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

Adiabatic Deprotonation as an Important Competing Pathway to ESIPT in Photoacidic 2-Phenylphenols

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SUPPORTING INFORMATION

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1. Experimental Information

- *MS analyses of irradiated compounds 1, 2, 5 and 6.*

[1,1'-biphenyl]-2-ol (1) after photolysis in $CH_3CN:D_2O$ (3:1).

A 15,2 mg sample of **1** in 40 mL of $CH_3CN:D_2O$ (1:3) solution was irradiated for 60 min. 1H NMR analysis showed an overall exchange of 27 % over possible 2'- and 4'-positions,[1] with 40% deuterium incorporation at 2'-position. Incorporation of deuterium at 4'-position was not detected. MS (after 13C correction) indicated an overall exchange of 22%. Relative product distribution obtained: **1** (51%), **1**-D (34%), **1**-D_2 (14%), and **1**-D_3 (1%).[2]

5-Methoxy-[1,1'-biphenyl]-2-ol (2) after photolysis in $CH_3CN:D_2O$ (3:1).

A 12 mg sample of **2** in 27 mL of $CH_3CN:D_2O$ (1:3) solution was irradiated for 60 min. 1H NMR analysis showed an overall exchange of 29 % over possible 2'- and 4'-positions,[1] with 44% deuterium incorporation at 2'-position. Incorporation of deuterium at 4'-position was not detected. MS (after 13C correction) indicated an overall exchange of 29%. Relative product distribution obtained: **2** (34%), **2**-D (44%) and **2**-D_2 (22%).[2]

6-Hydroxy-[1,1'-biphenyl]-3-carbonitrile (5) after photolysis in $CH_3CN:D_2O$ (3:1).

A 20 mg sample of **5** in 46,4 mL of $CH_3CN:D_2O$ (1:3) solution was irradiated for 60 min. 1H NMR analysis showed an overall exchange of 3 % over possible 2'- and 4'-positions,[1] with 4% deuterium incorporation at 2'-position. Incorporation of deuterium at 4'-position was not detected. MS (after 13C correction) indicated an overall exchange of 5%. Relative product distribution obtained: **5** (84%), **5**-D (14%) and **5**-D_2 (2%).[2]

3,5-di-*tert*-Butyl-[1,1'-biphenyl]-2-ol (6) after photolysis in $CH_3CN:D_2O$ (3:1).

A 15 mg sample of **6** in 24 mL of $CH_3CN:D_2O$ (1:3) solution was irradiated for 60 min. 1H NMR analysis showed an overall exchange of 67 % over possible 2'- and 4'-positions,[1] with 100% deuterium incorporation at 2'-position. MS (after 13C correction) indicated an overall exchange of 67%. Relative product distribution obtained: **6** (1%), **6**-D (3%), **6**-D_2 (83%), and **6**-D_3 (11%).[2]

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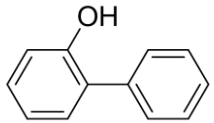
[1] Average overall deuterium incorporation (NMR), calculated as [2(%D-2') + (%D-4')]/3.

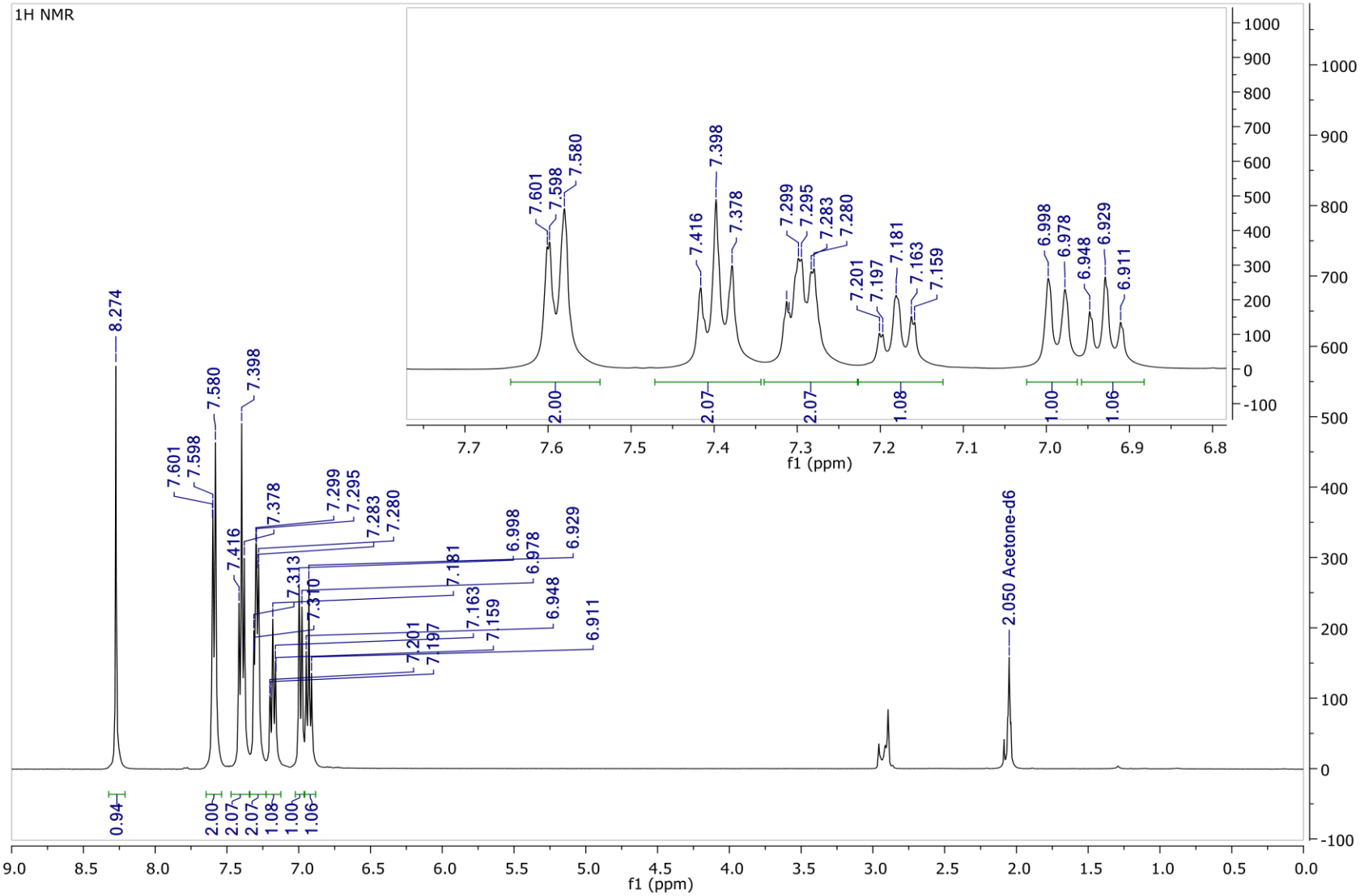
[2] Average overall deuterium incorporation (MS), calculated as [1(%1-D) + 2(%2-D) + 3(%3-D)]/3.

2. NMR spectra

[1,1'-biphenyl]-2-ol (*o*-phenylphenol) (1)

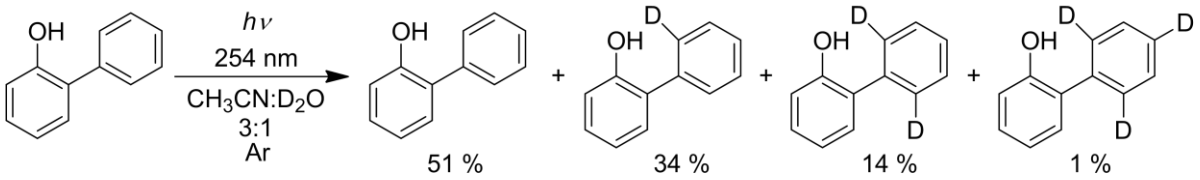


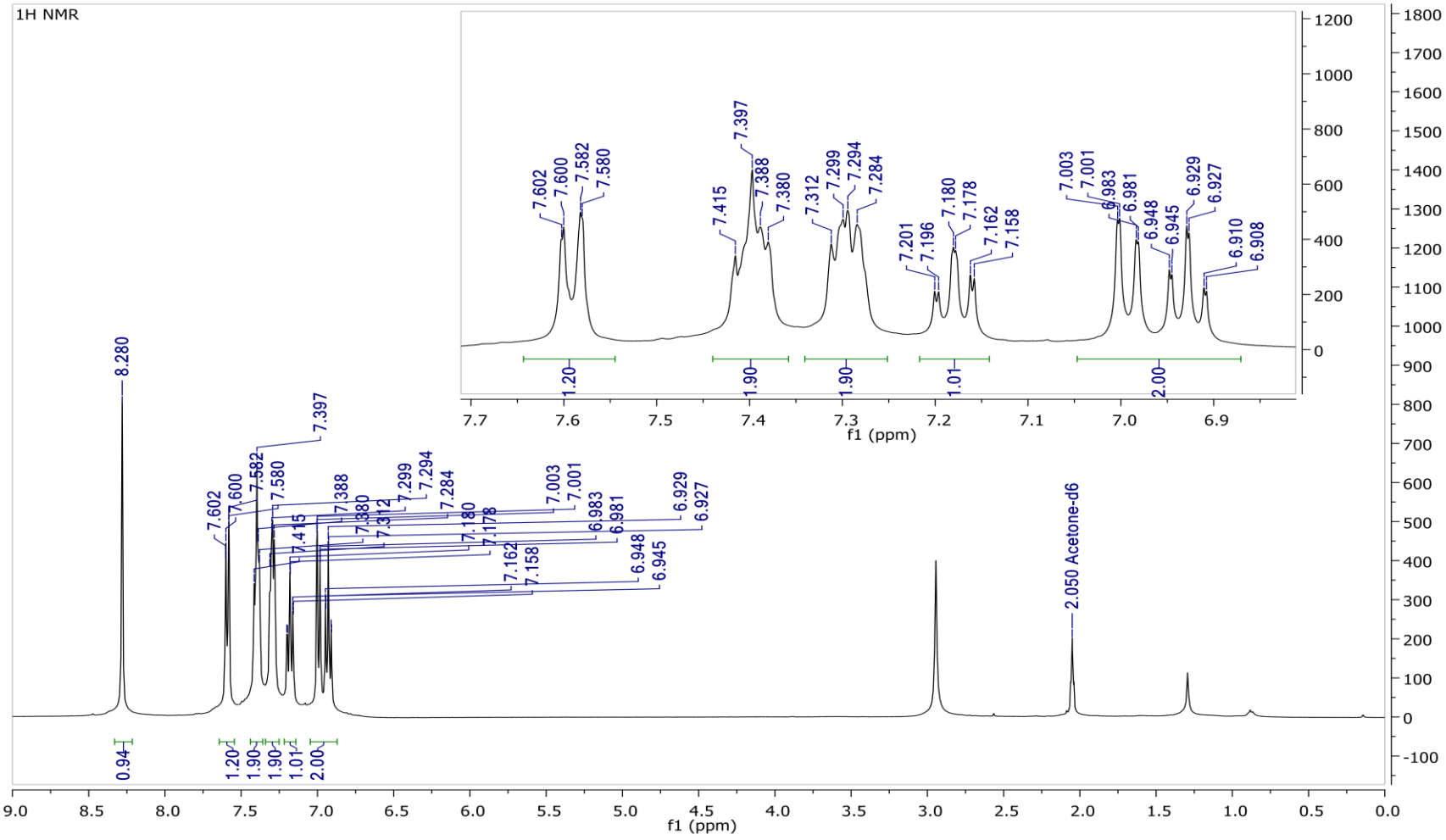
^{1}H NMR (400 MHz, $(CD_3)_2CO$)



[1,1'-biphenyl]-2-ol (1) after photolysis in $CH_3CN:D_2O$ (3:1)

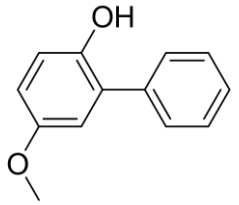
^1H NMR (400 MHz, $(CD_3)_2CO$)

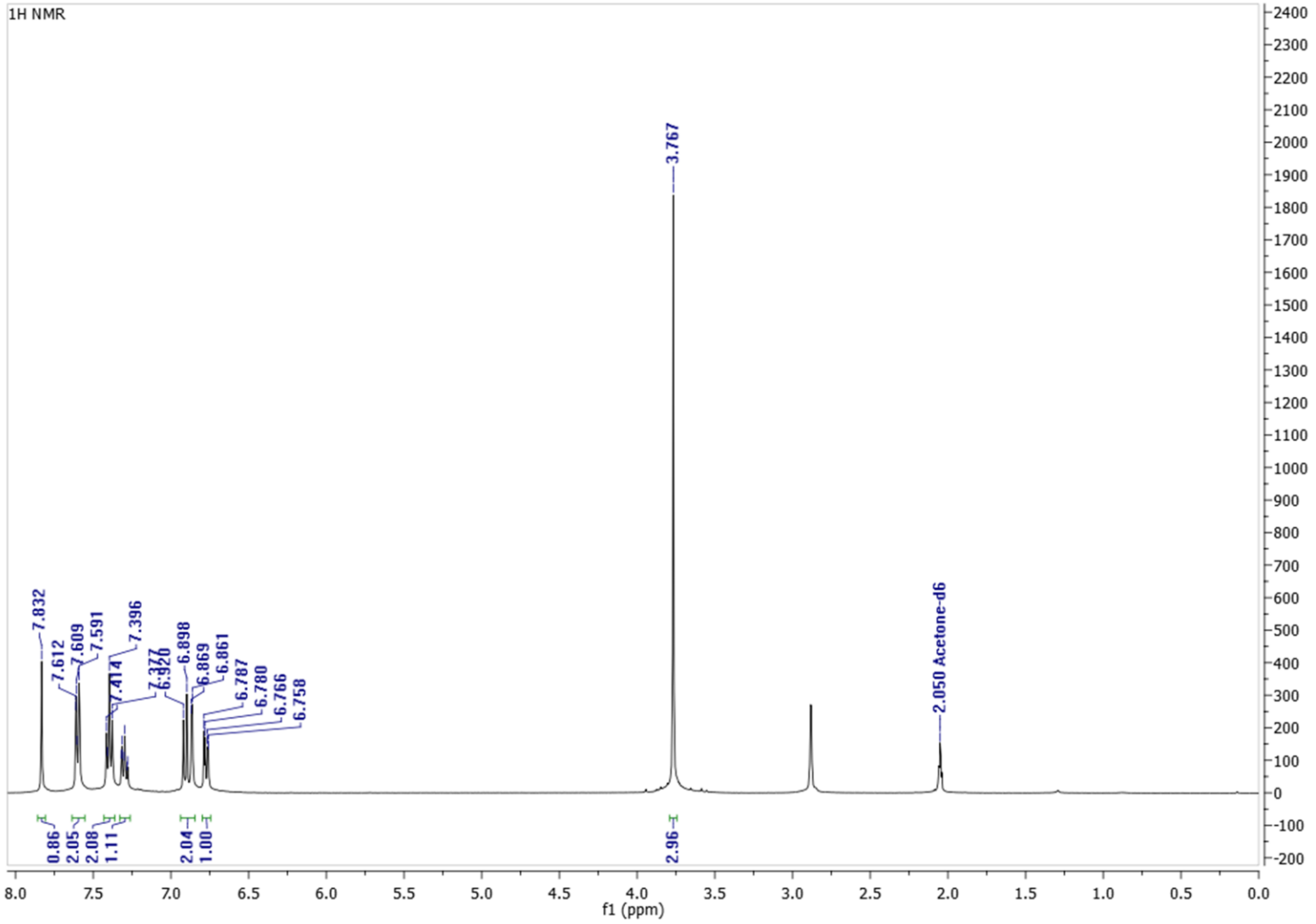


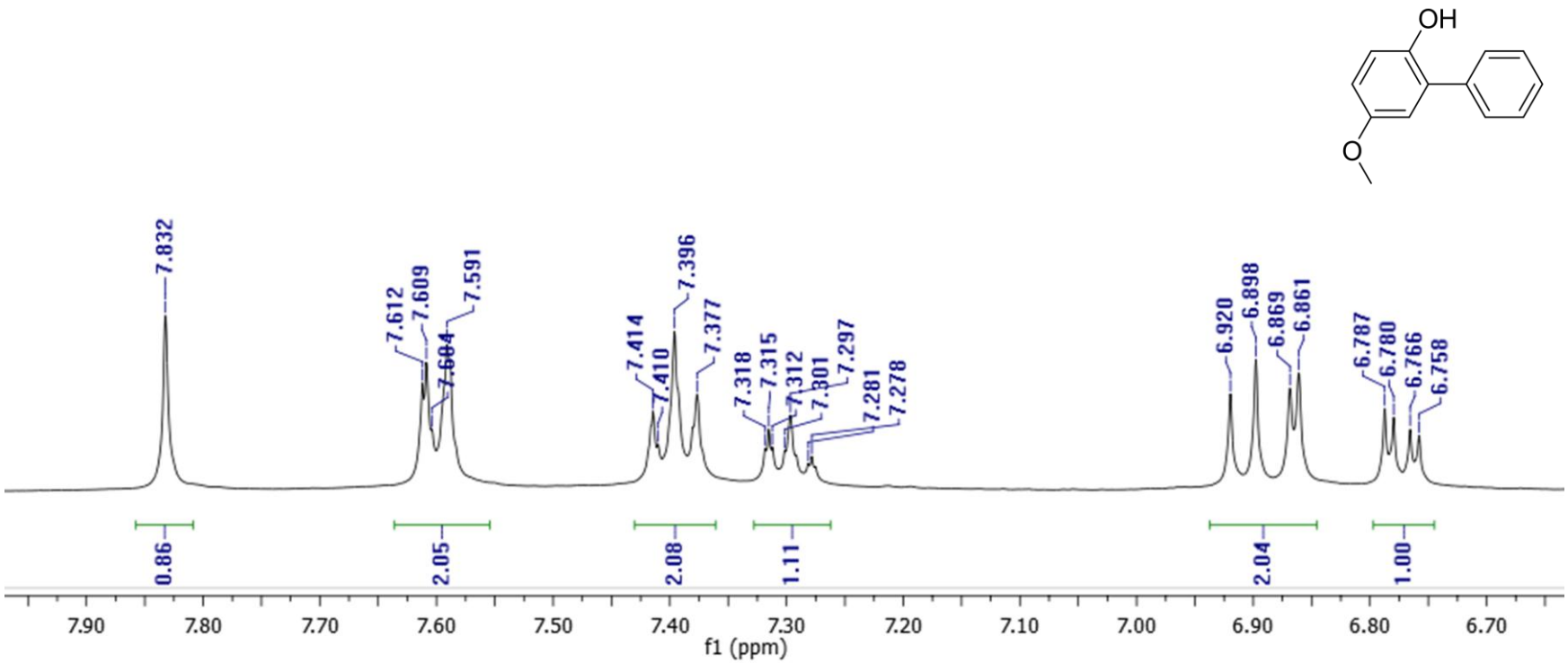


5-Methoxy-[1,1'-biphenyl]-2-ol (2)

^{1}H NMR (400 MHz, $(CD_3)_2CO$)






OH
O
7.832
7.612
7.609
7.604
7.591
7.414
7.410
7.396
7.377
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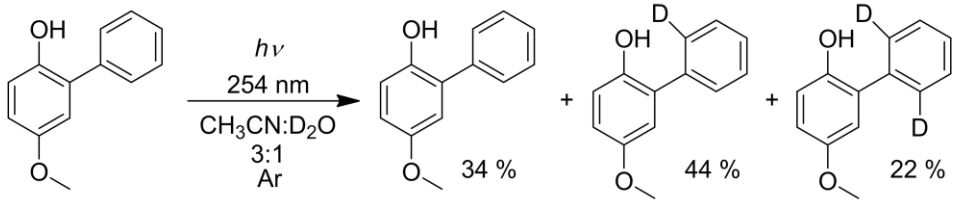
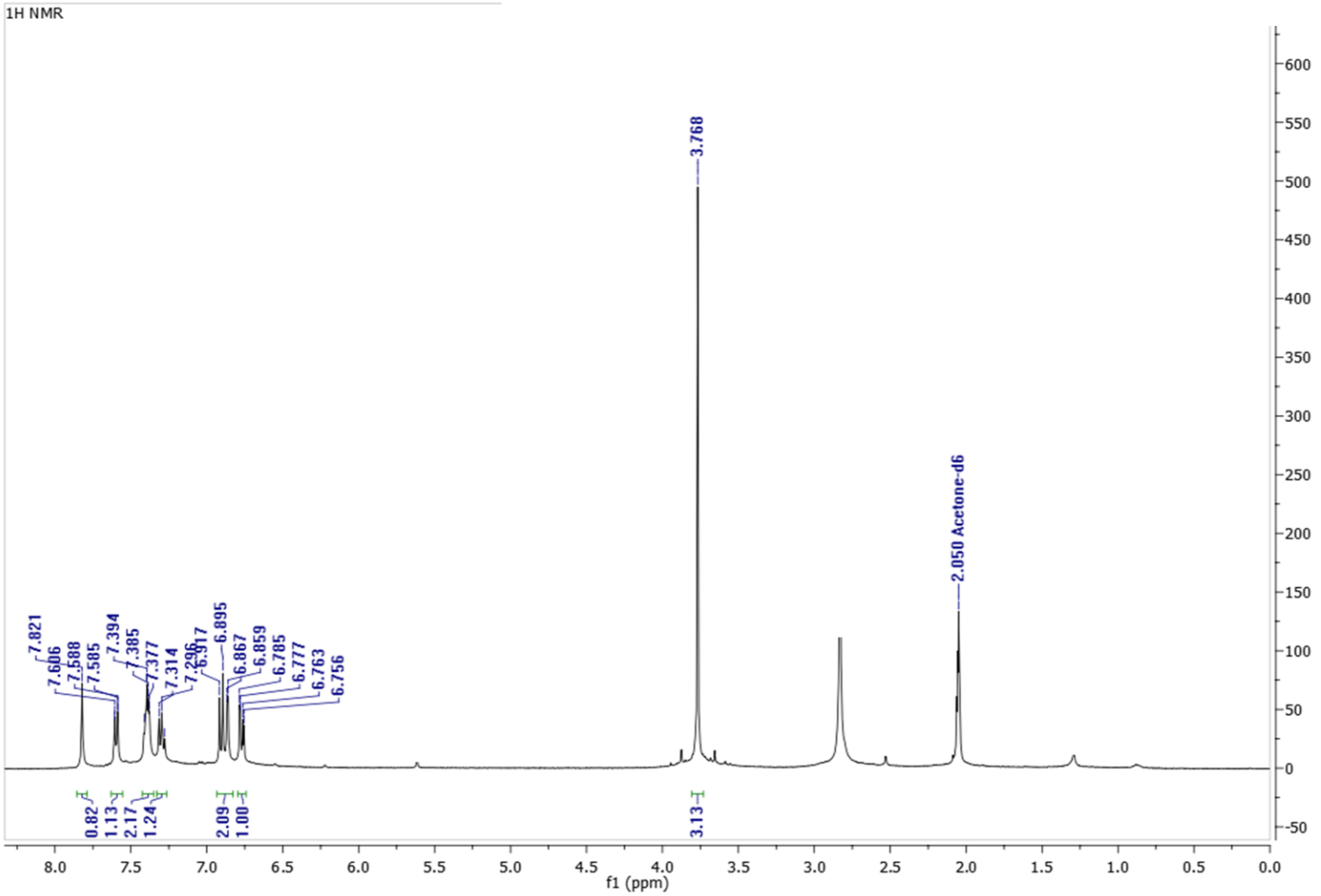
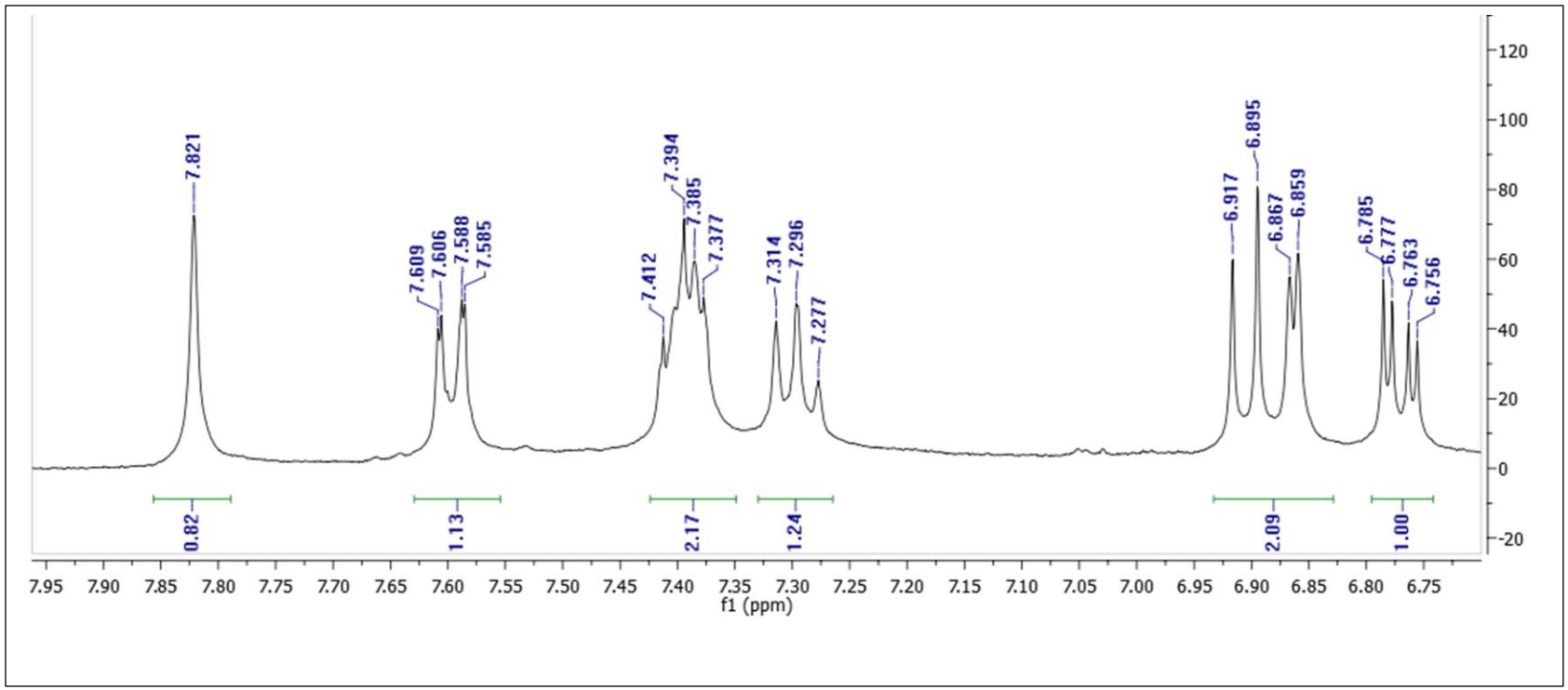
7.315
7.312
7.301
7.297
7.281
7.278
6.920
6.898
6.869
6.861
6.787
6.780
6.766
6.758
0.86
2.05
2.08
1.11
2.04
1.00
7.90
7.80
7.70
7.60
7.50
7.40
7.30
7.20
7.10
7.00
6.90
6.80
6.70
f1 (ppm)

5-Methoxy-[1,1'-biphenyl]-2-ol (2) after photolysis in $CH_3CN:D_2O$ (3:1)

^1H NMR (400 MHz, $(CD_3)_2CO$)



