Electronic Supplementary Material (ESI) for Photochemical & Photobiological Sciences.

Photocyclization of diarylethenes: the effect of imidazole on the oxidative photodegradation process.

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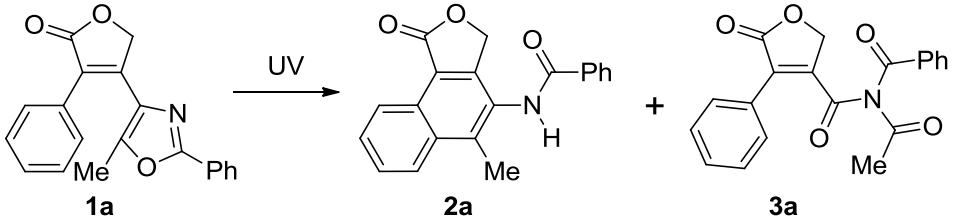
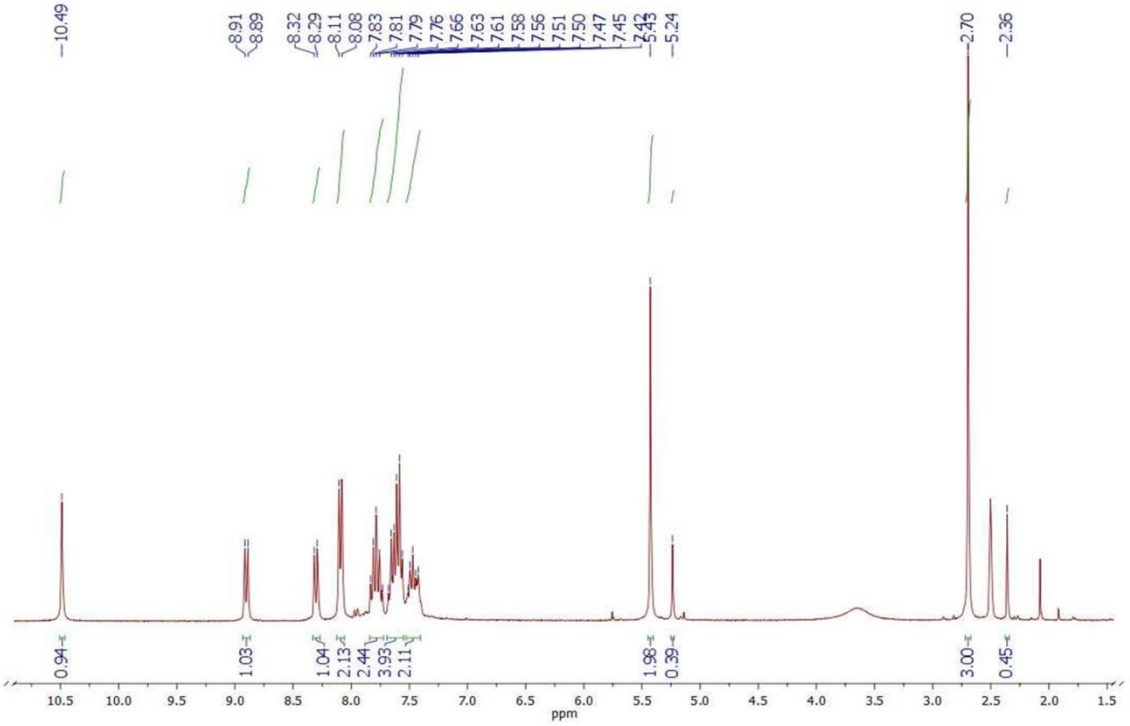
I.1. Diarylethene 1a

