Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information to:

Competition of Singlet and Triplet Recombination of Radical Pairs in Photoreactions of Carboxy Benzophenones and Aromatic Amino Acids

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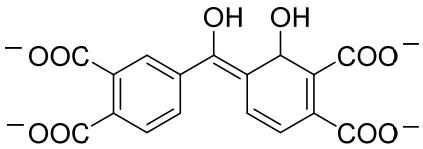
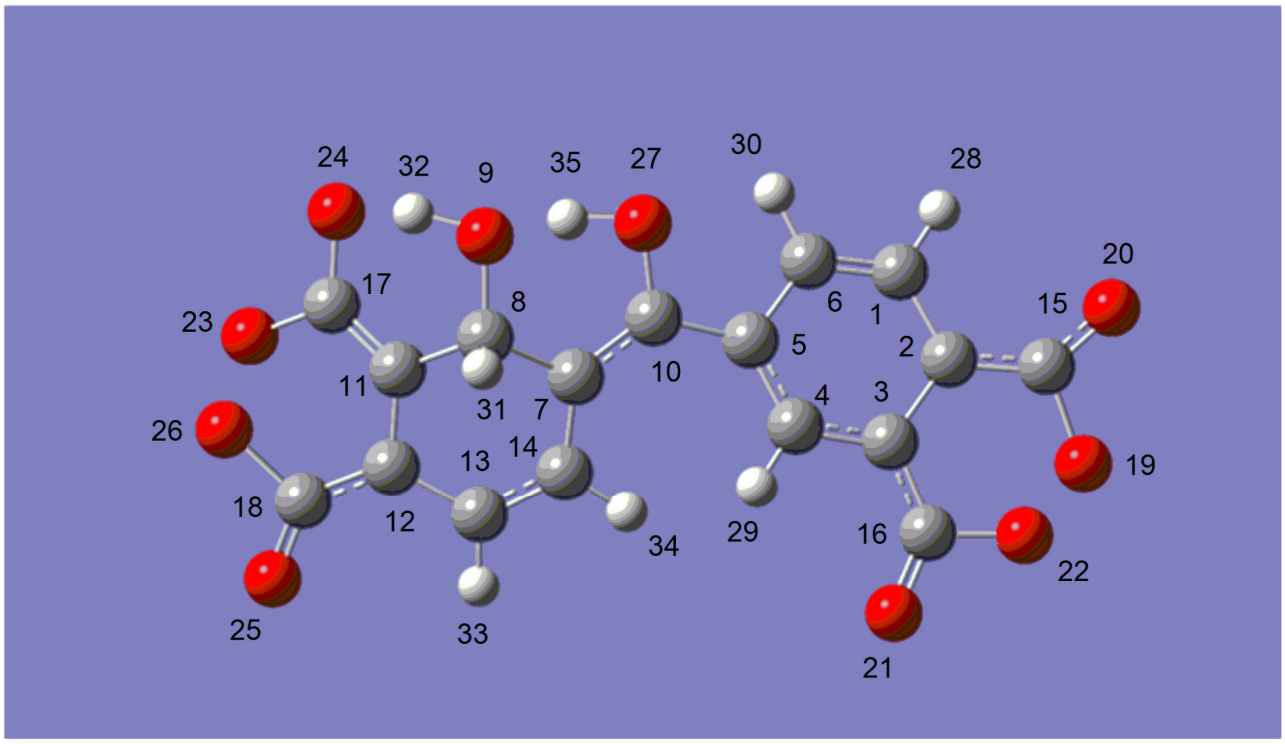
Cartesian coordinates and energy for TCBP·H_2O calculated using ORCA

