zero-point Energies= -1495.733065

Sum of electronic and thermal Free Energies= -1495.800797

The imaginary frequency: -140.49

The product complex for ketyl formation in HAT process between IPA and meta position of the compound **1** via the triplet surface:



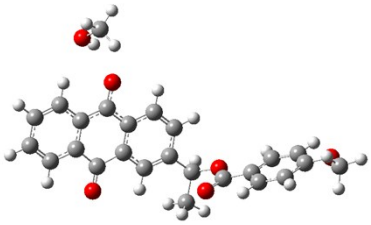
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.347219	-2.446054	-1.214925
2	6	0	5.137638	-3.035538	-0.888842
3	6	0	4.064719	-2.269251	-0.419
4	6	0	4.21436	-0.859521	-0.269538
5	6	0	5.459579	-0.277771	-0.618512
6	6	0	6.502165	-1.057058	-1.077959
7	6	0	2.793421	-2.948853	-0.090986
8	6	0	3.115337	-0.089677	0.216108
9	6	0	1.868824	-0.693117	0.555626
10	6	0	1.6981	-2.09421	0.402694
11	6	0	0.466264	-2.674709	0.732874
12	1	0	0.365164	-3.745169	0.602383
13	6	0	-0.577405	-1.905286	1.210565
14	6	0	-0.42108	-0.511933	1.372405
15	6	0	0.784457	0.077344	1.041969
16	1	0	7.170468	-3.051006	-1.576386
17	1	0	4.981764	-4.102933	-0.986296
18	1	0	5.611285	0.794038	-0.5356
19	1	0	7.446098	-0.590162	-1.335806
20	1	0	-1.525576	-2.368121	1.456293
21	1	0	0.914222	1.146099	1.155045
22	8	0	3.191543	1.25097	0.390453
23	8	0	2.659109	-4.166344	-0.223993
24	6	0	-1.54084	0.331306	1.939394
25	1	0	-1.328509	1.388621	1.777811
26	8	0	-2.745994	0.006413	1.1878
27	6	0	-3.673307	0.986238	1.058898
28	8	0	-3.549719	2.08656	1.550264
29	6	0	-4.841972	0.553823	0.253652

30	6	0	-4.928012	-0.709934	-0.351182
31	6	0	-5.896498	1.454088	0.090066
32	6	0	-6.040679	-1.057066	-1.094993
33	1	0	-4.113331	-1.412286	-0.236808
34	6	0	-7.021058	1.115918	-0.653598
35	1	0	-5.821527	2.428406	0.556913
36	6	0	-7.097822	-0.147926	-1.251432
37	1	0	-6.122595	-2.026859	-1.570083
38	1	0	-7.822406	1.833849	-0.761175
39	8	0	-8.144371	-0.585417	-1.99649
40	6	0	-9.255216	0.281847	-2.194817
41	1	0	-8.960181	1.19591	-2.720882
42	1	0	-9.958972	-0.276416	-2.809378
43	1	0	-9.73215	0.544121	-1.244551
44	6	0	-1.788795	0.085223	3.426968
45	1	0	-2.586573	0.737582	3.785528
46	1	0	-2.068432	-0.955603	3.605531
47	1	0	-0.881115	0.299617	3.996281
48	6	0	6.381958	3.923778	-0.530528
49	1	0	6.545663	4.993329	-0.740783
50	1	0	6.981499	3.352793	-1.242739
51	1	0	6.753969	3.732479	0.478735
52	6	0	4.935941	3.567928	-0.639558
53	1	0	4.079717	1.598692	0.208468
54	6	0	4.25385	3.531732	-1.972876
55	1	0	4.847683	2.976413	-2.701772
56	1	0	3.270622	3.053773	-1.909772
57	1	0	4.10201	4.548701	-2.371389
58	8	0	4.206119	4.063506	0.421815
59	1	0	3.270819	3.870716	0.286799

Sum of electronic and zero-point Energies= -1495.759991

Sum of electronic and thermal Free Energies= -1495.830266

The reaction complex for ketyl formation in HAT process between MeOH and para position of the compound **1** via the triplet surface:



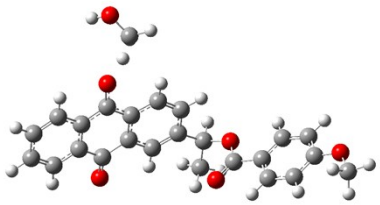
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.087752	-0.128998	-1.71644
2	6	0	-1.048048	0.602729	-1.458837
3	6	0	-2.107371	0.035197	-0.709788
4	6	0	-1.974762	-1.285391	-0.227908
5	6	0	-0.799963	-2.002547	-0.499457
6	6	0	0.234085	-1.4501	-1.235513
7	6	0	-3.308644	0.782414	-0.433499
8	6	0	-3.040826	-1.938182	0.556701
9	6	0	-4.251176	-1.130587	0.807194
10	6	0	-4.387108	0.19444	0.326274
11	6	0	-5.572243	0.919735	0.597371
12	1	0	-5.677939	1.931879	0.224847
13	6	0	-6.587239	0.329935	1.323388
14	6	0	-6.456539	-0.985093	1.801712
15	6	0	-5.301621	-1.700206	1.541921
16	1	0	0.891473	0.317151	-2.291727
17	1	0	-1.145926	1.615584	-1.831413
18	1	0	-0.744739	-3.00611	-0.098329
19	1	0	-7.49332	0.890978	1.523051
20	1	0	-7.259233	-1.437761	2.372254
21	1	0	-5.166441	-2.716279	1.893014
22	8	0	-2.929681	-3.092228	0.972224
23	8	0	-3.391642	2.009349	-0.861559
24	6	0	1.494252	-2.217662	-1.598121
25	6	0	1.6129	-3.63715	-1.056288
26	8	0	2.690903	-1.426354	-1.309628
27	1	0	0.821979	-4.262165	-1.47801
28	1	0	2.572766	-4.0572	-1.363766
29	1	0	1.548899	-3.664087	0.029941
30	6	0	2.978376	-1.115627	-0.019731

31	8	0	2.300918	-1.460136	0.920357
32	6	0	4.218989	-0.306361	0.091954
33	6	0	4.995139	0.063105	-1.017784
34	6	0	4.625519	0.098486	1.364796
35	6	0	6.142366	0.817025	-0.851976
36	1	0	4.691026	-0.249415	-2.007797
37	6	0	5.776387	0.857156	1.544246
38	1	0	4.022408	-0.191972	2.216177
39	6	0	6.542847	1.221137	0.430456
40	1	0	6.753634	1.109833	-1.696749
41	1	0	6.065424	1.156419	2.542325
42	1	0	1.541614	-2.266109	-2.689833
43	8	0	7.681572	1.957617	0.485433
44	6	0	8.151733	2.399683	1.753982
45	1	0	8.383741	1.554915	2.411077
46	1	0	9.062784	2.959844	1.551862
47	1	0	7.424103	3.055257	2.243951
48	6	0	-4.678613	5.022467	-0.439945
49	1	0	-3.809188	4.70766	0.148159
50	1	0	-5.382972	5.529378	0.220098
51	1	0	-4.34849	5.7332	-1.207909
52	8	0	-5.364225	3.913136	-1.010577
53	1	0	-4.731526	3.404289	-1.529456

Sum of electronic and zero-point Energies= -1417.131225

Sum of electronic and thermal Free Energies= -1417.197699

The transition state for ketyl formation in HAT process between MeOH and para position of the compound **1** via the triplet surface:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.056794	0.683874	1.26723
2	6	0	1.141263	1.25592	0.642922
3	6	0	2.254226	0.470681	0.245968
4	6	0	2.189909	-0.932568	0.473222
5	6	0	1.07129	-1.486181	1.110807
6	6	0	0.006672	-0.704328	1.526348
7	6	0	3.398141	1.034549	-0.404793
8	6	0	3.253944	-1.841269	0.005578
9	6	0	4.355877	-1.222121	-0.754176
10	6	0	4.425111	0.184012	-0.946031
11	6	0	5.526226	0.726849	-1.653529
12	1	0	5.583516	1.799068	-1.789903
13	6	0	6.507179	-0.100167	-2.160235
14	6	0	6.435768	-1.491456	-1.969011
15	6	0	5.375342	-2.03643	-1.266177
16	1	0	-0.788638	1.304388	1.54307
17	1	0	1.123045	2.311569	0.408614
18	1	0	1.076256	-2.559725	1.245271
19	1	0	7.341223	0.327343	-2.705669
20	1	0	7.212659	-2.133922	-2.367243
21	1	0	5.298316	-3.102162	-1.088109
22	8	0	3.217118	-3.054415	0.225743
23	8	0	3.555686	2.338884	-0.59548
24	6	0	-1.190371	-1.265683	2.274713
25	6	0	-1.235469	-2.77832	2.454925
26	8	0	-2.444465	-0.747676	1.724564
27	1	0	-0.398597	-3.102	3.078454
28	1	0	-2.160926	-3.050127	2.96693
29	1	0	-1.193267	-3.300412	1.500949
30	6	0	-2.795754	-1.083831	0.457294
31	8	0	-2.137665	-1.806918	-0.253212