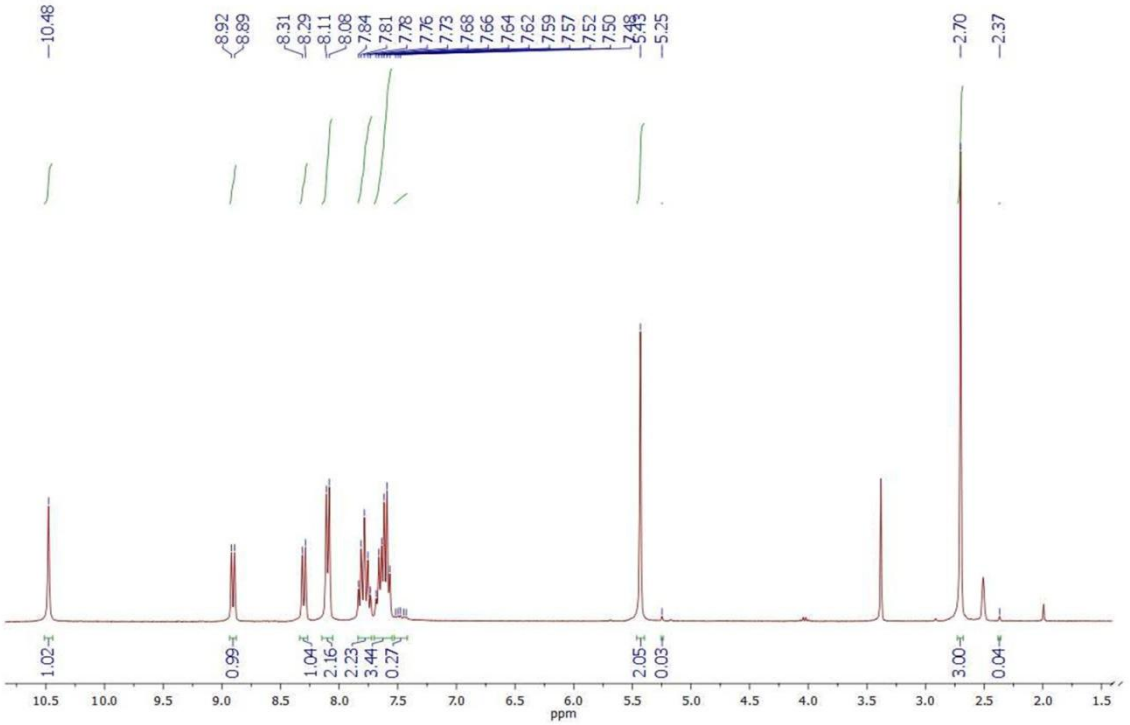


1a **2a** **3a**

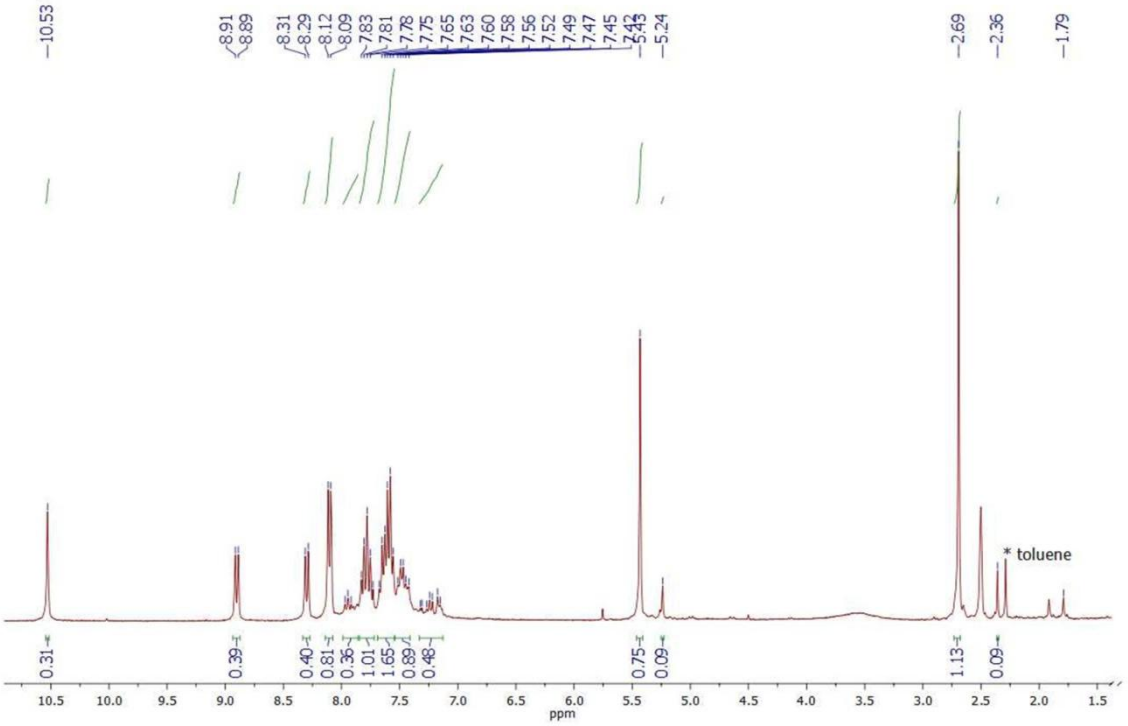
Solvent: MeCN



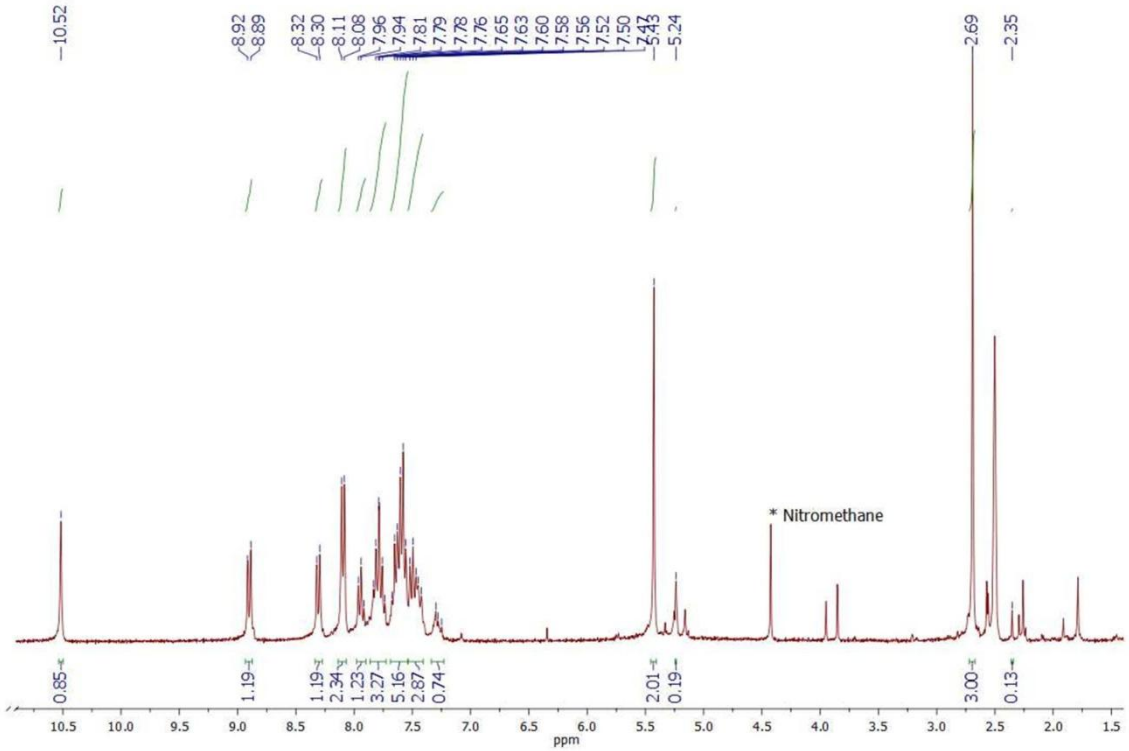
Solvent: DMF



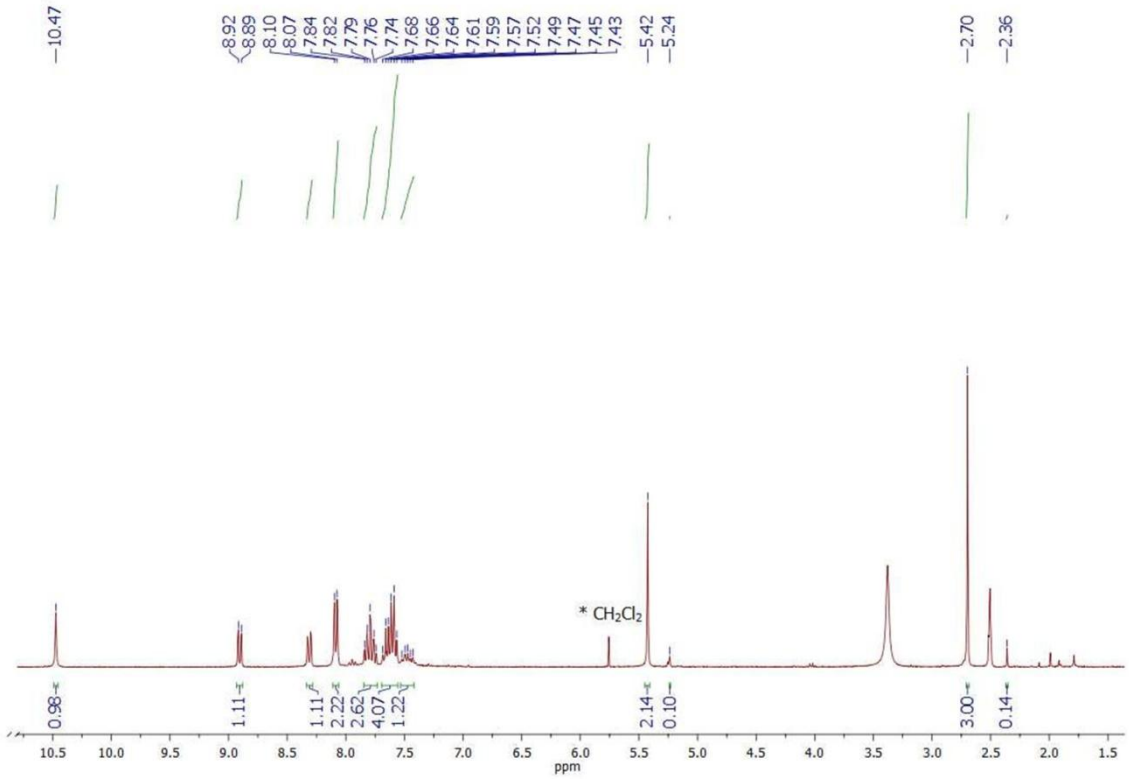
Solvent: toluene



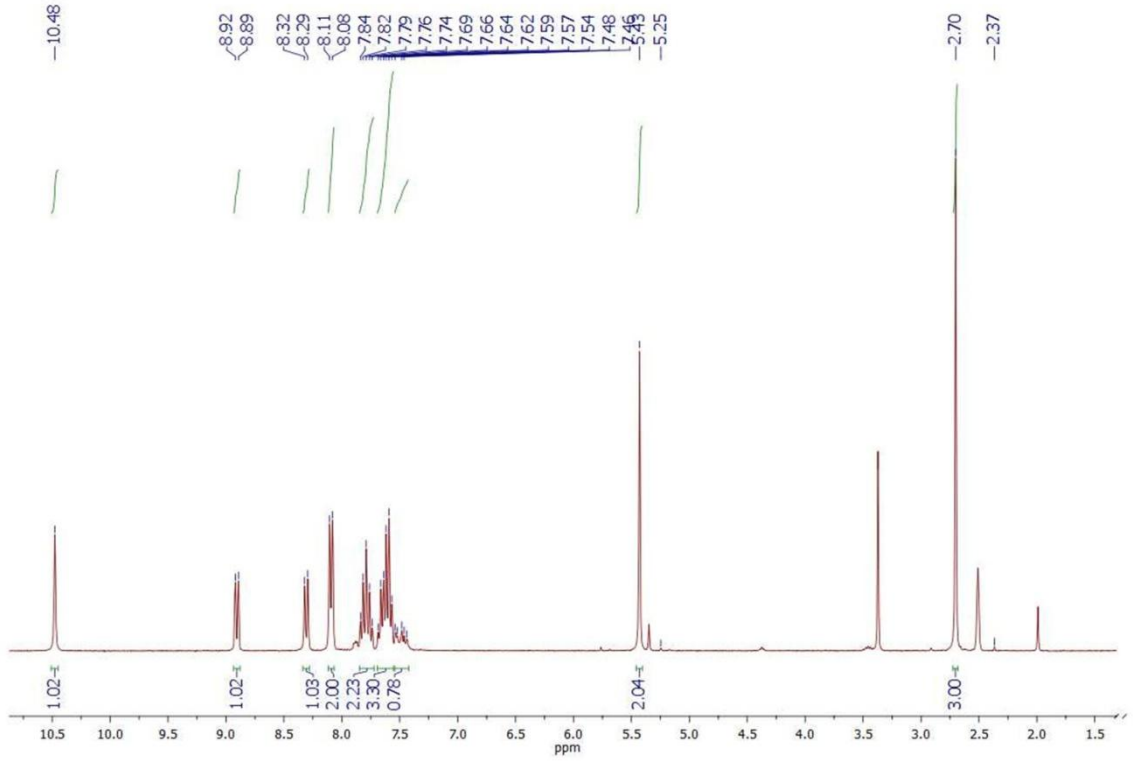
Solvent: CH_3NO_2



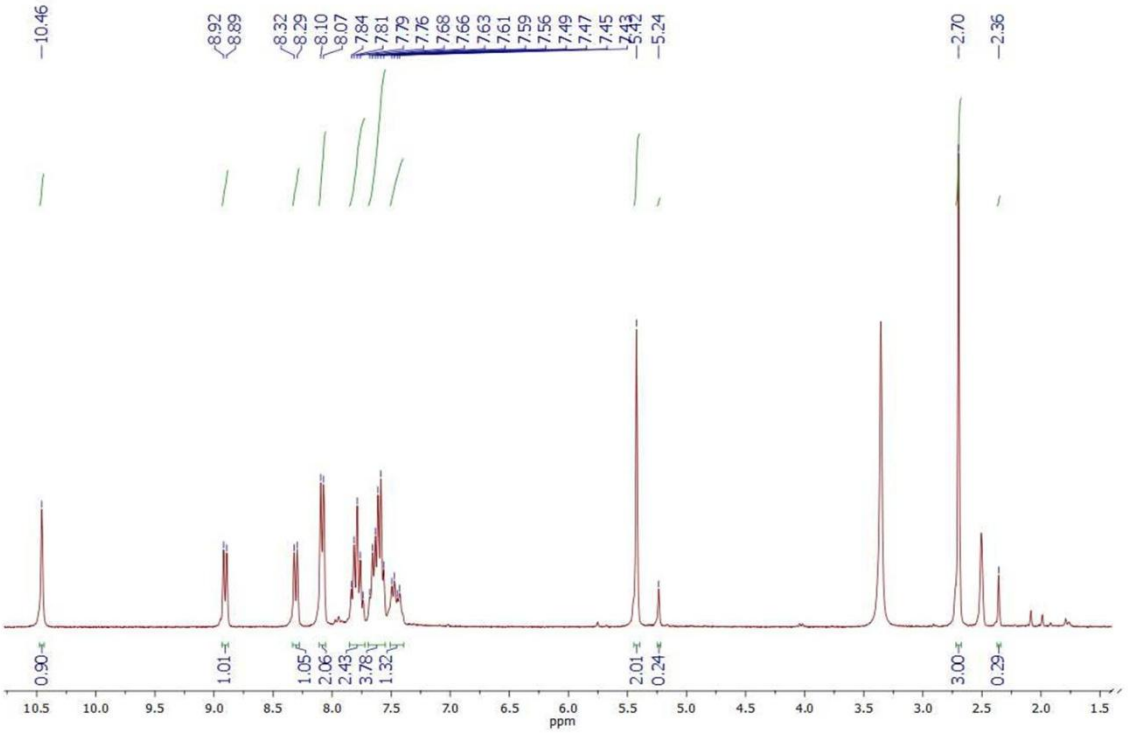
Solvent: CH_2Cl_2



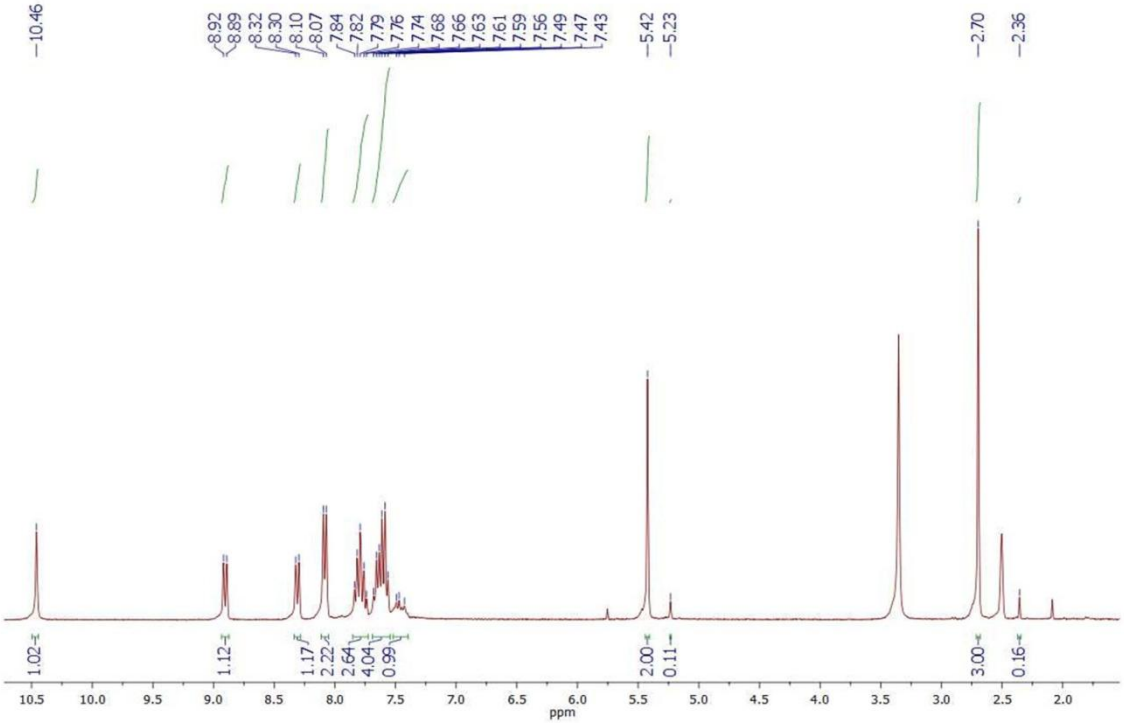
Solvent: EtOH



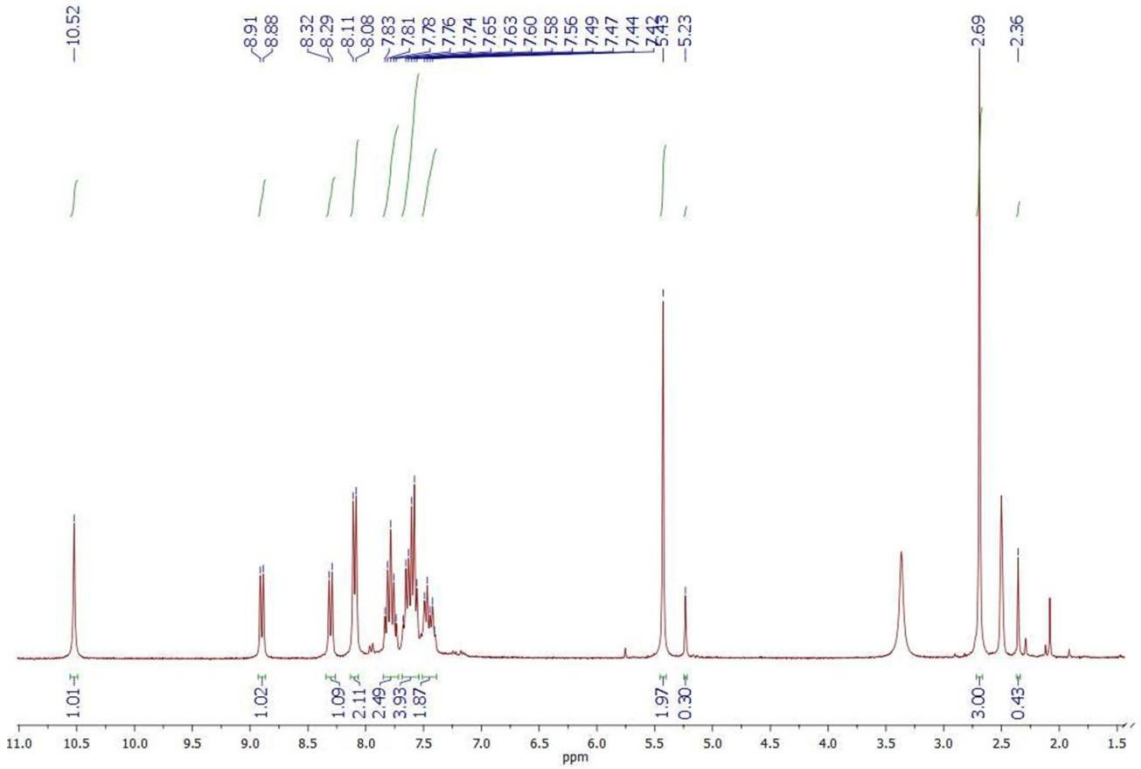
Solvent: EtOAc



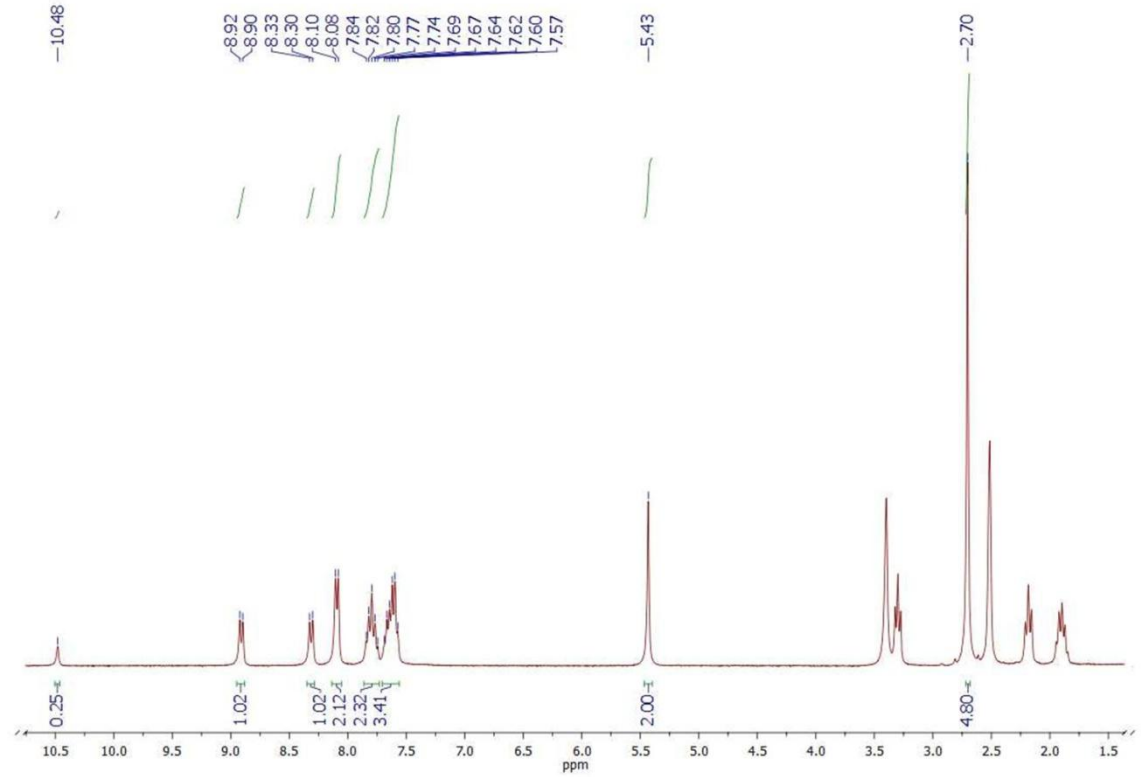
Solvent: $CHCl_3$



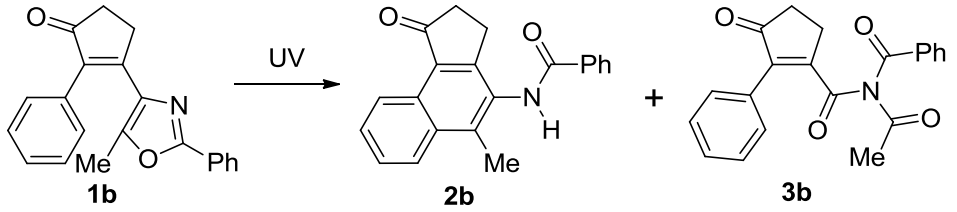
Solvent: acetone



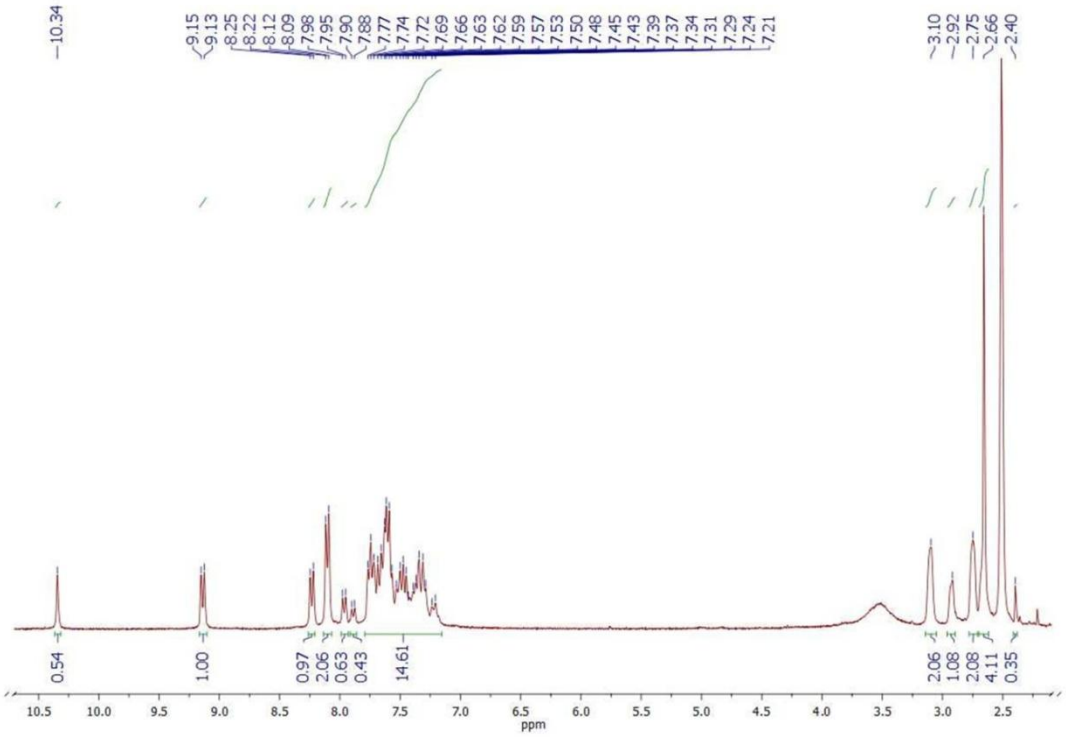
Solvent: *N*-methyl-2-pyrrolidone



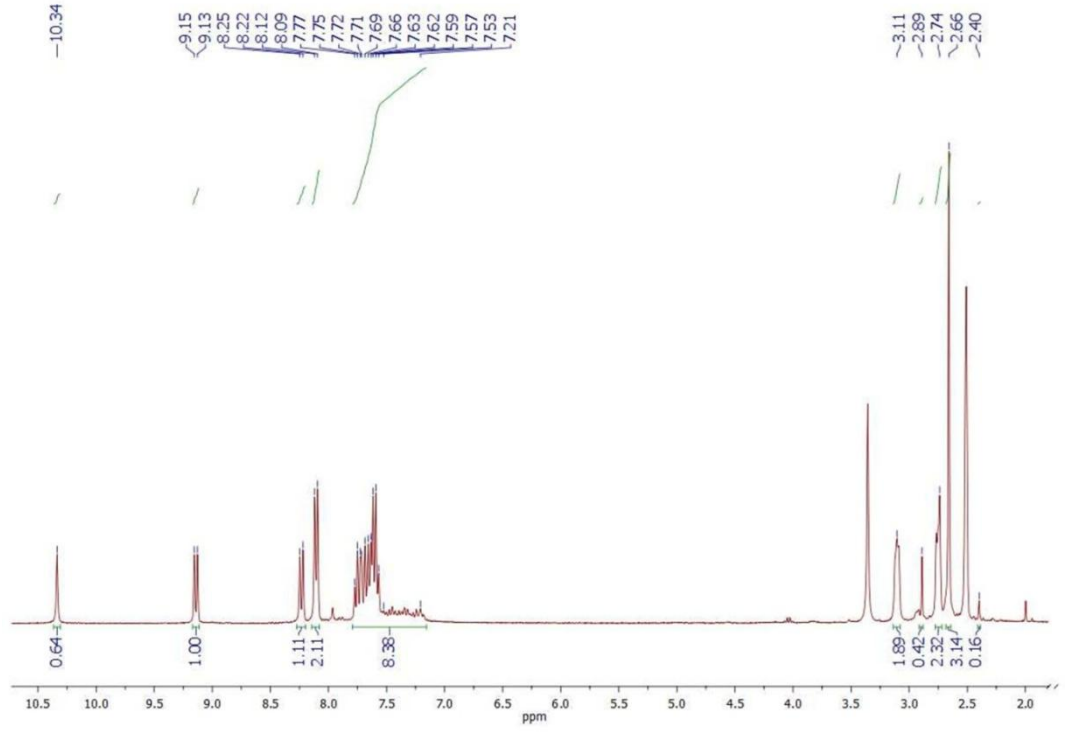
I.2. Diarylethene 1b



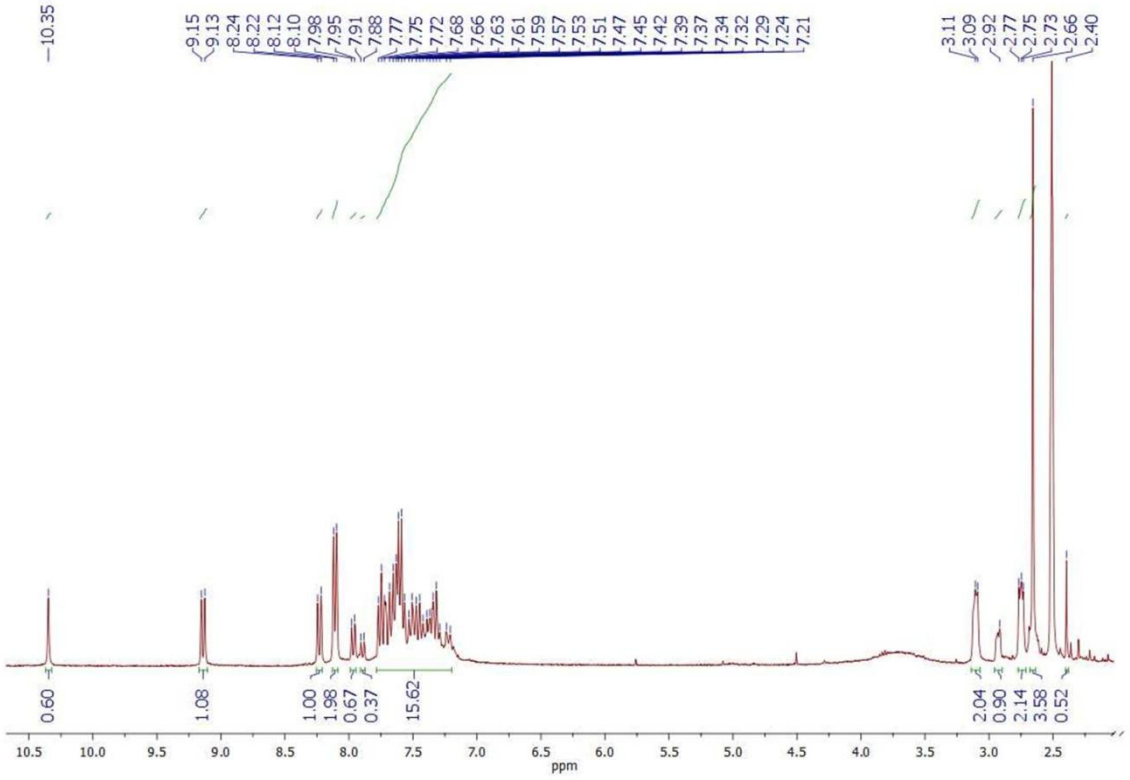
Solvent: MeCN



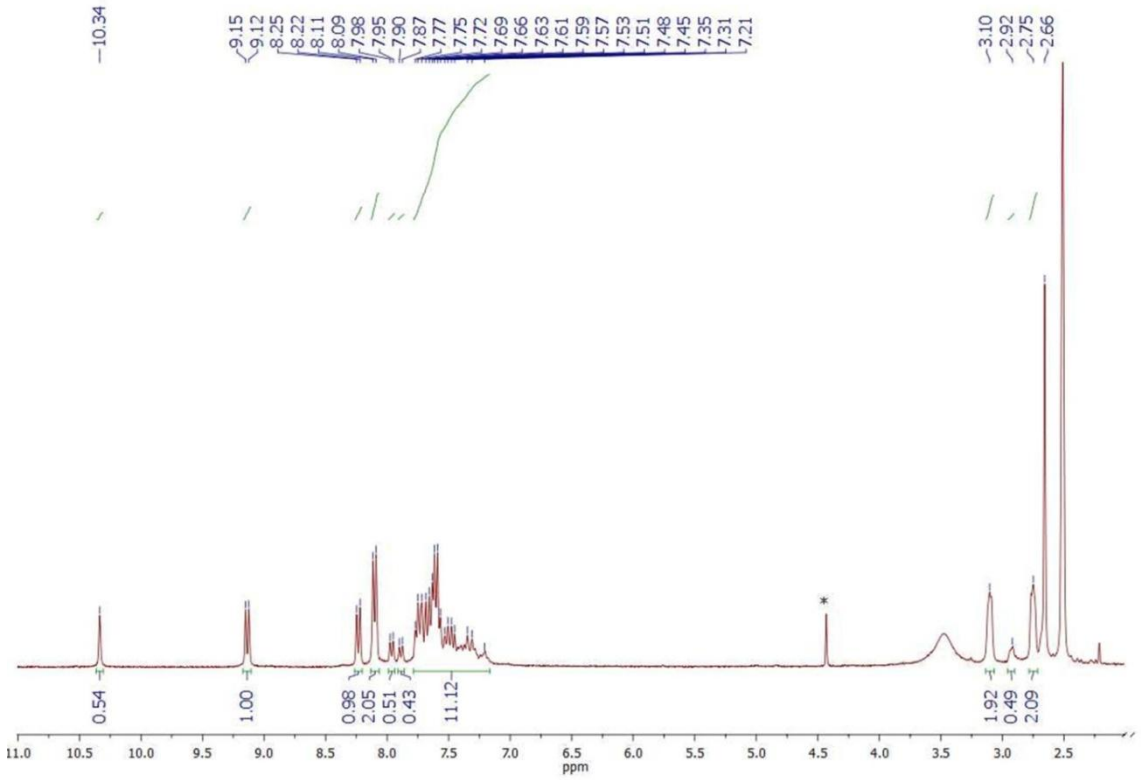
Solvent: DMF



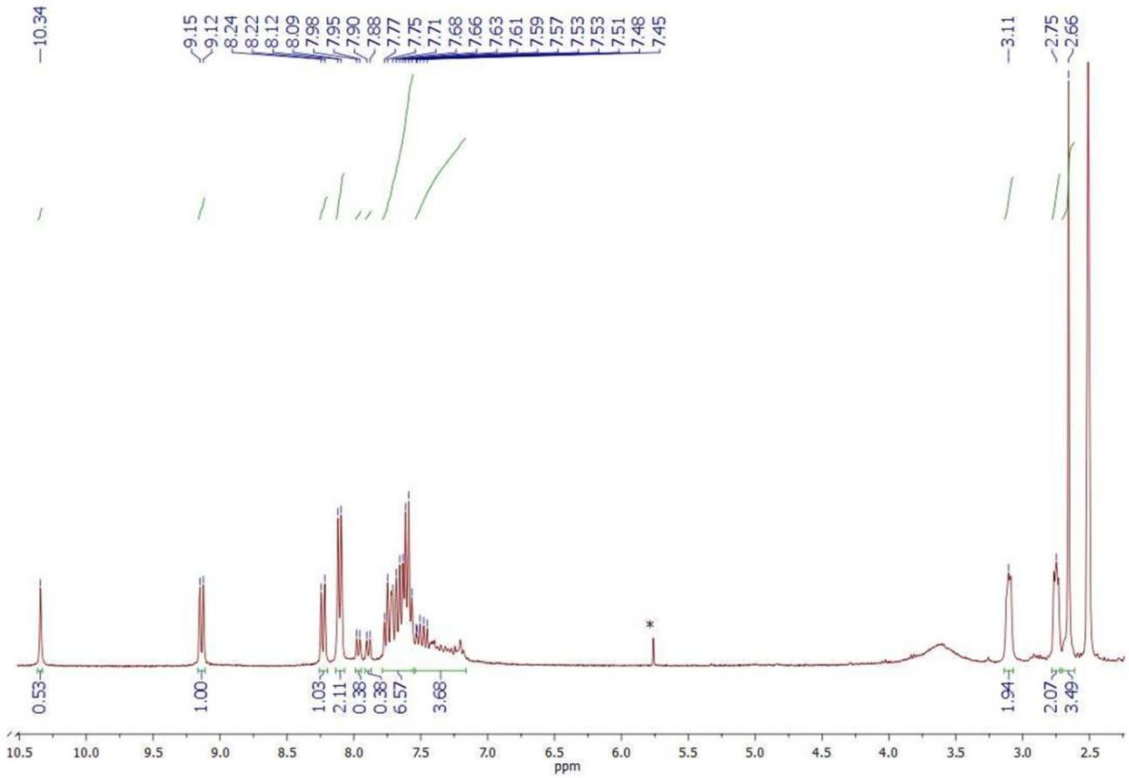
Solvent: toluene



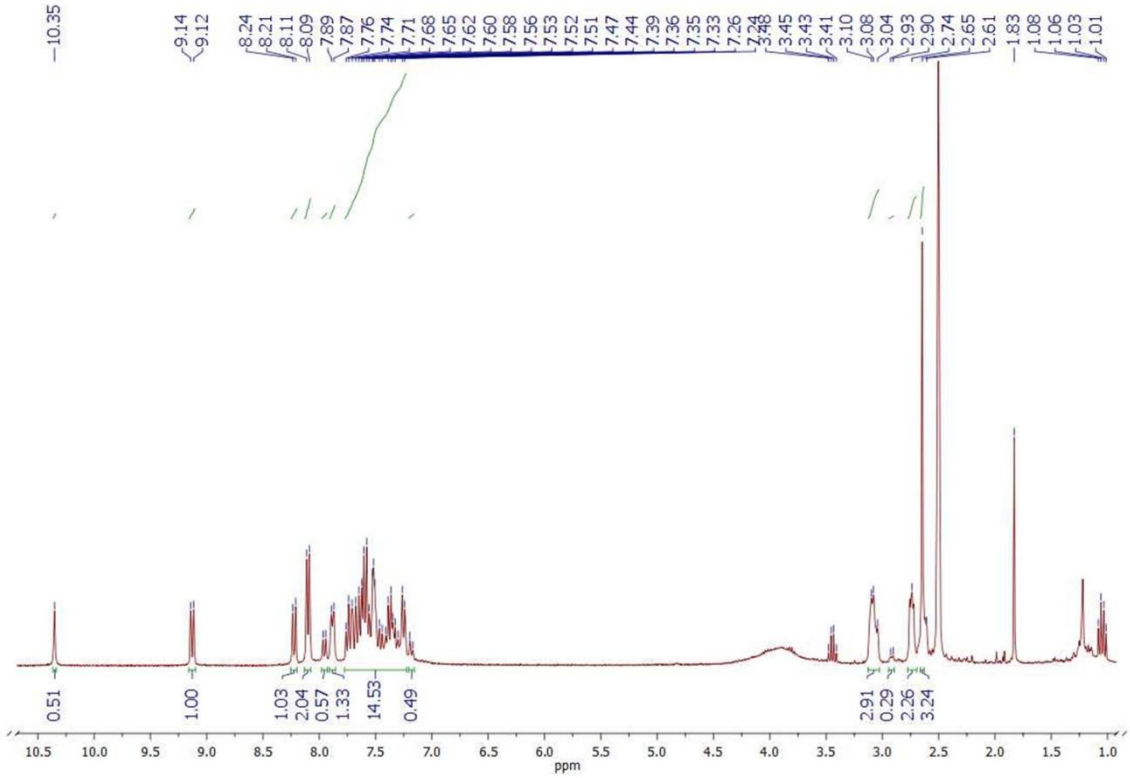
Solvent: $MeNO_2$



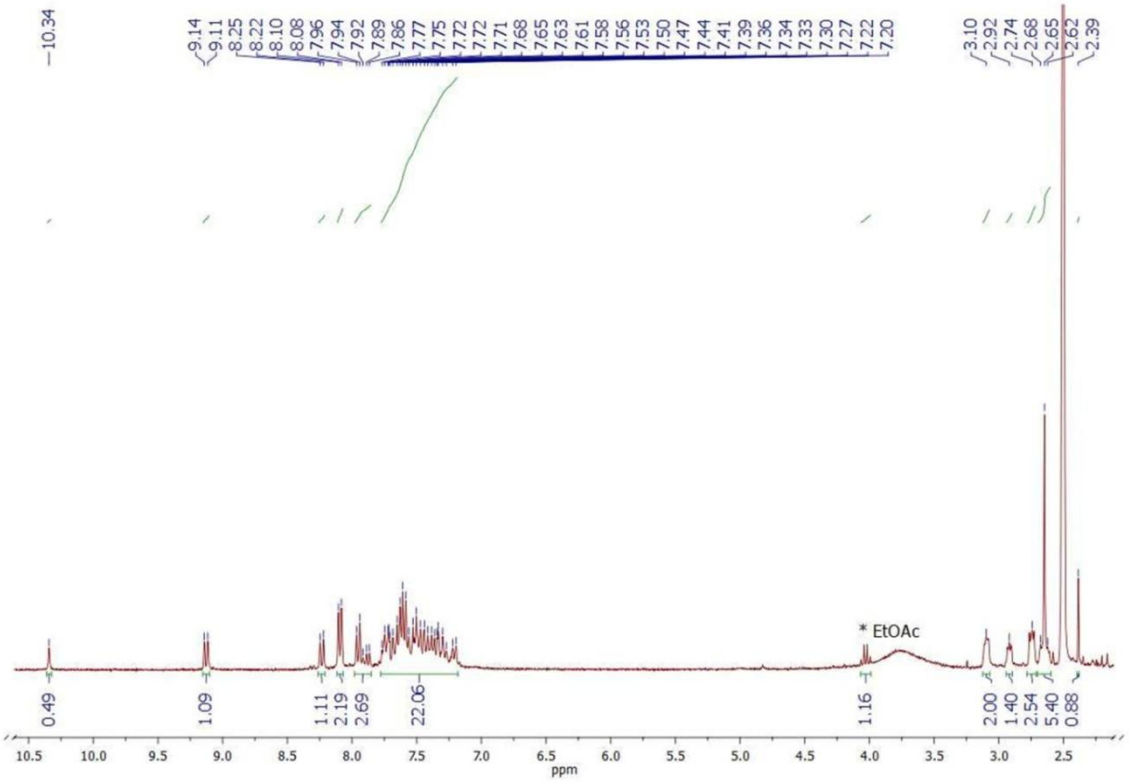
Solvent: CH_2Cl_2



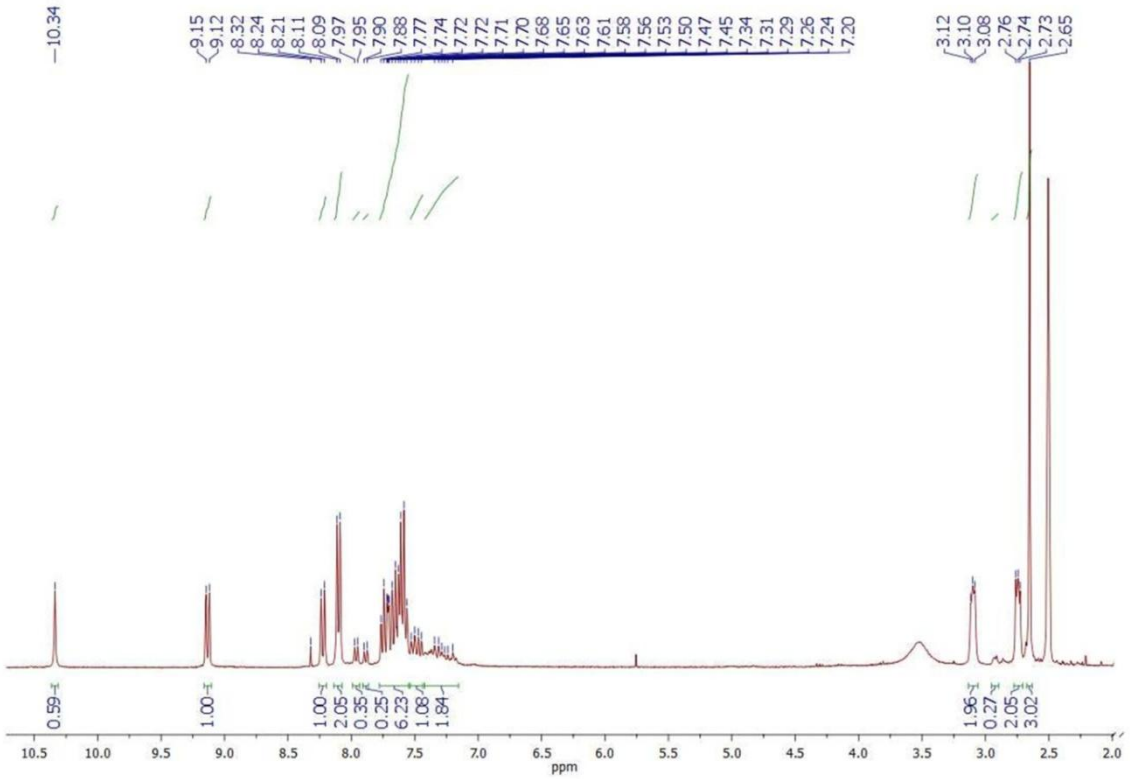
Solvent: EtOH



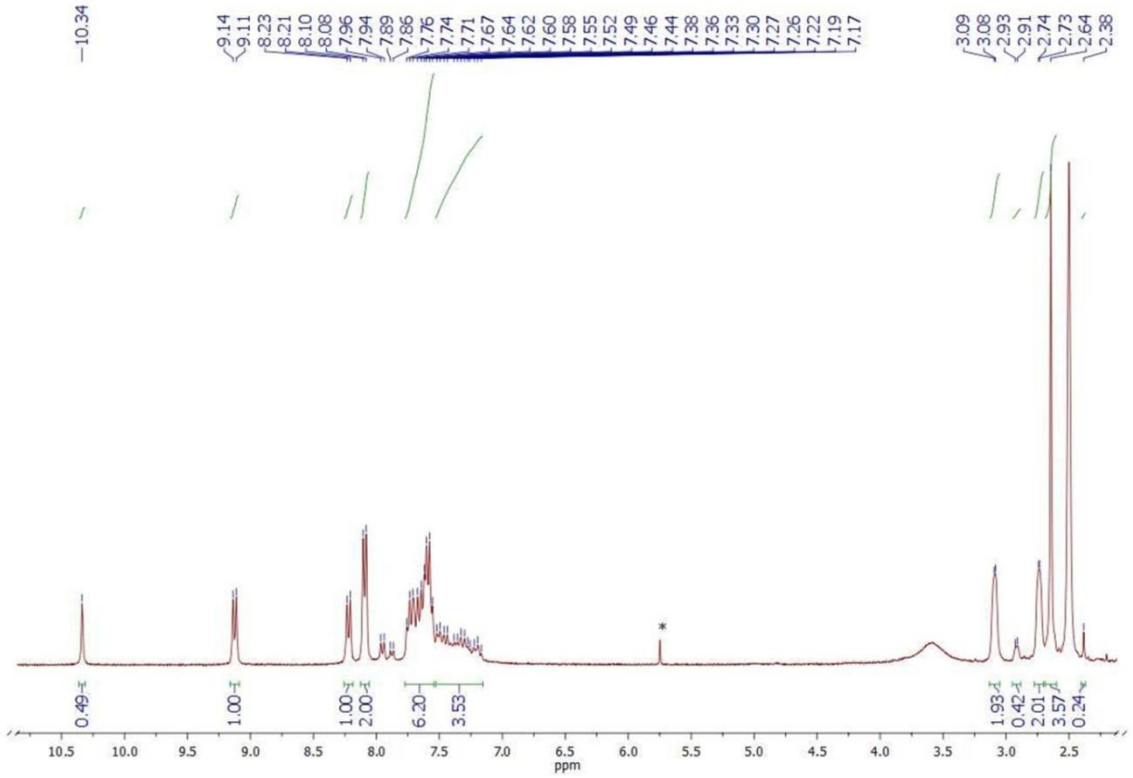
Solvent: EtOAc



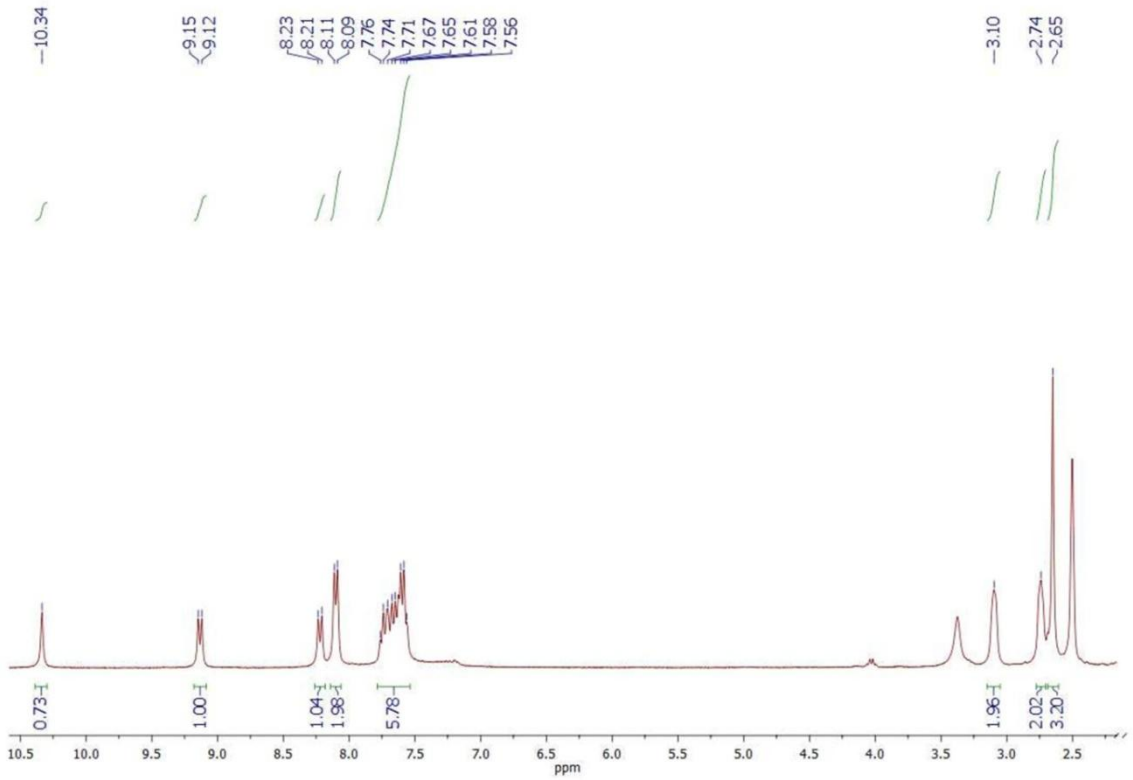
Solvent: $CHCl_3$



Solvent: acetone

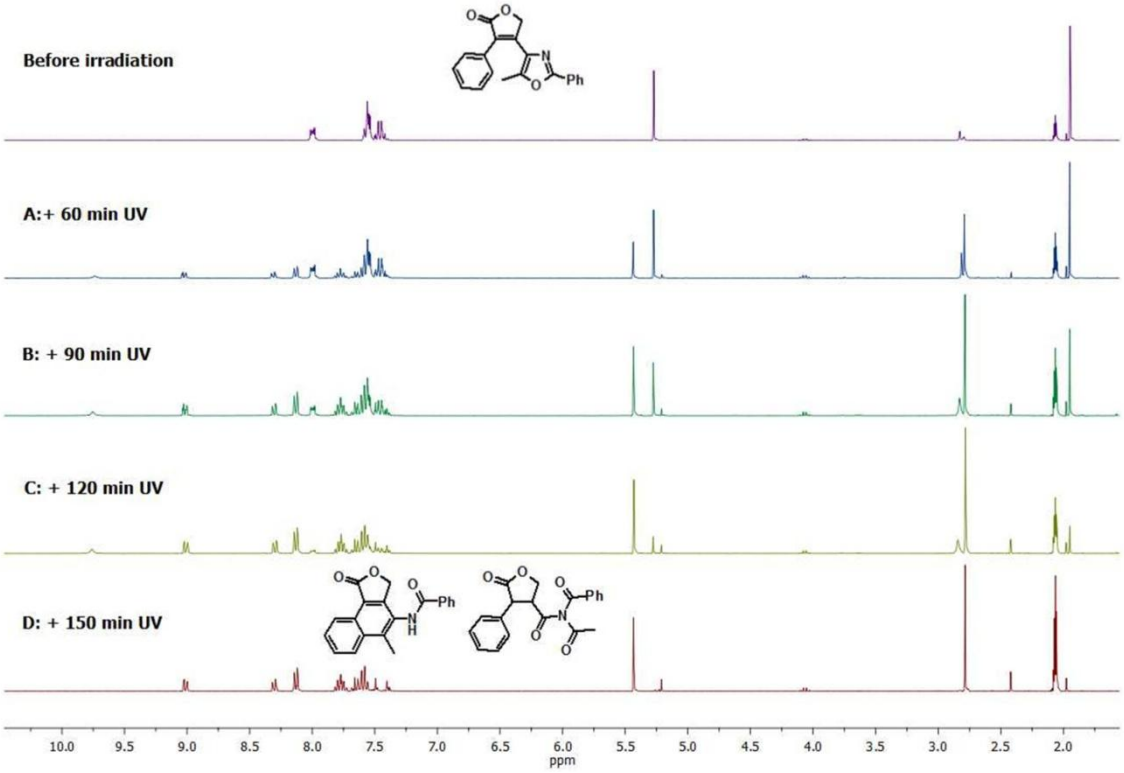


Solvent: *N*-methyl-2-pyrrolidone

