

Supplementary data

Green Photocatalytic N-Debenzylations with Molecular Oxygen Catalyzed by Recyclable Metal- free Tubular Carbon Nitride

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Number of figures: 1 [Figure S1]

References: 10

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General Information

All reagents were commercially available and used without further purification unless indicated otherwise. **1a** -**1ak** were prepared in laboratory. Silica gel column chromatography was performed with 200 – 300 mesh silica gels. TLC was performed using commercially prepared 100 - 400 mesh silica gel plates (GF254), and visualization was effected with UV light (254 nm).

¹H spectra was recorded on Bruker Avance 400 MHz spectrophotometers (¹H: 400 MHz, ¹³C: 101 MHz). Chemical shifts (δ) for ¹H are given in ppm relative to TMS. The residual solvent signals were used as references for ¹H and ¹³C NMR spectra and the chemical shifts converted to the TMS scale (CDCl₃: δ H = 7.26 ppm, DMSO-d₆: δ H = 2.50 ppm). The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, m = multiplet.

High performance liquid chromatography (HPLC) were carried out on an Agilent 1100. Gas chromatography mass spectrometry (GC-MS) were carried out on an Agilent 5975C Gas Chromatograph/Mass Selective. X-ray diffraction (XRD) patterns were recorded using a D8 Advance spectrometer, Cu K α radiation (λ = 0.154 nm), operating at 40 mA and 40 kV. FT-IR spectra were recorded using a Thermo Fisher 6700 spectrometer. SEM patterns were recorded using a NOVA Nano SEM 450 field emission transmission electron microscope. Specific surface areas of catalysts were carried out on Accelerated Surface Area Porosimetry System (Micromeritics Instrument Corporation). UV-vis diffuse reflectance spectra were recorded using a UV-550 UV spectrophotometer. EPR spectra was recorded using a Bruker E500 electron paramagnetic resonance spectrometer. PL spectra was recorded using a F-7100 fluorescence spectrometer. The light intensity was determined by a digital illuminometer (DL333205) made by Deli.

Experiments

Preparation of catalysts

CN-M: CN-M was prepared according to Xiao's literature¹. Melamine (20 g, 159 mmol) in a ceramic crucible was heated to 550 °C at a rate of 2.3 °C min⁻¹ in a muffle furnace in an air atmosphere. The temperature was maintained at 550°C for 4 hours and CN-M was obtained after cooling to room temperature.

CN-U: CN-U was prepared according to Zhang's literature². Urea (20 g, 333 mmol) in a ceramic crucible was heated to 550°C at a rate of 2.3 °C min⁻¹ in a muffle furnace in an air atmosphere. The temperature was maintained at 550°C for 4 hours and CN-U was obtained after cooling to room temperature.

CN-T: CN-T was prepared according to Wang's literature³. The mixture of melamine (1.0 g, 8 mmol) and urea (12.0 g, 200 mmol) was fully grounded with a mortar and then heated to 550°C at a rate of 2.3 °C min⁻¹ in a muffle furnace in an air atmosphere. The temperature was maintained at 550°C for 4 hours and CN-T was obtained after cooling to room temperature.

CN-G: CN-G was prepared according to Jun's literature⁴. Melamine (0.5 g, 4 mmol) and cyanuric acid (0.51 g, 4 mmol) were dissolved in 20 and 10 mL DMSO, respectively. After sonication for 30 min to dissolve them completely, the two solutions were mixed together to obtain a white precipitate. The precipitate was filtered, washed with water and ethanol, dried at 50 °C, and then calcined at 550 °C for 4 h with the heating rate of 2.3 °C min⁻¹.

CN-F: CN-F was prepared according to Yu's literature⁵. Melamine (0.5 g, 4 mmol), and the mixture of cyanuric acid (0.51 g, 4 mmol) and oxalic acid (0.1 g, 1 mmol) were dissolved in 20 and 10 mL DMSO, respectively. After sonication for 30 min to dissolve them completely, the two solutions were mixed together to obtain a white precipitate. The precipitate was filtered, washed with water and ethanol, dried at 50 °C and then calcined at 550 °C for 4 h with the heating rate of 2.3 °C min⁻¹.

TiO₂-F: TiO₂-F was prepared according to Yu's literature⁶. Potassium titanate oxalate (0.8 g, 2.2 mmol) and urea (2.4 g, 40 mmol) were added to the mixture of diethyleneglycol (60 ml) and deionized water (20 ml). The mixture was then sealed and stirred for 2 hours. After stirring, the dispersed mixture was loaded into a 100 ml a hydrothermal reactor and reacted at 180 °C for 12 hours. Finally, TiO₂-F was obtained by centrifugation, washing with anhydrous ethanol and deionized water, and vacuum drying overnight at 70 °C.

CN-M-Fe: CN-M-Fe was prepared according to Ahmad's literature⁷. The catalyst was synthesized via incipient wetness impregnation method using FeCl₃ as Fe source and CN-M as support. FeCl₃ (20 mg, 0.12 mmol) and CN-M (1.0 g) were dissolved into 20 mL of deionized water. The mixture was stirred vigorously at room temperature for 2 h, followed by stirring and heating at 80 °C until the water almost completely

evaporates. The sample was dried at 50 °C and then calcined at 550 °C for 4 h with the heating rate of 2.3 °C min⁻¹.

CN-M-Ni: CN-M-Ni was prepared according to Ahmad's literature⁷. The catalyst was synthesized via incipient wetness impregnation method using Ni(NO₃)₂·6H₂O as Ni source and CN-M as support. Ni(NO₃)₂·6H₂O (20 mg, 0.07 mmol) and CN-M (1.0 g) were dissolved into 20 mL of deionized water. The mixture was stirred vigorously at room temperature for 2 h, followed by stirring and heating at 80 °C until the water almost completely evaporates. The sample was dried at 50 °C and then calcined at 550 °C for 4 h with the heating rate of 2.3 °C min⁻¹.

General Photocatalytic N-debenzylation

The oven-dried schlenk tube (25 mL) equipped with a stirring bar, gas balloon and an inner light resource was charged with **1** (0.2 mmol, 1.0 equiv.), catalyst (5 mg), HCl (37%, 25 uL, 0.3 mmol) and acetone (2 mL). The light source (415 nm, 3W) was 4 centimeters higher than the liquid level, with an intensity of about 464 Lx. The reaction mixture in sealed tube was stirred at 25 °C for about 15 minutes and then reacted under light for 1 – 72 h. The yield was obtained via column separation, high performance liquid chromatography (HPLC) or Gas Chromatography-Mass Spectrometry (GC-MS).

Table S1. The light intensity for different light resources.

Light resource	Light intensity (Lx)
660nm, 3W	1738
620 nm, 3W	2156
590 nm, 3W	2991
550 nm, 3W	3970
450 nm, 3W	3186
415 nm, 3W	8192
385 nm, 3W	7400
395 nm, 30W	50500
254nm, 1W	--

Catalyst recovery experiments

The 1th cycle: The oven-dried quartz schlenk tube (50 mL) containing a stirring bar and a gas balloon was charged with **1a** (257.0 mg, 1.0 mmol, 1.0 equiv), CN-T (25.0 mg), HCl (125 μ l, 1.5 mmol, 1.5 equiv), and acetone (10 mL). the gas balloon was filled with a mixture of air and N₂ (V_{air}:V_{N₂} = 1:2). 20 W LEDs (wavelength: 395 nm) was used to illuminate the reaction solution from the side after pre-stirring for 15 min. the reaction temperature was 25 °C. The reaction time for each cycle was shown in Table S1. After reaction, the mixture was centrifuged to obtained recycled CN-T and reaction liquid. The reaction liquid was analyzed by HPLC. The recycled CN-T was further washed with acetone and dried at 50 °C in vacuum for 4 h.

The 2 – 4th cycles: the recycled CN-T and a small amount of fresh CN-T (if the catalyst loss is significant) is used in the next cycle. The recycled CN-T for 3 – 6th cycles are dried at 150 °C for 2 h. More detailed information is shown in Table S2.

Table S2. The results for the recycled experiments.

Cycle	Fresh CN-T (mg)	Recycled CN-T (mg)	Recovery rate (%)	Drying Temperature (°C)	Reaction time (°C)	Yield (%)
1	25	24.8	99	50	5	85
2	0	23.6	95	50	5	86
3	0	22	93	150	5.5	88
4	3	24.5	98	150	6	89
5	0	23.8	97	150	6	90
6	1.2	24.2	97	150	6	89

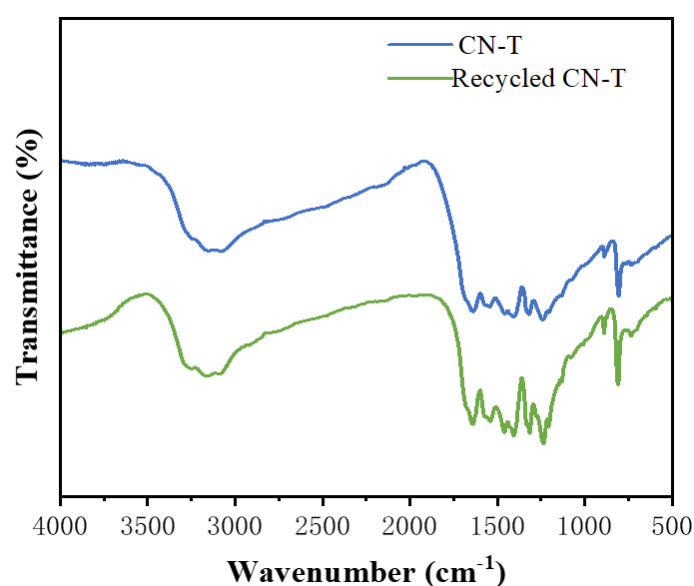


Figure S1. Fourier transform infrared (FT-IR) pattern for the recycled CN-T.

Electron paramagnetic resonance experiments

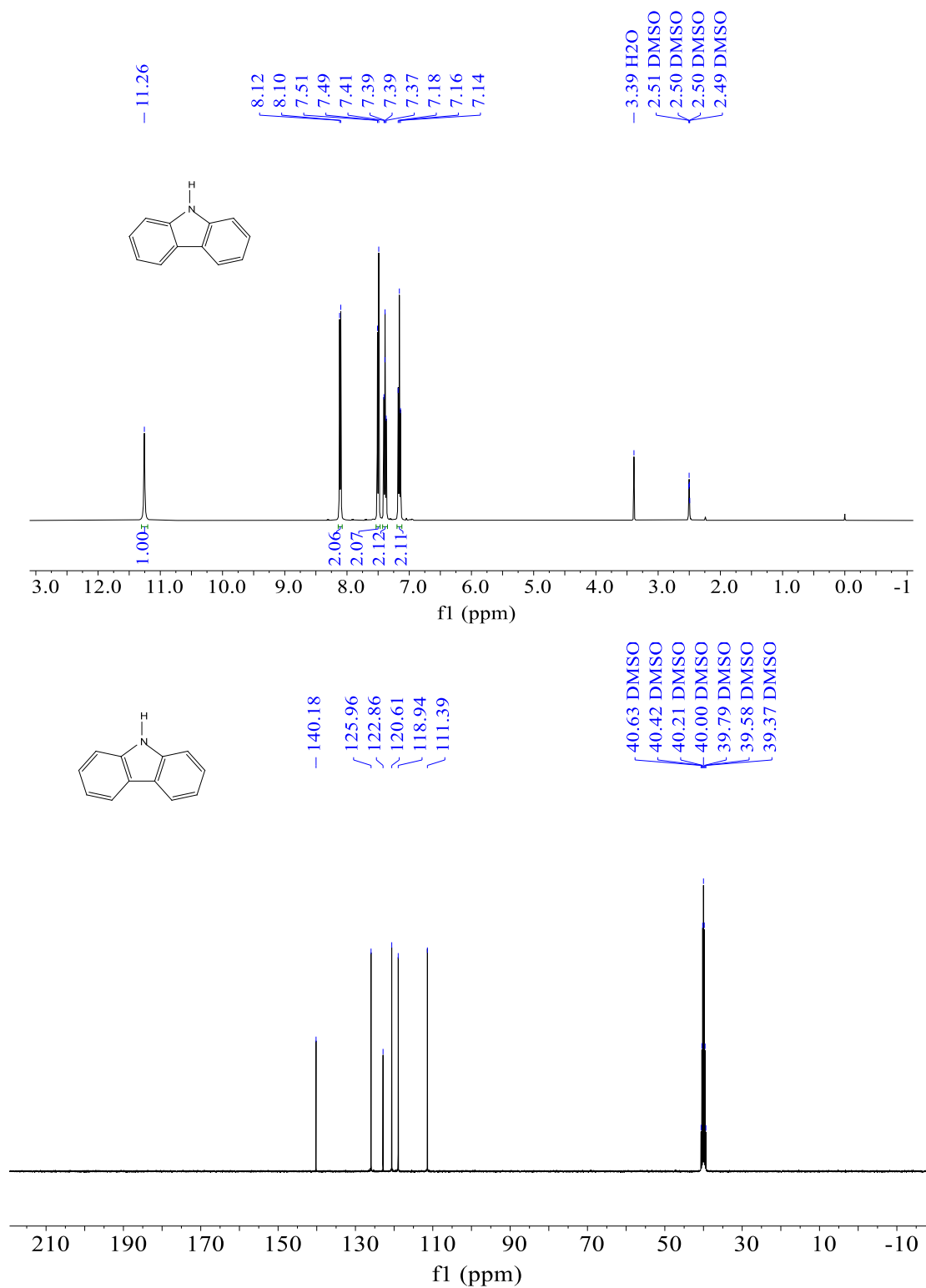
Electron paramagnetic resonance experiments were measured on Bruker E500 electron paramagnetic resonance spectrometer. A mixture of 1a (0.2 mmol), CN-T (5 mg), TEMP (2,2,6,6-tetramethyl-piperidine) (0.4mmol) or DMPO (5,5-dimethyl-1-pyrroline-N-oxide, 0.2 mmol) (0.4mmol) in acetone (2 mL) was stirred. 20 μ L of the mixture was quickly taken out into a small tube and analyzed by EPR. Afterwards, the mixture irradiated by a 100 W Xenon lamp for 2 min. Signal comparison reveals that molecular oxygen is activated to generate singlet oxygen and superoxide radicals.

