A Multi-Site Constrained Model of *trans*-4-(Dimethylamino)-4'-nitrostilbene for Structural Elucidation of the Radiative and Nonradiative Excited States

Cheng-Kai Lin, Yu-Fu Wang, Yuan-Chung Cheng,* and Jye-Shane Yang*

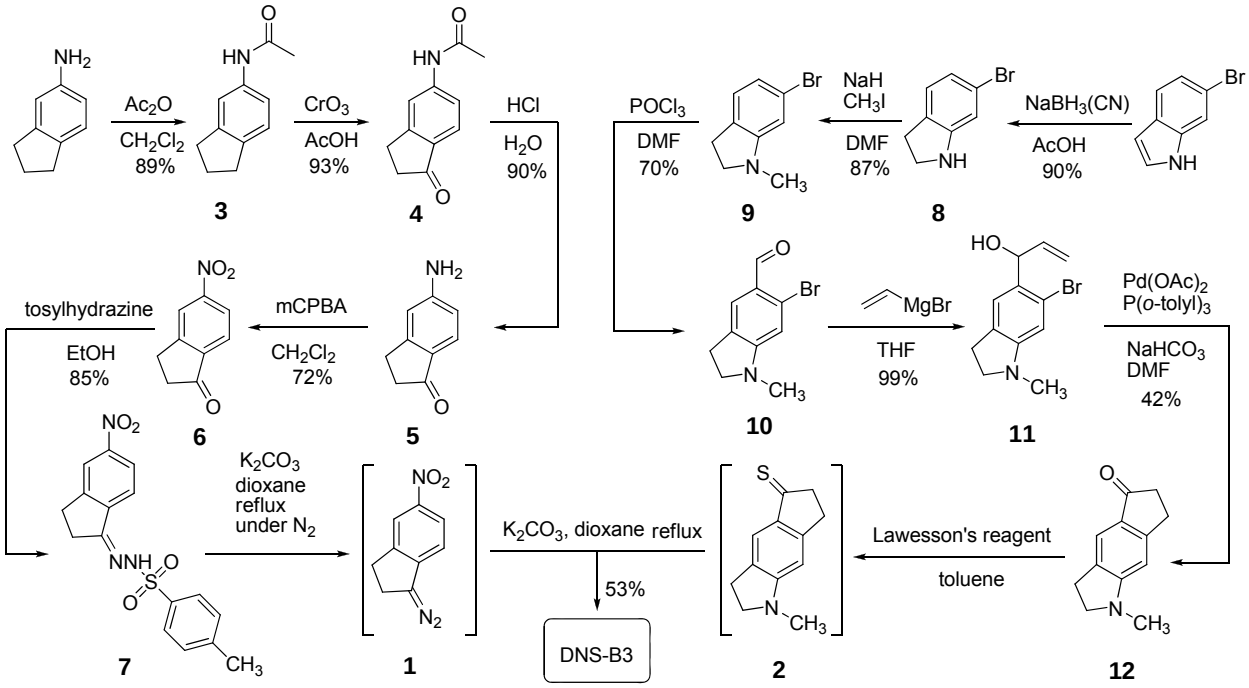
Department of Chemistry, National Taiwan University, Taipei, 10617

jsyang@ntu.edu.tw and yuanchung@ntu.edu.tw

Supporting Information (28 pages)

Contents:

Synthetic Scheme



Compound **2** (1-methyl-2,3,6,7-tetrahydrocyclopenta[f]indole-5(1H)-thione)**.** Anhydrous toluene (10 mL) was added to a mixture of compound **12** (0.31 g, 1.67 mmol) and Lawesson's reagent (0.68 g, 1.67 mmol) under N_2(g) and stirred at 100 °C for 3 h. After removal of the solvent, the crude product was purified by flash chromatography (SiO_2, *n*-hexane : EtOAc = 4 : 1) to afford a brown solid powder, which was not further purified. ESI-HRMS calcd for $C_{12}H_{13}NS$: 203.0769, found : 203.0763.

Compound **3** (5-acetamidoindane).[S1] To a solution of 5-aminoindane (2.00 g, 15.0 mmol) in 20 mL CH_2Cl_2 was added slowly with acetic anhydride (1.84 g, 18.0 mmol) and stirred at RT for 60 min. The reaction mixture was neutralized by adding NaOH solution, and extracted with CH_2Cl_2 for three times. The combined organic layers

were dried over $MgSO_4$ and solvent was removed under reduced pressure. The crude product was purified by flash chromatography (SiO_2, *n*-hexane : EtOAc = 1 : 1) to afford pale pink solid **3** with 89% yield; m.p: 104-105 °C, lit[S1] m.p: 105-106 °C; ^{1}H NMR (400 MHz $CDCl_3$): 1.99-2.06 (m, 2H), 2.10 (s, 1H), 2.80-2.84 (m, 4H), 7.09 (d, *J* = 8.0 Hz, 1H), 7.14 (d, *J* = 8.0 Hz, 1H), 7.41 (s, 1H), 7.87 (bs, 1H).

Compound **4** (5-acetamido-1-indanone).[S2] To a solution of compound **3** (1.00 g, 5.7 mmol) in 14 mL glacial acetic acid was added slowly with the chromium trioxide solution (2.35 g, 23.5 mmol, in 14 mL 50% glacial acetic acid/water mixture) in 20 min at 50 °C and then stirred for 60 min. The reaction mixture was added slowly with a cold NaOH solution until the solution became weakly basic. The mixture was extracted with EtOAc for three times. The combined organic layers were dried over $MgSO_4$ and solvent was removed under reduced pressure. The crude product was purified by flash chromatography (SiO_2, *n*-hexane : EtOAc = 1 : 4) to afford white solid with 93% yield; m.p: 165-166 °C, lit[S2] m.p: 170.5-171 °C; ^{1}H NMR (400 MHz $CDCl_3$): 2.20 (s, 3H), 2.64 (t, *J* = 6.0 Hz, 2H), 3.07 (t, *J* = 6.0 Hz, 2H), 7.26 (d, *J* = 8.4 Hz, 1H), 7.62 (d, *J* = 8.4 Hz, 1H), 7.96 (s, 1H), 8.36 (bs, 1H).

Compound **5** (5-aminoindan-1-one).[S3] A solution of compound **4** (1.00 g, 5.3 mmol) in 30 mL 6M HCl solution was stirred at 100 °C for 60 min. The reaction mixture was added slowly with a cold sodium hydroxide solution until the solution became weakly basic. The mixture was extracted with EtOAc for three times. The combined organic layers were dried over $MgSO_4$ and solvent was removed under reduced pressure. After removal of the solvent, the crude product was purified by flash chromatography (SiO_2, *n*-hexane : EtOAc = 1 : 1) to afford yellow solid with 90% yield; m.p : 187-189

°C lit[S3] m.p: 188-190 °C; ^{1}H NMR (400 MHz $CDCl_3$): 2.60 (t, *J* = 6.0 Hz, 2H), 2.97 (t, *J* = 6.0 Hz, 2H), 4.20 (bs, 2H), 6.56-6.59 (m, 2H), 7.55 (d, *J* = 8.8 Hz, 1H).

Compound **6** (5-nitroindan-1-one).[S4,S5] A mixture of compound **5** (0.92 g, 6.25 mmol) and mCPBA (5.39 g, 31.25 mmol) in CH_2Cl_2 was stirred at 50 °C for 3 h. Solvent was removed under reduced pressure. The crude product was purified by chromatography (SiO_2, *n*-hexane : CH_2Cl_2 = 1 : 1) to afford yellow solid with 72% yield; m.p : 125-126 °C; lit m.p: 131-132 °C; ^{1}H NMR (400 MHz $CDCl_3$): 2.80 (t, *J* = 6.0 Hz, 2H), 3.26 (t, *J* = 6.0 Hz, 2H), 7.87 (d, *J* = 8.4 Hz, 1H), 8.21 (d, *J* = 8.4 Hz, 1H), 8.32 (s, 1H) ppm.; ESI-HRMS calcd for $C_9H_7NO_3$: 177.0426, found : 177.0444.

Compound **7** (5-nitroindanone (*p*-tosyl)hydrazone, a mixture of both trans and cis isomers with respect to the C=N bond). *p*-Toluenesulfonylhydrazide (0.37 g, 2.0 mmol) was added to a stirred suspension of compound **6** (0.18 g, 1.0 mmol) in EtOH (10 mL). The resulting mixture was stirred at 65 °C for 2 h. Solvent was removed under reduced pressure. The crude product was purified by flash chromatography (SiO_2, *n*-hexane : EA = 2 : 1) to afford yellow solid with 85% yield; m.p: 158-160 °C; ^{1}H NMR (400 MHz $CDCl_3$): 2.40 (s, 3H), 2.74-2.80 (m, 3H), 3.05-3.18 (m, 3H), 7.22-7.33 (m, 2H), 7.76-7.79 (m, 1H), 7.89-7.91 (m, 1H), 7.96-8.11 (m, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): 21.6, 25.3, 27.0, 28.3, 120.8, 122.6, 122.8, 128.0, 129.7, 135.1, 138.3, 143.1, 144.5, 148.9, 149.4, 152.2, 158.7, 159.1 ppm. ESI-HRMS calcd for $C_{16}H_{15}N_3O_4S$: 345.0783, found : 345.0780.

Compound **8** (6-bromoindoline).[S6] After portion-wise addition of $NaBH_3(CN)$ (6.4 g, 102.0 mmol) to a solution of 6-bromoindoline (5.00 g, 25.5 mmol) in 100 mL glacial

acetic acid at 10-15 °C, the solution was stirred for 30 min. The solution was poured to a mixture of ice and NaOH and the solution become basic. The mixture was extracted with EtOAc for three times. The combined organic layers were washed with water and brine, and dried ($MgSO_4$). After removal of the solvent, the crude product was purified by flash chromatography (SiO_2, *n*-hexane : EtOAc = 3 : 1) to afford yellow solid with 90% yield; mp: 40-41 °C; ^{1}H-NMR ($CDCl_3$) 1.40-2.40 (br, 1H), 2.96 (t, *J* = 7.6 Hz, 2H), 3.56 (t, *J* =7.6, 2H), 6.72 (s, 1H), 6.77 (d, *J* = 8.0 Hz, 1H), 6.92 (d, *J* = 8.0 Hz, 1H) ppm.