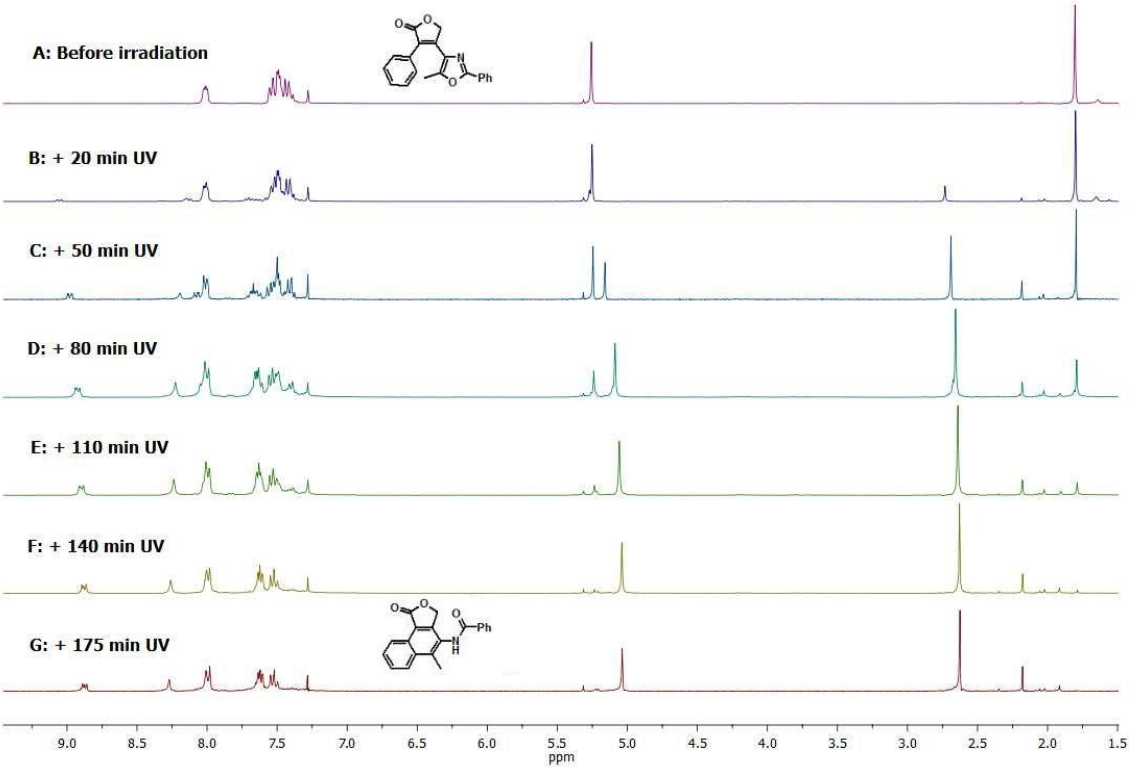


II. NMR monitoring of photoreactions of diarylethene 1a

Acetone-d_6, C = 0.063 M.



Solvent: $CDCl_3$, C = 0.063 M.



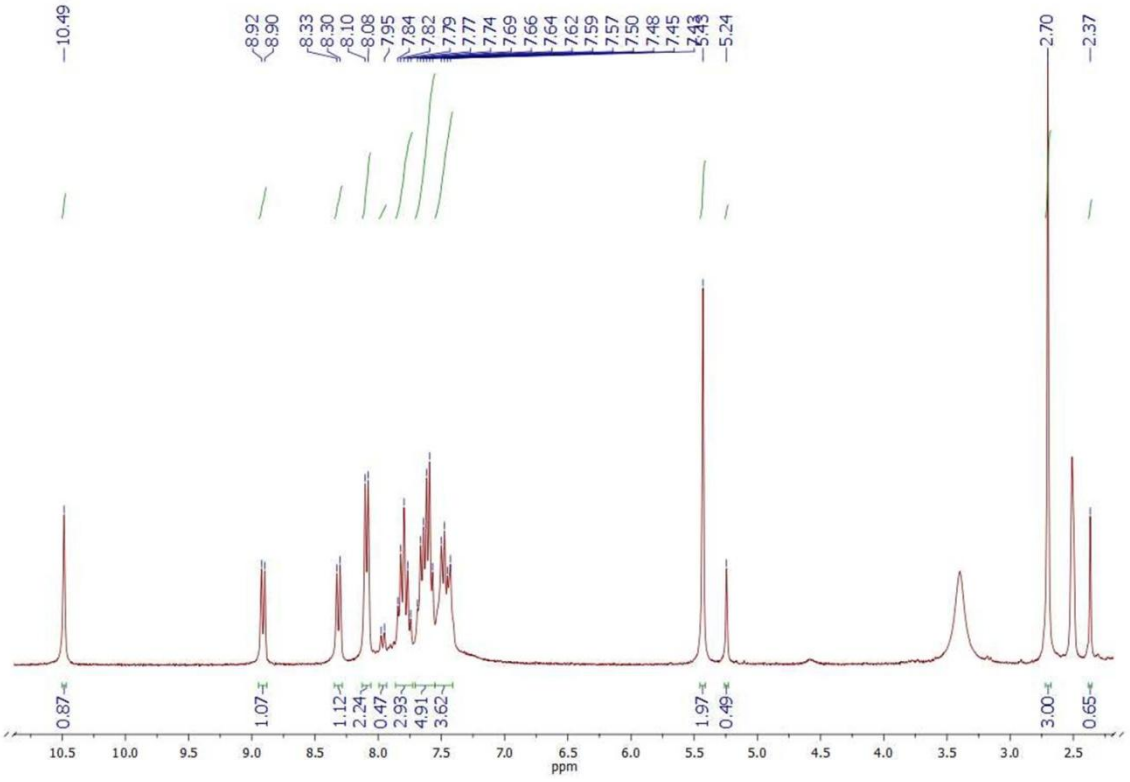
III. Photosensitizer effect (NMR spectra of reaction mixtures)

Table S1. The effect of UV sensitizers on the yields of photoproducts[a]

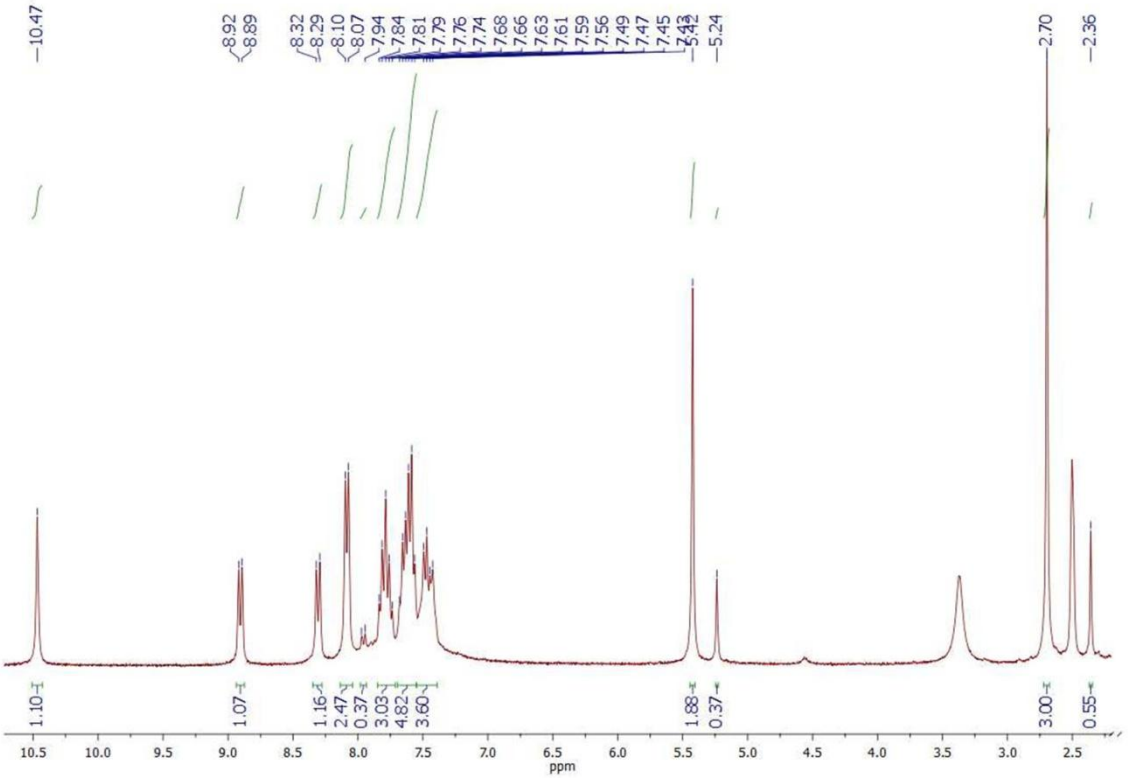
No.	Sensitizers	Time (h)	Yields	
			2a	**3a**
1	Coumarin 30	17	80	20
2	Perylenetetracarboxylic dianhydride	17	83	17
3	Erythrosin B	17	82	18
4	Coumarin 1	17	81	19
5	6-Ethoxy-3-methyl-1*H*-phenalen-1-one	17	80	20
6	Naphthalene[b]	17	69	30
7	Phenanthrene	15	78	22
8	Pyrene	26	81	19
9	4-Dimethylamino-4'-nitrostilbene	17	94	6
10	5,10,15,20-Tetrakis(4-bromophenyl)porphyrin	11	84	16
11	Benzophenone	36	85	15

[a] 0.1 eq. of sensitizer with 1 eq. of diarylethene in 2 ml acetone;
[b] Scaling down does not affect the yield of the by-product.

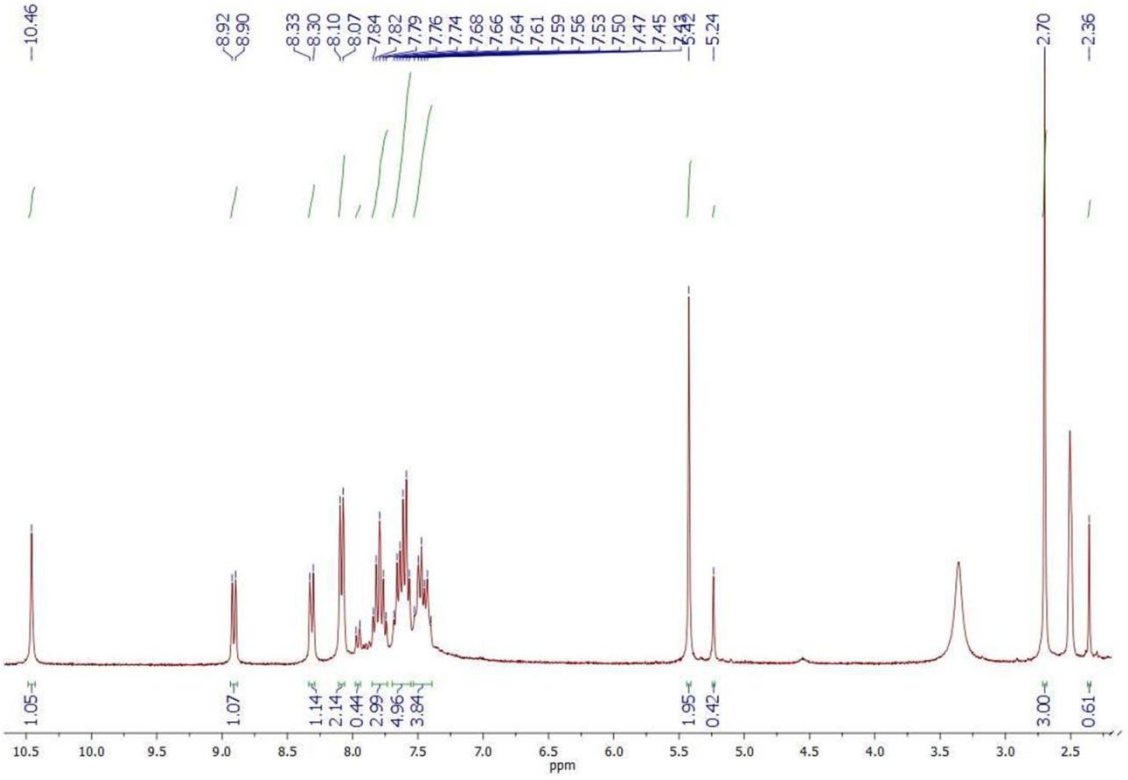
Sensitizer: coumarin 30



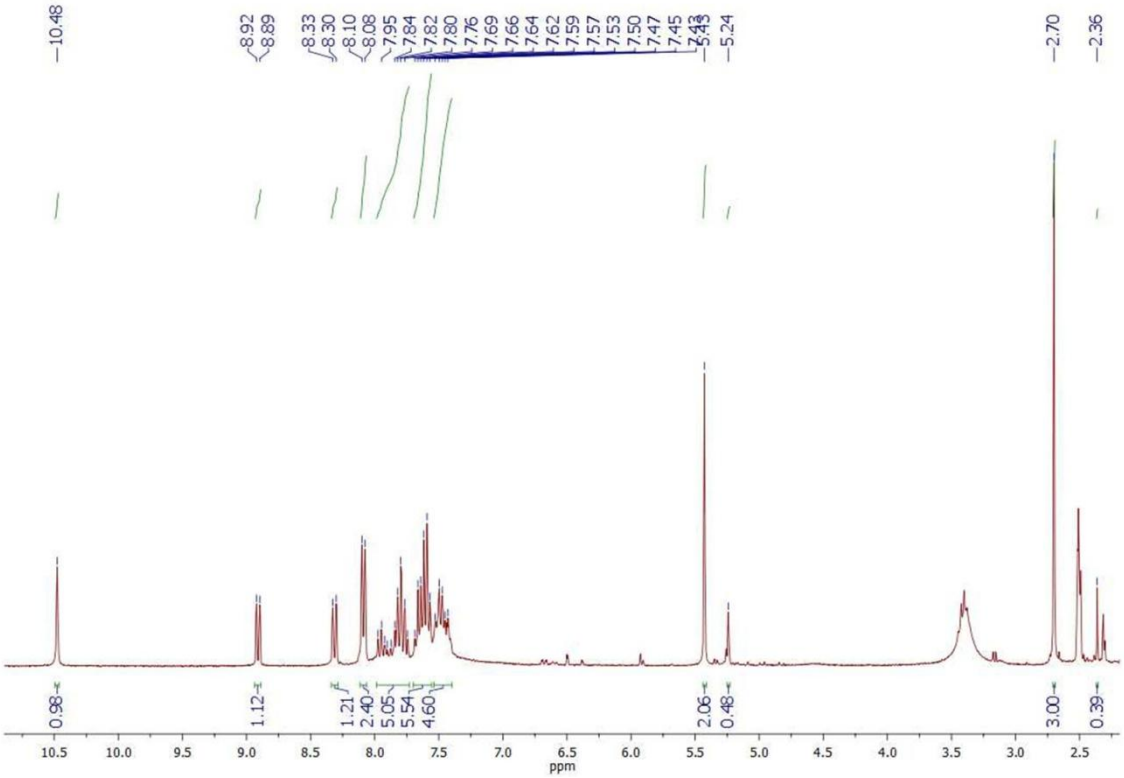
Sensitizer: perylenetetracarboxylic dianhydride



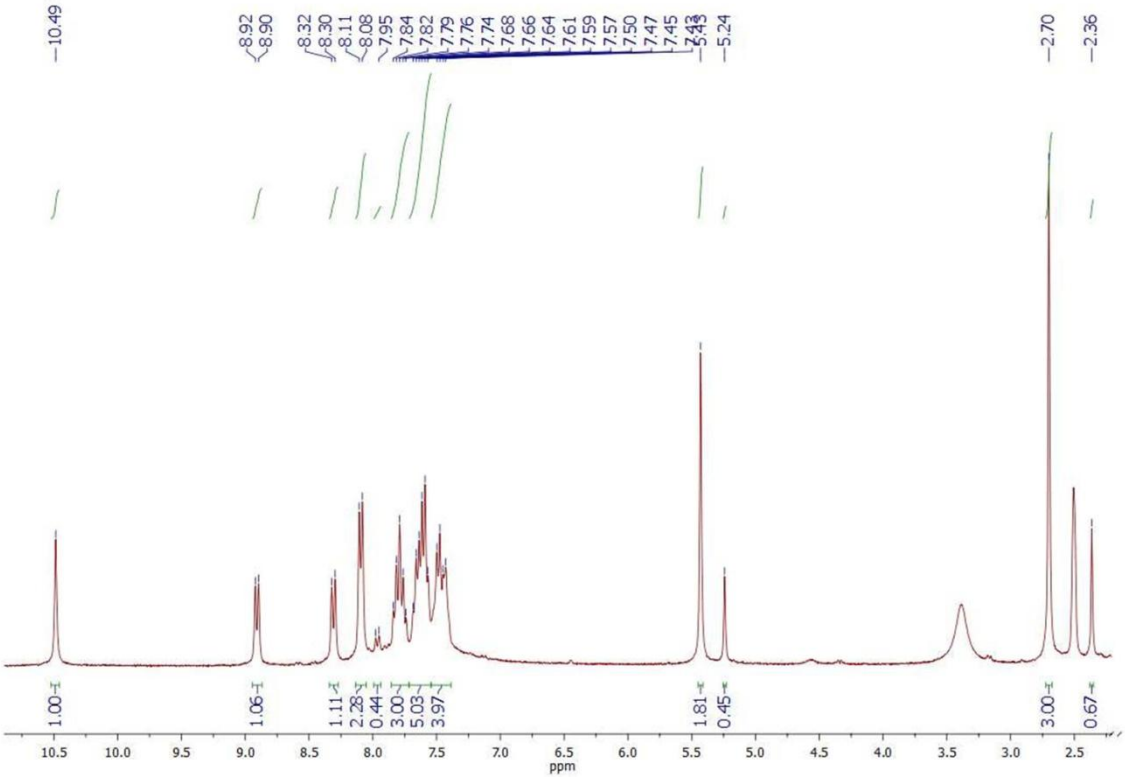
Sensitizer: erythrosine B



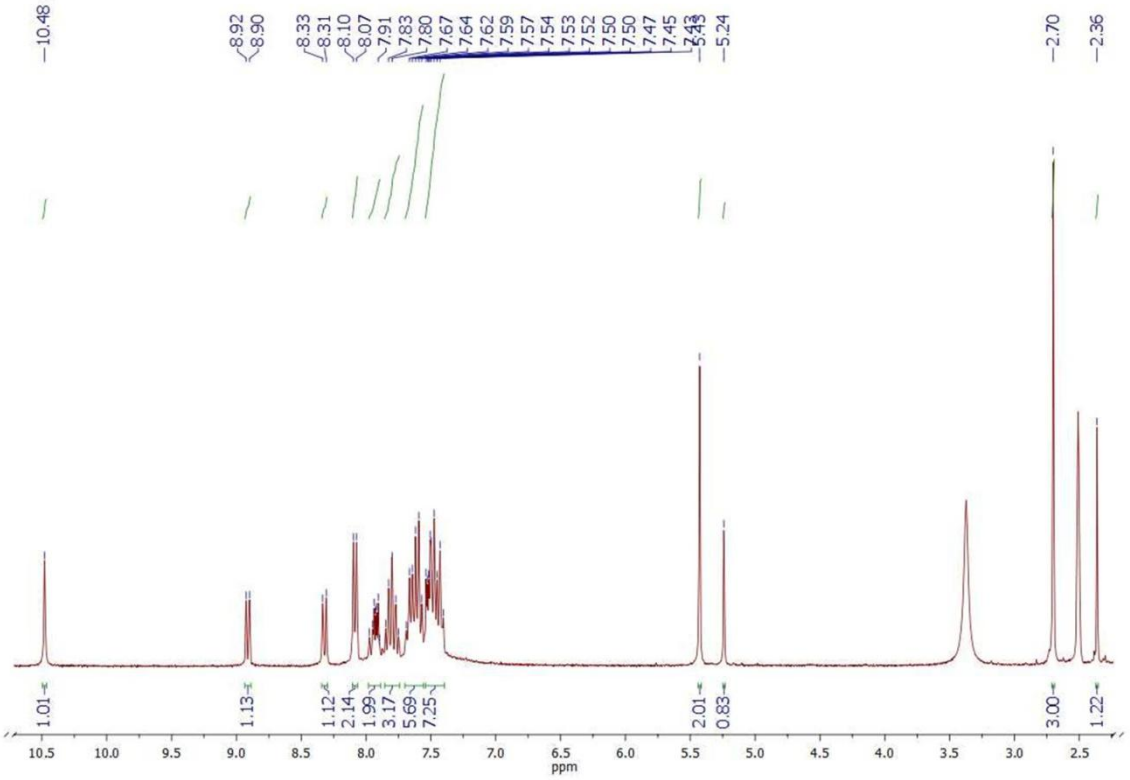
Sensitizer: coumarin 1



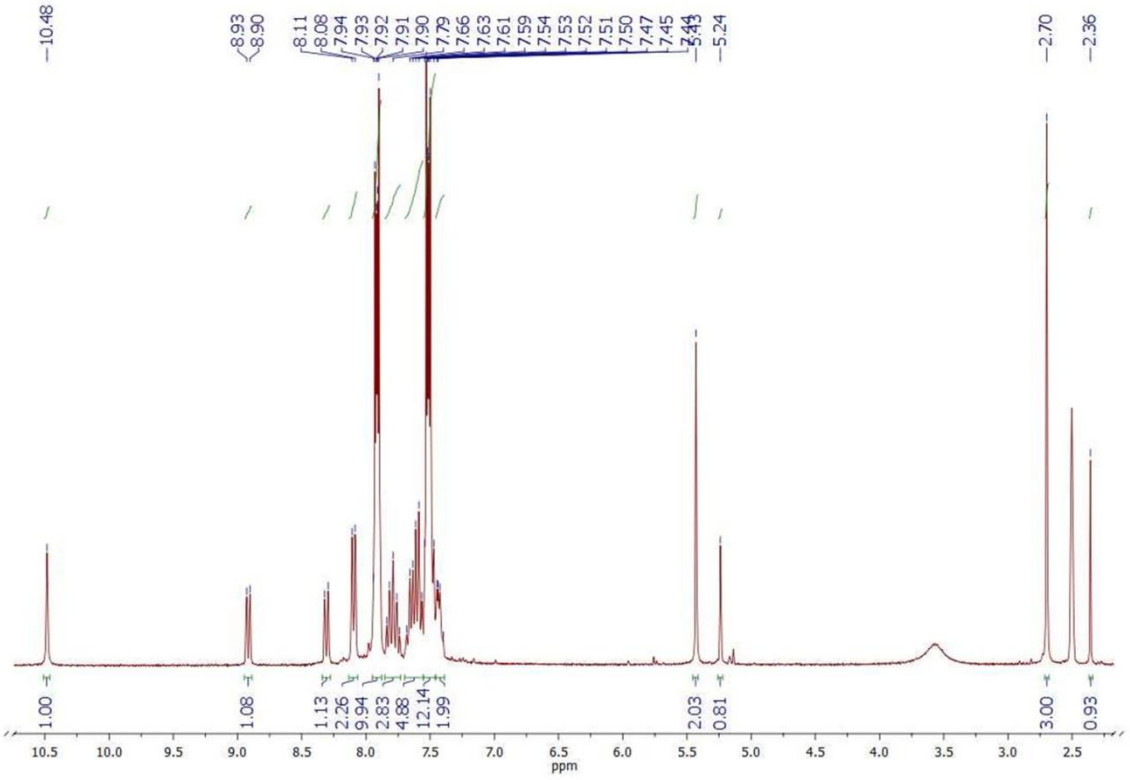
Sensitizer: 6-ethoxy-3-methyl-1*H*-phenalen-1-one