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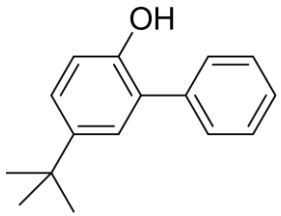
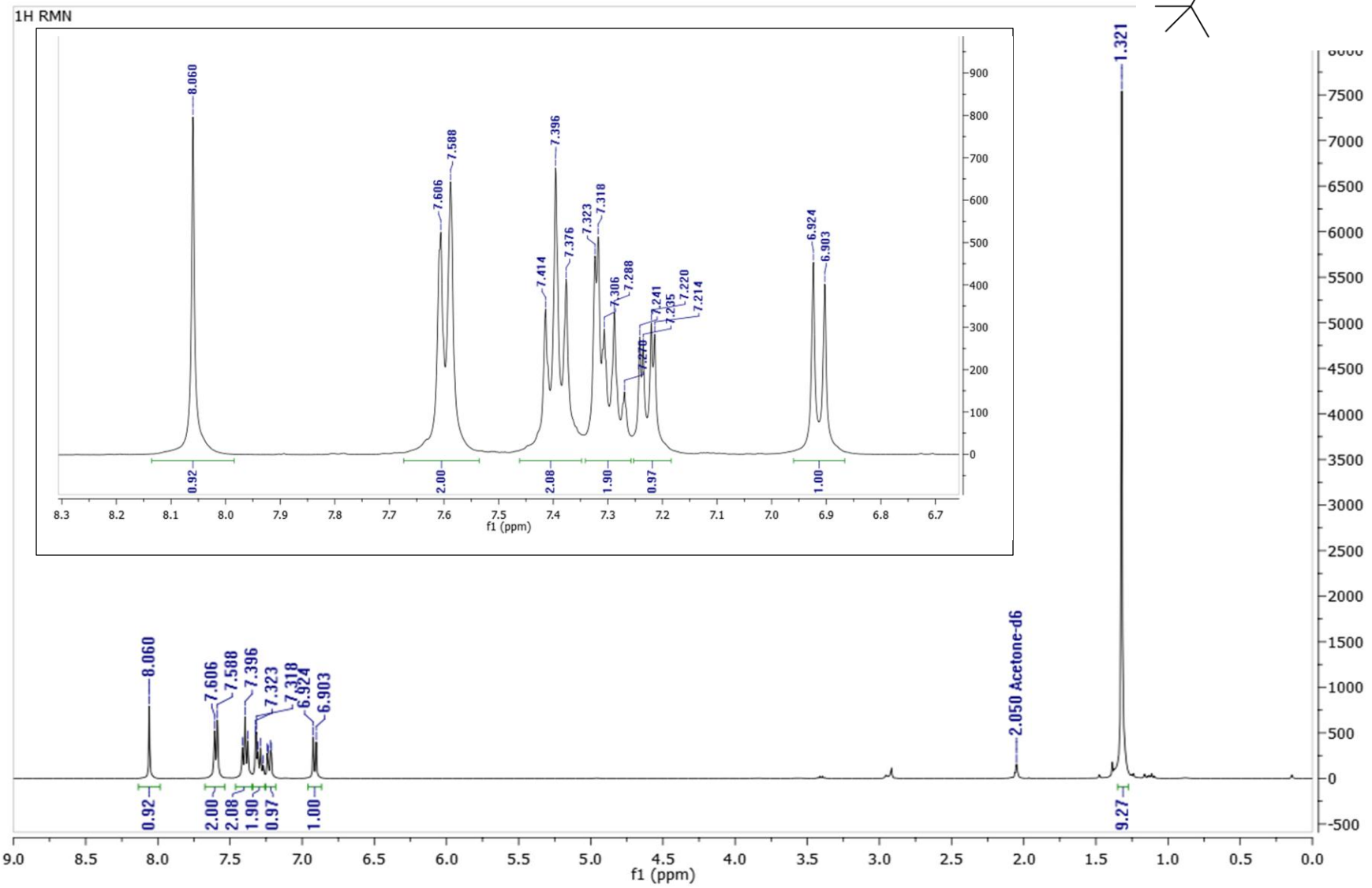
7.585
7.412
7.394
7.385
7.377
7.314
7.296
7.277
6.917
6.895
6.867
6.859
6.785
6.777
6.763
6.756
0.82
1.13
2.17
1.24
2.09
1.00
f1 (ppm)

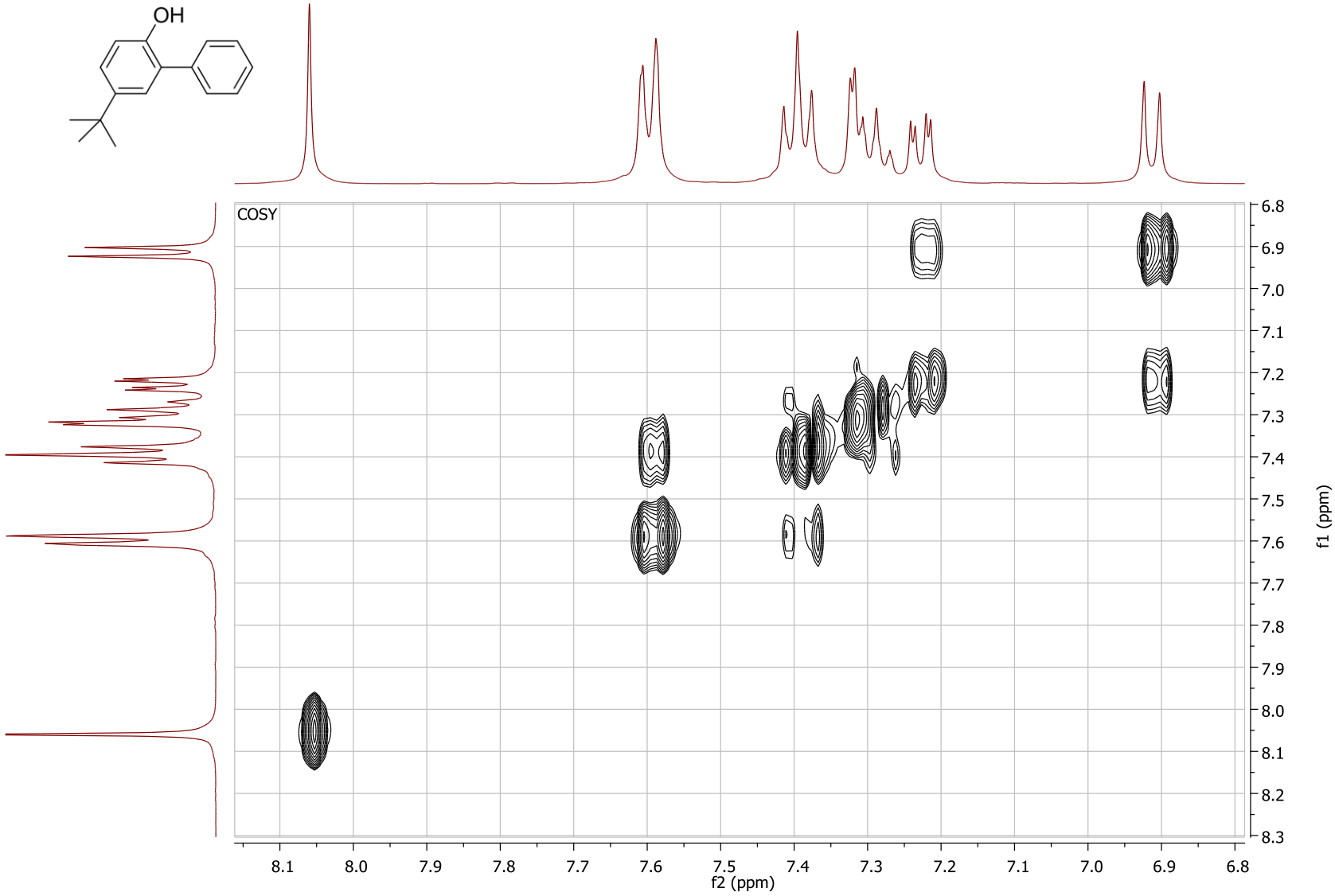
5-(*tert*-Butyl)-[1,1'-biphenyl]-2-ol (3)



^{1}H NMR (400 MHz, $(CD_3)_2CO$)

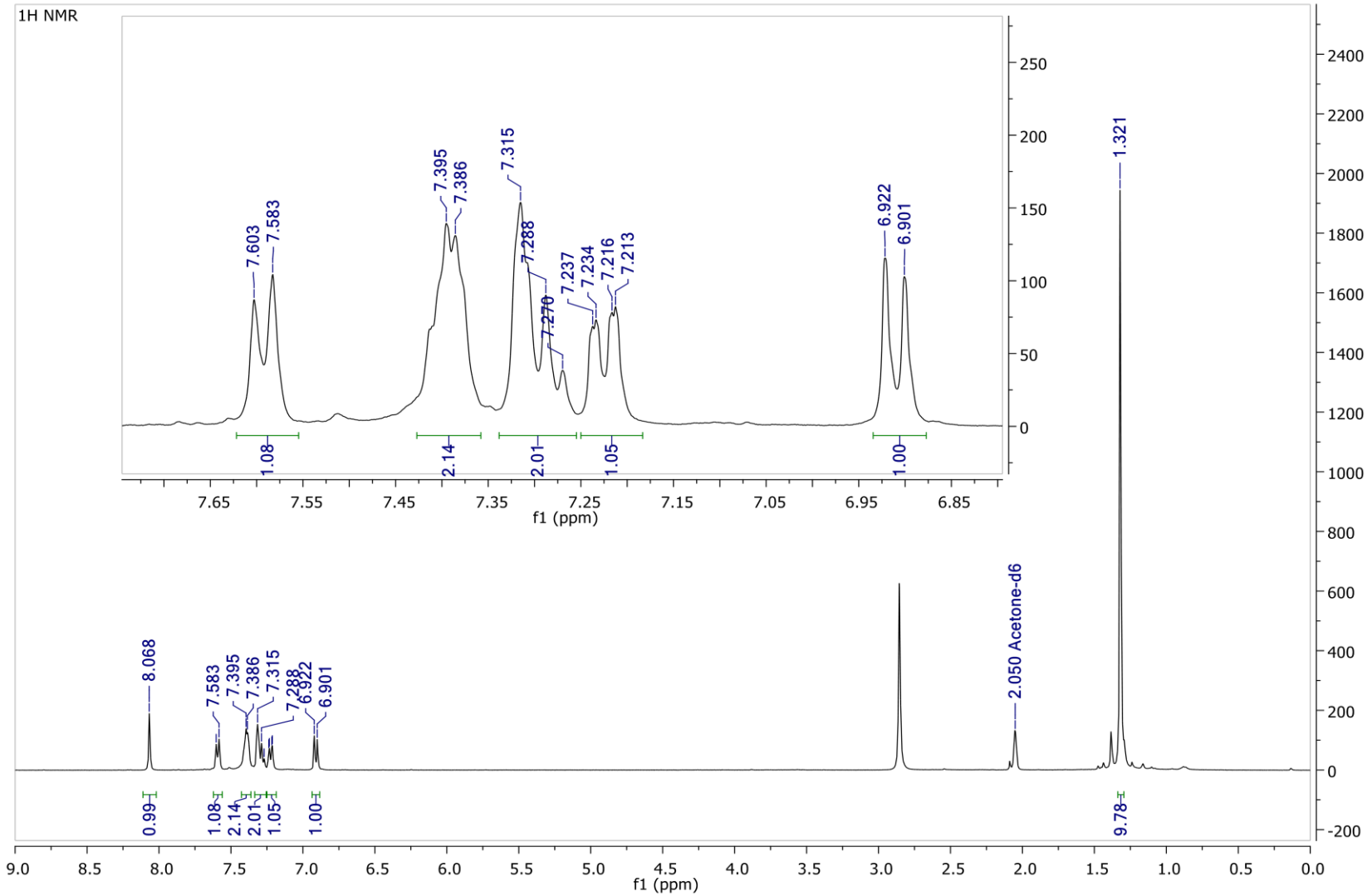


COSY ($(CD_3)_2CO$)


OH
COSY
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
f2 (ppm)
6.8
6.9
7.0
7.1
7.2
7.3
7.4
7.5
7.6
7.7
7.8
7.9
8.0
8.1
8.2
8.3
f1 (ppm)

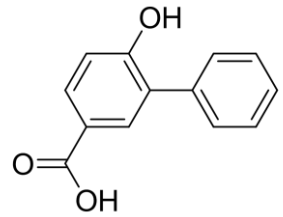
5-(*tert*-Butyl)-[1,1'-biphenyl]-2-ol (3) after photolysis in $CH_3CN:D_2O$ (3:1)

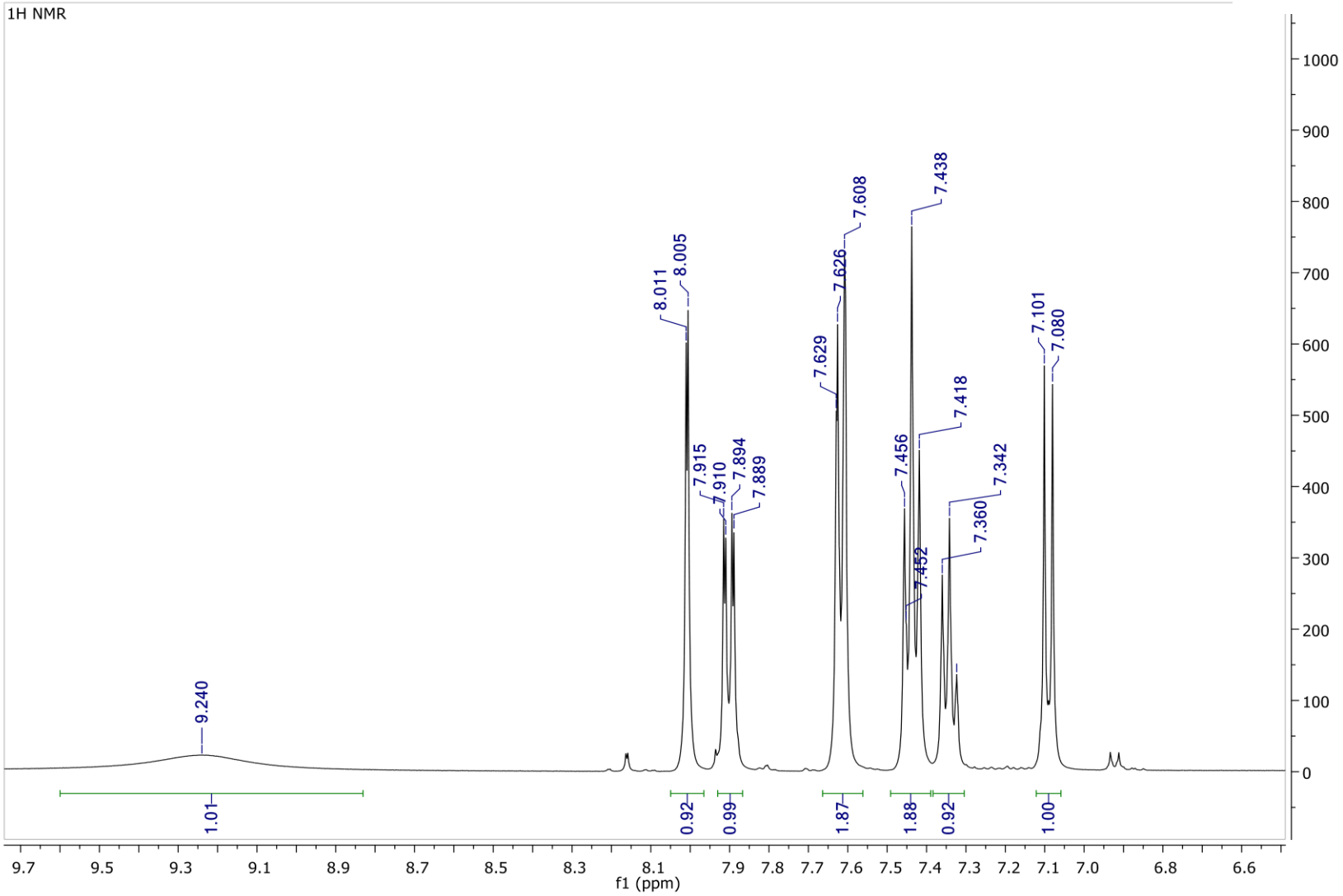
^{1}H NMR (400 MHz, $(CD_3)_2CO$)



6-Hydroxy-[1,1'-biphenyl]-3-carboxylic acid

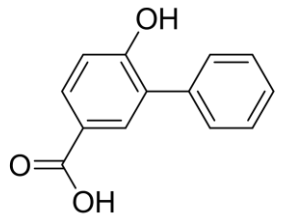
^{1}H NMR (400 MHz, $(CD_3)_2CO$)

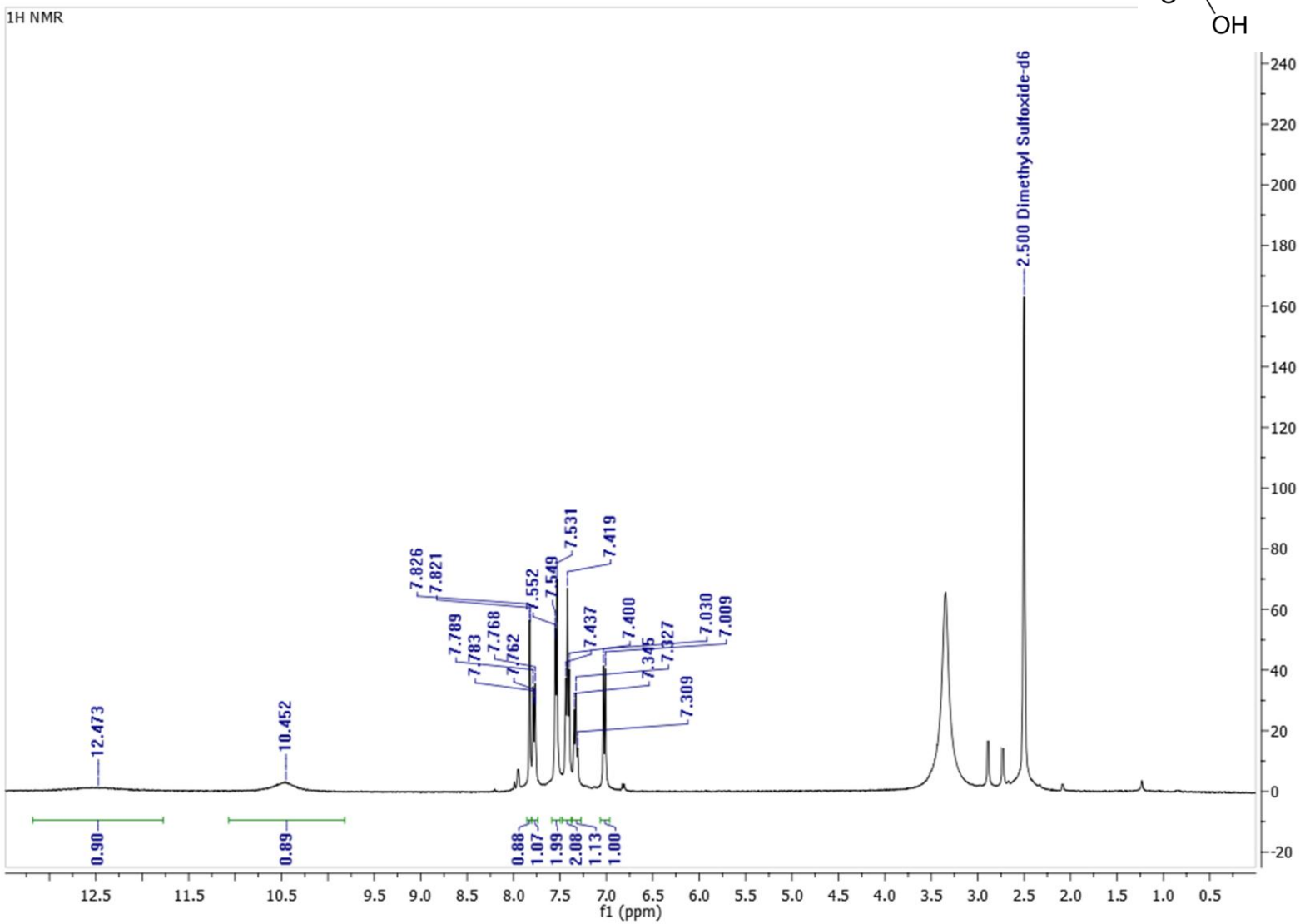




6-Hydroxy-[1,1'-biphenyl]-3-carboxylic acid

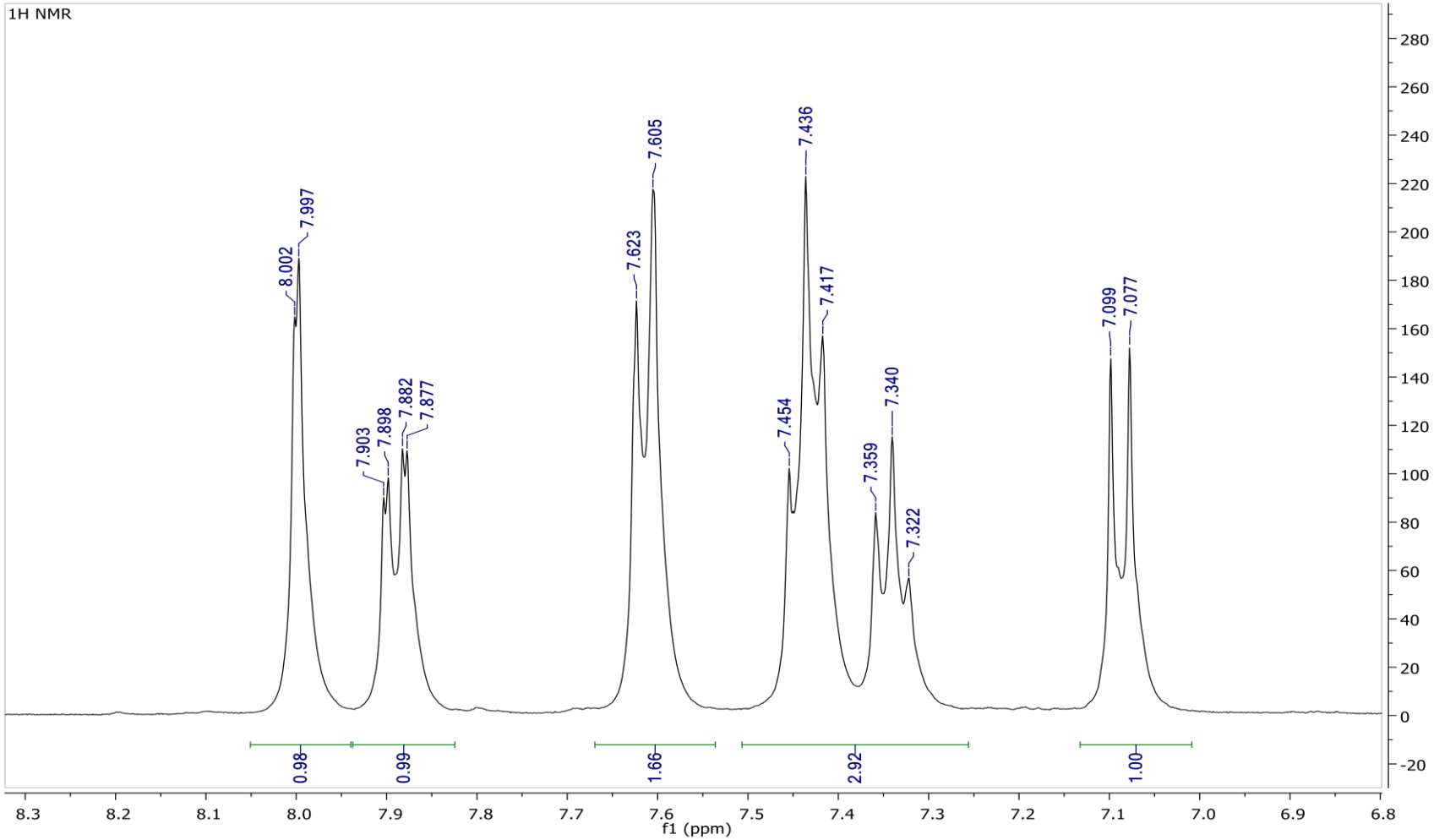
^{1}H NMR (400 MHz, $(CD_3)_2SO$)





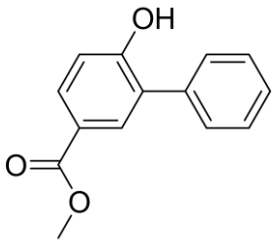
6-Hydroxy-[1,1'-biphenyl]-3-carboxylic acid after photolysis in $CH_3CN:D_2O$ (3:1)

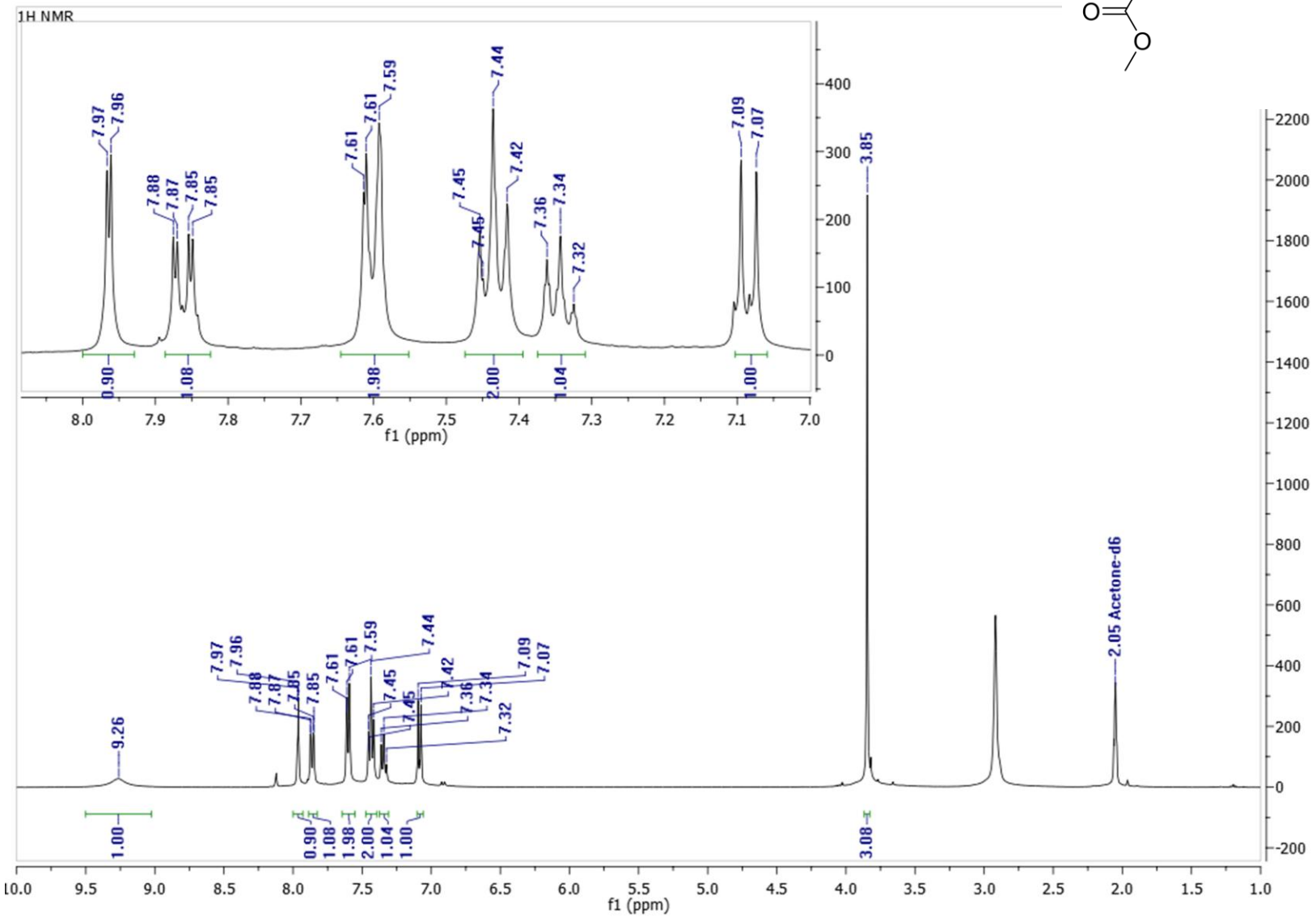
^1H NMR (400 MHz, $(CD_3)_2CO$)



Methyl 6-hydroxy-[1,1'-biphenyl]-3-carboxylate (4)

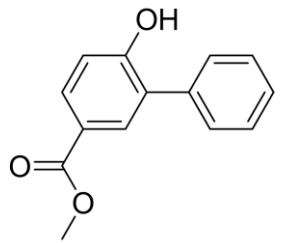
^{1}H NMR (400 MHz, $(CD_3)_2CO$)