Compound **9** (*N*-methyl-6-bromoindoline).[S7] To a solution of compound **8** (4.55 g, 23.0 mmol) in 20 mL DMF was added slowly with sodium hydride (60%. 1.84 g, 46.0 mmol) at 0 °C and then stirred for 10 min. Iodomethane (2.26 mL, 34.5 mmol) was then added and stirred at RT for 4 h. The reaction mixture was extracted with EtOAc for three times. The combined organic layers were dried over $MgSO_4$ and solvent was removed under reduced pressure. After removal of the solvent, the crude product was purified by flash chromatography (SiO_2, *n*-hexane : EtOAc = 3 : 1) to afford colorless liquid **9** with yield of 87%.; ^{1}H-NMR ($CDCl_3$) 2.71 (s, 1H), 2.87 (t, *J* = 8.0 Hz, 2H), 3.31 (t, *J* =8.0, 2H), 6.53 (s, 1H), 6.72 (d, *J* = 7.6 Hz, 1H), 6.87 (d, *J* = 7.6 Hz, 1H) ppm.

Compound **10** (*N*--methyl-6-bromoindoline-5-carbaldehyde). Phosphorus oxychloride (2.8 mL, 30 mmol) was added slowly into anhydrous DMF (10 mL) at 0 °C under N_2(g) and stir for 30 min. Compound **9** (4.68 g, 22 mmol) in anhydrous DMF (10 mL) was added to the above solution at 0 °C and the mixture was stirred at RT for 12 h. Cold NaOAc (aq) (0.1 M, 200 mL) was added to the mixture at 0 °C and the resulting

solution was stirred for 30 min. The crude product can be obtained by filtration, and further purification was performed with flash column chromatography (SiO_2, *n*-hexane : EtOAc = 4 : 1) to afford pale yellow solid with 70% yield; m.p: 104-105 °C; ^{1}H NMR (400 MHz $CDCl_3$): 2.80 (s, 3H), 2.89 (t, J = 8.5 Hz, 2H), 3.51 (t, J = 8.5 Hz, 2H), 6.36 (s, 1H), 7.47 (s, 1H), 9.96 (s, 1H) ppm; 13C NMR (100 MHz, $CDCl_3$): 26.8, 33.4, 54.6, 108.3, 122.6, 124.5, 129.6, 130.2, 157.9, 189.8 ppm. ESI-HRMS calcd for $C_{10}H_{10}BrNO$: 238.9946, found : 238.9946.

Compound **11** (1-(6-bromo-1-methylindolin-5-yl)prop-2-en-1-ol). To a solution of compound **10** (1.20 g, 5.0 mmol) in anhydrous THF was added slowly with vinylmagnesium bromide (1M slotion in THF, 6.0 mL, 6.0 mmol) under N_2(g) at 0 °C and the solution was stirred for 10 min. The solution was allowed to warm up to RT and the stirred at RT for 3 h. Saturated NH_4Cl(aq) (30 mL) was added slowly to the mixture at 0 °C and the resulting solution was stirred for 30 min before extraction with diethyl ether 3 times. The combined organic layers were dried over $MgSO_4$ and solvent was removed under reduced pressure to afford yellow solid with 99% yield; m.p: 80-81 °C; ^{1}H NMR (400 MHz $CDCl_3$): 2.56 (s, 1H), 2.69 (s, 3H), 2.84 (t, J = 8.1 Hz, 2H), 3.22-3.35 (m, 2H), 5.15 (d, J = 10.4 Hz, 1H), 5.35 (d, J = 17.2 Hz, 1H), 5.50 (s, 1H), 5.92-6.00 (m, 1H), 6.54 (s, 1H), 7.11 (s, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): 28,1, 35.7, 56.1, 73.2, 110.5, 114.3, 121.3, 123.4, 130.0, 130.4, 139.1, 153.8 ppm. ESI-HRMS calcd for $C_{12}H_{14}BrNO$: 267.0259, found : 267.0251.

Compound **12** (1-methyl-2,3,6,7-tetrahydrocyclopenta[f]indol-5(1H)-one). A mixture of Compound **11** (0.27 g, 1.0 mmol), $Pd(OAc)_2$ (0.011 g, 0.05 mmol), P(*o*-tolyl)$_3$ (0.030 g, 0.1 mmol) and $NaHCO_3$ (0.092 g, 1.1 mmol) in 2 mL anhydrous DMF was

stirred at 120 °C under N_2(g) for 48 h. The reaction mixture was purified by chromatography (SiO_2, *n*-hexane : EtOAc = 4 : 1) to afford colorless solid with 42% yield; m.p: 108-109 °C; ^{1}H NMR (400 MHz $CDCl_3$): 2.58 (t, *J* = 5.8 Hz, 2H), 2.83 (s, 3H), 2.92-2.98 (m, 4H), 3.51 (t, *J* = 8.3 Hz, 2H), 6.22 (s, 1H), 7.32 (s, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): 25.9, 27.1, 34.0, 36.5, 55.1, 100.9, 119.2, 127.0, 130.7, 158.8, 159.2, 204.1 ppm. ESI-HRMS calcd for $C_{12}H_{13}NO$: 187.0997, found : 187.0995.

Compound DNS-B3. A reaction mixture of compound **2** (0.12 g, 0.56 mmol), **7** (0.39 g, 1.13 mmol) and K_2CO_3 (0.23g, 1.68 mmol) in anhydrous dioxane was stirred at 110 °C under N_2(g) for 18 h. Solvent was removed under reduced pressure. The crude product was extracted with CH_2Cl_2 for three times. The combined organic layers were dried over $MgSO_4$ and solvent was removed under reduced pressure. The mixture was purified by flash chromatography (SiO_2, *n*-hexane : CH_2Cl_2 = 1 : 1) to afford black solid with 53% yield; m.p : 220-222 °C; ^{1}H NMR (400 MHz $CDCl_3$): 2.80 (s, 3H), 2.97 (t, J = 8.1 Hz, 2H), 3.04-3.07 (m, 2H), 3.12-.317 (m, 6H), 3.40 (t, J = 8.1 Hz, 2H), 6.411 (s, 1H), 7.34 (s, 1H), 7.54 (d, J = 8.5 Hz, 1H), 8.05-8.07 (m, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): 28.3, 30.6, 31.1, 32.1, 32.8, 35.4, 56.0, 102.9, 119.8, 121.0, 122.6, 123.0, 128.2, 129.6, 132.2, 142.4, 145.2, 147.3, 149.6, 150.9, 154.2 ppm. ESI-HRMS calcd for $C_{21}H_{20}N_2O_2$: 332.1525, found : 332.1512.