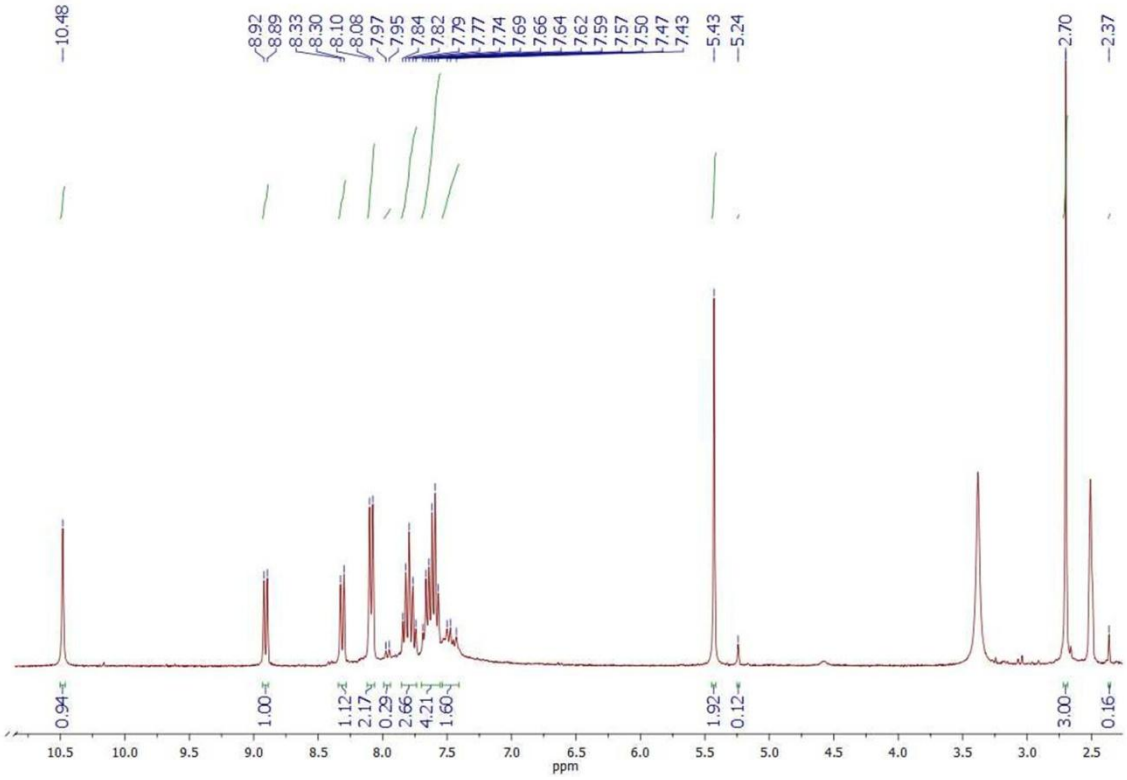
Sensitizer: naphthalene (0.1 eq.)



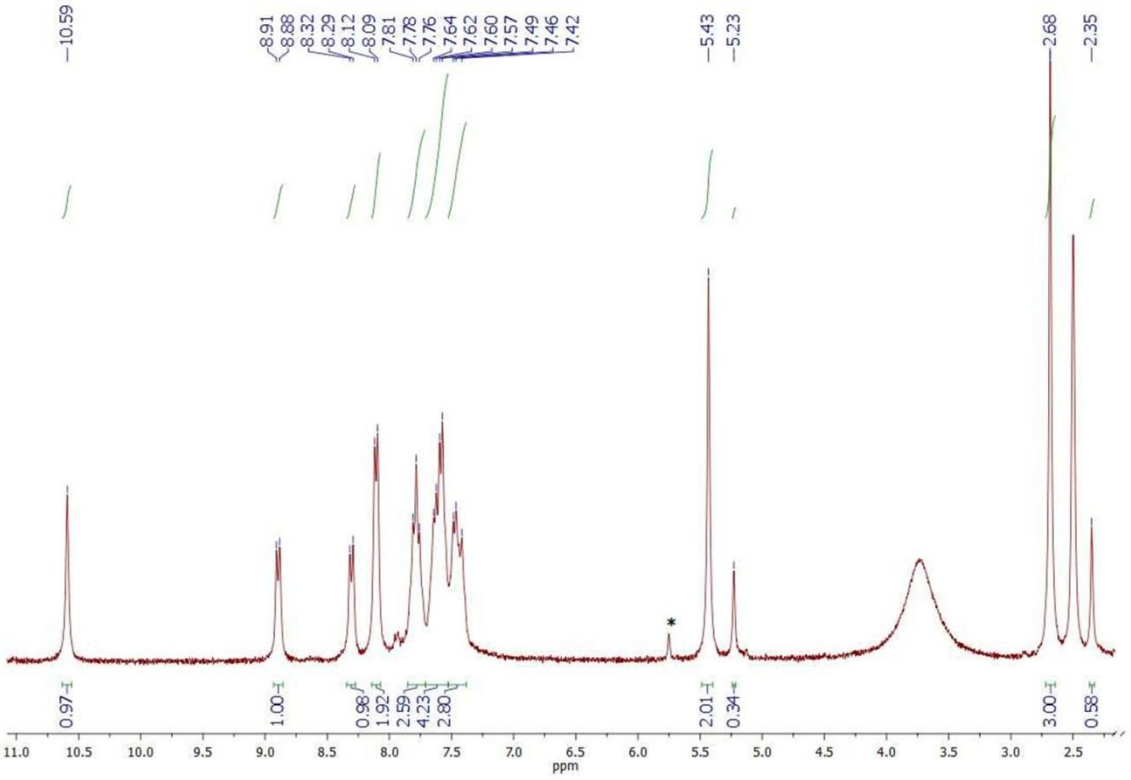
Sensitizer: naphthalene (1 eq.)



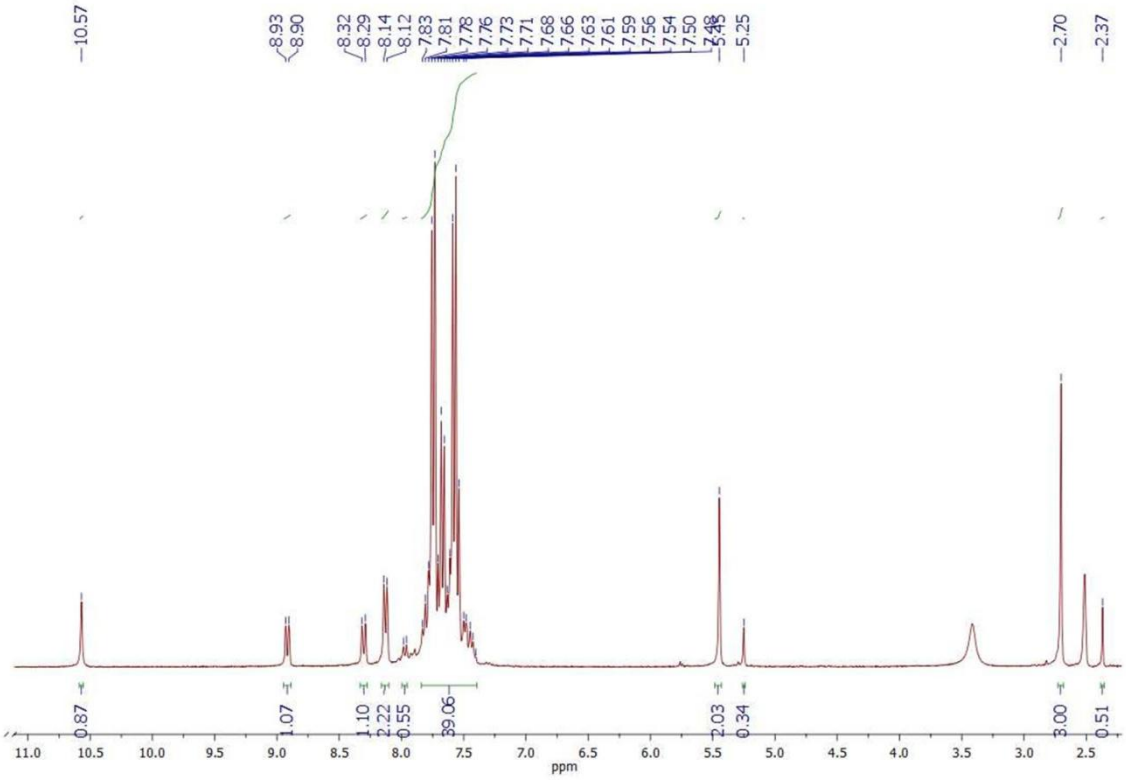
Sensitizer: 4-dimethylamino-4'-nitrostilbene



Sensitizer: 5,10,15,20-tetrakis(4-bromophenyl)porphyrin



Sensitizer: benzophenone

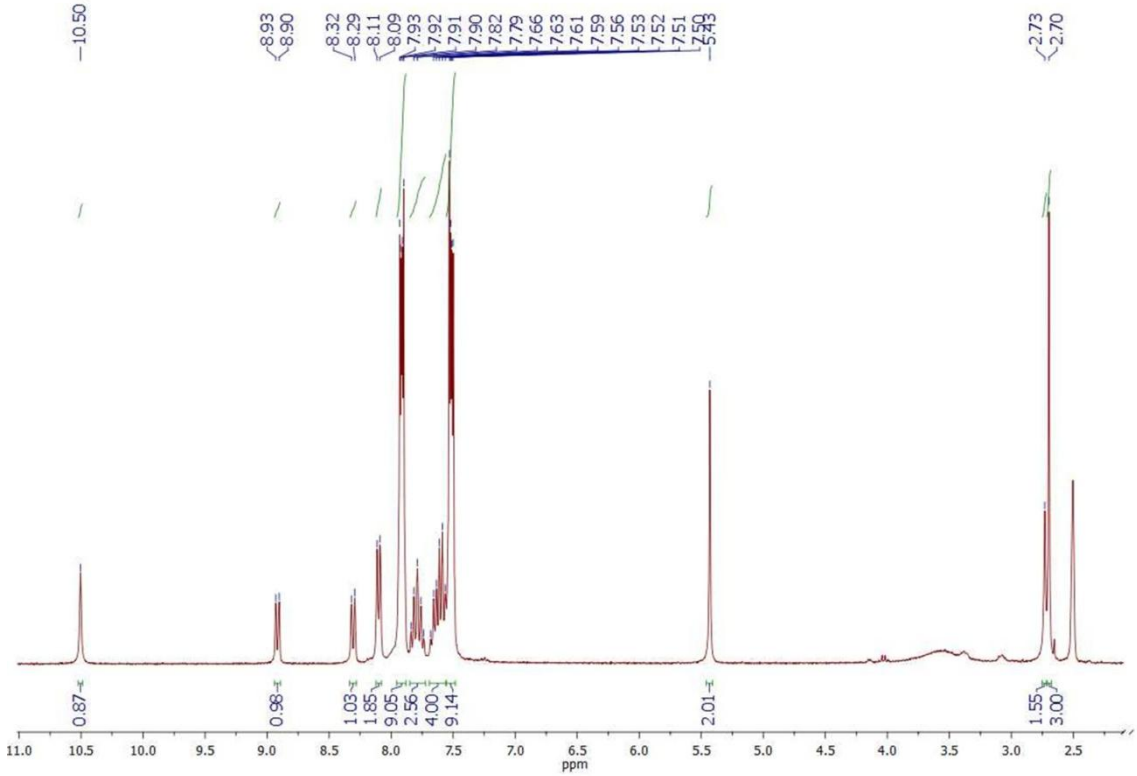


IV. Amine effect (NMR spectra of reaction mixtures)

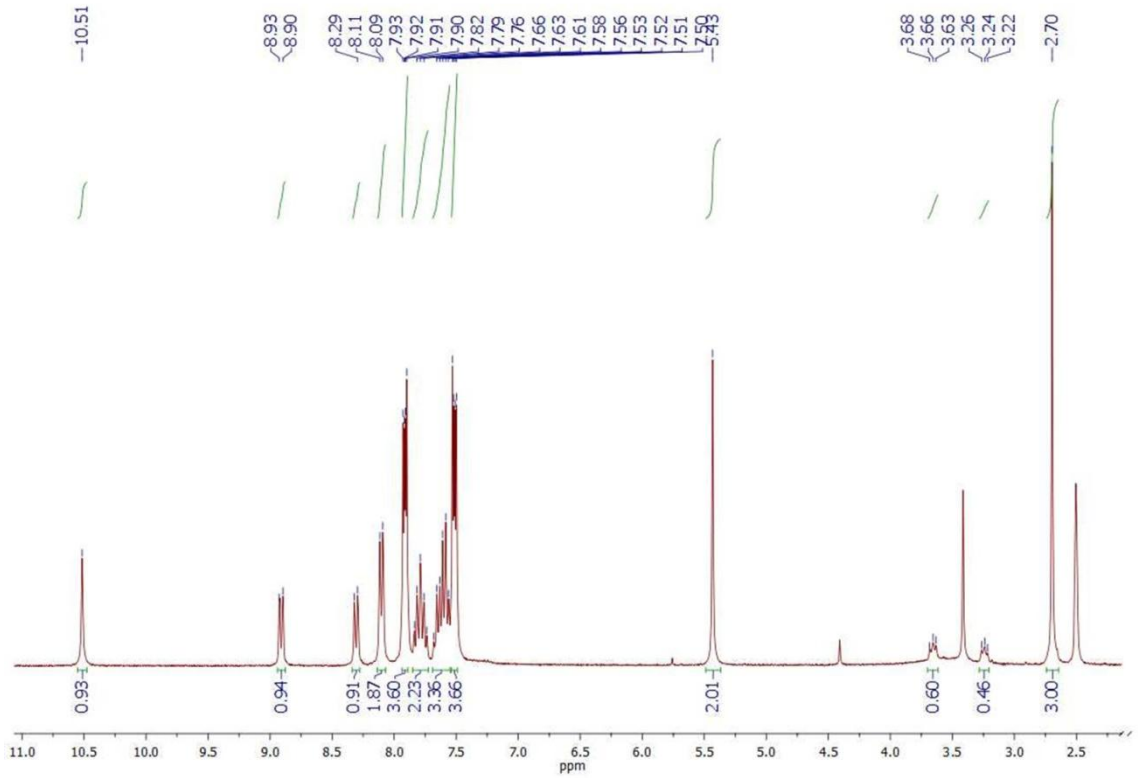
Table S2. ^{1}H NMR chemical shift signals (ppm) of tertiary amines after reaction completion.

Amines	Starting values	Values after photoreaction
Et_3N	0.93 (t, *J* = 7.2 Hz, 3H, CH_3)	1.20 (t, *J* = 7.2 Hz, 3H, CH_3)
	2.43 (q, *J* = 7.2 Hz, 2H, CH_2)	3.04 (q, *J* = 7.2 Hz, 2H, CH_2)
DABCO	2.73 (s, 12H, CH_2)	3.24 (m, 6H, CH_2)
		3.66 (m, 6H, CH_2)
1-Methylimidazole	3.66 (s, 3H, CH_3)	3.76 (s, 3H, CH_3)
	6.93 (s, 1H, H^{arom})	7.30 (s, 1H, H^{arom})
	7.14 (s, 1H, H^{arom})	7.43 (s, 1H, H^{arom})
	7.66 (s, 1H, H^{arom})	8.39 (s, 1H, H^{arom})

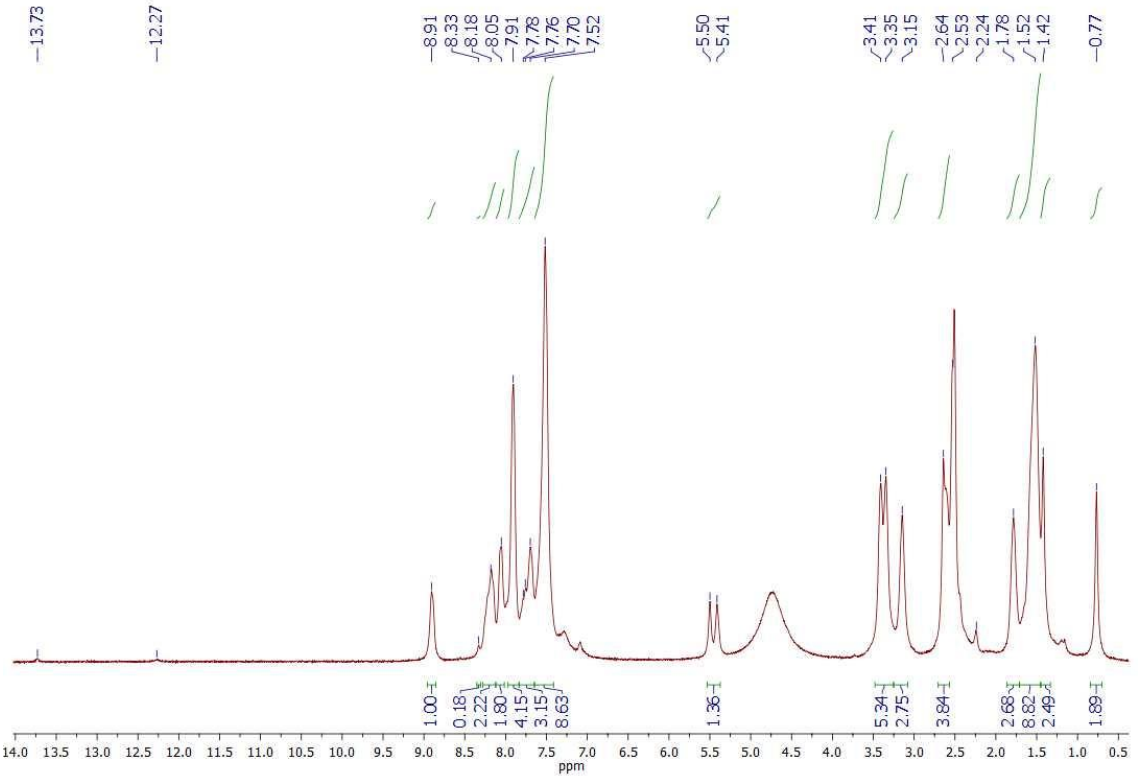
Amine: DABCO (1 eq.)



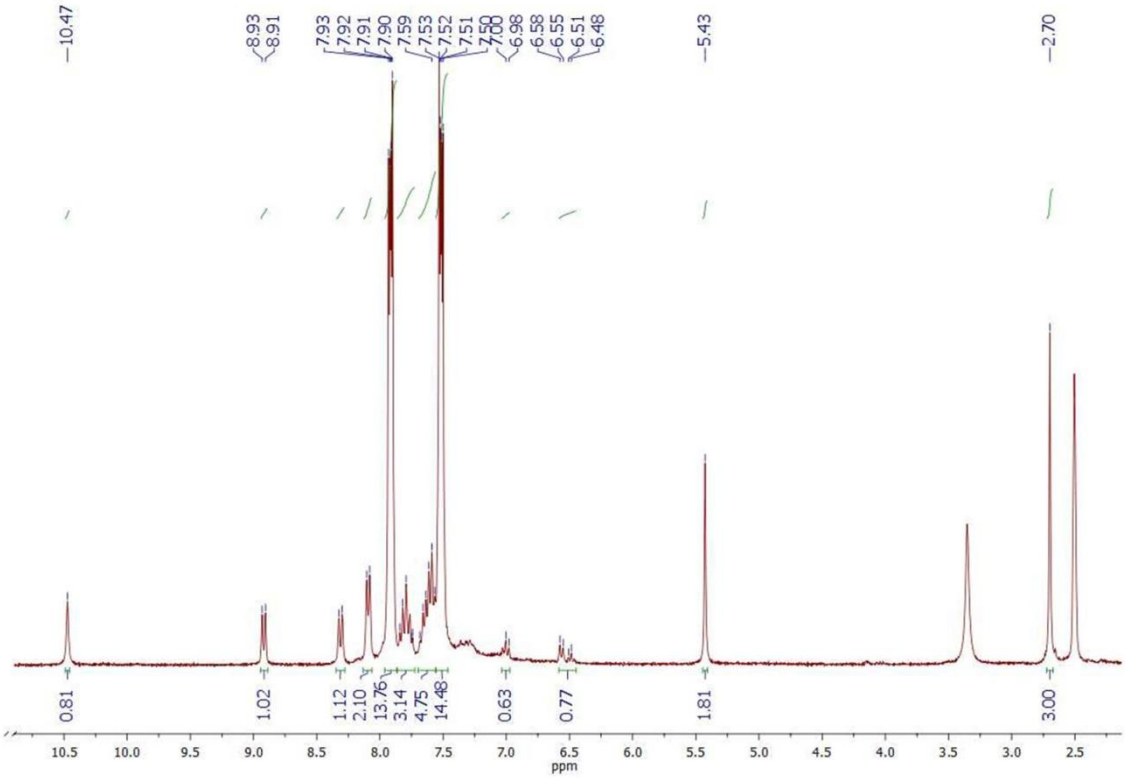
Amine: DABCO (0.1 eq.)