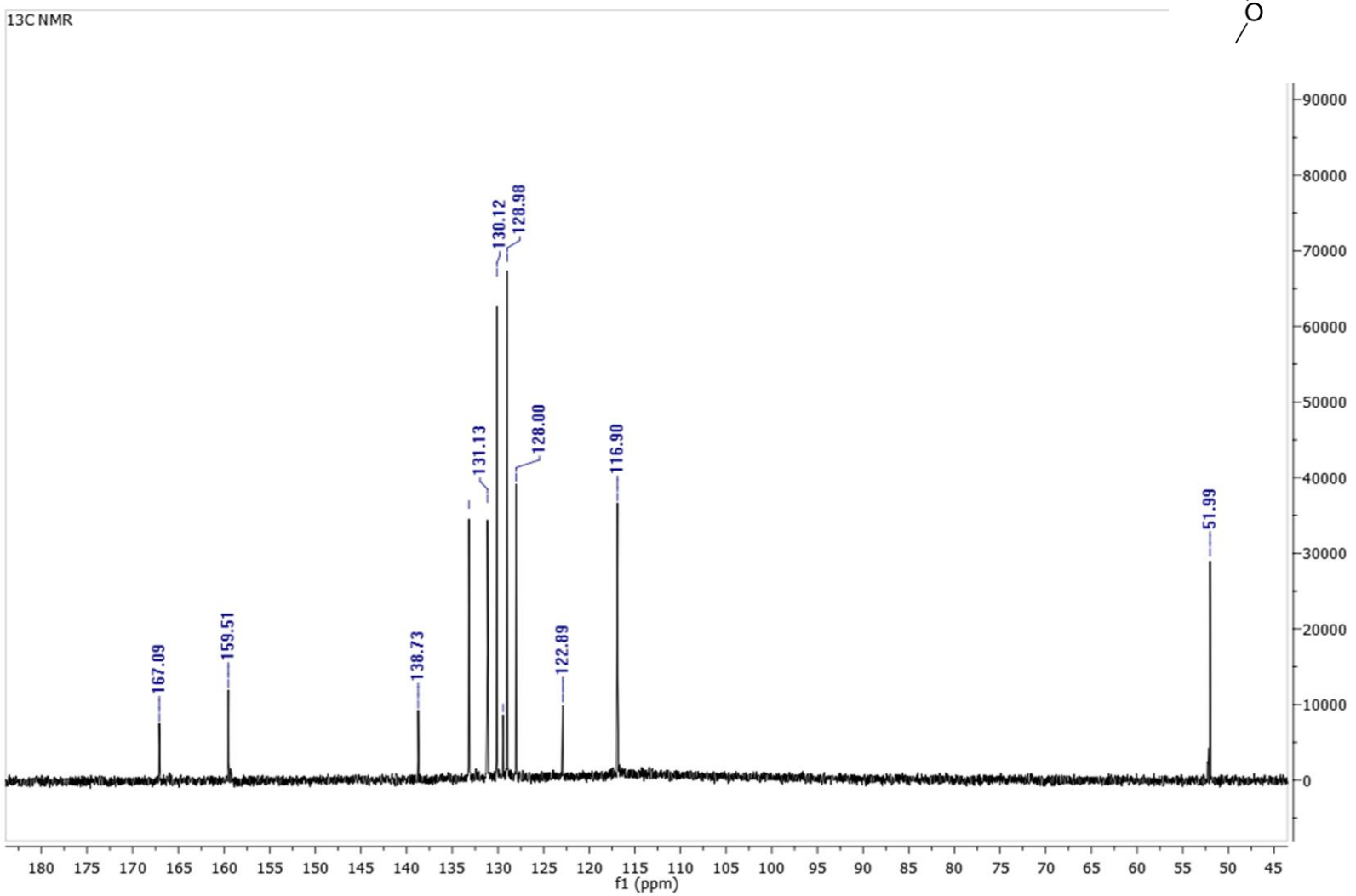




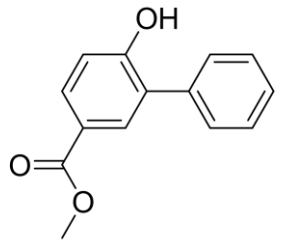
Methyl 6-hydroxy-[1,1'-biphenyl]-3-carboxylate (4)

^{13}C NMR (100 MHz, $(CD_3)_2CO$)





Methyl 6-hydroxy-[1,1'-biphenyl]-3-carboxylate (4)



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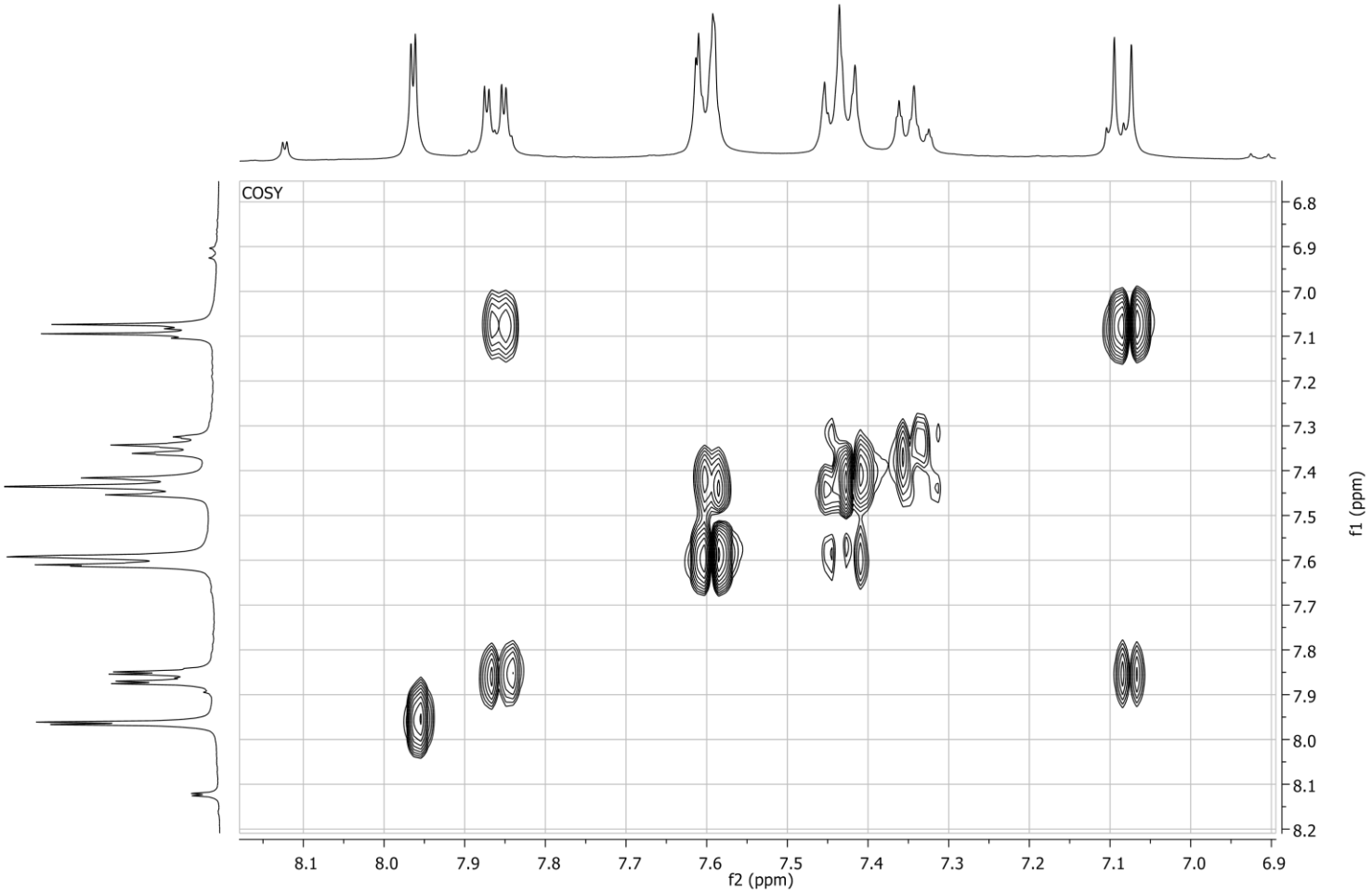
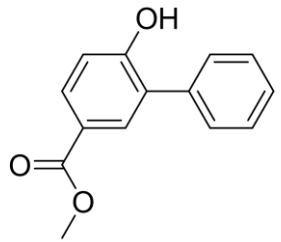
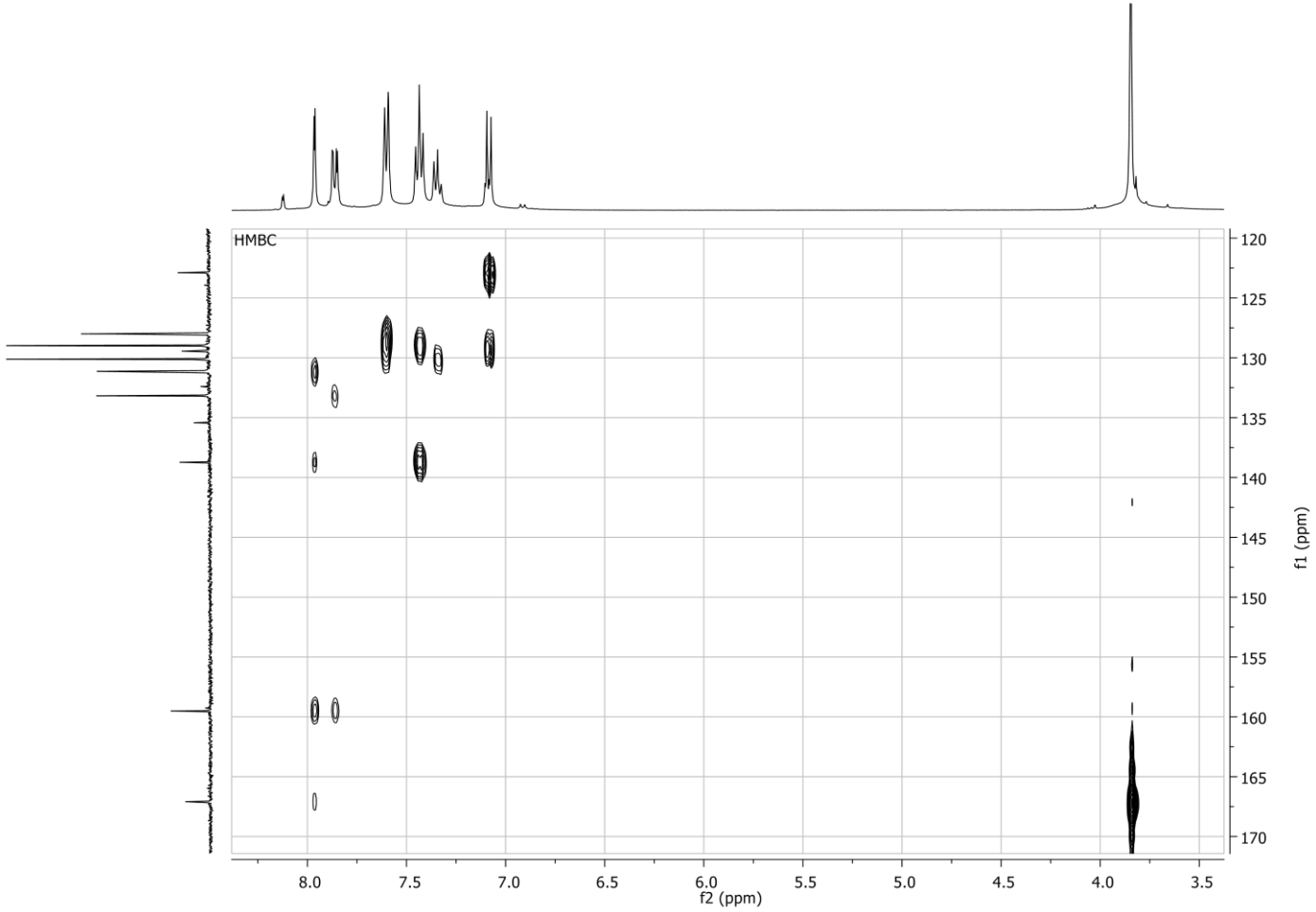


Methyl 6-hydroxy-[1,1'-biphenyl]-3-carboxylate (4)

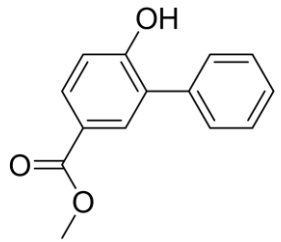


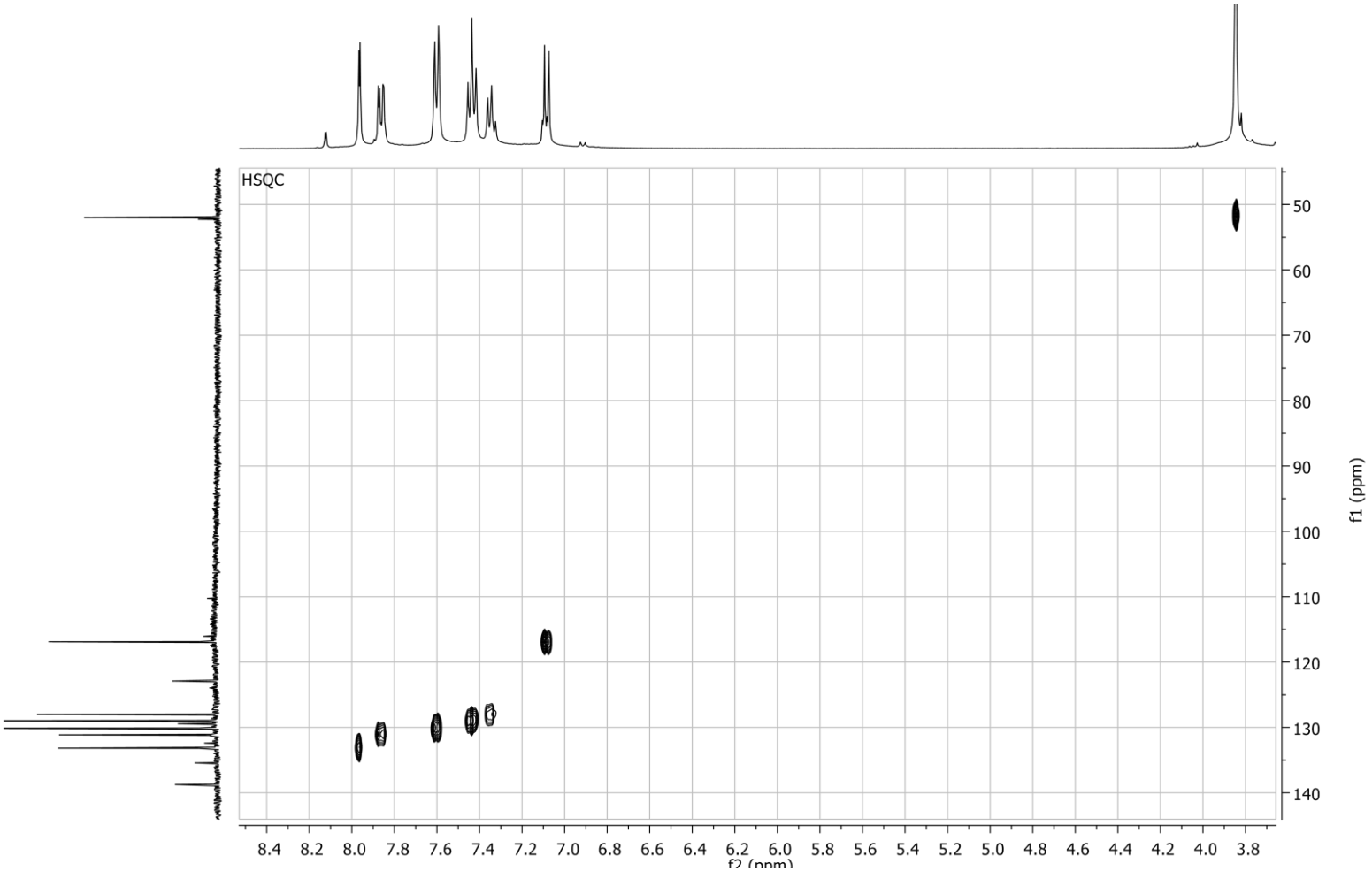
HMBC



Methyl 6-hydroxy-[1,1'-biphenyl]-3-carboxylate (4)

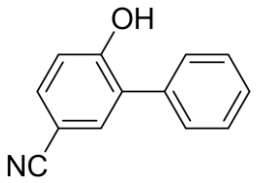
HSQC

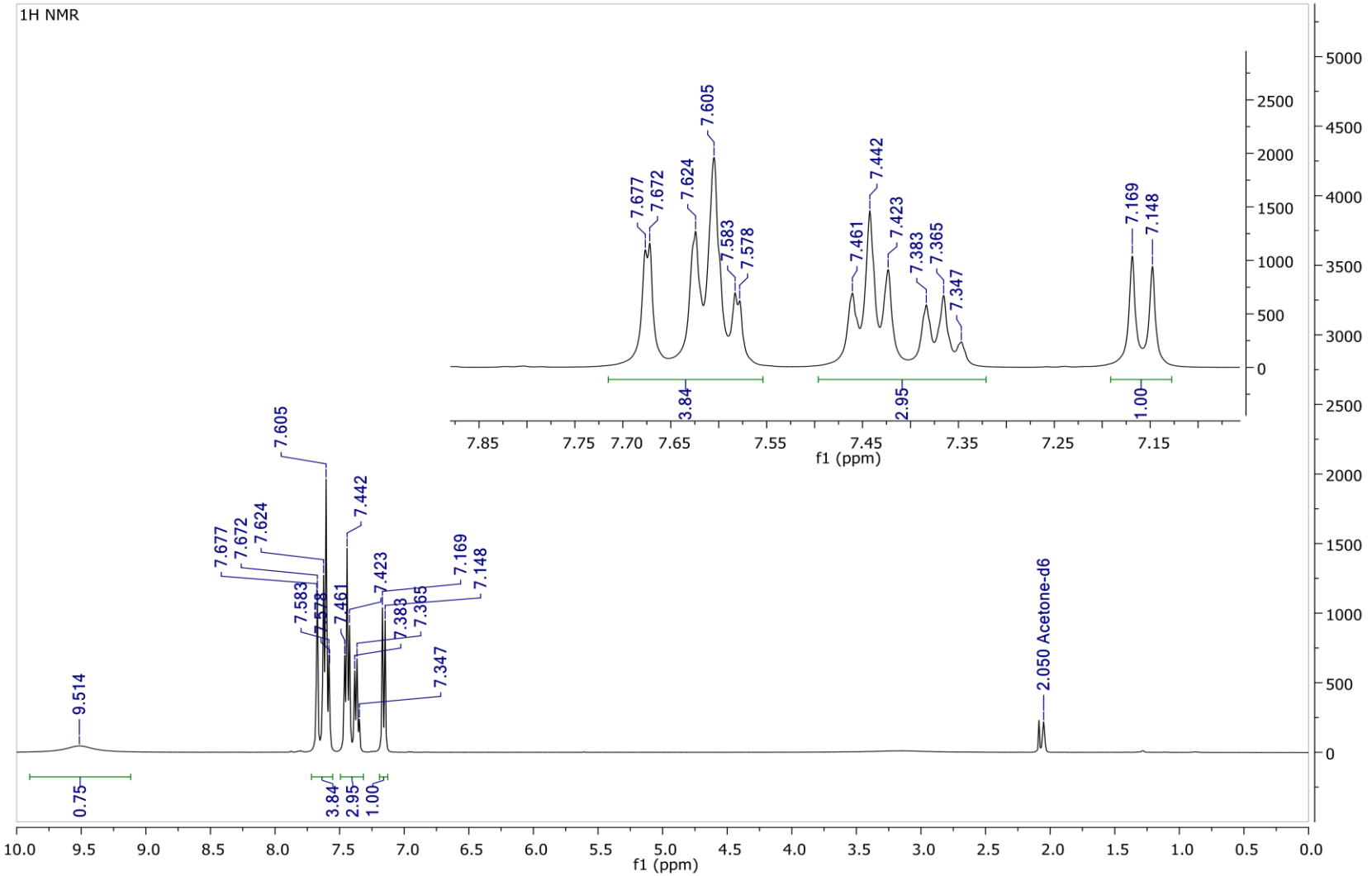




6-Hydroxy-[1,1'-biphenyl]-3-carbonitrile (5)

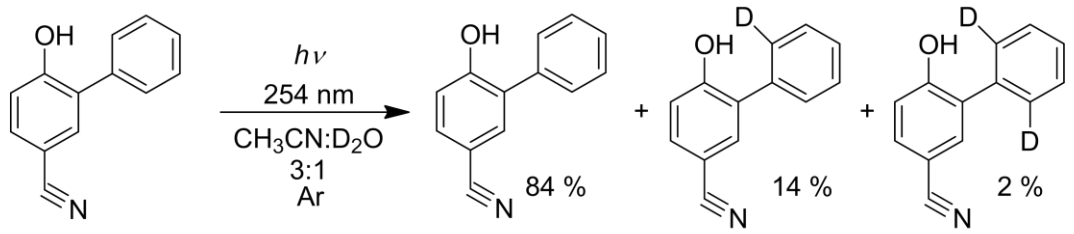
^{1}H NMR (400 MHz, $(CD_3)_2CO$)

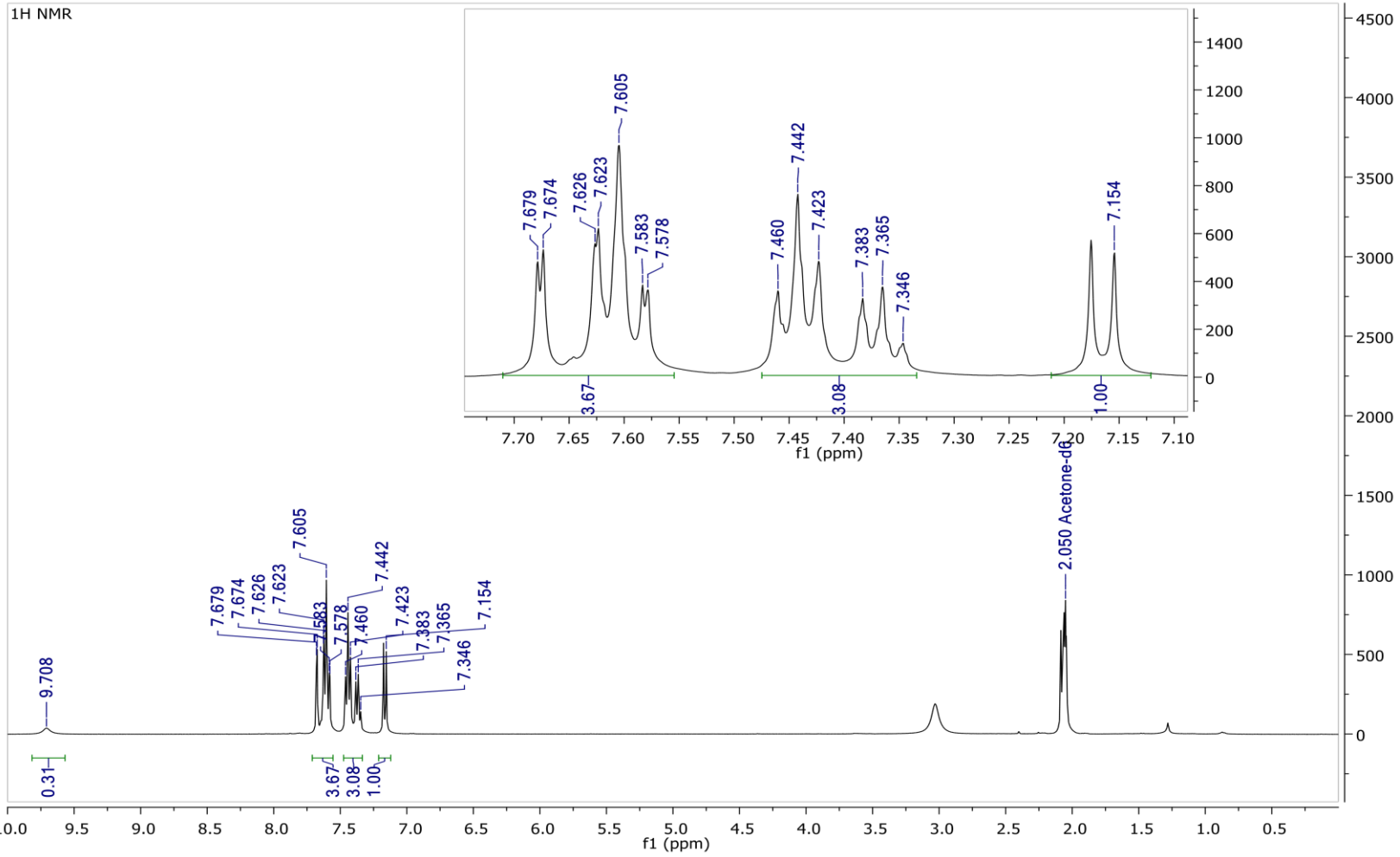




6-Hydroxy-[1,1'-biphenyl]-3-carbonitrile (5) after photolysis in $CH_3CN:D_2O$ (3:1)

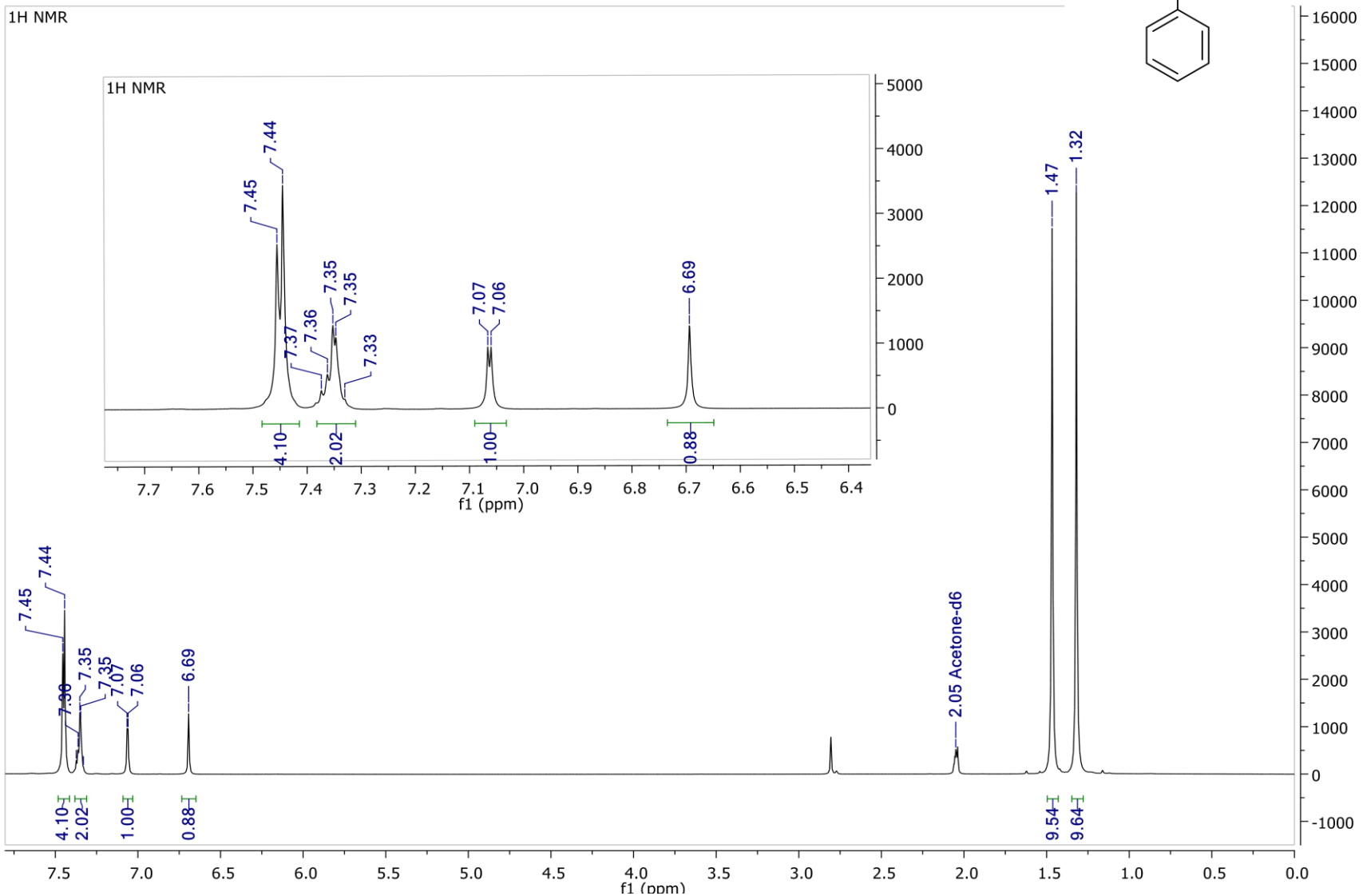
^1H NMR (400 MHz, $(CD_3)_2CO$)





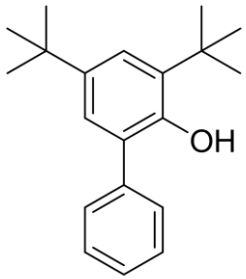
3,5-di-*tert*-Butyl-[1,1'-biphenyl]-2-ol (6)