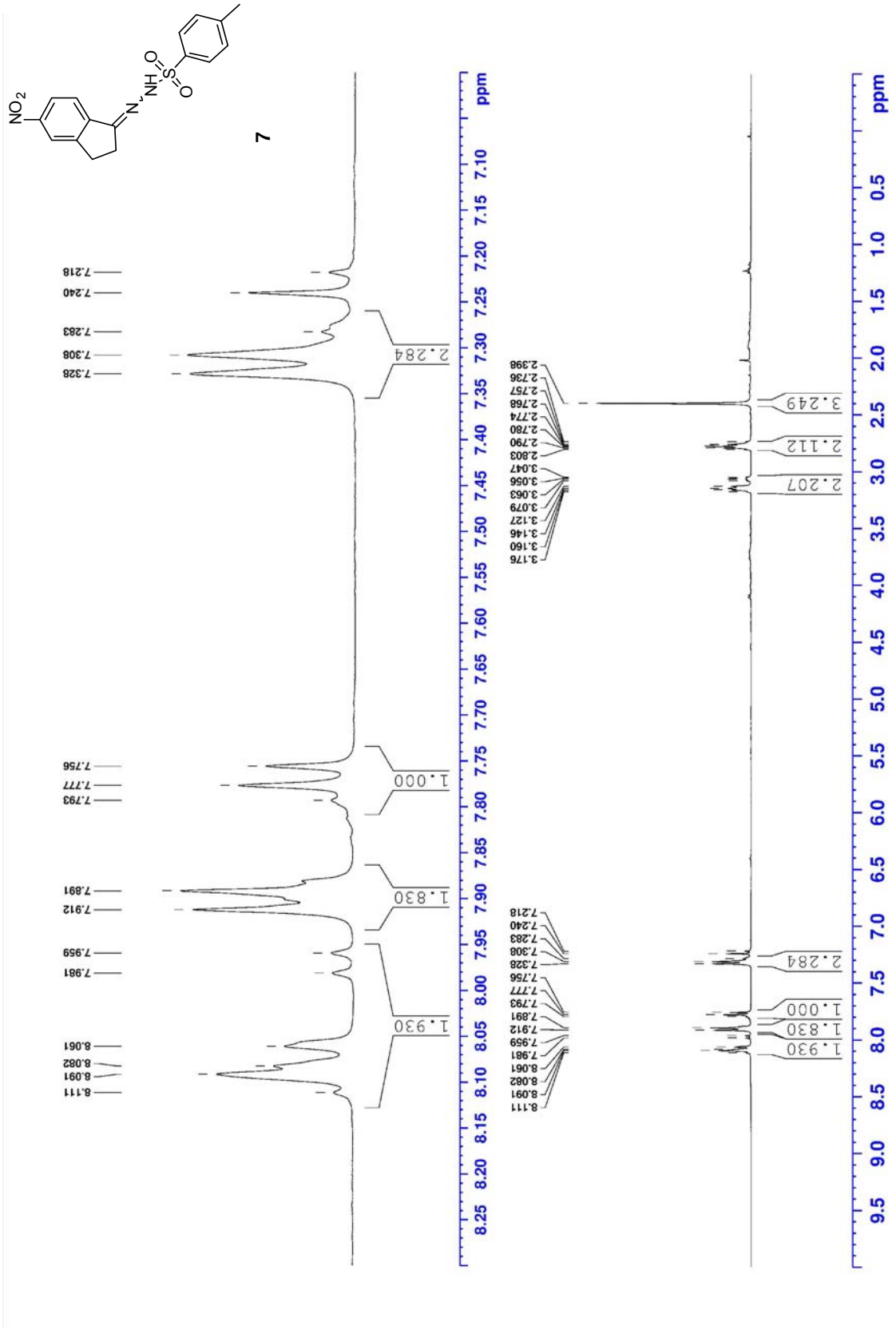


Figure S1 ^{1}H NMR spectrum of **7**

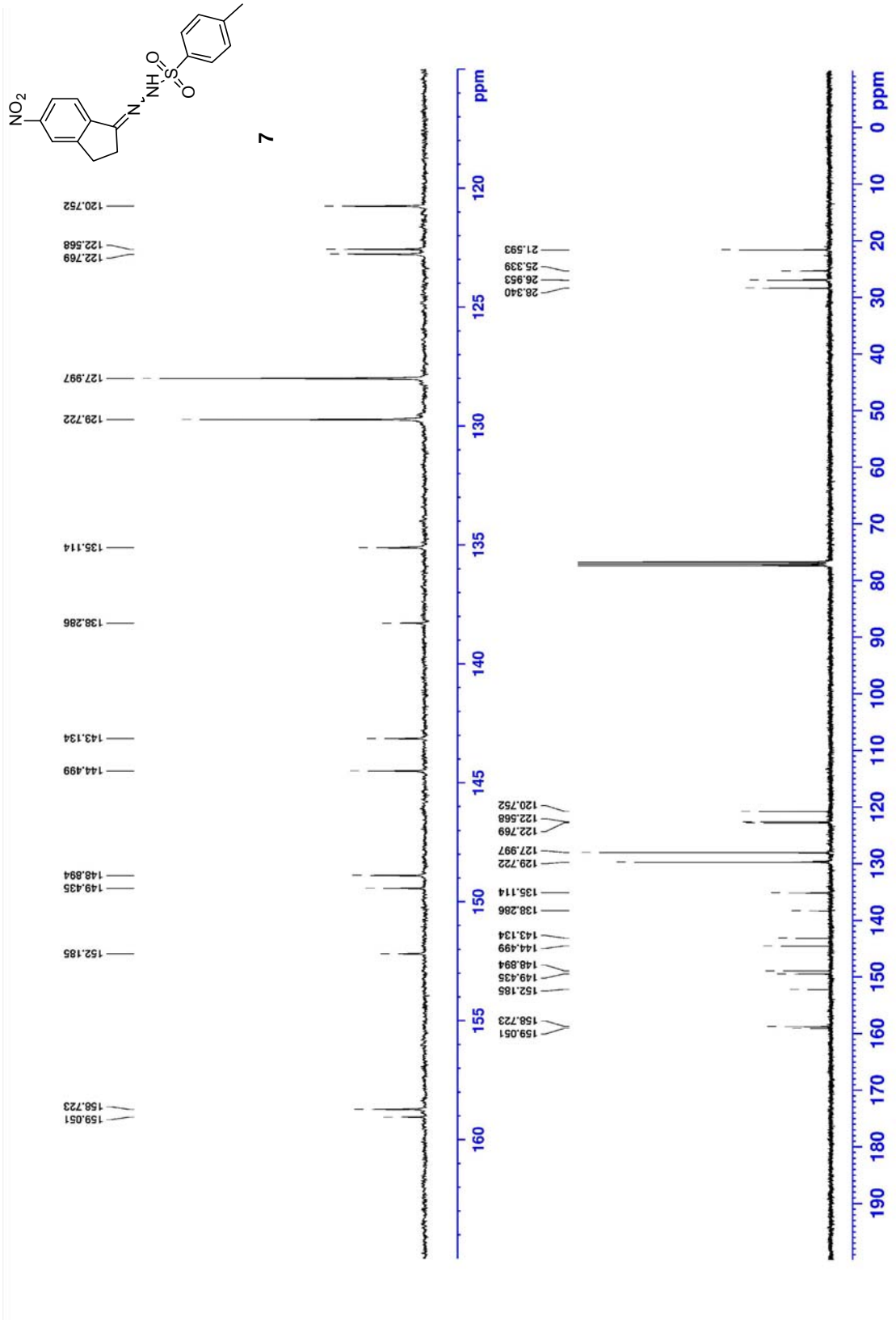


Figure S2 ^{13}C NMR spectrum of **7**

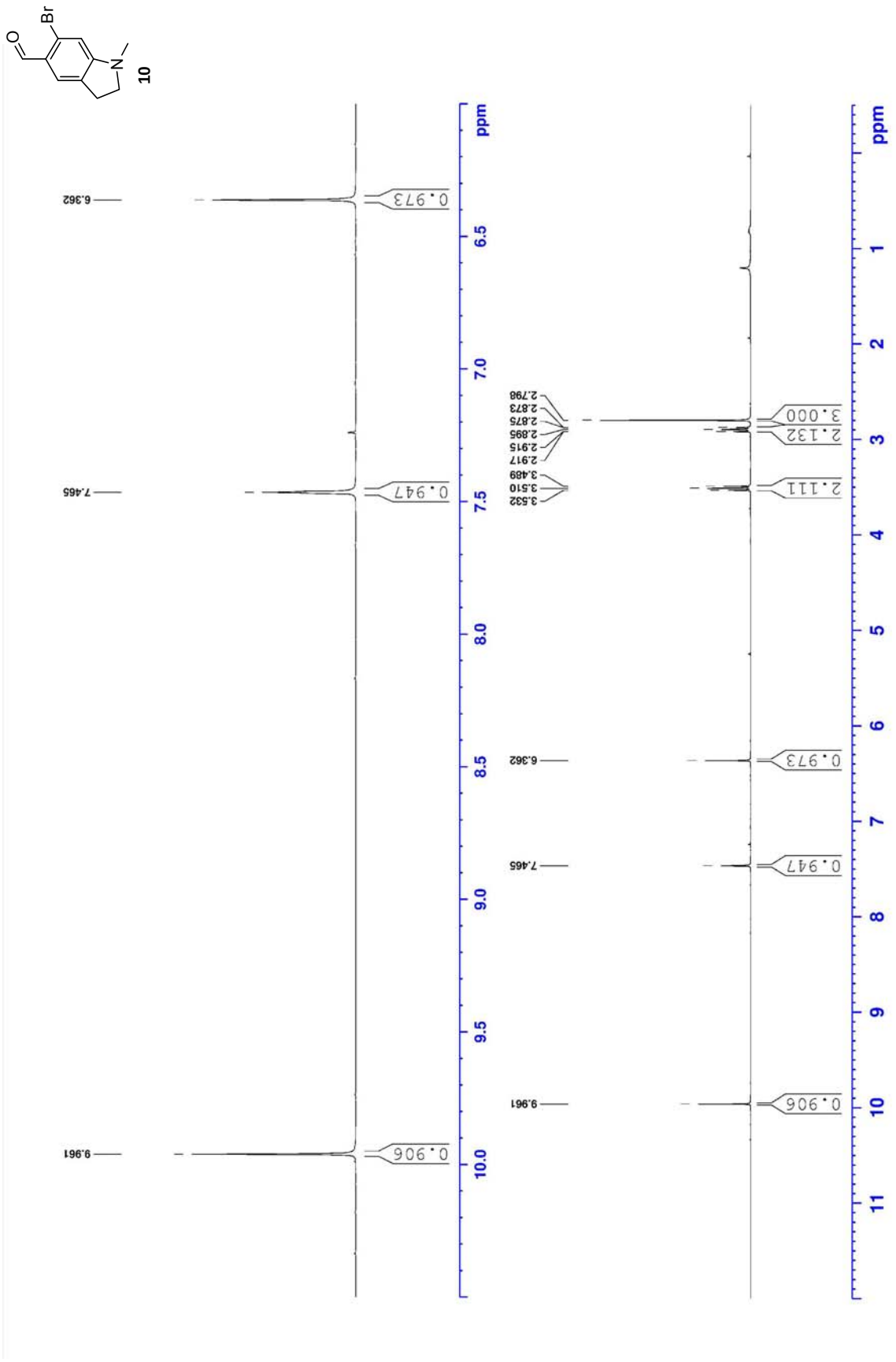


Figure S3 ^{1}H NMR spectrum of **10**

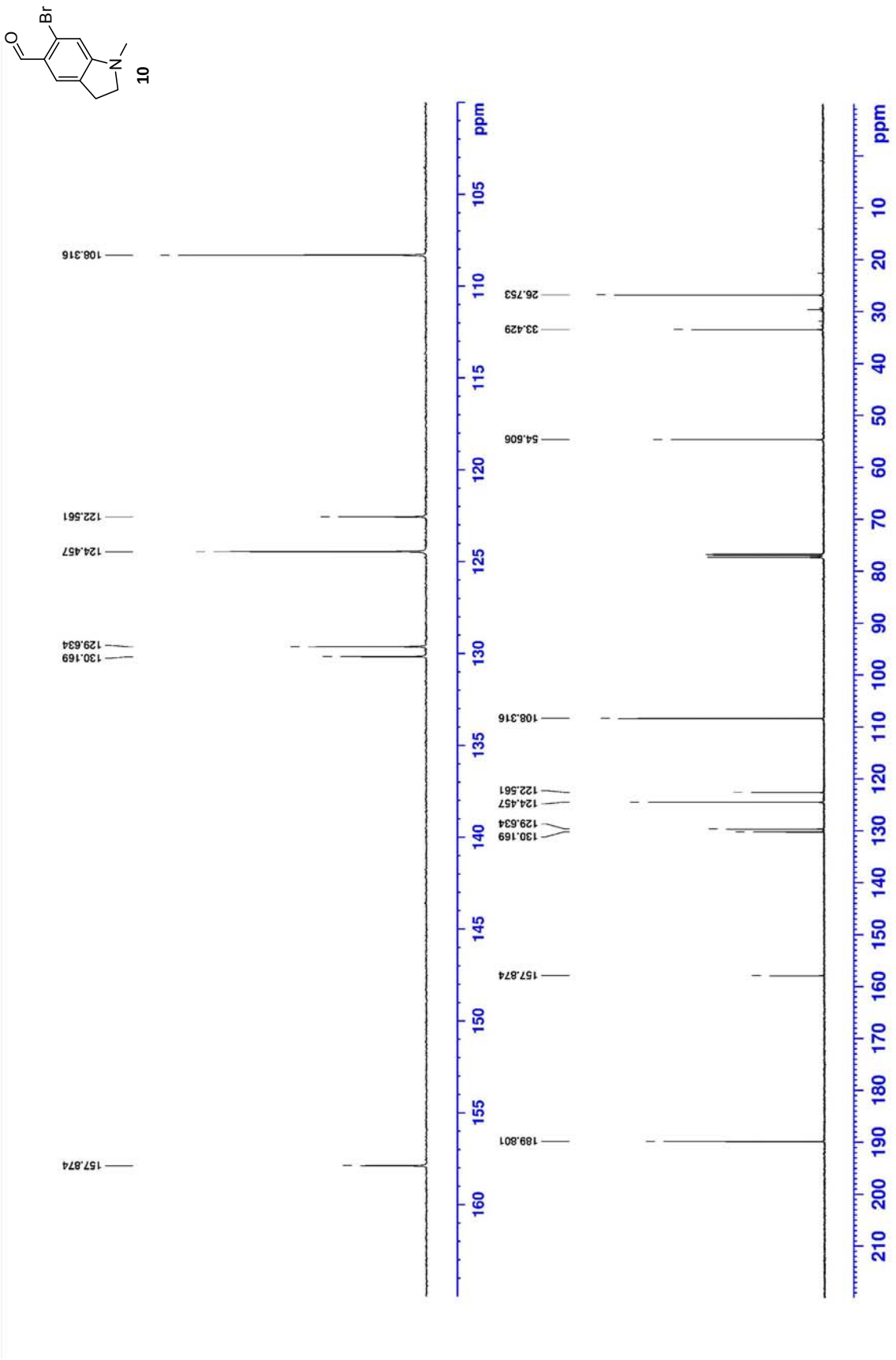


