Supporting Information

Photoactivatable Anthracenes

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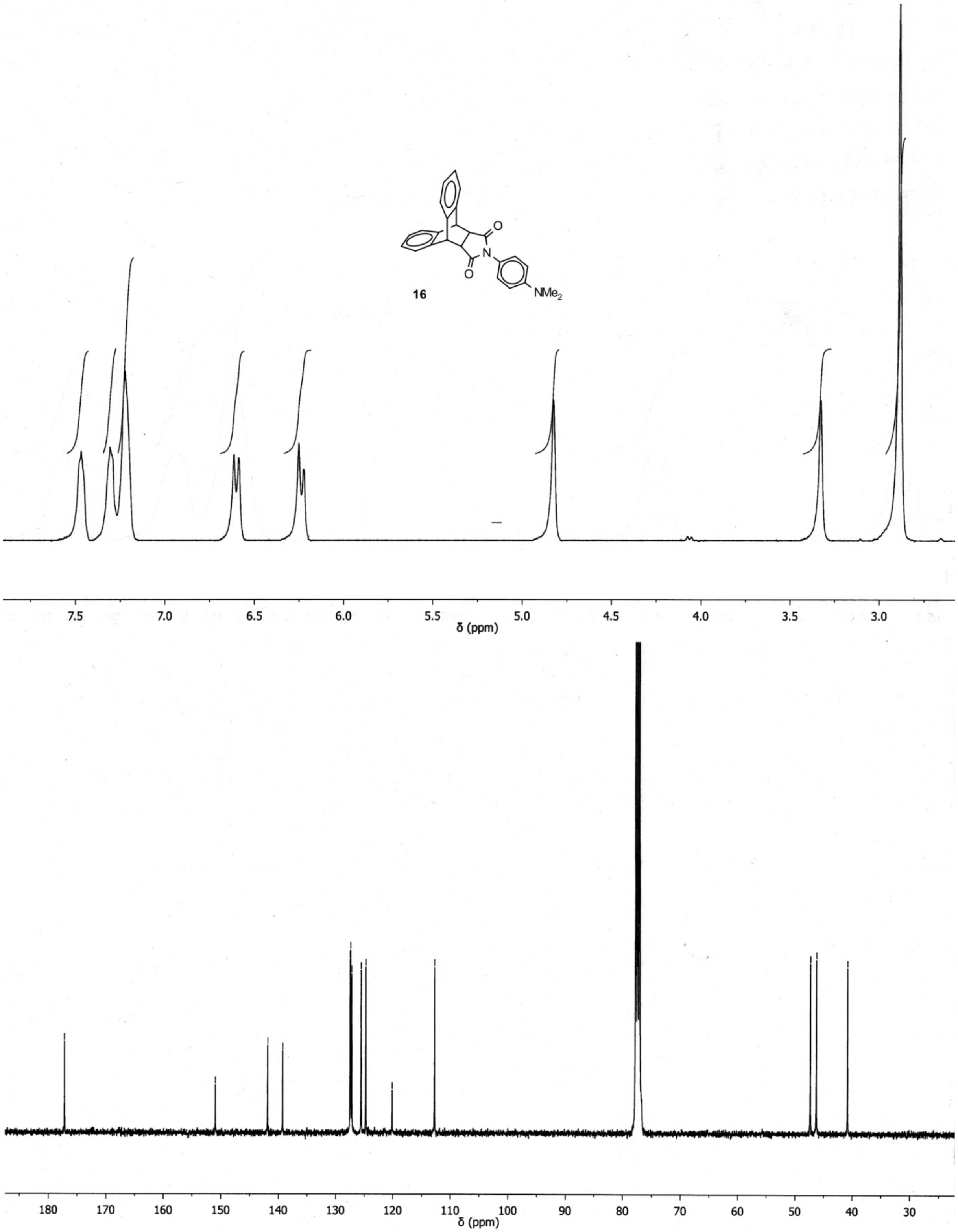

Figure S1. ^{1}H and ^{13}C NMR spectra of **16** in CD_3CN and $CDCl_3$ respectively at 25 °C.

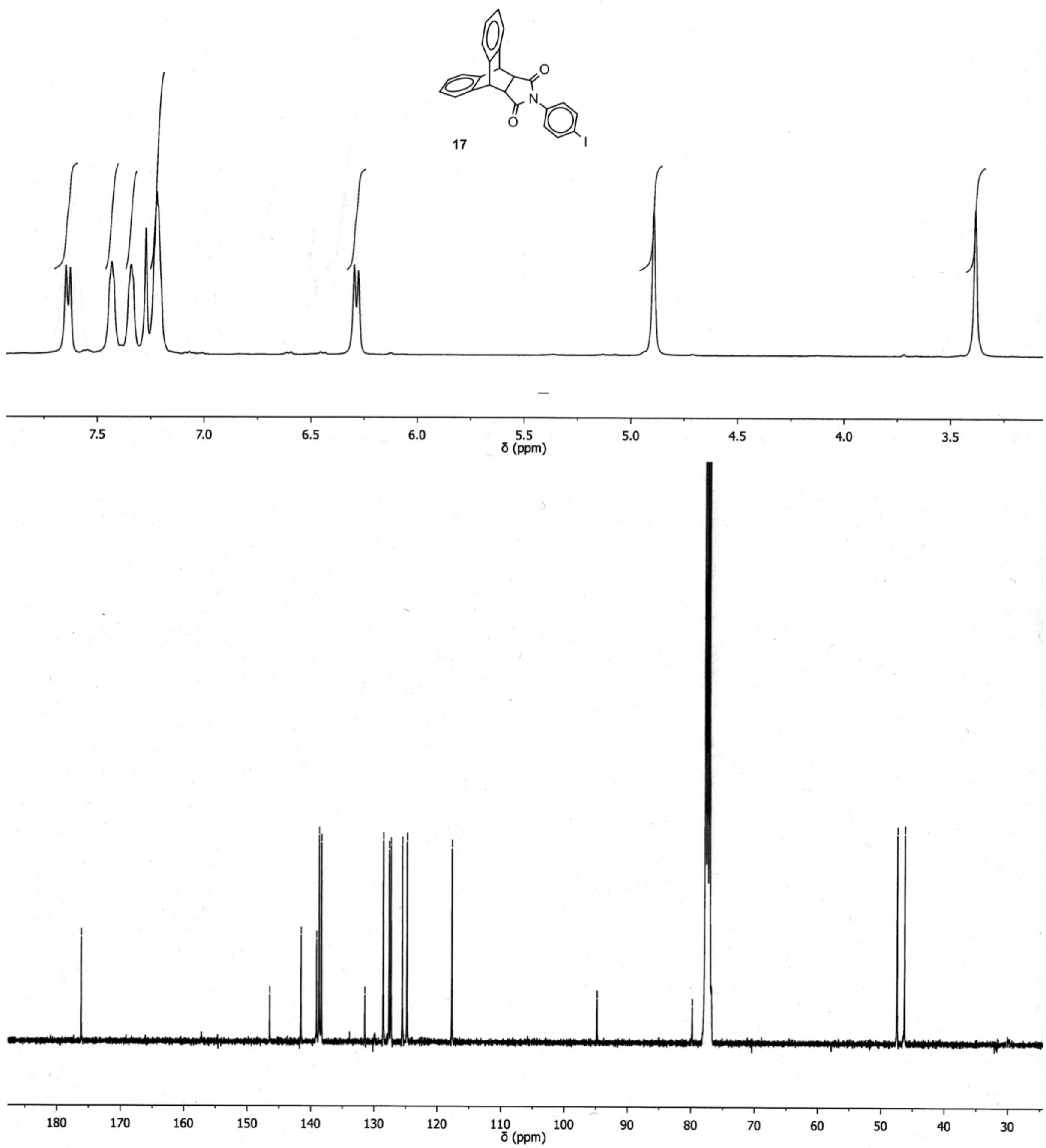

Figure S2. ^{1}H and ^{13}C NMR spectra of **17** in $CDCl_3$ at 25 °C.

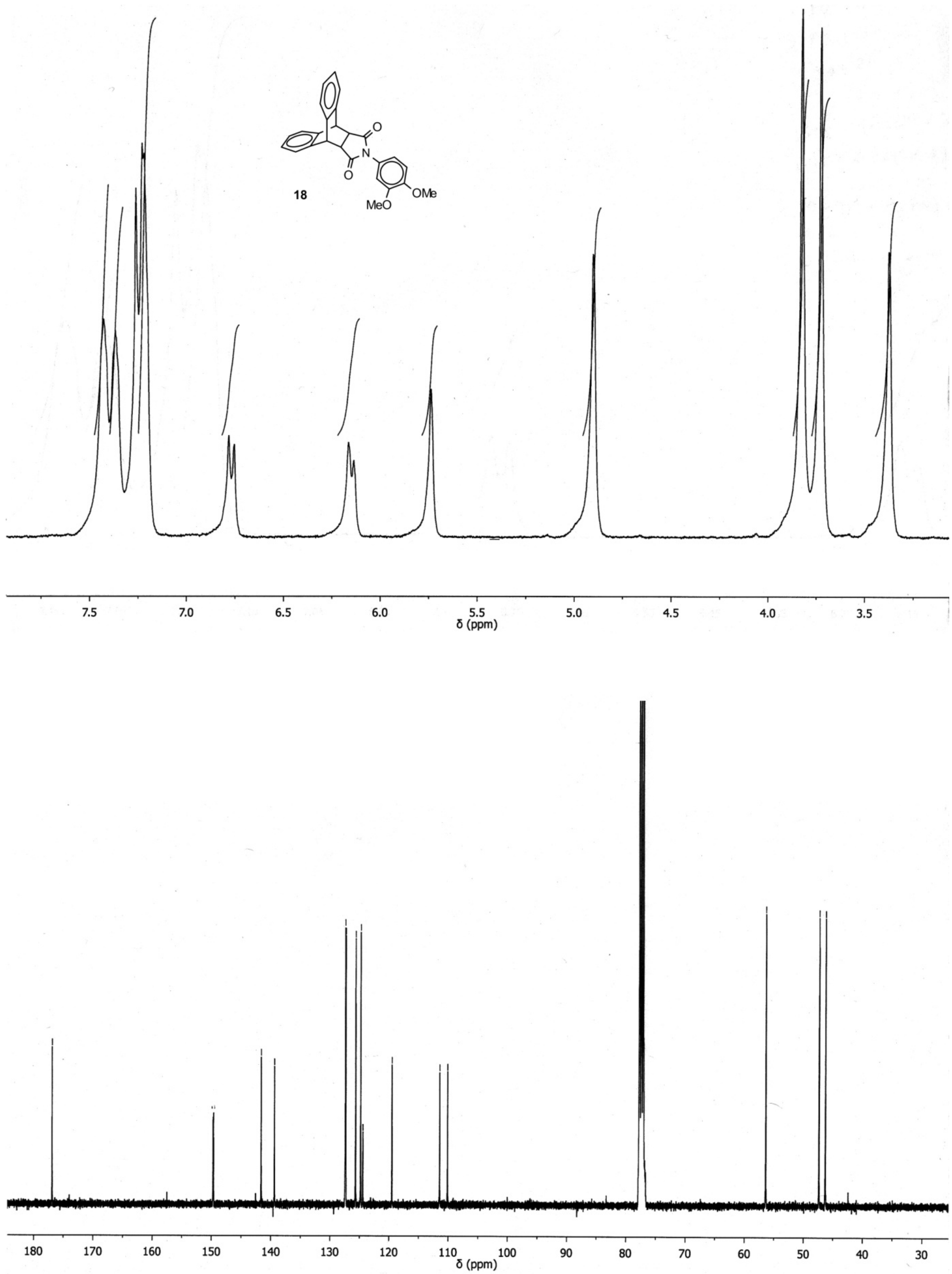

Figure S3. ^{1}H and ^{13}C NMR spectra of **18** in $CDCl_3$ at 25 °C.

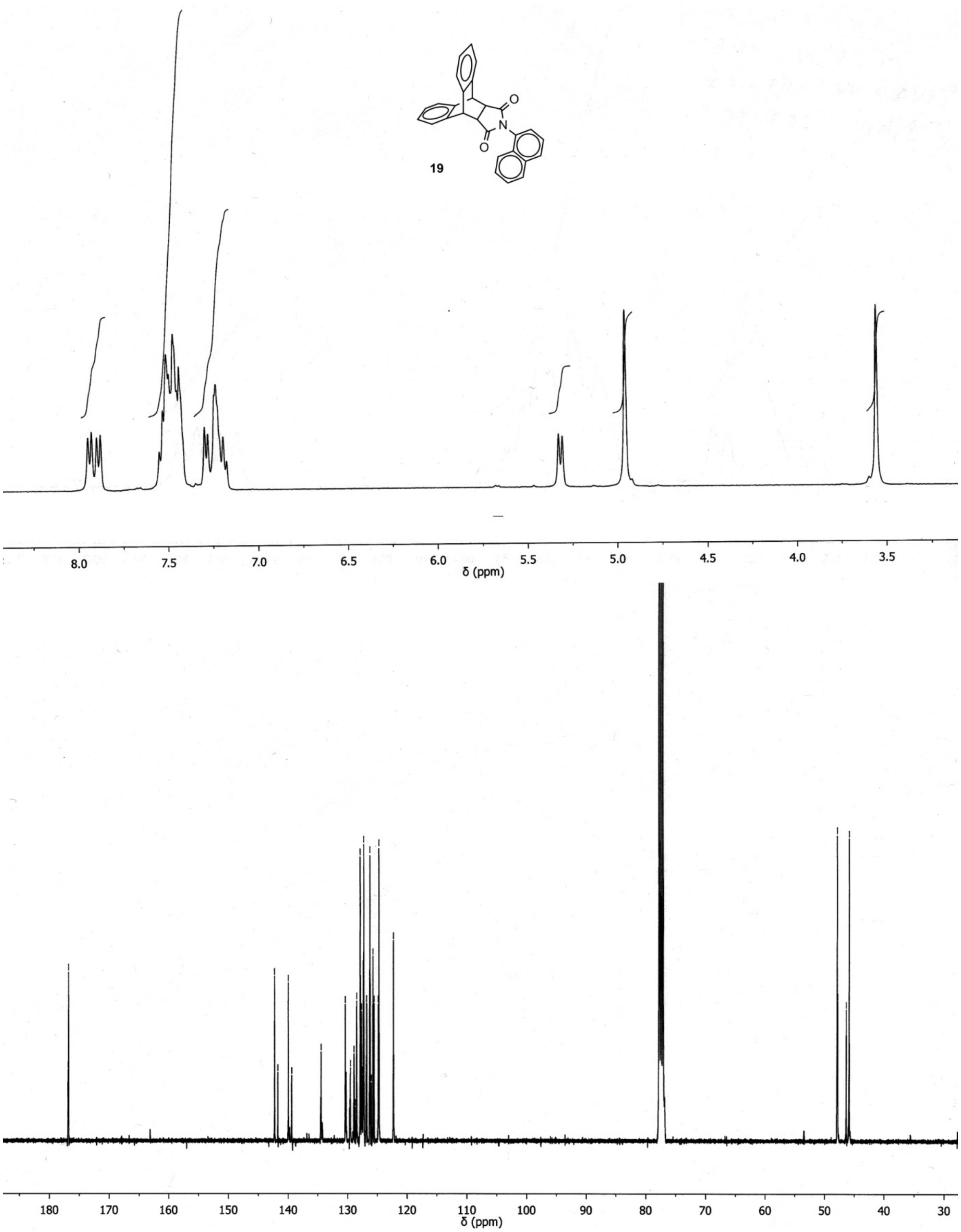

Figure S4. ^{1}H and ^{13}C NMR spectra of **19** in CD_3CN and $CDCl_3$ respectively at 25 °C.

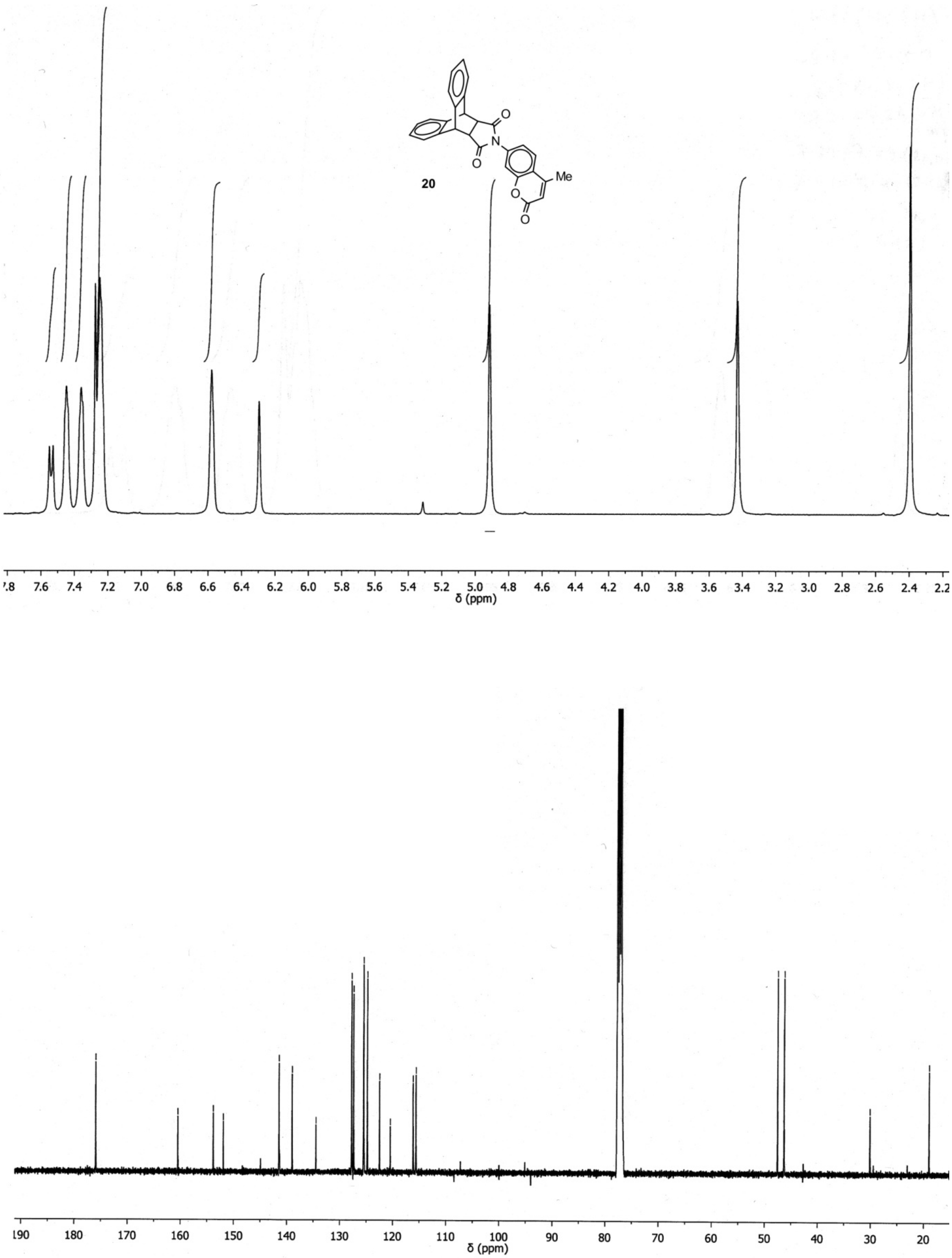

Figure S5. ^{1}H and ^{13}C NMR spectra of **20** in $CDCl_3$ at 25 °C.

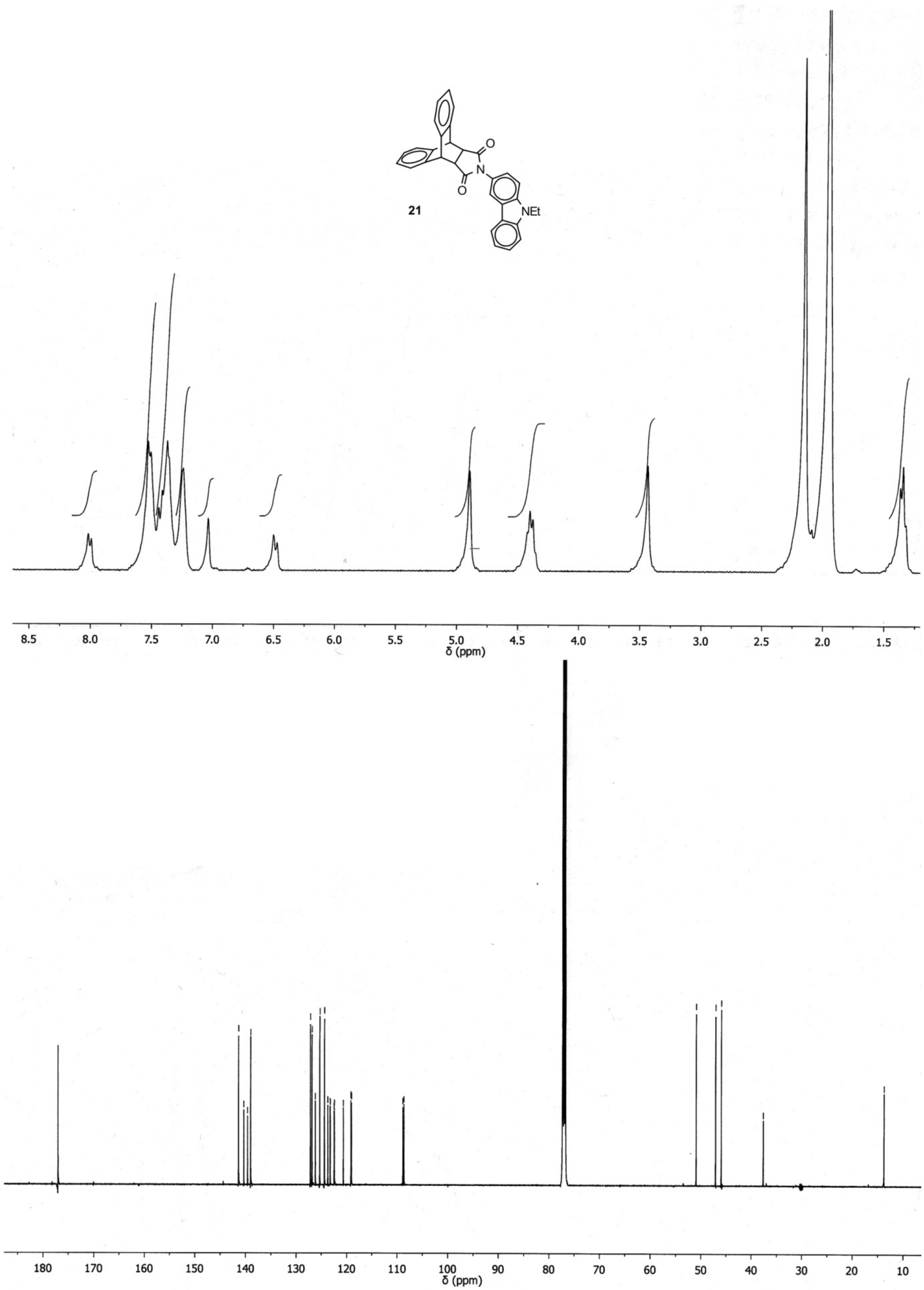

Figure S6. ^{1}H and ^{13}C NMR spectra of **21** in CD_3CN and $CDCl_3$ respectively at 25 °C.

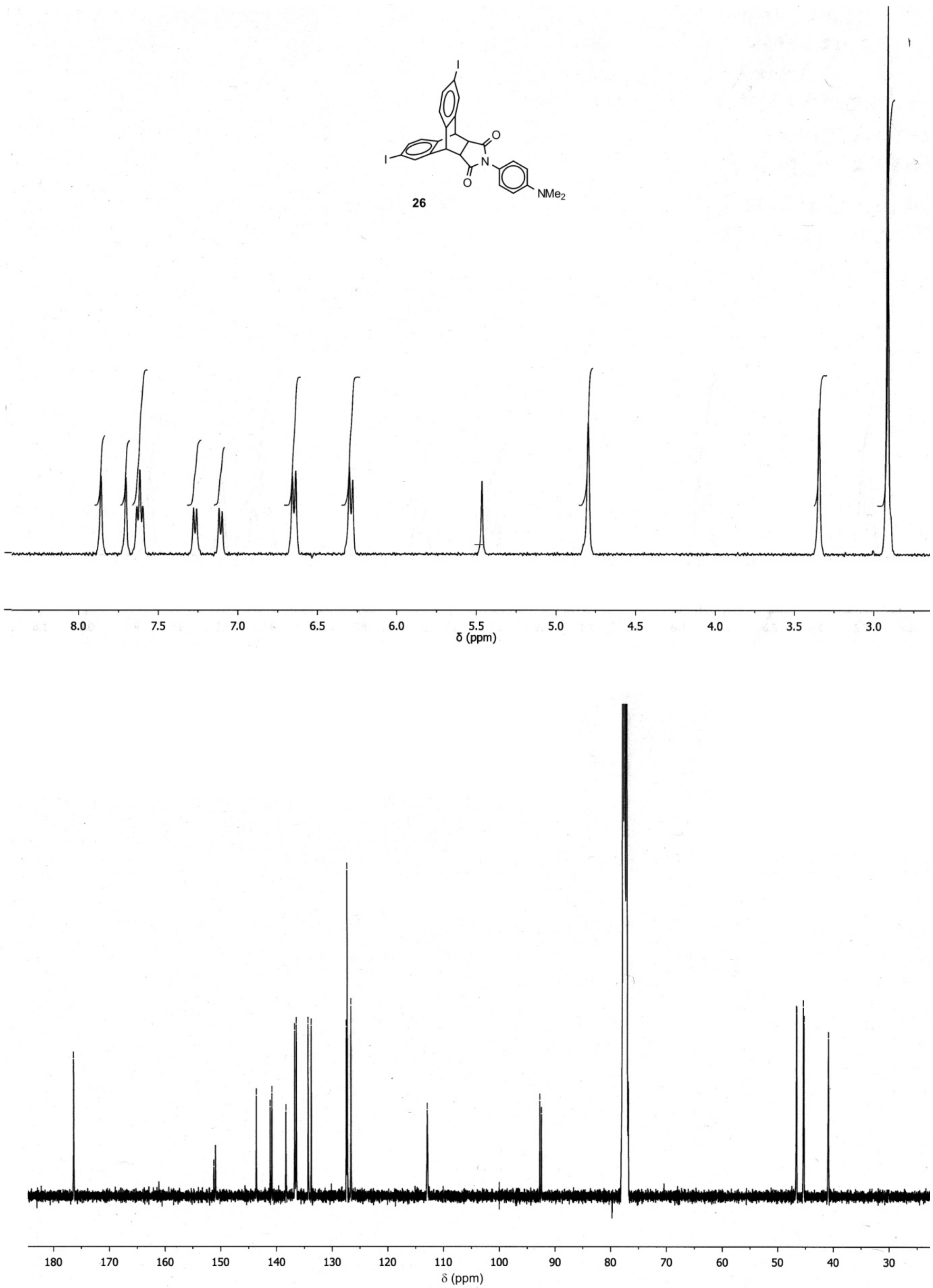

Figure S7. ^{1}H and ^{13}C NMR spectra of **26** in CD_3CN and $CDCl_3$ respectively at 25 °C.

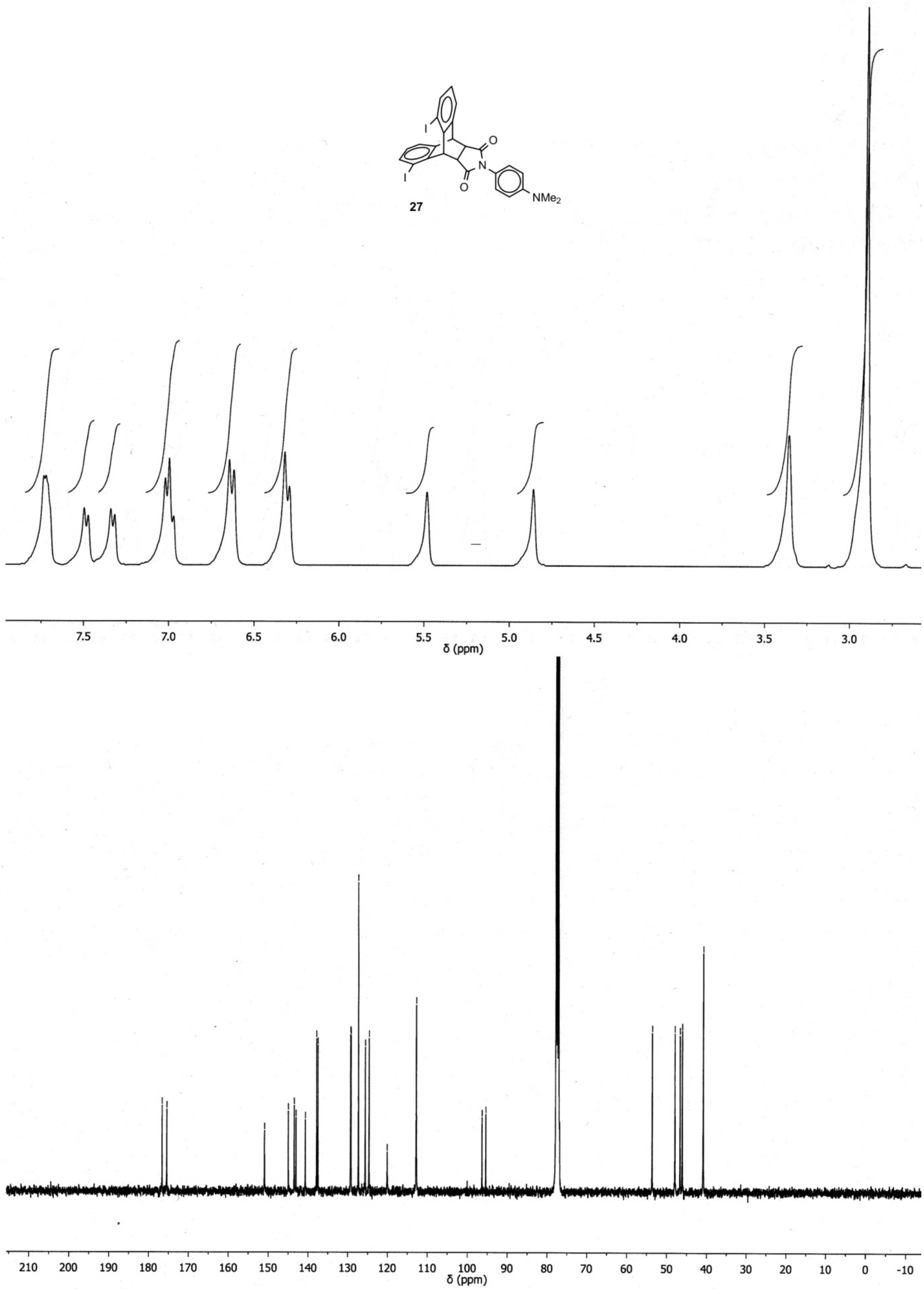

Figure S8. ^{1}H and ^{13}C NMR spectra of **27** in CD_3CN and $CDCl_3$ respectively at 25 °C.

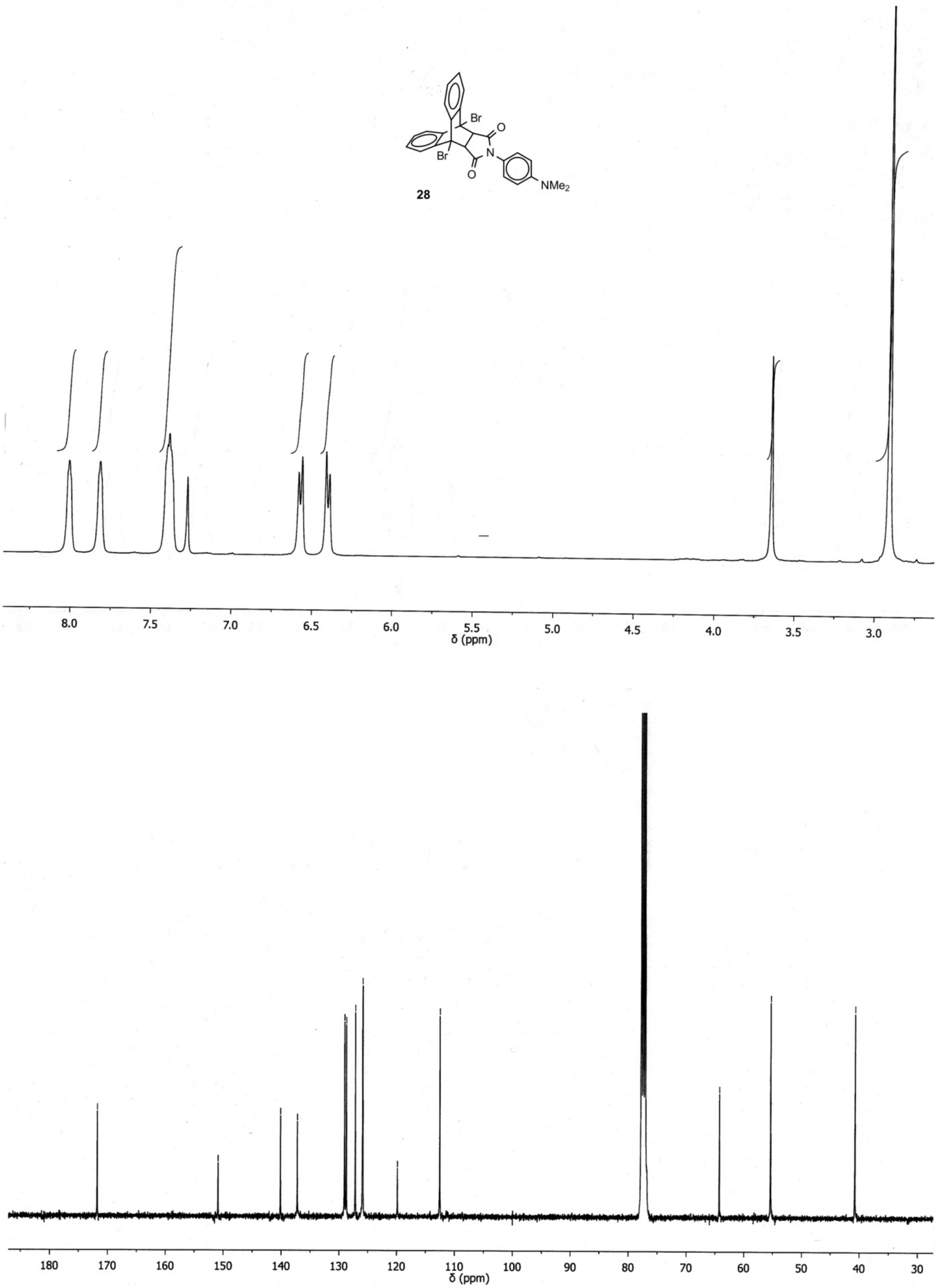

Figure S9. ^{1}H and ^{13}C NMR spectra of **28** in $CDCl_3$ at 25 °C.

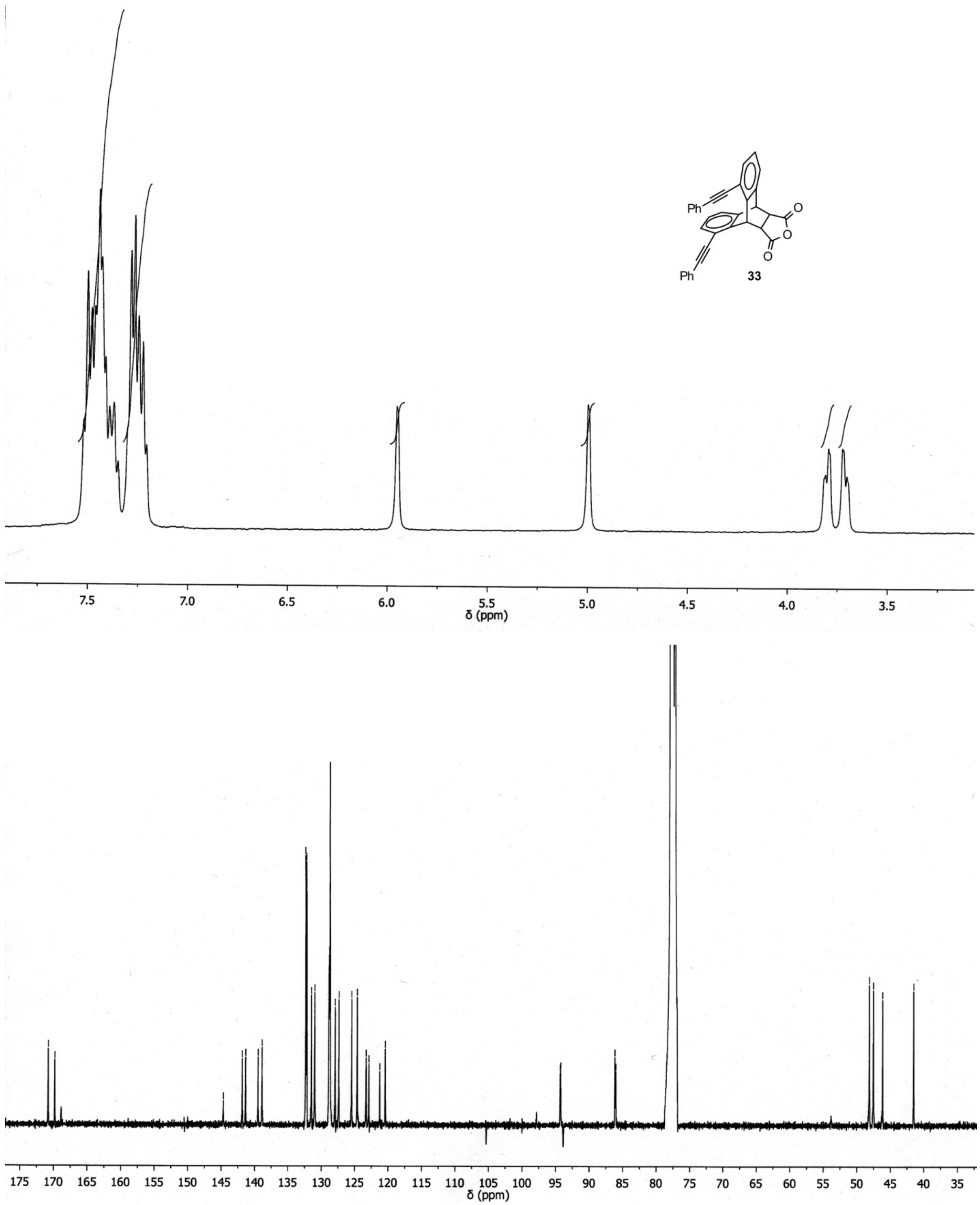

Figure S10. ^{1}H and ^{13}C NMR spectra of **33** in CD_3CN and $CDCl_3$ respectively at 25 °C.

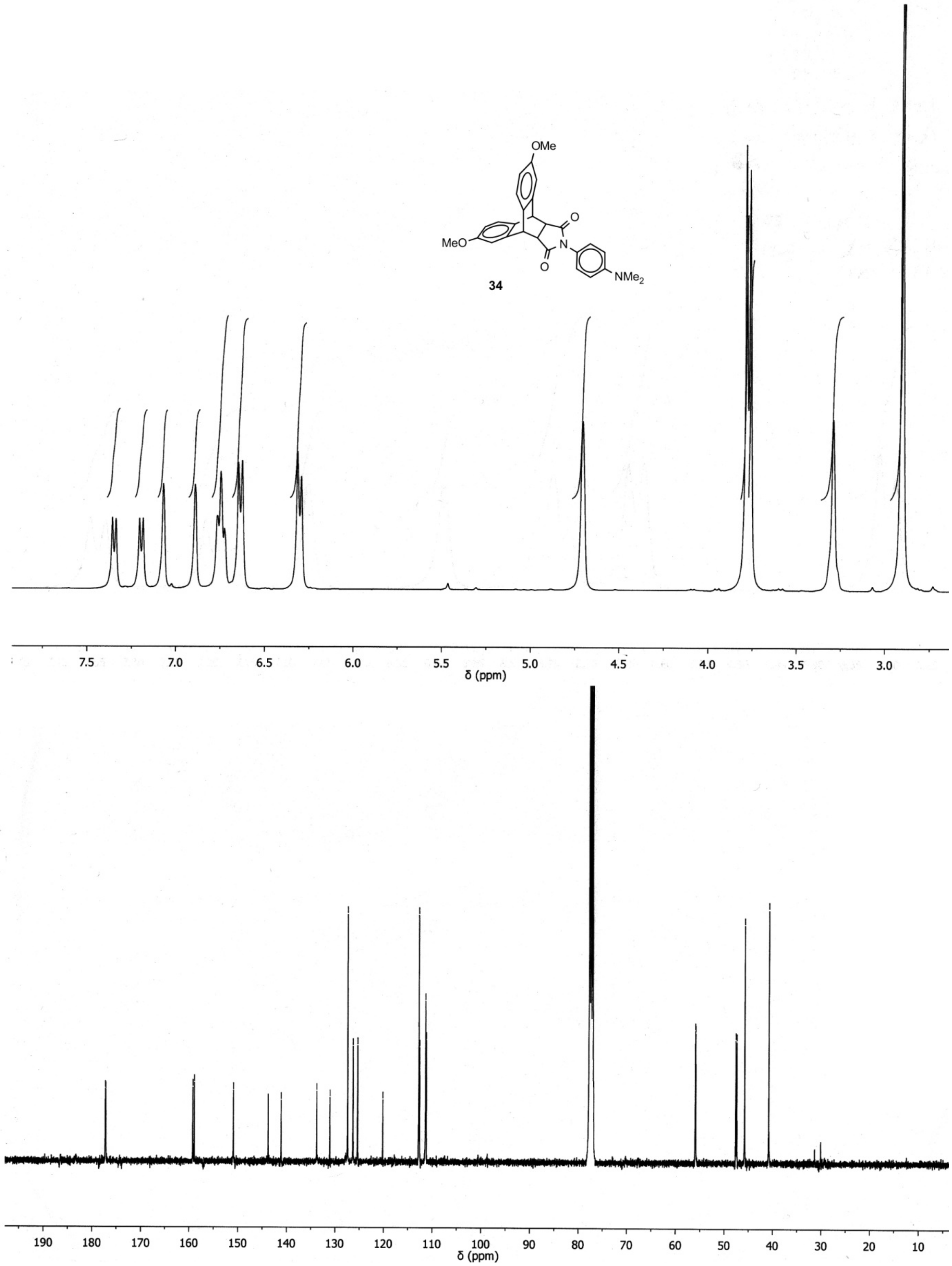

Figure S11. ^{1}H and ^{13}C NMR spectra of **34** in CD_3CN and $CDCl_3$ respectively at 25 °C.

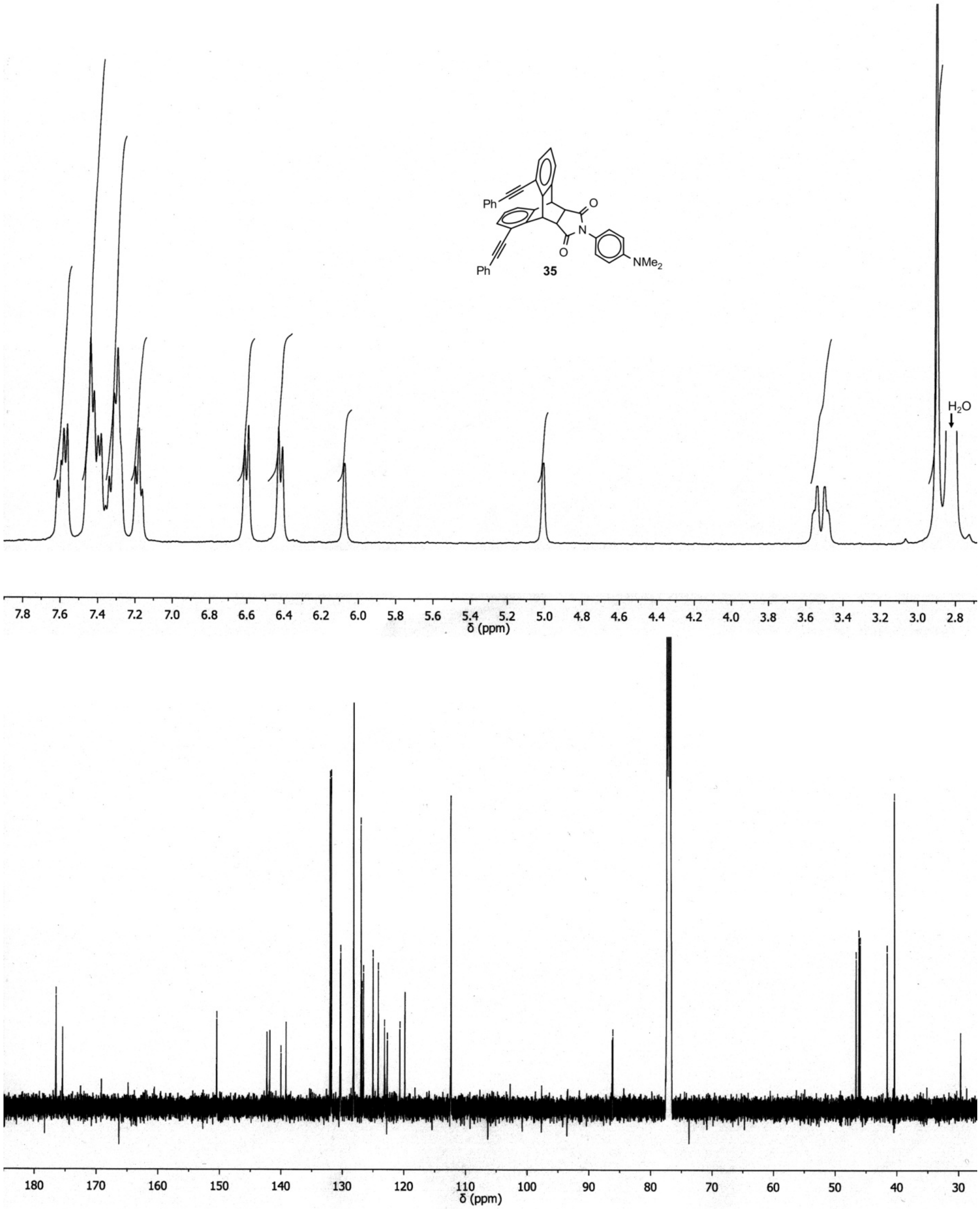

Figure S12. ^{1}H and ^{13}C NMR spectra of **35** in $[(CD_3)_2CO$ and $CDCl_3$ respectively at 25 °C.

Table S1. Crystallographic Data for **15**, **16**, **18** and **19**.

	15	**16**	**18**	**19**
Empirical Formula	$C_{25}H_{19}NO_3$	$C_{26}H_{22}N_2O_4$	$C_{26}H_{21}NO_4$	$C_{28}H_{19}NO_2$
Formula Weight	381.41	394.46	411.44	401.44
Crystal System	Triclinic	Triclinic	Orthorhombic	Monoclinic
Lattice Parameters:				
a (Å)	10.0356(4)	8.7939(4)	8.6359(3)	10.8929(6)
b (Å)	12.8316(5)	9.6279(4)	12.0457(5)	8.6496(5)
c (Å)	16.3402(7)	12.5660(6)	19.5543(8)	21.3698(13)
α (°)	80.535(1)	76.008(1)	90	90
β (°)	80.757(1)	78.669(1)	90	95.896(1)
γ (°)	74.556(1)	85.631(1)	90	90
V (Å^3)	1985.42(14)	1011.77(8)	2034.15(14)	2002.8
Space Group	$P\overline{1}$ (# 2)	$P\overline{1}$ (# 2)	$P2_12_12_1$ (# 19)	$P2_1/n$ (# 14)
Z Value	4	2	4	4
ρ_{calc} (g cm^{-3})	1.276	1.295	1.343	1.331
μ (Mo Kα) (mm^{-1})	0.084	0.082	0.091	0.084
T (K)	296	296	296	296
$2\Theta_{max}$ (°)	51.0	54.0	60.0	52.0
No. Obs. ($I > 2\sigma(I)$)	5765	3760	5379	2958
No. Parameters	525	274	282	280
Goodness of Fit	1.018	1.040	1.036	1.029
Max. Shift in Cycle	0.00	0.00	0.001	0.00
*Residuals**: R1; wR2	0.0398; 0.0985	0.0394; 0.1020	0.0381; 0.0992	0.0394; 0.0947
Absorption Correction, Max/min	Multi-scan 0.9900/0.9688	Multi-scan 0.7465/0.6896	Multi-scan 0.7465/0.6987	Multi-scan 0.9967/0.9689
Largest Peak in Final Diff. Map (e$^-$ Å^{-3})	0.161	0.188	0.225	0.173

* $R = \Sigma_{hkl}(||F_{obs}|-|F_{calc}||)/\Sigma_{hkl}|F_{obs}|$; $R_w = [\Sigma_{hkl}w(|F_{obs}|-|F_{calc}|)^2/\Sigma_{hkl}wF_{obs}^2]^{1/2}$, $w = 1/\sigma^2(F_{obs})$; $GOF = [\Sigma_{hkl}w(|F_{obs}|-|F_{calc}|)^2/(n_{data} - n_{vari})]^{1/2}$

Table S2. Crystallographic Data for **20**, **21**, **28** and **34**.

	20	**21**	**28**	**34**
Empirical Formula	$C_{28}H_{19}NO_4$	$C_{32}H_{24}N_2O_2$	$C_{26}H_{20}N_2O_2Br_2$	$C_{28}H_{26}N_2O_4$
Formula Weight	433.44	468.53	552.26	454.51
Crystal System	Triclinic	Triclinic	Monoclinic	Triclinic
Lattice Parameters:				
a (Å)	8.1852(4)	9.7650(4)	9.3468(4)	9.8381(8)
b (Å)	8.4437(4)	11.9476(5)	14.5715(6)	10.4824(9)
c (Å)	16.9210(9)	12.3011(5)	16.6456(6)	12.5322(11)
α (°)	97.887(1)	113.172(1)	90	74.656(1)
β (°)	93.333(1)	101.293(1)	105.260(1)	74.429(1)
γ (°)	111.291(1)	106.109(1)	90	71.299(1)
V (Å^3)	1071.93(9)	1189.59(8)	2187.15(15)	1156.45(17)
Space Group	$P\bar{1}$ (# 2)	$P\bar{1}$ (# 2)	$P2_1/n$ (# 14)	$P\bar{1}$ (# 2)
Z Value	2	2	4	2
ρ_{calc} (g cm^{-3})	1.343	1.308	1.677	1.305
μ (Mo Kα) (mm^{-1})	0.090	0.082	3.734	0.088
T (K)	296	296	100	296
$2\Theta_{max}$ (°)	54.0	55.0	58.0	55.0
No. Obs. ($I > 2\sigma(I)$)	3770	4623	5135	3115
No. Parameters	299	326	291	311
Goodness of Fit	1.020	1.030	1.019	1.027
Max. Shift in Cycle	0.00	0.001	0.003	0.00
*Residuals**: R1; wR2	0.0375; 0.0929	0.0396; 0.1018	0.0236; 0.0561	0.0455; 0.0994
Absorption Correction, Max/min	Multi-scan 0.9946/0.9631	Multi-scan 0.9919/0.9743	Multi-scan 0.7065/0.3311	Multi-scan 0.9930/0.9691
Largest Peak in Final Diff. Map (e$^-$ Å^{-3})	0.185	0.232	0.693	0.125

* $R = \Sigma_{hkl}(||F_{obs}| - |F_{calc}||)/\Sigma_{hkl}|F_{obs}|$; $R_w = [\Sigma_{hkl}w(|F_{obs}| - |F_{calc}|)^2/\Sigma_{hkl}wF_{obs}^2]^{1/2}$, $w = 1/\sigma^2(F_{obs})$; $GOF = [\Sigma_{hkl}w(|F_{obs}| - |F_{calc}|)^2/(n_{data} - n_{vari})]^{1/2}$

Table S3. Crystallographic Data for **35**.

	35
Empirical Formula	$C_{42}H_{30}N_2O_2 \cdot CH_3CN$
Formula Weight	635.73
Crystal System	Triclinic
Lattice Parameters:	
a (Å)	8.5020(3)
b (Å)	11.6522(4)
c (Å)	17.4372(6)
α (°)	104.952(1)
β (°)	92.109(1)
γ (°)	98.182(1)
V (Å^3)	1647.09(10)
Space Group	$P\bar{1}$ (# 2)
Z Value	2
ρ_{calc} (g cm^{-3})	1.282
μ (Mo Kα) (mm^{-1})	0.079
T (K)	100
$2\Theta_{max}$ (°)	55.0
No. Obs. ($I > 2\sigma(I)$)	6541
No. Parameters	445
Goodness of Fit	1.034
Max. Shift in Cycle	0.000
*Residuals**: R1; wR2	0.0393; 0.1005
Absorption Correction, Max/min	Multi-Scan 0.9906 / 0.9706
Largest Peak in Final Diff. Map (e$^-$ Å^{-3})	0.317

* $R = \Sigma_{hkl}(||F_{obs}|-|F_{calc}||)/\Sigma_{hkl}|F_{obs}|$; $R_w = [\Sigma_{hkl}w(|F_{obs}|-|F_{calc}|)^2/\Sigma_{hkl}wF_{obs}^2]^{1/2}$, $w = 1/\sigma^2(F_{obs})$; $GOF = [\Sigma_{hkl}w(|F_{obs}|-|F_{calc}|)^2/(n_{data} - n_{vari})]^{1/2}$

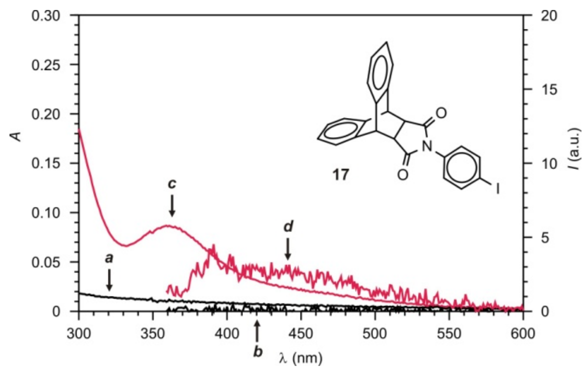

Figure S13. Absorption and emission spectra of **17** (40 μM, MeCN, 25 °C, λ_{Ex} = 350 nm) before (***a*** and ***b***) and after (***c*** and ***d***) ultraviolet irradiation (254 nm, 0.4 mW cm^{-2}, 5 min).

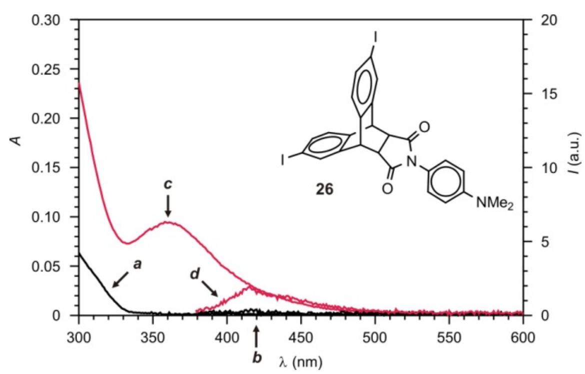

Figure S14. Absorption and emission spectra of **26** (40 μM, MeCN, 25 °C, λ_{Ex} = 373 nm) before (***a*** and ***b***) and after (***c*** and ***d***) ultraviolet irradiation (254 nm, 0.4 mW cm^{-2}, 5 min).

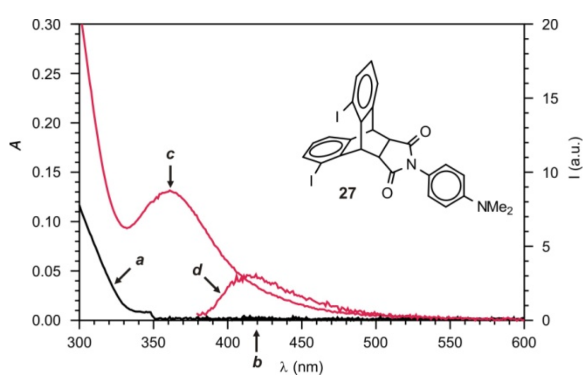

Figure S15. Absorption and emission spectra of **27** (20 μM, MeCN, 25 °C, λ_{Ex} = 370 nm) before (***a*** and ***b***) and after (***c*** and ***d***) ultraviolet irradiation (254 nm, 0.4 mW cm^{-2}, 5 min).

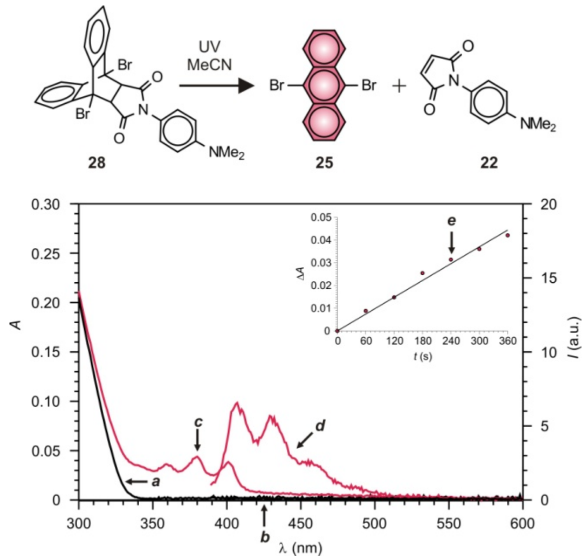

Figure S16. Absorption and emission spectra of **28** (40 μM, MeCN, 25 °C, λ_{Ex} = 370 nm) before (***a*** and ***b***) and after (***c*** and ***d***) ultraviolet (UV) irradiation (254 nm, 0.4 mW cm^{-2}, 6 min) and the corresponding absorbance evolution at 380 nm during photolysis.

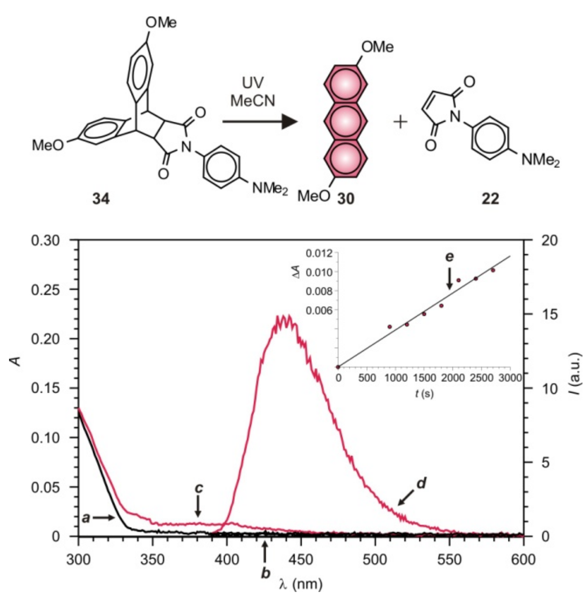

Figure S17. Absorption and emission spectra of **34** (30 μM, MeCN, 25 °C, λ_{Ex} = 350 nm) before (***a*** and ***b***) and after (***c*** and ***d***) ultraviolet (UV) irradiation (254 nm, 0.4 mW cm^{-2}, 50 min) and the corresponding absorbance evolution at 401 nm during photolysis.

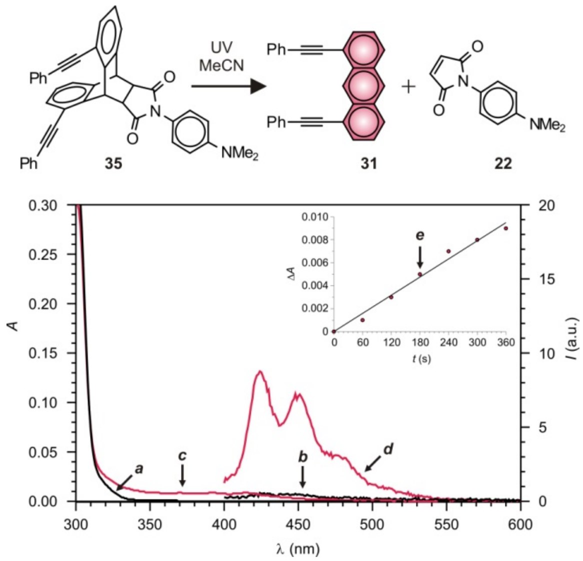

Figure S18. Absorption and emission spectra of **35** (10 μM, MeCN, 25 °C, λ_{Ex} = 390 nm) before (***a*** and ***b***) and after (***c*** and ***d***) ultraviolet (UV) irradiation (254 nm, 0.4 mW cm^{-2}, 6 min) and the corresponding absorbance evolution at 392 nm during photolysis.

Computed Coordinates of 16, 22, 36 and the corresponding transition state

16

O	-0.379391000	-0.937539000	-2.303695000
O	-0.419601000	-0.903116000	2.276467000
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N	-6.290079000	0.020345000	-0.094631000
C	2.454804000	-0.099257000	1.308207000
H	2.459384000	-0.073725000	2.397085000
C	3.816956000	-0.433554000	0.721857000
C	4.974495000	-0.719625000	1.436548000
H	4.964827000	-0.712829000	2.521451000
C	6.154130000	-1.012042000	0.742893000
H	7.062275000	-1.229568000	1.293767000
C	6.166742000	-1.023505000	-0.651359000
H	7.084694000	-1.249908000	-1.182027000
C	4.999883000	-0.742753000	-1.371003000
H	5.009908000	-0.753717000	-2.455858000
C	3.829575000	-0.445228000	-0.682239000
C	2.478109000	-0.120854000	-1.298465000
H	2.502188000	-0.113285000	-2.387372000
C	2.016984000	1.201879000	-0.712209000
C	1.623094000	2.328444000	-1.426690000
H	1.629588000	2.318635000	-2.511481000
C	1.222373000	3.475156000	-0.733358000
H	0.920782000	4.358979000	-1.284180000
C	1.209874000	3.486730000	0.661262000
H	0.898598000	4.379527000	1.191841000
C	1.597881000	2.351687000	1.380552000
H	1.585007000	2.359806000	2.465302000
C	2.004279000	1.213472000	0.691960000
C	1.489963000	-1.219414000	0.777852000
H	1.794284000	-2.177633000	1.202850000
C	1.503498000	-1.231945000	-0.767047000
H	1.814547000	-2.197226000	-1.170779000
C	0.057200000	-1.000495000	-1.174962000
C	0.036838000	-0.982532000	1.156603000
C	-2.134573000	-0.645642000	-0.030435000
C	-3.019212000	-1.721601000	-0.043999000

H	-2.634623000	-2.735284000	-0.043462000
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H	-5.044156000	-2.369775000	-0.054699000
C	-4.929149000	-0.198213000	-0.055009000
C	-4.009059000	0.878852000	-0.025303000
H	-4.361913000	1.899932000	-0.007375000
C	-2.639251000	0.652735000	-0.018409000
H	-1.956883000	1.494908000	0.001665000
C	-6.811596000	1.366237000	0.111947000
H	-6.571142000	1.760196000	1.108778000
H	-7.894278000	1.345132000	0.003404000
H	-6.417740000	2.059988000	-0.635315000
C	-7.206933000	-1.099391000	0.082372000
H	-7.047320000	-1.863976000	-0.682389000
H	-8.228256000	-0.738118000	-0.021670000
H	-7.106197000	-1.572065000	1.068898000

22 + 36

O	-0.782281000	-1.382081000	-2.198500000
O	-1.259364000	-2.230587000	2.279690000
N	-1.392449000	-1.632267000	0.033896000
N	-6.501582000	0.761090000	-0.092533000
C	3.956186000	1.170129000	1.352520000
H	4.070646000	1.305043000	2.423715000
C	4.733857000	0.206948000	0.699282000
C	5.678858000	-0.610073000	1.395923000
H	5.792067000	-0.475181000	2.466538000
C	6.426695000	-1.542800000	0.730092000
H	7.139879000	-2.155462000	1.269902000
C	6.277803000	-1.718768000	-0.677335000
H	6.879879000	-2.462752000	-1.186615000
C	5.384882000	-0.957427000	-1.381427000
H	5.271426000	-1.090364000	-2.452219000
C	4.583170000	0.028888000	-0.725590000
C	3.662487000	0.823227000	-1.419002000
H	3.549360000	0.689738000	-2.490504000
C	2.884570000	1.786188000	-0.765693000
C	1.942645000	2.606066000	-1.463105000
H	1.829646000	2.471321000	-2.533734000
C	1.198032000	3.541820000	-0.797938000

H	0.487768000	4.157255000	-1.338432000
C	1.347360000	3.718154000	0.609394000
H	0.748681000	4.465377000	1.117966000
C	2.237398000	2.954145000	1.314190000
H	2.352113000	3.088320000	2.384691000
C	3.035626000	1.964571000	0.659106000
C	0.553841000	-2.699690000	0.720844000
H	1.239623000	-3.181289000	1.402132000
C	0.692671000	-2.452960000	-0.580992000
H	1.520911000	-2.681548000	-1.235198000
C	-0.542453000	-1.761976000	-1.073716000
C	-0.781339000	-2.186697000	1.167637000
C	-2.690113000	-1.026425000	0.010082000
C	-3.820828000	-1.790189000	-0.275596000
H	-3.715371000	-2.849841000	-0.479498000
C	-5.082072000	-1.210412000	-0.296462000
H	-5.933518000	-1.838688000	-0.515486000
C	-5.256603000	0.171874000	-0.038158000
C	-4.095716000	0.924653000	0.267417000
H	-4.169964000	1.978773000	0.493230000
C	-2.840310000	0.332158000	0.283863000
H	-1.968233000	0.932493000	0.517291000
C	-6.673345000	2.133661000	0.367890000
H	-6.448559000	2.248687000	1.436981000
H	-7.705698000	2.434873000	0.200761000
H	-6.033332000	2.819709000	-0.192999000
C	-7.691767000	-0.072316000	-0.212331000
H	-7.653321000	-0.685505000	-1.116453000
H	-8.566430000	0.570908000	-0.287108000
H	-7.825385000	-0.738774000	0.650602000

Transition State

O	0.215353000	-0.923219000	2.425179000
O	0.240042000	-1.412952000	-2.129653000
N	0.561518000	-0.948797000	0.125828000
N	6.140119000	-0.062557000	0.119265000
C	-2.677506000	0.229713000	-1.396079000
H	-2.614032000	0.032517000	-2.461464000
C	-3.909149000	-0.090547000	-0.724406000
C	-5.029052000	-0.649183000	-1.374687000

H	-5.005919000	-0.790742000	-2.449787000
C	-6.151306000	-0.995977000	-0.645826000
H	-7.020134000	-1.402315000	-1.150821000
C	-6.172557000	-0.829704000	0.754192000
H	-7.057448000	-1.109709000	1.314156000
C	-5.071608000	-0.317417000	1.414255000
H	-5.080928000	-0.202407000	2.492711000
C	-3.930491000	0.077398000	0.684344000
C	-2.723814000	0.560317000	1.298038000
H	-2.689377000	0.615247000	2.381471000
C	-1.886990000	1.453460000	0.551648000
C	-1.072912000	2.443489000	1.146019000
H	-1.086816000	2.568422000	2.223096000
C	-0.297219000	3.266756000	0.353886000
H	0.299004000	4.049554000	0.808737000
C	-0.270041000	3.093892000	-1.046226000
H	0.347820000	3.744549000	-1.654405000
C	-1.021536000	2.101314000	-1.643904000
H	-0.995501000	1.962499000	-2.719042000
C	-1.863016000	1.282455000	-0.858877000
C	-1.597446000	-1.506007000	-0.532453000
H	-2.229158000	-2.185944000	-1.083176000
C	-1.604253000	-1.354249000	0.864952000
H	-2.251442000	-1.885149000	1.545495000
C	-0.216891000	-1.048928000	1.295480000
C	-0.201273000	-1.298509000	-1.002669000
C	1.974608000	-0.715032000	0.110095000
C	2.859019000	-1.779215000	-0.066364000
H	2.472243000	-2.783592000	-0.196428000
C	4.231283000	-1.568614000	-0.083606000
H	4.880293000	-2.419695000	-0.233113000
C	4.775536000	-0.273217000	0.095619000
C	3.859679000	0.793743000	0.261010000
H	4.215306000	1.807101000	0.381130000
C	2.488750000	0.570007000	0.268223000
H	1.811164000	1.405758000	0.392519000
C	6.659022000	1.299514000	0.087078000
H	6.393698000	1.829225000	-0.838456000
H	7.744262000	1.264843000	0.163296000
H	6.287020000	1.882044000	0.933626000

C	7.041177000	-1.137893000	-0.277393000
H	6.907743000	-2.017370000	0.357564000
H	8.068480000	-0.798711000	-0.157854000
H	6.897004000	-1.442690000	-1.323215000

Web Enhanced Object

Video S1. Animation of the vibration associated with the imaginary frequency of the transition state.

Table S3. Excitation energy (ΔE), wavelength (λ_{Cal}), oscillator strength (f_{Cal}) and main orbital pair with its contribution for electronic transitions from the ground state of **16** to the first ten singlet excited states.

	ΔE_{Cal} (eV)	λ_{Cal} (nm)	f_{Cal}	*Main Orbital Pair*	*Contribution* (%)
S_1	3.86	321	0.0037	[HOMO] $\rightarrow$ [LUMO]	97
S_2	4.30	288	0.0378	[HOMO] $\rightarrow$ [LUMO + 3]	95
S_3	4.36	285	0.0249	[HOMO] $\rightarrow$ [LUMO + 1]	97
S_4	4.44	280	0.0000	[HOMO] $\rightarrow$ [LUMO + 2]	98
S_5	4.69	264	0.0042	[HOMO] $\rightarrow$ [LUMO + 4]	90
S_6	4.80	259	0.1785	[HOMO] $\rightarrow$ [LUMO + 5]	43
S_7	4.87	254	0.0004	[HOMO – 1] $\rightarrow$ [LUMO]	96
S_8	4.93	251	0.0206	[HOMO – 6] $\rightarrow$ [LUMO]	62
S_9	4.95	250	0.3083	[HOMO] $\rightarrow$ [LUMO + 5]	50
S_{10}	5.02	247	0.0455	[HOMO – 1] $\rightarrow$ [LUMO + 2]	31