1. TCBP·H_2O hydroxylated at the position 2



E(HF)=-1385.8453386 a.u. = -37710.79046 eV

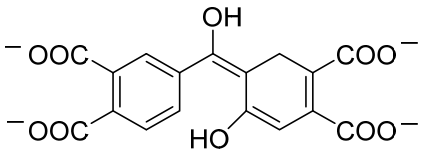


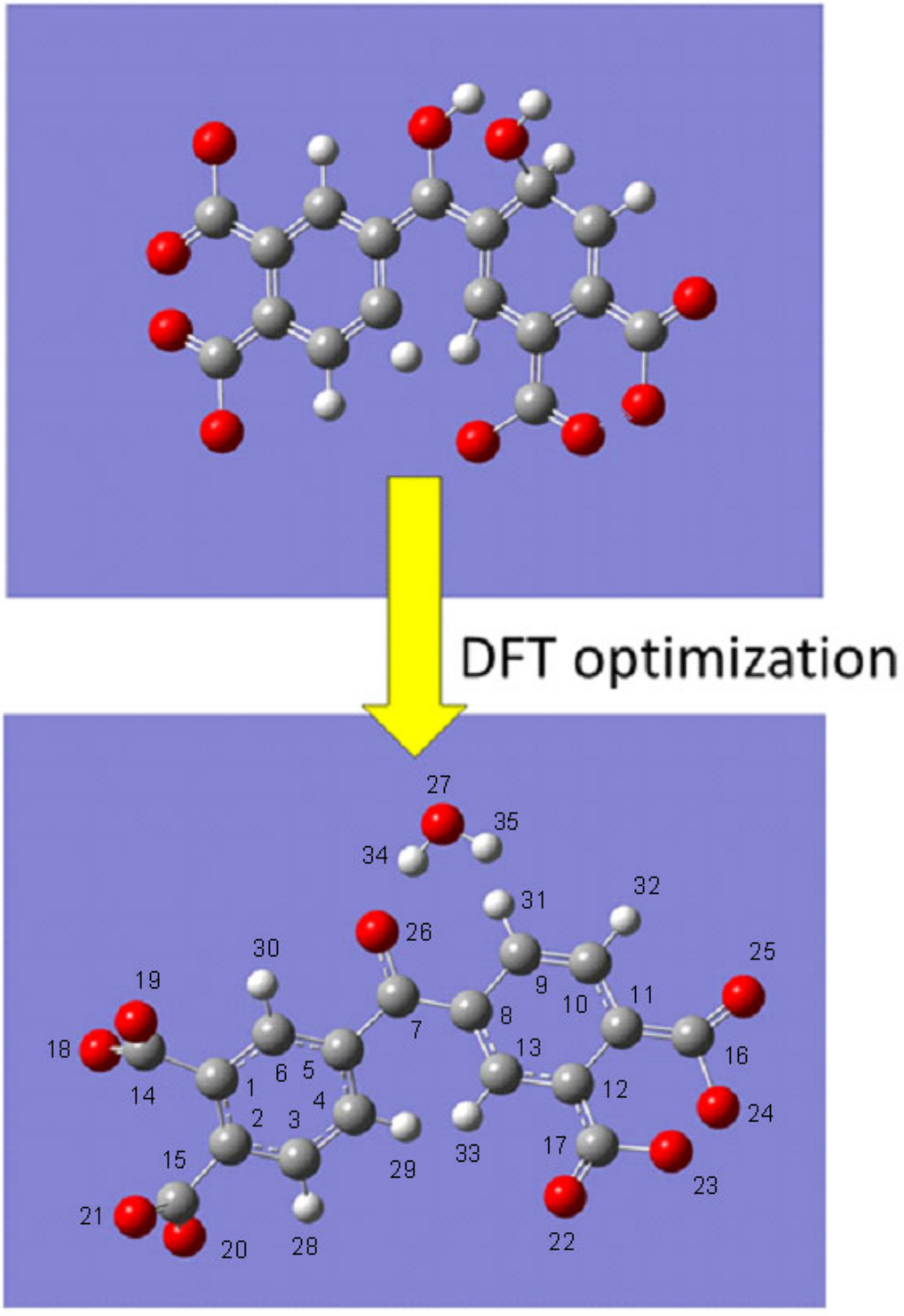
Standard orientation:

Center	Coordinates (Angstroms)		
Number	X	Y	Z
1	-3.604360	-1.788765	-0.736572
2	-4.361783	-0.594008	-0.397227
3	-3.536132	0.566508	0.122216
4	-2.135800	0.363844	0.364257
5	-1.436356	-0.818194	0.069440
6	-2.255600	-1.916861	-0.523065
7	1.097781	-0.242416	0.538259

8	2.476270	-0.833900	1.040955
9	2.559942	-2.306567	0.995625
10	0.005908	-1.127931	0.368499
11	3.661904	-0.193313	0.268526
12	3.657426	1.268504	0.046616
13	2.347919	1.901843	0.098559
14	1.165245	1.199648	0.289150
15	-5.781433	-0.551368	-0.407188
16	-4.144690	1.862631	0.280448
17	4.629080	-1.010669	-0.248370
18	4.879549	1.886045	-0.353623
19	-6.344454	0.749058	0.207998
20	-6.697741	-1.398286	-0.731536
21	-3.686071	2.998640	0.666632
22	-5.581882	1.918202	-0.239655
23	5.735692	-0.387359	-1.016069
24	4.640733	-2.384444	-0.217090
25	5.240191	3.088875	-0.610792
26	6.080914	0.889856	-0.365065
27	0.239882	-2.509023	0.431688
28	-4.163619	-2.639180	-1.163092
29	-1.593978	1.213277	0.807254
30	-1.727979	-2.844017	-0.778993
31	2.571357	-0.535567	2.130501
32	3.564960	-2.489429	0.348800
33	2.289503	2.986433	-0.080533
34	0.224419	1.755033	0.198984
35	1.348130	-2.547752	0.637902