DFT Calculations

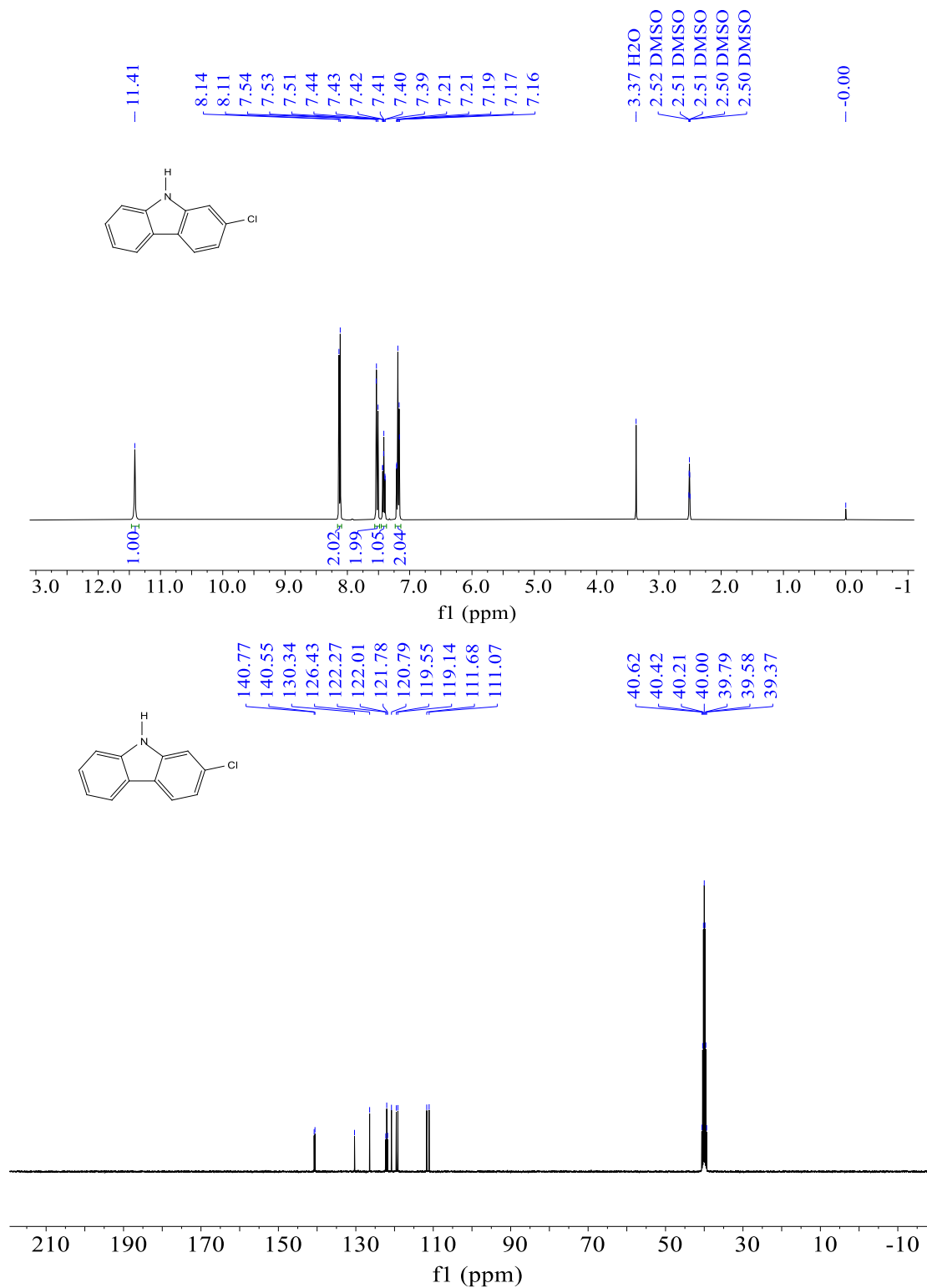
All calculations were carried out with Gaussian 16⁸. Geometry optimization and vibrational frequencies for all structures of reductants, products, transition states and intermediates were performed using M06-2x hybrid meta functiona^{9, 10} with a basis set of 6-311+G(d,p) for all atoms. Acetone was used as solvent and the self-consistent reaction field (SCRF) polarizable continuum model (PCM) model was applied to calculate the solvation energy corrections. Only one imaginary frequency corresponding to the reaction coordinates was found for the transition states. The more accurate electron energies were obtained from the frequency calculations at a level of M06-2x/def2tzvp.

Characterization for products

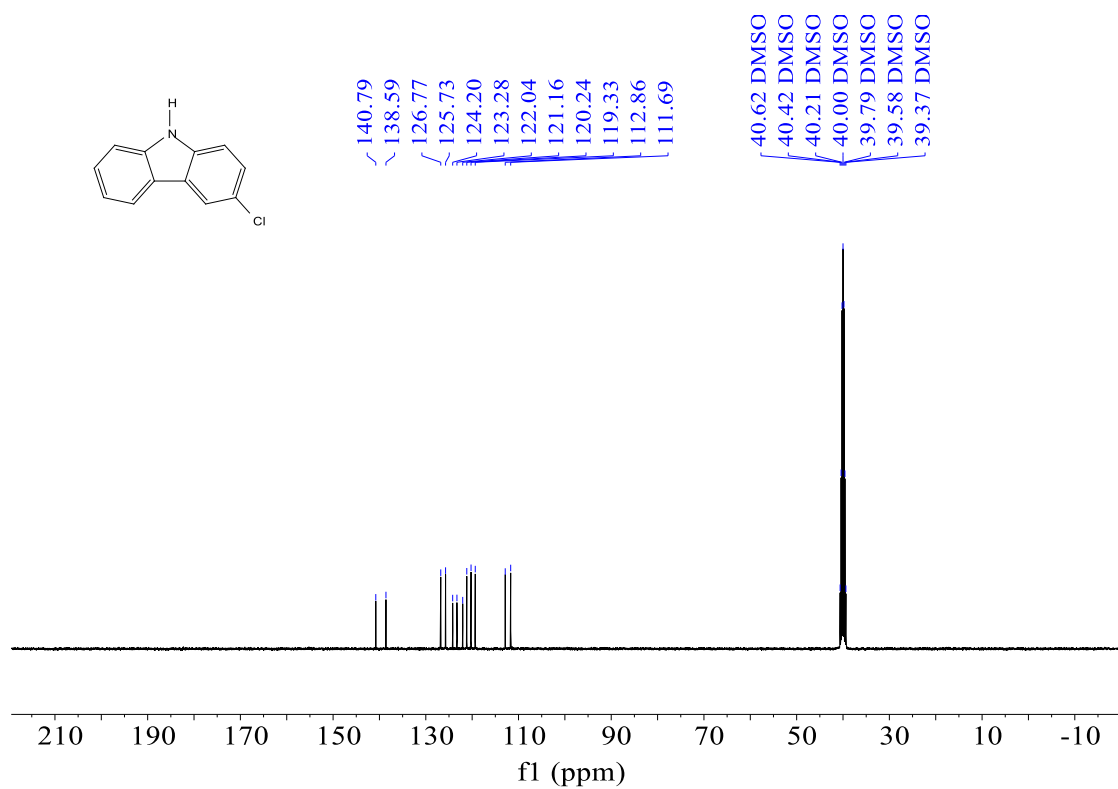
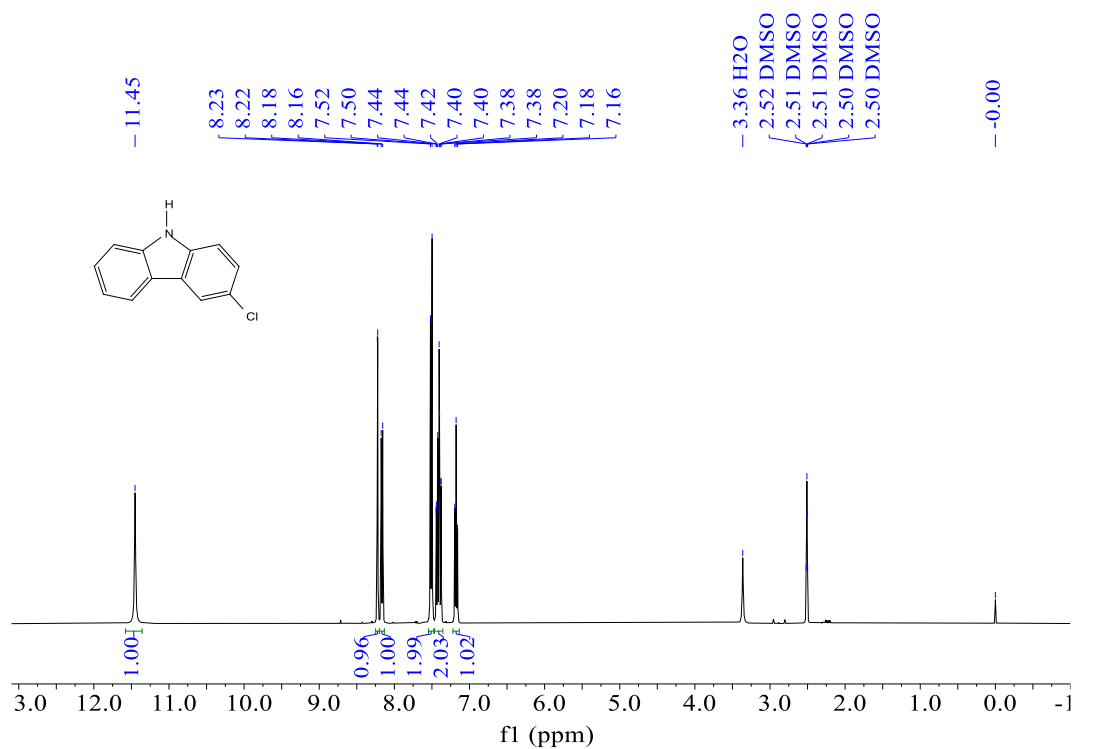
Carbazole (2a - 2r): White solid, 13.4 ~ 31.1 mg; $^1\text{H NMR}$ (400 MHz, $\text{DMSO-}d_6$) δ 11.26 (s, 1H), 8.12-8.10 (d, $J = 7.8$ Hz, 2H), 7.51-7.39 (d, $J = 8.1$ Hz, 2H), 7.41-7.39 (t, $J = 7.0$ Hz, 2H), 7.20 - 7.12 (m, 2H). $^{13}\text{C NMR}$ (101 MHz, $\text{DMSO-}d_6$) δ 140.18, 125.96, 122.86, 120.61, 118.94, 111.39.



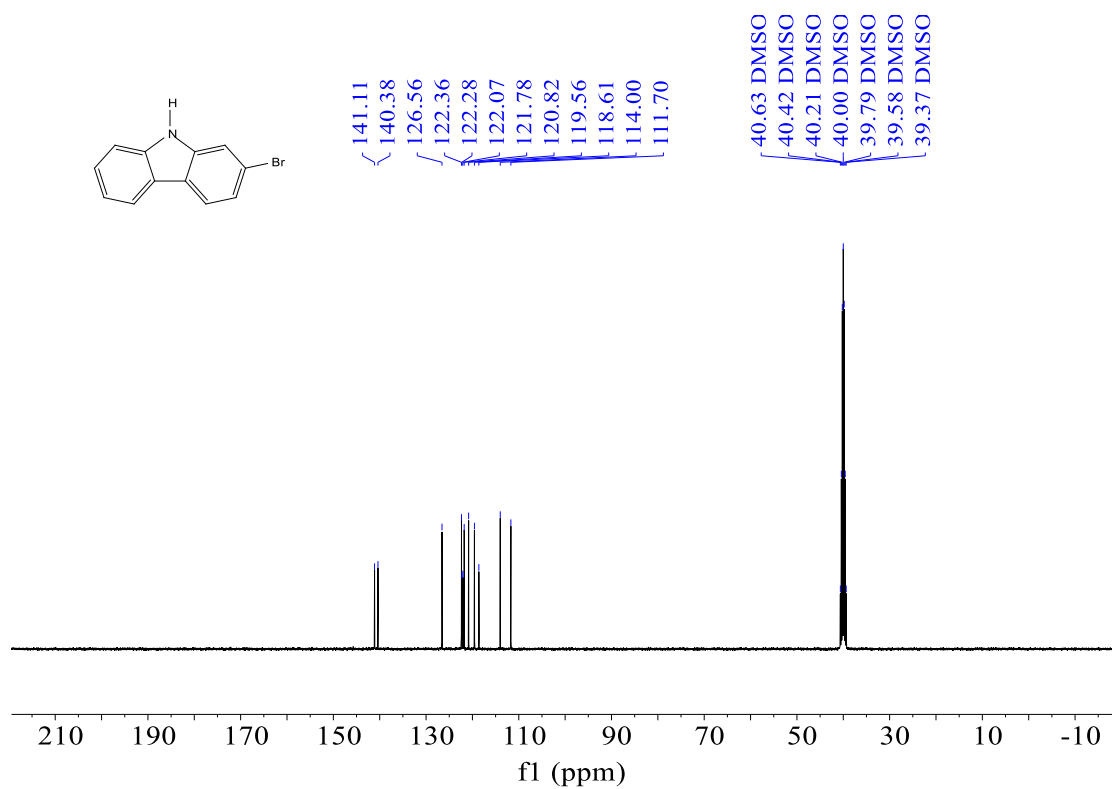
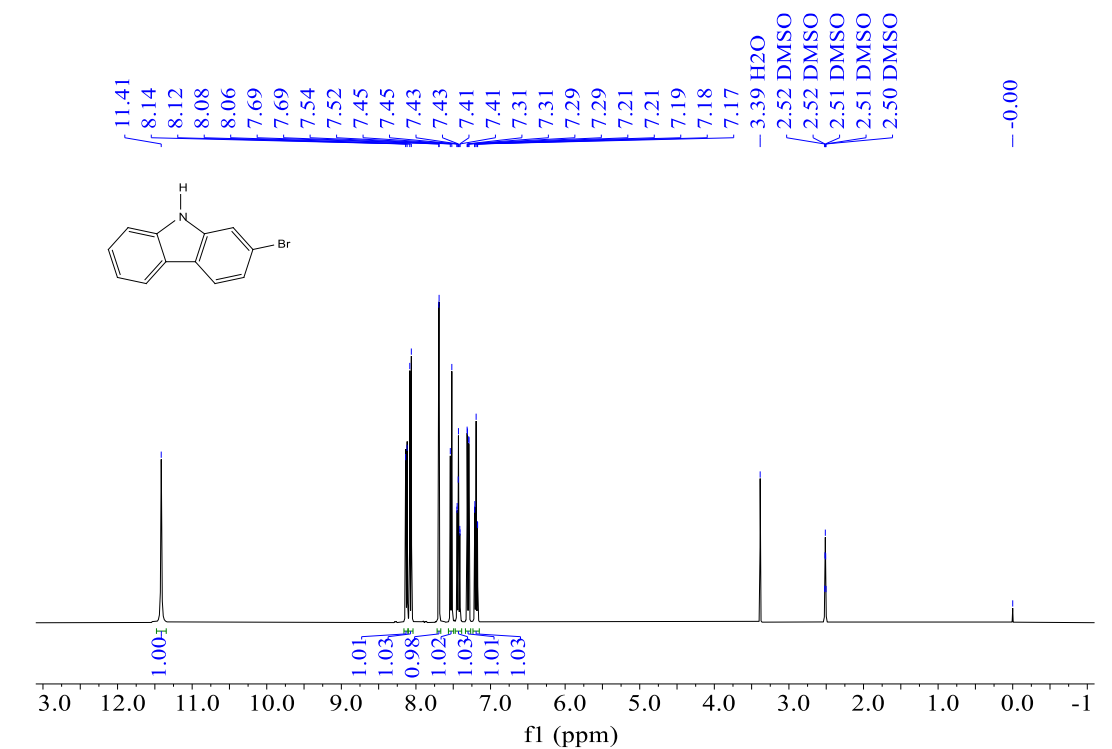
2-Chloro-9H-carbazole (2t): White solid, 32.6 mg; $^1\text{H NMR}$ (400 MHz, $\text{DMSO-}d_6$) δ 11.41 (s, 1H), 8.12 (d, $J = 8.2$ Hz, 2H), 7.56 – 7.48 (m, 2H), 7.46 – 7.37 (m, 1H), 7.23 – 7.14 (m, 2H). $^{13}\text{C NMR}$ (101 MHz, $\text{THF-}d_8$) δ 126.43, 122.01, 120.79, 119.55, 119.14, 111.68, 111.07.



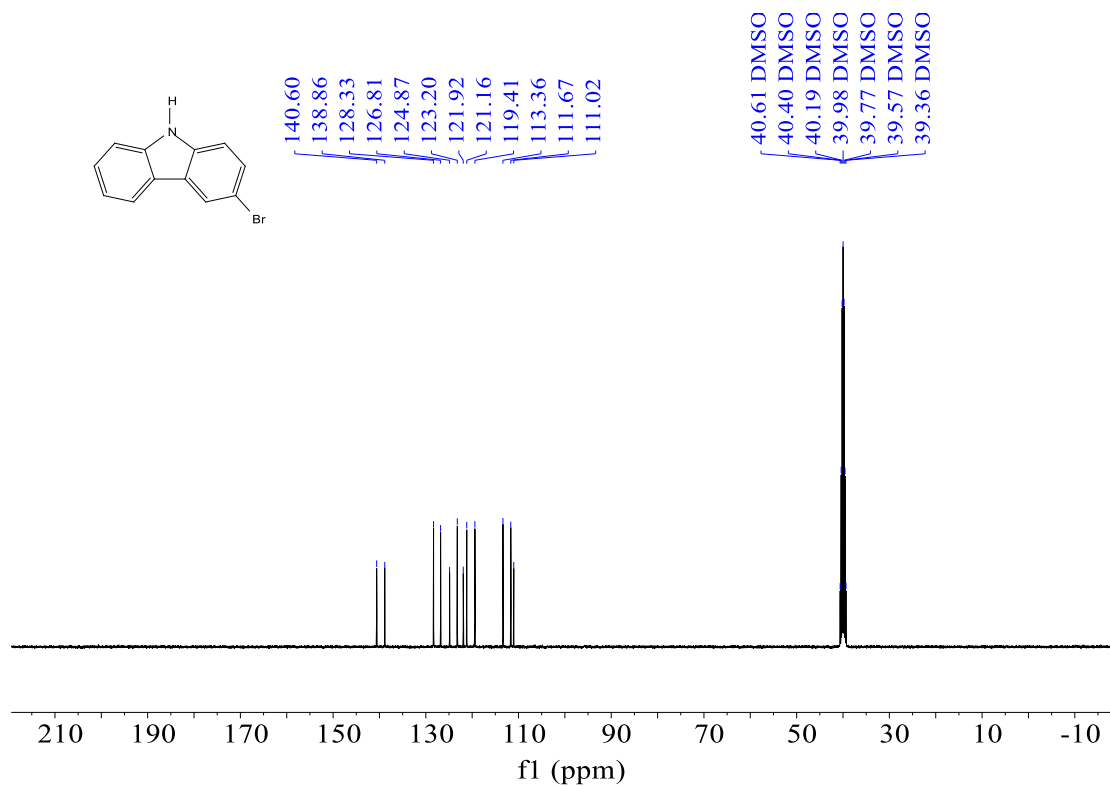
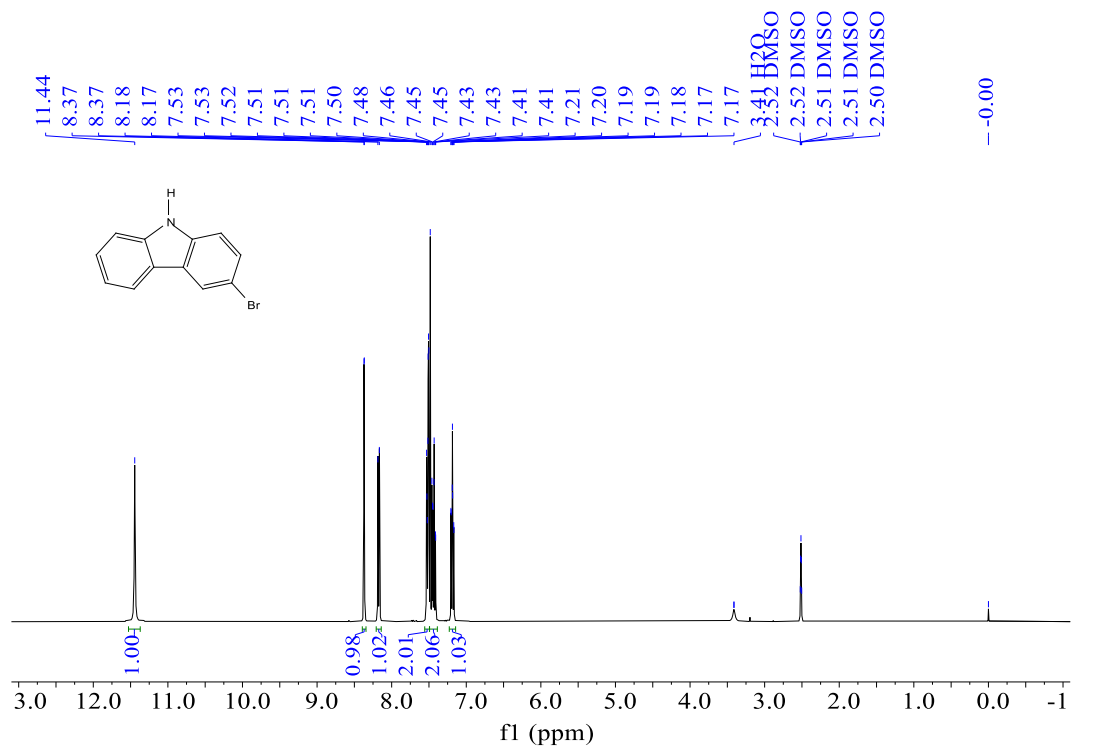
3-Chloro-9H-carbazole (2u): White solid, 35.0 mg; $^1\text{H NMR}$ (400 MHz, $\text{DMSO-}d_6$) δ 11.45 (s, 1H), 8.23-8.21 (d, $J = 2.1$ Hz, 1H), 8.18-8.16 (d, $J = 7.8$ Hz, 1H), 7.52-7.51 (d, $J = 8.6$ Hz, 2H), 7.47 – 7.35 (m, 2H), 7.20-7.16 (t, $J = 6.9$ Hz, 1H). $^{13}\text{C NMR}$ (101 MHz, $\text{DMSO-}d_6$) δ 140.79, 138.59, 126.77, 125.73, 124.20, 123.28, 122.04, 121.16, 120.24, 119.33, 112.86, 111.69.



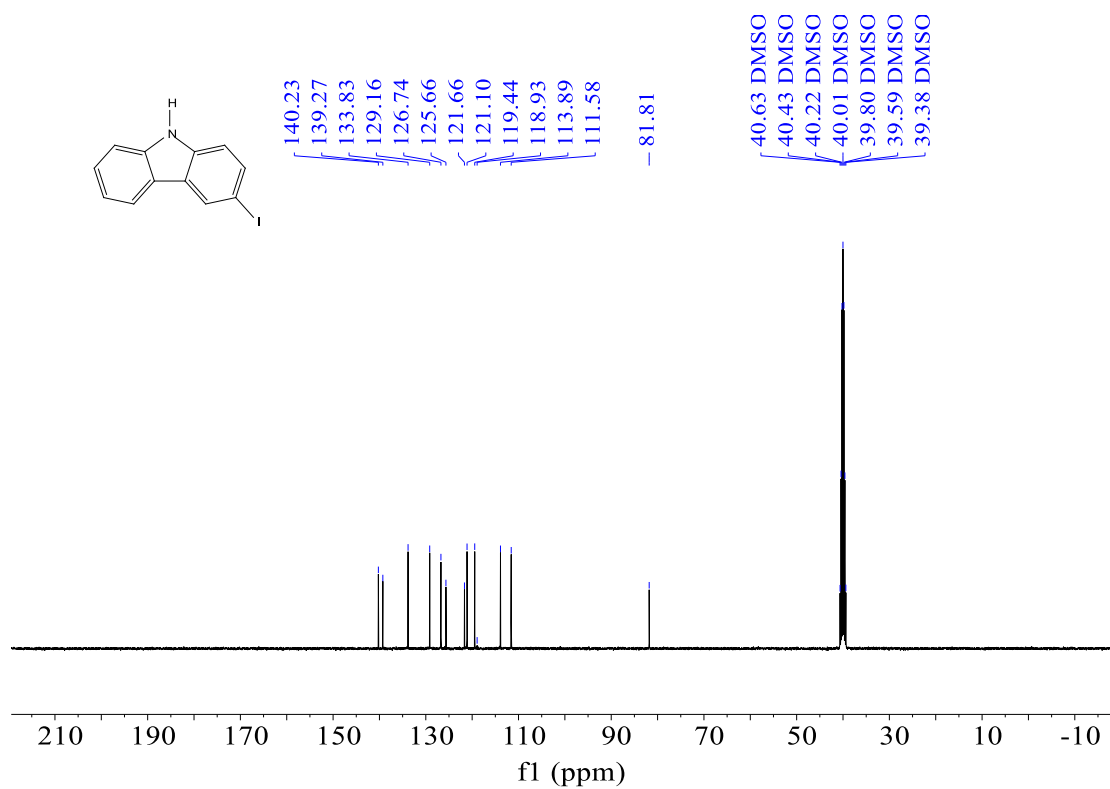
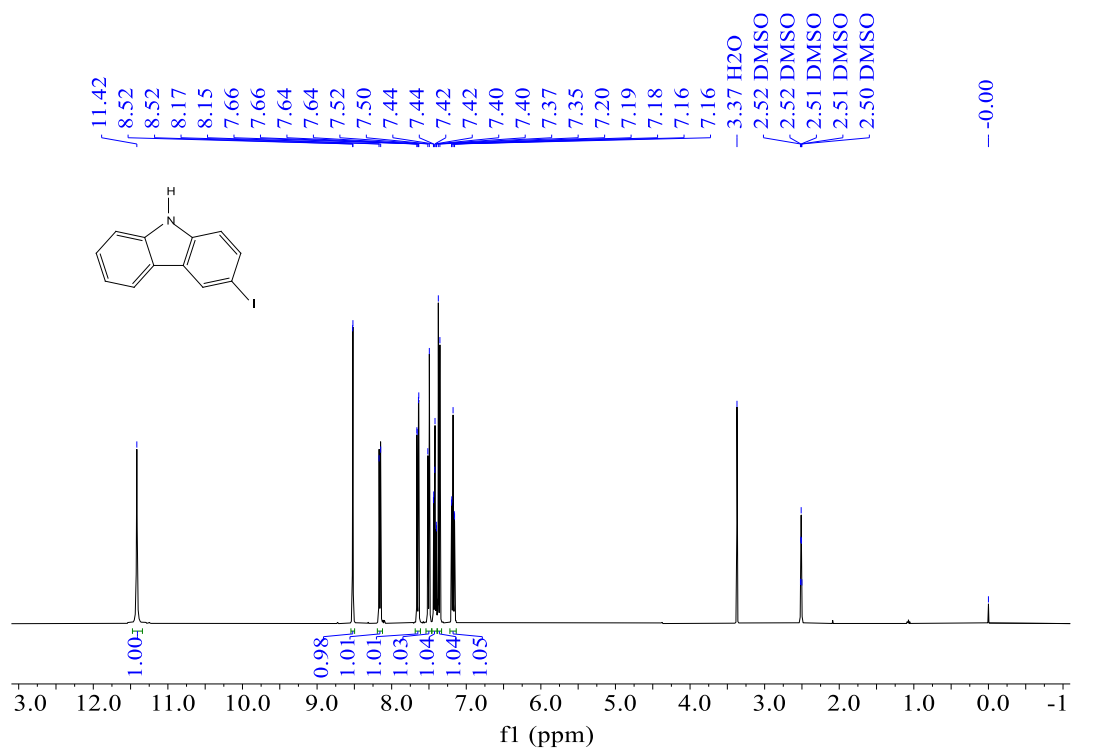
2-Bromo-9H-carbazole (2v): White solid, 39.2 mg; $^1\text{H NMR}$ (400 MHz, $\text{DMSO-}d_6$) δ 11.41 (s, 1H), 8.13 (d, $J = 7.8$ Hz, 1H), 8.07 (d, $J = 8.3$ Hz, 1H), 7.69 (d, $J = 1.7$ Hz, 1H), 7.53 (d, $J = 8.2$ Hz, 1H), 7.43 (m, $J = 8.2, 7.6, 1.2$ Hz, 1H), 7.30 (m, $J = 8.3, 1.8$ Hz, 1H), 7.24 – 7.14 (m, 1H). $^{13}\text{C NMR}$ (101 MHz, $\text{DMSO-}d_6$) δ 141.11, 140.38, 126.56, 122.36, 122.28, 122.07, 121.78, 120.82, 119.56, 118.61, 114.00, 111.70.



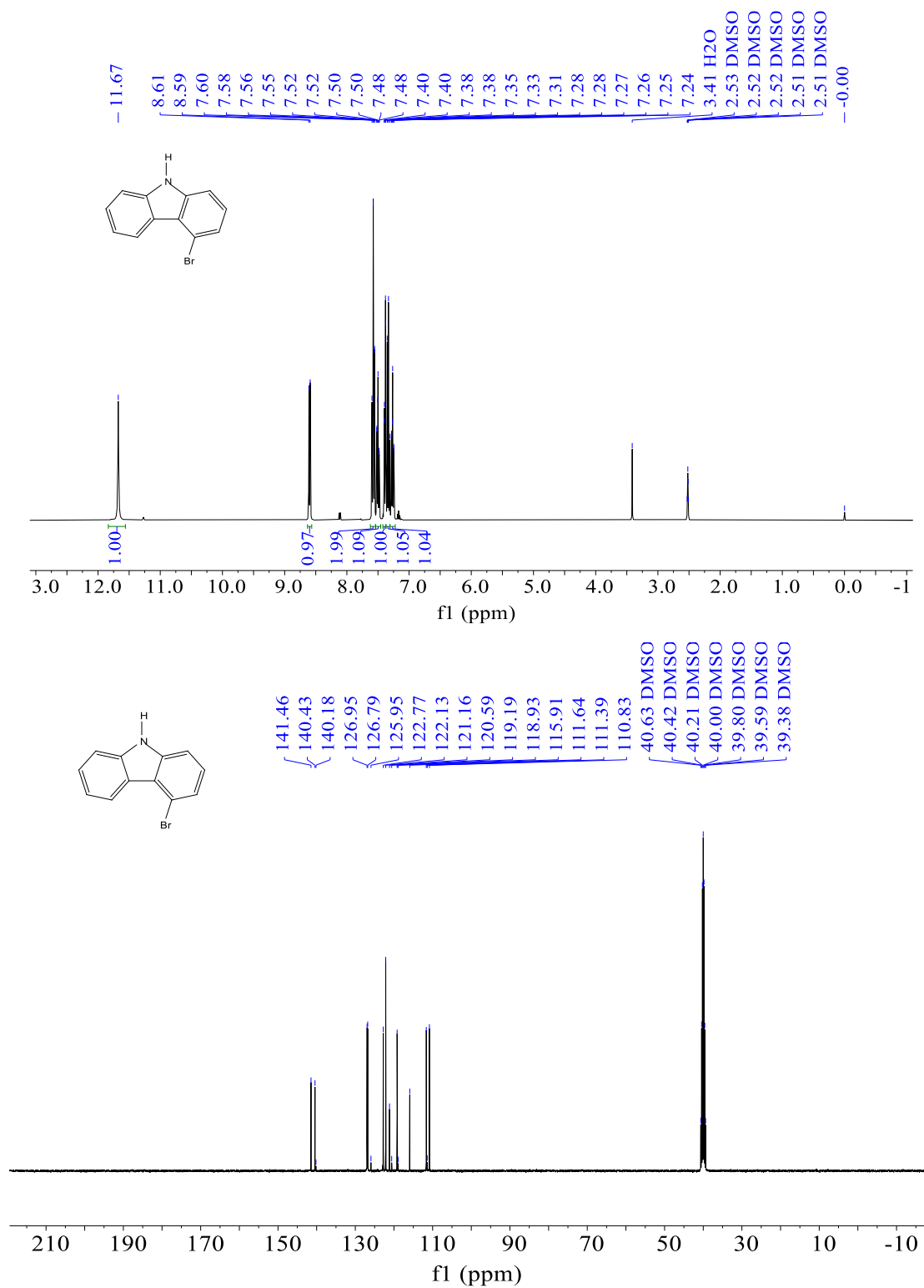
3-Bromo-9H-carbazole (2w, 2x): White solid, 38.2 ~ 44.1 mg; $^1\text{H NMR}$ (400 MHz, $\text{DMSO-}d_6$) δ 11.44 (s, 1H), 8.37 (d, $J = 1.9$ Hz, 1H), 8.18 (d, $J = 7.9$ Hz, 1H), 7.56 – 7.49 (m, 2H), 7.49 – 7.39 (m, 2H), 7.23 – 7.14 (m, 1H). $^{13}\text{C NMR}$ (101 MHz, $\text{DMSO-}d_6$) δ 140.60, 138.86, 128.33, 126.81, 124.87, 123.20, 121.92, 121.16, 119.41, 113.36, 111.67, 111.02.



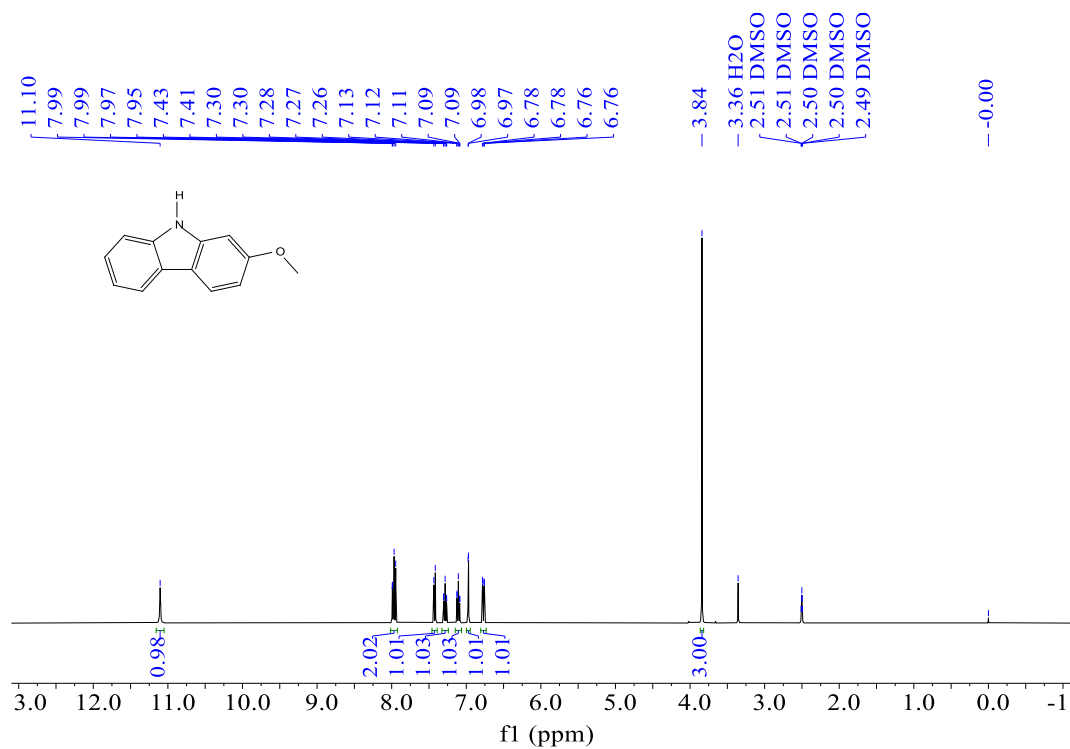
3-Iodo-9H-carbazole (2y): White solid, 45.7 mg; $^1\text{H NMR}$ (400 MHz, $\text{DMSO-}d_6$) δ 11.42 (s, 1H), 8.52 (d, $J = 1.7$ Hz, 1H), 8.16 (d, $J = 8.8$ Hz, 1H), 7.68 – 7.61 (m, 1H), 7.51 (d, $J = 8.1$ Hz, 1H), 7.46 – 7.39 (m, 1H), 7.36 (d, $J = 8.5$ Hz, 1H), 7.22 – 7.13 (m, 1H). $^{13}\text{C NMR}$ (101 MHz, $\text{DMSO-}d_6$) δ 140.23, 139.27, 133.83, 129.16, 126.74, 125.66, 121.66, 121.10, 119.44, 118.93, 113.89, 111.58, 81.81.

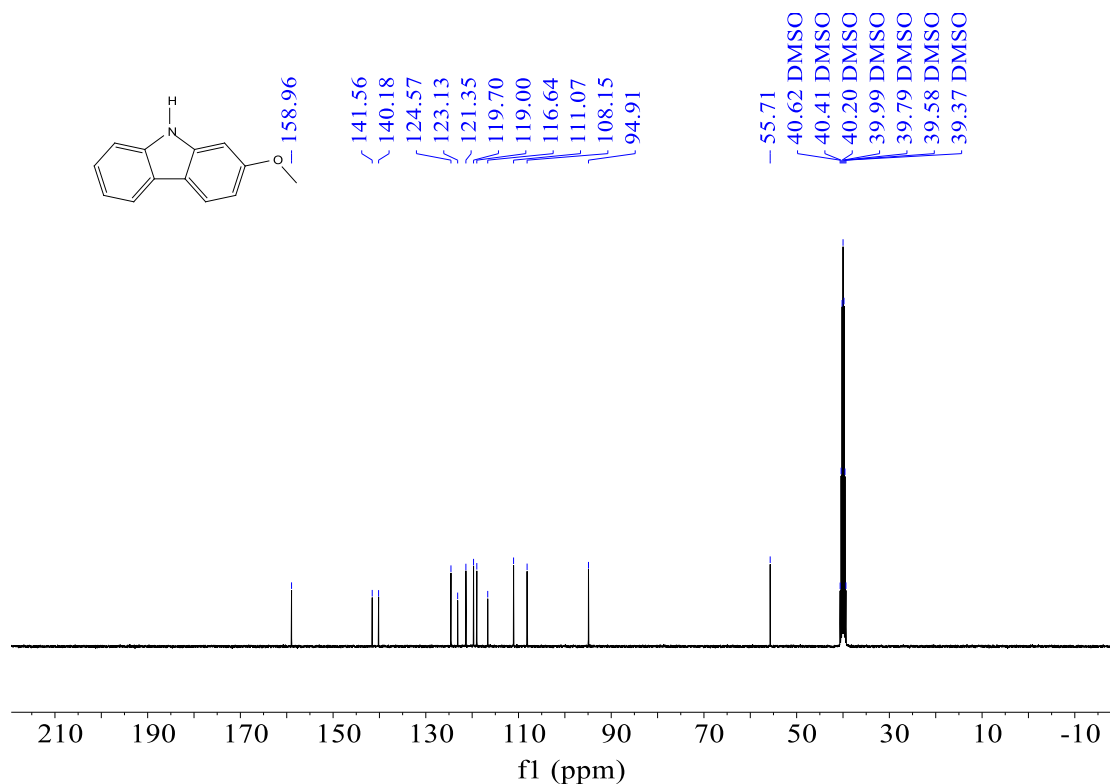


4-Bromo-9H-carbazole (2z): White solid, 35.3 mg; $^1\text{H NMR}$ (400 MHz, $\text{DMSO-}d_6$) δ 11.67 (s, 1H), 8.60 (d, $J = 8.1$ Hz, 1H), 7.61 – 7.54 (m, 2H), 7.54 – 7.47 (m, 1H), 7.39 (m, $J = 7.8, 1.1$ Hz, 1H), 7.33 (t, $J = 7.8$ Hz, 1H), 7.29 – 7.23 (m, 1H). $^{13}\text{C NMR}$ (101 MHz, $\text{DMSO-}d_6$) δ 141.46, 140.43, 126.95, 126.79, 122.77, 122.13, 121.16, 119.19, 115.91, 111.64, 110.83.

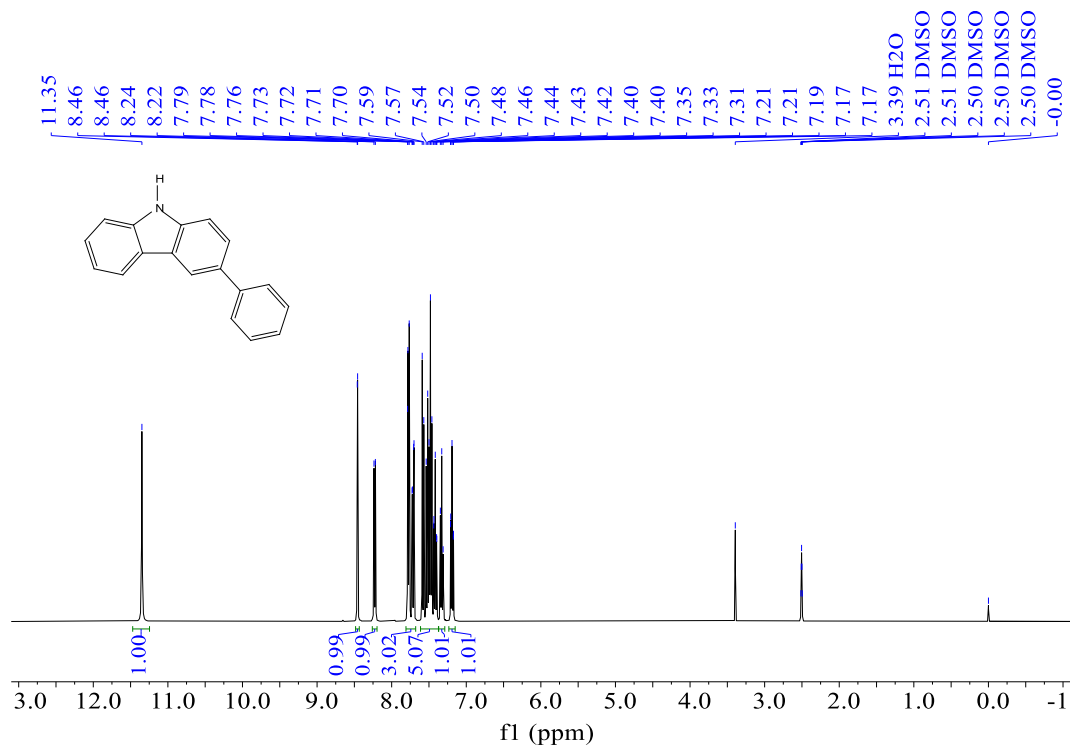


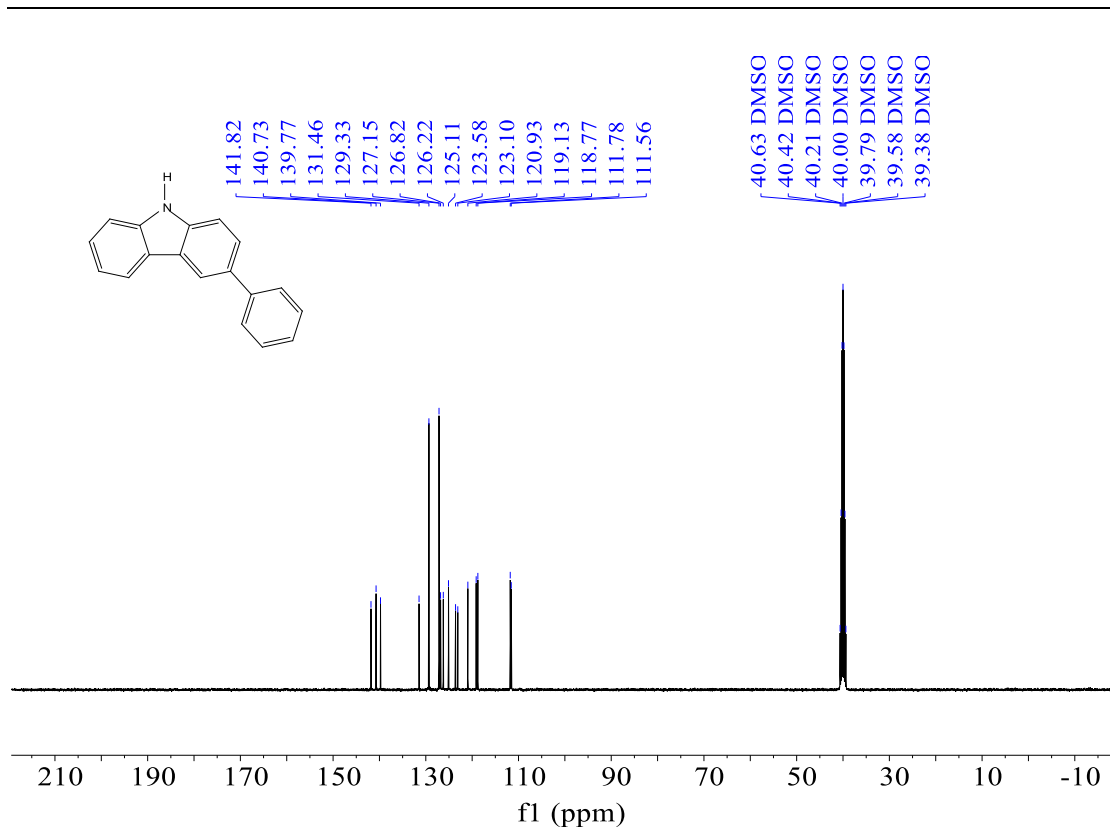
2-Methoxy-9H-carbazole (2aa): White solid, 31.0 mg; $^1\text{H NMR}$ (400 MHz, $\text{DMSO-}d_6$) δ 11.10 (s, 1H), 8.01 – 7.92 (m, 2H), 7.42 (d, $J = 8.0$ Hz, 1H), 7.33 – 7.24 (m, 1H), 7.15 – 7.06 (m, 1H), 6.97 (d, $J = 2.3$ Hz, 1H), 6.81 – 6.73 (m, $J = 8.5, 2.3$ Hz, 1H), 3.84 (s, 3H). $^{13}\text{C NMR}$ (101 MHz, $\text{DMSO-}d_6$) δ 158.96, 141.56, 140.18, 124.57, 123.13, 121.35, 119.70, 119.00, 116.64, 111.07, 108.15, 94.91, 55.71.



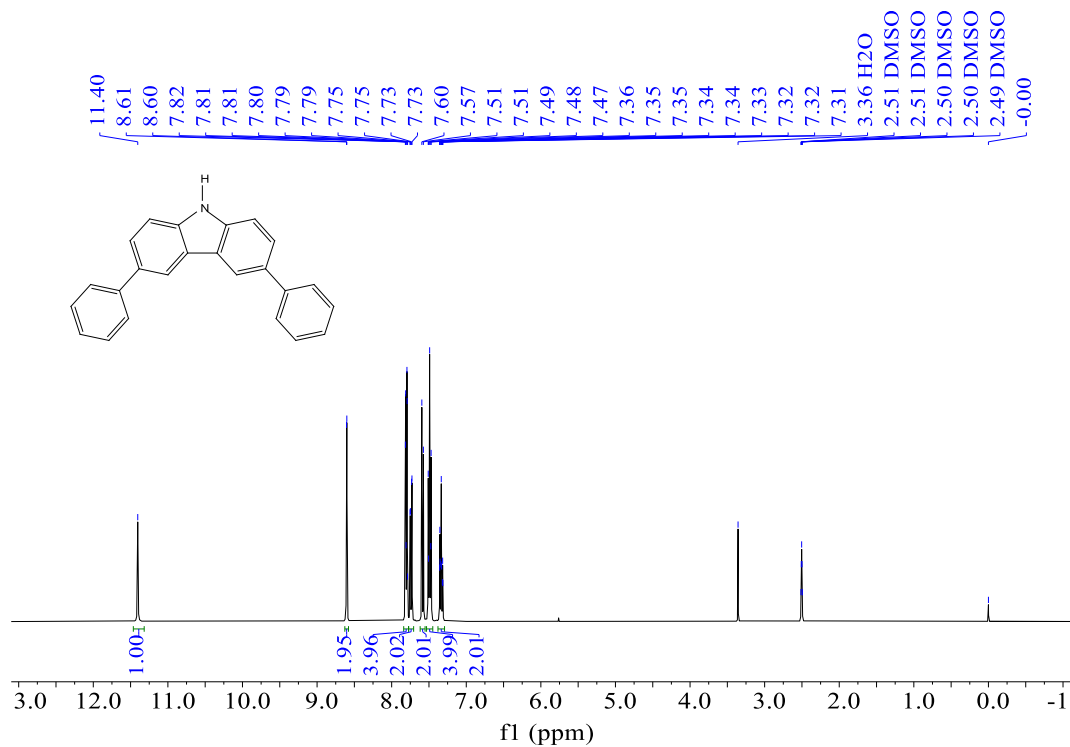


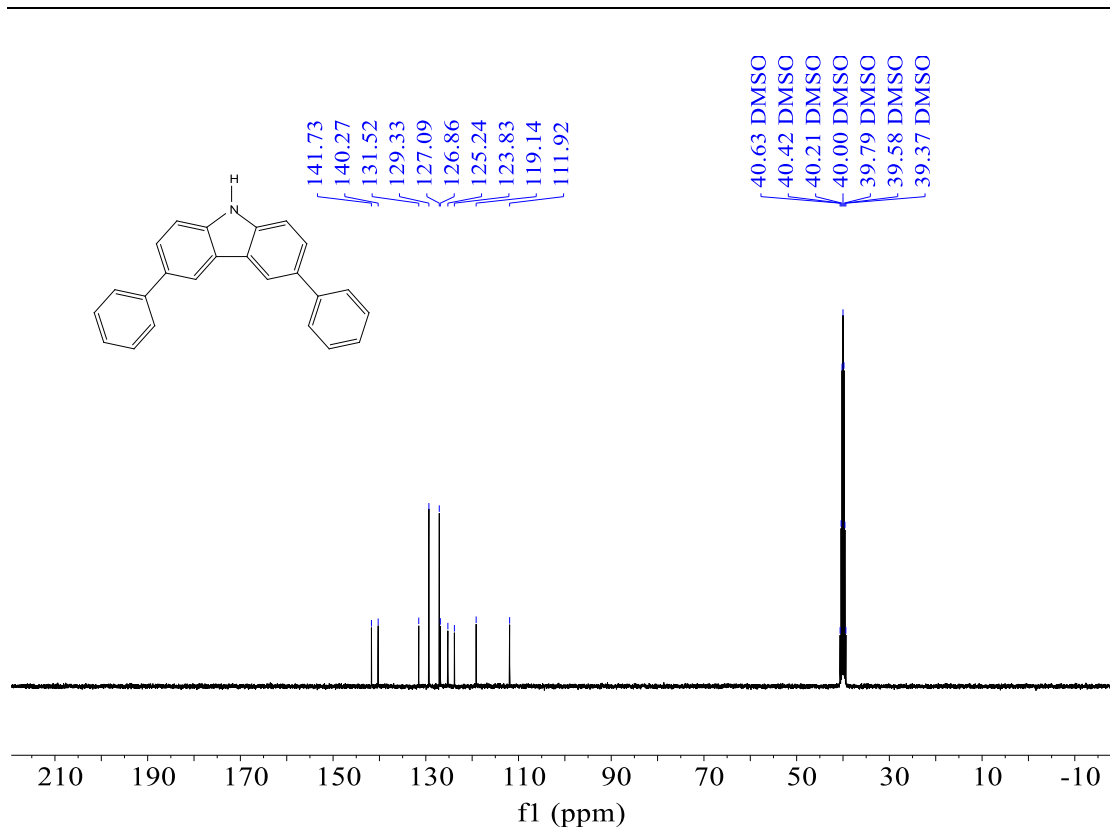
3-Phenyl-9H-carbazole (2ab): White solid, 38.4 mg; $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 11.35 (s, 1H), 8.46 (d, $J = 1.8$ Hz, 1H), 8.23 (d, $J = 7.4$ Hz, 1H), 7.81 – 7.68 (m, 3H), 7.61 – 7.37 (m, 5H), 7.33 (t, $J = 7.3$ Hz, 1H), 7.23 – 7.15 (m, 1H). $^{13}\text{C NMR}$ (101 MHz, DMSO- d_6) δ 141.82, 140.73, 139.77, 131.46, 129.33, 127.15, 126.82, 126.22, 125.11, 123.58, 123.10, 120.93, 119.13, 118.77, 111.78, 111.56.



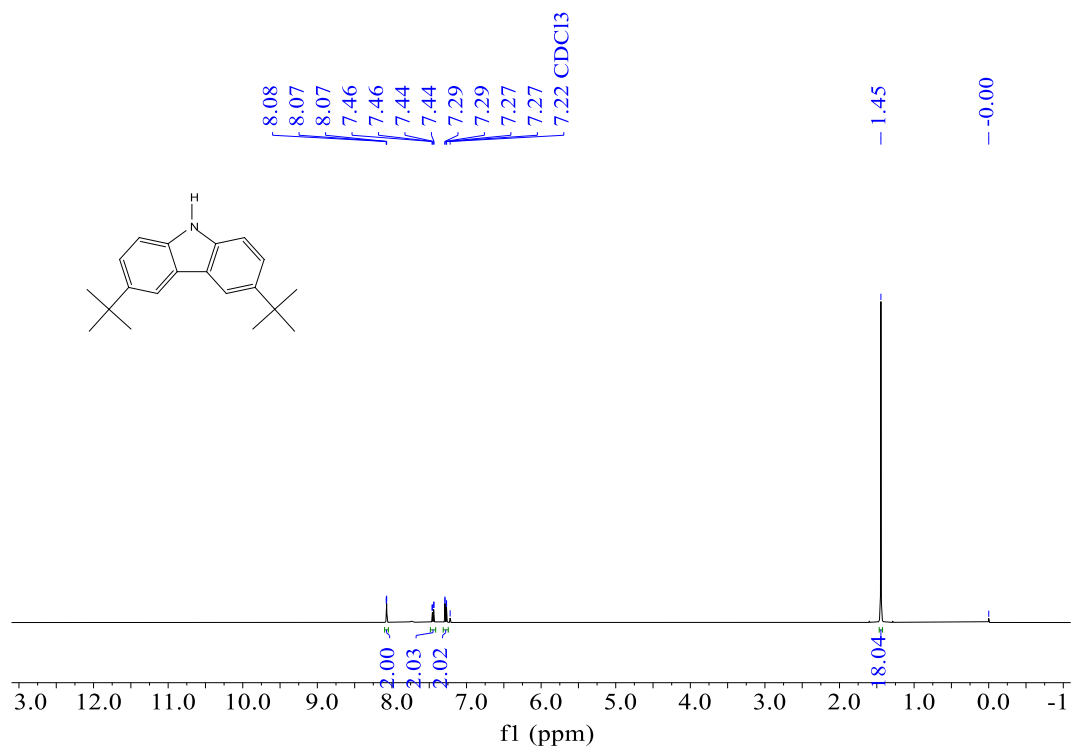


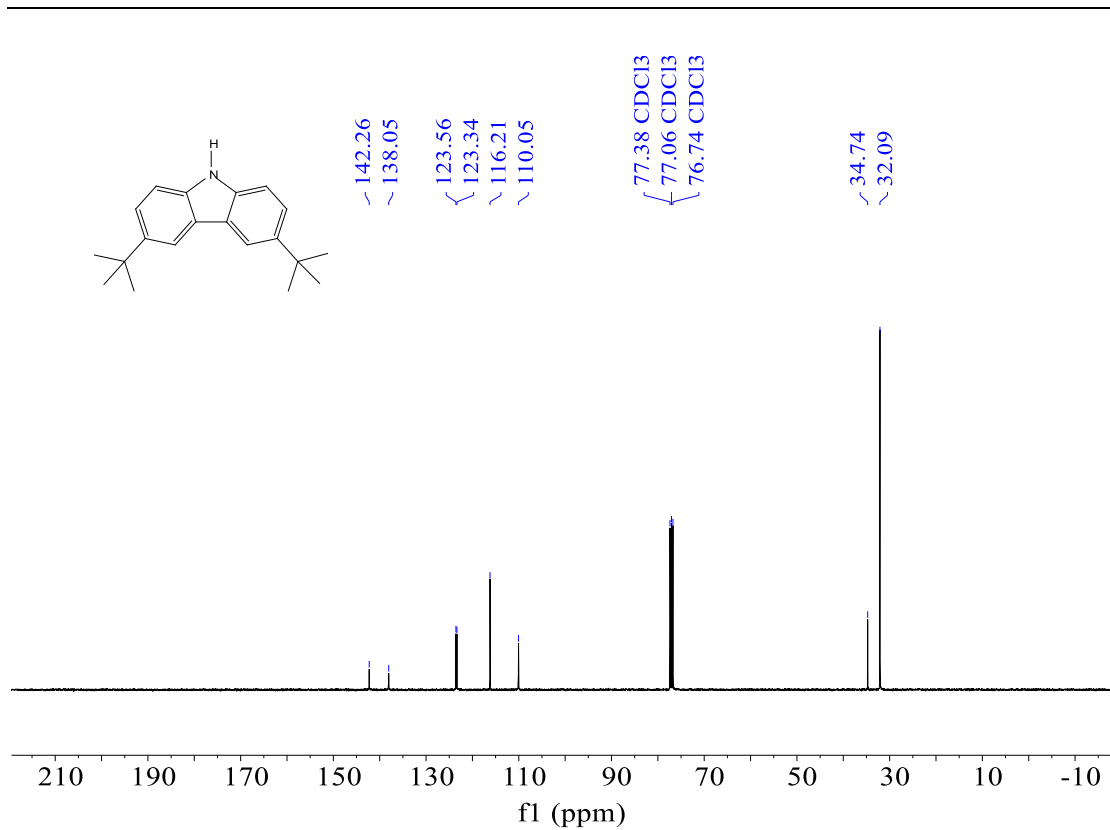
3,6-Diphenyl-9H-carbazole (2ac): White solid, 53.0 mg; ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 11.40 (s, 1H), 8.60 (d, $J = 1.8$ Hz, 2H), 7.84 – 7.77 (m, 4H), 7.77 – 7.71 (m, 2H), 7.59 (d, $J = 8.4$ Hz, 2H), 7.49 (t, $J = 7.7$ Hz, 4H), 7.38 – 7.29 (m, 2H). ^{13}C NMR (101 MHz, $\text{DMSO-}d_6$) δ 141.73, 140.27, 131.52, 129.33, 127.09, 126.86, 125.24, 123.83, 119.14, 111.92.



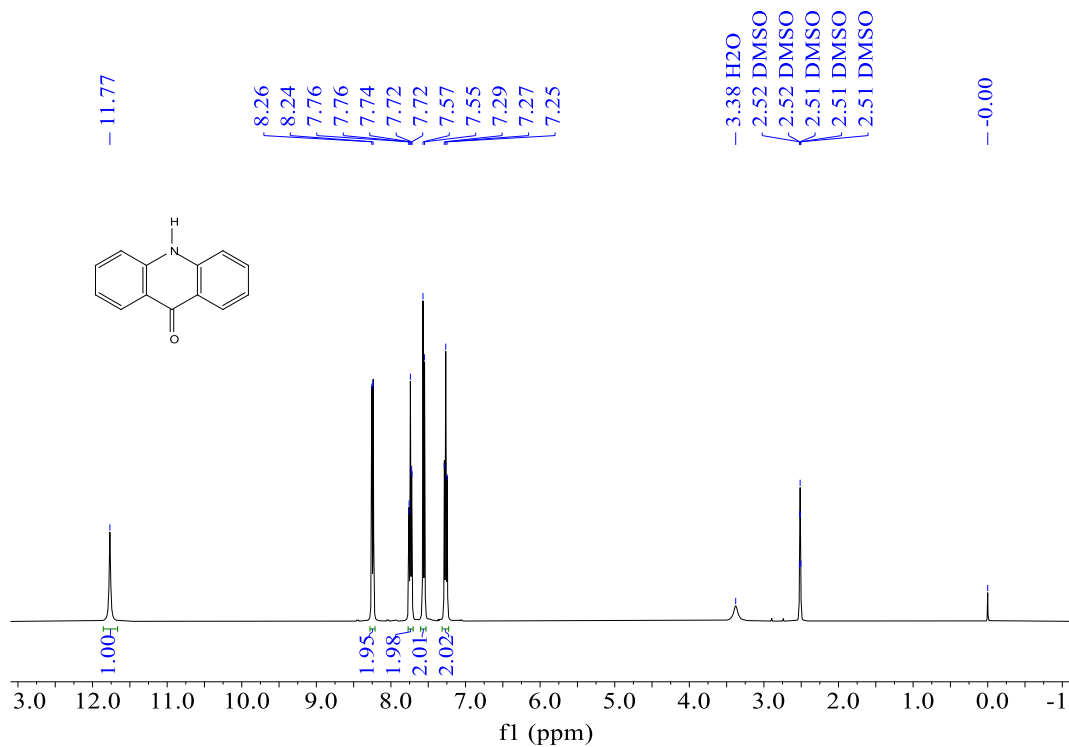


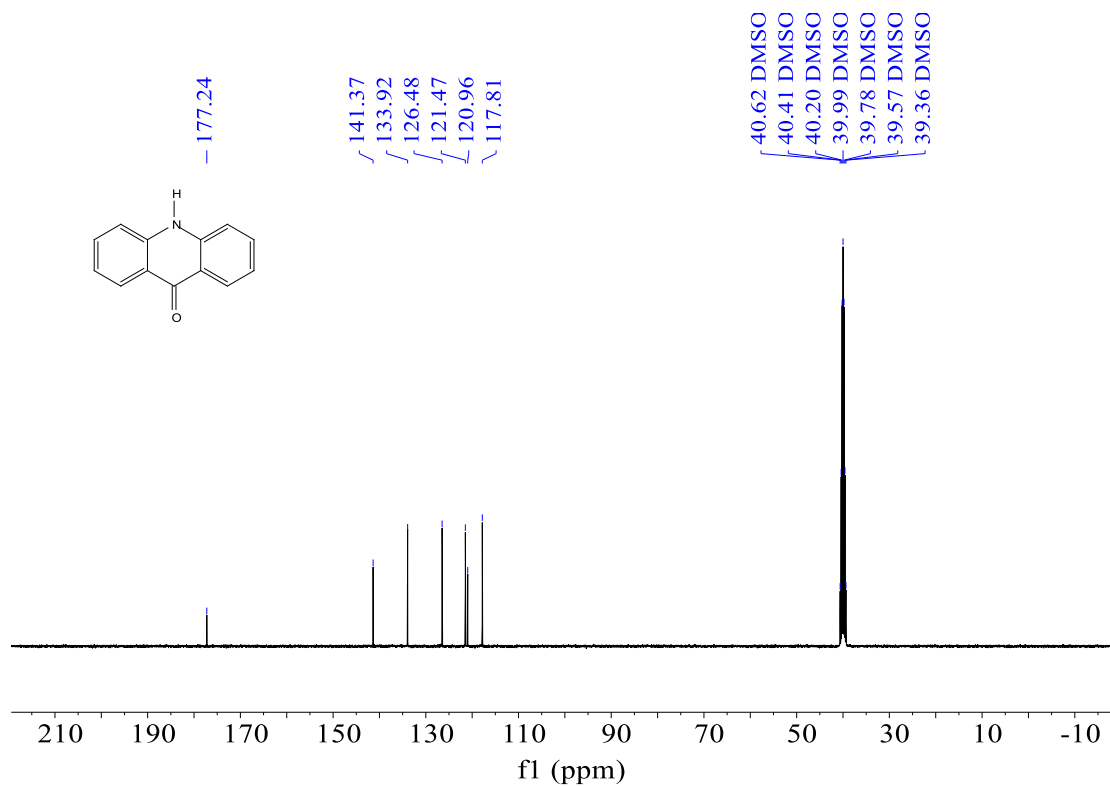
3,6-Di-tert-butylcarbazole (1ad, 1ae): White solid, 47.4 mg; ^1H NMR (400 MHz, Chloroform-*d*) δ 8.10 – 8.05 (m, 2H), 7.48 – 7.41 (m, $J = 8.5, 1.9$ Hz, 2H), 7.31 – 7.24 (m, 2H), 1.45 (s, 18H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 142.26, 138.05, 123.56, 123.34, 116.21, 110.05, 34.74, 32.09.



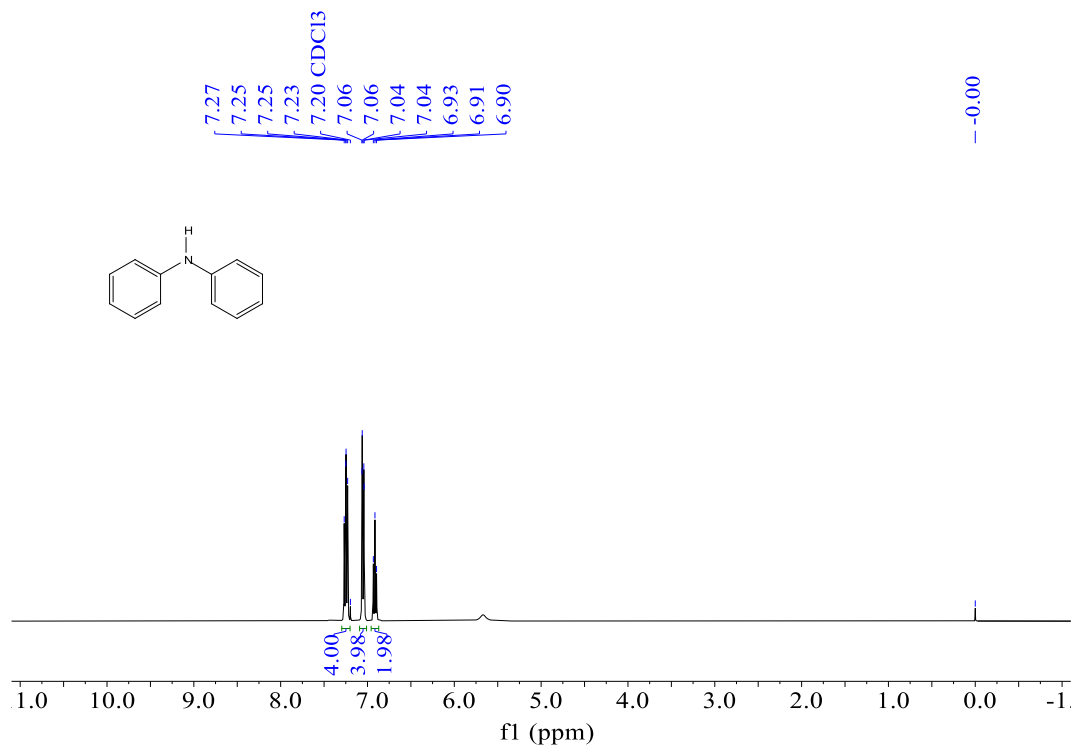


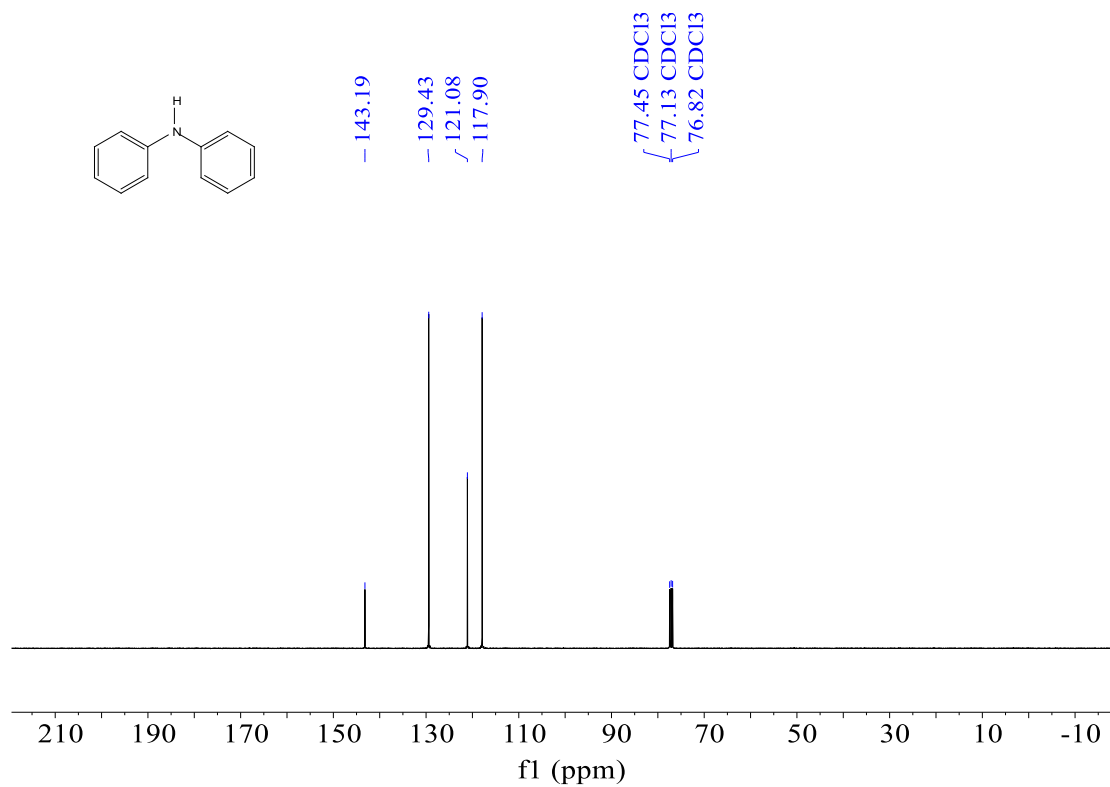
9(10H)-Acridinone (2af): Green solid, 33.2 mg; ^1H NMR (400 MHz, DMSO-*d*₆) δ 11.77 (s, 1H), 8.25 (d, *J* = 6.6 Hz, 2H), 7.77 – 7.70 (m, 2H), 7.56 (d, *J* = 8.3 Hz, 2H), 7.27 (t, *J* = 7.5 Hz, 2H). ^{13}C NMR (101 MHz, DMSO-*d*₆) δ 177.24, 141.37, 133.92, 126.48, 121.47, 120.96, 117.81.



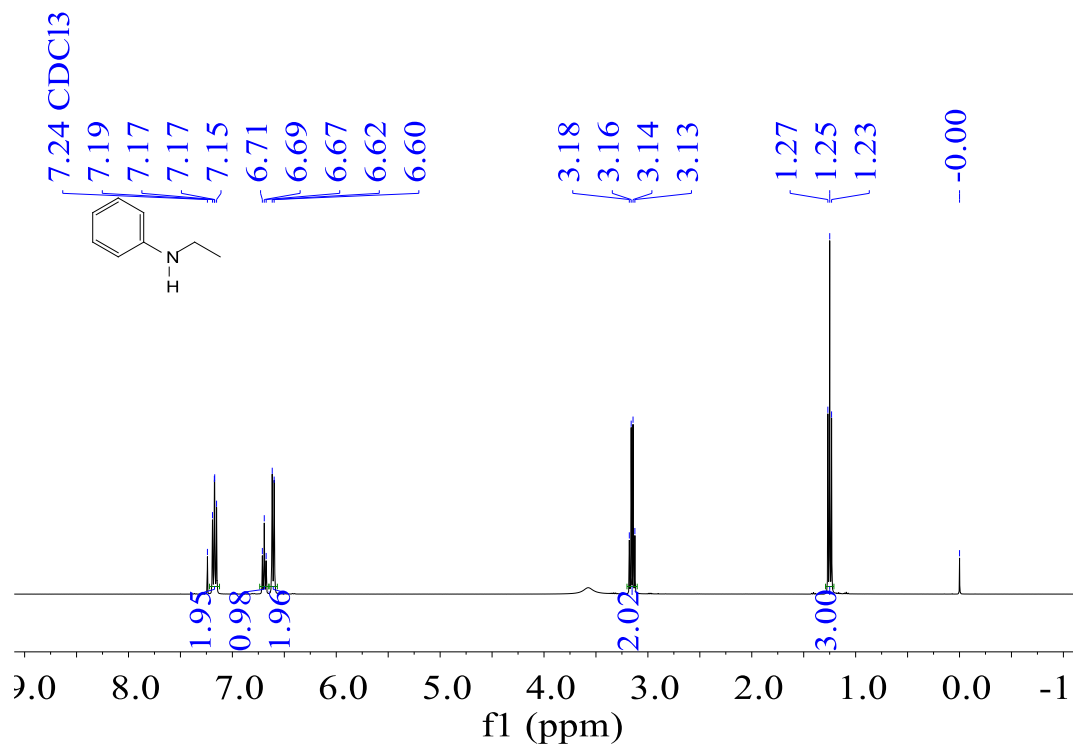


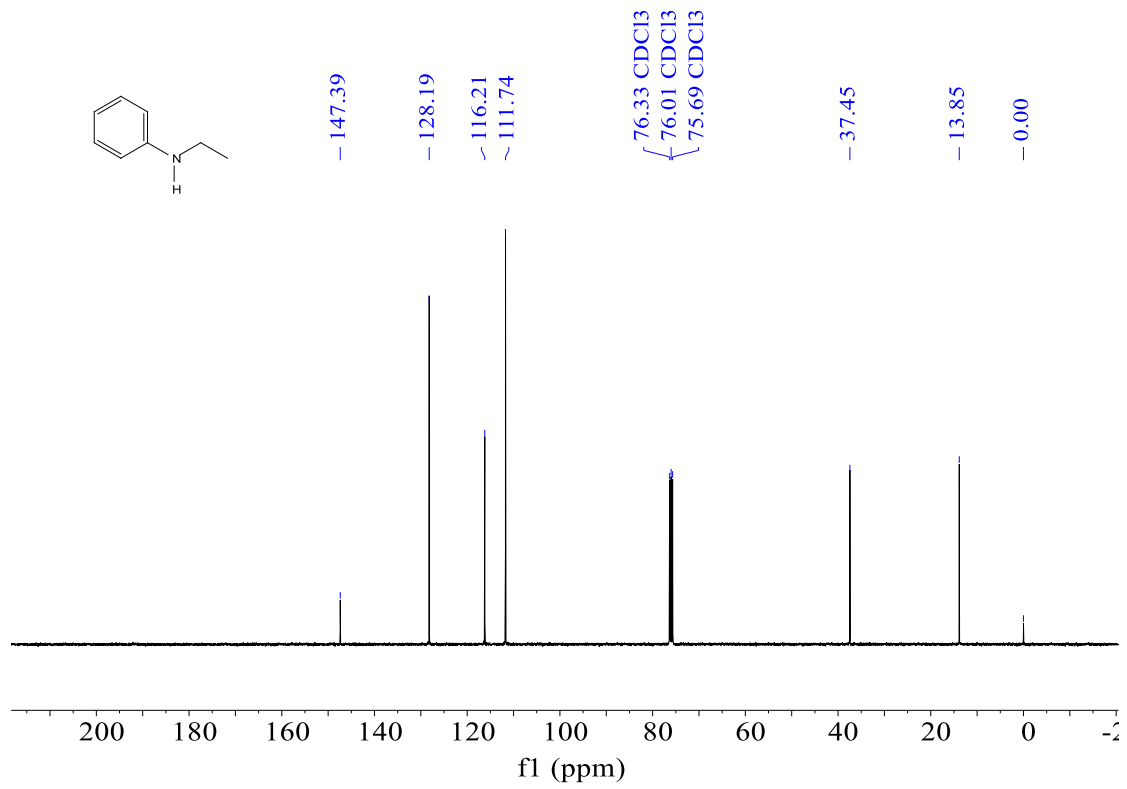
Diphenylamine (2ag): White solid, 27.4 mg; ^1H NMR (400 MHz, Chloroform-d) δ 7.30 – 7.20 (m, 4H), 7.09 – 7.01 (m, 4H), 6.91 (t, $J = 7.4$ Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-d) δ 143.19, 129.43, 121.08, 117.90.





N-ethylaniline (2ah): Colorless liquid, 20.1 mg; ^1H NMR (400 MHz, Chloroform-d) δ 7.22 – 7.12 (m, 2H), 6.69 (t, $J = 7.3$ Hz, 1H), 6.61 (d, $J = 7.3$ Hz, 2H), 3.20 – 3.10 (m, 2H), 1.25 (t, $J = 7.1$ Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-d) δ 147.39, 128.19, 116.21, 111.74, 37.45, 13.85.





Cartesian coordinates of optimized structures

1ah -636.532669

C	-4.37929900	0.37530100	0.70176700
C	-3.03618100	0.36276800	0.32625000
C	-2.43891900	1.50139700	-0.20866700
C	-3.20478700	2.65966800	-0.36335200
C	-4.54247200	2.67708900	0.01186400
C	-5.13400000	1.53240900	0.54675200
H	-4.83142500	-0.51765400	1.11731500
H	-2.44830600	-0.54099300	0.45162100
H	-2.73998300	3.54954800	-0.77515200
H	-5.12719900	3.58096600	-0.11374500
H	-6.17728100	1.54564400	0.83929200
C	-0.98753300	1.49296000	-0.62934600
H	-0.93544400	1.72594200	-1.69593100
H	-0.57727900	0.48097800	-0.49887000
N	-0.20733000	2.50683900	0.07825000
C	-0.30906400	2.42863300	1.54398800
H	0.16402700	3.30977100	1.97309300
H	-1.36636100	2.48766800	1.80726000
C	0.31202100	1.16316300	2.13367500
H	0.26522100	1.19491000	3.22398300
H	-0.21792600	0.26707100	1.80282200
H	1.36048700	1.07339100	1.83753200
C	1.07661300	2.77295900	-0.43750600
C	1.82407800	3.85224400	0.07051500
C	1.64274500	2.02194400	-1.47881500
C	3.07563700	4.15876700	-0.44083800
H	1.40978900	4.47341400	0.85432000
C	2.89741400	2.34612100	-1.99357200
H	1.11983000	1.17028500	-1.89191100
C	3.62687900	3.40991000	-1.48103100
H	3.62089400	5.00121200	-0.03054400
H	3.30494300	1.74538700	-2.79886400
H	4.60292200	3.65557500	-1.88074100

1al -326.888167

C	-4.71471700	0.34342800	0.15590500
C	-3.32309800	0.38763000	0.07794800

C	-2.65658200	1.60093500	-0.08422000
C	-3.40828000	2.77688200	-0.16080100
C	-4.79538700	2.73763100	-0.08244800
C	-5.45393900	1.51833500	0.07610000
H	-5.21773700	-0.60815300	0.28320000
H	-2.74977500	-0.53133000	0.14551600
H	-2.89314500	3.72379400	-0.27795200
H	-5.36603600	3.65706200	-0.14580600
H	-6.53536300	1.48764900	0.13852700
C	-1.14905100	1.65183100	-0.18483800
H	-0.86881600	1.98884500	-1.18724000
H	-0.75321800	0.63625100	-0.06415100
N	-0.59114900	2.61258500	0.77413600
H	-0.75341000	2.28170000	1.72069800
H	0.41546400	2.66803200	0.65714000

CN -777.200097

N	-2.07112800	-3.45282800	-0.00005700
C	-1.37709000	2.25022100	0.00005400
C	0.62940600	1.20611500	0.00008300
C	-1.48669200	0.00013200	0.00090000
C	0.62924600	-1.20628000	-0.00033400
C	2.54833900	-0.00019600	0.00016100
C	-1.37731700	-2.25002200	-0.00030800
N	-0.08628200	0.00001000	0.00015800
N	1.93664200	-1.20367700	-0.00071300
N	1.93666800	1.20357100	0.00011300
N	-0.05808300	2.35805300	-0.00081100
N	-2.13910000	1.15415200	0.00118100
N	-2.13915700	-1.15411800	0.00061600
N	-0.05817000	-2.35799100	-0.00090300
N	3.87161700	-0.00007400	0.00069400
N	-2.07089300	3.45292600	-0.00093700
H	4.37507700	-0.87408600	0.00045300
H	4.37478200	0.87410700	0.00082700

CN⁺ (VB) -776.930836

N	-2.07188300	-3.45216500	-0.00104200
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C	-1.38724500	2.27372400	0.00018500
C	0.62985400	1.19318800	-0.00120100
C	-1.47638200	0.00007400	0.00058100
C	0.62985600	-1.19329500	0.00040600
C	2.56468500	-0.00003700	0.00009500
C	-1.38735000	-2.27363300	-0.00007700
N	-0.08227000	-0.00002600	0.00012500
N	1.93026300	-1.20528100	0.00019700
N	1.93025500	1.20514100	-0.00132200
N	-0.05634900	2.35883800	-0.00183300
N	-2.14015600	1.14563200	0.00092600
N	-2.14021200	-1.14556500	0.00055800
N	-0.05648600	-2.35884200	-0.00007900
N	3.87262700	-0.00005100	0.00115600
N	-2.07165700	3.45232200	0.00094600
H	4.38024000	-0.87496100	0.00205300
H	4.38032800	0.87480600	0.00059700

CN⁻ (CB) -777.289366

N	2.13018400	-3.44107300	-0.00297300
C	1.36319500	2.26469000	-0.00086900
C	-0.65479800	1.22030100	-0.00775700
C	1.48470700	0.00909900	0.01179200
C	-0.63957500	-1.23104600	-0.00854600
C	-2.56597900	-0.02025800	0.01035900
C	1.39147800	-2.24929000	-0.00059900
N	0.10620100	0.00188200	0.02208400
N	-1.93490400	-1.21266000	-0.00930500
N	-1.94631600	1.18986300	-0.01160100
N	0.05725000	2.38164100	-0.01312600
N	2.14452600	1.16834500	0.00934500
N	2.15969400	-1.13859700	0.00907100
N	0.09050300	-2.38288100	-0.01256600
N	-3.96085800	-0.02077100	-0.08119400
N	2.07893200	3.46723100	-0.00262500
H	-4.37443300	-0.86124300	0.30185000
H	-4.37621700	0.80939700	0.32211000

$^1\text{O}_2$	-150.268924			
O	1.81084900	-1.09761000	-2.05399900	
O	1.32280100	-2.09159400	-1.62769600	
O_2^-	-150.443046			
O	1.83815400	-1.04199900	-2.07785000	
O	1.29549600	-2.14720500	-1.60384500	
H_2O_2	-151.558724			
H	1.09406800	-1.27191200	-1.85415500	
H	2.00267700	-3.31777500	-1.08233300	
O	2.00318500	-1.59921100	-1.85077300	
O	2.02265000	-2.43106600	-0.69876800	
Cl^-	-460.367846			
Cl	1.21362300	-2.31395200	-1.53233100	
Cl^\bullet	-460.133506			
Cl	1.21362300	-2.31395200	-1.53233100	
H_2O	-76.433271			
O	-1.91024900	3.15744400	2.31703100	
H	-1.07769400	3.39165200	2.73647600	
H	-2.34025000	4.00056100	2.14911500	
HOO^\bullet	-150.913908			
O	1.79329100	-1.09600300	-2.05468800	
O	1.77358300	-2.29298400	-1.54132300	
H	2.73303600	-0.85312000	-2.15885700	
HOO^-	-151.051623			
O	1.79471100	-1.02311100	-2.08595000	
O	1.76916400	-2.37359000	-1.50675300	
H	2.73603500	-0.84540600	-2.16216500	

Acetone	-193.145365		
O	-0.01071300	2.99888000	-1.68902900
C	-0.78031400	3.30053900	-2.57585900
C	-0.44015400	4.35655500	-3.59674500
H	-0.34092200	3.88321400	-4.57736600
H	-1.25152800	5.08376800	-3.67171900
H	0.49114100	4.85429300	-3.33439900
C	-2.12817300	2.63927800	-2.71549400
H	-2.90855500	3.37728100	-2.51072800
H	-2.27457800	2.29311500	-3.74084600
H	-2.21877200	1.80863100	-2.01857900

A-1ah	-636.333705		
C	-4.57267600	0.76371000	-0.33943600
C	-3.27753800	0.34804800	-0.05851600
C	-2.22929700	1.27015800	-0.04753400
C	-2.49253900	2.61294900	-0.30712700
C	-3.79435800	3.02870700	-0.58122100
C	-4.83425500	2.10735300	-0.60121900
H	-5.37914800	0.04046200	-0.34751600
H	-3.07692600	-0.69683000	0.15352500
H	-1.69656900	3.34918300	-0.29175800
H	-3.99033900	4.07581000	-0.77763700
H	-5.84521900	2.43279100	-0.81425700
C	-0.82898200	0.74860900	0.22475000
H	-0.41206800	0.24711700	-0.64709900
H	-0.86481700	0.00934000	1.02730100
N	0.08945500	1.79812600	0.66915200
C	0.07583600	2.05756400	2.11820900
H	0.24275300	3.11885100	2.28775600
H	-0.93633100	1.82812900	2.45414200
C	1.09726100	1.18869600	2.84856000
H	1.02354700	1.38439700	3.91826400
H	0.89971800	0.12982100	2.67763400
H	2.11275500	1.41164000	2.51984900
C	0.88564900	2.46858100	-0.18439500
C	1.89841900	3.35301800	0.30467100
C	0.72291900	2.32153900	-1.59855600
C	2.70648000	4.02387800	-0.57845900

H	2.05298700	3.47669800	1.36681300
C	1.53682600	3.01523600	-2.45858200
H	-0.06605900	1.69887300	-1.99649100
C	2.53697500	3.86334400	-1.96173200
H	3.48181400	4.67803200	-0.20209300
H	1.39830900	2.91115600	-3.52661100
H	3.17812900	4.40029900	-2.64897400

A-1al -326.650469

C	-4.59997700	0.44270100	0.41559300
C	-3.22274500	0.46638100	0.27155900
C	-2.59887700	1.63291800	-0.19657800
C	-3.34702400	2.79487300	-0.43918900
C	-4.72357700	2.76030500	-0.29131600
C	-5.34839700	1.58750100	0.13674600
H	-5.09306300	-0.46276800	0.74543700
H	-2.63170600	-0.41687200	0.48611800
H	-2.85069100	3.69958200	-0.77185200
H	-5.31248000	3.64270100	-0.50671200
H	-6.42454000	1.56705300	0.25844500
C	-1.08555700	1.65673500	-0.38427800
H	-0.77067900	2.39817600	-1.11311200
H	-0.67918400	0.67450800	-0.60876700
N	-0.71578200	2.06310700	0.93789700
H	-0.65805600	1.38285600	1.69258200
H	-0.75190500	3.04335100	1.20914300

B-1ah -635.895721

C	-4.37915300	0.02439300	-0.14648800
C	-2.99785200	0.09121700	-0.19094100
C	-2.31899600	1.32353700	-0.02310900
C	-3.10676600	2.48591300	0.16446100
C	-4.48984800	2.40548700	0.20839900
C	-5.13950700	1.17872200	0.06245700
H	-4.87272800	-0.93231500	-0.27374100
H	-2.41543400	-0.81047100	-0.34898700
H	-2.62238400	3.45306300	0.23243700
H	-5.07111800	3.31050900	0.34422400

H	-6.22049800	1.12366100	0.09920800
C	-0.89817800	1.34975600	-0.10010700
H	-0.37997000	0.50710800	-0.54675600
N	-0.11545900	2.40948500	0.32922800
C	-0.30453800	2.89853100	1.70460500
H	0.07157600	3.92041100	1.76276000
H	-1.37369500	2.94418900	1.89964100
C	0.35278400	1.98713300	2.73898800
H	0.19761100	2.38780000	3.74259000
H	-0.09646300	0.99267300	2.69258400
H	1.42580100	1.88571900	2.56946500
C	1.09672400	2.66152400	-0.33013000
C	2.16666400	3.32343300	0.29570600
C	1.24992400	2.27406300	-1.67303300
C	3.34429900	3.57086400	-0.40023400
H	2.09642800	3.64412100	1.32555200
C	2.43682800	2.51799900	-2.35074800
H	0.42193200	1.80989200	-2.19363100
C	3.49697500	3.16628700	-1.72277500
H	4.15402200	4.08196100	0.10771500
H	2.52388900	2.21083200	-3.38659600
H	4.41961600	3.35947300	-2.25556000

B-1al -326.255006

C	-4.93709200	0.98574700	0.38429900
C	-3.65019400	1.14410800	0.87477100
C	-2.70762600	1.96133600	0.19284800
C	-3.14649500	2.61063000	-0.99471200
C	-4.43217600	2.44292100	-1.46808700
C	-5.34541800	1.62571900	-0.78719900
H	-5.63591400	0.35735100	0.92547800
H	-3.37768300	0.64395700	1.79714900
H	-2.44858300	3.24421400	-1.53231800
H	-4.73583500	2.94992800	-2.37719600
H	-6.35306700	1.49628100	-1.16184500
C	-1.38187000	2.14266100	0.63857700
H	-0.72251700	2.81914200	0.11061500
N	-0.86967200	1.56806700	1.77372600
H	0.13269900	1.58299800	1.88269600

H	-1.29824800	0.72291200	2.12276100
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C-1ah -635.757496

C	-4.53795100	0.36518800	-0.63064900
C	-3.20370200	0.64583100	-0.88215700
C	-2.55548800	1.66833400	-0.17328000
C	-3.27971100	2.45740800	0.73325600
C	-4.62200900	2.19045900	0.95340100
C	-5.24538400	1.13628400	0.28810700
H	-5.02952800	-0.43992700	-1.16142300
H	-2.65394200	0.06811600	-1.61643500
H	-2.81616100	3.30143500	1.22657500
H	-5.18510000	2.80894800	1.64048000
H	-6.29220900	0.92827400	0.47328300
C	-1.16083500	1.89683300	-0.51269800
H	-0.86510500	1.67896600	-1.53619600
N	-0.20693300	2.32587500	0.24559700
C	-0.31688300	2.55752300	1.71211900
H	-0.39960800	3.63405000	1.87341500
H	-1.23679900	2.08131600	2.03989900
C	0.87179300	1.96636900	2.45398100
H	0.68265800	2.06920100	3.52266800
H	0.98146800	0.90550400	2.22375000
H	1.80239000	2.48092600	2.21825600
C	1.10019200	2.54956400	-0.34534200
C	1.63814100	3.82955400	-0.30155800
C	1.77954600	1.48349800	-0.91719600
C	2.89194600	4.04308900	-0.86149400
H	1.08472300	4.64397300	0.15059200
C	3.03344700	1.71264800	-1.47519800
H	1.34156700	0.49208700	-0.91238400
C	3.58806700	2.98792600	-1.44667500
H	3.32187200	5.03655200	-0.84321400
H	3.57639000	0.89008300	-1.92315300
H	4.56563200	3.16108500	-1.87914200

C-1al -326.118405

C	-4.94870900	0.96458200	0.37911700
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C	-3.66065500	1.08609400	0.86478600
C	-2.74052000	1.90451000	0.18804400
C	-3.12871400	2.59481800	-0.96955900
C	-4.42336700	2.46733500	-1.45019500
C	-5.32838400	1.65359600	-0.77633100
H	-5.66284000	0.33583700	0.89467900
H	-3.38367700	0.54703900	1.76282900
H	-2.41275800	3.22551600	-1.48379100
H	-4.72500300	2.99861600	-2.34332000
H	-6.34033700	1.55199500	-1.14946800
C	-1.38012100	2.08430700	0.62342700
H	-0.74094600	2.74403500	0.04468200
N	-0.83410900	1.53034400	1.65034700
H	0.13429300	1.71638000	1.88524900
H	-1.33384400	0.89296600	2.26106700

D-1ah -712.199664

C	-4.28794900	0.35660900	0.62214000
C	-2.98973200	0.47315800	0.13440200
C	-2.51836000	1.71103800	-0.29558200
C	-3.35057600	2.83157000	-0.25397400
C	-4.64494200	2.71230000	0.23609400
C	-5.11218200	1.47578700	0.67733400
H	-4.65446800	-0.60712300	0.95303100
H	-2.35118800	-0.40196200	0.08131800
H	-2.99669300	3.79075600	-0.61818100
H	-5.29063700	3.58105300	0.26806600
H	-6.12285900	1.38479800	1.05636400
C	-1.10927800	1.84137000	-0.81345200
H	-0.64303200	0.86003800	-0.91350100
N	-0.25507600	2.63427100	0.16884400
C	-0.27050000	2.09198600	1.59181700
H	0.27387200	2.83177500	2.17747400
H	-1.31456300	2.09903900	1.90168800
C	0.35076300	0.71748300	1.72971000
H	0.25667400	0.42413100	2.77569500
H	-0.16092800	-0.03716100	1.13175000
H	1.41045700	0.72144000	1.47731900
C	1.11934500	2.89351300	-0.31807900

C	1.62253400	4.17374400	-0.14483900
C	1.87395100	1.88029000	-0.89109300
C	2.92352300	4.44742800	-0.55349400
H	1.01252200	4.95185000	0.30209400
C	3.17239700	2.16790300	-1.29682300
H	1.47673400	0.88339500	-1.03123900
C	3.69767600	3.44565500	-1.12830600
H	3.32425100	5.44463900	-0.42422500
H	3.77113800	1.38658400	-1.74725800
H	4.70950500	3.66018200	-1.44867800
H	-0.71337400	3.55208000	0.21246000
O	-1.00434100	2.59817800	-1.97866600
H	-1.62869900	2.26028300	-2.63124400

D-1al -402.557291

C	-5.03246200	0.82252900	0.33149100
C	-3.74071800	0.80607800	0.82721100
C	-2.81459300	1.75874600	0.37701100
C	-3.19499700	2.71802900	-0.57079600
C	-4.49222800	2.72975100	-1.06194400
C	-5.40735000	1.78360700	-0.60973700
H	-5.75071300	0.08878800	0.67377200
H	-3.46679500	0.04999200	1.55347300
H	-2.47220300	3.45220900	-0.90819800
H	-4.78901000	3.47124000	-1.79228900
H	-6.42097000	1.79017400	-0.99211900
C	-1.45016400	1.81338400	0.84738600
H	-0.78756700	2.55281100	0.41379600
N	-0.93531700	1.03883600	1.73798900
H	0.03681600	1.13468200	2.00648500
H	-1.46868000	0.32149400	2.21619900
O	-1.84177600	4.22555400	1.95154800
H	-1.34791700	4.76935000	2.57265300
H	-2.74051700	4.56805600	1.97983000

2ah -366.632596

N	0.54390200	3.19671500	1.48198900
C	-0.08169700	1.81359400	1.48696800

H	0.70934800	1.12764400	1.78653900
H	-0.84545400	1.83925600	2.26254900
C	-0.65524400	1.47106000	0.12947900
H	-1.13195900	0.49329300	0.19672800
H	-1.41308500	2.19552100	-0.17540900
H	0.12120700	1.41965600	-0.63410400
C	1.67001000	3.35165900	0.54566800
C	1.46650700	4.02391000	-0.64837500
C	2.89095700	2.78824300	0.88365900
C	2.53214900	4.13622500	-1.53601700
H	0.50041300	4.45363500	-0.88835500
C	3.94683800	2.90984600	-0.01221100
H	3.02293600	2.27064000	1.82701400
C	3.76738300	3.58087200	-1.21893700
H	2.39197700	4.65955400	-2.47313900
H	4.90940500	2.48198700	0.23714800
H	4.59401000	3.67305300	-1.91223200
H	-0.17994800	3.88593700	1.25814900
H	0.85468300	3.42274800	2.43162800

2al -56.554919

N	-1.62892300	1.05562900	0.96745300
H	-1.24648000	0.11543000	0.96709700
H	-1.24647200	1.52597600	1.78153000
H	-1.24643000	1.52568900	0.15316200

E-1al -325.677172

C	-1.43141700	1.98568700	1.93439400
C	-1.80995100	1.36857600	0.74520500
C	-0.93747400	0.49522800	0.09472600
C	0.32343700	0.24201400	0.64498500
C	0.70049000	0.85704100	1.83008700
C	-0.17642500	1.72998200	2.47682800
H	-2.11333400	2.66276800	2.43448000
H	-2.78795000	1.56455500	0.31775900
H	0.99351300	-0.43774100	0.13227400
H	1.67757100	0.65982800	2.25486700
H	0.12153500	2.20852900	3.40228200

C	-1.36929000	-0.14424300	-1.16629200
H	-2.37629800	0.12733500	-1.50081300
N	-0.62843400	-0.94812600	-1.81314800
H	-1.10859100	-1.27700200	-2.65013700

F-1al -401.590763

C	-1.41670200	2.00772500	1.93444600
C	-1.84835200	1.37555500	0.77219200
C	-1.02259200	0.47709800	0.08881300
C	0.24905400	0.22643900	0.60384200
C	0.69026600	0.86186900	1.76455800
C	-0.14076100	1.75372000	2.43605900
H	-2.07336200	2.70092400	2.44881200
H	-2.83549000	1.58367200	0.37547700
H	0.88253800	-0.47250100	0.07308300
H	1.68501600	0.65786300	2.14603800
H	0.19963000	2.24608800	3.33994900
C	-1.53527100	-0.24182900	-1.16152700
N	-0.51441100	-0.83757700	-1.90290000
H	-0.96304200	-1.48075300	-2.55484400
H	-2.34529800	-0.91935700	-0.82712800
O	-2.32782900	0.75934500	-1.93909700
H	-1.67977800	1.05844100	-2.58844600

G-1al -402.125503

C	-1.41999900	2.15492300	1.59779100
C	-1.87837200	1.43819200	0.49405900
C	-1.27365600	0.23639100	0.13787300
C	-0.21177400	-0.24749400	0.90434600
C	0.24711300	0.46590600	2.00610000
C	-0.35665800	1.67264700	2.35403000
H	-1.89792900	3.08926200	1.86800200
H	-2.71740800	1.81190600	-0.08043300
H	0.25366100	-1.19264600	0.64008700
H	1.06970500	0.07907200	2.59594600
H	-0.00323400	2.22930000	3.21381200
C	-1.71694800	-0.54962500	-1.08473400
N	-0.78009900	-0.30952700	-2.17221700

H	-0.82634900	-1.05775400	-2.85687900
H	-1.78597600	-1.60819000	-0.80941800
O	-3.01314800	-0.20724400	-1.52591000
H	-2.92068100	0.58543700	-2.06810500
H	0.17396600	-0.25627900	-1.83326500

TS1 -829.449352, 1092.77i

C	-4.63949600	0.54769400	0.50716900
C	-3.34196500	0.42477600	0.03154700
C	-2.32699700	1.28085300	0.48688500
C	-2.65493600	2.28150900	1.40998900
C	-3.95561400	2.39699700	1.88871700
C	-4.94940100	1.52702500	1.44952300
H	-5.41055200	-0.12025600	0.14248200
H	-3.11096500	-0.33599700	-0.70834300
H	-1.90285600	2.99306900	1.73035300
H	-4.19469600	3.18013100	2.59824100
H	-5.96063600	1.62054100	1.82598500
C	-0.96122600	1.09715500	-0.06020300
H	-0.92671800	1.00472400	-1.14345400
H	-0.75566500	-0.33746000	0.16396300
N	0.12246200	1.79209100	0.46060900
C	0.45696400	1.63943600	1.88640000
H	0.89933900	2.57365900	2.23222800
H	-0.47491100	1.50516000	2.43272500
C	1.37849400	0.44936000	2.15767600
H	1.61710800	0.42412700	3.22198800
H	0.89206600	-0.49147900	1.90104800
H	2.30908600	0.50521300	1.59474000
C	1.00510100	2.48507900	-0.38797600
C	2.31848800	2.78156000	0.01147000
C	0.55636900	2.94273800	-1.63836800
C	3.16355500	3.47911200	-0.83934600
H	2.69206200	2.47279900	0.97683900
C	1.41647700	3.63134600	-2.48105300
H	-0.47489300	2.80495000	-1.93403600
C	2.72644000	3.89710900	-2.09340400
H	4.17505000	3.69314100	-0.51665100
H	1.04965100	3.98057800	-3.43842100

H	3.39331000	4.43865900	-2.75242100
C	-1.16427900	-2.19631500	1.03106100
C	-1.09167200	-3.67210100	0.91555400
H	-0.82714700	-3.97420800	-0.09414800
H	-0.32271900	-4.01282800	1.61762400
H	-2.03522200	-4.11775200	1.23472800
C	-1.80055600	-1.59211100	2.23009500
H	-2.88521400	-1.67942100	2.09598700
H	-1.53587000	-2.17194700	3.11504000
H	-1.55038700	-0.54176000	2.35978900
O	-0.68083800	-1.51361800	0.10938100

TS2 -786.789577, 987.51i

C	-4.29866200	1.17028800	-1.18656800
C	-3.18431200	0.74603400	-0.46592300
C	-2.24278800	1.67261500	-0.00245000
C	-2.42883500	3.03406300	-0.28070400
C	-3.54113400	3.45130500	-0.99398300
C	-4.47508300	2.52016400	-1.45604800
H	-5.02258900	0.44350700	-1.53424200
H	-3.05206400	-0.30647600	-0.24165500
H	-1.71900900	3.76483400	0.08649100
H	-3.68902500	4.50704900	-1.18705900
H	-5.33995000	2.85445400	-2.01660800
C	-1.09831500	1.14644400	0.77984200
H	-0.68365100	0.24069700	0.02696200
H	-1.41785700	0.51992000	1.61470900
N	-0.04214500	1.97335200	1.15686800
C	0.77291900	1.47235100	2.27726200
H	1.36944200	2.29686800	2.66318400
H	0.09040000	1.16814100	3.07205700
C	1.67572900	0.31613100	1.85485400
H	2.28743200	-0.00909000	2.69785400
H	1.08530000	-0.53705300	1.51194200
H	2.33910800	0.62688600	1.04454600
C	0.62933500	2.78271600	0.19983800
C	1.31517600	3.92109300	0.63917200
C	0.61231800	2.48040300	-1.16596500
C	1.97843500	4.73507100	-0.26934600
H	1.30604400	4.18489400	1.68955900

C	1.27060200	3.31058900	-2.06840200
H	0.08729500	1.60901500	-1.53552300
C	1.96003000	4.43567500	-1.62961900
H	2.50007900	5.61492000	0.08806900
H	1.24762700	3.06426300	-3.12344600
H	2.47413600	5.07412100	-2.33749100
O	-1.17017400	-0.29058900	-1.97713700
O	-0.46842400	-0.58708000	-0.96655700

TS3 -1096.701415, 148.09i

C	-4.37606000	1.32326100	-0.92644200
C	-3.26821000	0.89553300	-0.21015600
C	-2.25390700	1.79618500	0.16179400
C	-2.39551800	3.14547900	-0.20265400
C	-3.50958800	3.56797400	-0.91845800
C	-4.50074000	2.66334400	-1.29110700
H	-5.14447100	0.61050100	-1.20161600
H	-3.17729300	-0.14912000	0.06993200
H	-1.64888800	3.87172900	0.09250900
H	-3.60587800	4.61495800	-1.18158900
H	-5.36403800	2.99916500	-1.85265800
C	-1.12605200	1.26729400	0.93216200
H	-0.61921900	0.05893500	-0.07310300
H	-1.38164900	0.51515700	1.67488200
N	-0.01990400	2.00947400	1.28148200
C	0.76666100	1.53147400	2.43160100
H	1.31054100	2.37759400	2.84800800
H	0.06255400	1.19342400	3.19193100
C	1.73368600	0.41963100	2.03905000
H	2.33532200	0.13035600	2.90218800
H	1.19372600	-0.45985000	1.68345700
H	2.40514600	0.75868200	1.24687700
C	0.64311100	2.86670900	0.35949200
C	1.30054500	4.00782000	0.82923800
C	0.64104200	2.59044300	-1.01071400
C	1.95043600	4.85392700	-0.06095700
H	1.28118200	4.25138700	1.88411800
C	1.28915700	3.44621300	-1.89338900
H	0.13432700	1.71134600	-1.38726700
C	1.94856800	4.57918800	-1.42588000

H	2.45014700	5.73817200	0.31604700
H	1.28188200	3.21876000	-2.95268900
H	2.45345200	5.24238300	-2.11738700
Cl	-0.24776700	-1.01690200	-0.89859500

TS4 -712.141904, 1426.49i

C	-3.34481800	-0.33518700	-0.14026100
C	-2.38107200	0.51912400	-0.66342400
C	-2.43494800	1.88406700	-0.38327300
C	-3.47781900	2.40171500	0.38436900
C	-4.44209800	1.54423100	0.90072800
C	-4.37062400	0.17641800	0.64877700
H	-3.29861800	-1.39513500	-0.35657100
H	-1.59137500	0.12133300	-1.29186900
H	-3.54865100	3.46770500	0.56518300
H	-5.25251100	1.94574100	1.49626500
H	-5.12344600	-0.48798500	1.05511300
C	-1.33490000	2.74825800	-0.91016100
H	-0.89142200	2.34544900	-1.81797900
N	-0.25376300	3.22650600	-0.01134500
C	-0.49015000	3.18956200	1.46518500
H	0.21081600	3.91431600	1.88072500
H	-1.49388100	3.57539800	1.64220100
C	-0.29776600	1.82758400	2.11327700
H	-0.49122200	1.92488900	3.18268300
H	-0.98587100	1.08256300	1.71137300
H	0.72524300	1.47045600	1.98764000
C	1.09549300	2.85309200	-0.39143100
C	2.07083200	3.84378400	-0.39336500
C	1.41561800	1.53700800	-0.70905500
C	3.38032300	3.51298100	-0.72573800
H	1.80137000	4.86305200	-0.14057800
C	2.72506300	1.21577000	-1.05151000
H	0.65510800	0.76437200	-0.67578600
C	3.70729100	2.20165800	-1.05891200
H	4.14155800	4.28322100	-0.73206500
H	2.97612900	0.19271700	-1.30251400
H	4.72658500	1.94790700	-1.32273100
H	-0.85183900	4.37949400	-0.61982600

O	-1.81459800	4.13289600	-1.19192800
H	-1.88407200	4.36312000	-2.13423100

TS5 -402.506072, 1547.42i

C	-5.09709700	1.03761800	0.69318300
C	-3.92509300	1.50382300	1.27584500
C	-3.06489900	2.31511100	0.53504300
C	-3.37516800	2.66024200	-0.77823500
C	-4.54743500	2.18553600	-1.35746200
C	-5.40722100	1.37583400	-0.62232600
H	-5.77113800	0.41440200	1.26761000
H	-3.69205100	1.25152500	2.30409500
H	-2.70554400	3.29725700	-1.34540200
H	-4.79028600	2.45443400	-2.37791100
H	-6.32331200	1.01206800	-1.07160600
C	-1.77159200	2.78970400	1.11270900
H	-1.36792900	3.66315900	0.60875500
N	-0.74212300	1.76455000	1.32957900
H	-1.02154200	2.30027400	2.58928400
H	0.15426900	1.97220000	0.89856300
O	-1.89732100	3.07717800	2.57055300
H	-1.03647700	0.82040000	1.09337000
H	-1.73520300	3.99999500	2.82811400

TS6 -477.158556, 888.47i

C	-4.02166200	3.33913600	1.43119100
C	-4.16581900	2.70096900	0.20239100
C	-3.28373000	1.68705500	-0.16821400
C	-2.24346700	1.32935700	0.69391000
C	-2.10606300	1.96236400	1.92393400
C	-2.99562600	2.96850200	2.29532600
H	-4.71390300	4.12317600	1.71415400
H	-4.96929100	2.98602000	-0.46785900
H	-1.53177200	0.56723600	0.38920800
H	-1.29801000	1.67916500	2.58783200
H	-2.88527500	3.46460600	3.25211600
C	-3.42200000	0.99788100	-1.48629200
H	-2.35966800	1.27445600	-2.08957900
H	-4.19833300	1.37940000	-2.14542500

N	-3.33239200	-0.37272000	-1.45907400
H	-3.15903000	-0.85558400	-0.58850700
H	-3.78549200	-0.92104900	-2.17535900
O	-1.19047100	0.70745500	-2.45226500
O	-1.37569700	-0.52958300	-2.18153400

TS7 -401.581416, 274.27i

C	-1.51636300	1.79309300	2.04357900
C	-1.99159500	1.07310100	0.95136100
C	-1.11928600	0.35201300	0.13478800
C	0.24356500	0.35842300	0.43751800
C	0.72441100	1.08343800	1.52328200
C	-0.15354800	1.80331100	2.33218600
H	-2.20782500	2.34594100	2.66944500
H	-3.05225000	1.07427200	0.72014100
H	0.91591500	-0.21702000	-0.18735100
H	1.78588600	1.08289000	1.74515400
H	0.22061800	2.36340000	3.18134200
C	-1.65614300	-0.44621700	-1.00974600
N	-0.90784300	-1.37558300	-1.53506300
H	-1.47220300	-1.93275400	-2.17352600
H	-2.74612800	-0.49885000	-1.02785600
O	-1.86867500	1.11845600	-2.26970000
H	-1.01425800	0.99864300	-2.69560700

TS8 -478.048126, 1008.89i

C	-1.01753700	2.17875700	1.32311000
C	-1.53914500	1.46672200	0.24592800
C	-1.22457400	0.12037500	0.06613900
C	-0.39365600	-0.50627200	0.99480500
C	0.12922300	0.19981800	2.07496100
C	-0.17903800	1.54847700	2.23983300
H	-1.26584500	3.22672000	1.44857400
H	-2.19699700	1.95717200	-0.46274100
H	-0.14533500	-1.55523900	0.86174300
H	0.77498100	-0.30074800	2.78756400
H	0.22588500	2.10188600	3.07911900
C	-1.69572600	-0.64264400	-1.16138700

N	-0.83349800	-0.36381400	-2.25813600
H	-0.84741300	-1.15037300	-2.90240700
H	-1.75171300	-1.70780400	-0.89059400
O	-3.07047700	-0.28905800	-1.46562800
H	-2.98422800	0.29682100	-2.22651500
O	1.48153900	0.41697300	-1.70499400
H	1.48952000	0.53653900	-0.75128400
H	0.36748000	0.02976100	-1.95928700

TS9 -402.071219, 1510.68i

C	-1.36550600	2.17998100	1.63218200
C	-1.88627200	1.46019500	0.55888500
C	-1.33852100	0.22873500	0.21262900
C	-0.27215700	-0.28482800	0.95236600
C	0.24973200	0.43327100	2.02281100
C	-0.29731700	1.66927700	2.36387800
H	-1.79702700	3.13730900	1.90053900
H	-2.72496600	1.83459300	-0.01543600
H	0.14796500	-1.25133000	0.68988600
H	1.07697400	0.02885900	2.59419600
H	0.10535100	2.22785500	3.20064300
C	-1.89355500	-0.54812100	-0.96636600
N	-1.02965400	-0.32010900	-2.21746900
H	-0.67766600	-1.16183700	-2.66687200
H	-1.86837300	-1.62380200	-0.74325500
O	-3.06475600	-0.09452600	-1.50852300
H	-2.13461800	0.04929900	-2.50714300
H	-0.28742100	0.36945700	-2.12186500

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