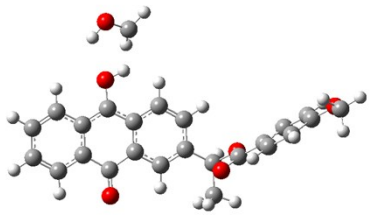
32	6	0	-4.080091	-0.454927	0.053441
33	6	0	-4.836014	0.361746	0.908827
34	6	0	-4.549092	-0.694035	-1.239598
35	6	0	-6.024292	0.921422	0.476083
36	1	0	-4.483654	0.549544	1.914265
37	6	0	-5.741455	-0.136359	-1.686598
38	1	0	-3.960832	-1.32621	-1.893251
39	6	0	-6.48701	0.678058	-0.825759
40	1	0	-6.620444	1.553123	1.123124
41	1	0	-6.077938	-0.339059	-2.694059
42	1	0	-1.201384	-0.80517	3.267155
43	8	0	-7.661815	1.274408	-1.153168
44	6	0	-8.192354	1.072643	-2.458199
45	1	0	-8.407066	0.014887	-2.643625
46	1	0	-9.120883	1.639666	-2.490064
47	1	0	-7.511303	1.448272	-3.229181
48	6	0	2.970368	3.942212	1.406151
49	1	0	3.069155	3.207804	0.476928
50	1	0	2.032724	4.484066	1.285058
51	1	0	2.963702	3.279304	2.27861
52	8	0	4.017859	4.843398	1.371195
53	1	0	4.833349	4.392559	1.619108

Sum of electronic and zero-point Energies= -1417.120458

Sum of electronic and thermal Free Energies= -1417.184344

The imaginary frequency: -380.89

The product complex for ketyl formation in HAT process between MeOH and para position of the compound **1** via the triplet surface:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.06129	0.392437	1.41741
2	6	0	1.148044	1.063158	0.903094
3	6	0	2.244085	0.3558	0.345089
4	6	0	2.188574	-1.066134	0.352925
5	6	0	1.066178	-1.719667	0.873476
6	6	0	-0.004317	-1.017374	1.404489
7	6	0	3.3842	1.005171	-0.206989
8	6	0	3.302377	-1.881565	-0.176554
9	6	0	4.45715	-1.145161	-0.728993
10	6	0	4.482947	0.276329	-0.747019
11	6	0	5.60638	0.931797	-1.307269
12	1	0	5.624763	2.012995	-1.337886
13	6	0	6.66014	0.200041	-1.816786
14	6	0	6.632999	-1.204462	-1.7896
15	6	0	5.539379	-1.862614	-1.252536
16	1	0	-0.764536	0.957422	1.8348
17	1	0	1.150349	2.148088	0.953381
18	1	0	1.075128	-2.800777	0.837494
19	1	0	7.513593	0.714639	-2.243912
20	1	0	7.465061	-1.770188	-2.192494
21	1	0	5.485433	-2.943906	-1.223213
22	8	0	3.269163	-3.112419	-0.153653
23	8	0	3.484275	2.361443	-0.252791
24	6	0	-1.209913	-1.696271	2.032681
25	6	0	-1.265427	-3.216392	1.935581
26	8	0	-2.455123	-1.077943	1.577255
27	1	0	-0.435367	-3.654844	2.494754
28	1	0	-2.19597	-3.569156	2.385036
29	1	0	-1.220787	-3.557206	0.902975

30	6	0	-2.798646	-1.179925	0.267387
31	8	0	-2.133213	-1.762084	-0.556876
32	6	0	-4.082137	-0.491359	-0.023843
33	6	0	-4.841548	0.160645	0.960287
34	6	0	-4.547991	-0.500351	-1.340006
35	6	0	-6.030401	0.785121	0.630402
36	1	0	-4.491607	0.16863	1.983866
37	6	0	-5.741267	0.124174	-1.684114
38	1	0	-3.9574	-1.006426	-2.093695
39	6	0	-6.490515	0.772855	-0.694933
40	1	0	-6.629353	1.291603	1.37721
41	1	0	-6.075637	0.100909	-2.712201
42	1	0	-1.223254	-1.422484	3.091784
43	8	0	-7.666439	1.413753	-0.914955
44	6	0	-8.195598	1.440409	-2.236001
45	1	0	-8.40385	0.430153	-2.60365
46	1	0	-9.127367	1.998935	-2.16919
47	1	0	-7.51656	1.949142	-2.928315
48	6	0	2.776927	4.547542	1.805031
49	1	0	2.659583	2.782197	0.027526
50	1	0	2.098801	5.325618	2.12796
51	1	0	3.047703	3.74396	2.483797
52	8	0	3.698864	4.97859	0.900111
53	1	0	4.283586	4.244758	0.671972

Sum of electronic and zero-point Energies= -1417.144145

Sum of electronic and thermal Free Energies= -1417.210123