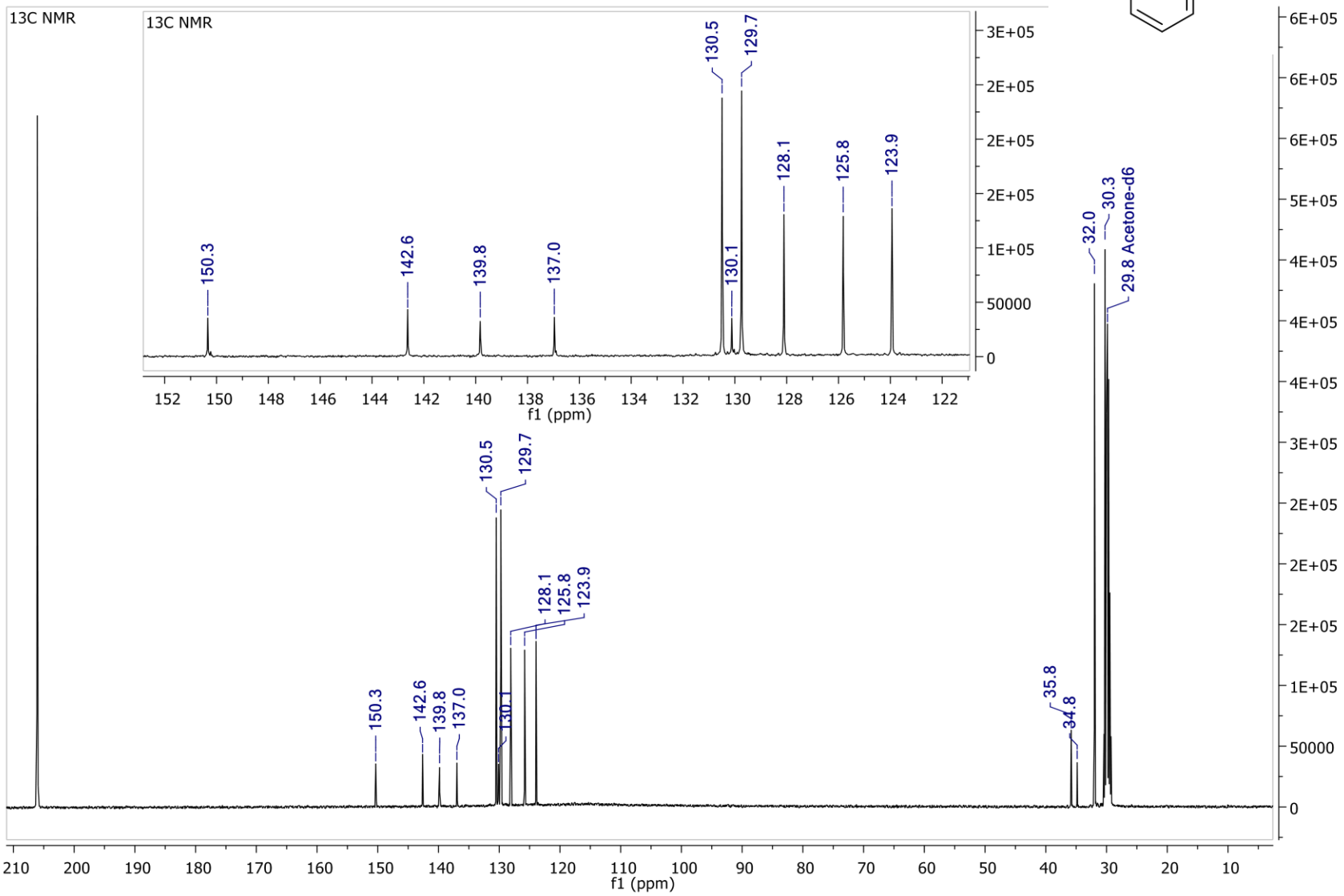
^{1}H NMR (400 MHz, $(CD_3)_2CO$)



3,5-di-*tert*-Butyl-[1,1'-biphenyl]-2-ol (6)

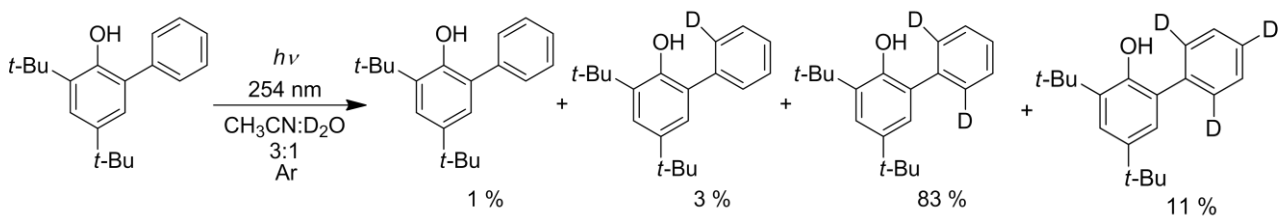
^{13}C NMR (100 MHz, $(CD_3)_2CO$)

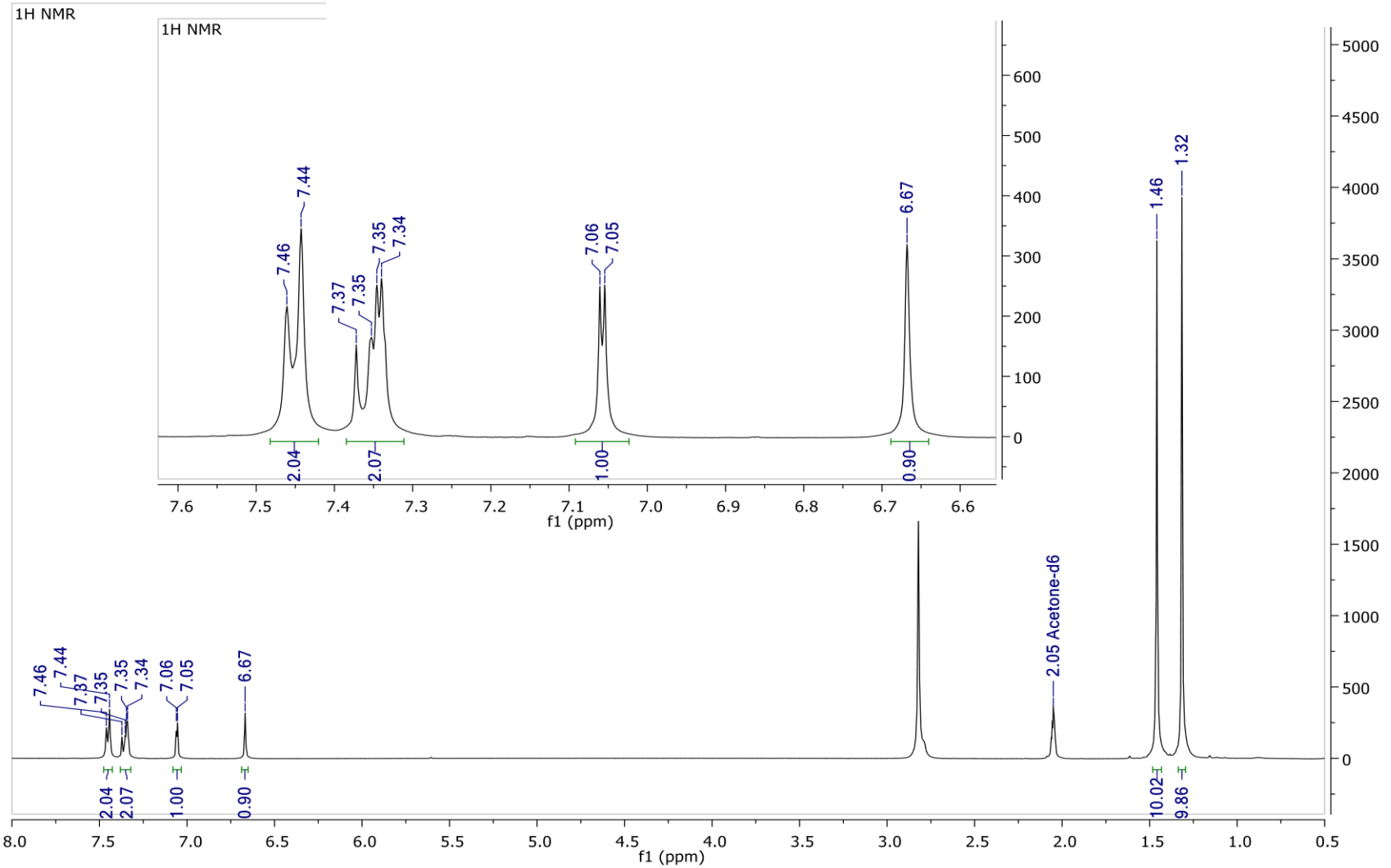




3,5-di-*tert*-Butyl-[1,1'-biphenyl]-2-ol (6) after photolysis in $CH_3CN:D_2O$ (3:1)

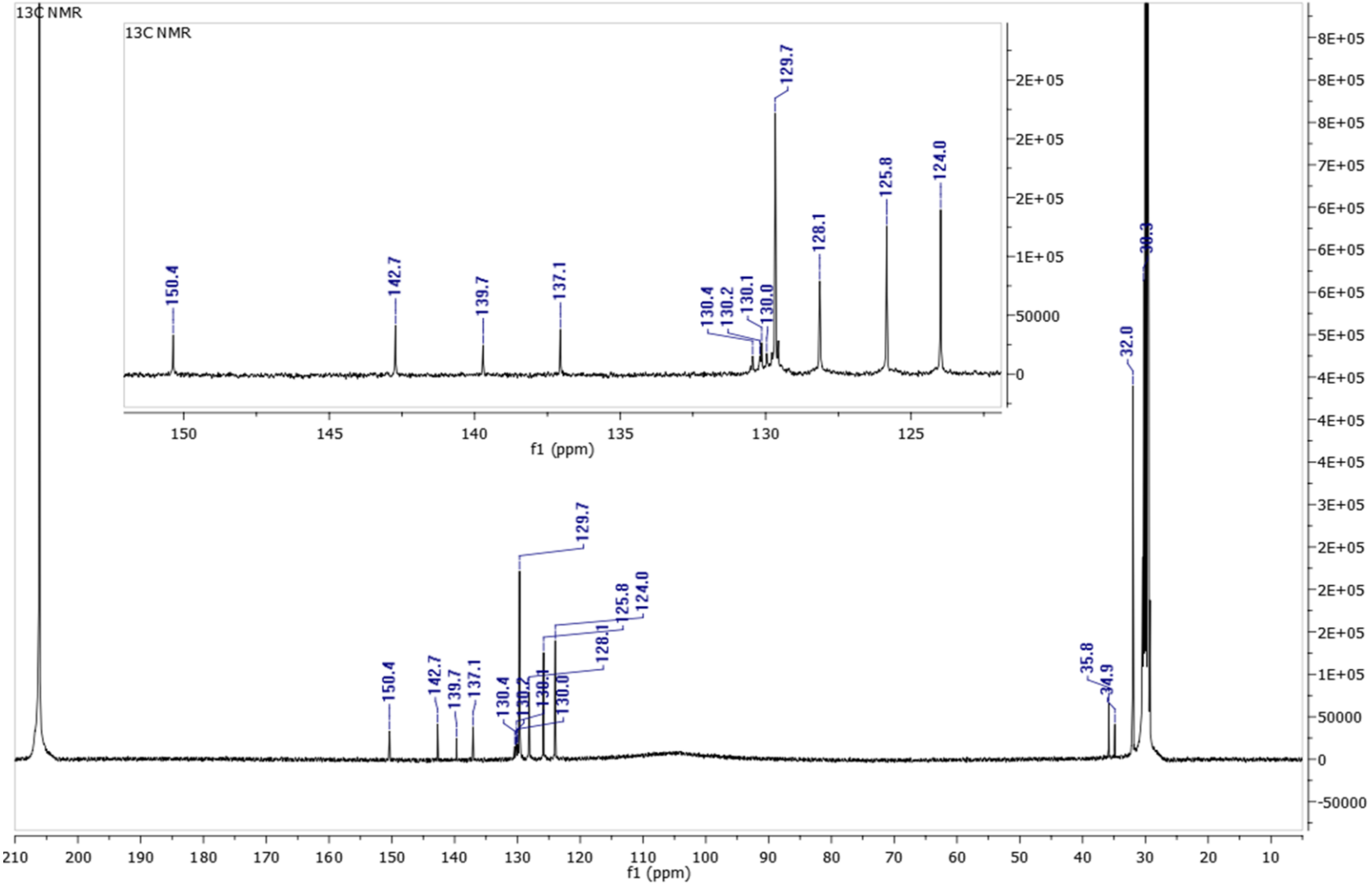
^{1}H NMR (400 MHz, $(CD_3)_2CO$)



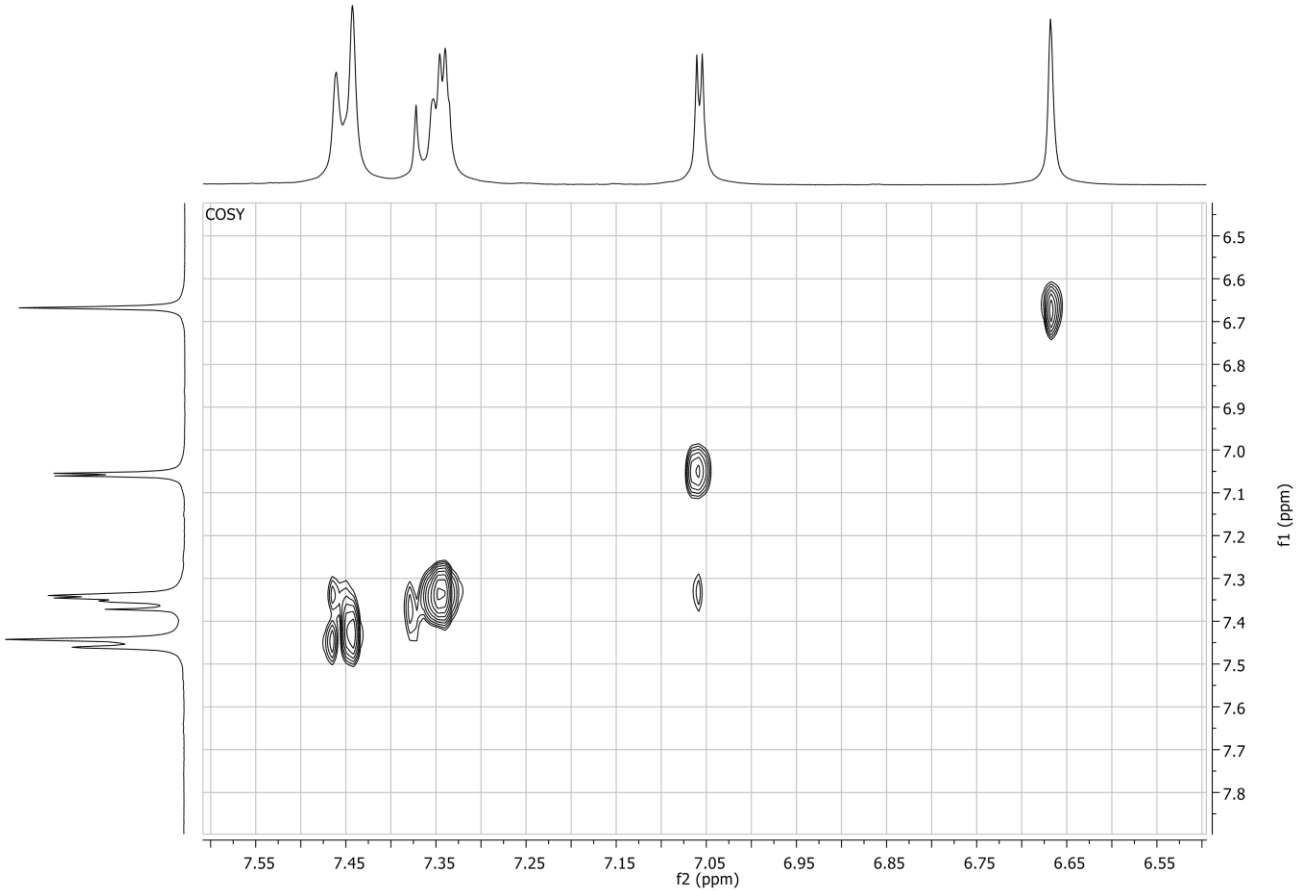


3,5-di-*tert*-Butyl-[1,1'-biphenyl]-2-ol (6) after photolysis in $CH_3CN:D_2O$ (3:1)

^{13}C NMR (100 MHz, $(CD_3)_2CO$)



COSY


COSY
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6.6
6.7
6.8
6.9
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7.1
7.2
7.3
7.4
7.5
7.6
7.7
7.8
f1 (ppm)
7.55
7.45
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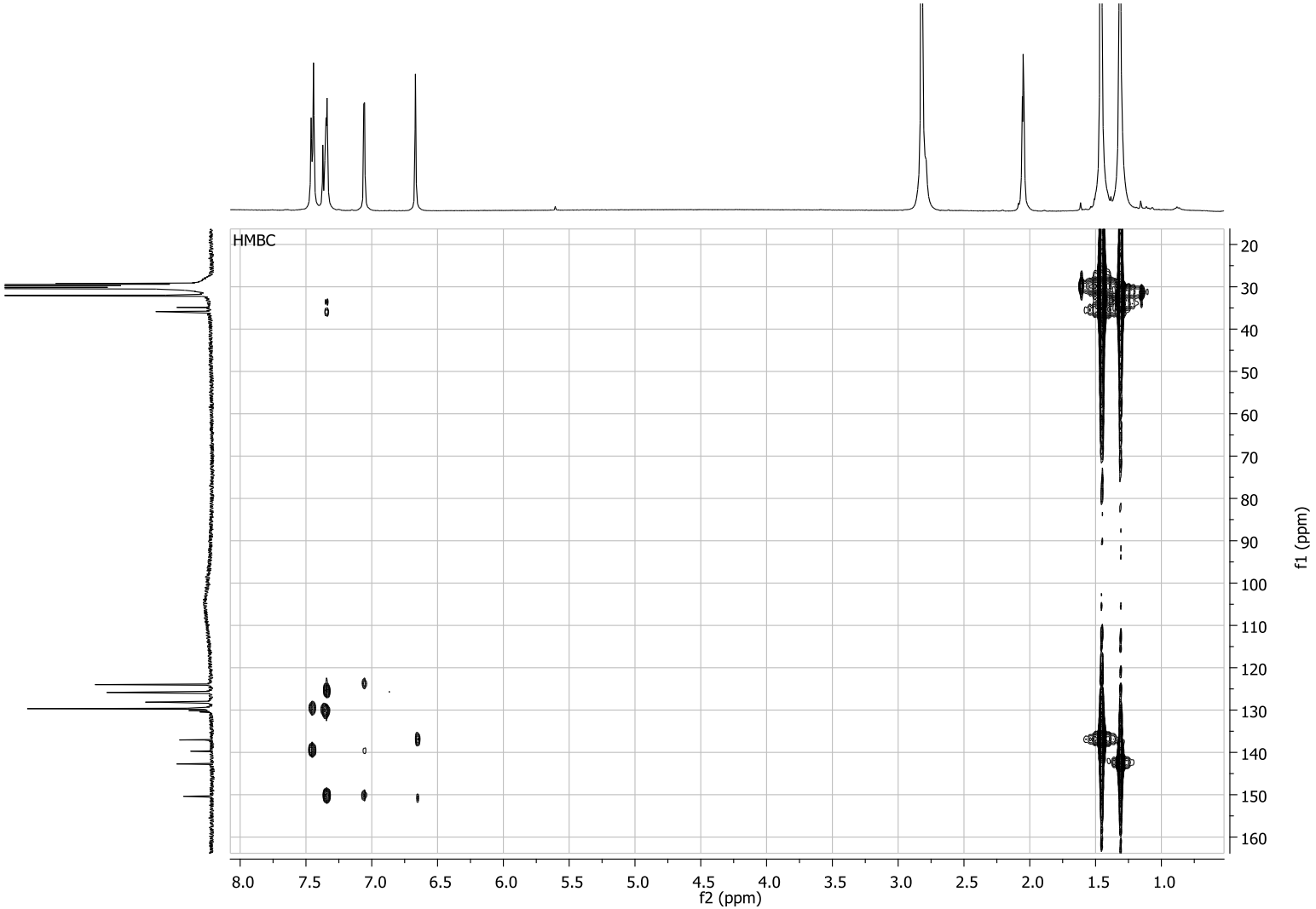
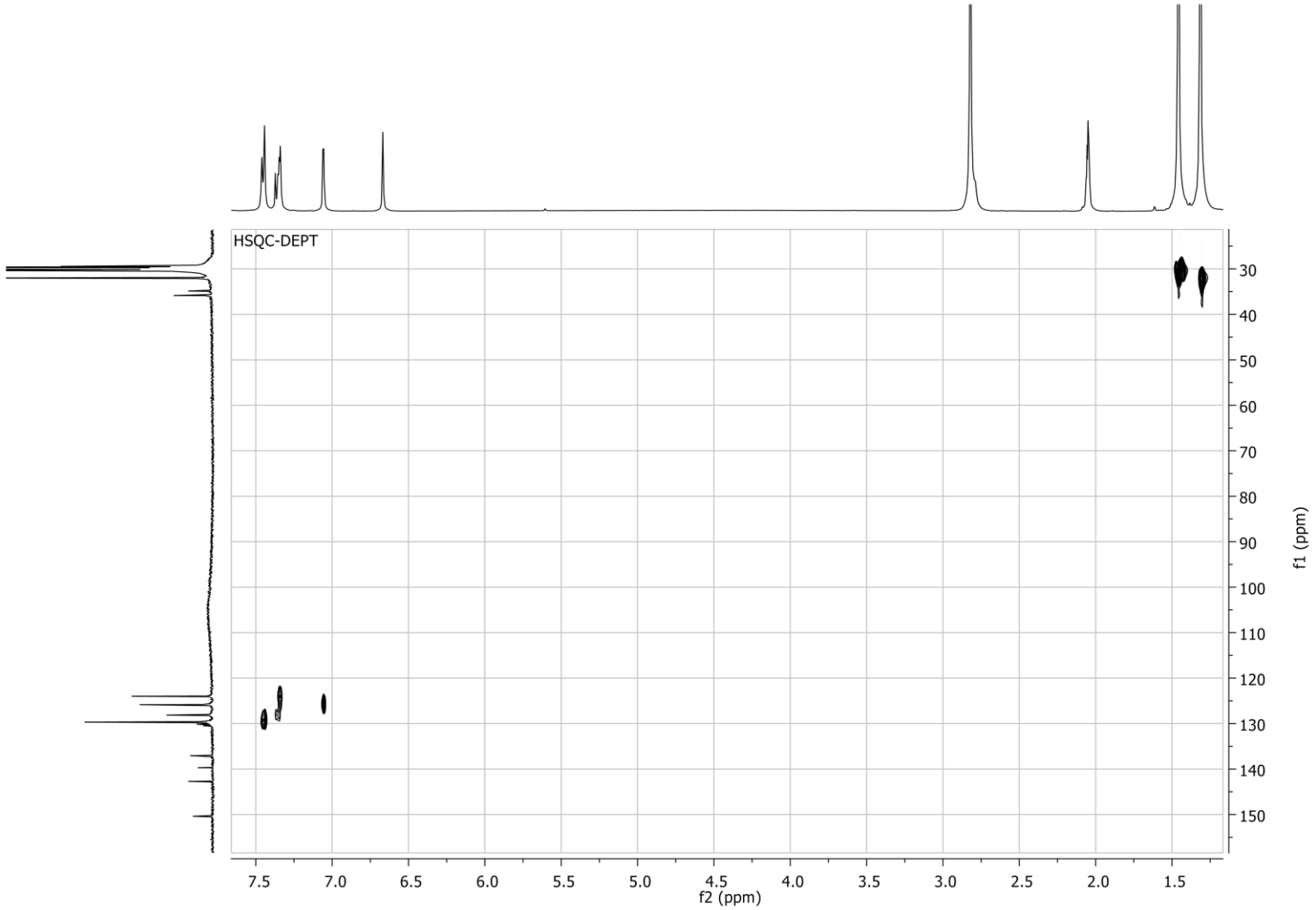
6.85
6.75
6.65
6.55
f2 (ppm)

HMBC



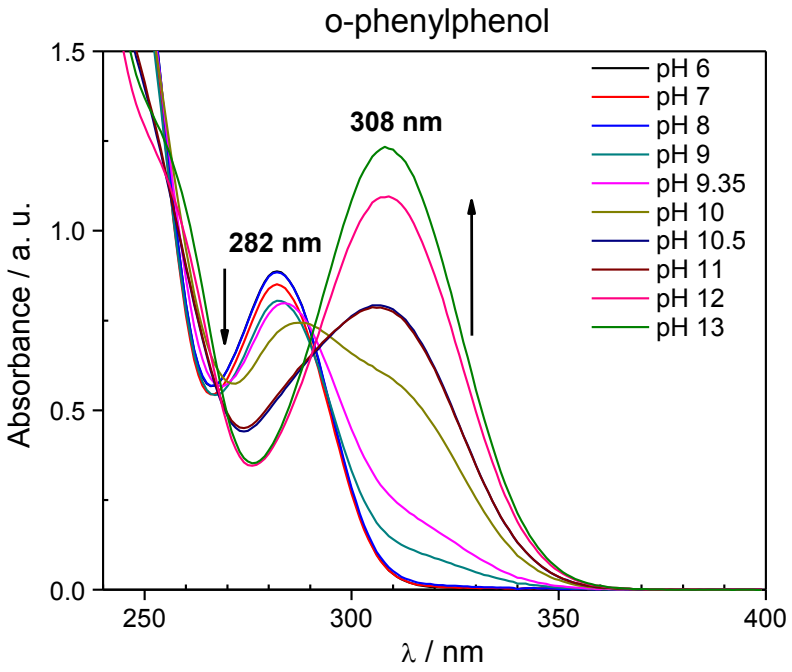
HSQC

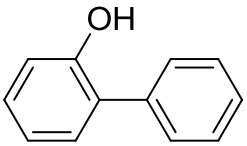

HSQC-DEPT
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
f2 (ppm)
30
40
50
60
70
80
90
100
110
120
130
140
150
f1 (ppm)

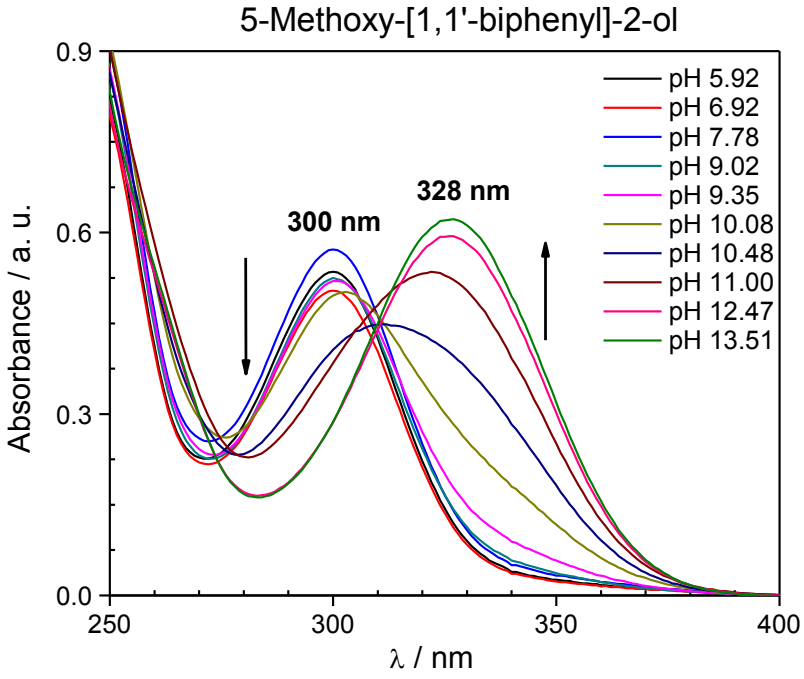
3. UV-visible absorption and fluorescence spectra

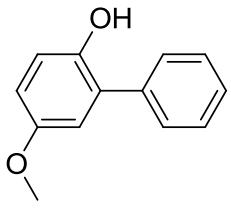
3.1. UV-Visible absorption spectra at different pH.

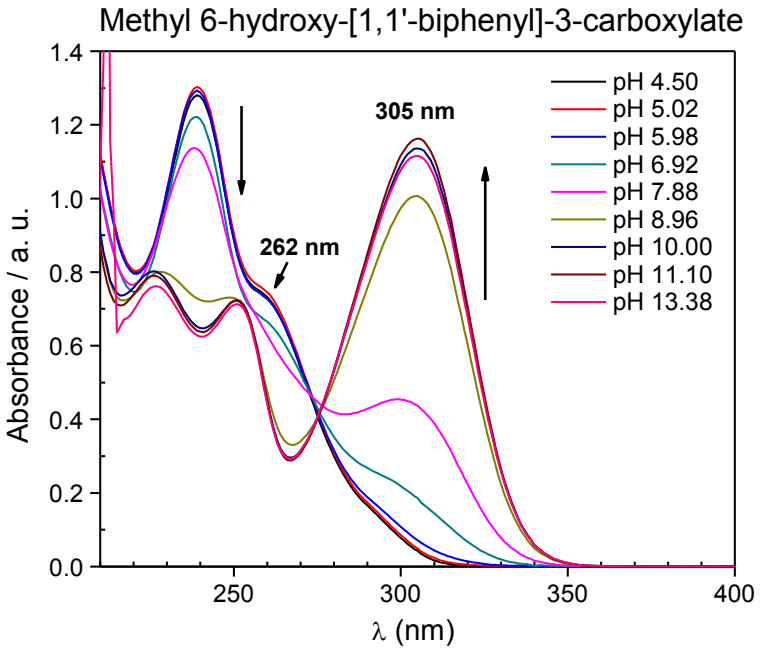
The pH was adjusted using different buffers solutions at ≈ 0.05M.

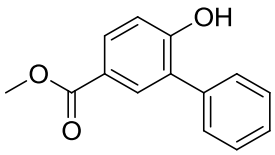


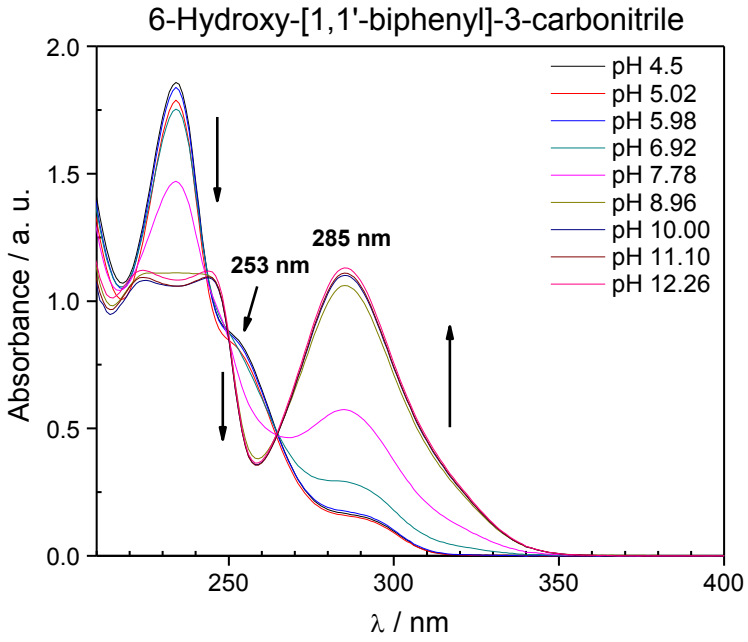


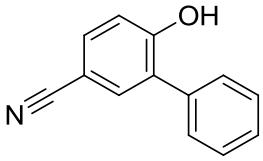




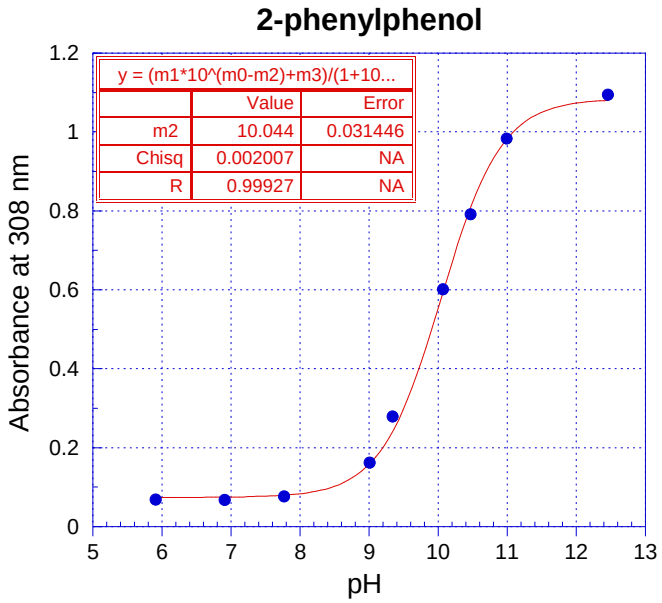

Methyl 6-hydroxy-[1,1'-biphenyl]-3-carboxylate
Absorbance / a. u.
λ (nm)
305 nm
262 nm
pH 4.50
pH 5.02
pH 5.98
pH 6.92
pH 7.88
pH 8.96
pH 10.00
pH 11.10
pH 13.38

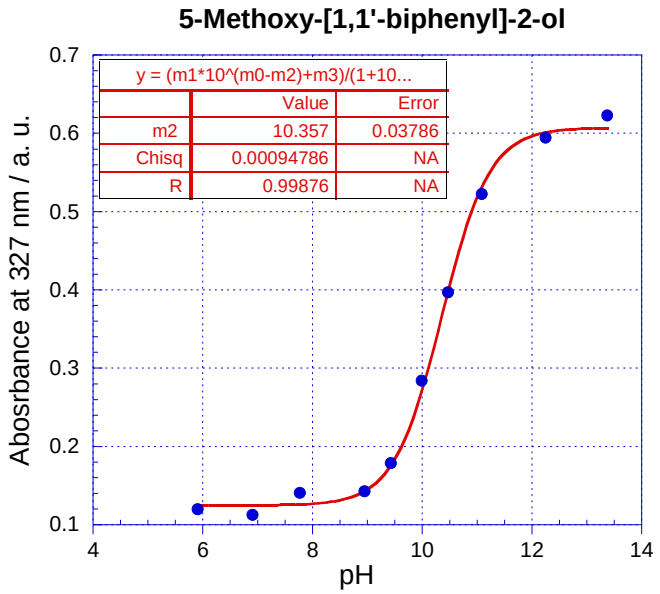

OH
O
O

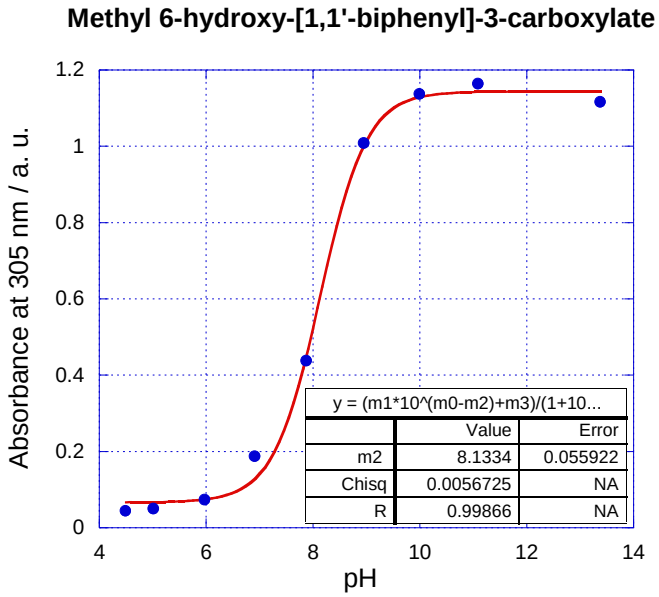

6-Hydroxy-[1,1'-biphenyl]-3-carbonitrile
Absorbance / a. u.
λ / nm
285 nm
253 nm
pH 4.5
pH 5.02
pH 5.98
pH 6.92
pH 7.78
pH 8.96
pH 10.00
pH 11.10
pH 12.26

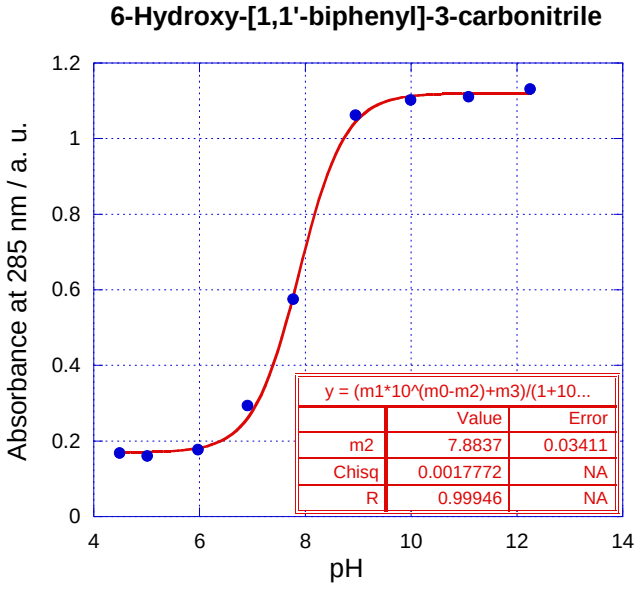

OH
N

3.2 Determination of pKa by UV-Visible absorption.

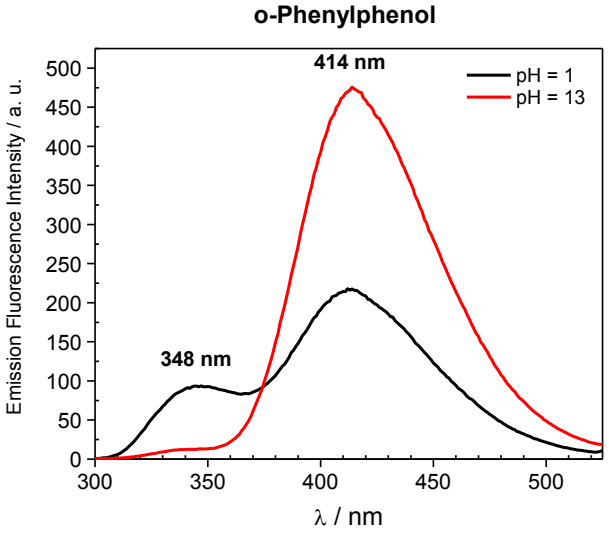




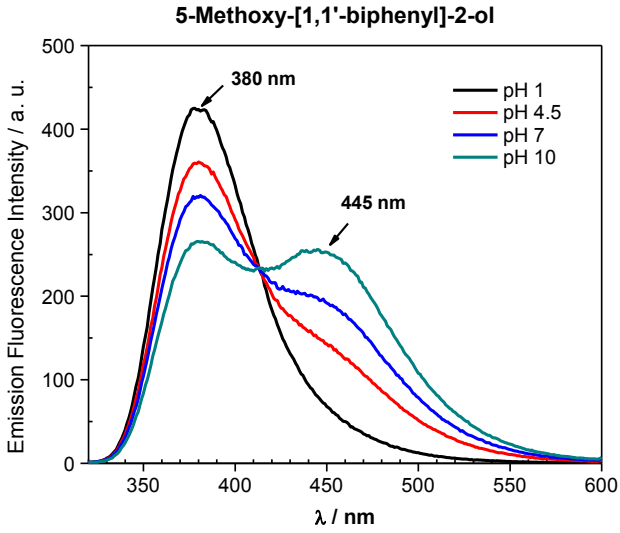




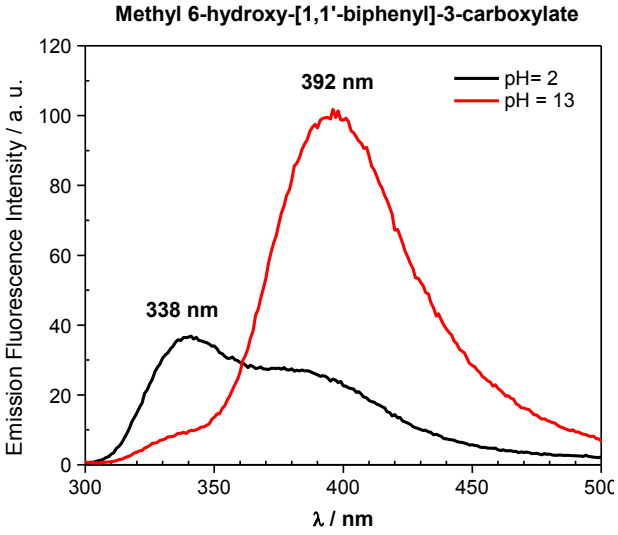
3.3. Emission fluorescence spectra at different pH



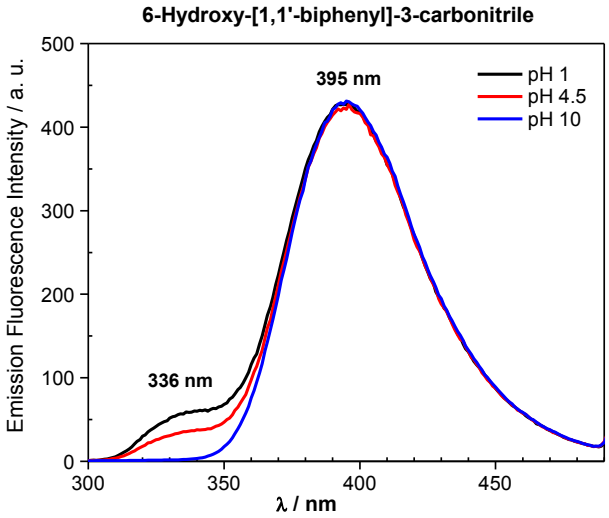
λ_{exc} (pH=1) = 283 nm; Abs (283 nm) = 0.141.
λ_{exc} (pH=13) = 283 nm; Abs (283 nm) = 0.141.



λ_{exc} (pH=1) = 300 nm; Abs (300 nm) = 0.327.
λ_{exc} (pH=4.5) = 300 nm; Abs (300 nm) = 0.141.
λ_{exc} (pH=7) = 300 nm; Abs (300 nm) = 0.214.
λ_{exc} (pH=10) = 327 nm; Abs (327 nm) = 0.376.

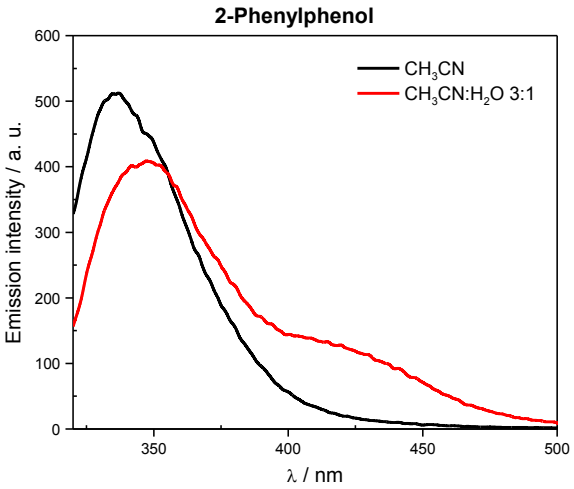


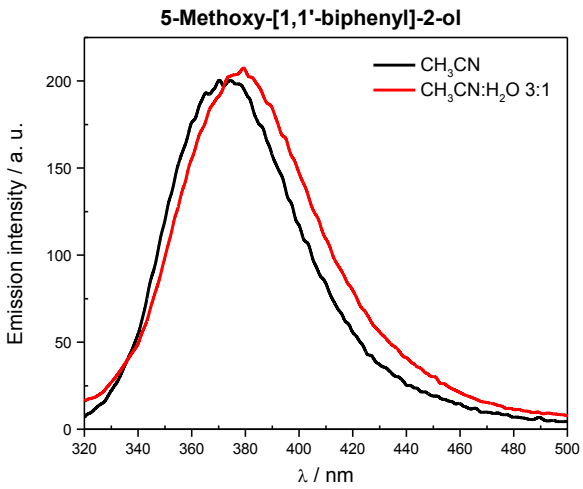
λ_{exc} (pH=2) = 267 nm; Abs (267 nm) = 0.094.
λ_{exc} (pH=13) = 305 nm; Abs (305 nm) = 0.133.

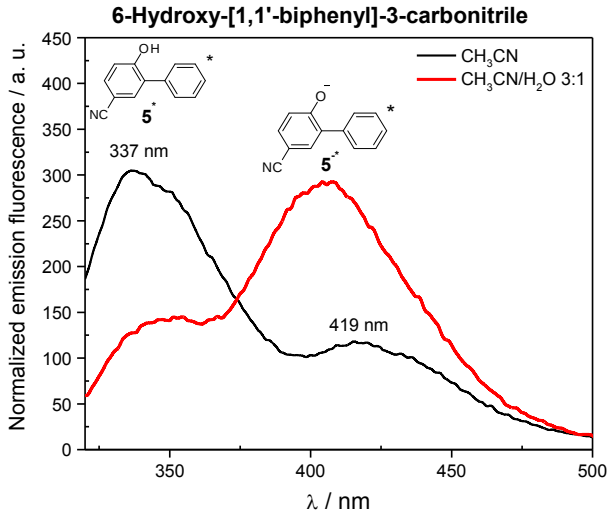


λ_{exc} (pH=1) = 267 nm; Abs (267 nm) = 0.364.
λ_{exc} (pH=4.5) = 267 nm; Abs (267 nm) = 0.301.
λ_{exc} (pH=10) = 267 nm; Abs (267 nm) = 0.285.

3.4 Fluorescence spectra at different solvents, λ_{exc} = 290 nm.







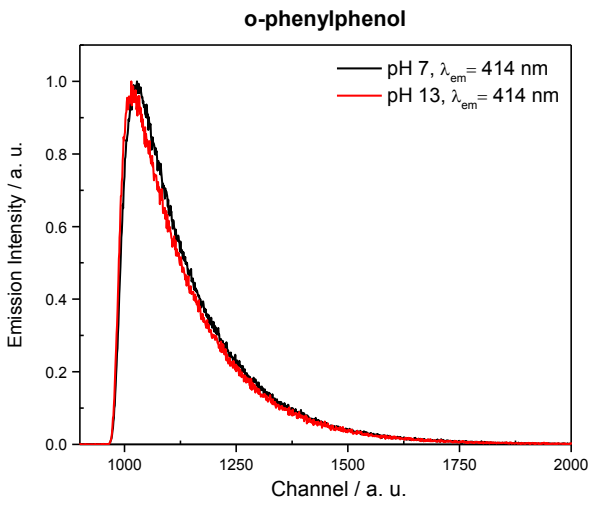
3.5 Fluorescence lifetimes of compounds 1, 2 and 5.

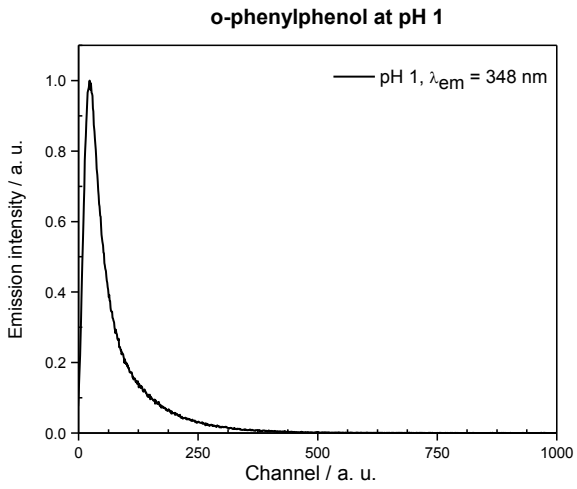
Fluorescence lifetimes of undeprotonated and deprotonated species for compounds **1**, **2** and **5** in water are presented in Table 3.5. The excitation wavelength was 267 nm. Firstly, fluorescence lifetimes of deprotonated species were determined at pH=13 for **1** and **5**, where the deprotonated form (A^-) was the dominant one. Consequently, lifetimes of deprotonated species were determined using mono-exponential fitting of the decay curves. The observed decay at pH=1 (for **1** and **5**) was fitted to a biexponential decay function for each compound giving a short component and a large one corresponding to the undeprotonated and deprotonated species, respectively.
However for compound **2**, the undeprotonated form (AH) was the dominant one at pH=1 and the fluorescence lifetime was determined using a mono-exponential fitting of the decay curve. At pH=13, the observed decay was fitted to a biexponential function. Corrected lifetime values are shown in the following table.

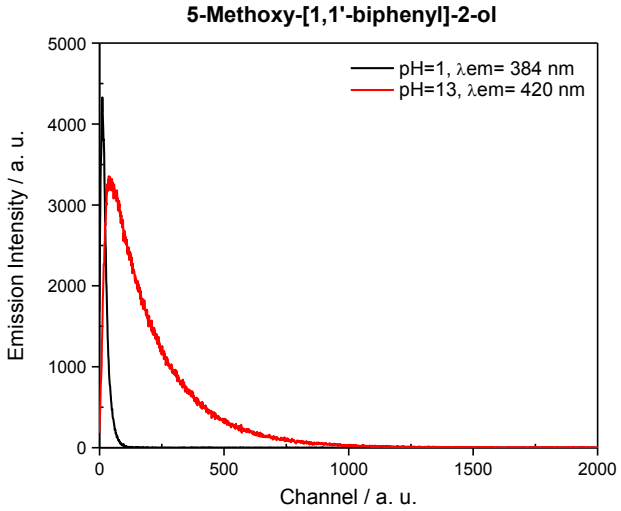
Table 3.5 Fluorescence lifetime values for compounds **1**, **2** and **5**.

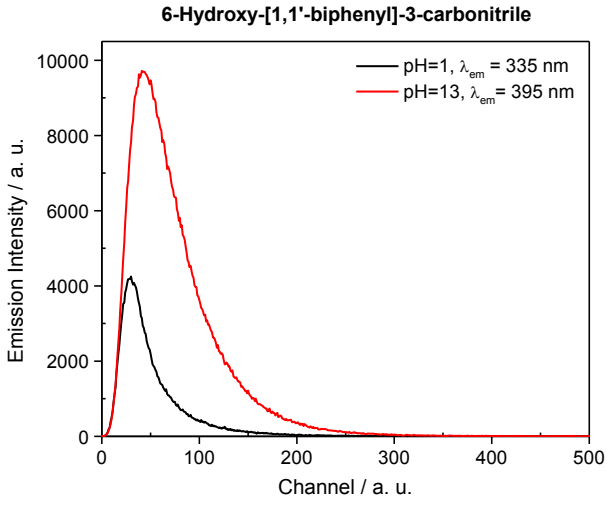
R	τ (AH)[a] / ns	τ (A^-)[b] / ns
H (**1**)	0.256 ± 0.003 0.313[c] ± 0.005 ns	3.722 ± 0.006 3.73[c] ± 0.01 ns
OCH_3 (**2**)	1.881 ± 0.006	5.079 ± 0.009
CN (**5**)	0.102 ± 0.005	1.07 ± 0.04 1.12[a] ± 0.01

[a] Fluorescence lifetime measured at pH=1. [b] Fluorescence lifetime measured at pH =13. [c] Fluorescence lifetime measured at pH =7.









4. Theoretical calculations

4.1 pK_a Calculation

For the computation of pK_a the method reported by Thapa *et al. (J. Phys. Chem. A* **2017**, *121, 24*, 4698-4706) was followed. Geometries of **1-5** were fully optimized in water (SMD model) at B3LYP/6-311++G(d,p) level of theory. Harmonic frequencies were calculated in order to confirm structures were minima on ground-state PES, and to get thermal corrections for free energies. According to the reported procedure, three explicit water molecules were included directly hydrogen-bonded to the site being protonated or deprotonated (Fig. S1).

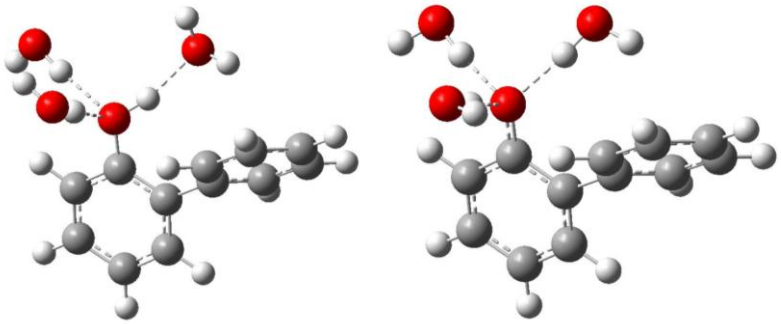


Figure S1. Optimized structures of the micro-solvated protonated and deprotonated species of **1** compound.

The pK_a for the considered acid-base reaction is given by

$$pK_a = \frac{\Delta G^*_{aq}}{2.303\ RT} = \frac{G^*_{aq,RO^-} + G^*_{aq,H^+} - G^*_{aq,ROH}}{2.303\ RT}$$

where $G^*_{aq,ROH}$ and G^*_{aq,RO^-} are the standard free energies of protonated and deprotonated phenols in aqueous solution, respectively. The free energy of a proton in aqueous solution is calculated as

$$G^*_{aq,H^+} = G^0_{H^+,g} + \Delta G^*_{H^+,aq} + \Delta G^{1atm \rightarrow 1M}$$

Where $G^0_{g,H^+} = H^0_{g,H^+}$ - TS^0_{g,H^+} is the gas phase free energy of proton at 298.15 K (from H^0_{g,H^+} = $5RT/2$ = 1.48 $kcal/mol$ and S^0_{g,H^+} = 26.05 $cal/(mol \bullet K)$, $\Delta G^0_{aq,H^+}$ = -265.9 kcal/mol is the aqueous phase solvation free energy of the proton and $\Delta G^{1atm \rightarrow 1M}$ = $RT\ log(24.4)$ = 1.89 kcal/mol is the correction term necessary for the change in standard state from 1 atm to 1mol/L.

Table S1. Calculation of pK_a of 2-phenylphenol derivatives in water using explicit water molecules and SMD model

Compound	Substituent	G° (a.u.) phenol [a]	G°(a.u.) anion [a]	Predicted pK_a	Experiment pK_a	MSE[b]	St. Dev.[c]
1	H	-767.90313	-767.45156	9.59	10.04		
2	OMe	-882.43057	-881.97989	9.18	10.36		
3	*t*-Bu	-925.09233	-924.64056	9.68	-	1.32	0.68
4	COOMe	-995.82022	-995.37536	6.50	8.13		
5	CN	-860.17885	-859.73541	5.85	7.88		

[a] Standard free energy (Hartree). [b] Mean signed error. [c] Standard deviation

As the pK_a of *t*-butyl containing derivative **3** could not be experimentally determined due to the poor solubility of **3** in water, the theoretical pK_a estimation was necessary. For this reason, the method proposed by Ugur *et al.* (*J. Chem. Inf. Model*. **2014**, *54*, 8, 2200-2213) was employed for the prediction of the pK_a since it allows to obtain accurate and fast results. Nevertheless, for the application of this method it is necessary to have a trustworthy set of experimental pK_a's. In our case, we determined the linear relationship between atomic charges and experimental pK_a's for a training set including 2-phenylphenols **1, 2, 4** and **5**. The NPA (Natural Population Analysis) atomic charge of the O atom for the anionic forms of the aforementioned 2-phenylphenols was associated with the experimental pK_a of each molecule in order to establish a linear fit (Fig. S2). The equation obtained by least-squares fit was then used for the pK_a prediction for derivative **3**.

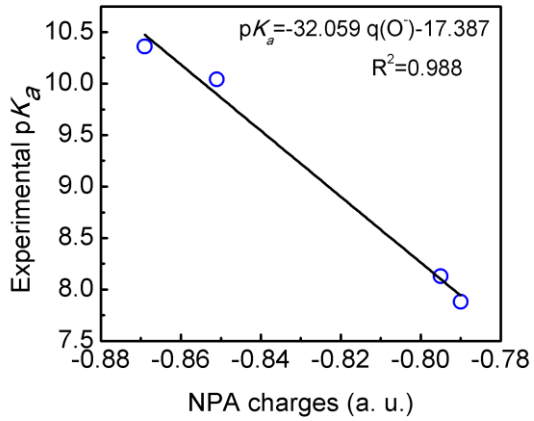


Figure S2. Experimental pK_a *vs.* NPA charges.

Table S2. NPA computed charges and predicted pK_a values

Compound	NPA atomic charge O^- (a. u.)	pK_a (Pred.)
1	-0.851	9.89
2	-0.869	10.47
3	-0.859	**10.15**
4	-0.795	8.10
5	-0.790	7.94

If we compare the two methodologies employed for the calculation of the pK_a of **3**, is evident that the latter one affords a more reasonable result (Table S2), at least higher than the value obtained for **1**, as could be expected for a phenol having an electron donating group.

4.2 pK_a^* calculation

As the experimental determination of pKa* was achieved by using the Förster cycle, the same method was applied for the theoretical determination. For that purpose, the absorption and

fluorescence vertical transition energies of undeprotonated and deprotonated species were calculated using PCM solvation model (solvent=water) with the linear response (LR) scheme at CAM-B3LYP/6-31+G(d) level of theory. The absorption energies for the undeprotonated species of **1**, **2** and **3** derivatives were computed at B3LYP/6-31+G(d) level, since the vertical transition energies predicted by the long range corrected functional CAM-B3LYP are blue-shifted, compared with the experimental values. In a few cases the computed energies were refined using the non-equilibrium state specific correction in order to obtain deeper accuracy. The results of the calculations are shown in Table S4.

Table S3. Experimental and theoretical determined absorption and emission energies at CAM-B3LYP/6-31+G(d) level of theory

	Phenol absorption (nm)		Phenol emission (nm)		Phenoxide absorption (nm)		Phenoxide emission (nm)	
	Exp	Theo	Exp	Theo	Exp	Theo	Exp	Theo
H	282	271[a] (251)	348	345	308	300 (331)[b]	414	398
OMe	300	302 [a] (274)	380	364 (347)[b]	328	326 (357)[b]	445	432
t-Bu	-	282[a] (258)	-	343	-	326 (335)[b]	-	383 [b]
COOMe	262	251	338	342	305	307	392	380
CN	253	250	336	344	285	308	395	380

[a] Calculated with B3LYP/6-31+G(d). In parenthesis, values obtained with LR-CAM-B3LYP/6-31+G(d). [b] Calculated using the non-equilibrium state specific correction. In parenthesis, values obtained using linear response formalism.

pK_a^* can be obtained using the following equation, in the same manner as for the experimental determination:

$$\Delta pKa^* = pKa - pKa^* = \frac{0.625\ (\nu ArOH - \nu ArO^-)}{T}$$

Table S4. Theoretically simulated p*Ka** values for compounds **1-5.**

Substituent	λ average phenol [a]	λ average phenoxide[a]	ΔE (cm^{-1})[b]	pK_a*$_{[c]}^{(Theo)}$	pK_a*$_{(Exp)}$	MSE	St. Dev.
H	308	349	-3814.237	2.07	1.59		
OMe	333	379	-3644.806	2.74	2.96		
t-Bu	312.5	354.5	-3791.255	2.22	-	-0.04	0.27
COOMe	296.5	343.5	-4614.731	-1.51	-1.56		
CN	297	344	-4600.266	-1.73	-1.62		

[a] $\lambda_{aver}=(\lambda_{Abs}+\lambda_{Em})/2$ [b] $\lambda_{aver\ phenoxide} - \lambda_{aver\ phenol}$ [c] $pK_a^* = pK_a + (\Delta E * 0.00209)$

4.3. Theoretical modeling of ESIPT process

All DFT and TD-DFT calculations were performed with Gaussian 09 package. Geometry optimizations were fully calculated by using the range-separated correction of the B3LYP functional, CAM (Coulomb-Attenuating Method), with the 6-31+G(d) basis set. The minima were characterized by Hessian diagonalization and further harmonic frequency analyses to obtain the

zero-point and thermal corrections for the energies, enthalpies and free energies. All optimizations and frequency analyses were performed within the PCM model for acetonitrile.

Table S5. Total energies,[(a)] zero point and thermal corrections to the standard free energy in atomic units.

Structures	E_{el}[b]	ZPE[c]	E_{el}+ ZPE	G°
1 enol form S_0	-538.25269	0.18786	-538.06483	-538.10093
1 enol form S_1	-538.09489	0.18420	-537.91069	-537.94686
1 keto form S_0	-538.19565	0.18630	-538.00935	-538.04579
1 keto form S_1	-538.12712	0.18513	-537.94198	-537.97839
2 enol form S_0	-652.73354	0.22069	-652.51284	-652.55249
2 enol form S_1	-652.58385	0.21751	-652.36633	-652.40552
2 keto form S_0	-652.67429	0.21913	-652.45516	-652.49549
2 keto form S_1	-652.61713	0.21928	-652.39784	-652.43700
5 enol form S_0	-630.46447	0.18673	-630.27774	-630.31638
5 enol form S_1	-630.30438	0.18304	-630.12134	-630.16000
5 keto form S_0	-630.40826	0.18490	-630.22336	-630.26250
5 keto form S_1	-630.33300	0.18315	- 630.14985	-630.18950

[a] All energies in Hartree. [b] Total electronic energies. [c] Zero-Point Energy corrections

4.3.1. Potential energy surfaces

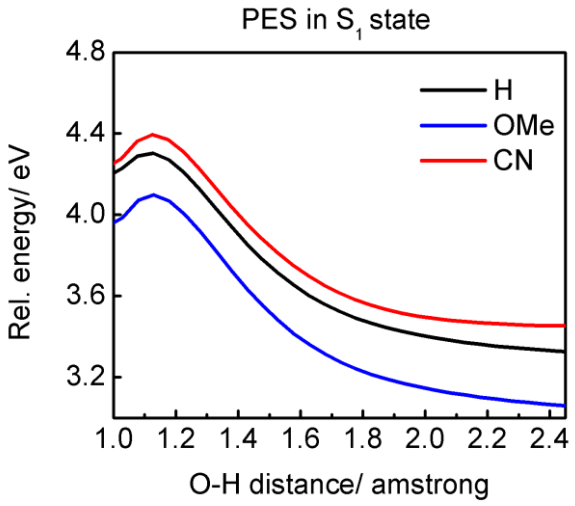


Figure S3. Relaxed scan of the S_1 state along the O-H stretching coordinate for compounds **1, 2** and **5.**

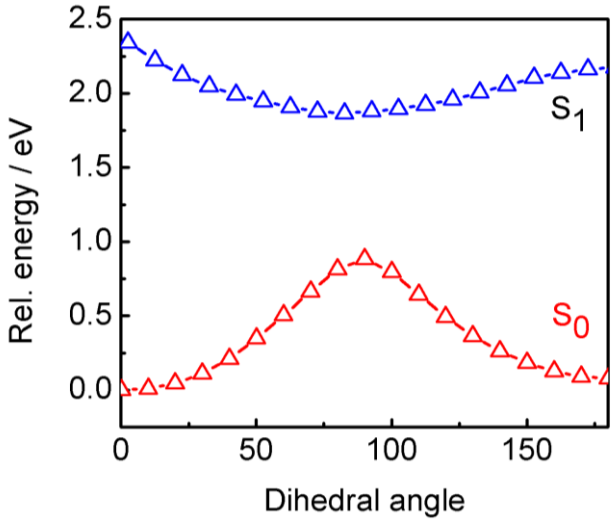


Figure S4. Potential energy surfaces for torsion rotation around the C2-C1' bond of **1** in S_0 and S_1 states.

4.3.2. Vertical excitations

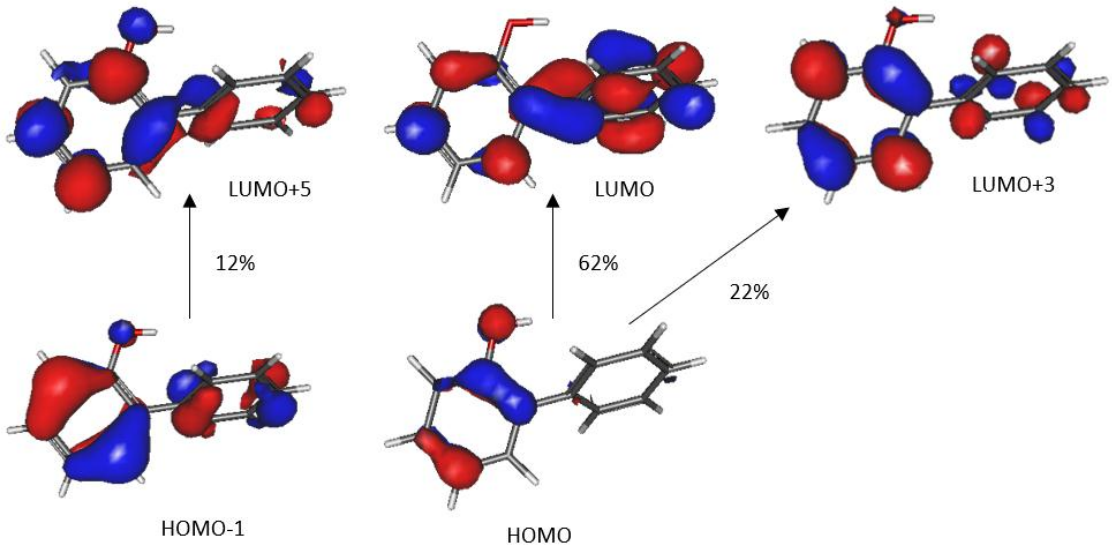


Figure S5. Molecular orbitals involved in the vertical transition to the S_1 state of **1** at ground state equilibrium geometry.

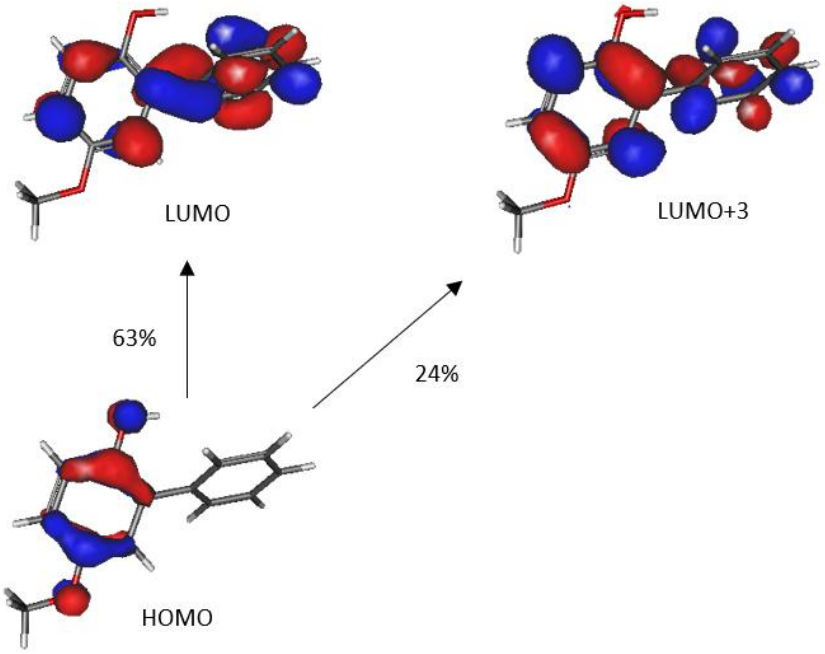


Figure S6. Molecular orbitals involved in the vertical transition to the S_1 state of **2** at ground state equilibrium geometry.

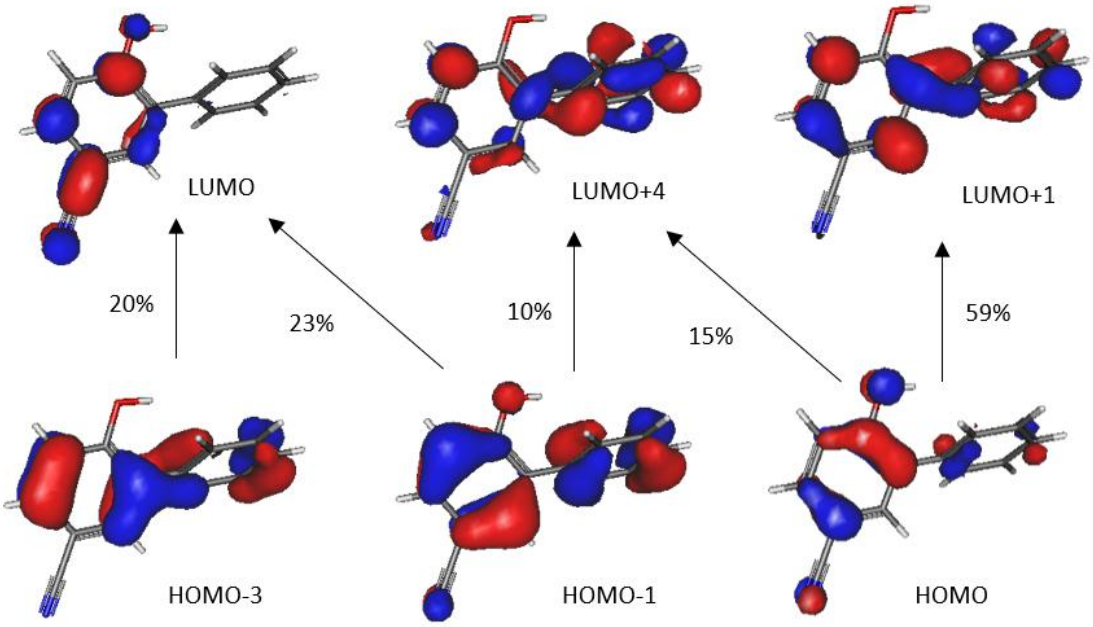


Figure S7. Molecular orbitals involved in the vertical transition to the S_1 state of **5** at ground state equilibrium geometry**.**

4.3.3. Non-covalent interactions (NCI) analysis

For analyzing the OH--π interaction the RDG function has been used

$$\boldsymbol{RDG}\ (r) = \frac{1}{2(3\pi^2)^{1/3}} \frac{|\nabla\rho(r)|}{\rho(r)^{4/3}} \qquad (1)$$

where ρ(r) is the total electron density and the RDG (r) is the reduced density gradient of the exchange contribution. According to Atoms in Molecules (AIM) theory the nature of a weak interaction depends on both the λ_2 eigenvalue and the electron density:

$$\Omega\ (r) = \textbf{Sign}\ (\lambda_2(r))\rho(r) \qquad (2)$$

When λ_2>0 the interaction is bonding, and the opposite if λ_2<0. In Fig. **S8** (top) the visual diagram of RDG isosurfaces (isovalue=0.6) shows the existence of a weak bonding interaction between the OH and the aromatic system in both S_0 and S_1 state. In the Fig. **S8** (bottom) the scatter plots of RDG function vs. Ω(r) function are shown for **1** in S_0 and S_1 states. It is important to note that the left spike shifts to the left in S_1, indicating a strengthening in the OH–π interaction upon excitation.

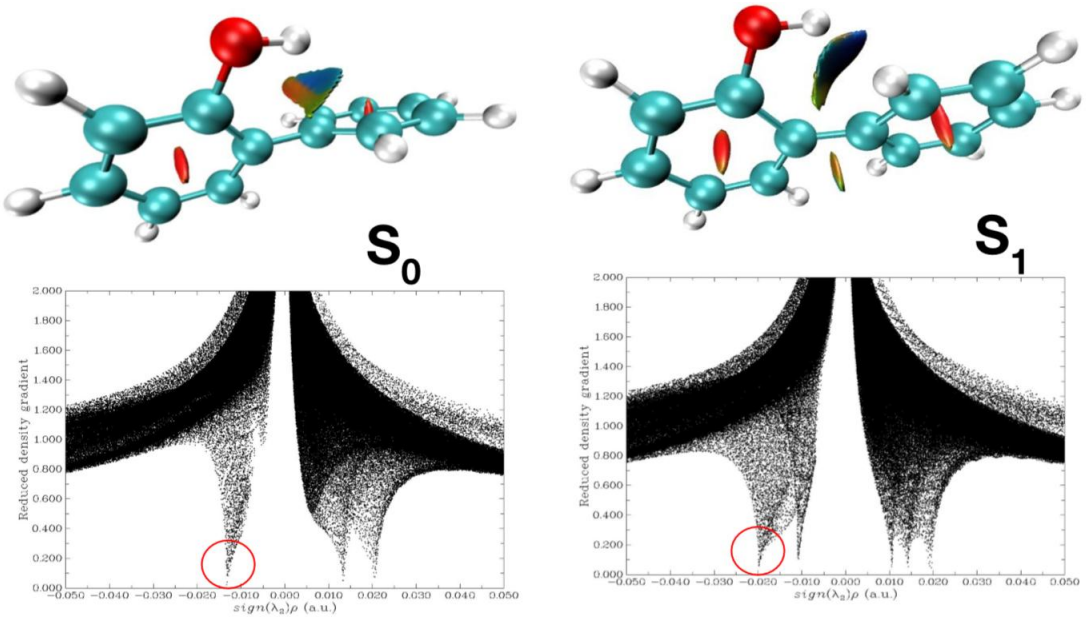


Figure S8. Top: Color-filled isosurface graph at equilibrium geometries for **1** (isovalue=0.6, color code: blue=strong attraction; green=vdW interactions, red=strong repulsion). Bottom: RDG scatter plot (isovalue=0.6). The left spike correspond to the attractive OH-π interaction.

4.3.4. IR frequencies

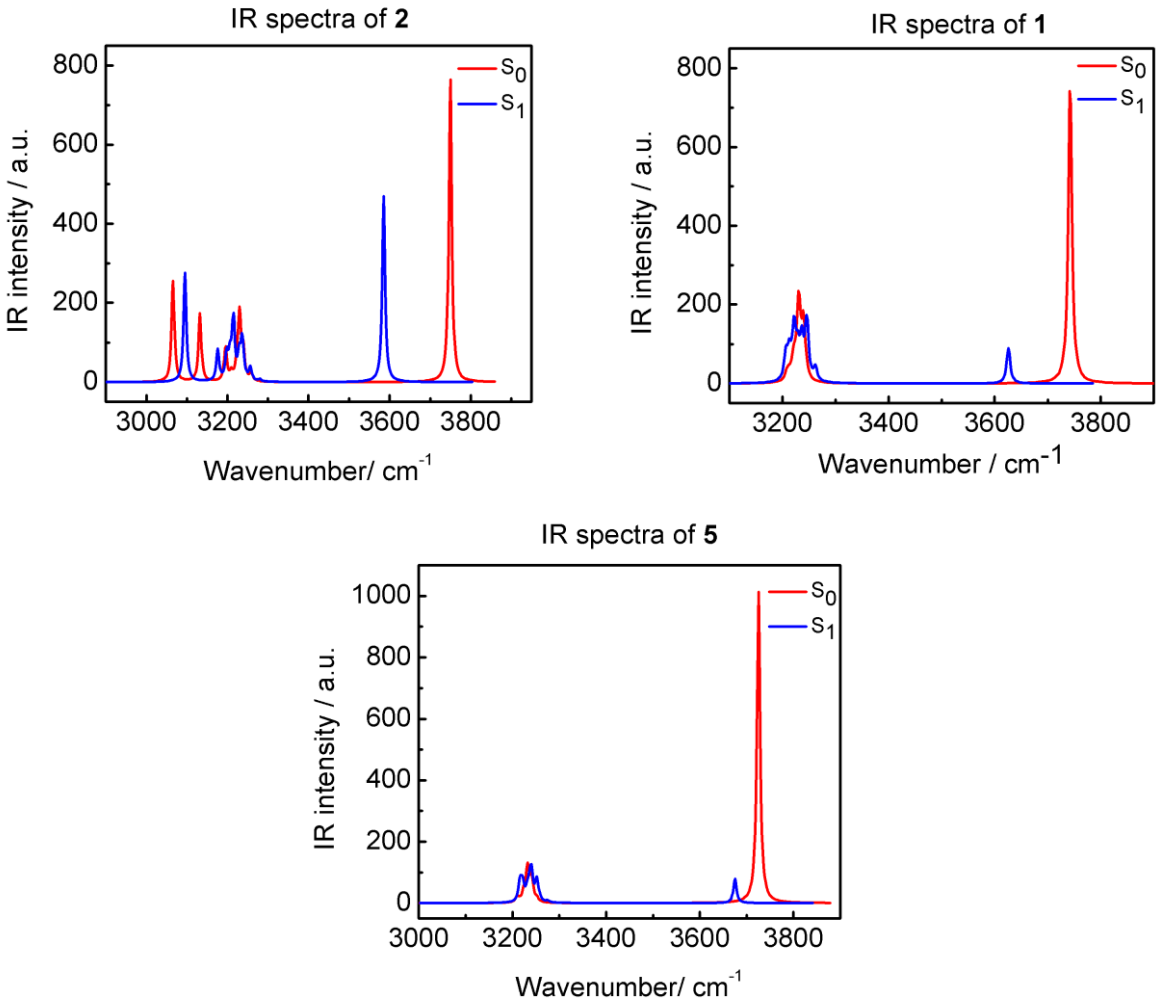


Figure S9. IR spectra of **1, 2** and **5** in S_0 and S_1 states depicting the red shifting of O-H stretching mode upon excitation.

4.3.5 Relevant optimized structures

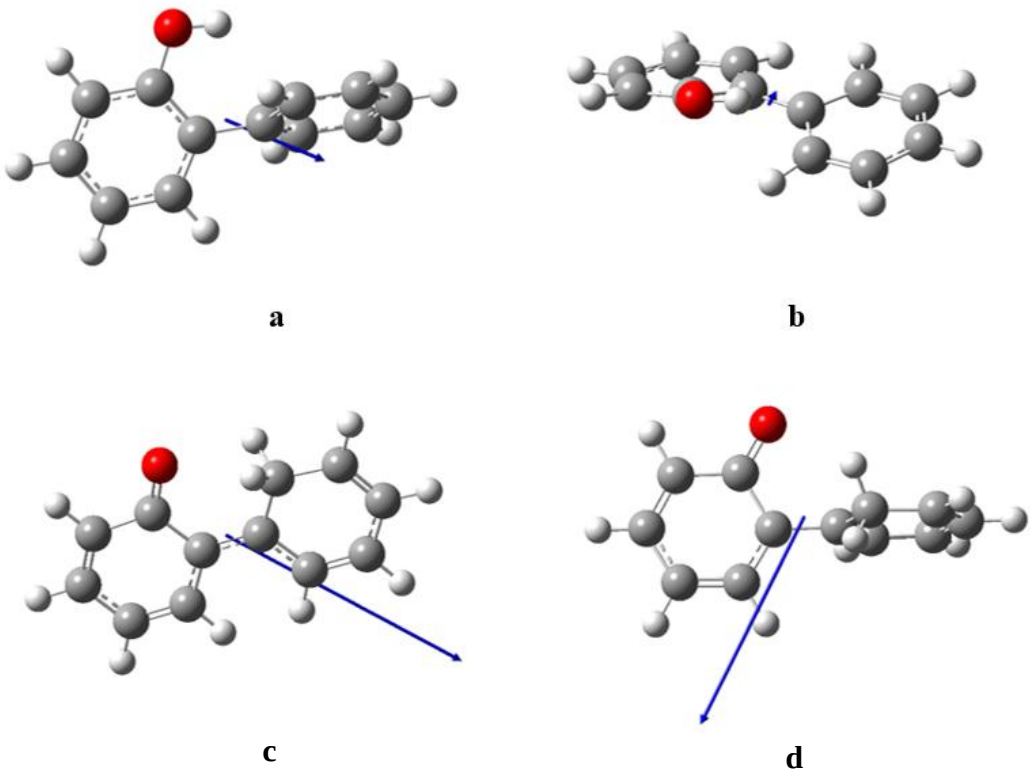


Figure S10. Structures of enol and keto forms along S_0 and S_1 surfaces for **1**. a) Enol S_0 form (E). b) Enol S_1 form (E*). c) Keto S_0 form (K). d) Keto S_1 form (K*).

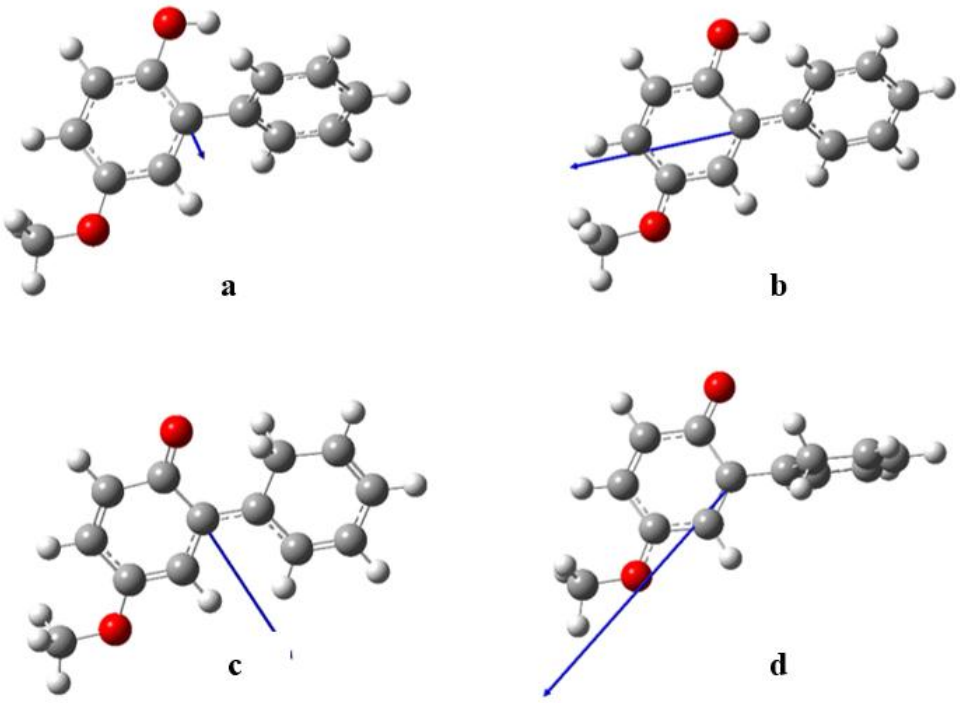


Figure S11. Structures of enol and keto forms along S_0 and S_1 surfaces for **2**. a) Enol S_0 form (E). b) Enol S_1 form (E*). c) Keto S_0 form (K). d) Keto S_1 form (K*).

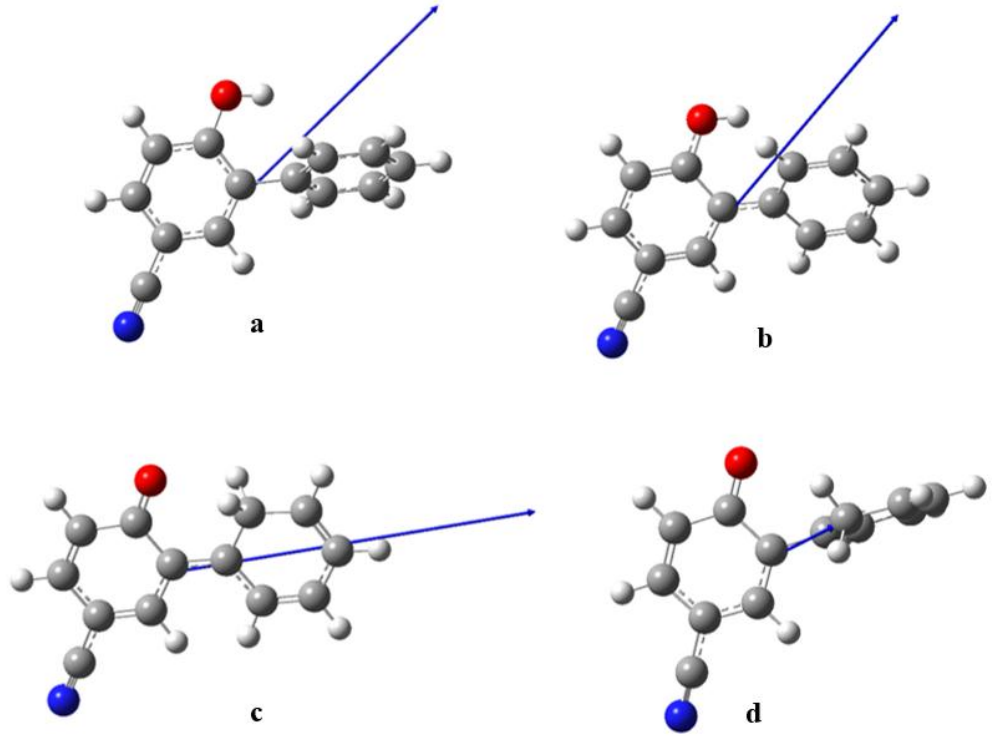


Figure S12. Structures of enol and keto forms along S_0 and S_1 surfaces for **5**. a) Enol S_0 form (E). b) Enol S_1 form (E*). c) Keto S_0 form (K). d) Keto S_1 form (K*).

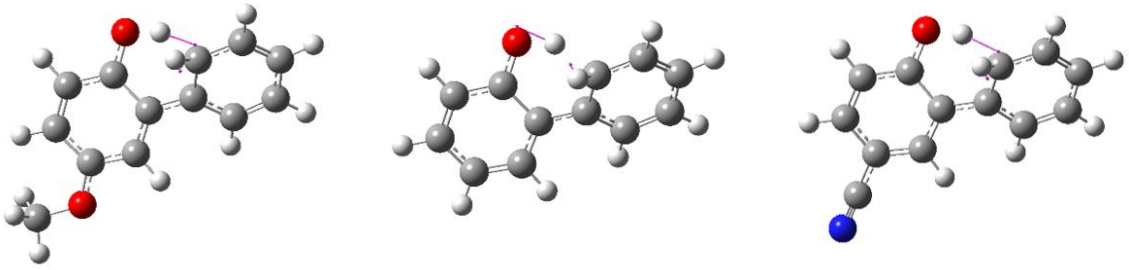


Figure S13. Structures of S1 transition state for **2, 1** and **5** showing the displacement vectors over the imaginary frequency mode. The obtained imaginary frequency values (-973.56 cm^{-1}, -1110.35 cm^{-1} and -1112.74 cm^{-1} for **1**, **2** and **5**, respectively) are in reasonable agreement with the expectable for proton transfer transition states.

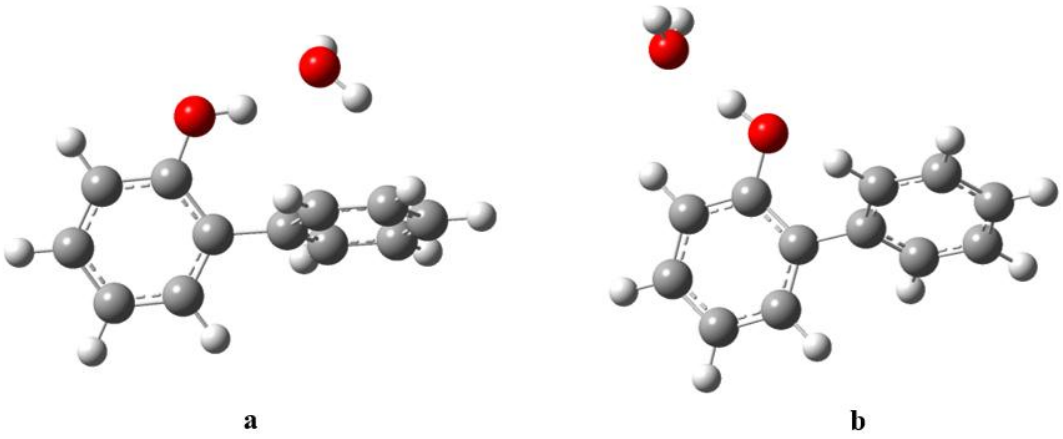


Figure S14. Structures of *syn* **1-W** and *anti* **1-W** conformers. Similar structures were found for **2** and **5**.

4.4 XYZ coordinates of all stationary points

1. 2-phenylphenol **(1)**, enol form (S0)

C	-2.7287470000	-1.4704020000	0.4225530000
C	-1.3403110000	-1.4010050000	0.4027910000
C	-0.6691170000	-0.2188300000	0.0724630000
C	-1.4407460000	0.9048630000	-0.2603250000
C	-2.8328590000	0.8461210000	-0.2423580000
C	-3.4743980000	-0.3370550000	0.1016520000
H	-3.2237020000	-2.3983720000	0.6906400000
H	-0.7512050000	-2.2765900000	0.6610250000
H	-3.3965380000	1.7345300000	-0.5095470000
H	-4.5596150000	-0.3735460000	0.1145470000
C	0.8188490000	-0.1678810000	0.0555910000
C	1.5187720000	0.7537610000	0.8450020000
C	1.5495020000	-1.0545930000	-0.7441950000
C	2.9114360000	0.7901020000	0.8311510000
H	0.9712650000	1.4301590000	1.4964590000
C	2.9405590000	-1.0224010000	-0.7538600000
H	1.0199900000	-1.7699420000	-1.3668550000
C	3.6260830000	-0.0972960000	0.0312480000
H	3.4364620000	1.5080580000	1.4540870000
H	3.4904370000	-1.7178880000	-1.3810000000
H	4.7114960000	-0.0704540000	0.0208350000
O	-0.8822550000	2.0957120000	-0.6350900000
H	0.0853070000	2.0160430000	-0.6697500000

2. 2-phenylphenol **(1)**, enol form (S1)

C	3.6309310000	-0.0154460000	0.0349840000
C	2.8542220000	1.0750540000	0.4528670000
C	1.4770680000	1.0019320000	0.4854950000

C	0.7813140000	-0.1987100000	0.0476650000
C	1.6188390000	-1.3388040000	-0.2614790000
C	2.9868300000	-1.2298020000	-0.2895640000
C	-0.6178860000	-0.2759330000	-0.0532710000
C	-1.3638970000	-1.5128580000	-0.0082130000
C	-2.7217850000	-1.5056100000	0.1956890000
C	-3.4620780000	-0.2940600000	0.2743110000
C	-2.8162230000	0.9214130000	0.0552660000
C	-1.4490160000	0.9327810000	-0.1791360000
O	-0.9119990000	2.0725050000	-0.6332480000
H	-3.2462430000	-2.4497090000	0.3098560000
H	-0.8323310000	-2.4561230000	-0.0227130000
H	-3.3670580000	1.8526240000	-0.0320690000
H	-4.5350070000	-0.3221910000	0.4323740000
H	0.9251540000	1.8032170000	0.9681380000
H	1.1578470000	-2.2773850000	-0.5466540000
H	3.3441060000	1.9816120000	0.7981040000
H	3.5832400000	-2.0937750000	-0.5692710000
H	4.7137180000	0.0556570000	0.0112930000
H	0.0426530000	1.9662900000	-0.8107590000

3. 2-phenylphenol **(1)**, keto form (S0)

C	3.6553760000	-0.1053450000	0.0002310000
C	2.9857590000	1.0590670000	0.0007670000
C	1.5019910000	1.1242760000	0.0004610000
C	0.7499880000	-0.1735810000	-0.0000360000
C	1.5455930000	-1.3707790000	-0.0008820000
C	2.9053480000	-1.3355650000	-0.0007590000
C	-0.6518580000	-0.2114900000	0.0001780000
C	-1.3679190000	-1.4651160000	0.0007170000
C	-2.7242720000	-1.5353350000	0.0006360000
C	-3.5004110000	-0.3319210000	-0.0000830000
C	-2.8964770000	0.8829500000	-0.0004940000
C	-1.4503380000	1.0267650000	-0.0001930000
O	-0.9387910000	2.1714480000	-0.0005050000
H	-3.2240320000	-2.4983910000	0.0011890000
H	-0.8131170000	-2.3946580000	0.0014750000
H	-3.4695570000	1.8054640000	-0.0009780000
H	-4.5851540000	-0.4008910000	-0.0002440000
H	1.1578270000	1.7399890000	0.8453920000
H	1.0662840000	-2.3398750000	-0.0018410000
H	3.5126870000	2.0090540000	0.0013720000
H	3.4508090000	-2.2749670000	-0.0015080000
H	4.7396290000	-0.1411220000	0.0004260000
H	1.1582790000	1.7402520000	-0.8445030000

4. 2-phenylphenol **(1)**, keto form (S1)

C	3.6114640000	-0.0713910000	-0.0135030000
C	2.9677950000	0.1841950000	1.1468620000
C	1.4766520000	0.1763630000	1.2492080000

C	0.7827510000	-0.2013530000	-0.0280340000
C	1.5045070000	-0.4507680000	-1.1872760000
C	2.8887890000	-0.3863370000	-1.2112900000
C	-0.6796250000	-0.2565960000	-0.0043790000
C	-1.3878620000	-1.4415480000	0.2030090000
C	-2.7721260000	-1.4465670000	0.2201810000
C	-3.5090770000	-0.2432370000	0.0450640000
C	-2.8612200000	0.9403980000	-0.1430540000
C	-1.4141070000	0.9932130000	-0.1692030000
O	-0.7987130000	2.0780660000	-0.3185540000
H	-3.3059960000	-2.3794970000	0.3649300000
H	-0.8411550000	-2.3696450000	0.3384740000
H	-3.3972410000	1.8734090000	-0.2823930000
H	-4.5935900000	-0.2793980000	0.0622390000
H	1.1498360000	-0.4842700000	2.0720030000
H	0.9644050000	-0.7035130000	-2.0957840000
H	3.5275570000	0.4071720000	2.0500980000
H	3.4277480000	-0.5911640000	-2.1285270000
H	4.6969020000	-0.0481280000	-0.0475420000
H	1.1135930000	1.1722840000	1.5694260000

5. 2-phenylphenol **(1)**, TS (S1)

-973.56 cm^{-1}

C	-3.5591520000	-0.0141930000	-0.1187200000
C	-2.8207200000	-1.0685870000	0.3664250000
C	-1.4157250000	-0.9717590000	0.5603690000
C	-0.7629130000	0.3022020000	0.1825950000
C	-1.5856090000	1.4030200000	-0.1964760000
C	-2.9408000000	1.2520190000	-0.3614620000
C	0.6450850000	0.3361650000	0.0682320000
C	1.4645790000	1.4968280000	0.1611070000
C	2.8341700000	1.3961390000	0.1596270000
C	3.4871640000	0.1343210000	0.0498490000
C	2.7471470000	-1.0176550000	-0.0935350000
C	1.3439800000	-0.9317040000	-0.1728600000
O	0.6506860000	-1.9750640000	-0.5545490000
H	3.4366700000	2.2924260000	0.2675900000
H	0.9964490000	2.4659290000	0.2959640000
H	3.2131940000	-1.9878190000	-0.2312190000
H	4.5711450000	0.0893470000	0.0590380000
H	-1.0139630000	-1.5009860000	1.4338100000
H	-1.1202190000	2.3526870000	-0.4442910000
H	-3.3262180000	-1.9875220000	0.6541400000
H	-3.5429880000	2.0914130000	-0.6922920000
H	-4.6301800000	-0.1203260000	-0.2651210000
H	-0.4126260000	-1.7954060000	-0.2721300000

6. 4-methoxy-2-phenylphenol **(2)**, enol form (S0)

C	-2.3250060000	-0.4577950000	0.0878350000
C	-0.9657260000	-0.7683710000	0.1225730000

C	0.0112700000	0.2134880000	-0.0269930000
C	-0.4002700000	1.5404870000	-0.2355120000
C	-1.7514630000	1.8524970000	-0.2719560000
C	-2.7201390000	0.8641050000	-0.1072130000
H	-0.6717210000	-1.8007050000	0.2865840000
H	-2.0481000000	2.8829470000	-0.4406180000
H	-3.7664150000	1.1425120000	-0.1396760000
C	1.4544960000	-0.1505940000	0.0155080000
C	2.3225970000	0.4557000000	0.9323080000
C	1.9682010000	-1.1184300000	-0.8553460000
C	3.6702080000	0.1050460000	0.9742860000
H	1.9360050000	1.1881580000	1.6362170000
C	3.3132660000	-1.4717580000	-0.8106410000
H	1.3069390000	-1.5913710000	-1.5756060000
C	4.1692130000	-0.8588850000	0.1024950000
H	4.3271830000	0.5811060000	1.6960290000
H	3.6948700000	-2.2241270000	-1.4944870000
H	5.2192660000	-1.1332620000	0.1353170000
O	0.4864500000	2.5705730000	-0.4283740000
H	1.3939530000	2.2269130000	-0.4621230000
O	-3.1847920000	-1.5071780000	0.2569970000
C	-4.5778460000	-1.2397670000	0.2408390000
H	-4.8904300000	-0.8247550000	-0.7237860000
H	-5.0699490000	-2.1989050000	0.3994190000
H	-4.8576680000	-0.5500010000	1.0446460000

7. 4-methoxy-2-phenylphenol **(2)**, enol form (S1)

C	-2.3341100000	-0.4426040000	0.0286450000
C	-0.9886580000	-0.8219390000	-0.0491450000
C	0.0492030000	0.1426840000	-0.0412310000
C	-0.4070860000	1.5274410000	-0.1770410000
C	-1.7532560000	1.8961820000	-0.0773540000
C	-2.7397650000	0.9229320000	0.0514250000
H	-0.7629680000	-1.8795110000	0.0082790000
H	-2.0085840000	2.9449050000	-0.1863760000
H	-3.7834030000	1.2033430000	0.0909300000
C	1.4366520000	-0.1729110000	0.0336140000
C	2.4137880000	0.7289120000	0.5841140000
C	1.9275670000	-1.4448290000	-0.4100740000
C	3.7632910000	0.4075790000	0.5858370000
H	2.0976100000	1.6149710000	1.1283890000
C	3.2731510000	-1.7396760000	-0.3971970000
H	1.2302140000	-2.1699340000	-0.8168220000
C	4.2190160000	-0.8117520000	0.0805090000
H	4.4697980000	1.1086550000	1.0229240000
H	3.6079400000	-2.7034840000	-0.7719350000
H	5.2768160000	-1.0543940000	0.0866710000
O	0.4455090000	2.4907750000	-0.5226000000
H	1.3538530000	2.1365170000	-0.6125800000
O	-3.2094230000	-1.4545390000	0.0957260000
C	-4.6086530000	-1.1962780000	0.2323500000

H	-4.9868480000	-0.6524370000	-0.6368000000
H	-5.0797320000	-2.1760800000	0.2865210000
H	-4.8102290000	-0.6368900000	1.1490700000

8. 4-methoxy-2-phenylphenol **(2)**, keto form (S0)

C	2.3242590000	-0.4506070000	-0.0004260000
C	1.0042030000	-0.7732530000	0.0042570000
C	-0.0400350000	0.2200020000	0.0034090000
C	0.3622370000	1.6340600000	0.0014860000
C	1.7877880000	1.9082750000	-0.0068020000
C	2.7231960000	0.9263560000	-0.0074370000
H	0.7617760000	-1.8277850000	0.0086520000
H	2.0782240000	2.9540450000	-0.0108350000
H	3.7742100000	1.1918610000	-0.0126680000
C	-1.3942770000	-0.1453750000	0.0028780000
C	-2.4881920000	0.8823600000	0.0029890000
C	-1.8094850000	-1.5210740000	0.0033480000
C	-3.8894090000	0.3876880000	-0.0051640000
H	-2.3333580000	1.5800800000	-0.8342290000
C	-3.1202420000	-1.8827280000	-0.0009200000
H	-1.0689850000	-2.3089170000	0.0061860000
C	-4.1927950000	-0.9204500000	-0.0066650000
H	-4.6702800000	1.1430230000	-0.0096190000
H	-3.3706940000	-2.9397880000	-0.0005240000
H	-5.2208340000	-1.2671570000	-0.0124110000
O	-0.4532160000	2.5868780000	0.0077500000
H	-2.3422190000	1.5667380000	0.8532260000
O	3.2248630000	-1.4824100000	0.0009180000
C	4.6143420000	-1.1859490000	-0.0002480000
H	4.9037770000	-0.6227340000	0.8934530000
H	5.1215940000	-2.1504710000	0.0038850000
H	4.9040540000	-0.6304600000	-0.8986740000

9. 4-methoxy-2-phenylphenol **(2)**, keto form (S1)

C	2.3373870000	-0.4651440000	-0.0064750000
C	0.9777790000	-0.8027100000	0.0098180000
C	0.0030540000	0.1728520000	0.0611350000
C	0.3828380000	1.5778050000	0.0678890000
C	1.7961750000	1.8803260000	0.0570800000
C	2.7417410000	0.8974790000	0.0210360000
H	0.7095390000	-1.8542500000	-0.0103990000
H	2.0819920000	2.9266890000	0.0813740000
H	3.7926430000	1.1580670000	0.0140000000
C	-1.4289390000	-0.1501880000	0.0602130000
C	-2.1285940000	-0.1651520000	-1.2674090000
C	-2.1222200000	-0.3930510000	1.2353210000
C	-3.5800350000	-0.5135470000	-1.1830010000
H	-1.6081690000	-0.8462570000	-1.9643160000
C	-3.4802600000	-0.6801550000	1.2366220000
H	-1.5823610000	-0.3568980000	2.1779190000

C	-4.1974150000	-0.7437220000	-0.0024910000
H	-4.1332620000	-0.5754680000	-2.1151410000
H	-3.9959090000	-0.8723000000	2.1697780000
H	-5.2557470000	-0.9877650000	0.0164200000
O	-0.4857040000	2.4885730000	0.0707550000
H	-2.0042470000	0.8248480000	-1.7476830000
O	3.1967450000	-1.4918130000	-0.0439470000
C	4.6043320000	-1.2439330000	-0.0621210000
H	4.9160030000	-0.7167520000	0.8432390000
H	5.0713460000	-2.2264680000	-0.0944950000
H	4.8847810000	-0.6727020000	-0.9508750000

10. 4-methoxy-2-phenylphenol **(2)**, TS (S1)

-1110.35 cm^{-1}

C	-2.3706730000	-0.4107300000	0.0464740000
C	-1.0521920000	-0.8560180000	0.1104100000
C	0.0234510000	0.0418700000	0.0566910000
C	-0.3143570000	1.4505330000	-0.1731520000
C	-1.6556710000	1.8871450000	-0.1571970000
C	-2.6835010000	0.9758490000	-0.0716210000
H	-0.8798680000	-1.9163610000	0.2580440000
H	-1.8525630000	2.9454370000	-0.2914080000
H	-3.7106480000	1.3133710000	-0.1117020000
C	1.4034900000	-0.2896660000	0.1618870000
C	2.3408870000	0.7517540000	0.6091390000
C	1.9256050000	-1.5304670000	-0.2918860000
C	3.7359020000	0.4873150000	0.4610200000
H	2.0599450000	1.3378300000	1.4931220000
C	3.2786790000	-1.7298190000	-0.4190450000
H	1.2377550000	-2.3088880000	-0.6114470000
C	4.1971260000	-0.6905090000	-0.0703400000
H	4.4467530000	1.2328250000	0.8104250000
H	3.6539370000	-2.6742170000	-0.8009700000
H	5.2638770000	-0.8579310000	-0.1885480000
O	0.6295140000	2.2932410000	-0.5002830000
H	1.6071840000	1.8286670000	-0.2022970000
O	-3.3135770000	-1.3625110000	0.1281350000
C	-4.6973980000	-1.0073060000	0.1167110000
H	-4.9639070000	-0.5148430000	-0.8221280000
H	-5.2383410000	-1.9479620000	0.2033160000
H	-4.9397090000	-0.3634790000	0.9662220000

11. 4-cyano-2-phenylphenol **(5)**, enol form (S0)

C	-2.5169630000	-0.4064250000	0.0802860000
C	-1.1611330000	-0.7457080000	0.1146990000
C	-0.1726090000	0.2238530000	-0.0192910000
C	-0.5745720000	1.5583270000	-0.2086490000
C	-1.9268780000	1.9040870000	-0.2414120000
C	-2.8970600000	0.9306150000	-0.0951880000
H	-0.8695690000	-1.7808150000	0.2602060000

H	-2.1979200000	2.9434430000	-0.3917920000
H	-3.9474630000	1.1995970000	-0.1205150000
C	1.2683590000	-0.1486530000	0.0146060000
C	2.1315200000	0.4102360000	0.9651190000
C	1.7808880000	-1.0750050000	-0.9003400000
C	3.4773680000	0.0523790000	0.9965290000
H	1.7441590000	1.1079800000	1.7031500000
C	3.1240950000	-1.4357030000	-0.8646380000
H	1.1223300000	-1.5096570000	-1.6467420000
C	3.9766530000	-0.8703890000	0.0815910000
H	4.1323250000	0.4904140000	1.7434960000
H	3.5066300000	-2.1561390000	-1.5813140000
H	5.0253590000	-1.1503140000	0.1067290000
O	0.3137410000	2.5664200000	-0.3845030000
H	1.2237360000	2.2230360000	-0.3902620000
C	-3.5123660000	-1.4248450000	0.2308770000

12. 4-cyano-2-phenylphenol **(5)**, enol form (S1)

C	-2.4932800000	-0.3853780000	0.0630830000
C	-1.1983330000	-0.7853690000	-0.1830990000
C	-0.1234630000	0.1793140000	-0.1377420000
C	-0.5648730000	1.5835140000	-0.1864120000
C	-1.8694360000	1.9602390000	0.0911990000
C	-2.8465430000	0.9833590000	0.2617830000
H	-0.9811100000	-1.8379040000	-0.3059590000
H	-2.1246900000	3.0145730000	0.0730640000
H	-3.8774730000	1.2546460000	0.4558780000
C	1.2275900000	-0.1732390000	0.0010700000
C	2.2305790000	0.7479930000	0.5061100000
C	1.6938180000	-1.5037810000	-0.3295740000
C	3.5627900000	0.3995520000	0.5362610000
H	1.9251810000	1.6806150000	0.9695970000
C	3.0296260000	-1.8173790000	-0.2936290000
H	0.9879350000	-2.2472310000	-0.6798800000
C	3.9899290000	-0.8691580000	0.1141840000
H	4.2870590000	1.1064770000	0.9306390000
H	3.3504230000	-2.8122900000	-0.5881740000
H	5.0425600000	-1.1320050000	0.1420970000
O	0.2761280000	2.5386290000	-0.5955310000
H	1.1423970000	2.1684470000	-0.8473480000
C	-3.5294400000	-1.3754150000	0.1227500000
N	-4.3735860000	-2.1671240000	0.1740630000

13. 4-cyano-2-phenylphenol **(5)**, keto form (S0)

C	2.5219330000	-0.3808610000	0.0007690000
C	1.1954100000	-0.7245840000	0.0028510000
C	0.1534510000	0.2491240000	0.0030330000
C	0.5384320000	1.6694370000	0.0051240000
C	1.9615390000	1.9689230000	-0.0025570000
C	2.9077650000	1.0021030000	-0.0031150000

H	0.9504610000	-1.7781050000	0.0038910000
H	2.2310750000	3.0200020000	-0.0065220000
H	3.9627240000	1.2576690000	-0.0070180000
C	-1.2038110000	-0.1499580000	0.0016730000
C	-2.3056420000	0.8601300000	0.0030290000
C	-1.5966410000	-1.5214470000	-0.0006540000
C	-3.6998910000	0.3611840000	0.0000070000
H	-2.1571010000	1.5573660000	-0.8361830000
C	-2.9102130000	-1.8940140000	-0.0026000000
H	-0.8538390000	-2.3070410000	-0.0012590000
C	-3.9920780000	-0.9520720000	-0.0025180000
H	-4.4847180000	1.1117970000	0.0002850000
H	-3.1463750000	-2.9542920000	-0.0044450000
H	-5.0152090000	-1.3112990000	-0.0044830000
O	-0.2920630000	2.6036640000	-0.0027810000
H	-2.1593880000	1.5511280000	0.8478930000
C	3.5253030000	-1.3986380000	0.0002040000
N	4.3479340000	-2.2160710000	-0.0001990000

14. 4-cyano-2-phenylphenol **(5)**, keto form (S1)

C	2.5211570000	-0.4077280000	-0.0536360000
C	1.1781770000	-0.7753770000	-0.0753020000
C	0.1834570000	0.1868280000	0.0587020000
C	0.5604280000	1.5954930000	0.1753880000
C	1.9707550000	1.9279970000	0.1827680000
C	2.9165580000	0.9578120000	0.0756730000
H	0.9058720000	-1.8200520000	-0.1792340000
H	2.2383230000	2.9734240000	0.2897740000
H	3.9724940000	1.2037810000	0.0890010000
C	-1.2409160000	-0.1464290000	0.0523000000
C	-2.0063050000	0.1638740000	-1.2011440000
C	-1.8711620000	-0.6859560000	1.1619770000
C	-3.4336390000	-0.2664550000	-1.1564890000
H	-1.4984910000	-0.2652480000	-2.0828570000
C	-3.2238050000	-1.0015370000	1.1453620000
H	-1.2895360000	-0.8702540000	2.0609720000
C	-3.9926170000	-0.7954540000	-0.0429910000
H	-4.0208180000	-0.1398490000	-2.0607830000
H	-3.6908700000	-1.4322230000	2.0229190000
H	-5.0392520000	-1.0852690000	-0.0474580000
O	-0.3229260000	2.4776250000	0.2557410000
H	-1.9424900000	1.2555940000	-1.3826330000
C	3.5278770000	-1.4184550000	-0.1597590000
N	4.3440530000	-2.2355120000	-0.2475320000

15. 4-cyano-2-phenylphenol **(5)**, TS (S1)

-1112.74 cm^{-1}

C	-2.5510000000	-0.3109250000	0.0350160000
C	-1.2645970000	-0.8059470000	0.0478320000
C	-0.1522370000	0.0788220000	0.0285360000

C	-0.4576280000	1.5027240000	-0.1682780000
C	-1.7789960000	1.9829720000	-0.0916260000
C	-2.8228170000	1.0934220000	-0.0122870000
H	-1.1019260000	-1.8741000000	0.1298880000
H	-1.9480630000	3.0502240000	-0.1843250000
H	-3.8496320000	1.4401960000	-0.0105980000
C	1.1977330000	-0.2948960000	0.1743970000
C	2.1768580000	0.7340600000	0.5952050000
C	1.6846460000	-1.5799130000	-0.2152990000
C	3.5535790000	0.4457390000	0.4026220000
H	1.9297390000	1.3237700000	1.4867390000
C	3.0279520000	-1.8036820000	-0.3703370000
H	0.9788560000	-2.3593010000	-0.4861040000
C	3.9723500000	-0.7633500000	-0.1041210000
H	4.2914510000	1.1804820000	0.7147950000
H	3.3790910000	-2.7711270000	-0.7142750000
H	5.0314420000	-0.9582790000	-0.2437470000
O	0.5095430000	2.3129060000	-0.4996450000
H	1.4805610000	1.8239030000	-0.2071690000
C	-3.6540260000	-1.2243690000	0.0960360000
N	-4.5512520000	-1.9552790000	0.1436810000

16. 2-phenylphenol + 1 explicit water (**1-W**), *syn* conformer S_0 (B3LYP/6-31+G(d,p)/scrf=acetonitrile)

C	-3.0679010000	-1.5042860000	-0.0475110000
C	-1.6741780000	-1.5645950000	-0.0325520000
C	-0.8783660000	-0.4071480000	0.0470660000
C	-1.5322210000	0.8458110000	0.0792340000
C	-2.9336700000	0.9079890000	0.0746680000
C	-3.6976510000	-0.2563500000	0.0164130000
H	-3.6527130000	-2.4174380000	-0.0987350000
H	-1.1770330000	-2.5303760000	-0.0598730000
H	-3.4058150000	1.8854320000	0.1016860000
H	-4.7816600000	-0.1871400000	0.0119880000
C	0.6063260000	-0.5373960000	0.1025720000
C	1.3414490000	-0.0073270000	1.1786000000
C	1.3003330000	-1.2302800000	-0.9049420000
C	2.7300610000	-0.1568530000	1.2386680000
H	0.8225300000	0.5172650000	1.9757240000
C	2.6885110000	-1.3822020000	-0.8453670000
H	0.7482860000	-1.6416670000	-1.7451770000
C	3.4094370000	-0.8424040000	0.2247650000
H	3.2794150000	0.2558460000	2.0799320000
H	3.2061570000	-1.9159560000	-1.6371360000
H	4.4882810000	-0.9571240000	0.2712680000
O	-0.8780580000	2.0443920000	0.1205850000
H	0.0597800000	2.0023330000	-0.1689920000
O	1.6932730000	2.5912780000	-0.7722840000
H	1.7528430000	2.7737940000	-1.7204200000
H	2.3854370000	1.9399110000	-0.5863510000

17. 2-phenylphenol + 1 explicit water (**1-W**), *anti* conformer S_0 (B3LYP/6-31+G(d,p)/scrf=acetonitrile)

C	1.6343740000	-2.6928280000	-0.2415950000
C	0.3590620000	-2.1259860000	-0.2016780000
C	0.1587620000	-0.7391590000	-0.0820860000
C	1.3055020000	0.0855890000	0.0041200000
C	2.5896640000	-0.4795730000	-0.0355970000
C	2.7537890000	-1.8598250000	-0.1589040000
H	1.7501620000	-3.7674580000	-0.3431700000
H	-0.5127860000	-2.7689360000	-0.2828970000
H	3.4541720000	0.1736670000	0.0391100000
H	3.7555740000	-2.2787810000	-0.1901310000
C	-1.2264280000	-0.1927340000	-0.0351340000
C	-1.6184950000	0.9049790000	-0.8238210000
C	-2.1970660000	-0.8010450000	0.7824210000
C	-2.9347680000	1.3712170000	-0.8000070000
H	-0.8887520000	1.3895390000	-1.4631830000
C	-3.5139060000	-0.3334530000	0.8090320000
H	-1.9148390000	-1.6393900000	1.4129810000
C	-3.8894180000	0.7554340000	0.0168340000
H	-3.2156800000	2.2156040000	-1.4234450000
H	-4.2429340000	-0.8170780000	1.4532250000
H	-4.9120380000	1.1209850000	0.0362490000
O	1.1320530000	1.4305320000	0.1493010000
H	1.9962770000	1.8944610000	0.2270010000
O	3.4930870000	2.8538750000	0.3770350000
H	3.5955930000	3.3118820000	1.2233520000
H	3.6076990000	3.5345450000	-0.3012930000

18. 4-methoxy-2-phenylphenol + 1 explicit water (**2-W**), *syn* conformer S_0 (B3LYP/6-31+G(d,p)/scrf=acetonitrile)

C	-2.6466970000	-0.4011310000	-0.0015590000
C	-1.3205410000	-0.8470030000	0.0078170000
C	-0.2395490000	0.0432050000	0.0802140000
C	-0.5126070000	1.4312310000	0.1114880000
C	-1.8385780000	1.8706300000	0.1093760000
C	-2.9084240000	0.9722760000	0.0598070000
H	-1.1325680000	-1.9161360000	-0.0140430000
H	-2.0289550000	2.9393280000	0.1331260000
H	-3.9212230000	1.3566060000	0.0606180000
C	1.1477830000	-0.5017280000	0.1266370000
C	2.0265200000	-0.1587890000	1.1703150000
C	1.5960930000	-1.4000800000	-0.8576570000
C	3.3180380000	-0.6906930000	1.2212760000
H	1.6948900000	0.5217060000	1.9489800000
C	2.8870080000	-1.9332480000	-0.8073130000
H	0.9322390000	-1.6707750000	-1.6736850000
C	3.7547460000	-1.5775400000	0.2303850000
H	3.9801310000	-0.4169010000	2.0376830000
H	3.2159100000	-2.6203910000	-1.5815270000

H	4.7590580000	-1.9887350000	0.2693130000
O	0.4568210000	2.4008280000	0.1569130000
H	1.3239140000	2.1084470000	-0.1988830000
O	3.0176160000	2.1898230000	-0.9099400000
H	3.0596880000	2.3063920000	-1.8693740000
H	3.5048010000	1.3737450000	-0.7241290000
O	-3.6102150000	-1.3792370000	-0.0629600000
C	-4.9798150000	-0.9749650000	-0.0624700000
H	-5.5620530000	-1.8952680000	-0.1141920000
H	-5.2337660000	-0.4336780000	0.8564410000
H	-5.2097090000	-0.3486460000	-0.9323280000

19. 4-methoxy-2-phenylphenol + 1 explicit water (**2-W**), *anti* conformer S_0 (B3LYP/6-31+G(d,p)/scrf=acetonitrile)

C	-2.1955290000	-1.0890580000	0.0764960000
C	-0.8078960000	-1.2743200000	0.0739610000
C	0.0871430000	-0.1969610000	0.0222340000
C	-0.4475910000	1.1130510000	-0.0344410000
C	-1.8332990000	1.2955560000	-0.0327060000
C	-2.7132450000	0.2082720000	0.0242570000
H	-0.4238970000	-2.2880130000	0.1336170000
H	-2.2330730000	2.3040360000	-0.0838590000
H	-3.7804800000	0.3942440000	0.0270480000
C	1.5530980000	-0.4648370000	0.0139620000
C	2.4368520000	0.2336660000	0.8572160000
C	2.0839830000	-1.4647250000	-0.8217070000
C	3.8014490000	-0.0636520000	0.8685290000
H	2.0499420000	1.0077280000	1.5106510000
C	3.4499000000	-1.7607510000	-0.8132720000
H	1.4235420000	-2.0054150000	-1.4935450000
C	4.3153440000	-1.0616780000	0.0332240000
H	4.4638970000	0.4835690000	1.5335170000
H	3.8364900000	-2.5332720000	-1.4720940000
H	5.3772990000	-1.2896840000	0.0410210000
O	0.4147250000	2.1733070000	-0.1150570000
H	-0.0774850000	3.0212920000	-0.1834470000
O	-0.8623410000	4.6292820000	-0.3096640000
H	-0.7101590000	5.0904910000	-1.1466970000
H	-0.6128380000	5.2588580000	0.3816210000
O	-2.9548660000	-2.2340820000	0.1396800000
C	-4.3754200000	-2.0977630000	0.1566380000
H	-4.7398290000	-1.6122120000	-0.7563770000
H	-4.7721830000	-3.1119190000	0.2105040000
H	-4.7101040000	-1.5285680000	1.0320170000

20. 4-cyano-2-phenylphenol + 1 explicit water (**5-W**), *syn* conformer S_0 (B3LYP/6-31+G(d,p)/scrf=acetonitrile)

C	-2.8428020000	-0.2886070000	0.0111980000
C	-1.5283010000	-0.7848300000	0.0185810000
C	-0.4226410000	0.0702110000	0.0519450000

C	-0.6575890000	1.4679240000	0.0485450000
C	-1.9739370000	1.9634930000	0.0569300000
C	-3.0596720000	1.1027480000	0.0406270000
H	-1.3625300000	-1.8572010000	0.0182890000
H	-2.1196090000	3.0385200000	0.0593160000
H	-4.0698070000	1.4977600000	0.0416060000
C	0.9519250000	-0.5082950000	0.0965620000
C	1.8033820000	-0.2547370000	1.1861800000
C	1.4055470000	-1.3476900000	-0.9348290000
C	3.0814960000	-0.8185000000	1.2362000000
H	1.4621150000	0.3784460000	2.0001920000
C	2.6831190000	-1.9120540000	-0.8846150000
H	0.7582650000	-1.5488450000	-1.7835620000
C	3.5266420000	-1.6459240000	0.1988130000
H	3.7256350000	-0.6159080000	2.0867620000
H	3.0199550000	-2.5542440000	-1.6929710000
H	4.5202230000	-2.0822100000	0.2376220000
O	0.3226800000	2.3983470000	0.0380990000
H	1.2233510000	2.0612580000	-0.1805090000
O	2.9494790000	2.1470050000	-0.6726020000
H	3.1183760000	2.3992910000	-1.5912210000
H	3.4250880000	1.3148280000	-0.5347880000
C	-3.9498890000	-1.1929170000	-0.0145420000
N	-4.8545710000	-1.9284930000	-0.0363260000

21. 4-cyano-2-phenylphenol + 1 explicit water (**5-W**), *anti* conformer S_0 (B3LYP/6-31+G(d,p)/scrf=acetonitrile)

C	2.3037960000	-1.2209080000	-0.0863570000
C	0.9022790000	-1.3387160000	-0.0844640000
C	0.0697410000	-0.2177480000	-0.0278500000
C	0.6820990000	1.0613880000	0.0323910000
C	2.0839310000	1.1812240000	0.0297270000
C	2.8927650000	0.0555830000	-0.0300300000
H	0.4543570000	-2.3250530000	-0.1439260000
H	2.5280080000	2.1699710000	0.0824270000
H	3.9724710000	0.1599500000	-0.0330370000
C	-1.4093620000	-0.3974430000	-0.0142150000
C	-2.2494380000	0.3364510000	-0.8710700000
C	-1.9933360000	-1.3493080000	0.8407920000
C	-3.6286220000	0.1180910000	-0.8762800000
H	-1.8194980000	1.0731300000	-1.5407310000
C	-3.3739880000	-1.5654640000	0.8376810000
H	-1.3641630000	-1.9142110000	1.5226840000
C	-4.1974130000	-0.8326510000	-0.0218720000
H	-4.2592970000	0.6897890000	-1.5511730000
H	-3.8041500000	-2.3019060000	1.5103610000
H	-5.2706830000	-0.9989610000	-0.0253500000
O	-0.1125940000	2.1497750000	0.1128530000
H	0.4137530000	2.9842810000	0.1749850000
O	1.2636270000	4.4941000000	0.2965940000
H	1.1346940000	4.9682740000	1.1304600000

H	1.0621150000	5.1336090000	-0.4014270000
C	3.1208480000	-2.3917370000	-0.1535780000
N	3.7891890000	-3.3460620000	-0.2071570000

22. 4,6 di-*tert*-butyl-2-phenylphenol, *syn* conformer S_0 (B3LYP/6-31+G(d,p)/scrf=acetonitrile)

C	1.2148130000	1.3367830000	0.0509810000
C	-0.1845410000	1.3061740000	0.0427670000
C	-0.8988430000	0.1031030000	0.0105100000
C	-0.1894570000	-1.1156880000	-0.0377300000
C	1.2217920000	-1.1411890000	-0.0315060000
C	1.8772710000	0.1012480000	0.0182610000
H	-0.7546130000	2.2299110000	0.0777410000
H	2.9570130000	0.0994220000	0.0275670000
C	-2.3930040000	0.1250700000	0.0065470000
C	-3.1353740000	-0.4895130000	1.0331430000
C	-3.0927090000	0.7875060000	-1.0185120000
C	-4.5332380000	-0.4450810000	1.0316380000
H	-2.6156620000	-0.9815870000	1.8511510000
C	-4.4887610000	0.8362370000	-1.0171810000
H	-2.5354880000	1.2613940000	-1.8214990000
C	-5.2141950000	0.2172970000	0.0064100000
H	-5.0865810000	-0.9200140000	1.8365790000
H	-5.0096860000	1.3526950000	-1.8183020000
H	-6.2995720000	0.2529790000	0.0056140000
O	-0.8699790000	-2.3098710000	-0.1178710000
H	-1.8229490000	-2.1345450000	-0.1544310000
C	1.9594950000	2.6864970000	0.1008700000
C	1.5733830000	3.5366870000	-1.1344840000
C	1.5618350000	3.4516350000	1.3872210000
C	3.4910200000	2.5140360000	0.1019650000
H	1.8588230000	3.0287620000	-2.0625330000
H	0.4970120000	3.7309130000	-1.1736090000
H	2.0869340000	4.5048900000	-1.1049950000
H	1.8329990000	2.8795690000	2.2816000000
H	2.0804190000	4.4165310000	1.4302940000
H	0.4860420000	3.6490630000	1.4266400000
H	3.9686900000	3.4989760000	0.1371170000
H	3.8381720000	1.9471910000	0.9726620000
H	3.8459390000	2.0070040000	-0.8018340000
C	2.0175910000	-2.4664640000	-0.0875080000
C	1.6642820000	-3.3543990000	1.1326990000
C	1.7004880000	-3.2236810000	-1.4023600000
C	3.5427000000	-2.2311900000	-0.0527670000
H	1.9280220000	-2.8464250000	2.0675360000
H	0.6016140000	-3.6003940000	1.1621810000
H	2.2327860000	-4.2909450000	1.0879980000
H	1.9812680000	-2.6189230000	-2.2723250000
H	2.2756550000	-4.1563070000	-1.4417940000
H	0.6407460000	-3.4707180000	-1.4825150000
H	4.0515460000	-3.2001690000	-0.0875400000
H	3.8912810000	-1.6460270000	-0.9104620000

H	3.8621260000	-1.7246880000	0.8643340000

23. 4,6 di-*tert*-butyl-2-phenylphenol, *anti* conformer S_0 (B3LYP/6-31+G(d,p)/scrf=acetonitrile)

C	1.1432820000	1.3709190000	0.0560350000
C	-0.2533420000	1.2722590000	0.0484000000
C	-0.9162940000	0.0409960000	0.0010240000
C	-0.1472870000	-1.1420010000	-0.0520460000
C	1.2649470000	-1.1016080000	-0.0398050000
C	1.8634450000	0.1708750000	0.0157240000
H	-0.8629910000	2.1693680000	0.0965530000
H	2.9418160000	0.2209780000	0.0273180000
C	-2.4086200000	0.0167460000	-0.0058830000
C	-3.1424300000	-0.7605000000	0.9087770000
C	-3.1207140000	0.8255480000	-0.9097150000
C	-4.5384890000	-0.7264860000	0.9203740000
H	-2.6153490000	-1.3890790000	1.6187540000
C	-4.5184800000	0.8586850000	-0.9012760000
H	-2.5747660000	1.4254030000	-1.6324670000
C	-5.2340480000	0.0823570000	0.0146200000
H	-5.0837880000	-1.3302980000	1.6405030000
H	-5.0455180000	1.4877460000	-1.6132140000
H	-6.3199250000	0.1059450000	0.0230980000
O	-0.8729040000	-2.3099640000	-0.1375430000
H	-0.2859270000	-3.0694410000	-0.2227760000
C	1.8192960000	2.7554760000	0.1133050000
C	1.3979130000	3.5868140000	-1.1236420000
C	1.3761630000	3.4980690000	1.3979510000
C	3.3575000000	2.6603980000	0.1235380000
H	1.7108800000	3.0935330000	-2.0507140000
H	0.3136360000	3.7293320000	-1.1670430000
H	1.8644090000	4.5784230000	-1.0918910000
H	1.6722870000	2.9406630000	2.2936870000
H	1.8439190000	4.4884430000	1.4436210000
H	0.2915330000	3.6399440000	1.4324260000
H	3.7848560000	3.6679140000	0.1657220000
H	3.7268850000	2.1082100000	0.9945320000
H	3.7433910000	2.1757110000	-0.7798720000
C	2.1356840000	-2.3839590000	-0.0902640000
C	1.8474370000	-3.2897560000	1.1377560000
C	1.9011180000	-3.1574980000	-1.4166480000
C	3.6463510000	-2.0637310000	-0.0429830000
H	2.0899830000	-2.7586760000	2.0640690000
H	0.8072090000	-3.6184100000	1.2213930000
H	2.4682300000	-4.1910200000	1.0902440000
H	2.1589780000	-2.5266360000	-2.2735610000
H	2.5378660000	-4.0482800000	-1.4455810000
H	0.8720100000	-3.4975890000	-1.5714140000
H	4.2084140000	-3.0027180000	-0.0723780000
H	3.9674510000	-1.4611330000	-0.8985310000
H	3.9271570000	-1.5402310000	0.8764110000

24. 2-phenylphenol with 3 explicit water molecules (**1-3W)** in S_0 (B3LYP/6-311+G(d,p)/SMD=water)

C	1.1862690000	0.4982470000	-0.0451460000
C	2.4182420000	1.1546070000	-0.0262270000
C	2.4760360000	2.5398620000	0.0907550000
C	1.2969890000	3.2802340000	0.1751020000
C	0.0717290000	2.6196710000	0.1625720000
C	-0.0155950000	1.2217730000	0.0716460000
H	3.3232950000	0.5653280000	-0.1190140000
H	3.4392820000	3.0371110000	0.1048790000
H	1.3300960000	4.3602300000	0.2591480000
H	-0.8467330000	3.1893890000	0.2500520000
O	1.2214950000	-0.8754670000	-0.1702890000
H	0.4378420000	-1.2498850000	-0.6439350000
O	-0.6442900000	-2.1710760000	-1.6853170000
H	-1.5438060000	-2.0385800000	-1.3558640000
H	-0.4855150000	-3.1199130000	-1.5939000000
O	1.9077330000	-2.4541080000	2.1289380000
H	1.6638480000	-1.9069780000	1.3602440000
H	2.7086850000	-2.9137060000	1.8490710000
O	3.5510590000	-2.2303390000	-1.2121980000
H	2.7948270000	-1.7208880000	-0.8685990000
H	4.2007470000	-1.5611410000	-1.4590190000
C	-1.3504640000	0.5613160000	0.1154720000
C	-2.3601810000	0.9386900000	-0.7812670000
C	-1.6366870000	-0.4234300000	1.0729860000
C	-3.6194230000	0.3422060000	-0.7283530000
H	-2.1538200000	1.6957250000	-1.5297210000
C	-2.8964130000	-1.0171730000	1.1277800000
H	-0.8721770000	-0.7194600000	1.7822340000
C	-3.8915420000	-0.6387990000	0.2253460000
H	-4.3861250000	0.6424220000	-1.4340280000
H	-3.1015140000	-1.7723020000	1.8785260000
H	-4.8706690000	-1.1026460000	0.2668610000

25. Anion of 2-phenylphenol with 3 explicit water molecules (**1-3W**) in S_0 (B3LYP/6-311+G(d,p)/SMD=water)

C	1.2702530000	0.3009880000	0.0233780000
C	2.5409660000	0.9260850000	0.0371230000
C	2.6838600000	2.3067070000	0.1157220000
C	1.5559880000	3.1281240000	0.1791090000
C	0.2943830000	2.5354910000	0.1716230000
C	0.1197490000	1.1453750000	0.1070880000
H	3.4187440000	0.2907050000	-0.0250790000
H	3.6781140000	2.7423550000	0.1245430000
H	1.6552370000	4.2058000000	0.2412260000
H	-0.5877210000	3.1649740000	0.2357190000
O	1.1763740000	-1.0185490000	-0.0873020000
O	-0.4729090000	-2.1253230000	-1.9250750000
H	-1.3489040000	-1.7413300000	-1.7985180000

H	0.0879210000	-1.6875450000	-1.2334240000
O	1.4085590000	-2.4532290000	2.1923430000
H	1.3003720000	-1.9118790000	1.3690720000
H	0.5282400000	-2.4786110000	2.5850600000
O	3.2024840000	-2.3721020000	-1.2544410000
H	2.4945260000	-1.8389810000	-0.8042190000
H	4.0306840000	-2.0163550000	-0.9119250000
C	-1.2624290000	0.5903160000	0.1109800000
C	-2.2263550000	1.0796150000	-0.7852740000
C	-1.6551210000	-0.4058080000	1.0198530000
C	-3.5330620000	0.5911510000	-0.7773050000
H	-1.9457520000	1.8419910000	-1.5038950000
C	-2.9606850000	-0.8932020000	1.0311170000
H	-0.9351750000	-0.7940320000	1.7305150000
C	-3.9064470000	-0.3992030000	0.1308440000
H	-4.2567380000	0.9822170000	-1.4844290000
H	-3.2410340000	-1.6581760000	1.7472820000
H	-4.9211800000	-0.7813580000	0.1383090000

26. 4-OMe-2-phenylphenol with 3 explicit water molecules (**2-3W)** in S_0 (B3LYP/6-311+G(d,p)/SMD=water)

C	-0.5120750000	0.8224820000	-0.0812150000
C	-1.7959870000	1.3558000000	-0.0980810000
C	-2.9224970000	0.5364950000	-0.0218550000
C	-2.7513540000	-0.8455910000	0.0549680000
C	-1.4628530000	-1.3829620000	0.0777150000
C	-0.3260780000	-0.5701920000	0.0293840000
H	-1.9150750000	2.4297440000	-0.1837870000
H	-3.9061060000	0.9853160000	-0.0352850000
H	-1.3481720000	-2.4575160000	0.1618360000
O	0.5439600000	1.7163410000	-0.1601580000
H	1.3055800000	1.3681180000	-0.6860660000
O	2.6536790000	1.0625750000	-1.7725150000
H	3.0862890000	0.2572030000	-1.4567810000
H	3.3232340000	1.7535500000	-1.6809960000
O	1.3973500000	3.0674920000	2.2051680000
H	1.1062240000	2.5934240000	1.4038970000
H	1.1189270000	3.9794530000	2.0580070000
O	0.1189210000	4.4081490000	-1.0982490000
H	0.2069590000	3.4872510000	-0.7905290000
H	-0.7898720000	4.4702580000	-1.4161090000
C	1.0233290000	-1.1983990000	0.1005910000
C	1.3716850000	-2.2349950000	-0.7770350000
C	1.9612880000	-0.7873170000	1.0596370000
C	2.6252780000	-2.8409220000	-0.7022890000
H	0.6607820000	-2.5602880000	-1.5283680000
C	3.2130860000	-1.3950040000	1.1355970000
H	1.7066680000	0.0042370000	1.7547780000
C	3.5510980000	-2.4220460000	0.2533210000
H	2.8784170000	-3.6377750000	-1.3928180000
H	3.9228820000	-1.0684770000	1.8875770000

H	4.5259910000	-2.8928980000	0.3119060000
O	-3.7846420000	-1.7552920000	0.1217850000
C	-5.1255270000	-1.2498910000	0.1156550000
H	-5.7712660000	-2.1248130000	0.1704180000
H	-5.3077110000	-0.6068780000	0.9812740000
H	-5.3342460000	-0.6987840000	-0.8055620000

27. Anion of **2-3W** in S_0 (B3LYP/6-311+G(d,p)/SMD=water)

C	-0.4694470000	0.9193360000	0.0054280000
C	-1.7916370000	1.4062760000	-0.0040070000
C	-2.9083760000	0.5690950000	0.0252780000
C	-2.7244950000	-0.8120700000	0.0598780000
C	-1.4286780000	-1.3272630000	0.0770990000
C	-0.3012360000	-0.4982540000	0.0627880000
H	-1.9388850000	2.4805620000	-0.0447820000
H	-3.8985470000	1.0060630000	0.0179970000
H	-1.3005050000	-2.4036980000	0.1213550000
O	0.5645410000	1.7604790000	-0.0617760000
O	2.5260240000	1.3380820000	-1.8645140000
H	2.8480970000	0.4379650000	-1.7345320000
H	1.8058520000	1.4411540000	-1.1871910000
O	1.3573390000	2.8835810000	2.2492800000
H	1.0699810000	2.4413060000	1.4070330000
H	1.8889320000	2.2208020000	2.7052430000
O	0.1986430000	4.1360140000	-1.2739670000
H	0.2804720000	3.2626310000	-0.8033250000
H	-0.5288260000	4.5873350000	-0.8305710000
C	1.0479470000	-1.1284460000	0.0910000000
C	1.3755160000	-2.1496080000	-0.8148960000
C	2.0161930000	-0.7465130000	1.0336990000
C	2.6262900000	-2.7665470000	-0.7831830000
H	0.6475080000	-2.4547360000	-1.5586110000
C	3.2647690000	-1.3645080000	1.0690250000
H	1.7849790000	0.0315370000	1.7514310000
C	3.5775520000	-2.3757210000	0.1588750000
H	2.8570920000	-3.5494580000	-1.4975320000
H	3.9941040000	-1.0577980000	1.8110240000
H	4.5505120000	-2.8537120000	0.1851220000
O	-3.7540120000	-1.7443120000	0.0895270000
C	-5.0954750000	-1.2501400000	0.0747410000
H	-5.2967910000	-0.6757170000	-0.8346760000
H	-5.7381900000	-2.1293680000	0.0966660000
H	-5.2996060000	-0.6294480000	0.9526020000

28. 4-COOMe-2-phenylphenol with 3 explicit water molecules (**4-3W)** in S_0 (B3LYP/6-311+G(d,p)/SMD=water)

C	0.2550910000	1.0225740000	-0.1133050000
C	-0.8534880000	1.8757260000	-0.1211500000
C	-2.1389260000	1.3637970000	-0.0630170000
C	-2.3369110000	-0.0228790000	-0.0056980000

C	-1.2218180000	-0.8668780000	0.0166240000
C	0.0839480000	-0.3741430000	-0.0163390000
H	-0.6859360000	2.9438680000	-0.1914680000
H	-2.9840980000	2.0389410000	-0.0747050000
H	-1.3726130000	-1.9371320000	0.0855430000
O	1.4813310000	1.6214520000	-0.1924270000
H	2.1943470000	1.0539190000	-0.5841300000
O	3.5813100000	0.4908500000	-1.4781660000
H	3.7458530000	-0.4266960000	-1.2203960000
H	4.3776940000	0.9682630000	-1.2096930000
O	2.4649340000	2.9116940000	2.2118650000
H	2.1278080000	2.4783570000	1.4084090000
H	2.4019240000	3.8548770000	2.0182760000
O	1.8123460000	4.3381780000	-1.1763640000
H	1.6468610000	3.4317690000	-0.8627180000
H	0.9687880000	4.6226320000	-1.5483960000
C	1.2309770000	-1.3217850000	0.0700730000
C	1.3674910000	-2.3589510000	-0.8625910000
C	2.1743760000	-1.2136040000	1.1021640000
C	2.4261800000	-3.2616990000	-0.7708290000
H	0.6476280000	-2.4513180000	-1.6683610000
C	3.2296270000	-2.1191550000	1.1958320000
H	2.0775340000	-0.4230940000	1.8379620000
C	3.3612230000	-3.1438430000	0.2576210000
H	2.5207890000	-4.0548740000	-1.5041640000
H	3.9470140000	-2.0255510000	2.0035300000
H	4.1841990000	-3.8460850000	0.3292490000
C	-3.6856390000	-0.6305190000	0.0445540000
O	-3.9013850000	-1.8337070000	0.0838340000
O	-4.6753210000	0.2787980000	0.0432360000
C	-6.0291870000	-0.2294770000	0.0898910000
H	-6.6655210000	0.6522470000	0.0810510000
H	-6.2293760000	-0.8511830000	-0.7829980000
H	-6.1862670000	-0.8020550000	1.0042060000

29. Anion of **4-3W** in S_0 (B3LYP/6-311+G(d,p)/SMD=water)

C	0.2993570000	1.1199100000	-0.0356880000
C	-0.8733540000	1.9245280000	-0.0583170000
C	-2.1412290000	1.3791470000	-0.0278440000
C	-2.3144990000	-0.0162750000	0.0254870000
C	-1.1676640000	-0.8268780000	0.0571480000
C	0.1203750000	-0.3036200000	0.0408170000
H	-0.7464040000	3.0005790000	-0.1115230000
H	-3.0041130000	2.0331370000	-0.0483800000
H	-1.2942580000	-1.9020420000	0.1122030000
O	1.4844100000	1.6728070000	-0.1040400000
O	3.3495160000	0.7595730000	-1.8890380000
H	3.3938910000	-0.1998900000	-1.7955910000
H	2.6727040000	1.0352430000	-1.2249850000
O	2.5971490000	2.5768240000	2.2380640000
H	2.1968590000	2.2297190000	1.4073830000

H	2.9534950000	1.7966880000	2.6791830000
O	1.7276530000	4.1974350000	-1.1096140000
H	1.5912170000	3.2928800000	-0.7315080000
H	0.9175920000	4.6744350000	-0.8943470000
C	1.2853010000	-1.2311320000	0.0837350000
C	1.3863960000	-2.2874970000	-0.8343100000
C	2.2927080000	-1.0965460000	1.0520980000
C	2.4587060000	-3.1789190000	-0.7889810000
H	0.6245430000	-2.4042620000	-1.5974450000
C	3.3623190000	-1.9882300000	1.1007960000
H	2.2328710000	-0.2948500000	1.7789000000
C	3.4522630000	-3.0322810000	0.1785620000
H	2.5181160000	-3.9846620000	-1.5126460000
H	4.1256480000	-1.8693480000	1.8622180000
H	4.2871490000	-3.7232770000	0.2146000000
C	-3.6353200000	-0.6517820000	0.0585800000
O	-3.8346670000	-1.8627090000	0.1065660000
O	-4.6582980000	0.2330420000	0.0310390000
C	-5.9948090000	-0.3133530000	0.0606580000
H	-6.6576650000	0.5486620000	0.0314620000
H	-6.1661710000	-0.9503110000	-0.8078050000
H	-6.1548990000	-0.8809160000	0.9780290000

30. 4-CN-2-phenylphenol with 3 explicit water molecules (**5-3W)** in S_0 (B3LYP/6-311+G(d,p)/SMD=water)

C	-0.6297020000	0.8507420000	-0.1018150000
C	-1.8867890000	1.4663980000	-0.0974370000
C	-3.0427730000	0.7105070000	-0.0195630000
C	-2.9466590000	-0.6881570000	0.0471260000
C	-1.6873170000	-1.3024240000	0.0582110000
C	-0.5125770000	-0.5516140000	0.0030430000
H	-1.9379560000	2.5457160000	-0.1743930000
H	-4.0132910000	1.1904480000	-0.0217130000
H	-1.6213860000	-2.3808620000	0.1344410000
O	0.4491390000	1.6802430000	-0.2014020000
H	1.2585830000	1.2637120000	-0.5988380000
O	2.7025810000	0.9983600000	-1.5193030000
H	3.1239810000	0.1842390000	-1.2112740000
H	3.3514670000	1.6932980000	-1.3455360000
O	1.2851050000	3.1029590000	2.1869030000
H	0.9926810000	2.6305310000	1.3881570000
H	1.0337370000	4.0207210000	2.0269520000
O	0.2074370000	4.4248530000	-1.1594040000
H	0.2306230000	3.5031520000	-0.8489770000
H	-0.6945410000	4.5488640000	-1.4788830000
C	0.8051680000	-1.2441080000	0.0724820000
C	1.1380210000	-2.2323660000	-0.8634890000
C	1.7180900000	-0.9432380000	1.0935990000
C	2.3601020000	-2.8991490000	-0.7857350000
H	0.4421950000	-2.4706320000	-1.6602200000
C	2.9377820000	-1.6127980000	1.1721630000

H	1.4694270000	-0.1881050000	1.8306630000
C	3.2638940000	-2.5902510000	0.2308960000
H	2.6058750000	-3.6575420000	-1.5206290000
H	3.6309450000	-1.3737280000	1.9708930000
H	4.2139530000	-3.1091100000	0.2913090000
C	-4.1246140000	-1.4847910000	0.1163130000
N	-5.0851650000	-2.1320750000	0.1727040000

31. Anion of **5-3W** in S_0 (B3LYP/6-311+G(d,p)/SMD=water)

C	-0.5791940000	0.9597590000	-0.0258770000
C	-1.8716290000	1.5554970000	-0.0442770000
C	-3.0292780000	0.8064090000	-0.0066250000
C	-2.9515710000	-0.5984430000	0.0506770000
C	-1.6872950000	-1.2138380000	0.0779760000
C	-0.5101720000	-0.4740850000	0.0521680000
H	-1.9285060000	2.6370430000	-0.0991890000
H	-3.9979560000	1.2926290000	-0.0231200000
H	-1.6324340000	-2.2950150000	0.1363180000
O	0.4916240000	1.7060990000	-0.0962940000
O	2.6017570000	1.2105280000	-1.7748940000
H	2.9287870000	0.3211540000	-1.5932190000
H	1.8436420000	1.3220790000	-1.1532070000
O	1.4072920000	2.8213910000	2.2419010000
H	1.0810290000	2.4018880000	1.4124590000
H	1.8598330000	2.1102190000	2.7107180000
O	0.3773090000	4.1904860000	-1.2252670000
H	0.3593950000	3.3018990000	-0.7915240000
H	-0.3514710000	4.6752500000	-0.8206840000
C	0.7957440000	-1.1885900000	0.0839720000
C	1.0483290000	-2.2420880000	-0.8078760000
C	1.7922420000	-0.8529930000	1.0140460000
C	2.2567000000	-2.9379270000	-0.7738020000
H	0.2962040000	-2.5102650000	-1.5417450000
C	2.9985060000	-1.5496880000	1.0508660000
H	1.6176330000	-0.0491270000	1.7190750000
C	3.2379810000	-2.5934020000	0.1552040000
H	2.4313630000	-3.7453930000	-1.4765120000
H	3.7522850000	-1.2782960000	1.7819670000
H	4.1784850000	-3.1323210000	0.1826560000
C	-4.1298810000	-1.3847520000	0.0920660000
N	-5.0978620000	-2.0278480000	0.1259050000