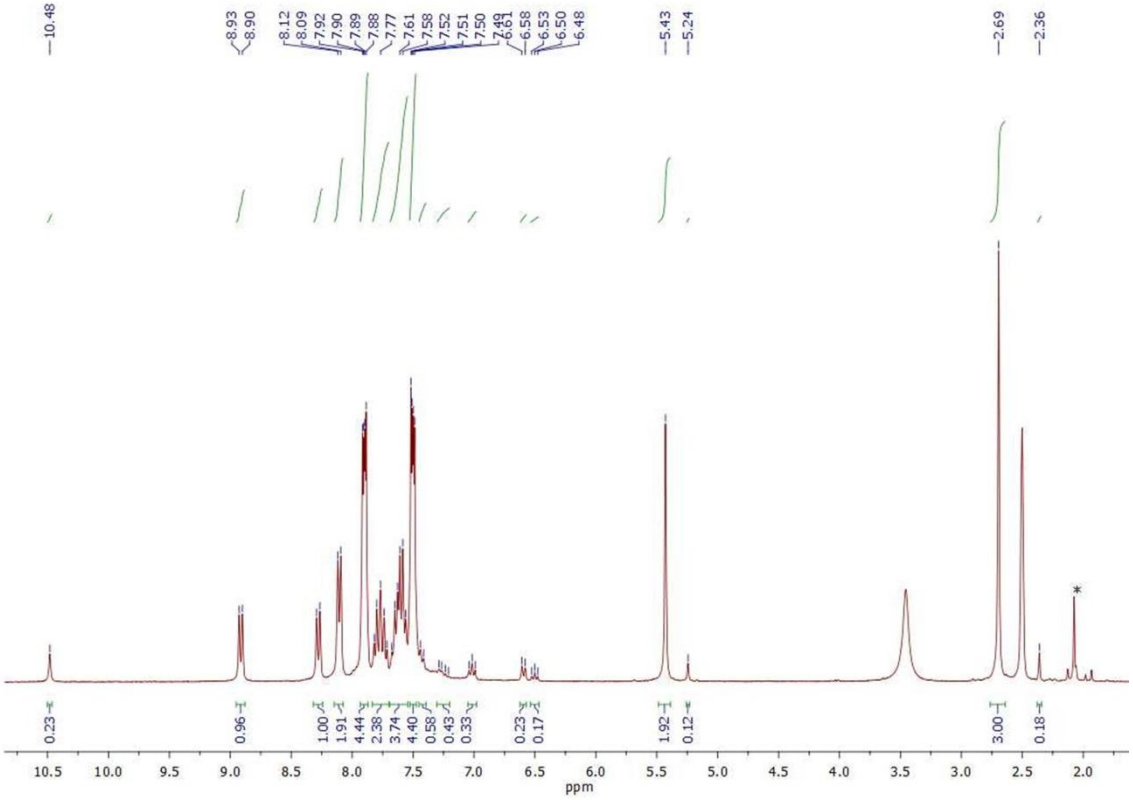
Amine: DBU



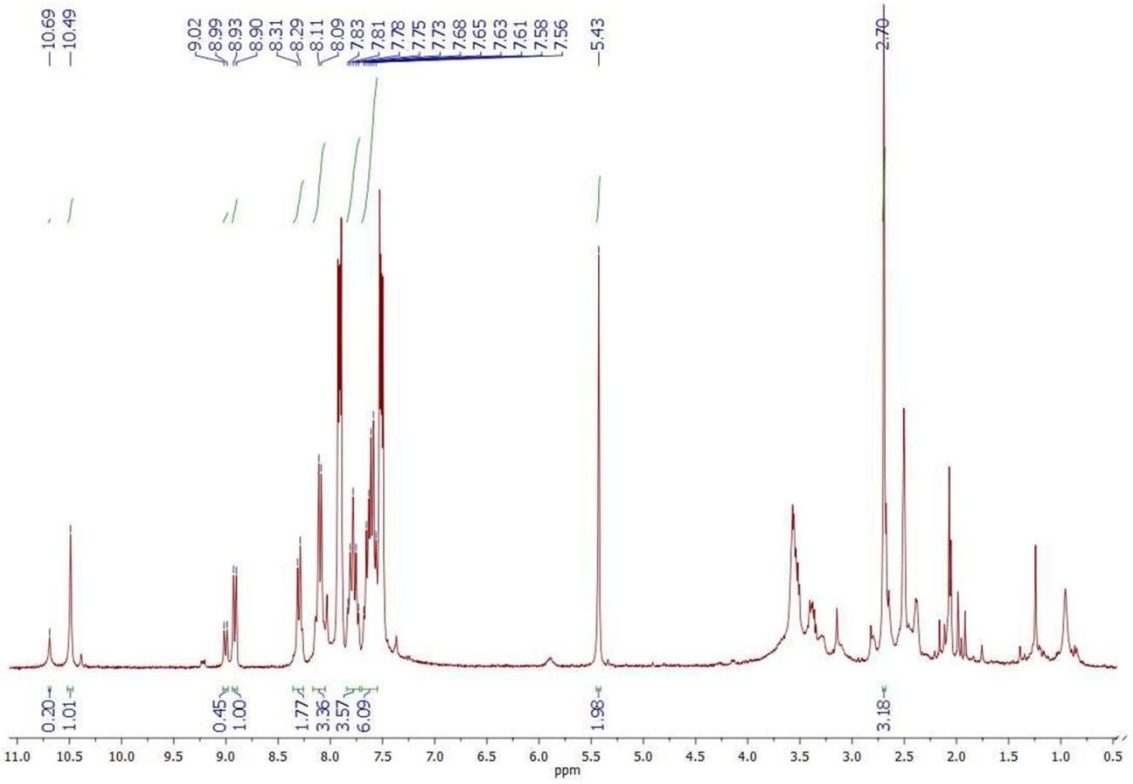
Amine: aniline (1 eq.)



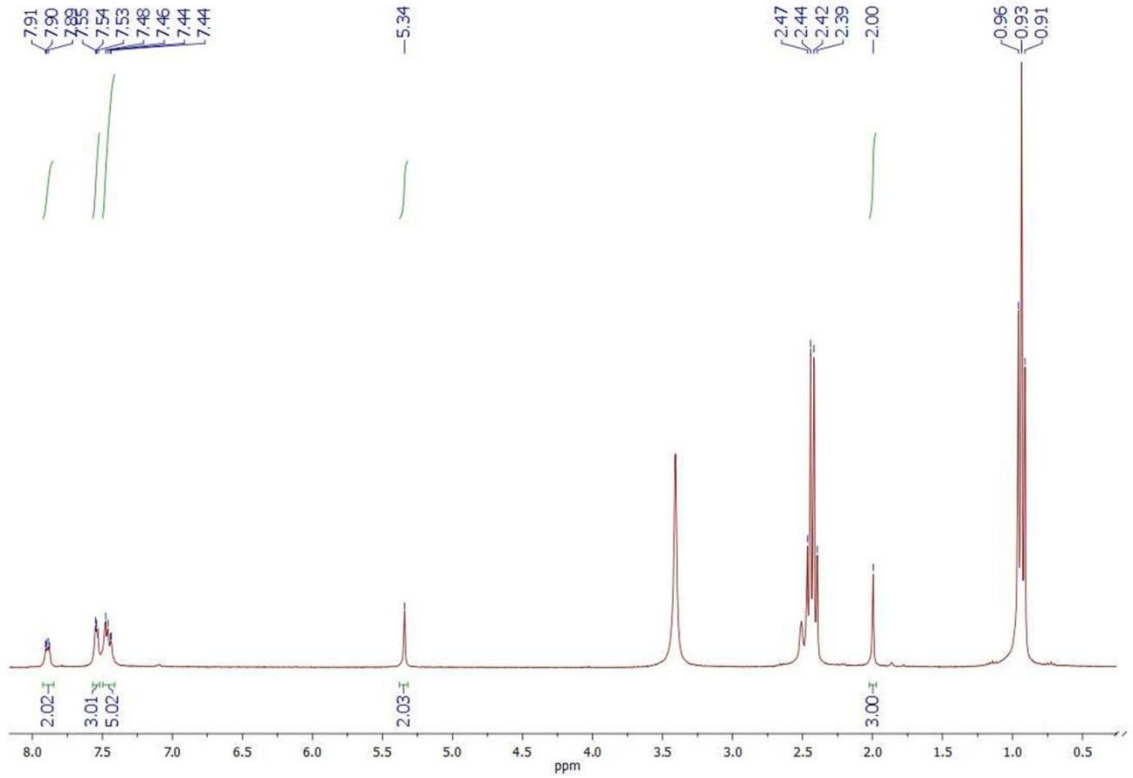
Amine: aniline (0.1 eq.)



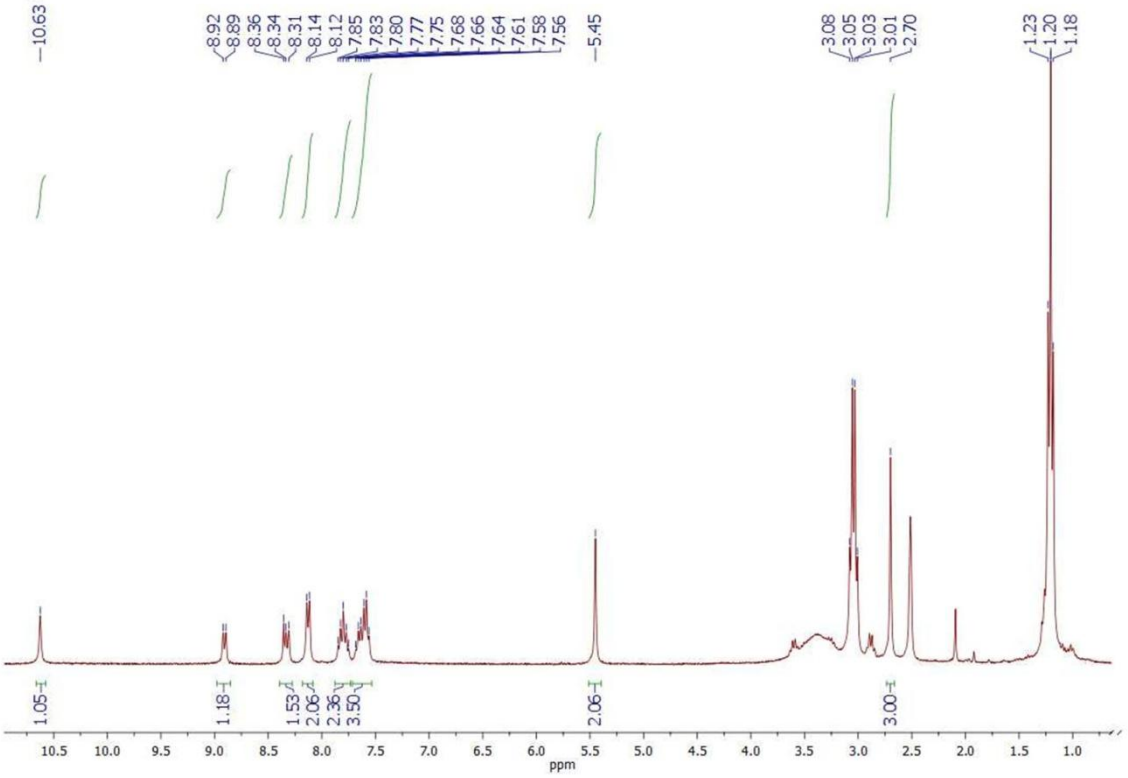
Amine: morpholine



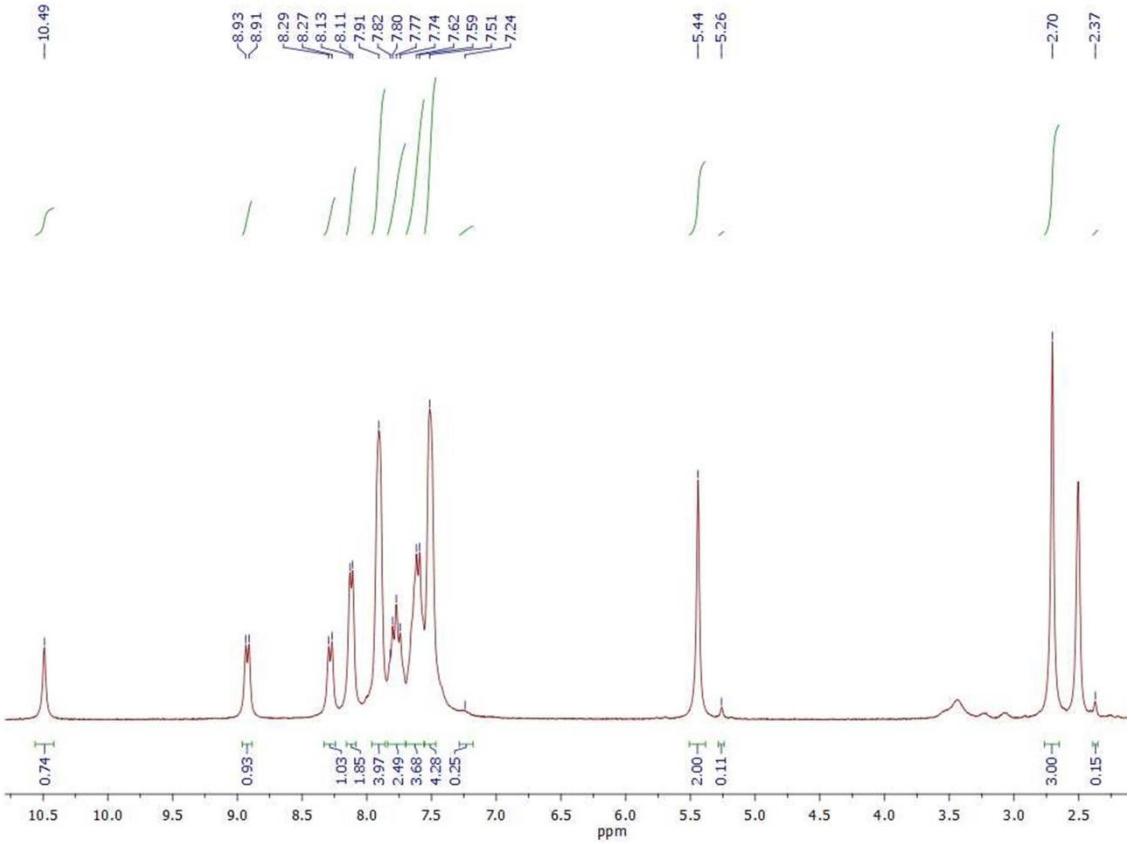
Amine: Et_3N (before irradiation)



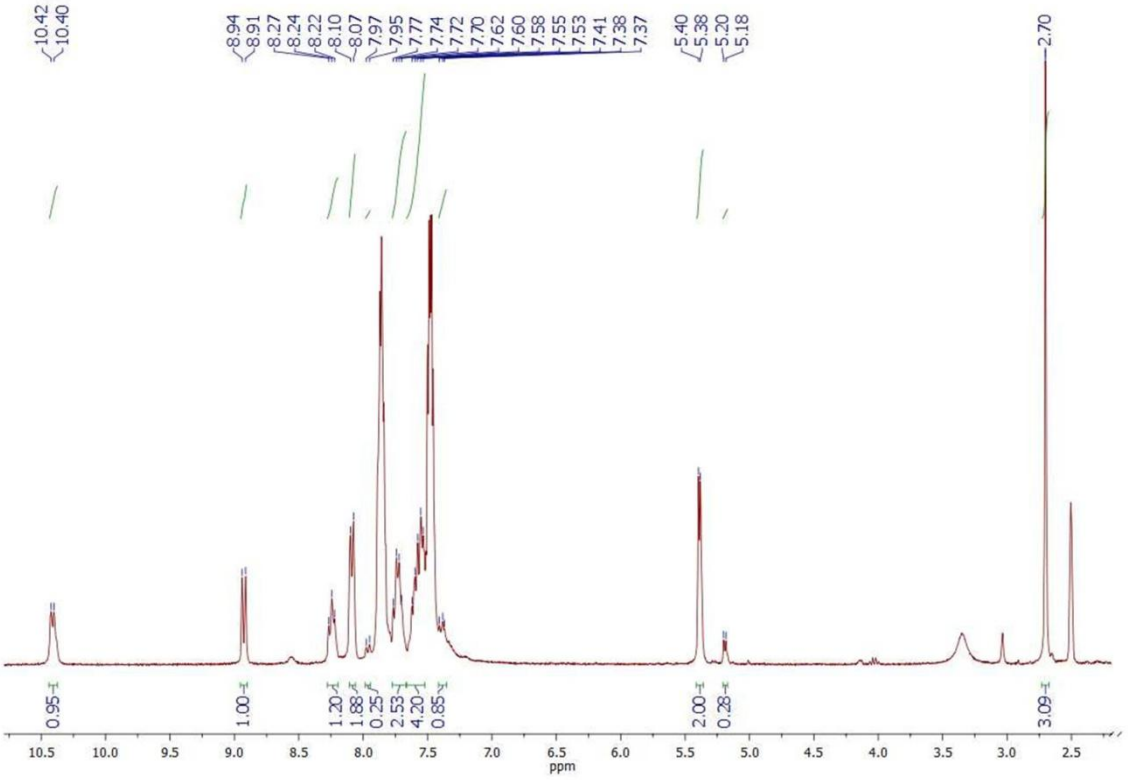
Amine: Et_3N (after irradiation)



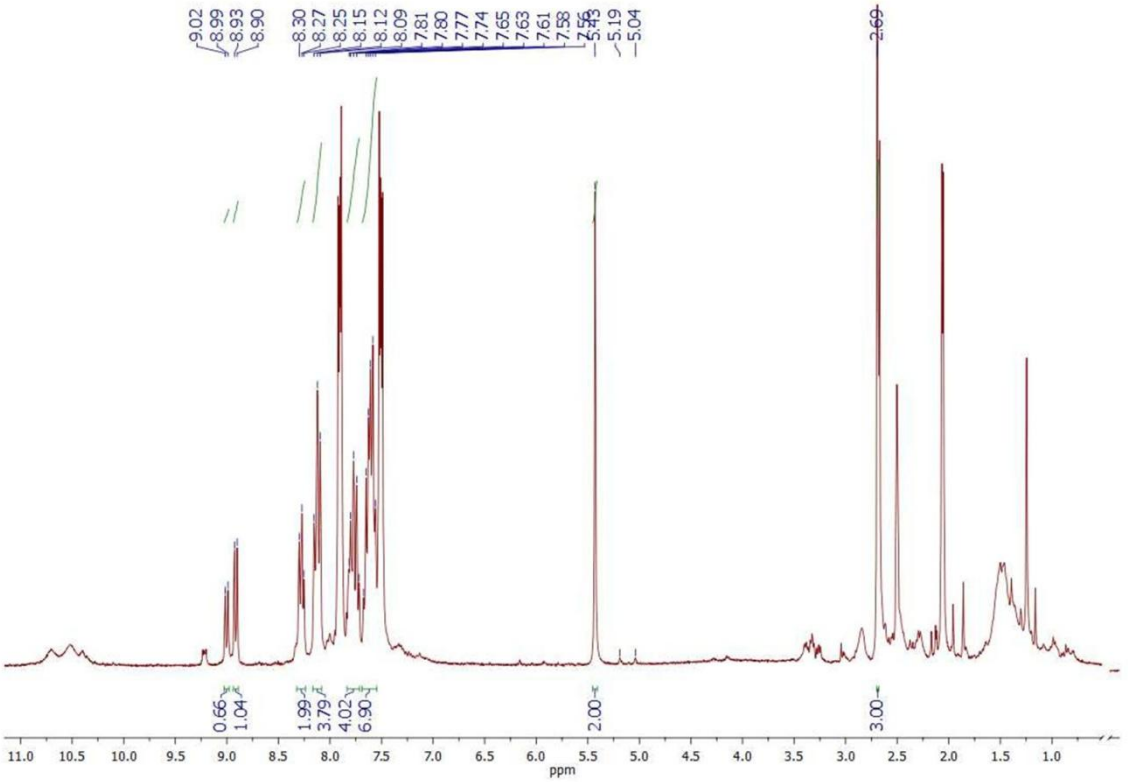
Amine: Et_3N (0.1 eq.)



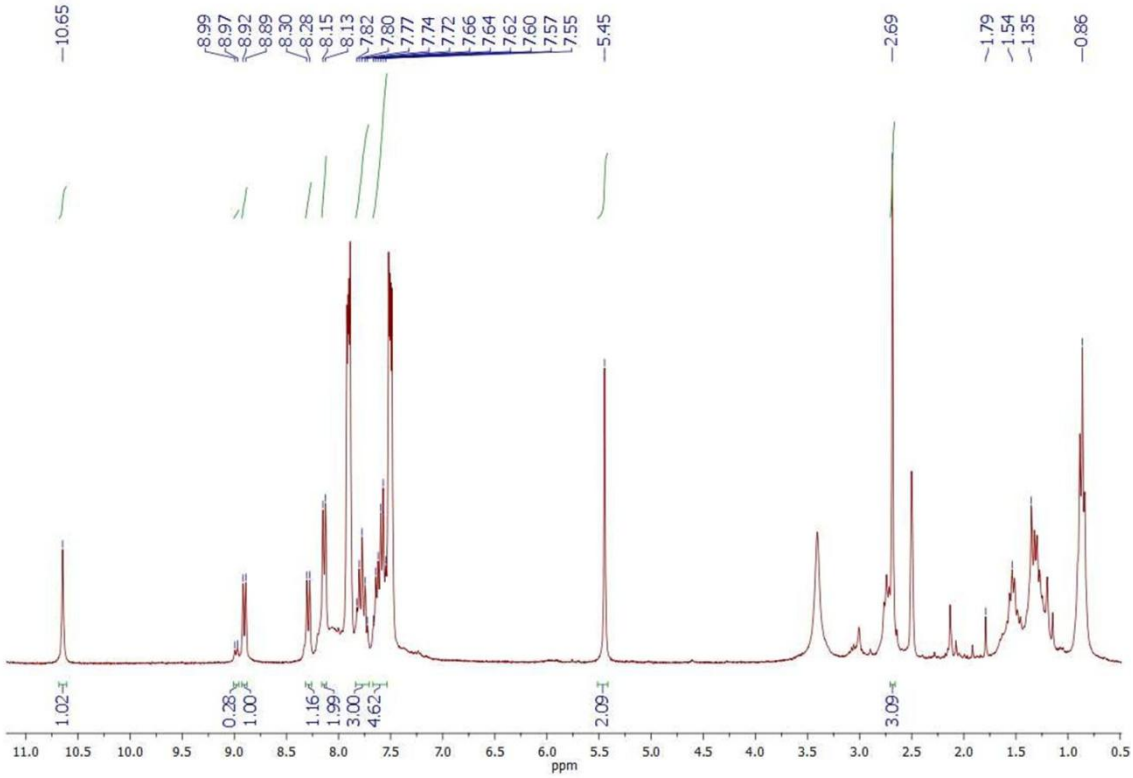
Amine: pyridine



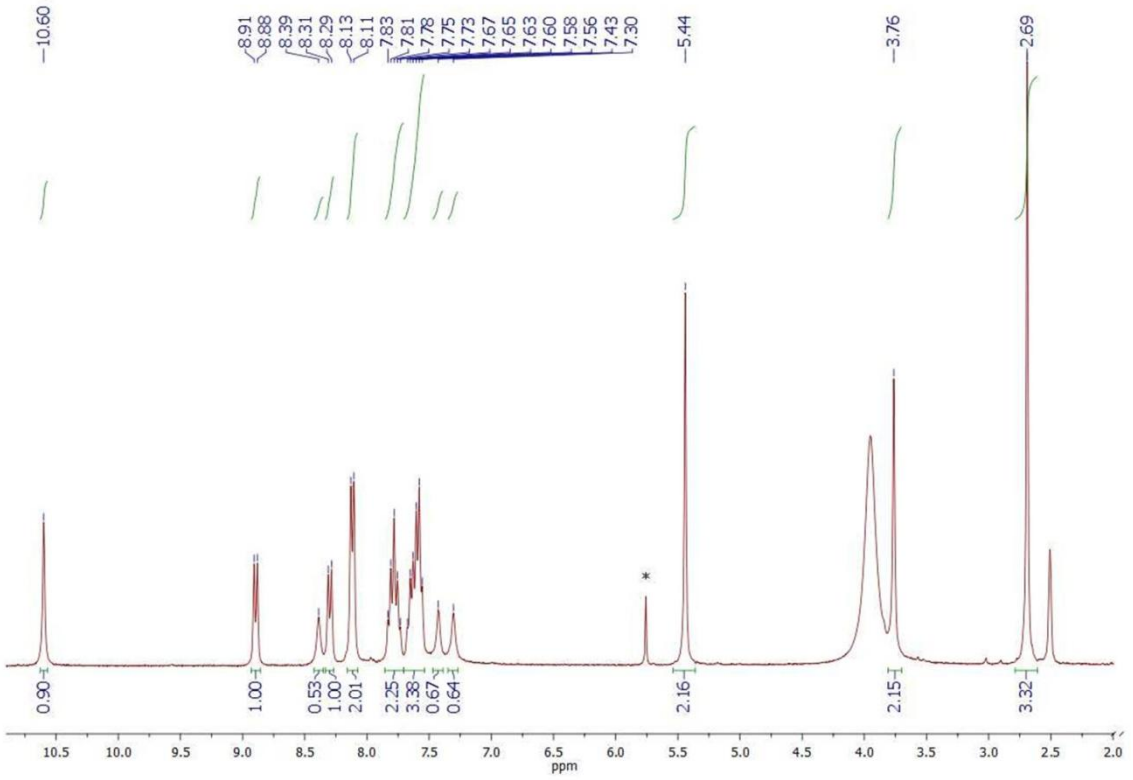
Amine: piperidine



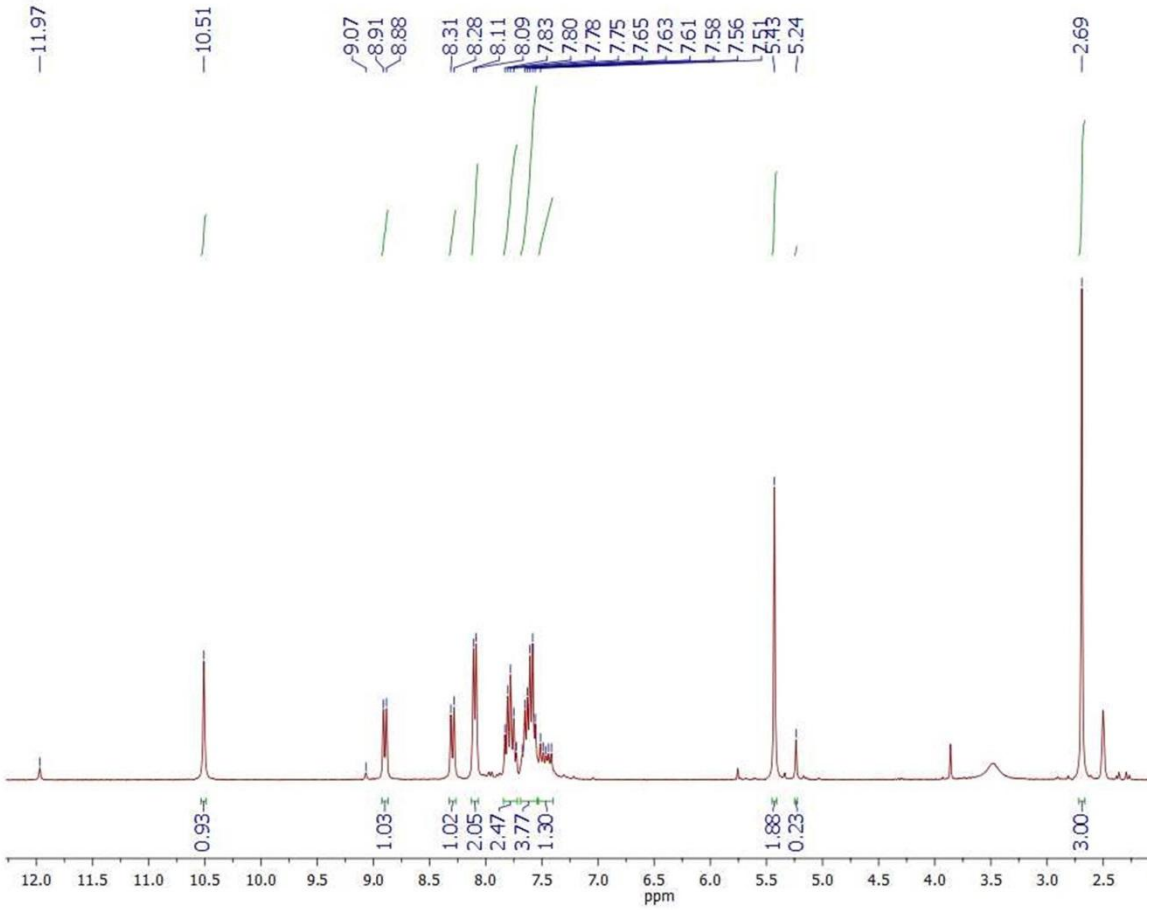
Amine: *n*-butylamine



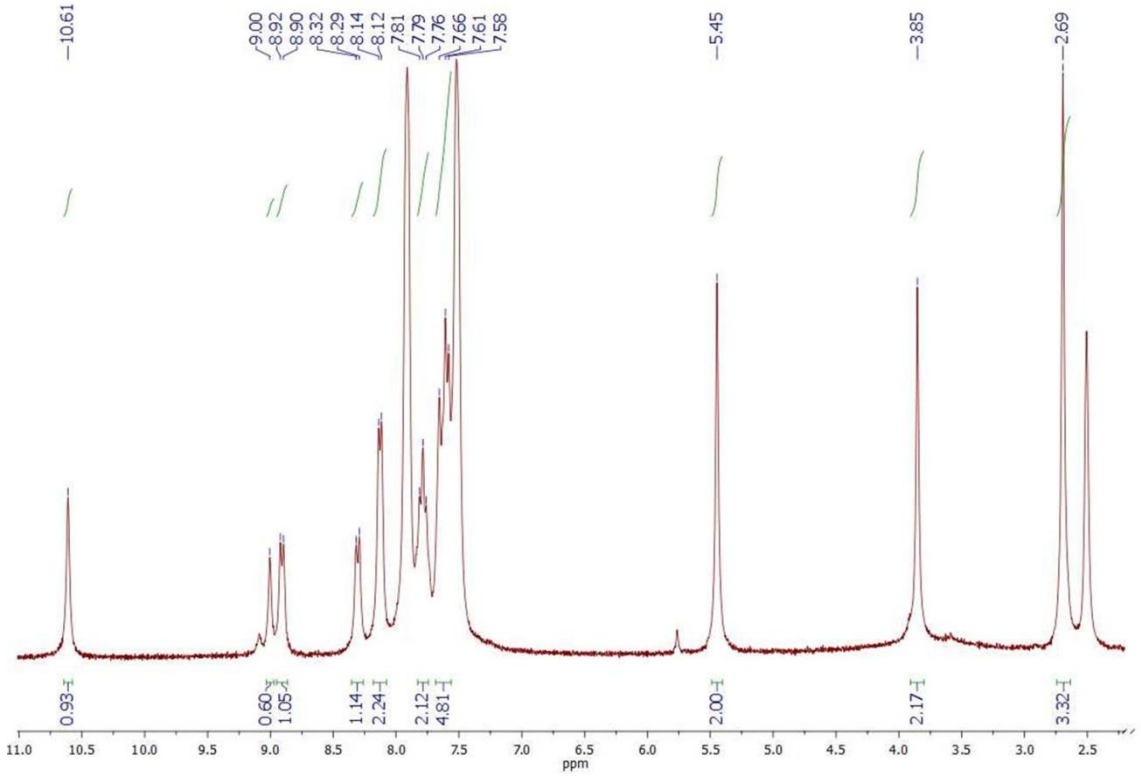
Amine: 1-methylimidazole (without naphthalene)