2. TCBP·H_2O hydroxylated at the position 6





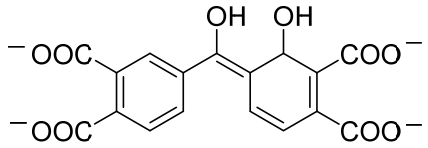
E(HF)=-1405.0369167 a.u. = -38233.020150 eV

Standard orientation:

Center	Coordinates (Angstroms)		
Number	X	Y	Z
1	-3.594517	0.276775	0.250750
2	-3.555411	-0.942658	-0.468768
3	-2.337046	-1.346193	-1.048551
4	-1.167972	-0.601289	-0.897769
5	-1.190513	0.599814	-0.157797
6	-2.416764	1.016509	0.396945
7	-0.009432	1.484694	-0.018977
8	1.371939	0.952168	-0.061964
9	2.426505	1.808665	-0.447782
10	3.731654	1.329800	-0.485889
11	4.047493	0.001538	-0.129985
12	3.008847	-0.844378	0.323598
13	1.691610	-0.363197	0.327692
14	-4.879235	0.867901	0.820389
15	-4.744663	-1.884343	-0.604558
16	5.487794	-0.446325	-0.334362
17	3.248457	-2.247924	0.873758
18	-5.949240	0.721282	0.125579
19	-4.776192	1.519877	1.926286
20	-5.111395	-2.178478	-1.800816
21	-5.217760	-2.369829	0.484556
22	2.284270	-3.092258	0.737771
23	4.360759	-2.468022	1.476583
24	5.677559	-1.349765	-1.225348
25	6.390431	0.187217	0.324551

26	-0.206190	2.732297	0.131907
27	1.175592	5.052813	-0.395390
28	-2.317610	-2.262129	-1.630845
29	-0.253729	-0.933046	-1.376007
30	-2.455509	1.940209	0.961780
31	2.212145	2.839251	-0.709299
32	4.536317	1.986318	-0.802886
33	0.919335	-1.039826	0.671070
34	0.711437	4.228521	-0.101812
35	0.912463	5.230267	-1.317802

Absorption spectrum via transition electric dipole moments for TCBP·H_2O hydroxilated at the position 2 calculated using ORCA



State	Energy, cm^{-1}	Wavelength, nm	Fosc (oscillator strength)
1	10041.2	995.9	0.017835204
2	12745.7	784.6	0.079368749
3	13237.1	755.5	0.018747708
4	16601.6	602.4	0.021943696
5	16856.1	**593.3**	**0.136633706**
6	19012.6	**526.0**	**0.152057856**
7	20700.9	483.1	0.026712145
8	22248.4	449.5	0.080181374
9	23614.8	**423.5**	**0.128538486**
10	24440.0	**409.2**	**0.271614569**
11	25489.9	392.3	0.075555868

12	27489.6	363.8	0.000143159
13	27685.1	361.2	0.006550786
14	29145.3	343.1	0.014680630
15	29744.7	**336.2**	**0.169395357**
16	29860.8	334.9	0.000250141
17	30335.9	329.6	0.000131516
18	30574.6	327.1	0.018288760
19	31700.3	315.5	0.085900911
20	32157.0	311.0	0.025197909

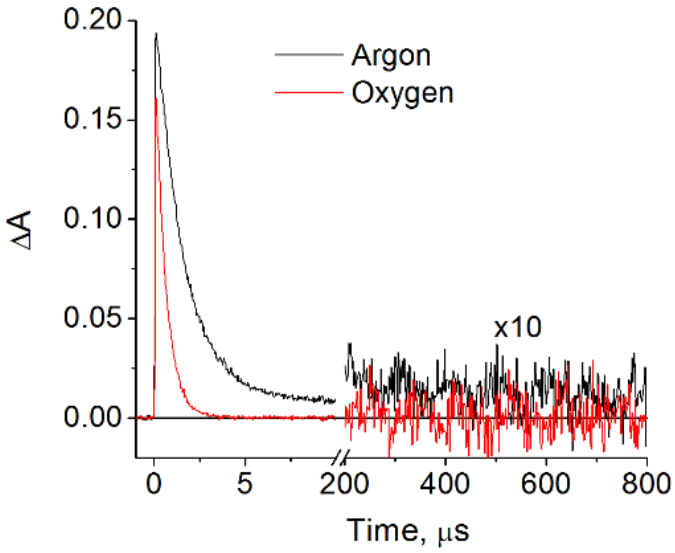


Figure S1. TA signal evolution recorded at 600 nm for 5 mM of TCBP in buffered solution, pH 7.4, after the excitation at 355 nm with laser pulse energy 20 mJ under argon (black curve), and oxygen (red curve).