Figure S4 ^{13}C NMR spectrum of **10**

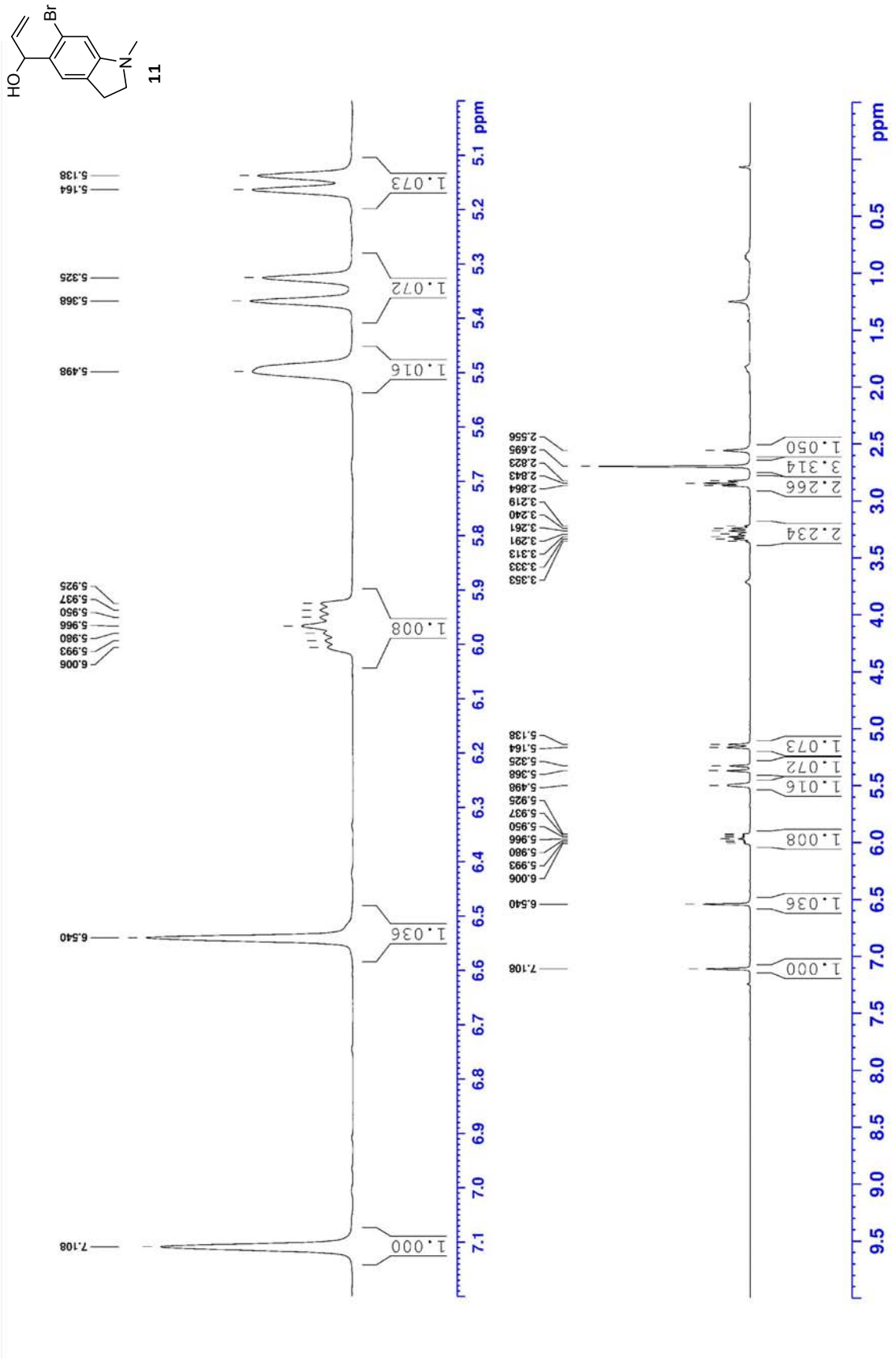


Figure S5 ^{1}H NMR spectrum of **11**

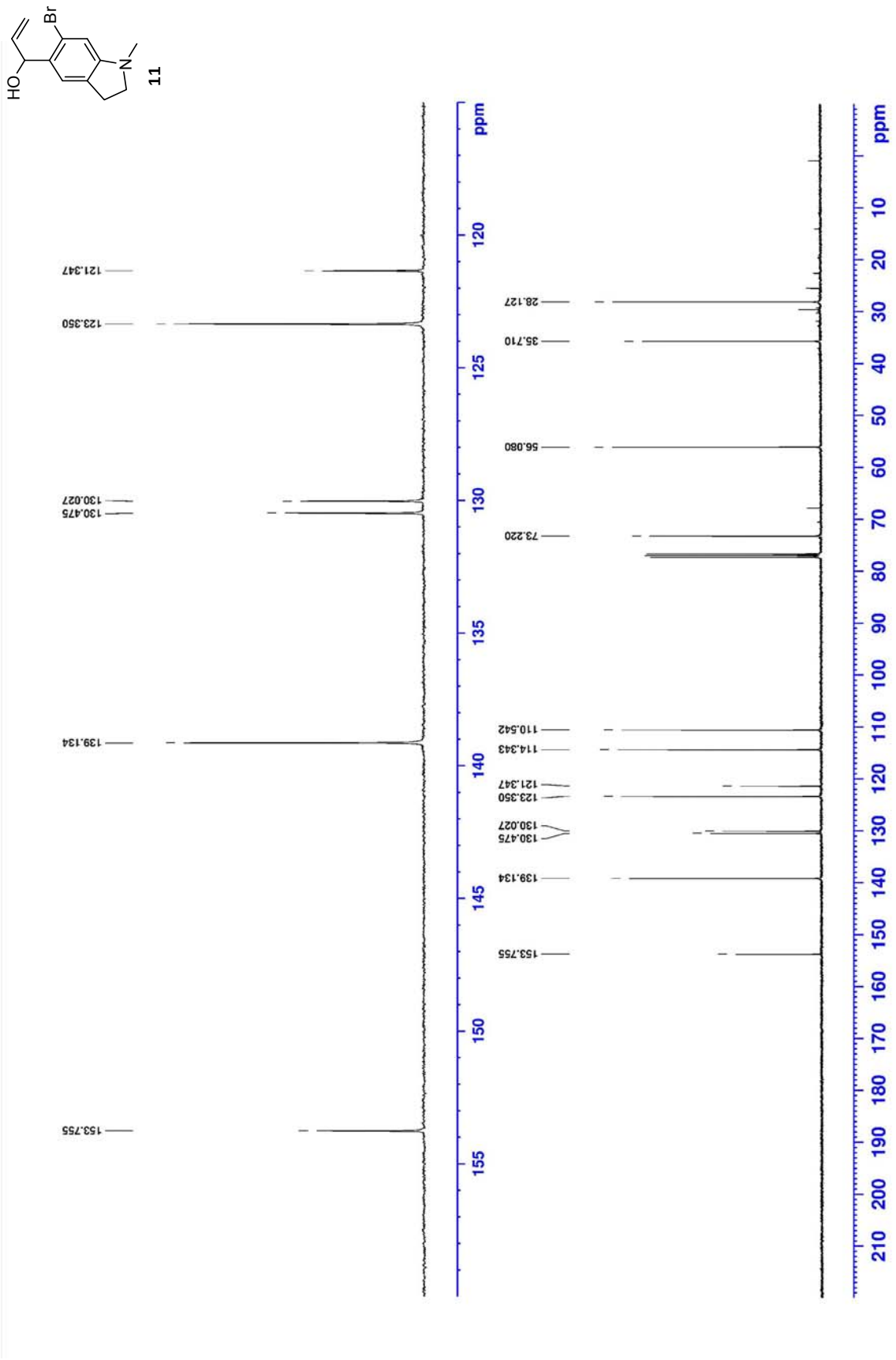


Figure S6 ^{13}C NMR spectrum of **11**

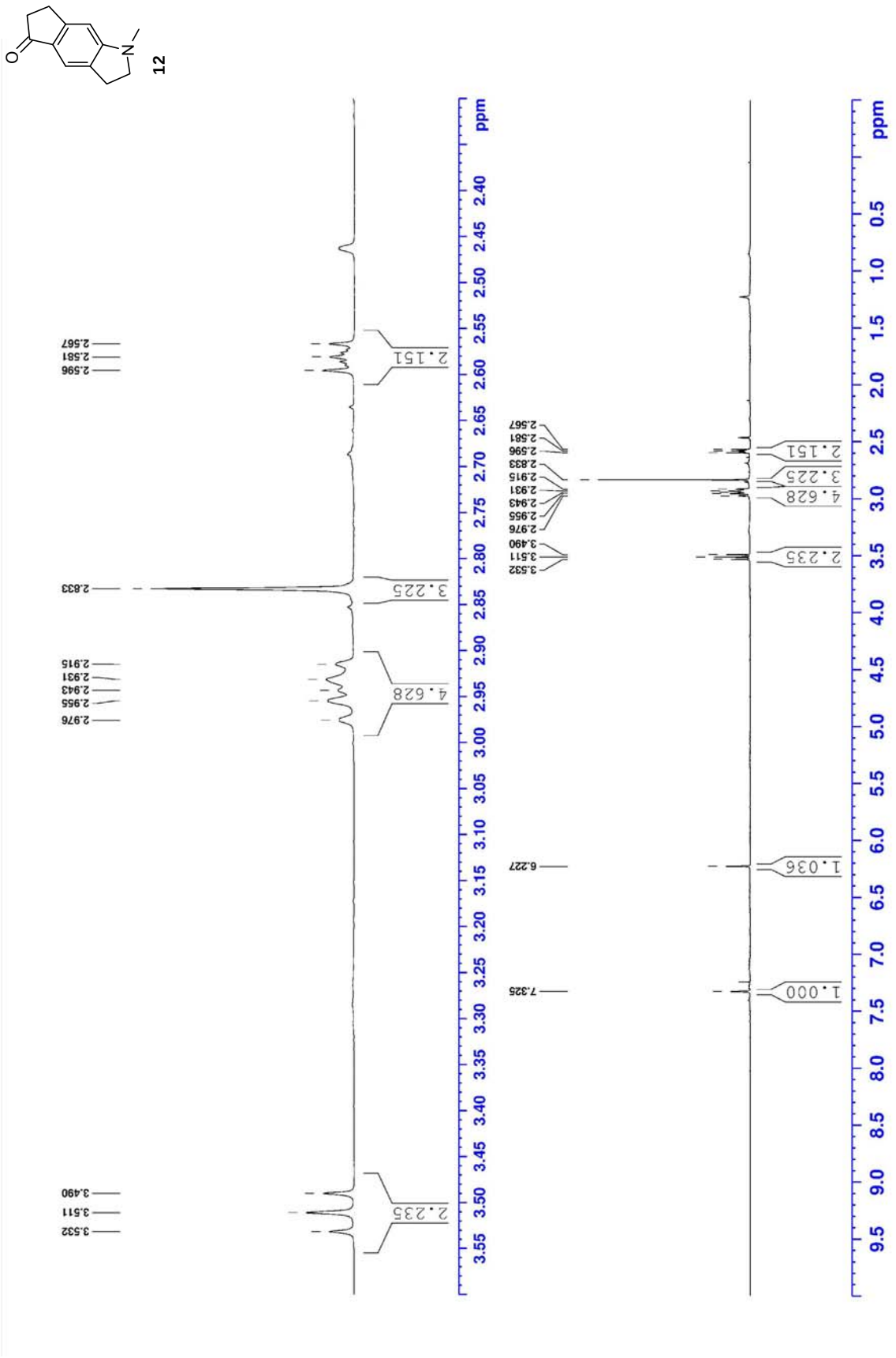


Figure S7 ^{1}H NMR spectrum of **12**

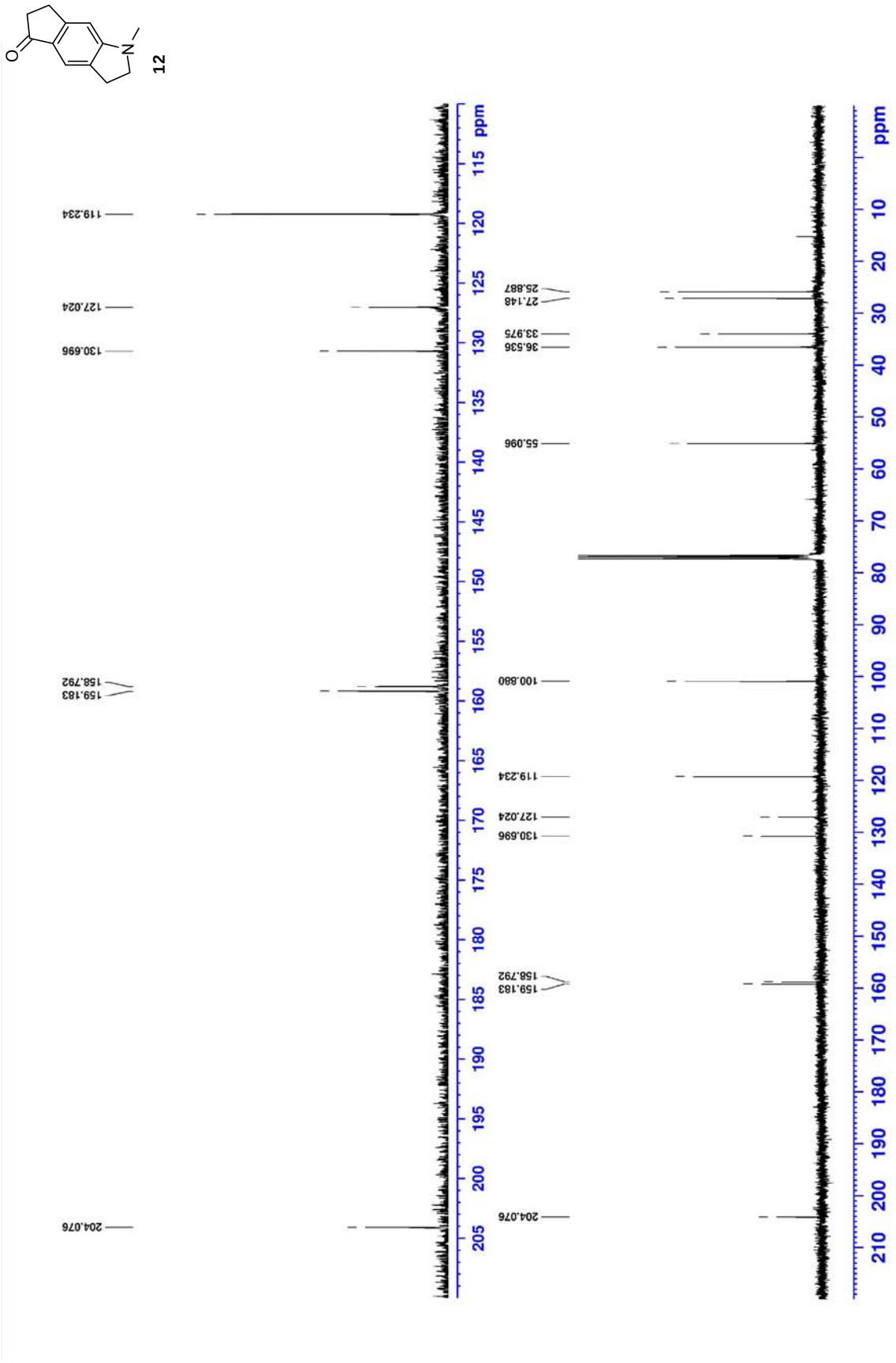


Figure S8 ^{13}C NMR spectrum of 12

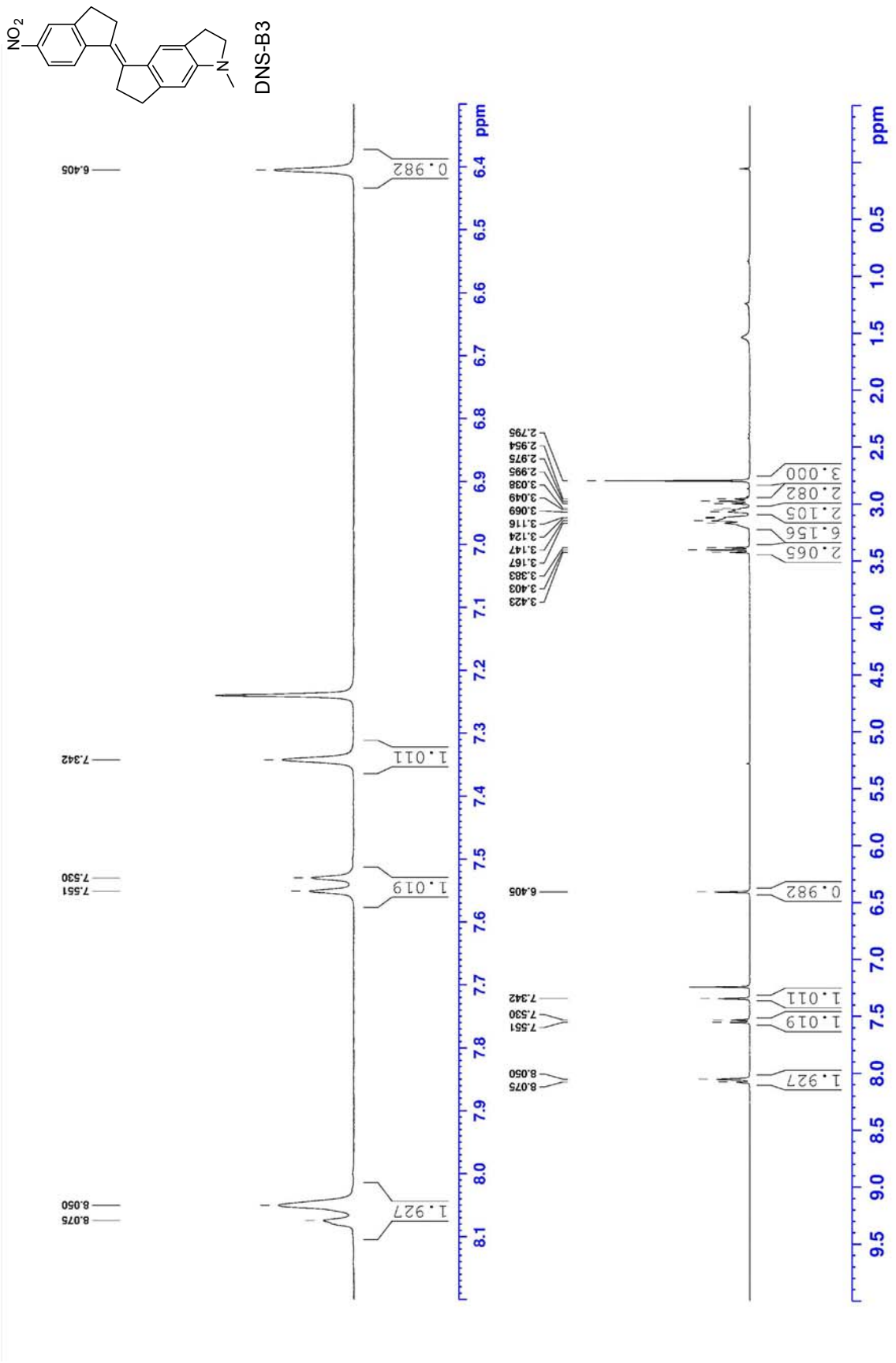


Figure S9 ^{1}H NMR spectrum of DNS-B3

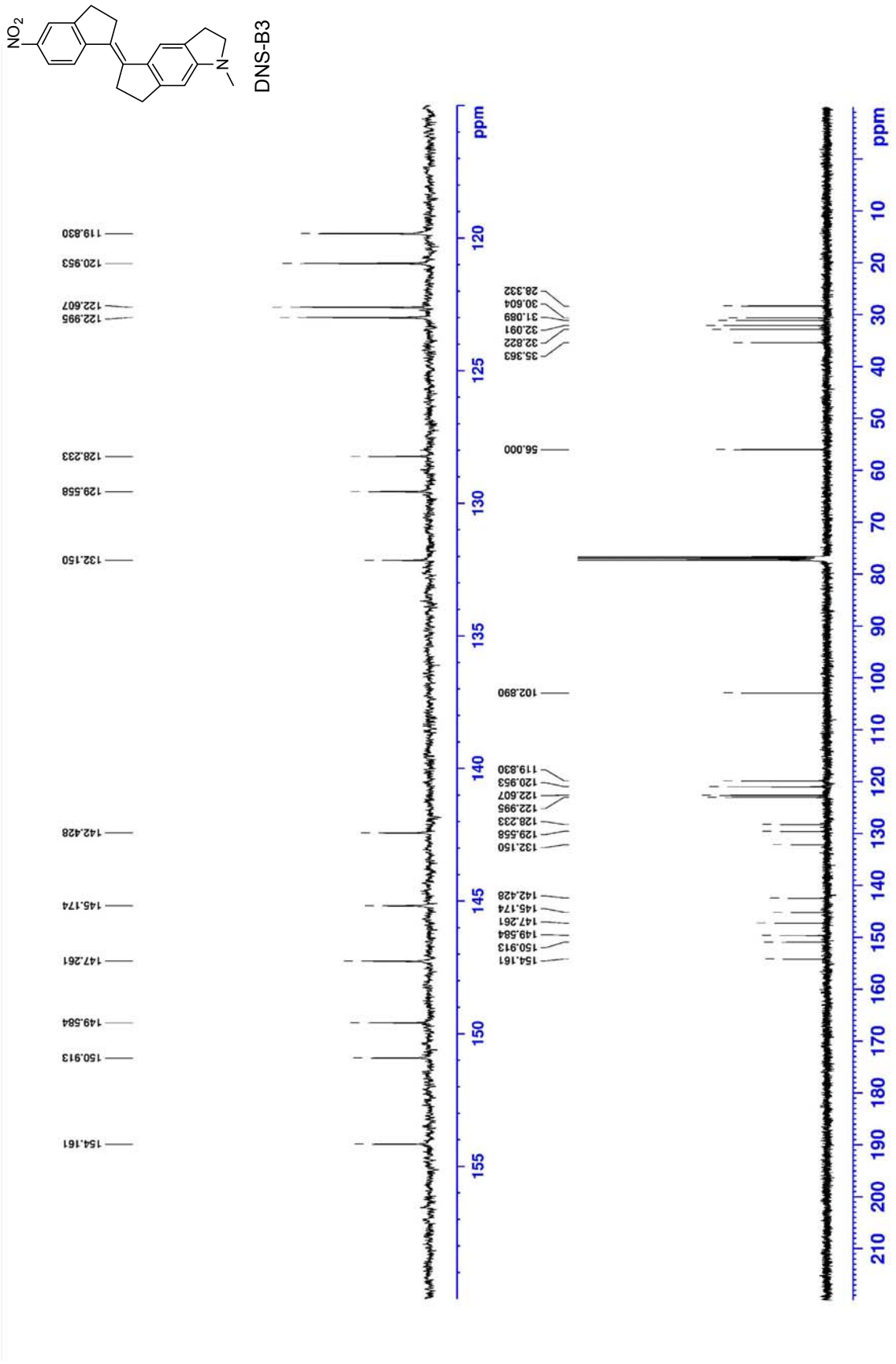


Figure S10 ^{13}C NMR spectrum of DNS-B3

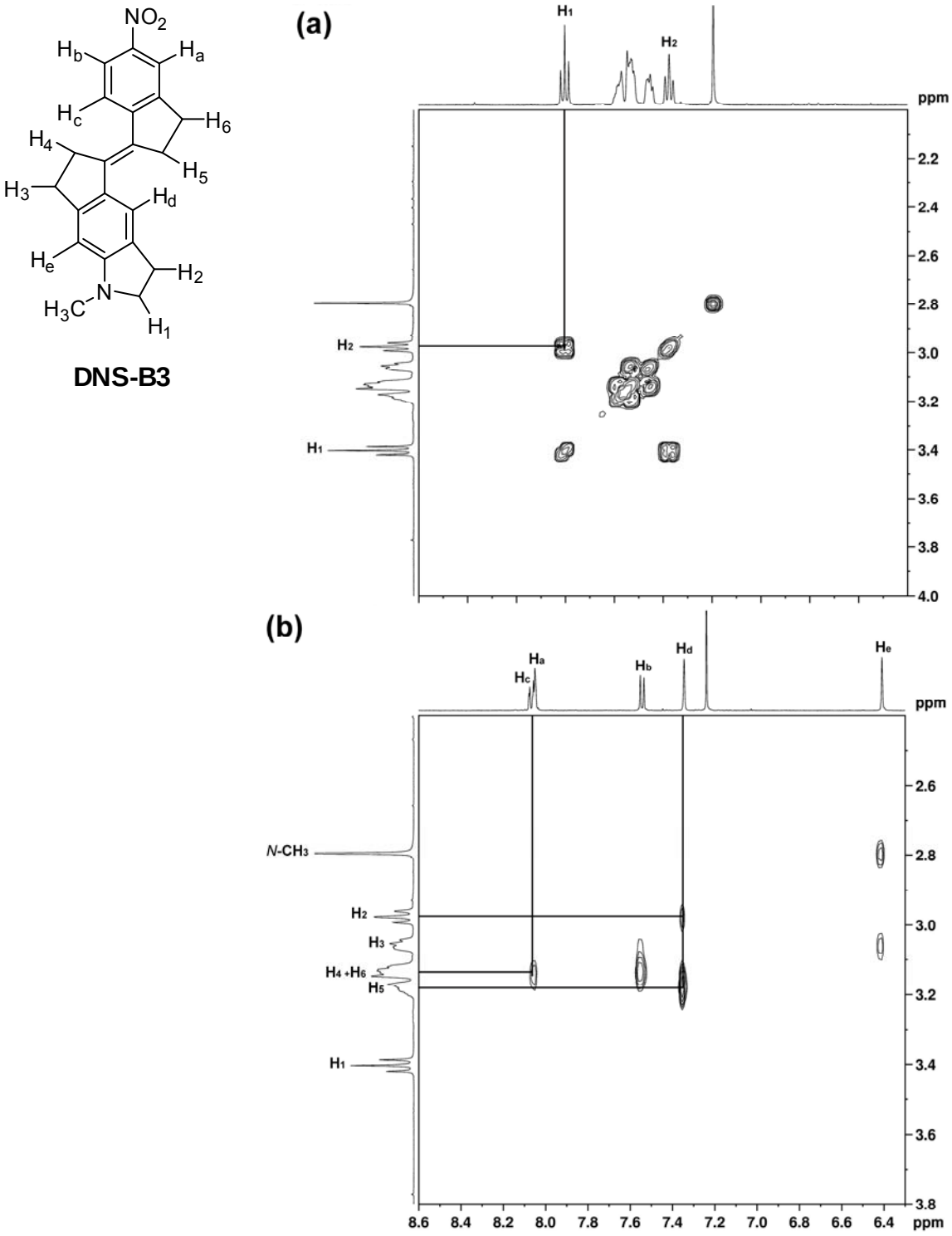


Figure S11. (a) COSY and (b) NOESY of DNS-B3 for the configuration determination. The trans configuration can be verified according to the presence of NOE signals between H_c and H_d and the nearby ethylene bridge proton (H_4 and H_5, respectively).

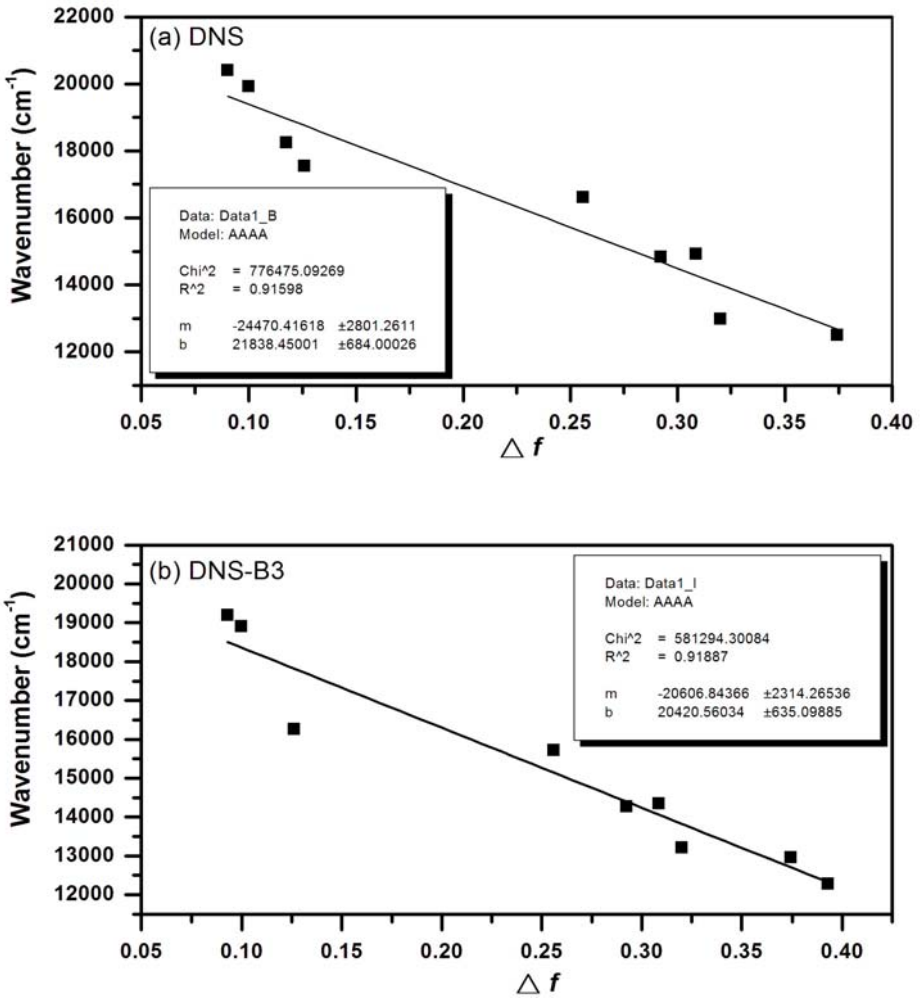


Figure S12. The Lippert-Mataga Plots of (a) DNS and (b) DNS-B3

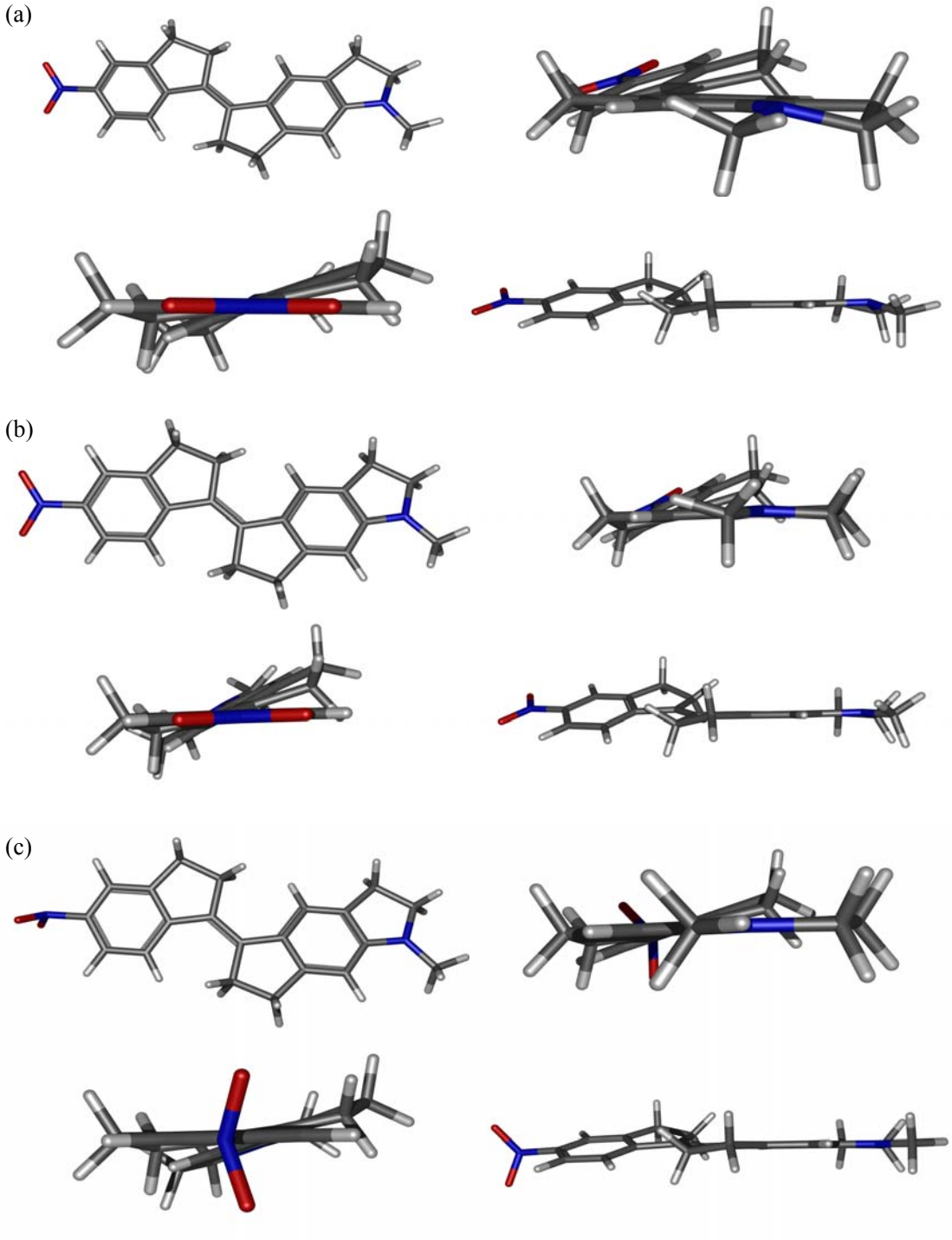
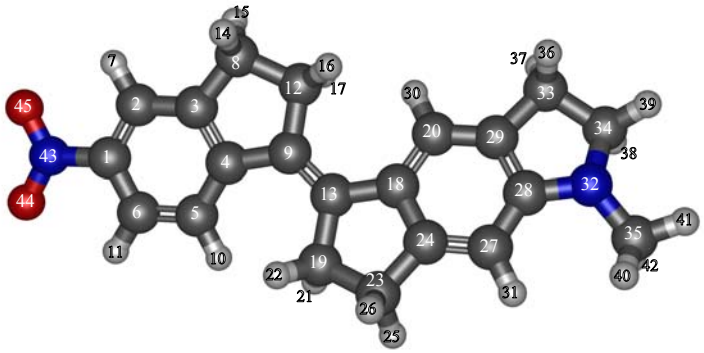


Figure S13. Equilibrium DFT structures of (a) the ground state (b) the planar radiative S_1 excited state (c) the S1 NO_2-twisted intramolecular charge transfer state (TICT). All structures are optimized with DFT (TDDFT) calculation with the B3LYP functional and 6-31G* basis set using the GAMESS electronic structure package. Bulk solvent effects are included using the equilibrium PCM solvation model in the DCM solvent.

TABLE S1. Fluorescence decay times (τ_f) for DNS-B3 determined at different emission wavelengths.