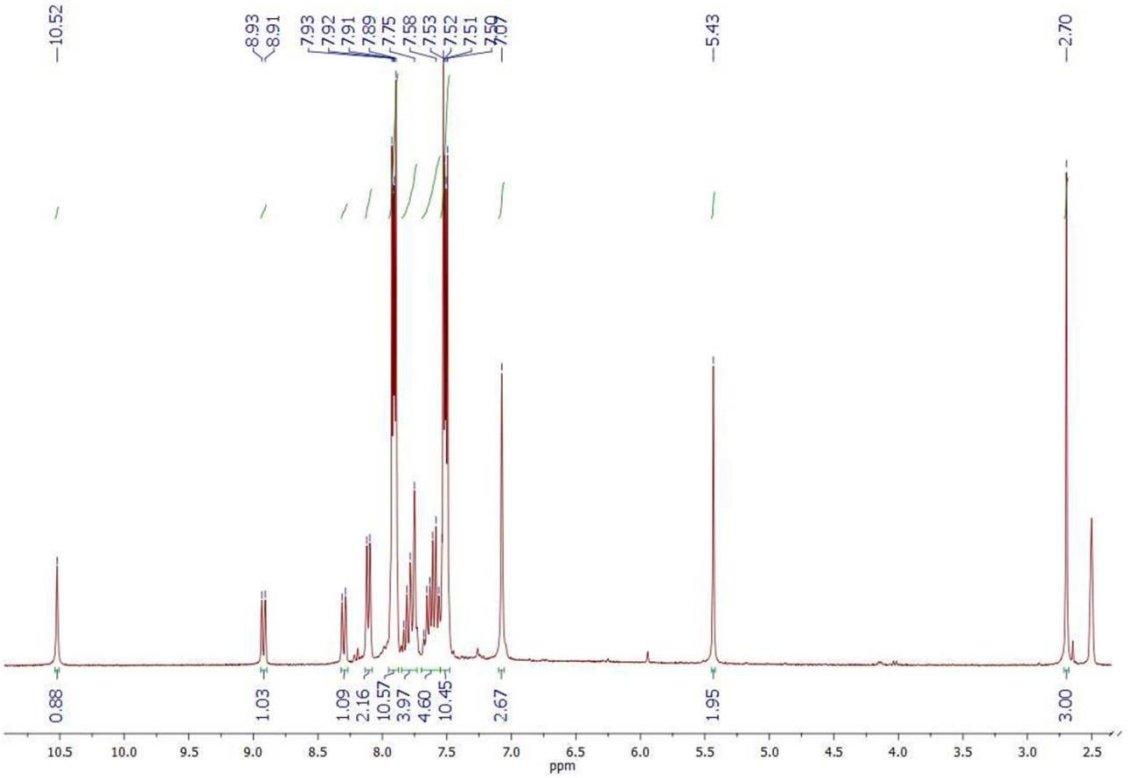
Amine: 1-methylimidazole (0.1 eq.)



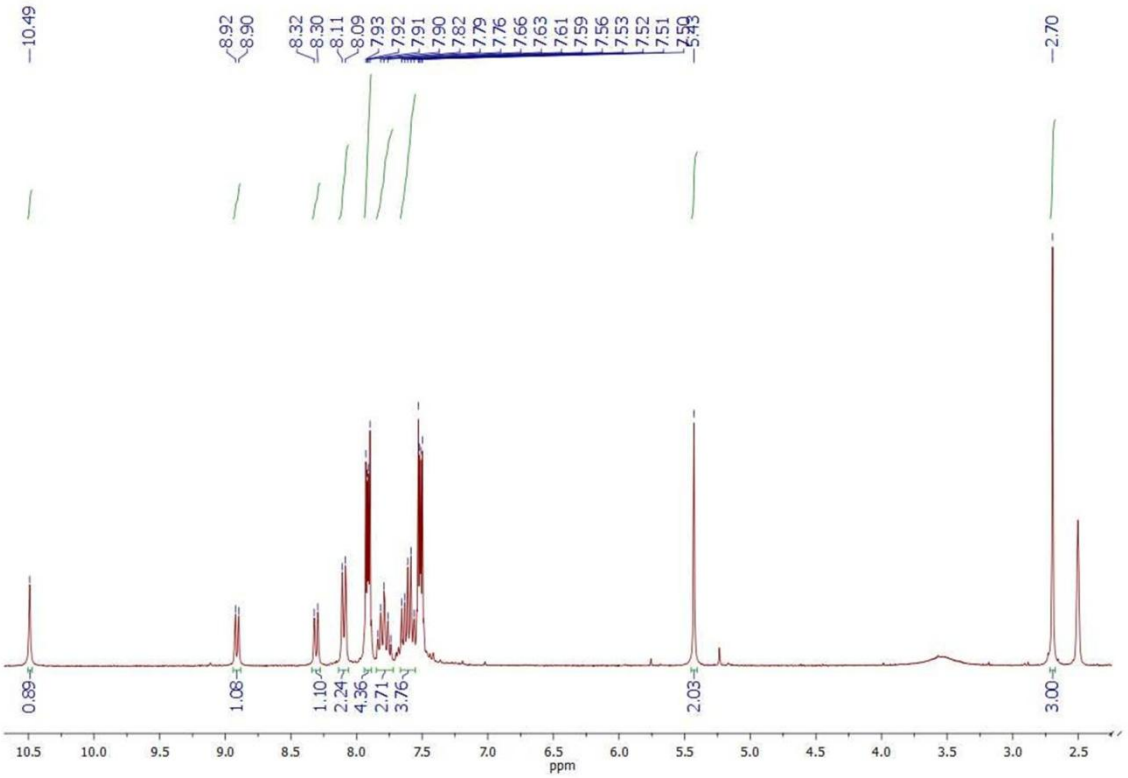
Amine: 1-methylimidazole (1 eq.)



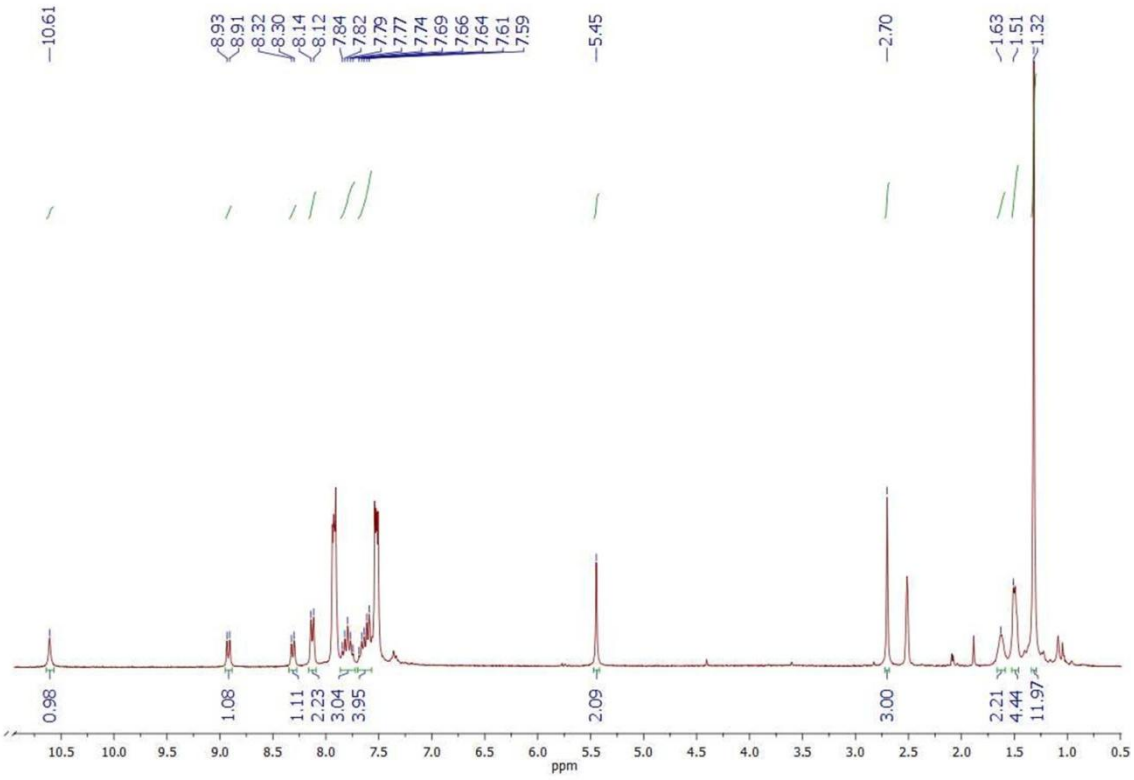
Amine: imidazole (1 eq.)



Amine: imidazole (0.1 eq.)

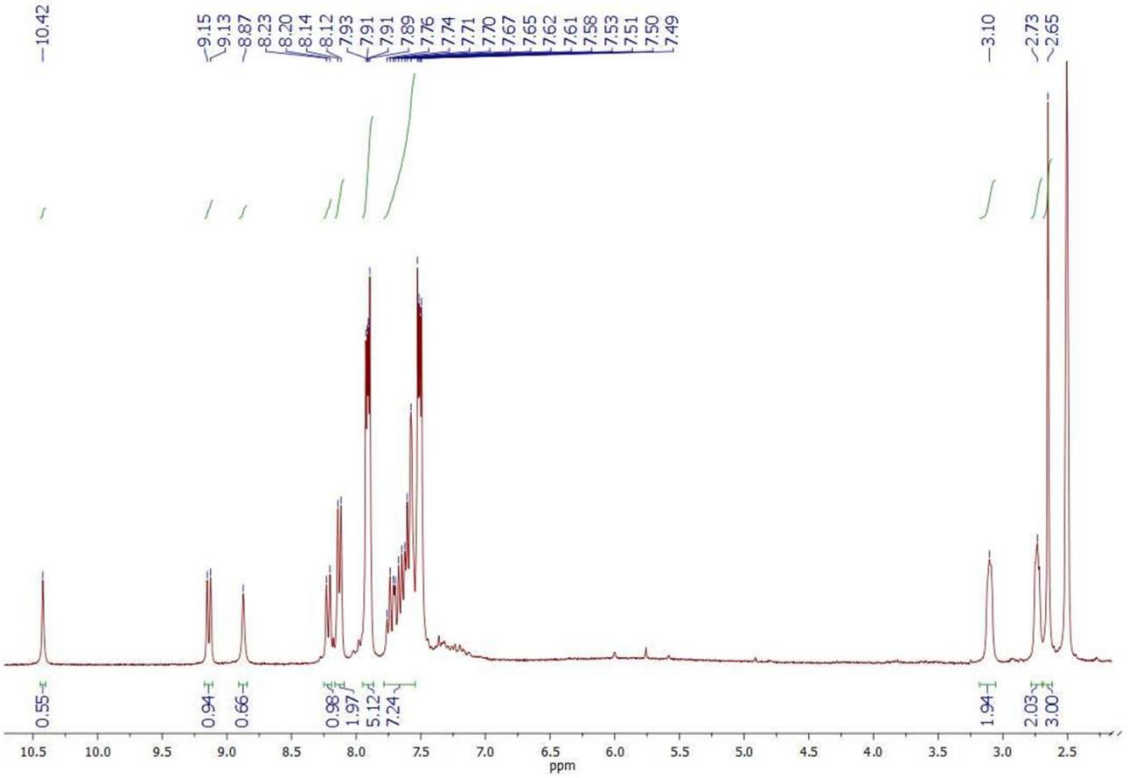


Amine: 2,2,6,6-tetramethylpiperidine

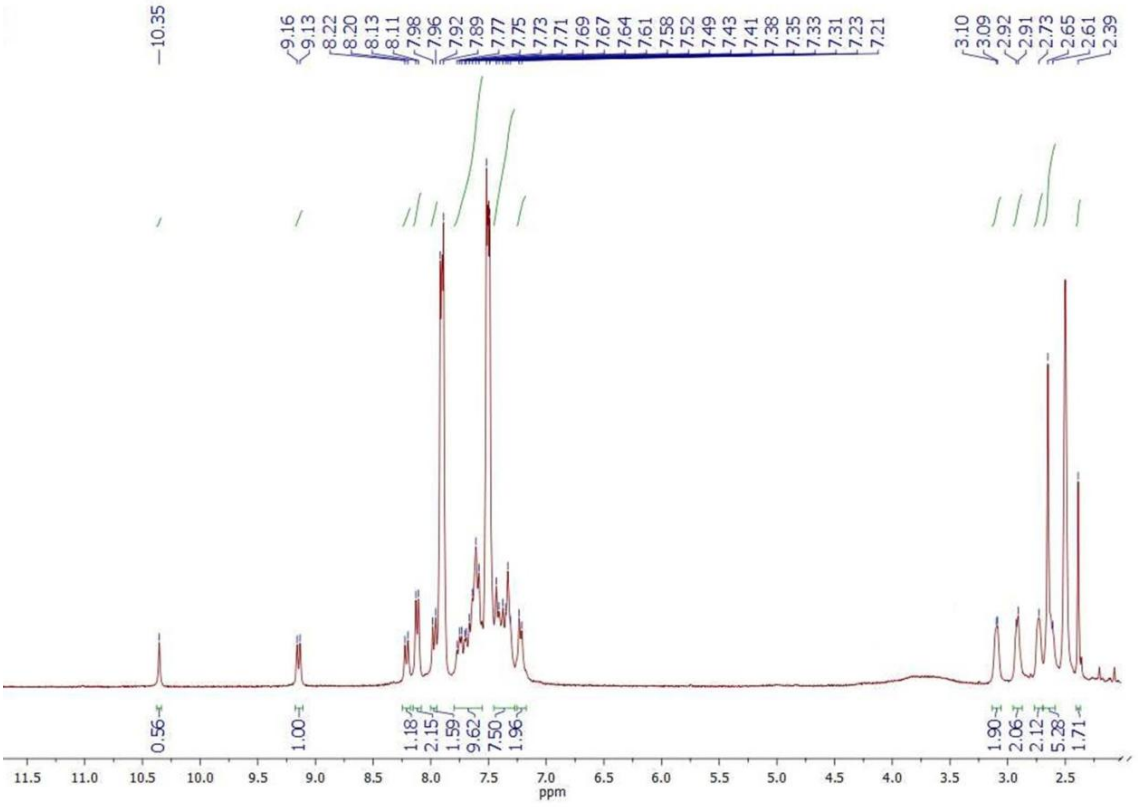


V. Effect of imidazole on the photoreaction of diarylethene 1b

^{1}H NMR spectra of photoreaction of **1b** (40 mg in 2 ml of MeCN, 1 eq. of imidazole)

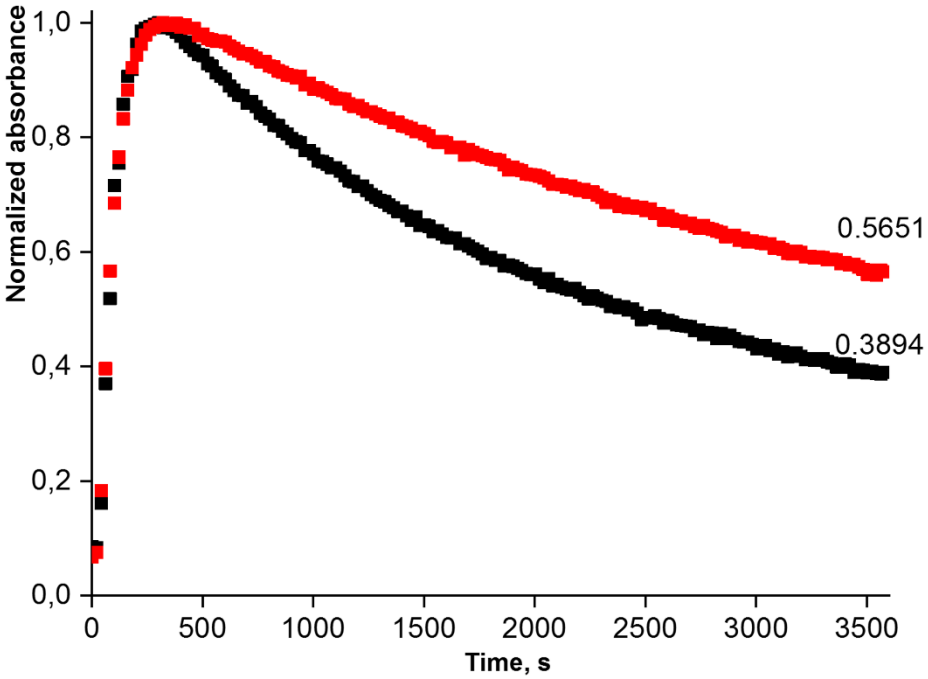


^{1}H NMR spectra of photoreaction of **1b** (40 mg in 2 ml of MeCN)

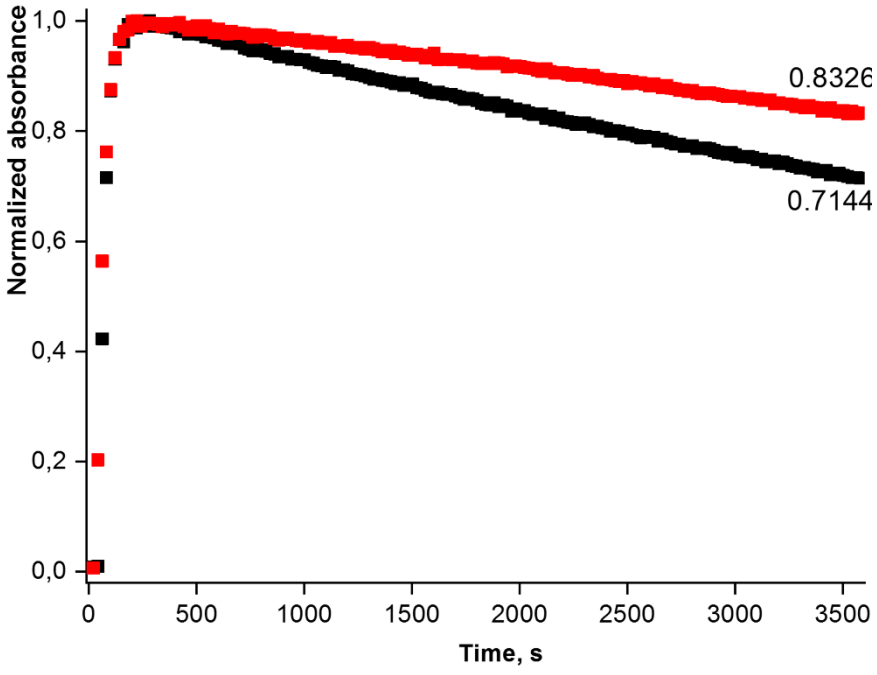


VI. Photostability of photochromic compounds

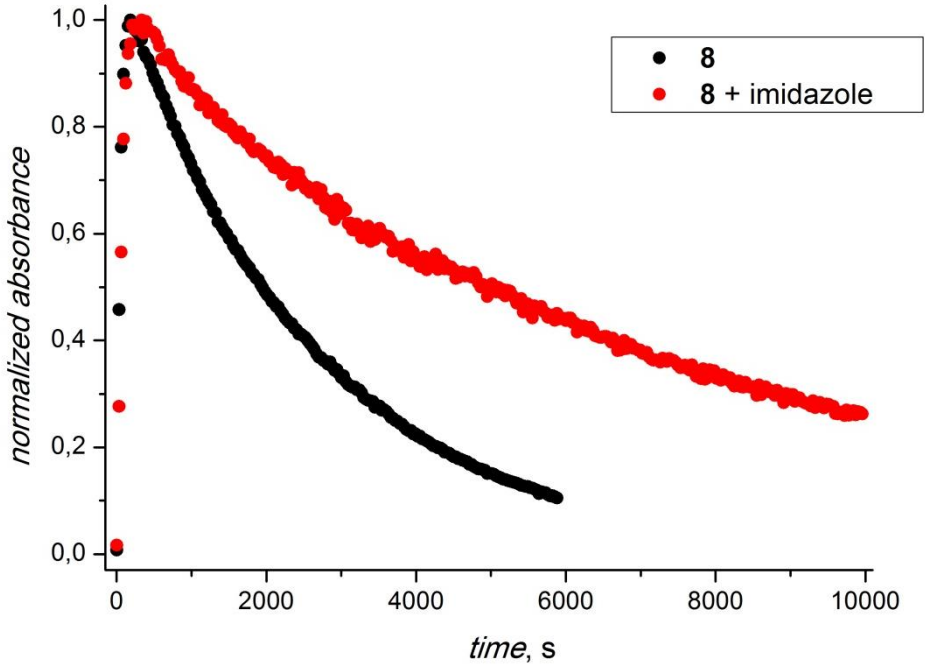
Dependence of the normalized optical density at the absorption maximum of photoinduced isomer **B** of diarylethene **5** on the irradiation time without (black points) and with imidazole (red points) (solvent – acetonitrile, C = $1.4 \cdot 10^{-5}$ M, C(imidazole) = $1.03 \cdot 10^{-3}$ M, λ^{irr} = 365 nm, T = 293 K).



Dependence of the normalized optical density at the absorption maximum of photoinduced isomer **B** of diarylethene **6** on the irradiation time without (black points) and with imidazole (red points) (solvent – acetonitrile, C = $1.4 \cdot 10^{-5}$ M, C(imidazole) = $1.03 \cdot 10^{-3}$ M, λ^{irr} = 365 nm, T = 293 K).

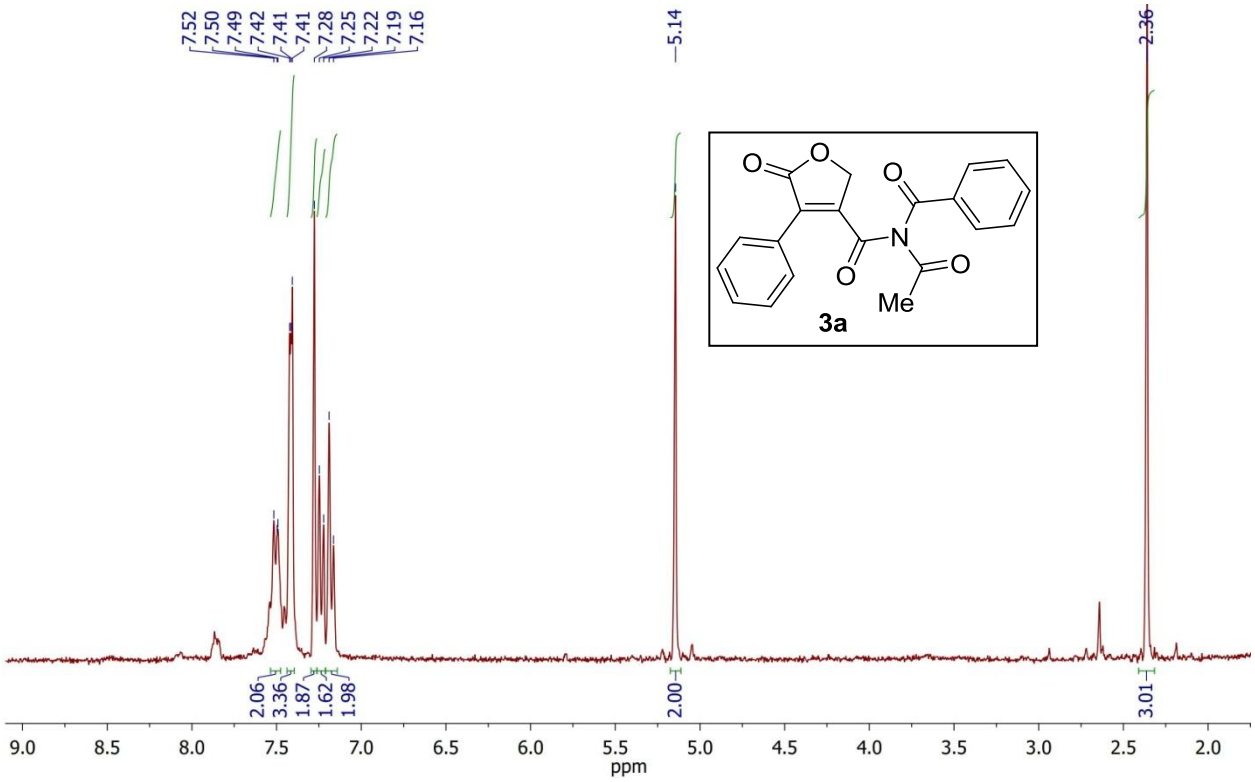


Dependence of the normalized optical density at the absorption maximum of photoinduced isomer **B** of spiropyran **8** on the irradiation time without (black points) and with imidazole (red points) (solvent – acetonitrile, C = $1.4 \cdot 10^{-5}$ M, C(imidazole) = $1.03 \cdot 10^{-3}$ M, λ^{irr} = 365 nm, T = 293 K).

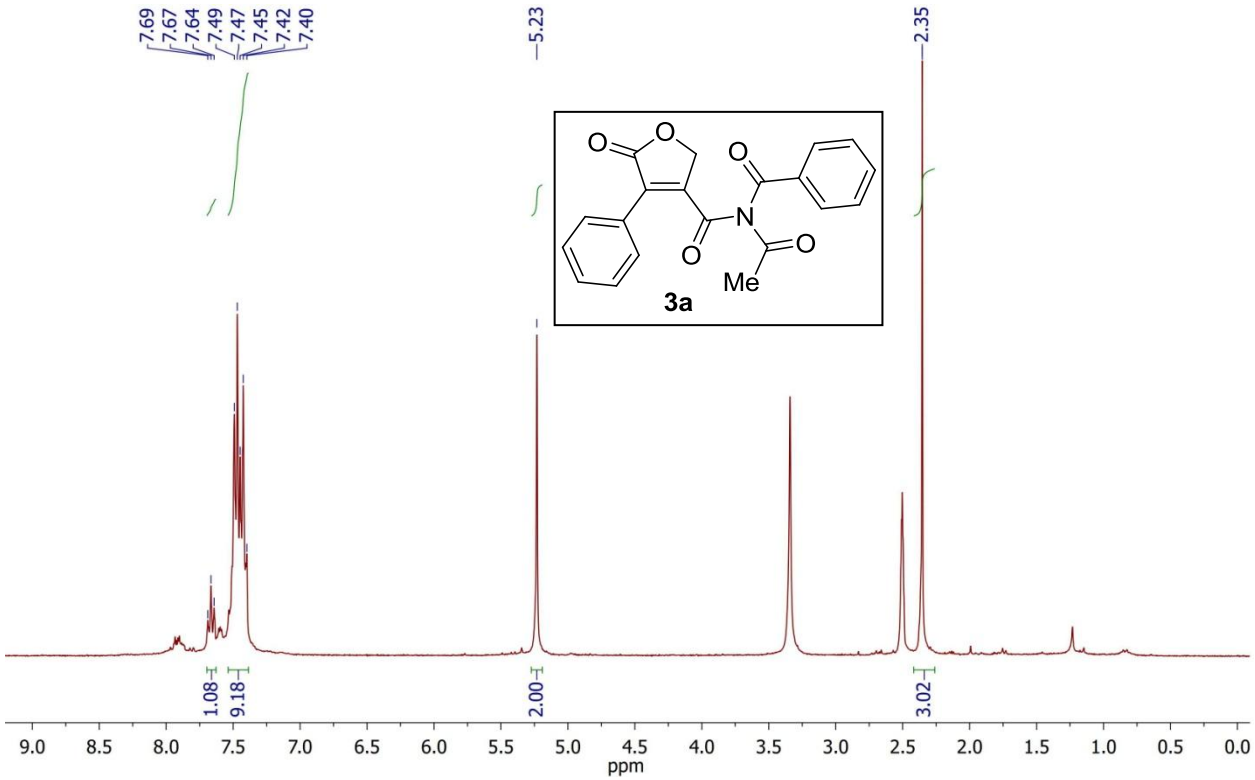


VII. Copies of NMR spectra

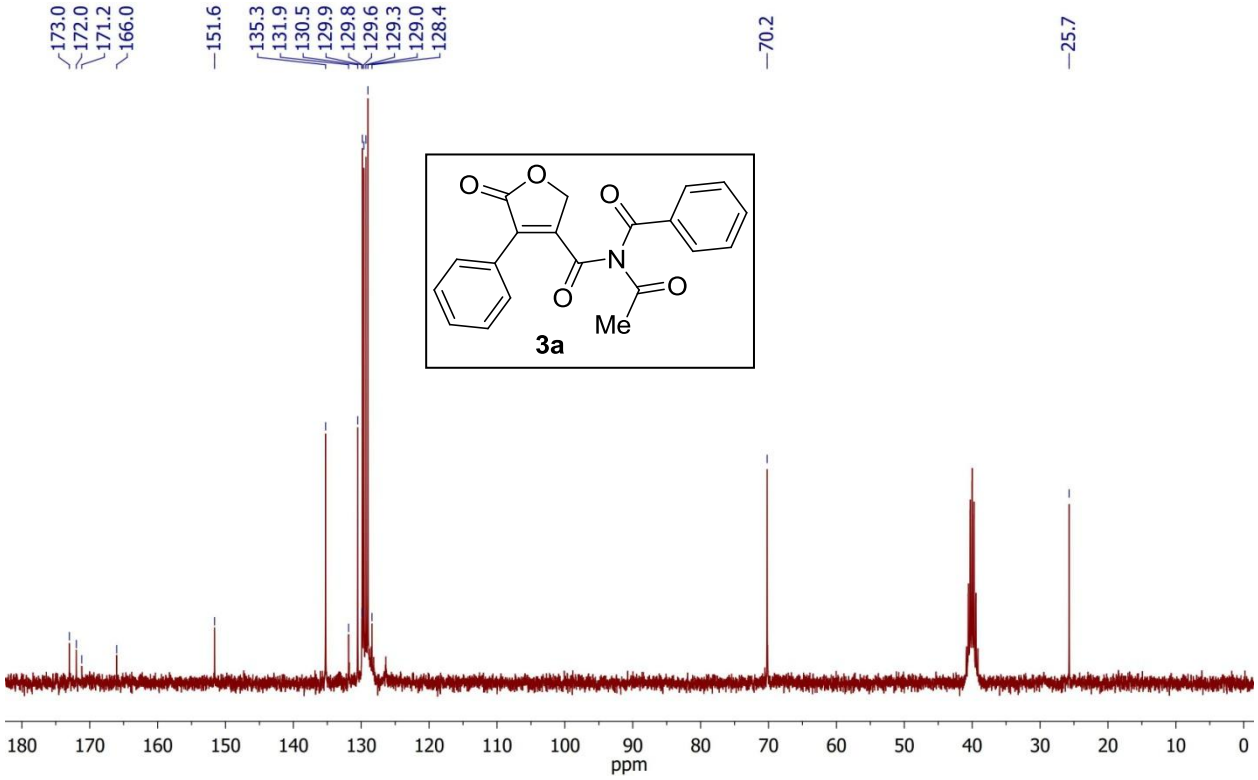
^{1}H NMR spectrum of compound 3a ($CDCl_3$)



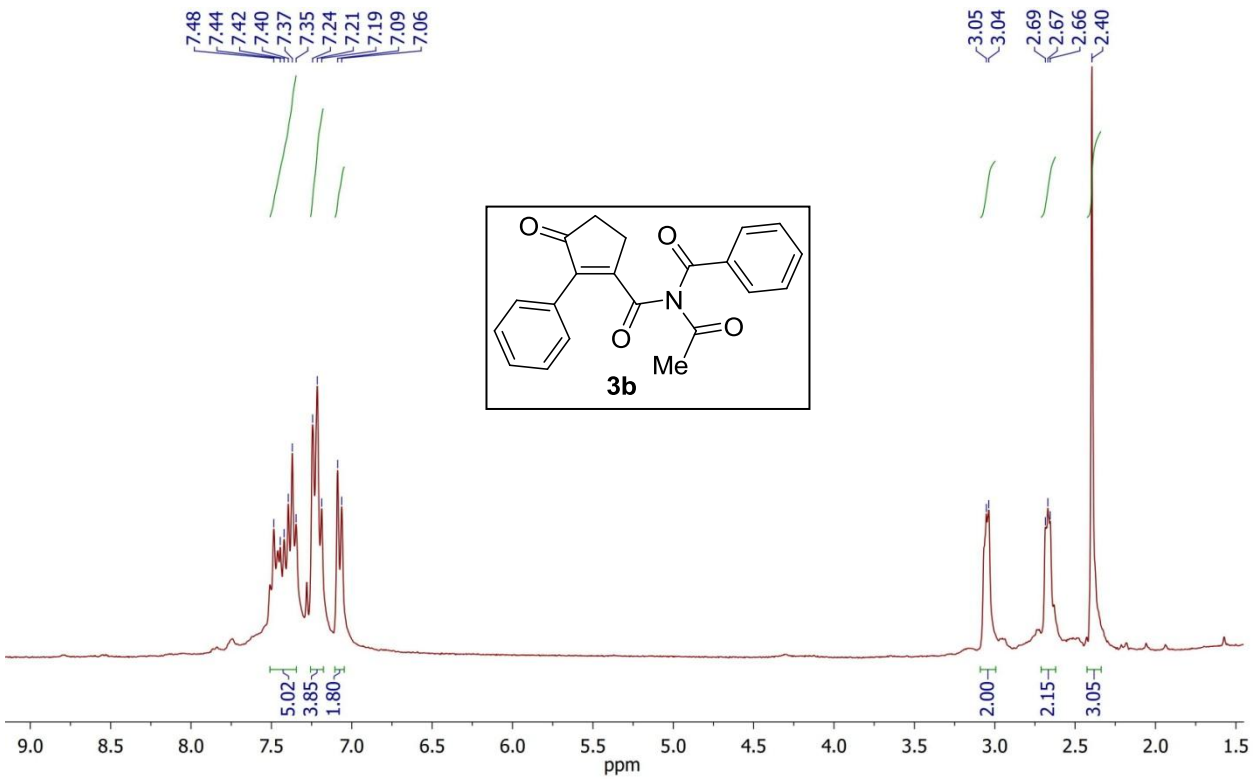
^{1}H NMR spectrum of compound 3a (DMSO-d_6)



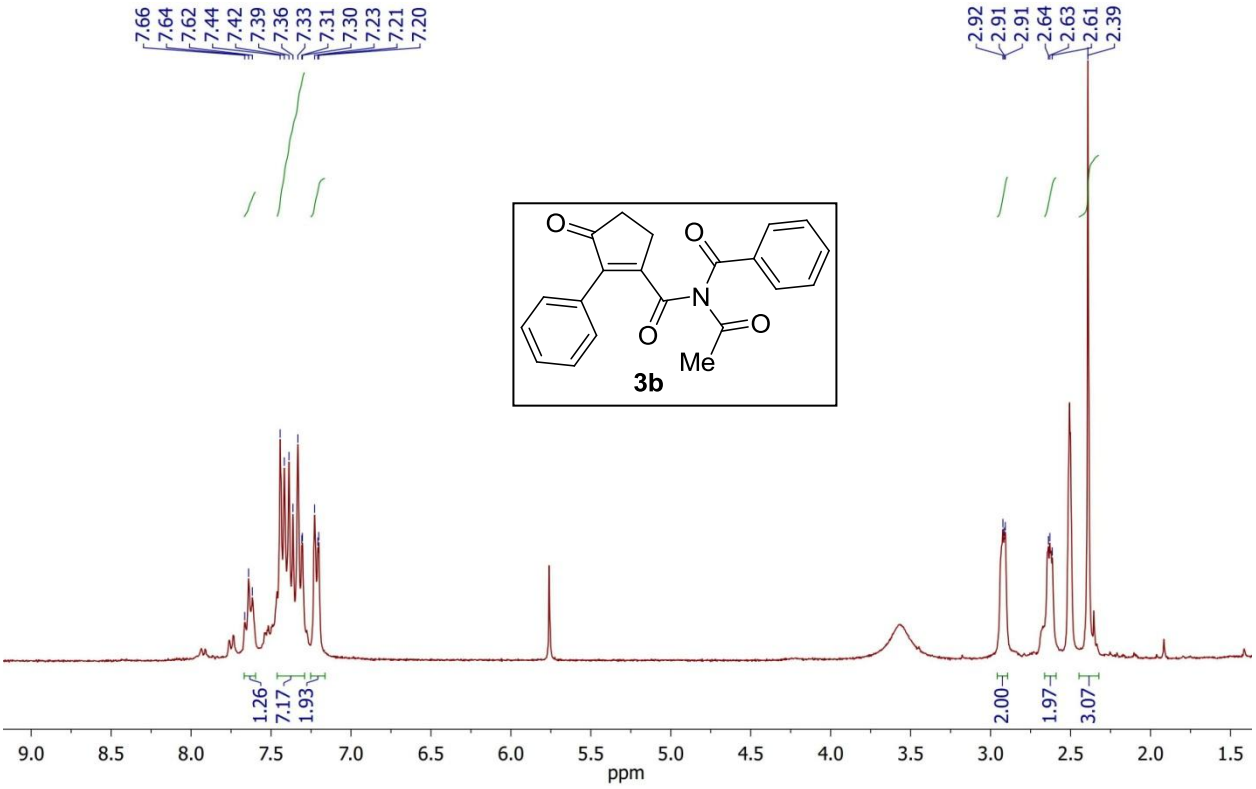
^{13}C NMR spectrum of compound 3a (DMSO-d_6)



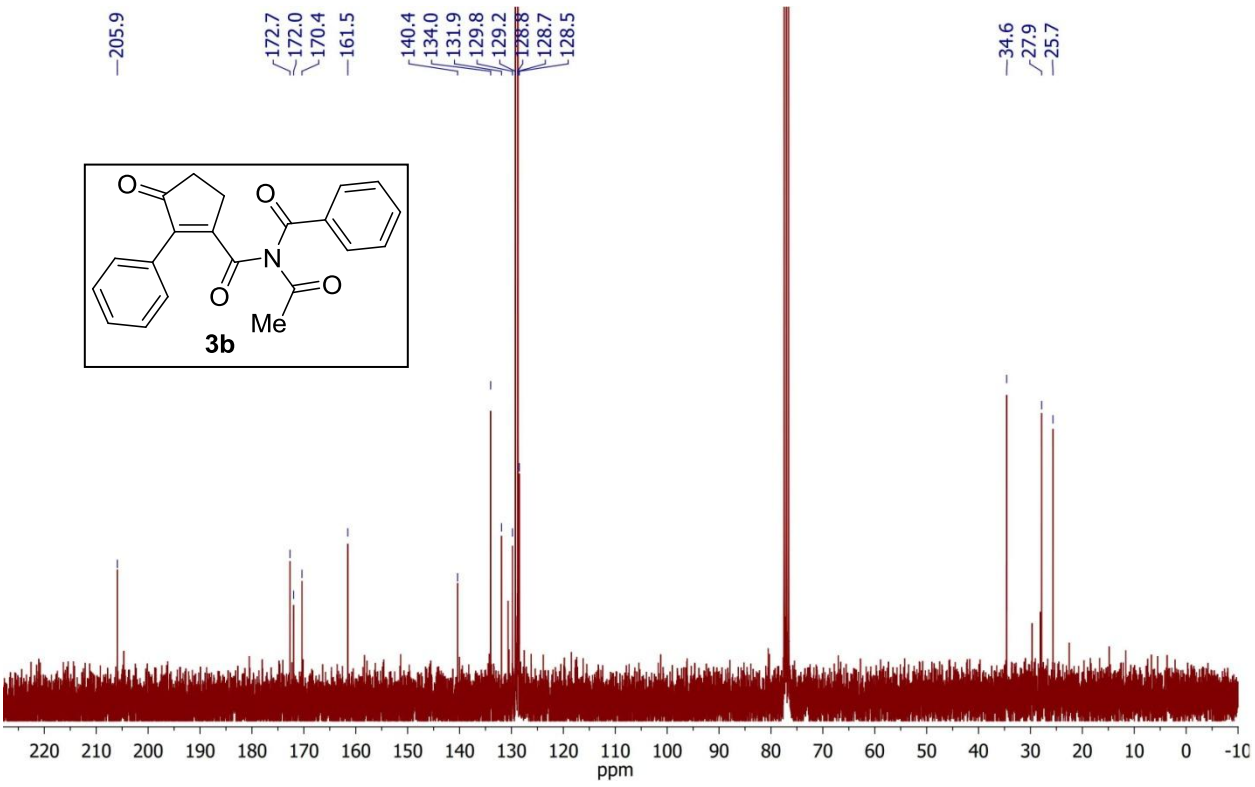
^{1}H NMR spectrum of compound 3b ($CDCl_3$)



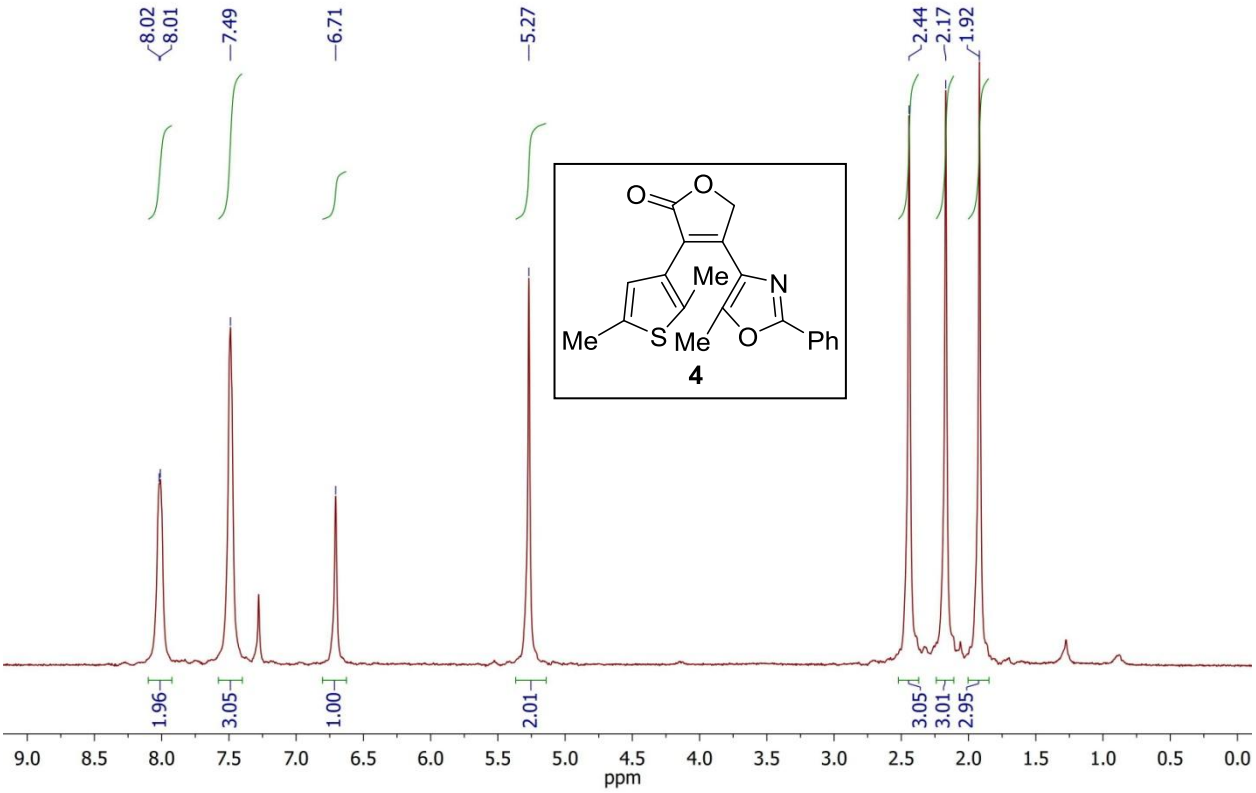
^{1}H NMR spectrum of compound 3b (DMSO-d_6)



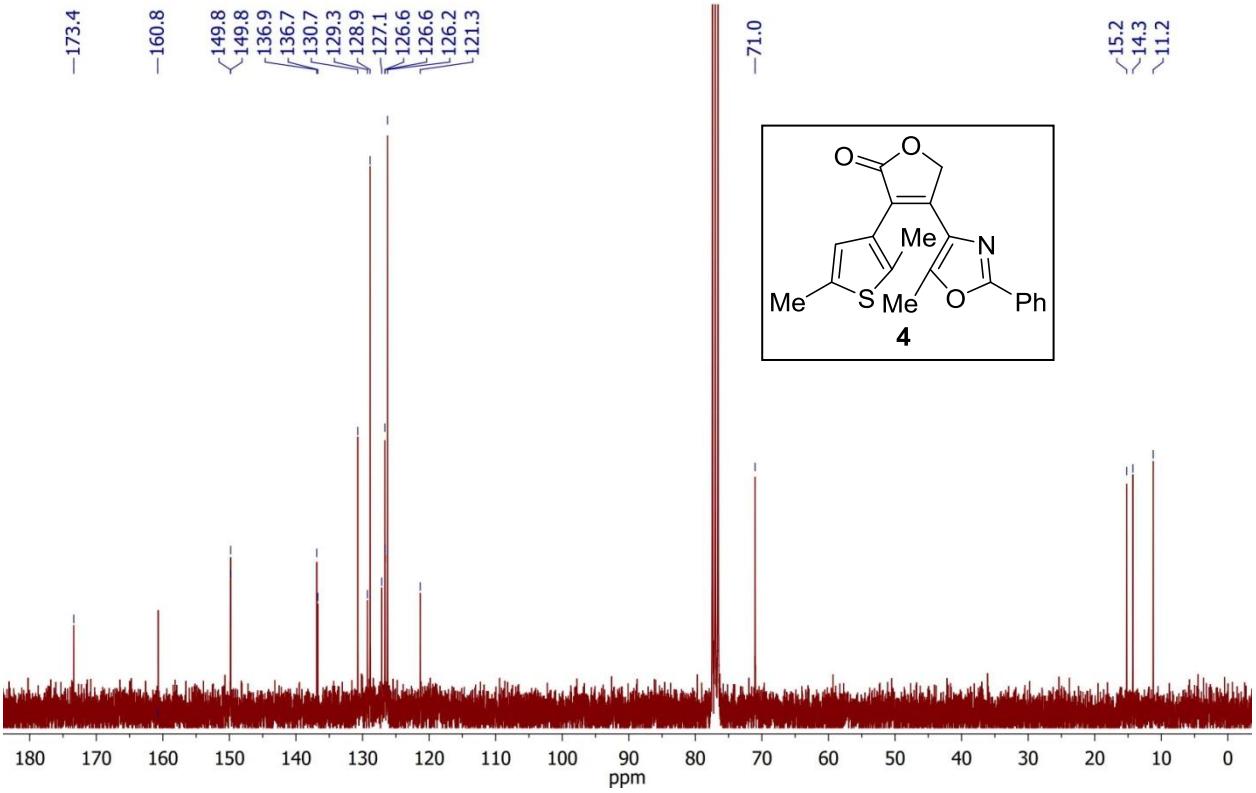
^{13}C NMR spectrum of compound 3b ($CDCl_3$)