Solvent	Ex (nm)	Em (nm)	τ (ns)
n-Hex	425	500	1.00
		550	0.99
		600	1.01
		650	1.04
Toluene	450	600	2.10
		650	2.21
		700	2.18
THF	500	650	1.02
		700	1.00
		750	1.04
		800	1.10

Table S2. Selected DFT structural parameters of DNS-B3 [a]



	Ground state	S_1-planar state	S_1-twisted state
α: ϕ(C5-C4-C9-C13)	-12.7°	-15.6°	-9.2°
β: ϕ(C9-C13-C18-C20)	-12.3°	-14.6°	-9.3°
τ: ϕ(C4-C9-C13-C18)	178.3°	177.9°	176.5°
φ: ϕ(O44-N43-C1-C6)	0.1°	0.6°	74.2°
θ: ϕ(C29-C28-N32-C34)	-16.3°	-5.0°	-1.5°
ϕ(C27-C28-N32-C35)	19.9°	4.0°	0.0°
ϕ(C28-N32-C35-C34)	140.9°	170.1°	178.0°
ϕ(C1-N43-O44-O45)	179.8°	-179.5°	143.6°
∠(C28-N32-C34)	108.6°	111.9°	112.4°
∠(N32-C34-C33)	103.9°	104.8°	104.6°
∠(C28-N32-C35)	122.2°	126.7°	125.2°
∠(C34-N32-C35)	118.7°	120.8°	122.4°
∠(O44-N43-O45)	122.9°	122.7°	123.0°
∠(O44-N43-C1)	118.6°	118.7°	113.8°
r(C28-N32)	1.384 Å	1.362 Å	1.345 Å
r(N32-C35)	1.450 Å	1.446 Å	1.454 Å
r(N32-C34)	1.475 Å	1.470 Å	1.475 Å
r(C1-N43)	1.449 Å	1.435 Å	1.443 Å
r(N43-O44)	1.240 Å	1.271 Å	1.315 Å
r(C33-C34)	1.546 Å	1.549 Å	1.550 Å

[a] The geometry optimization calculations are carried out with DFT/TD-DFT in the B3LYP/6-31G* level[S8] using the GAMESS software.[S9] Bulk solvent effects are included using the equilibrium PCM solvation model in the DCM solvent.[S10]

Table S3. Calculated electronic properties of DNS-B3[a]

	Ground state	S_1-planar state	S_1-twisted state
S_0 energy	0 (eV)	0.13314 (eV)	1.45391 (eV)
S_1 energy	2.195151 (eV)	2.054385 (eV)	1.822882 (eV)
$S_0 \rightarrow S_1$ excitation energy	2.195151 (eV)	1.921245 (eV)	0.368972 (eV)
S_1 electronic configuration	HOMO → LUMO	HOMO → LUMO	HOMO → LUMO
S_1 transition dipole	3.883290 (Debye)	3.963903 (Debye)	0.037740 (Debye)
Oscillator strength of S_1 excitation	0.811000	0.739597	0.000013
Ground state dipole moment (μ_g) [b]	13.653790 (Debye)	15.885711 (Debye)	12.443758 (Debye)

[a] The optimized geometries are obtained with DFT/TD-DFT in the B3LYP/6-31G* level[S8] using the GAMESS software.[S9] Bulk solvent effects are included using the equilibrium PCM solvation model in the DCM solvent.[S10] [b] The calculations include PCM solvation in the DCM solvent, thus the ground-state dipole moments are expected to be different from those calculated in the gas phase.

Table S4. xyz-coordinates for the ground state structure

atom	x	y	z
C	-2.545546046	5.521975748	-0.655702151
C	-1.300344143	5.436806183	-0.014081630
C	-0.718521554	4.190213521	0.123027446
C	-1.357203527	3.015199532	-0.356329009
C	-2.602628111	3.137259432	-1.010207925
C	-3.192649504	4.386419600	-1.157719341
H	-0.822466149	6.335727497	0.357947841
C	0.597403653	3.852163462	0.782435282
C	-0.517701330	1.848535409	-0.091776482
H	-3.106188206	2.275618899	-1.428267629
H	-4.145583029	4.495263996	-1.661460920
C	0.831108064	2.366567358	0.407687227
C	-0.859132397	0.530470993	-0.215981744
H	0.518022601	3.973840419	1.871215244
H	1.411600085	4.505574694	0.450928546
H	1.204438452	1.788481549	1.259087554
H	1.591441116	2.292360657	-0.382762040
C	-0.015695796	-0.642360763	0.012759780
C	-2.250478772	0.018581854	-0.583368877
C	1.387298576	-0.758067014	0.188252066
H	-2.427327048	0.143760617	-1.660624856
H	-3.041697252	0.570931459	-0.066630248
C	-2.258553868	-1.485433919	-0.215991420
C	-0.802701889	-1.817475882	0.001135644
H	-2.716746867	-2.106143489	-0.994833115
H	-2.834491694	-1.662306594	0.702838562
C	-0.255887557	-3.086557750	0.176682431
C	1.129628971	-3.174934659	0.370575525
C	1.939262702	-2.011363840	0.359214971
H	2.034118952	0.111183331	0.160434268
H	-0.886014937	-3.971239779	0.150741030
N	1.901462868	-4.300787660	0.599137804
C	3.375585672	-2.432840649	0.601353447
C	3.316297949	-3.958617369	0.362249458
C	1.442476502	-5.634226041	0.263231669
H	3.671782791	-2.213217433	1.636341613
H	4.096901592	-1.938620444	-0.056805783
H	3.596539308	-4.206139546	-0.675600782
H	3.965543774	-4.529865260	1.033236773
H	0.450540801	-5.808329898	0.690100621
H	2.128619814	-6.368997530	0.695280941
H	1.391642719	-5.803250716	-0.825497043
N	-3.176157319	6.817589667	-0.804719650
O	-4.275469123	6.881432497	-1.374020796
O	-2.591890846	7.813697859	-0.353604301

Table S5. xyz-coordinates for the S_1-planar state structure

atom	x	y	z
C	-2.553304913	5.546334114	-0.633236792
C	-1.331415255	5.427337481	0.047615949
C	-0.756240609	4.165908045	0.163054573
C	-1.372247200	3.021251224	-0.384900253
C	-2.585673933	3.163386585	-1.078442743
C	-3.175544669	4.421003639	-1.202470729
H	-0.862556600	6.313158164	0.459105278
C	0.539604938	3.806626977	0.848040327
C	-0.523623052	1.827238443	-0.129227781
H	-3.069727808	2.314098506	-1.546816735
H	-4.108116779	4.553169957	-1.736364191
C	0.809334634	2.352434681	0.385797586
C	-0.865190187	0.515574427	-0.265310812
H	0.422706186	3.849315360	1.939810928
H	1.356837429	4.489700715	0.591856807
H	1.221268086	1.733294818	1.188135531
H	1.549754414	2.356879104	-0.428116425
C	-0.008079370	-0.657190052	-0.05063572
C	-2.255193659	-0.004146518	-0.626468856
C	1.396389021	-0.764541460	0.070771062
H	-2.424900218	0.063431106	-1.710372489
H	-3.049925257	0.572609846	-0.143815891
C	-2.265941935	-1.489428732	-0.185342004
C	-0.807001625	-1.838148595	-0.018587499
H	-2.772183207	-2.143043974	-0.904137336
H	-2.790824044	-1.609986850	0.772673938
C	-0.261528872	-3.097083123	0.163516903
C	1.138460741	-3.179440717	0.314877196
C	1.955951448	-2.013663996	0.256603423
H	2.037714297	0.105834744	0.001179683
H	-0.888848154	-3.982900044	0.178751226
N	1.908185864	-4.283615161	0.522345589
C	3.400410085	-2.416270196	0.441336066
C	3.342286844	-3.962562425	0.505237775
C	1.456544854	-5.656990701	0.556840274
H	3.812921017	-1.995184161	1.366172765
H	4.037407562	-2.068479935	-0.379027871
H	3.809145240	-4.433758180	-0.370614837
H	3.822528476	-4.376433036	1.399154956
H	0.402102861	-5.702315386	0.835592111
H	2.038650139	-6.210814206	1.300565334
H	1.587472877	-6.145245563	-0.419578146
N	-3.163623007	6.838381410	-0.763004323
O	-4.267450389	6.933017541	-1.385466134
O	-2.571935964	7.842606794	-0.256861048

Table S6. xyz-coordinates for the S_1-twisted state structure

atom	x	y	z
C	0.886725377	0.100156080	3.716209054
C	1.081273328	-0.122086020	2.355480473
C	-0.026172131	-0.185709736	1.514404706
C	-1.339378284	-0.026785053	2.019650188
C	-1.519774045	0.196277943	3.404426509
C	-0.410143617	0.251636263	4.234687336
H	2.090993984	-0.234958301	1.969802918
C	-0.037681223	-0.419812325	0.028864510
C	-2.297246449	-0.090250451	0.922612433
H	-2.502988156	0.349021463	3.828876863
H	-0.526863052	0.434926095	5.298203589
C	-1.508458517	-0.165480316	-0.375832306
C	-3.682900446	-0.113485488	1.006822491
H	0.258399941	-1.451179142	-0.204014399
H	0.663921085	0.233832916	-0.501172285
H	-1.895799736	-0.944361226	-1.040214909
H	-1.589733797	0.786009823	-0.919030198
C	-4.623537955	-0.106694610	-0.079911017
C	-4.461669186	-0.187071683	2.315254324
C	-4.436782253	0.098702034	-1.479541902
H	-4.408109462	0.772760824	2.845050067
H	-4.050583596	-0.944931916	2.989011054
C	-5.923013782	-0.499381226	1.917968631
C	-5.953239923	-0.305988988	0.425620585
H	-6.647915910	0.142771996	2.429534727
H	-6.186750675	-1.534167700	2.171416802
C	-7.061192904	-0.326807907	-0.392762957
C	-6.844850685	-0.128014372	-1.775039030
C	-5.530793548	0.083197618	-2.303585025
H	-3.456766864	0.283692964	-1.897949658
H	-8.058526840	-0.481718619	0.005862088
N	-7.761379546	-0.097932267	-2.759554582
C	-5.637039587	0.265323938	-3.801792556
C	-7.159789432	0.176872652	-4.077538496
C	-9.193287132	-0.270937552	-2.578091015
H	-5.089919522	-0.517438126	-4.338455453
H	-5.226069022	1.226526061	-4.127491189
H	-7.571809643	1.111509537	-4.474772119
H	-7.421079953	-0.629056306	-4.771624398
H	-9.408314430	-1.239291381	-2.113231066
H	-9.677458817	-0.234387505	-3.555034960
H	-9.606255663	0.525946983	-1.948631151
N	2.030034856	0.193348796	4.591426764
O	2.195960604	-0.858587848	5.362956723
O	2.280468393	1.421258064	4.989954483

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