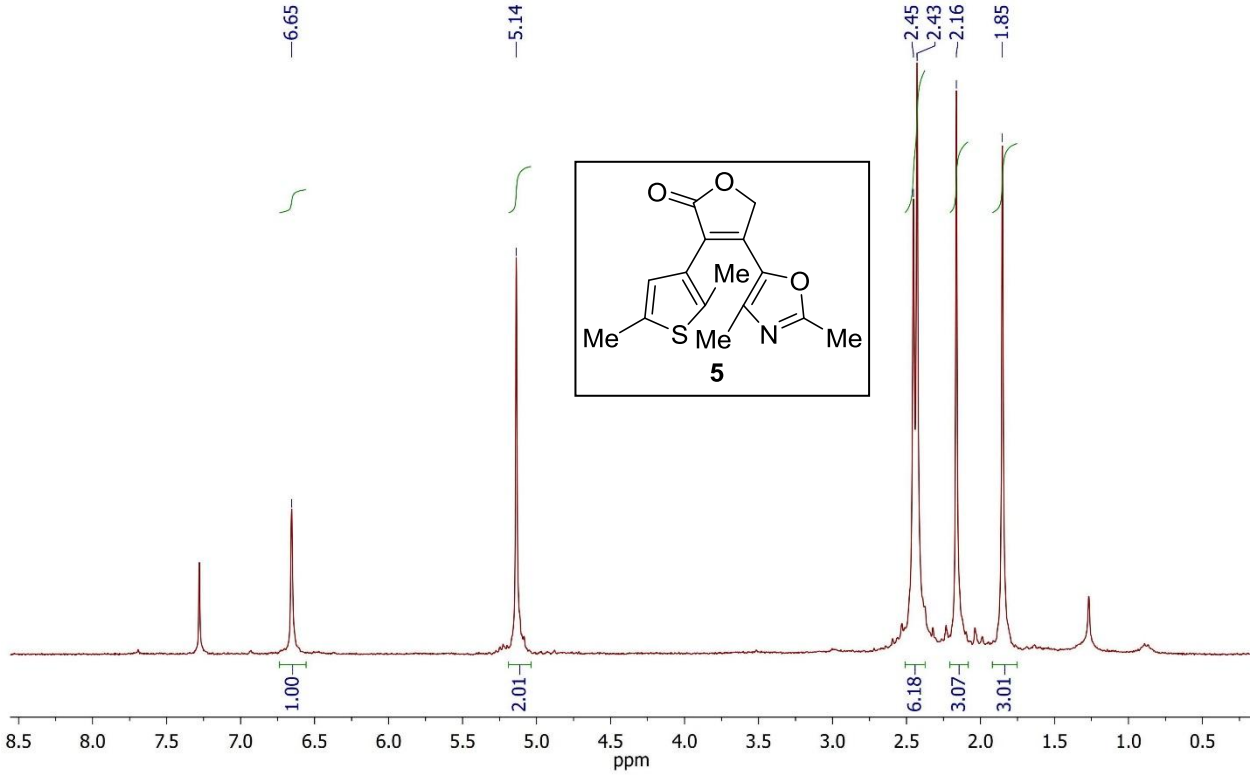
^{1}H NMR spectrum of compound 4



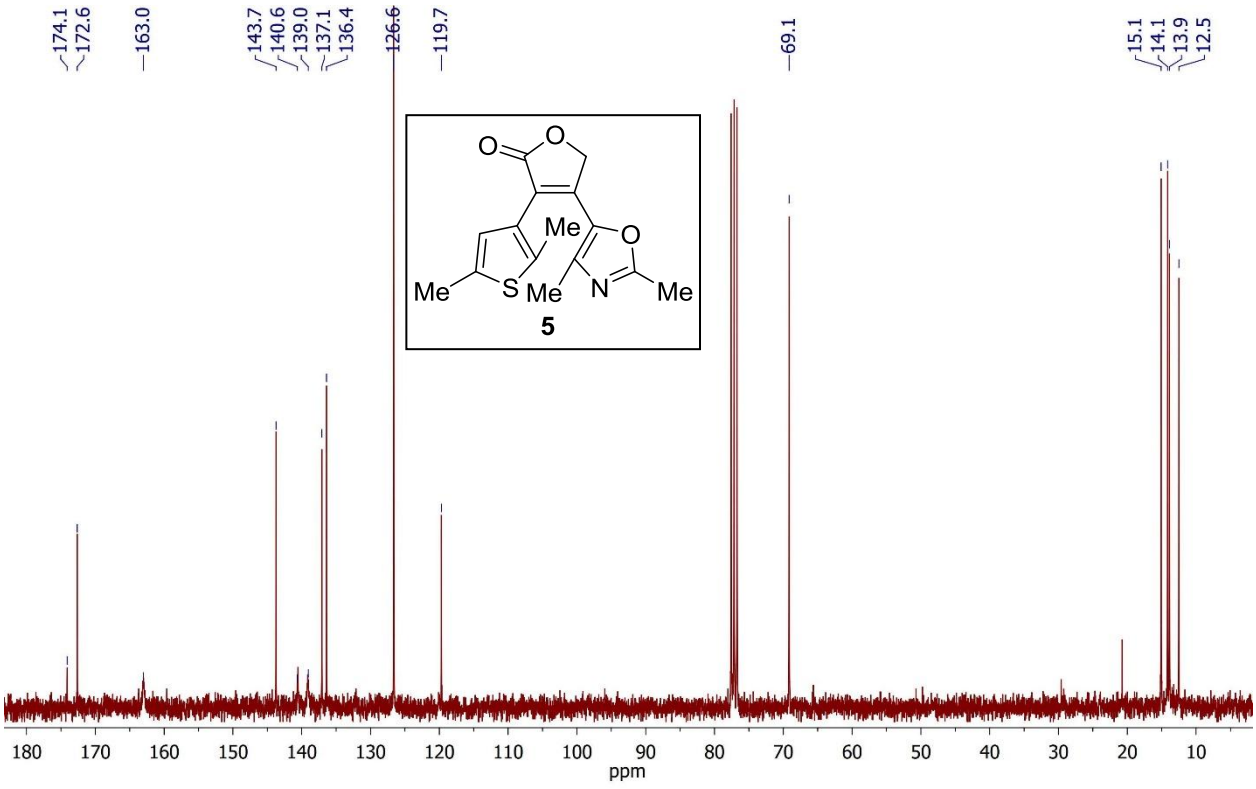
^{13}C NMR spectrum of compound 4



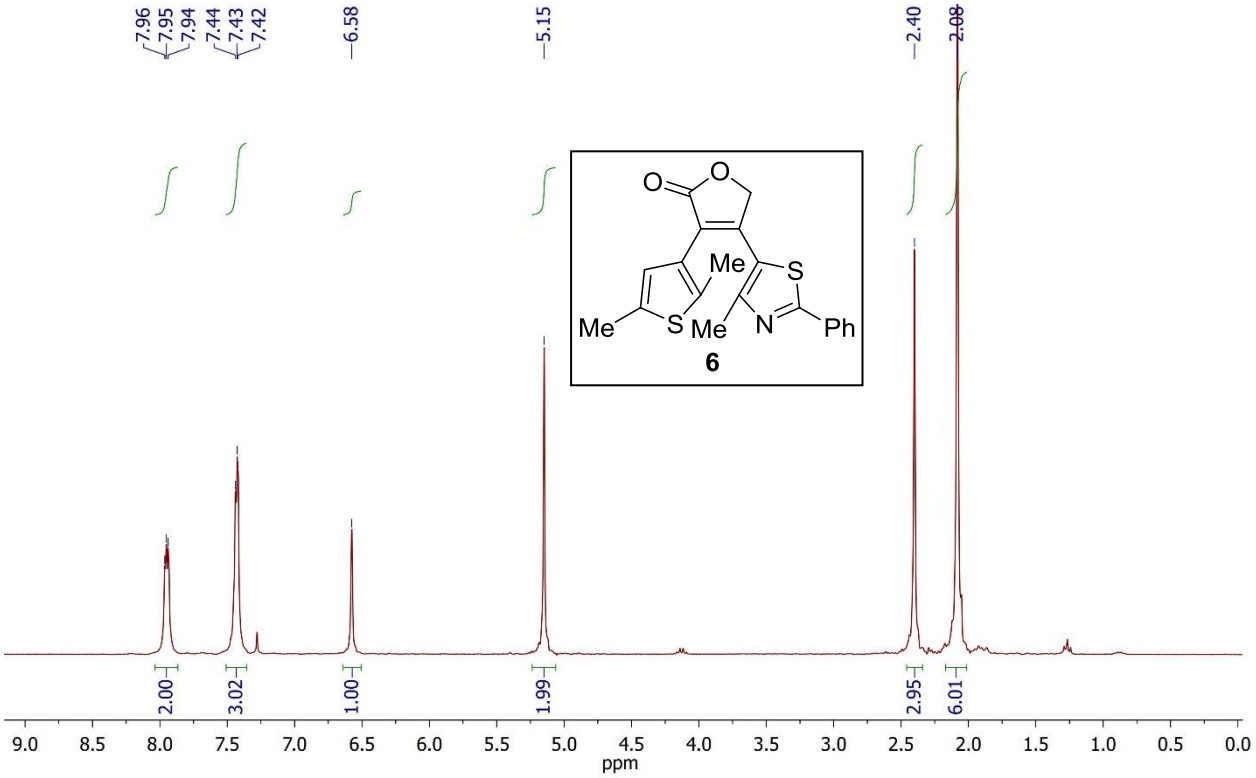
^{1}H NMR spectrum of compound 5



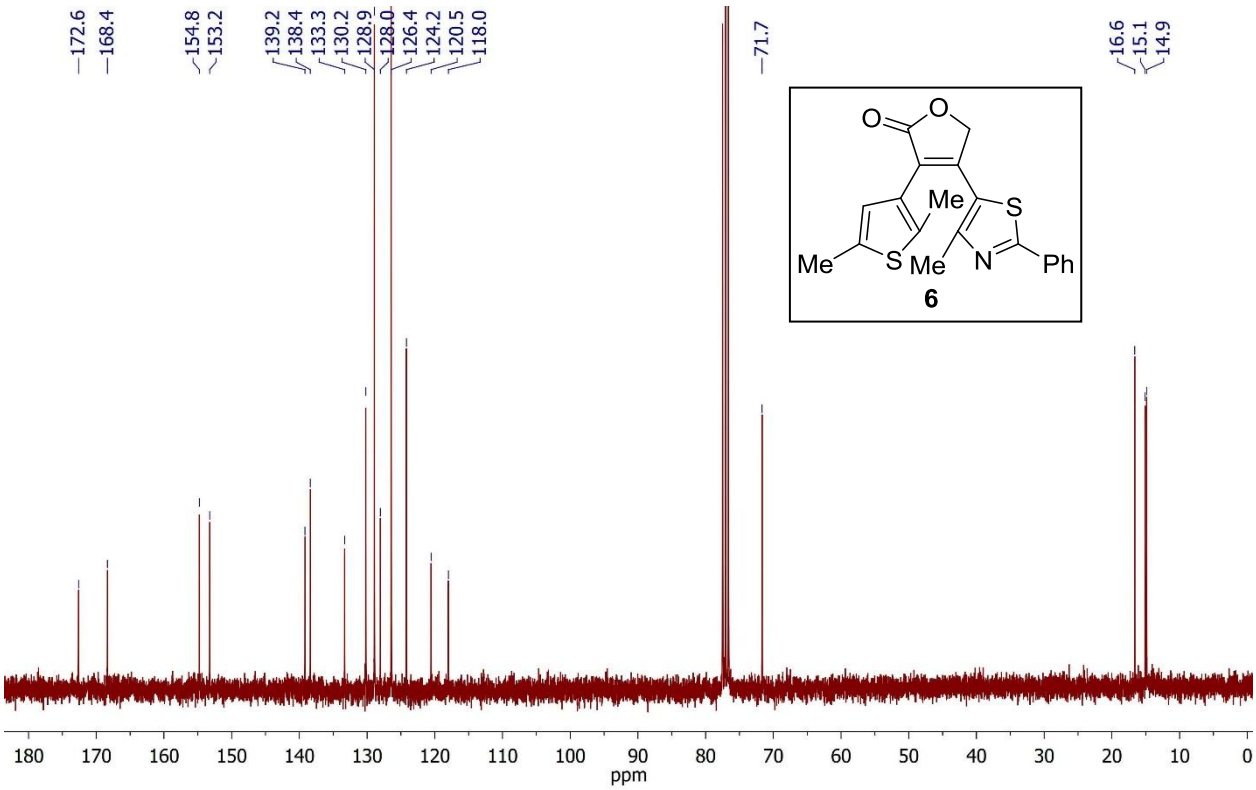
^{13}C NMR spectrum of compound 5



^{1}H NMR spectrum of compound 6

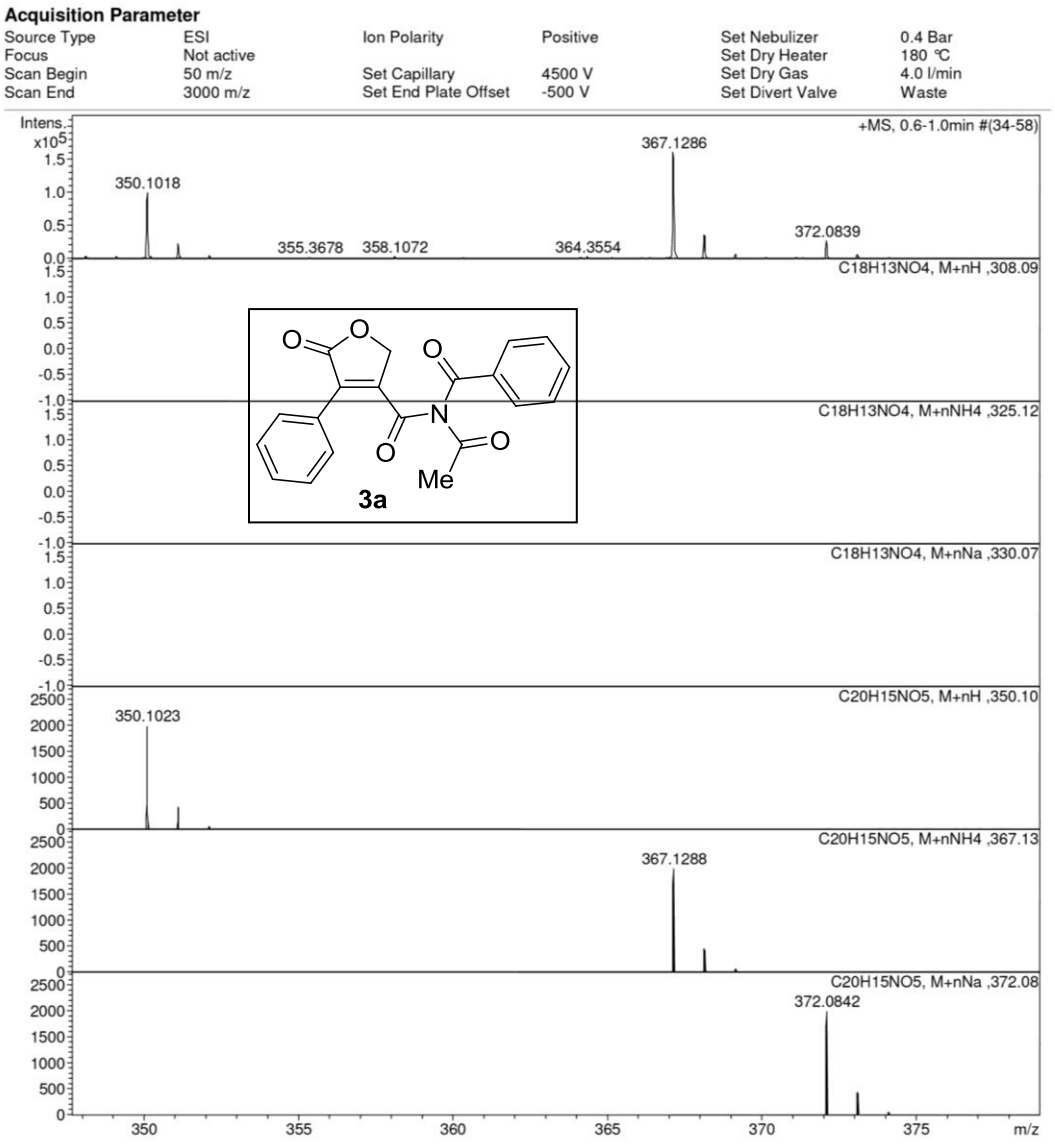


^{13}C NMR spectrum of compound 6

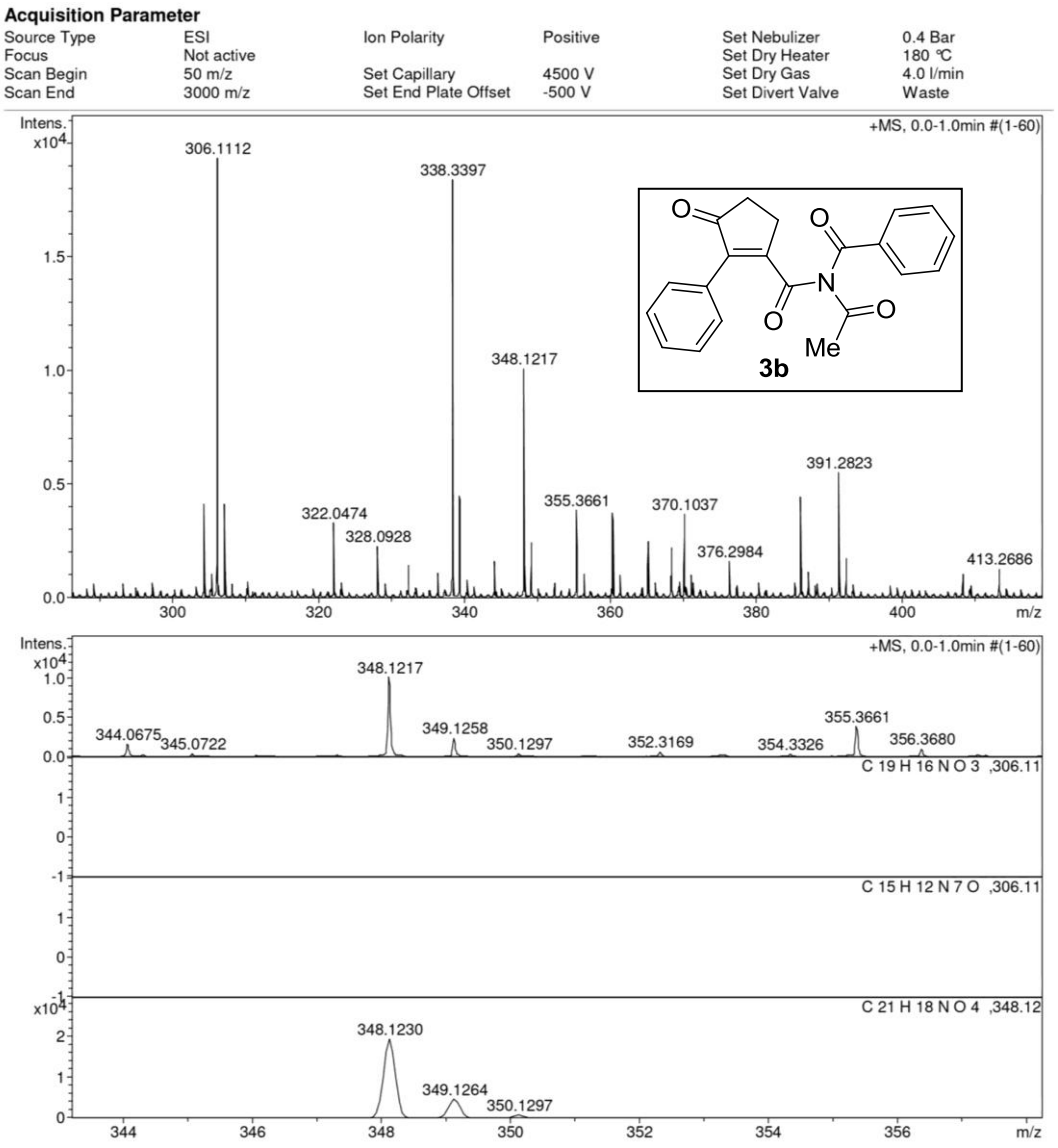


VIII. Copies of HRMS spectra

Compound 3a



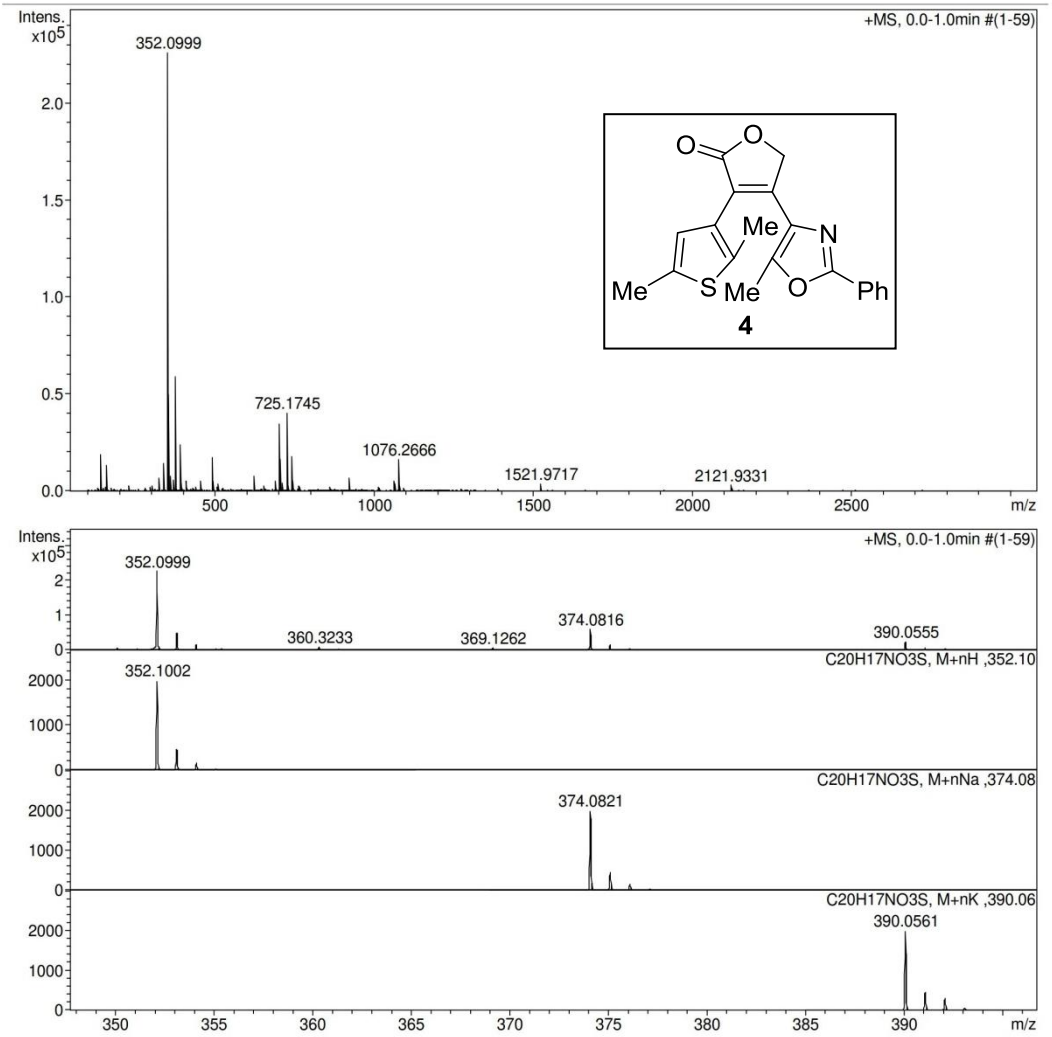
Compound 3b


Acquisition Parameter
Source Type ESI
Ion Polarity Positive
Set Nebulizer 0.4 Bar
Focus Not active
Set Dry Heater 180 °C
Scan Begin 50 m/z
Set Capillary 4500 V
Set Dry Gas 4.0 l/min
Scan End 3000 m/z
Set End Plate Offset -500 V
Set Divert Valve Waste
+MS, 0.0-1.0min #(1-60)
306.1112
338.3397
348.1217
322.0474
328.0928
355.3661
370.1037
376.2984
391.2823
413.2686
3b
C 19 H 16 N O 3 ,306.11
C 15 H 12 N 7 O ,306.11
C 21 H 18 N O 4 ,348.12
348.1230
349.1264
350.1297
344.0675
345.0722
349.1258
352.3169
354.3326
356.3680
m/z

Compound 4

Acquisition Parameter

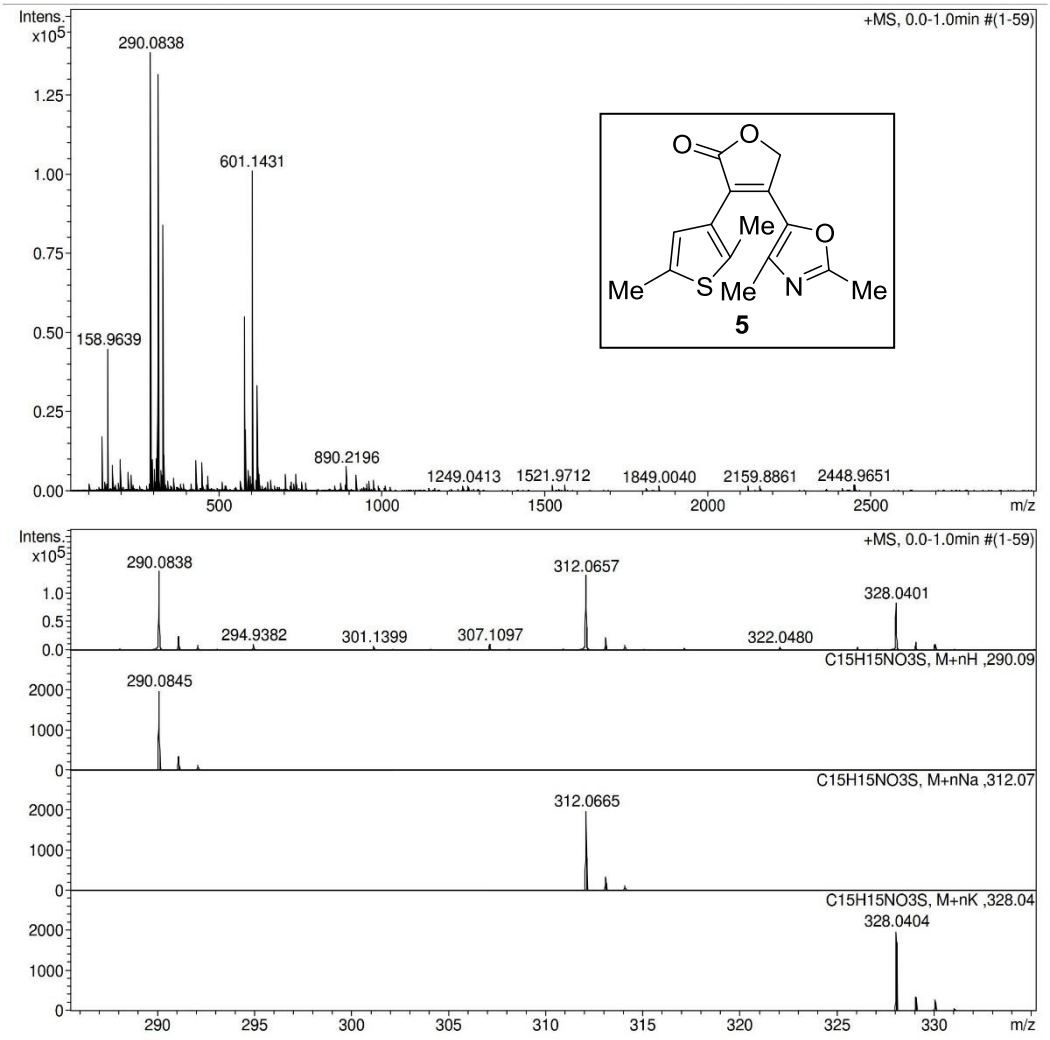
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



Compound 5

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 ℃
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



Compound 6

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste