Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supplementary Information

Mild diazenylation of C_{sp2}-H and C_{sp3}-H bond via arylazo sulfones

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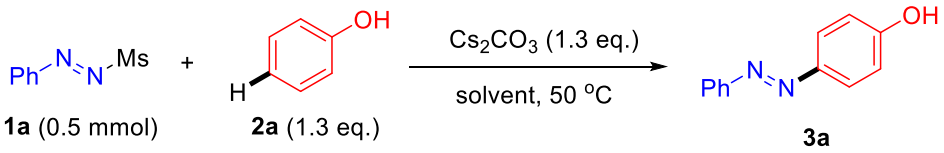
General Information

All glassware was oven dried at 100 ^{o}C for hours and cooled down under vacuum. Solvents were obtained from commercial sources. All the starting materials (including arylazo sulfones,[1-2] phenolic derivatives, indole derivatives, pyrrole derivatives,[3] Octabenzone, Estrone, 1,3-dicarbonyl compounds,[4-8] etc.) were obtained from commercial sources or synthesized according to literature methods (>95% purity). The thin layer chromatography (TLC) employed glass 0.25 mm silica gel plates. Purification of reaction products was carried out by flash chromatography on silica gel (300~400 mesh). ^{1}H NMR spectra were recorded at 500 or 400 MHz, ^{13}C NMR spectra were recorded at 125 or 100 MHz, and in $CDCl_3$ or DMSO-d_6 (containing 0.03% TMS) solutions with Bruker Advance III spectrometers. ^{1}H NMR spectra were recorded with Me_4Si (δ = 0.00), $CDCl_3$ (δ = 7.26) or DMSO-d_6 (δ = 2.50) as the internal reference and ^{13}C NMR spectra were recorded with $CDCl_3$ (δ = 77.16) or DMSO-d_6 (δ = 39.52) as the internal reference. High-resolution mass spectra were obtained using a Bruker Maxis Impact mass spectrometer with a TOF (for ESI) analyzer.

All density functional theory (DFT) calculations were performed with Gaussian09 program,[9] M06-2X method,[10] SMD solvation model[11] (*N*,*N*-dimethylformamide and ethanol were used as solvent for the reactions of **4a** and **2a** respectively) associated with a (99,590) grid. Geometry optimization, frequency analysis and intrinsic reaction coordinate (IRC) analysis[12] were performed with 6-31G(d) basis set. Based on the solution-phase optimized structures, solution-phase single-point energy calculation was performed with 6-311++G(d,p) basis set. No imaginary frequency was found for energetic minima while only one imaginary frequency was found for transition states. IRC analysis was performed to ensure that the optimized transition states connect with correct intermediates. The thermodynamic correction to Gibbs free energy (ΔG_{cor}), solution-phase single-point energy (ΔE_{sol}) and an extra 1.89 kcal/mol which accounts for the standard state change from 1 atm. to 1 M at 298.15 K[13-15] were added up to get the solution-phase Gibbs free energy of every species (ΔG_{sol}) referring to 1 M and 298.15 K.

Table S1 Optimization studies of solvent for the synthesis of **3a**[a]



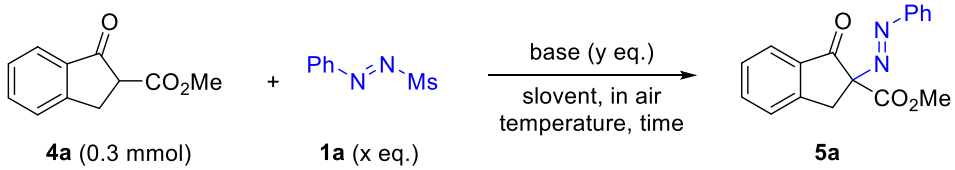
1a (0.5 mmol) **2a** (1.3 eq.) **3a**

entry	solvent	time	yield (%)
1	THF	4 h	73
2	MeCN	3 h	75
3	DMF	2 h	30
4	DCE	1 h	85
5	EtOAc	8 h	69
6	PhMe	6 h	60
7	MeOH	15 min	92
8	**EtOH**	**15 min**	**92**

[a] **1a** (92 mg, 0.5 mmol), PhOH (61 mg, 0.65 mmol), Cs_2CO_3 (212 mg, 0.65 mmol), solvent (5 mL), 50 °C, in air.

The solvent has a significant effect on the substitution-arylation reaction. Tetrahydrofuran (THF), acetonitrile (MeCN), *N,N*-dimethylformamide (DMF), 1,2-dichloroethane (DCE), ethyl acetate (EtOAc), or toluene (PhMe) can also be used in this reaction, but the yield is not as good as that of alcohol (e.g., EtOH or MeOH) as the solvent. This outcome may be attributed to the solubility of the alcohol solvent towards the reagents and potential hydrogen bonding interactions.

Table S2 Optimization studies for the synthesis of **5a**[a]



4a (0.3 mmol) **1a** (x eq.) **5a**

entry	x	base	y	slovent	temp. (°C)	time	yield (%)
1	1.3	DABCO	2.0	DMF	70	1 h	59
2	1.3	DABCO	2.0	MeOH	70	5 min	63
3	1.3	DABCO	2.0	THF	70	8 h	54
4	1.3	DABCO	2.0	MeCN	70	5 h	20
5	1.3	DABCO	2.0	DCE	70	5 h	48
6	1.3	DABCO	2.0	PhMe	70	5 h	24
7	1.3	DABCO	2.0	DMSO	70	30 min	49
8	1.3	DABCO	2.0	DMF/H_2O (5/1)	70	15 min	57
9	1.3	DABCO	2.0	EtOAc	70	3 h	40
10	1.3	pyridine	2.0	DMF	70	5 h	53
11	1.3	Et_3N	2.0	DMF	70	30 min	47
12	1.3	DBU	2.0	DMF	70	10 min	trace
13	1.3	$NaHCO_3$	2.0	DMF	70	40 min	71
14	1.3	Cs_2CO_3	2.0	DMF	70	30 min	n.d.
15	1.3	NaOH	2.0	DMF	70	30 min	10
16	1.3	$KHCO_3$	2.0	DMF	70	30 min	70
17	1.3	$NaHCO_3$	1.5	DMF	70	40 min	30
18	1.3	$NaHCO_3$	2.5	DMF	70	40 min	61
19	1.3	$NaHCO_3$	3.0	DMF	70	40 min	25
20	1.3	$NaHCO_3$	2.0	DMF	70	40 min	73[b]
21	**1.5**	**$NaHCO_3$**	**2.0**	**DMF**	**70**	**30 min**	**86**
22	1.1	$NaHCO_3$	2.0	DMF	70	30 min	60
23	0.9	$NaHCO_3$	2.0	DMF	70	30 min	57
24	1.5	$NaHCO_3$	2.0	DMF	90	15 min	60
25	1.5	$NaHCO_3$	2.0	DMF	50	1 h	71

[a] solvent (3 mL), in air, n.d. = no detected. [b] under N_2.

The substitution-alkylation of arylazo sulfone **1a** has also been carefully investigated (Table S2). Through the solvent screening (entries 1-9), we found that methanol (MeOH) as the solvent, the best yield can be achieved within five minutes. However, MeOH as a solvent has a significant disadvantage, which is that MeOH will further participate in the reaction to produce the ring-opening products (for details, see the next page, Page S7). Based on the above investigation results, we finally decided to use DMF as a solvent for follow-up research. A number of common organic and inorganic bases could be used for this reaction (entries 10-16), of which sodium bicarbonate showed the best effect, with a yield of 71% to **5a** (entry 13). Subsequently, increasing or decreasing the dosage of $NaHCO_3$ was investigated (entries 17-19), but no better results were achieved than with 2-equivalent $NaHCO_3$. If the reaction was carried out under N_2, there was little difference from that under air, which indicates that the reaction is not sensitive to air. Next, we tried to optimize the amount of **1a** (entries 21-23). We found that the best reaction results were achieved when 1.5 equivalent **1a** was used (entry 21). Finally, we also investigated the reaction temperature and found that 70 ^{o}C was the best reaction temperature (entries 24 and 25 vs entry 21).

Unexpected discoveries and corresponding control experiments

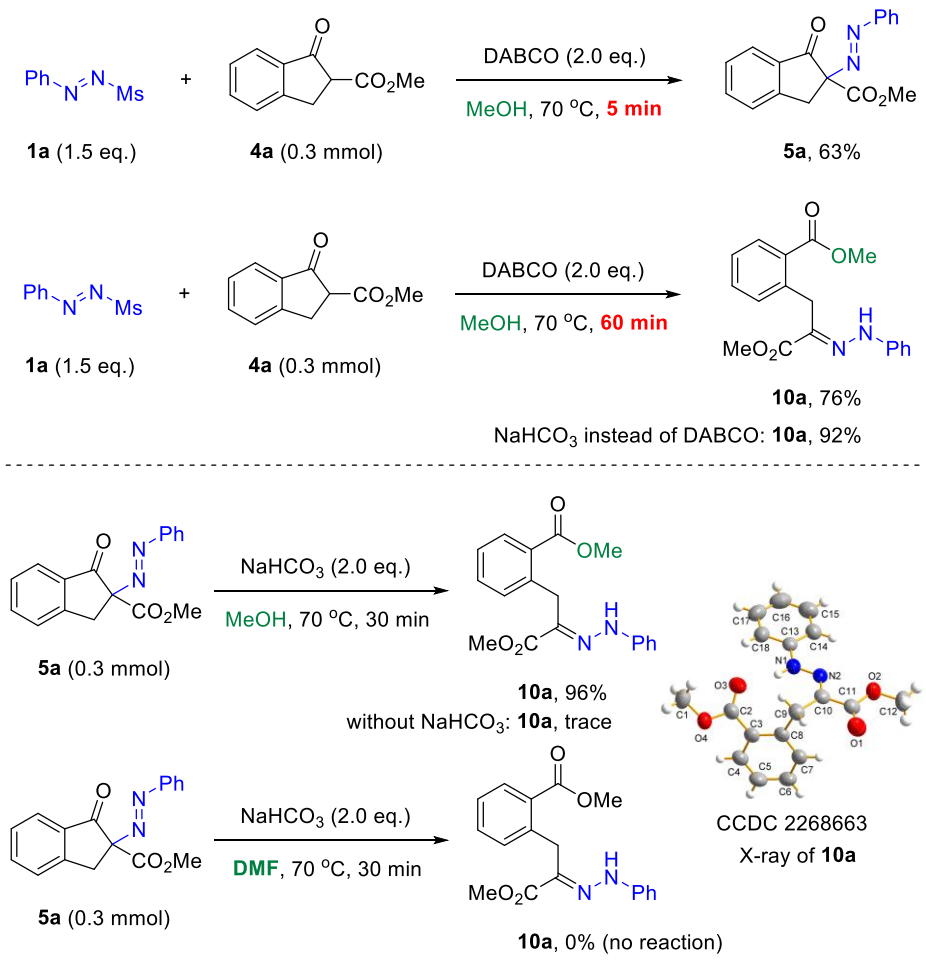
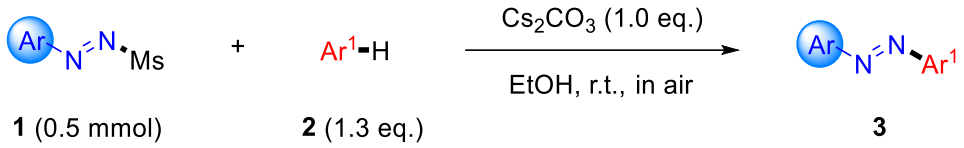


Figure S1 Formation of hydrazone derivatives and the control experiments

When optimizing the reaction conditions for the alkylation of azo, an interesting ring-opening reaction was found (Figure S1). When methanol was used as the solvent, the alkylated azo **5a** can be rapidly generated within minutes (5 min, 63%). However, when the reaction time was prolonged, the azo product **5a** was gradually transformed into the ring-opening product **10a** (60 min, 76%; the yield increased to 92% after the DABCO was changed to $NaHCO_3$). Control experiments have demonstrated the involvement of alcohol solvent in the reaction. Quantitative conversion of **5a** to **10a** can be achieved when methanol is utilized as the solvent, whereas no reaction occurs upon replacement of methanol with DMF. The present ring-opening reaction provides an intriguing pathway for the synthesis of hydrazone derivatives, which is being followed up in our laboratory.

General procedure for the synthesis of 3



In an oven-dried bottle (25 mL) equipped with a stir bar, **1** (0.5 mmol), Cs_2CO_3 (162.9 mg, 0.5 mmol), EtOH (5 mL) and **2** (0.65 mmol) were added. Then, the mixture was stirred at room temperature. After the reaction finished as monitored with TLC, the resulting mixture was concentrated under reduced pressure and pure product was obtained by flash column chromatography on silica gel (petroleum ether/ethyl acetate = 20:1–1:1).

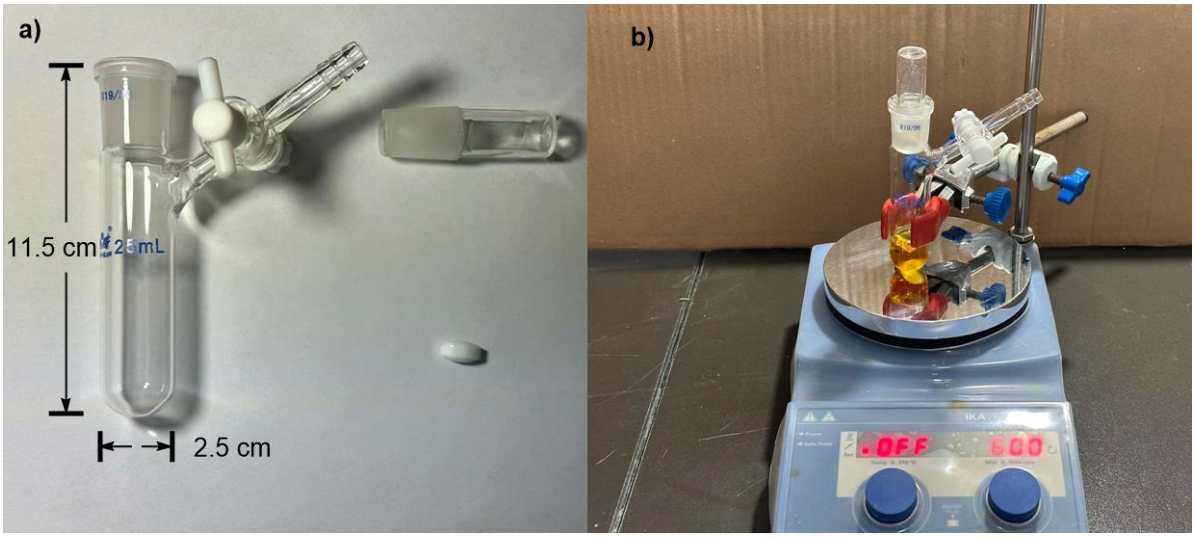
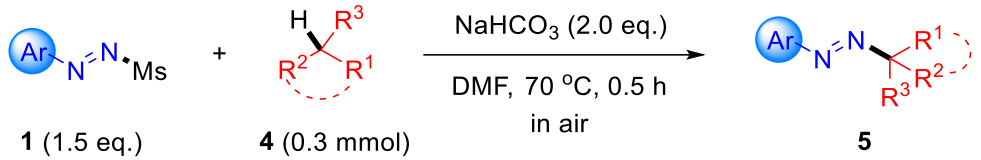


Figure S2 Set-up of Experiments (the photographs come from our lab). a) Experimental equipment. b) Reaction process diagram.

General procedure for the synthesis of 5



1 (1.5 eq.) **4** (0.3 mmol) **5**

In an oven-dried bottle (25 mL) equipped with a stir bar, **4** (0.3 mmol), $NaHCO_3$ (50.4 mg, 0.6 mmol), DMF (3 mL) and **1** (0.45 mmol) were added. Then, the mixture was stirred in the 70 °C oil bath. After the reaction finished as monitored with TLC, the reaction mixture was washed with water and extracted with ethyl acetate (15 mL×3). The organic layers were combined, dried over Na_2SO_4, and concentrated in vacuum. The pure product was obtained by flash column chromatography on silica gel (petroleum ether:ethyl acetate = 15:1-3:1).

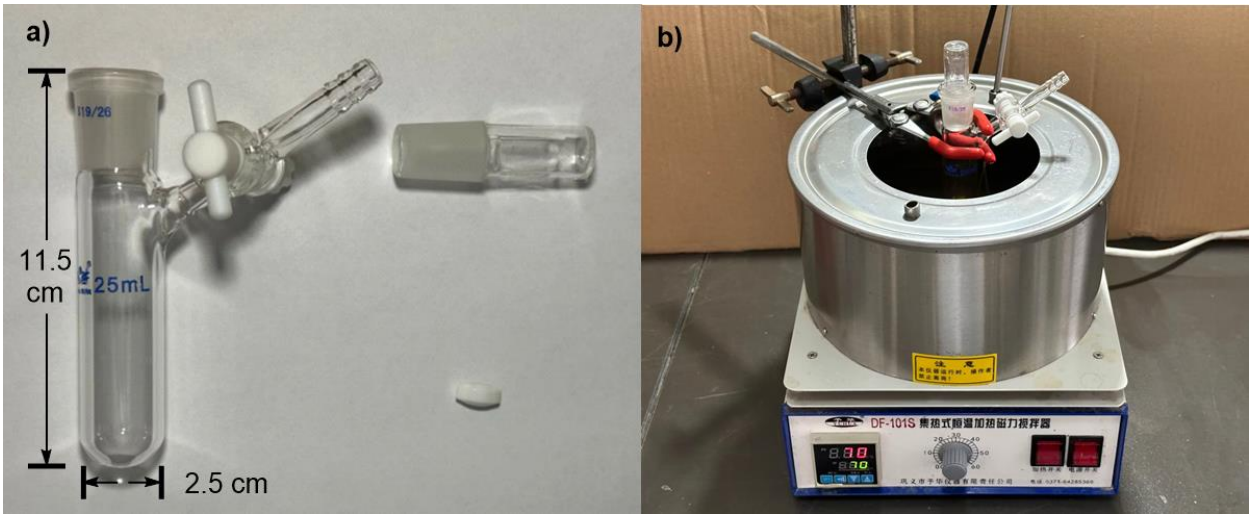
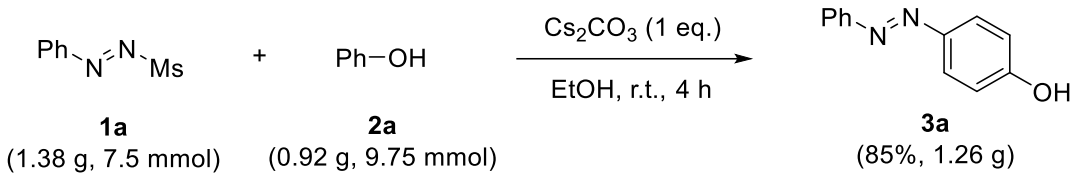


Figure S3 Set-up of Experiments (the photographs come from our lab). a) Experimental equipment. b) Reaction process diagram.

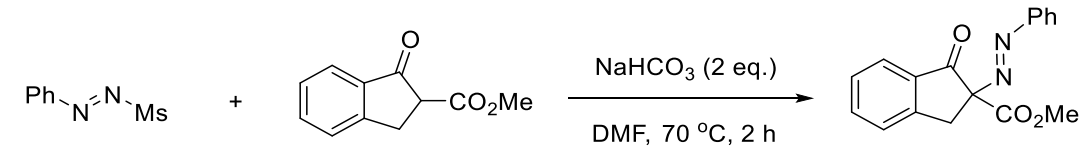
Scale-up Reaction



1a (1.38 g, 7.5 mmol) **2a** (0.92 g, 9.75 mmol) **3a** (85%, 1.26 g)

In an oven-dried bottle (250 mL) equipped with a stir bar, **1a** (1.38 g, 7.5 mmol), Cs_2CO_3 (2.44 g, 7.5 mmol), EtOH (75 mL) and **2a** (0.92 g, 9.75 mmol) were added. Then, the mixture was stirred at room temperature for about 4 hours. After the reaction finished as monitored with TLC, the resulting mixture was concentrated under reduced pressure and the pure **3a** (84%, 1.26 g) was obtained by flash column chromatography on silica gel (petroleum ether/ethyl acetate = 10: 1).

Note: The corresponding experimental device is basically the same as Supplementary Figure 2, except that the volume of the reaction vessel increases correspondingly.

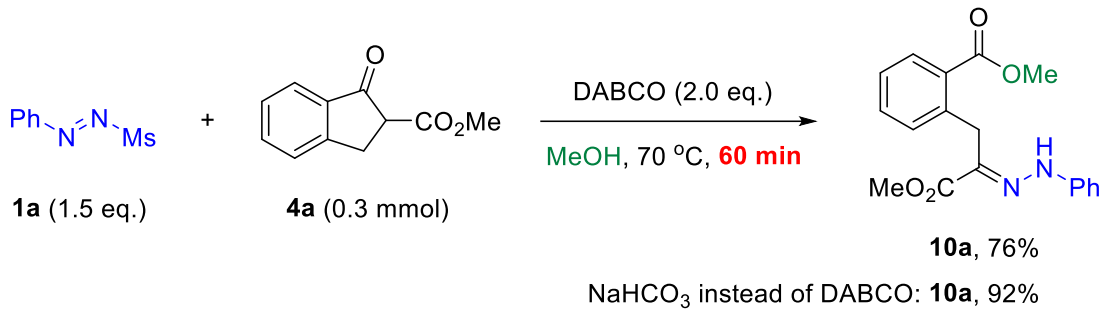


1a (1.24 g, 6.75 mmol) **4a** (0.86 g, 4.5 mmol) **5a** (79%, 1.05 g)

In an oven-dried bottle (250 mL) equipped with a stir bar, **4a** (0.86 g, 4.5 mmol), $NaHCO_3$ (0.76 g, 9 mmol), DMF (45 mL) and **1a** (1.24 g, 6.75 mmol) were added. Then, the mixture was stirred in the 70 °C oil bath for about 2 hours. After the reaction finished as monitored with TLC, the reaction mixture was washed with water and extracted with ethyl acetate (50 mL×3). The organic layers were combined, dried over Na_2SO_4, and concentrated in vacuum. The pure **5a** (79%, 1.05 g) was obtained by flash column chromatography on silica gel (petroleum ether: ethyl acetate = 10:1).

Note: The corresponding experimental device is basically the same as Supplementary Figure 3, except that the volume of the reaction vessel increases correspondingly.

Synthesis and characterization of hydrazine 10a

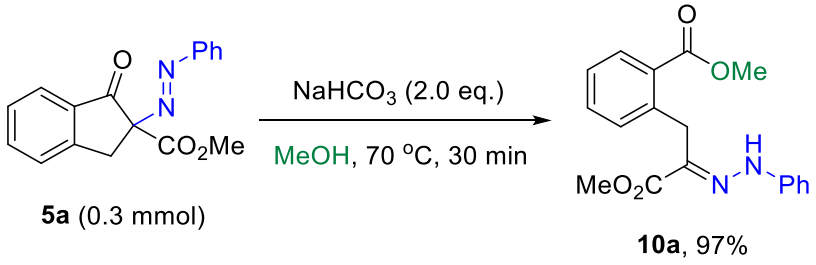


In an oven-dried seal tube (25 mL) equipped with a stir bar, **4a** (57.0 mg, 0.3 mmol), DABCO (67.3 mg, 0.6 mmol), MeOH (3 mL) and **1a** (82.9 mg, 0.45 mmol) were added. Then the vessel was sealed at atmospheric pressure of air and the resulting mixture was stirred in a 70 ℃ oil bath for 60 minutes. The resulting mixture was concentrated under reduced pressure and pure product **10a** (76%, 74.4 mg) was obtained by flash column chromatography on silica gel (petroleum ether: ethyl acetate = 12:1).

Note: When DABCO is replaced with $NaHCO_3$, the yield of **10a** can be increased to 92% (90.1 mg).

Methyl (*E*)-2-(3-methoxy-3-oxo-2-(2-phenylhydrazineylidene)propyl)benzoate (10a).

Compound **10a** was prepared in 76% yield (74 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 12/1); Yellow solid; mp 89-91 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.47 (s, 1H), 7.83-7.81 (m, 1H), 7.54-7.52 (m, 1H), 7.45-7.42 (m, 1H), 7.28-7.26 (m, 1H), 7.25-7.19 (m, 4H), 6.93-6.89 (m, 1H), 4.31 (s, 2H), 4.04 (s, 3H), 3.94 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 170.8, 167.4, 143.8, 138.1, 133.0, 132.5, 131.4, 130.4, 129.3, 129.0, 126.9, 121.9, 114.1, 53.1, 52.7, 27.4; HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{18}H_{19}N_2O_4$: 327.1339, Found 327.1337.



In an oven-dried seal tube (25 mL) equipped with a stir bar, $NaHCO_3$ (50.4 mg, 0.6 mmol), MeOH (3 mL), **5a** (88.3 mg, 0.3 mmol) were added. Then the vessel was sealed at atmospheric pressure of air and the resulting mixture was stirred in a 70 ℃ oil bath for 0.5 h. The resulting mixture was

concentrated under reduced pressure and pure **10a** (97%, 95.0 mg) was obtained by flash column chromatography on silica gel (petroleum ether: ethyl acetate = 12:1).

Possible ring-opening mechanism

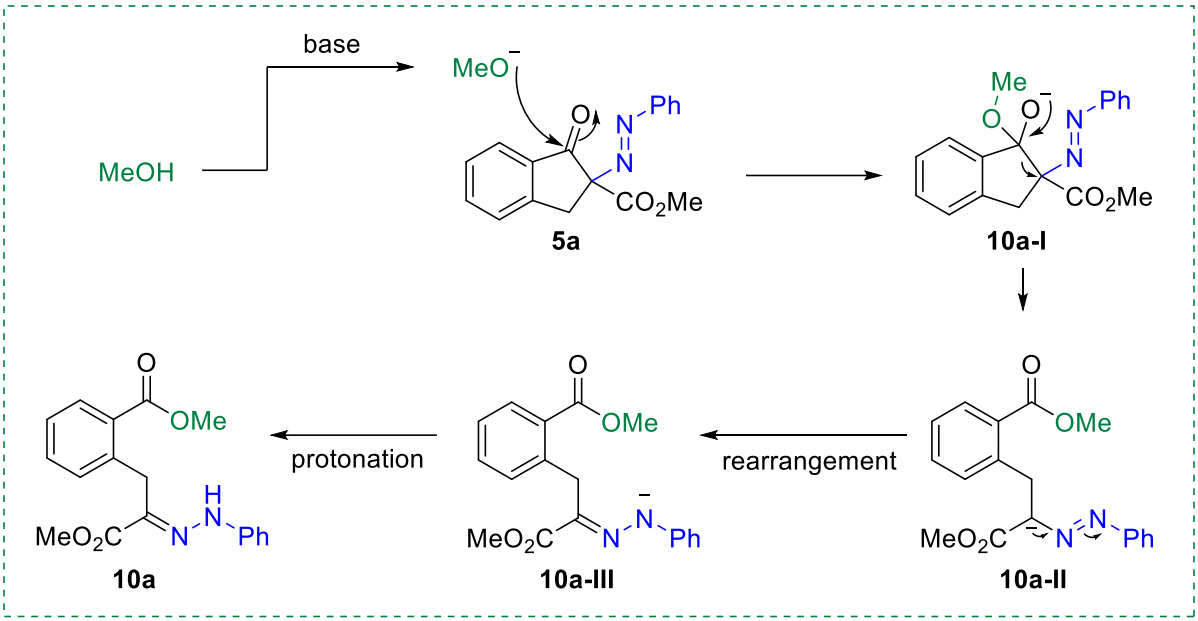
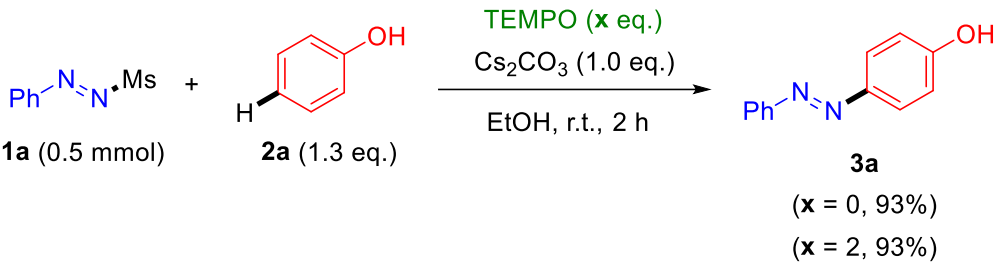
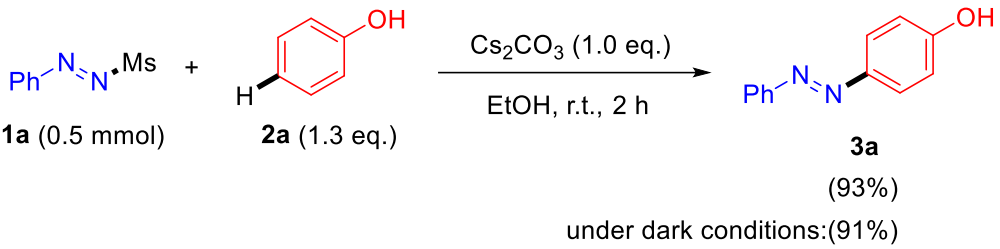


Figure S4 Possible reaction mechanism of ring-opening reaction

Hydrazone **10a** may be generated by nucleophilic addition, intramolecular elimination, rearrangement, and protonation processes, as shown in the figure above.

Mechanistic experiment





When 2,2,6,6-tetramethylpiperidin-1-yl)oxyl (TEMPO) was added to the reaction of **1a** and **2a** under the standard conditions, the reaction was not suppressed (with 0 equiv of TEMPO: **3a**, 93%; with 2 equiv of TEMPO: **3a**, 93%).

Light has no obvious effect on the reaction, and **3a** can be obtained with almost the same yield (91%) under dark conditions.

These results suggest that radical intermediates may not be involved in the substitution reaction.

X-ray crystal structure of 3o

The displacement ellipsoids are drawn at the 50% probability level. Single crystals suitable for X-ray analysis were obtained by slow evaporation of the mixed solution of ethyl acetate/petroleum ether (1/10, v/v). Supplementary crystallographic data was deposited at the Cambridge Crystallographic Data Centre (CCDC) under the number CCDC 2263570 (**3o**) and can be obtained free of charge from via www.ccdc.cam.ac.uk/data_request.cif.

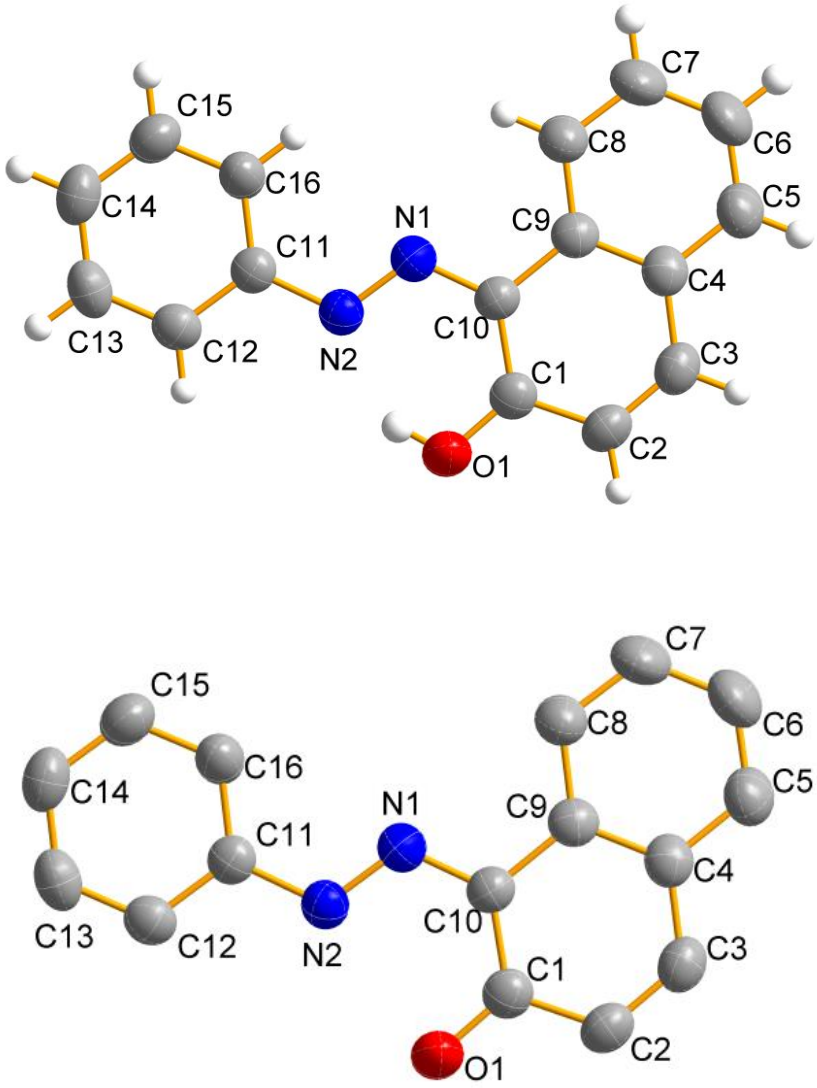


Figure S5 X-ray ORTEP illustration of (*E*)-1-(phenyldiazenyl)naphthalen-2-ol (**3o**) (50% probability ellipsoids)

Table S3 Crystal data and structure refinement for **3o**

Identification code	Zgao_a	
Empirical formula	$C_{16}H_{12}N_2O$	
Formula weight	248.28	
Temperature	295(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 5.8326(8) Å	α= 90 °
	b = 17.478(3) Å	β= 91.997(4) °
	c = 24.849(3) Å	γ = 90 °
Volume	2531.7(6) $Å^3$	
Z	8	
Density (calculated)	1.303 mg/m^3	
Absorption coefficient	0.083 mm^{-1}	
F(000)	1040	
Crystal size	0.520 x 0.200 x 0.160 mm^3	
Theta range for data collection	2.47 to 24.14 °	
Index ranges	-7<=h<=7, -21<=k<=21, -30<=l<=30	
Reflections collected	51542	
Independent reflections	4970 [R(int) = 0.0911]	
Completeness to theta = 25.242 °	100.0 %	
Max. and min. transmission	1.000 and 1.000	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4970 / 1 / 346	
Goodness-of-fit on F^2	1.006	
Final R indices [I>2sigma(I)]	R1 = 0.0604, wR2 = 0.1492	
R indices (all data)	R1 = 0.1336, wR2 = 0.1922	
Largest diff. peak and hole	0.560 and -0.197 e.$Å^{-3}$	

X-ray crystal structure of 10a

The displacement ellipsoids are drawn at the 50% probability level. Single crystals suitable for X-ray analysis were obtained by slow evaporation of the mixed solution of ethyl acetate/petroleum ether (1/5, v/v). Supplementary crystallographic data was deposited at the Cambridge Crystallographic Data Centre (CCDC) under the number CCDC 2268663 (**10a**) and can be obtained free of charge from via www.ccdc.cam.ac.uk/data_request.cif.

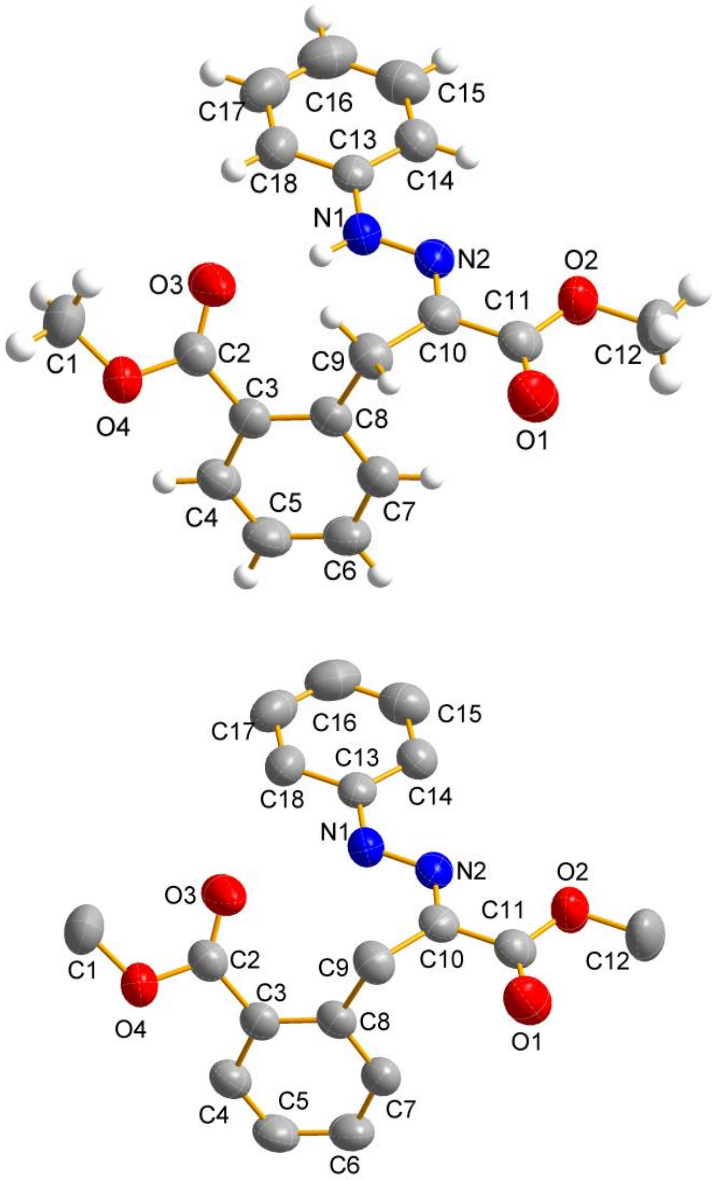


Figure S6 X-ray ORTEP illustration of methyl (*E*)-2-(3-methoxy-3-oxo-2-(2-phenylhydrazineylidene)propyl)benzoate (**10a**) (50% probability ellipsoids)

Table S4 Crystal data and structure refinement for **10a**

Identification code	Zhao07223_0m	
Empirical formula	$C_{18}H_{18}N_2O_4$	
Formula weight	326.34	
Temperature	295(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 4.7435(7) Å	α= 90 °
	b = 16.733(2) Å	β= 90.221(4) °
	c = 20.701(3) Å	γ = 90 °
Volume	1643.1(4) $Å^3$	
Z	4	
Density (calculated)	1.319 mg/m^3	
Absorption coefficient	0.094 mm^{-1}	
F(000)	688	
Crystal size	0.420 x 0.220 x 0.060 mm^3	
Theta range for data collection	2.63 to 27.23 °	
Index ranges	-6<=h<=6, -21<=k<=21, -27<=l<=27	
Reflections collected	19601	
Independent reflections	3852 [R(int) = 0.0283]	
Completeness to theta = 25.000 °	99.4 %	
Max. and min. transmission	0.994 and 0.994	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3852 / 0 / 219	
Goodness-of-fit on F^2	1.027	
Final R indices [I>2sigma(I)]	R1 = 0.0424, wR2 = 0.1048	
R indices (all data)	R1 = 0.0645, wR2 = 0.1196	
Largest diff. peak and hole	0.164 and -0.139 e.$Å^{-3}$	

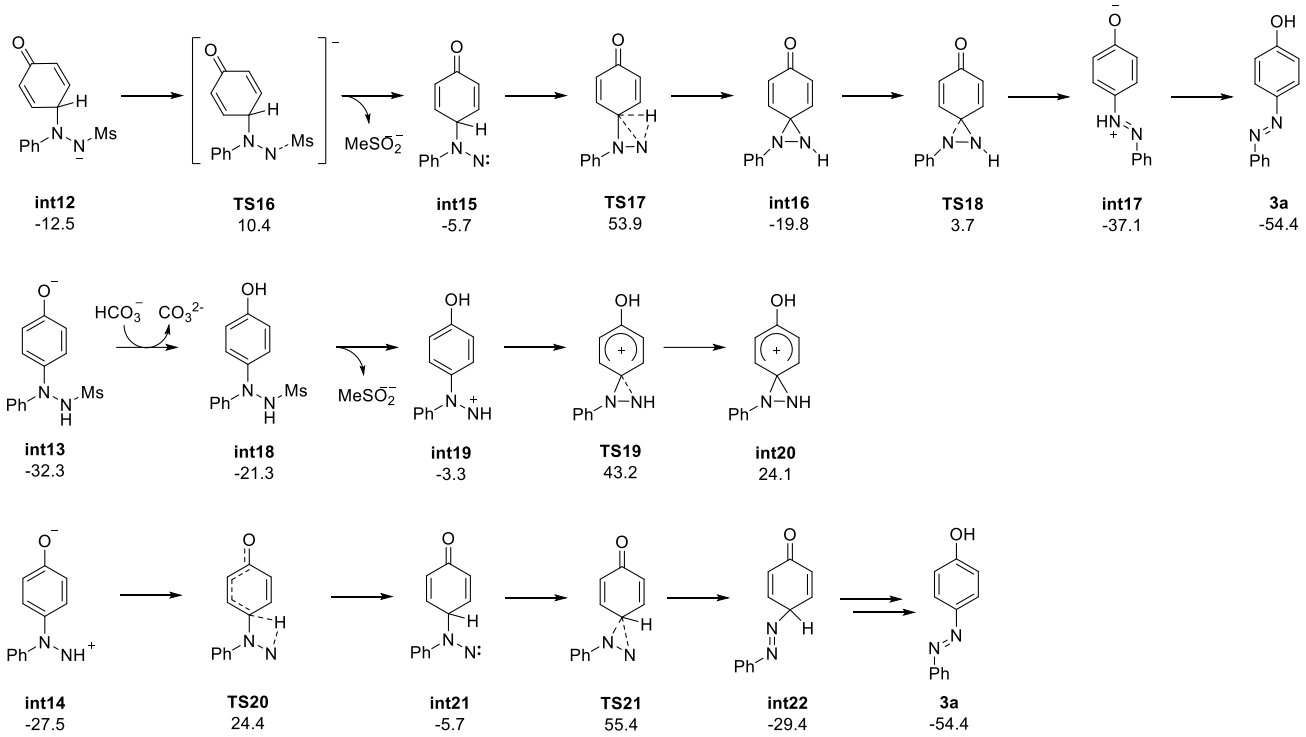


Figure S7 Calculated relative solution-phase Gibbs free energies of unfavorable mechanisms of cross-coupling of **1a** and **2a** (in kcal/mol).

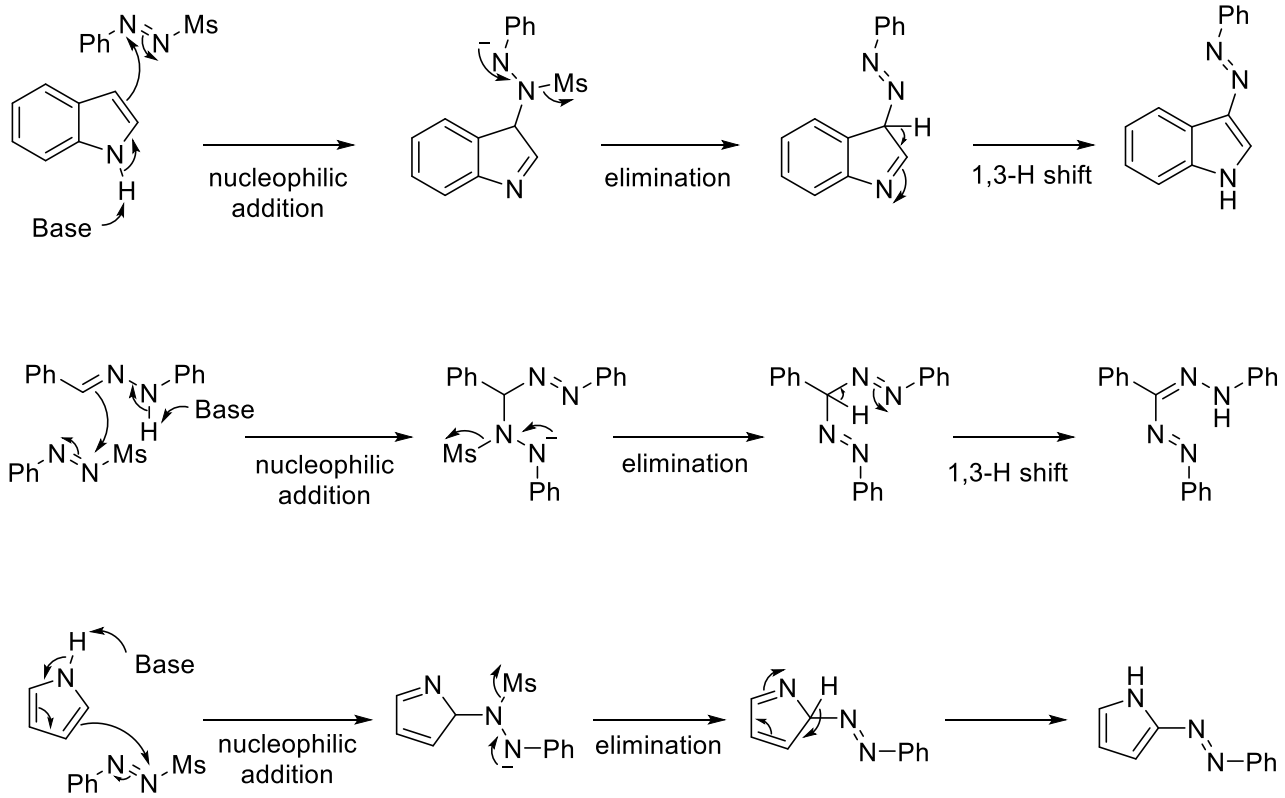
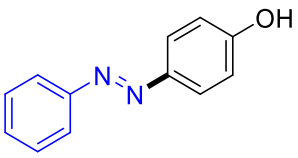


Figure S8 The possible mechanism of arylation for other aromatic compounds

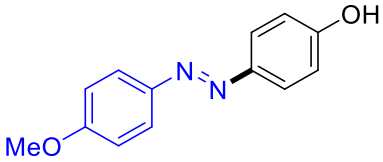
Detail descriptions for products 3



3a

(*E*)-4-(Phenyldiazenyl)phenol (3a).[16]

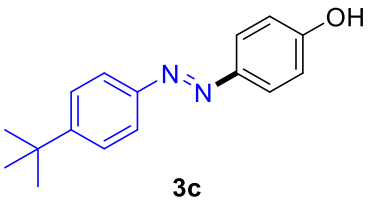
Compound **3a** was prepared in 93% yield (92 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 10/1); Yellow solid; mp 155-157 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.89-7.87 (m, 4H), 7.52-7.49 (m, 2H), 7.46-7.43 (m, 1H), 6.96-6.93 (m, 2H), 5.36 (s, br, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 158.4, 152.8, 147.4, 130.6, 129.2, 125.1, 122.7, 116.0; HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{12}H_{11}N_2O$: 199.0866, Found 199.0868. Analytical data for **3a** was consistent with that previously reported.[16]



3b

(*E*)-4-((4-Methoxyphenyl)diazenyl)phenol (3b).[17]

Compound **3b** was prepared in 90% yield (103 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 11/1); Yellow solid; mp 138-140 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.88-7.86 (m, 2H), 7.82 (d, *J* = 8.8 Hz, 2H), 7.01-6.99(m, 2H), 6.92 (d, *J* = 8.8 Hz, 2H), 4.19 (s, br, 1H), 3.88 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.7, 158.2, 147.2, 147.1, 124.7, 124.5, 116.0, 114.3, 55.7; HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{13}H_{13}N_2O_2$: 229.0972, Found 229.0967. Analytical data for **3b** was consistent with that previously reported.[17]

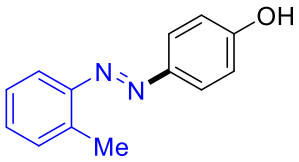


3c

(*E*)-4-((4-(*Tert*-butyl)phenyl)diazenyl)phenol (3c).[18]

Compound **3c** was prepared in 83% yield (106 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 11/1); Yellow solid; mp 124-126 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ

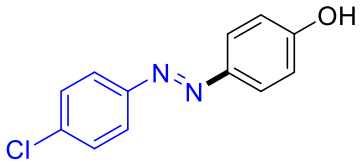
7.86 (d, *J* = 8.7 Hz, 2H), 7.81 (d, *J* = 8.5 Hz, 2H), 7.52 (d, *J* = 8.5 Hz, 2H), 6.93 (d, *J* = 8.7 Hz, 2H), 5.30 (s, br, 1H), 1.37 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 158.2, 154.1, 150.8, 147.4, 126.1, 125.0, 122.4, 115.9, 35.1, 31.4; HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{16}H_{19}N_2O$: 255.1492, Found 255.1492. Analytical data for **3c** was consistent with that previously reported.[18]



3d

(*E*)-4-(*o*-Tolyldiazenyl)phenol (3d).[19]

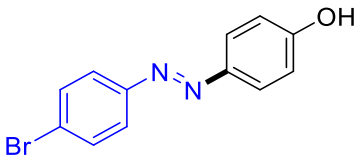
Compound **3d** was prepared in 88% yield (93 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 10/1); Yellow solid; mp 101-103 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.87 (d, *J* = 8.8 Hz, 2H), 7.58 (d, *J* = 7.9 Hz, 1H), 7.32-7.31 (m, 2H), 7.25-7.23 (m, 1H), 6.93 (d, *J* = 8.8 Hz, 2H), 4.13 (s, br, 1H), 2.69 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 158.5, 151.0, 147.7, 137.6, 131.3, 130.5, 126.6, 125.2, 116.0, 115.6, 17.6; HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{13}H_{13}N_2O$: 213.1022, Found 213.1017. Analytical data for **3d** was consistent with that previously reported.[19]



3e

(*E*)-4-((4-Chlorophenyl)diazenyl)phenol (3e).[20]

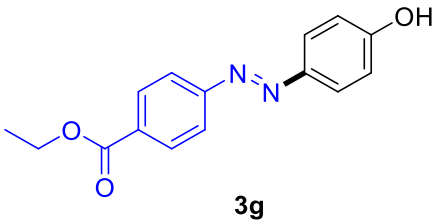
Compound **3e** was prepared in 93% yield (108 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 9/1); Yellow solid; mp 149-151 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 10.41 (s, br, 1H), 7.83-7.80 (m, 4H), 7.61 (d, *J* = 7.9 Hz, 2H), 6.95 (d, *J* = 8.3 Hz, 2H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 161.3, 150.7, 145.1, 134.8, 129.4, 125.0, 123.7, 116.0; HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{12}H_{10}ClN_2O$: 233.0476, Found 233.0480. Analytical data for **3e** was consistent with that previously reported.[20]



3f

(*E*)-4-((4-Bromophenyl)diazenyl)phenol (3f).[20]

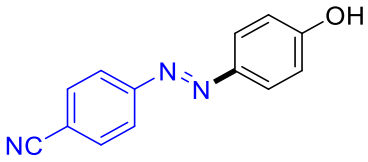
Compound **3f** was prepared in 72% yield (100 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 9/1); Yellow solid; mp 147-149 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.87 (d, *J* = 8.6 Hz, 2H), 7.75 (d, *J* = 8.5 Hz, 2H), 7.62 (d, *J* = 8.5 Hz, 2H), 6.94 (d, *J* = 8.6 Hz, 2H), 5.41 (s, 1H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 161.3, 151.0, 145.1, 132.4, 125.1, 124.0, 123.6, 116.0; HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{12}H_{10}BrN_2O$: 276.9971, Found 276.9969. Analytical data for **3f** was consistent with that previously reported.[20]



3g

Ethyl (*E*)-4-((4-hydroxyphenyl)diazenyl)benzoate (3g).[21]

Compound **3g** was prepared in 73% yield (99 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 8/1); Yellow solid; mp 160-162 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.18 (d, *J* = 8.4 Hz, 2H), 7.92-7.89 (m, 4H), 6.98 (d, *J* = 8.7 Hz, 2H), 6.23 (s, br, 1H), 4.42 (q, *J* = 7.1 Hz, 2H), 1.43 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.6, 159.4, 155.5, 147.2, 131.5, 130.7, 125.6, 122.5, 116.1, 61.5, 14.5; HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{15}H_{15}N_2O_3$: 271.1077, Found 271.1085. Analytical data for **3g** was consistent with that previously reported.[21]

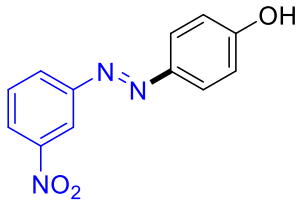


3h

(*E*)-4-((4-Hydroxyphenyl)diazenyl)benzonitrile (3h).[22]

Compound **3h** was prepared in 41% yield (46 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 7/1); Yellow solid; mp 175-177 °C; ^{1}H NMR (500 MHz, DMSO-d_6):

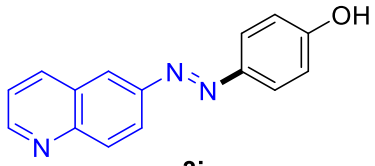
δ 10.51 (s, 1H), 8.02-8.01 (m, 2H), 7.93-7.91 (m, 2H), 7.86-7.83 (m, 2H), 6.98-6.96 (m, 2H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 162.1, 154.3, 145.3, 133.7, 125.6, 122.7, 118.5, 116.2, 112.2; HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{13}H_{10}N_3O$: 224.0818, Found 224.0820. Analytical data for **3h** was consistent with that previously reported.[22]



3i

(*E*)-4-((3-Nitrophenyl)diazenyl)phenol (3i).[23]

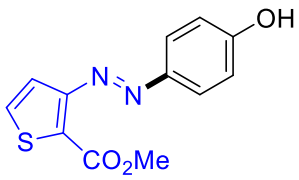
Compound **3i** was prepared in 39% yield (47 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 7/1); Yellow solid; mp 165-167 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 10.53 (s, 1H), 8.47-8.46 (m, 1H), 8.34-8.31 (m, 1H), 8.27-8.24 (m, 1H), 7.89-7.83 (m, 3H), 6.99-6.96 (m, 2H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 162.0, 152.5, 148.6, 145.0, 130.9, 129.4, 125.6, 124.4, 116.1, 115.1; HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{12}H_{10}N_3O_3$: 244.0717, Found 244.0725. Analytical data for **3i** was consistent with that previously reported.[23]



3j

(*E*)-4-(Quinolin-6-yldiazenyl)phenol (3j).

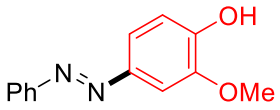
Compound **3j** was prepared in 58% yield (72 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 3/1); Yellow solid; mp 253-255 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 10.38 (s, 1H), 8.96-8.95 (m, 1H), 8.56 (d, J = 8.3 Hz, 1H), 8.48 (d, J = 2.0 Hz, 1H), 8.20 (dd, J = 9.1, 2.2 Hz, 1H), 8.12 (d, J = 9.1 Hz, 1H), 7.88 (d, J = 8.8 Hz, 2H), 7.63-7.60 (m, 1H), 6.98 (d, J = 8.8 Hz, 2H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 161.3, 151.5, 149.5, 148.6, 145.3, 137.2, 130.3, 128.2, 125.5, 125.0, 122.2, 120.7, 116.0; HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{15}H_{12}N_3O$: 250.0975, Found 250.0973.



3k

Methyl (*E*)-3-((4-hydroxyphenyl)diazenyl)thiophene-2-carboxylate (3k).

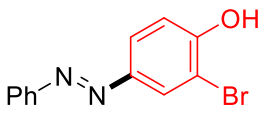
Compound **3k** was prepared in 50% yield (66 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 3/1); Yellow solid; mp 148-150 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 10.43 (s, 1H), 7.90 (d, J = 5.4 Hz, 1H), 7.83-7.80 (m, 2H), 7.39 (d, J = 5.4 Hz, 1H), 6.98-6.95 (m, 2H), 3.88 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 161.7, 161.1, 156.3, 145.6, 131.9, 127.9, 125.4, 118.6, 116.1, 52.4; HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{12}H_{11}N_2O_3S$: 263.0485, Found 263.0480.



3l

(*E*)-2-Methoxy-4-(phenyldiazenyl)phenol (3l).[24]

Compound **3l** was prepared in 86% yield (98 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 10/1); Yellow solid; mp 68-70 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.89-7.88 (m, 2H), 7.63-7.61 (m, 1H), 7.52-7.49 (m, 3H), 7.46-7.43 (m, 1H), 7.07 (d, J = 8.4 Hz, 1H), 5.99 (s, br, 1H), 3.99 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 152.8, 149.0, 147.2, 146.9, 130.5, 129.2, 122.7, 121.5, 114.3, 102.0, 56.2; HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{13}H_{13}N_2O_2$: 229.0972, Found 229.0976. Analytical data for **3l** was consistent with that previously reported.[24]



3m

(*E*)-2-Bromo-4-(phenyldiazenyl)phenol (3m).

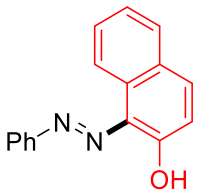
Compound **3m** was prepared in 83% yield (115 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 10/1); Yellow solid; mp 77-79 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.12 (d, J = 2.2 Hz, 1H), 7.90-7.88 (m, 3H), 7.53-7.45 (m, 3H), 7.16 (d, J = 8.7 Hz, 1H), 5.46 (s, br,

1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 154.8, 152.6, 147.4, 131.0, 129.2, 125.9, 125.7, 122.9, 116.3, 111.3; HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{12}H_{10}BrN_2O$: 276.9971, Found 276.9978.

3n

(*E*)-4-Methoxy-2-(phenyldiazenyl)phenol (3n).

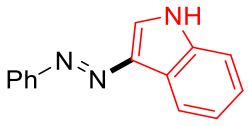
Compound **3n** was prepared in 44% yield (50 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 15/1); Yellow solid; mp 70-72 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 12.46 (s, 1H), 7.88-7.86 (m, 2H), 7.54-7.51 (m, 2H), 7.49-7.47 (m, 1H), 7.45 (d, *J* = 2.7 Hz, 1H), 7.01-6.96 (m, 2H), 3.87 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 153.0, 150.8, 147.3, 137.1, 131.3, 129.5, 122.4, 121.8, 119.0, 114.8, 56.1; HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{13}H_{13}N_2O_2$: 229.0972, Found 229.0977.



3o

(*E*)-1-(Phenyldiazenyl)naphthalen-2-ol (3o).[25]

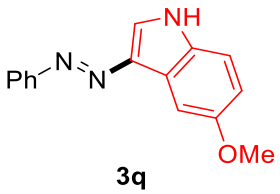
Compound **3o** was prepared in 81% yield (101 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 20/1); Yed solid; mp 128-130 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.54 (d, *J* = 8.1 Hz, 1H), 7.73-7.67 (m, 3H), 7.59-7.53 (m, 2H), 7.49-7.46 (m, 2H), 7.39-7.37 (m, 1H), 7.31-7.29 (m, 1H), 6.86-6.84 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 172.2, 144.8, 140.2, 133.7, 130.1, 129.7, 129.0, 128.7, 128.1, 127.5, 125.8, 125.0, 121.8, 118.7; HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{16}H_{13}N_2O$: 249.1022, Found 249.1023. Analytical data for **3o** was consistent with that previously reported.[25]



3p

(*E*)-3-(Phenyldiazenyl)-1*H*-indole (3p).[26]

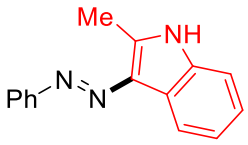
Compound **3p** was prepared in 71% yield (79 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 10/1); Yellow solid; mp 132-134 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.61-8.57 (m, 2H), 8.00 (d, *J* = 3.0 Hz, 1H), 7.91-7.89 (m, 2H), 7.53-7.49 (m, 2H), 7.42-7.32 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 154.0, 137.0, 136.4, 130.6, 129.3, 129.1, 124.5, 123.2, 123.2, 122.0, 119.1, 111.5; HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{14}H_{12}N_3$: 222.1026, Found 222.1028. Analytical data for **3p** was consistent with that previously reported.[26]



3q

(*E*)-5-Methoxy-3-(phenyldiazenyl)-1*H*-indole (3q).

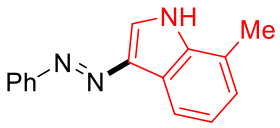
Compound **3q** was prepared in 66% yield (83 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 10/1); Yellow solid; mp 122-124 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.56 (s, 1H), 8.10 (d, *J* = 1.6 Hz, 1H), 7.96 (d, *J* = 1.0 Hz, 1H), 7.86 (d, *J* = 7.9 Hz, 2H), 7.51-7.47 (m, 2H), 7.39-7.36 (m, 1H), 7.26-7.24 (m, 1H), 6.97-6.94 (m, 1H), 3.91 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.8, 153.9, 136.8, 131.3, 131.2, 129.2, 129.1, 121.9, 119.5, 114.3, 112.3, 104.9, 55.9; HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{15}H_{14}N_3O$: 252.1131, Found 252.1136.



3r

(*E*)-2-Methyl-3-(phenyldiazenyl)-1*H*-indole (3r).[27]

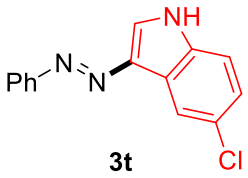
Compound **3r** was prepared in 83% yield (98 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 10/1); Yellow solid; mp 173-175 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.52 (d, *J* = 7.6 Hz, 1H), 8.12 (s, 1H), 7.87 (d, *J* = 7.9 Hz, 2H), 7.47-7.44 (m, 2H), 7.34-7.31 (m, 1H), 7.26-7.21 (m, 3H), 2.74 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 154.3, 143.0, 135.1, 133.0, 129.0, 128.7, 123.6, 123.0, 122.6, 121.8, 119.7, 110.6, 11.6; HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{15}H_{14}N_3$: 236.1182, Found 236.1186. Analytical data for **3r** was consistent with that previously reported.[27]



3s

(*E*)-7-Methyl-3-(phenyldiazenyl)-1*H*-indole (3s).

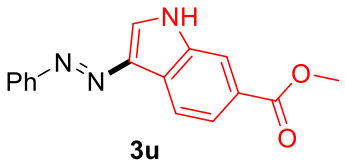
Compound **3s** was prepared in 75% yield (88 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 10/1); Yellow solid; mp 111-113 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.49 (s, 1H), 8.44 (d, *J* = 8.0 Hz, 1H), 8.00 (d, *J* = 3.0 Hz, 1H), 7.91-7.89 (m, 2H), 7.52-7.49 (m, 2H), 7.41-7.38 (m, 1H), 7.27-7.24 (m, 1H), 7.14 (d, *J* = 7.2 Hz, 1H), 2.51 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 153.9, 137.4, 135.9, 130.3, 129.3, 129.1, 125.2, 123.3, 122.0, 120.9, 120.5, 118.6, 16.5; HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{15}H_{14}N_3$: 236.1182, Found 236.1182.



3t

(E)-5-Chloro-3-(phenyldiazenyl)-1*H*-indole (3t).

Compound **3t** was prepared in 77% yield (98 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 8/1); Yellow solid; mp 127-129 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.62 (s, 1H), 8.57 (s, 1H), 8.00 (d, *J* = 3.0 Hz, 1H), 7.90 (d, *J* = 7.5 Hz, 2H), 7.53-7.49 (m, 2H), 7.43-7.39 (m, 1H), 7.27-7.25 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.7, 136.3, 134.6, 131.4, 129.6, 129.2, 128.8, 124.8, 122.7, 122.0, 119.8, 112.5; HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{14}H_{11}ClN_3$: 256.0636, Found 256.0634.

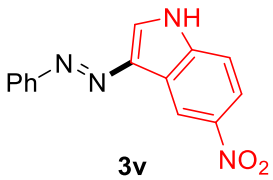


3u

Methyl (*E*)-3-(phenyldiazenyl)-1*H*-indole-6-carboxylate (3u).

Compound **3u** was prepared in 69% yield (96 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 5/1); Yellow solid; mp 163-165 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.15 (s, 1H), 8.58 (d, *J* = 8.4 Hz, 1H), 8.17 (d, *J* = 0.6 Hz, 1H), 8.15 (d, *J* = 3.0 Hz, 1H), 7.99 (dd, *J* = 8.4, 1.4 Hz, 1H), 7.91-7.89 (m, 2H), 7.52-7.49 (m, 2H), 7.42-7.40 (m, 1H), 3.97 (s, 3H); ^{13}C NMR

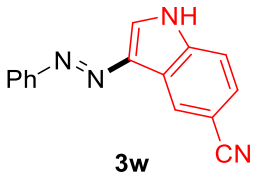
(125 MHz, $CDCl_3$): δ 167.9, 153.7, 136.7, 135.8, 132.8, 129.7, 129.2, 125.9, 124.1 ,122.8, 122.3, 122.1, 113.8, 52.3; HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{16}H_{14}N_3O_2$: 280.1081, Found 280.1085.



3v

(*E*)-5-Nitro-3-(phenyldiazenyl)-1*H*-indole (3v).

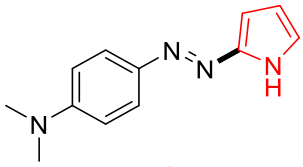
Compound **3v** was prepared in 60% yield (80 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 2/1); Yellow solid; mp 234-236°C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 12.67 (s, br, 1H), 9.21 (d, J = 2.3 Hz, 1H), 8.65 (s, 1H), 8.16 (dd, J = 9.0, 2.4 Hz, 1H), 7.85-7.83 (m, 2H), 7.69 (d, J = 9.0 Hz, 1H), 7.58-7.55 (m, 2H), 7.48-7.45 (m, 1H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 152.8, 143.1, 139.5, 136.5, 135.9, 129.7, 129.3, 121.6, 119.1, 118.7, 117.3, 113.0; HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{14}H_{11}N_4O_2$: 267.0877, Found 267.0875.



3w

(*E*)-3-(Phenyldiazenyl)-1*H*-indole-5-carbonitrile (3w).

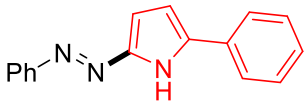
Compound **3w** was prepared in 51% yield (63 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 2/1); Yellow solid; mp 177-179 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 12.56 (s, br, 1H), 8.78 (s, 1H), 8.59 (s, 1H), 7.88 (d, J = 7.7 Hz, 2H), 7.69-7.64 (m, 2H), 7.56-7.53 (m, 2H), 7.46-7.43 (m, 1H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 152.9, 138.2, 135.4, 134.9, 129.6, 129.2, 127.3, 126.7, 121.6, 120.2, 117.8, 113.7, 104.6; HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{15}H_{11}N_4$: 247.0978, Found 247.0984.



3y

(*E*)-4-((1H-pyrrol-2-yl)diazenyl)-N,N-dimethylaniline (3y).[28]

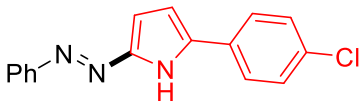
Compound **3y** was prepared in 53% yield (57 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 5/1); Rufous solid; mp 159-160 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.27 (s, br, 1H), 7.75 (d, *J* = 9.0 Hz, 2H), 6.84-6.82 (m, 2H), 6.74 (d, *J* = 9.0 Hz, 2H), 6.34-6.34 (m, 1H), 3.06 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 151.6, 146.2, 143.5, 124.0, 119.9, 112.1, 111.9, 111.0, 40.5; HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{12}H_{15}N_4$: 215.1291, Found 215.1294. Analytical data for **3y** was consistent with that previously reported.[28]



3z

(*E*)-2-Phenyl-5-(phenyldiazenyl)-1*H*-pyrrole (3z).

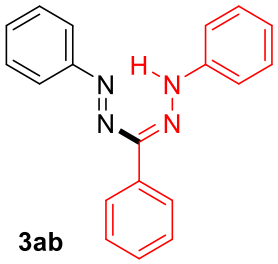
Compound **3z** was prepared in 90% yield (111 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 20/1); Yellow solid; mp 116-118 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.53 (s, br, 1H), 7.82 (d, *J* = 7.8 Hz, 2H), 7.63 (d, *J* = 7.7 Hz, 2H), 7.50-7.42 (m, 4H), 7.39-7.32 (m, 2H), 7.08 (d, *J* = 3.7 Hz, 1H), 6.74 (d, *J* = 3.7 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 152.9, 146.5, 135.8, 131.2, 129.6, 129.2, 128.2, 124.9, 122.1, 118.0, 109.7; HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{16}H_{14}N_3$: 248.1182, Found 248.1187.



3aa

(*E*)-2-(4-Chlorophenyl)-5-(phenyldiazenyl)-1*H*-pyrrole (3aa).

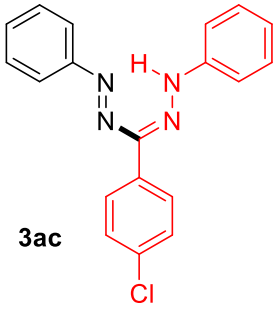
Compound **3aa** was prepared in 93% yield (131 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 20/1); Yellow solid; mp 122-124 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.49 (s, br, 1H), 7.82 (d, *J* = 7.6 Hz, 2H), 7.54 (d, *J* = 8.5 Hz, 2H), 7.50-7.47 (m, 2H), 7.40-7.37 (m, 3H), 7.07 (d, *J* = 4.0 Hz, 1H), 6.70 (d, *J* = 4.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 152.8, 146.6, 134.5, 133.9, 129.8, 129.4, 129.3, 126.1, 122.2, 117.9, 109.9; HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{16}H_{13}ClN_3$: 282.0793, Found 282.0797.



3ab

(*Z*,*E*)-1,3,5-triphenylformazan (3ab).[29]

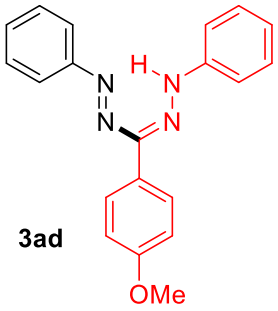
Compound **3ab** was prepared in 61% yield (92 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 400/1); Red solid; mp 170-171 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 15.41 (s, 1H), 8.13-8.12 (m, 2H), 7.68-7.66 (m, 4H), 7.45-7.42 (m, 6H), 7.34-7.27 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 148.0, 141.3, 137.6, 129.8, 129.6, 128.5, 128.3, 127.8, 127.6, 126.6, 126.0, 120.2, 118.9; HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{19}H_{17}N_4$: 301.1448, Found 301.1450. Analytical data for **3ab** was consistent with that previously reported.[29]



3ac

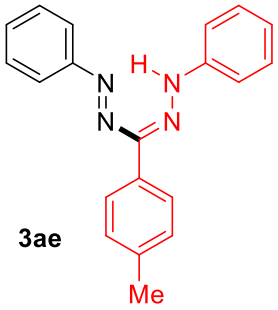
(*Z*,*E*)-3-(4-chlorophenyl)-1,5-diphenylformazan (3ac).[30]

Compound **3ac** was prepared in 33% yield (55 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 400/1); Red solid; mp 205-206 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 15.45 (s, 1H), 8.07 (d, *J* = 8.6 Hz, 2H), 7.67 (d, *J* = 7.6 Hz, 4H), 7.48-7.45 (m, 4H), 7.39 (d, *J* = 8.7 Hz, 2H), 7.31-7.28 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 147.8, 140.4, 136.1, 133.6, 129.6, 128.7, 127.8, 127.2, 119.0; HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{19}H_{16}ClN_4$: 335.1058, Found 335.1063. Analytical data for **3ac** was consistent with that previously reported.[30]



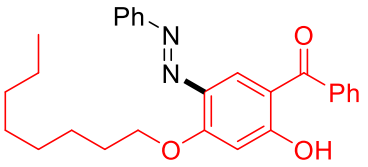
(*Z*,*E*)-3-(4-methoxyphenyl)-1,5-diphenylformazan (3ad).[31]

Compound **3ad** was prepared in 57% yield (94 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 200/1); Red solid; mp 158-159 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 15.20 (s, 1H), 8.05 (d, *J* = 9.0 Hz, 2H), 7.66-7.64 (m, 4H), 7.44-7.41 (m, 4H), 7.24 (d, *J* = 8.7 Hz, 2H), 6.96 (d, *J* = 9.0 Hz, 2H), 3.85 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 159.6, 148.1, 141.4, 130.7, 130.3, 129.7, 129.5, 128.3, 127.4, 126.7, 118.8, 115.2, 114.0; HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{20}H_{19}N_4O$: 331.1553, Found 331.1546. Analytical data for **3ad** was consistent with that previously reported.[31]



(Z,E)-1,5-diphenyl-3-(p-tolyl)formazan (3ae).[31]

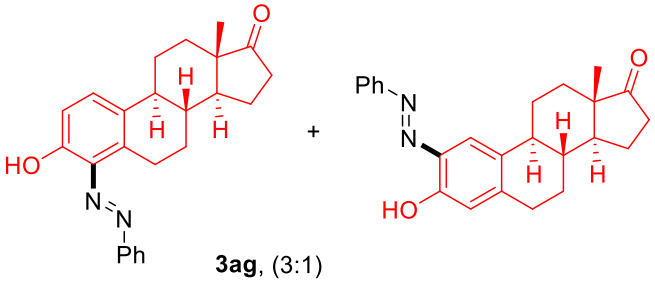
Compound **3ae** was prepared in 59% yield (93 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 400/1); Red solid; mp 155-156 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 15.34 (s, 1H), 8.05 (d, *J* = 8.3 Hz, 2H), 7.71-7.69 (m, 4H), 7.48-7.45 (m, 4H), 7.30-7.27 (m, 4H), 2.43 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 148.1, 141.5, 137.6, 134.8, 130.5, 129.5, 129.3, 129.3, 129.2, 127.5, 126.0, 118.9, 113.0; HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{20}H_{19}N_4$: 315.1604, Found 315.1599. Analytical data for **3ae** was consistent with that previously reported.[31]



3af

(*E*)-(2-Hydroxy-4-(octyloxy)-5-(phenyldiazenyl)phenyl)(phenyl)methanone (3af).

Compound **3af** was prepared in 74% yield (159 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 15/1); Yellow solid; mp 79-81 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 12.89 (s, 1H), 8.03 (s, 1H), 7.81-7.80 (m, 2H), 7.71-7.69 (m, 2H), 7.61-7.58 (m, 1H), 7.54-7.51 (m, 2H), 7.47-7.40 (m, 3H), 6.68 (s, 1H), 4.24 (t, *J* = 6.6 Hz, 2H), 1.98-1.92 (m, 2H), 1.54-1.51 (m, 2H), 1.42-1.39 (m, 2H), 1.35-1.28 (m, 6H), 0.88 (t, *J* = 6.7 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 200.9, 168.2, 163.2, 153.0, 138.0, 135.8, 132.1, 130.7, 129.3, 129.1, 128.6, 123.0, 122.2, 112.2, 101.6, 69.8, 31.9, 29.4, 29.4, 29.0, 26.1, 22.8, 14.2; HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{27}H_{31}N_2O_3$: 431.2329, Found 431.2337.



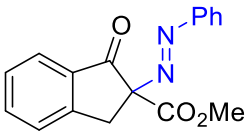
3ag, (3:1)

(8*R*,9*S*,13*S*,14*S*)-3-Hydroxy-13-methyl-4-((*E*)-phenyldiazenyl)-6,7,8,9,11,12,13,14,15,16-decahydro-17*H*-cyclopenta[*a*]phenanthren-17-one and **(8*R*,9*S*,13*S*,14*S*)-3-Hydroxy-13-methyl-2-((*E*)-phenyldiazenyl)-6,7,8,9,11,12,13,14,15,16-decahydro-17*H*-cyclopenta[*a*]phenanthren-17-one (3ag).**

Compound **3ag** was prepared in 70% yield (131 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 10/1); Yellow solid; mp 159-161 °C; ^{1}H NMR (500 MHz, $CDCl_3$): major isomer: δ 13.58 (s, 1H), 7.85-7.83 (m, 2H), 7.53-7.50 (m, 2H), 7.47-7.44 (m, 1H), 7.33 (d, *J* = 8.8 Hz, 1H), 6.84 (d, *J* = 8.8 Hz, 1H), 3.69-3.65 (m, 1H), 3.25-3.19 (m, 1H), 2.55-2.50 (m, 1H), 2.44-2.41 (m, 1H), 2.34-2.30 (m, 1H), 2.20-2.07 (m, 3H), 2.05-1.98 (m, 1H), 1.69-1.61 (m, 3H), 1.58-1.47 (m, 3H), 0.94 (s, 3H), minor isomer: δ 12.74 (s, 1H), 6.76 (s, 1H), 2.98-2.93 (m, 2H), other peaks are

overlapped with the signals of the major isomer; ^{13}C NMR (125 MHz, $CDCl_3$): δ 220.9, 220.8, 151.4, 151.0, 150.8, 150.8, 143.6, 139.4, 136.2, 134.7, 132.2, 131.8, 131.6, 130.9, 130.3, 129.5, 129.5, 122.3, 122.2, 117.7, 115.9, 50.6, 50.5, 48.1, 48.1, 44.1, 43.8, 38.2, 38.1, 36.0, 36.0, 31.8, 31.6, 26.4, 26.3, 26.0, 25.9, 21.7, 21.7, 14.0, 14.0; HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{24}H_{27}N_2O_2$: 375.2067, Found 375.2072.

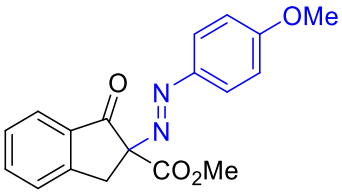
Detail descriptions for products 5



5a

Methyl (*E*)-1-oxo-2-(phenyldiazenyl)-2,3-dihydro-1*H*-indene-2-carboxylate (5a).[32]

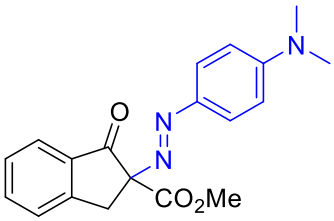
Compound **5a** was prepared in 86% yield (76 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 10/1); Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.82 (d, *J* = 7.7 Hz, 1H), 7.75-7.72 (m, 2H), 7.67-7.64 (m, 1H), 7.53 (d, *J* = 7.7 Hz, 1H), 7.44-7.41 (m, 4H),3.96-3.89 (m, 2H), 3.86 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 196.6, 169.0, 152.3, 151.5, 136.0, 134.6, 131.8, 129.1, 128.3, 126.6, 125.4, 123.0, 87.8, 53.4, 36.0; HRMS (ESI) m/z $[M+Na]^+$ Calcd for $C_{17}H_{14}N_2NaO_3$: 317.0897, Found 317.0895. Analytical data for **5a** was consistent with that previously reported.[32]



5b

Methyl (*E*)-2-((4-methoxyphenyl)diazenyl)-1-oxo-2,3-dihydro-1*H*-indene-2-carboxylate (5b).

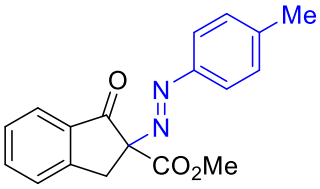
Compound **5b** was prepared in 87% yield (85 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 10/1); Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.81 (d, *J* = 7.7 Hz, 1H), 7.75-7.72 (m, 2H), 7.66-7.63 (m, 1H), 7.52 (d, *J* = 7.7 Hz, 1H), 7.43-7.40 (m, 1H), 6.93-6.90 (m, 2H), 3.94-3.83 (m, 8H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 197.1, 169.3, 162.6, 152.4, 145.8, 135.9, 134.7, 128.2, 126.6, 125.3, 125.0, 114.1, 87.2, 55.7, 53.3, 36.1; HRMS (ESI) m/z $[M+Na]^+$ Calcd for $C_{18}H_{16}N_2NaO_4$: 347.1002, Found 347.1007.



5c

Methyl (*E*)-2-((4-(dimethylamino)phenyl)diazenyl)-1-oxo-2,3-dihydro-1*H*-indene-2-carboxylate (5c).

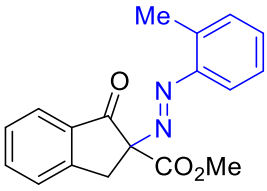
Compound **5c** was prepared in 67% yield (68 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 3/1); Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.10 (d, *J* = 7.8 Hz, 1H), 7.63 (d, *J* = 9.2 Hz, 2H), 7.50-7.47 (m, 1H), 7.36-7.33 (m, 1H), 7.23 (d, *J* = 7.5 Hz, 1H), 6.61 (d, *J* = 9.2 Hz, 2H), 3.85-3.80 (m, 5H), 3.04 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 196.1, 167.4, 153.3, 141.3, 135.1, 134.2, 129.9, 128.2, 127.9, 125.8, 125.2, 111.2, 100.5, 53.4, 40.3, 33.4; HRMS (ESI) m/z $[M+Na]^+$ Calcd for $C_{19}H_{19}N_3NaO_3$: 360.1319, Found 360.1327.



5d

Methyl (*E*)-1-oxo-2-(p-tolyldiazenyl)-2,3-dihydro-1*H*-indene-2-carboxylate (5d).

Compound **5d** was prepared in 82% yield (76 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 8/1); Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.81 (d, *J* = 7.7 Hz, 1H), 7.66-7.63 (m, 3H), 7.52 (d, *J* = 7.8 Hz, 1H), 7.43-7.40 (m, 1H), 7.22 (d, *J* = 8.2 Hz, 2H), 3.94-3.84 (m, 5H), 2.38 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 196.8, 169.2, 152.3, 149.6, 142.4, 135.9, 134.6, 129.7, 128.2, 126.6, 125.3, 123.1, 87.6, 53.3, 36.0, 21.6; HRMS (ESI) m/z $[M+Na]^+$ Calcd for $C_{18}H_{16}N_2NaO_3$: 331.1053, Found 331.1056.

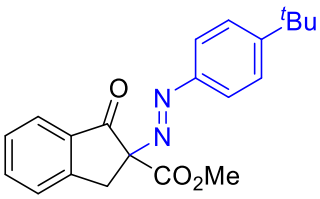


5e

Methyl (*E*)-1-oxo-2-(o-tolyldiazenyl)-2,3-dihydro-1*H*-indene-2-carboxylate (5e).

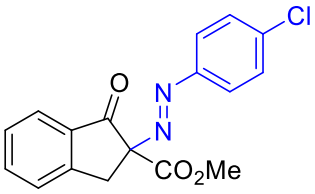
Compound **5e** was prepared in 81% yield (75 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 8/1); Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.81 (d, *J* = 7.7 Hz, 1H), 7.67-7.64 (m, 1H), 7.53 (d, *J* = 7.8 Hz, 1H), 7.44-7.40 (m, 2H), 7.34-7.31 (m, 1H), 7.24 (d, *J* = 7.7 Hz, 1H), 7.20-7.17 (m, 1H), 3.89-3.87 (m, 5H), 2.44 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 196.7,

169.1, 152.0, 149.6, 137.8, 135.9, 134.6, 131.6, 131.2, 128.2, 126.5, 126.5, 125.2, 115.9, 88.3, 53.3, 36.2, 17.2; HRMS (ESI) m/z $[M+Na]^+$ Calcd for $C_{18}H_{16}N_2NaO_3$: 331.1053, Found 331.1054.



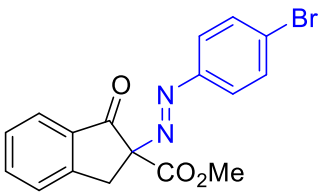
5f

Methyl (*E*)-2-((4-(*tert*-butyl)phenyl)diazenyl)-1-oxo-2,3-dihydro-1*H*-indene-2-carboxylate (5f). Compound **5f** was prepared in 84% yield (88 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 8/1); Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.81 (d, *J* = 7.7 Hz, 1H), 7.68-7.63 (m, 3H), 7.52 (d, *J* = 7.7 Hz, 1H), 7.46-7.40 (m, 3H), 3.95-3.84 (m, 5H), 1.32 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 196.8, 169.2, 155.4, 152.3, 149.4, 135.9, 128.2, 126.6, 126.0, 125.3, 122.8, 87.6, 53.3, 36.0, 35.1, 31.3; HRMS (ESI) m/z $[M+Na]^+$ Calcd for $C_{21}H_{22}N_2NaO_3$: 373.1523, Found 373.1530.



5g

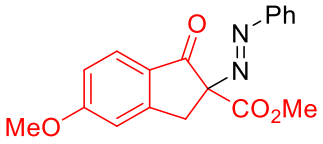
Methyl (*E*)-2-((4-chlorophenyl)diazenyl)-1-oxo-2,3-dihydro-1*H*-indene-2-carboxylate (5g). Compound **5g** was prepared in 80% yield (79 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 12/1); Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.82 (d, *J* = 7.7 Hz, 1H), 7.70-7.65 (m, 3H), 7.53 (d, *J* = 7.7 Hz, 1H), 7.45-7.40 (m, 3H), 3.94-3.85 (m, 5H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 196.3, 168.9, 152.2, 149.8, 137.9, 136.1, 134.4, 129.3, 128.3, 126.6, 125.4, 124.3, 87.8, 53.4, 36.1; HRMS (ESI) m/z $[M+Na]^+$ Calcd for $C_{17}H_{13}ClN_2NaO_3$: 351.0507, Found 351.0512.



5h

Methyl (*E*)-2-((4-bromophenyl)diazenyl)-1-oxo-2,3-dihydro-1*H*-indene-2-carboxylate (5h).

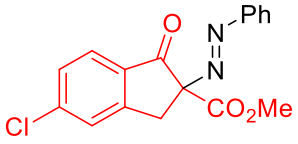
Compound **5h** was prepared in 82% yield (92 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 12/1); Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.81 (d, *J* = 7.8 Hz, 1H), 7.68-7.65 (m, 1H), 7.62-7.56 (m, 4H), 7.53 (d, *J* = 7.7 Hz, 1H), 7.45-7.42 (m, 1H), 3.94-3.85 (m, 5H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 196.3, 168.9, 152.2, 150.2, 136.1, 134.4, 132.4, 128.4, 126.6, 126.4, 125.4, 124.6, 87.9, 53.4, 36.1; HRMS (ESI) m/z $[M+Na]^+$ Calcd for $C_{17}H_{13}BrN_2NaO_3$: 395.0002, Found 395.0004.



5i

Methyl (*E*)-5-methoxy-1-oxo-2-(phenyldiazenyl)-2,3-dihydro-1*H*-indene-2-carboxylate (5i).

Compound **5i** was prepared in 78% yield (76 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 10/1); Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.75-7.72 (m, 3H), 7.44-7.43 (m, 3H), 6.95-6.94 (m, 2H), 3.91 (s, 3H), 3.87-3.78 (m, 5H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 194.5, 169.2, 166.4, 155.5, 151.6, 131.6, 129.0, 127.6, 127.2, 123.0, 116.4, 109.7, 88.2, 55.9, 53.3, 35.8; HRMS (ESI) m/z $[M+Na]^+$ Calcd for $C_{18}H_{16}N_2NaO_4$: 347.1002, Found 347.1008.

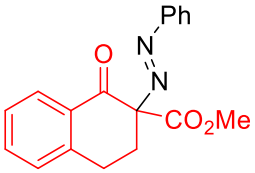


5j

Methyl (*E*)-5-chloro-1-oxo-2-(phenyldiazenyl)-2,3-dihydro-1*H*-indene-2-carboxylate (5j).

Compound **5j** was prepared in 70% yield (69 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 10/1); Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.75-7.72 (m, 3H), 7.53 (s, 1H), 7.45-7.40 (m, 4H), 3.93-3.82 (m, 5H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 195.2, 168.7,

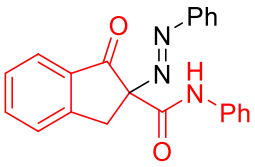
153.7, 151.4, 142.7, 132.9, 131.9, 129.2, 129.1, 126.9, 126.4, 123.1, 87.8, 53.5, 36.6; HRMS (ESI) m/z $[M+Na]^+$ Calcd for $C_{17}H_{13}ClN_2NaO_3$: 351.0507, Found 351.0512.



5k

Methyl (*E*)-1-oxo-2-(phenyldiazenyl)-1,2,3,4-tetrahydronaphthalene-2-carboxylate (5k).[32]

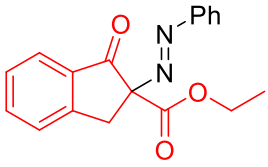
Compound **5k** was prepared in 70% yield (65 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 12/1); Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.10 (d, *J* = 7.9 Hz, 1H), 7.71-7.69 (m, 2H), 7.52-7.43 (m, 4H), 7.36-7.33 (m, 1H), 7.23 (d, *J* = 7.7 Hz, 1H), 3.80 (s, 3H), 3.13-3.05 (m, 2H), 2.99-2.93 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 191.6, 168.7, 151.6, 142.9, 134.0, 131.9, 131.6, 129.1, 128.9, 128.2, 127.2, 122.9, 85.2, 53.0, 31.1, 25.1; HRMS (ESI) m/z $[M+Na]^+$ Calcd for $C_{18}H_{16}N_2NaO_3$: 331.1053, Found 331.1056. Analytical data for **5k** was consistent with that previously reported.[32]



5l

(*E*)-1-oxo-*N*-phenyl-2-(phenyldiazenyl)-2,3-dihydro-1*H*-indene-2-carboxamide (5l).

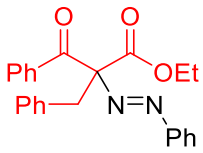
Compound **5l** was prepared in 43% yield (46 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 5/1); Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.43 (s, 1H), 7.77-7.72 (m, 3H), 7.69-7.65 (m, 3H), 7.60 (d, *J* = 7.8 Hz, 1H), 7.48-7.46 (m, 3H), 7.42-7.39 (m, 1H), 7.37-7.34 (m, 2H), 7.16-7.13 (m, 1H), 4.20 (d, *J* = 17.6 Hz, 1H), 3.97 (d, *J* = 17.6 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 198.2, 164.2, 154.1, 151.3, 137.7, 136.4, 133.4, 132.1, 129.3, 129.2, 128.1, 126.7, 125.5, 124.9, 123.0, 120.3, 90.0, 33.4; HRMS (ESI) m/z $[M+Na]^+$ Calcd for $C_{22}H_{17}N_3NaO_2$: 378.1213, Found 378.1206.



5m

Ethyl (*E*)-1-oxo-2-(phenyldiazenyl)-2,3-dihydro-1*H*-indene-2-carboxylate (5m).

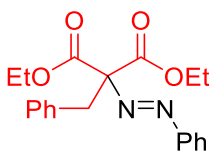
Compound **5m** was prepared in 80% yield (74 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 10/1); Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.82 (d, *J* = 7.7 Hz, 1H), 7.74-7.72 (m, 2H), 7.67-7.64 (m, 1H), 7.53 (d, *J* = 7.7 Hz, 1H), 7.45-7.41 (m, 4H), 4.33 (q, *J* = 7.1 Hz, 2H), 3.94 (d, *J* = 17.6 Hz, 1H), 3.86 (d, *J* = 17.5 Hz, 1H), 1.29 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 196.7, 168.5, 152.3, 151.6, 135.9, 134.7, 131.7, 129.1, 128.2, 126.6, 125.3, 123.0, 87.7, 62.4, 36.0, 14.3; HRMS (ESI) m/z $[M+Na]^+$ Calcd for $C_{18}H_{16}N_2NaO_3$: 331.1053, Found 331.1055.



5n

Ethyl (*E*)-2-benzyl-3-oxo-3-phenyl-2-(phenyldiazenyl)propanoate (5n).

Compound **5n** was prepared in 72% yield (83 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 15/1); Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.74-7.69 (m, 4H), 7.46-7.42 (m, 4H), 7.36-7.33 (m, 2H), 7.21-7.19 (m, 3H), 7.14-7.12 (m, 2H), 4.16-4.03 (m, 2H), 3.79 (d, *J* = 14.0 Hz, 1H), 3.65 (d, *J* = 14.0 Hz, 1H), 0.98 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 192.9, 169.6, 151.9, 135.3, 134.7, 132.9, 131.9, 130.7, 129.7, 129.2, 128.5, 128.2, 127.1, 122.8, 88.9, 61.7, 42.7, 13.8; HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{24}H_{23}N_2O_3$: 387.1703, Found 387.1706.



5o

Diethyl (*E*)-2-benzyl-2-(phenyldiazenyl)malonate (5o).

Compound **5o** was prepared in 59% yield (63 mg) according to the general procedure. R_f = 0.2 (petroleum ether/ethyl acetate = 15/1); Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.75-7.73 (m, 2H), 7.49-7.47 (m, 3H), 7.25-7.20 (m, 5H), 4.28-4.20 (m, 4H), 3.58 (s, 2H), 1.22 (t, *J* = 7.2 Hz, 6H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 168.0, 151.6, 135.0, 131.8, 130.8, 129.2, 128.2, 127.1, 123.0, 86.1, 61.9, 41.7, 14.2; HRMS (ESI) m/z $[M+Na]^+$ Calcd for $C_{20}H_{22}N_2NaO_4$: 377.1472, Found 377.1477.

Calculated energies and details of optimized structures

Table S5 Calculated thermodynamic corrections to Gibbs free energy (ΔG_{cor}), solution-phase single-point energies (ΔE_{sol}), solution-phase Gibbs free energies (ΔG_{sol}) and imaginary frequencies (ImF, in cm^{-1}). All ΔG_{sol} refer to 1 M and 298.15 K except the ΔG_{sol} of CO_2 refers to $9.59*10^{-3}$ M and 298.15 K (in Hartree).

species	ΔG_{cor}	ΔE_{sol}	ΔG_{sol}	ImF
Energies in DMF				
4a	0.152166	-650.8167188	-650.6615409	N.A.
HCO_3^-	0.001223	-264.542819	-264.5385841	N.A.
CO_2	-0.008939	-188.5768283	-188.5827554	N.A.
H_2O	0.003561	-76.42929907	-76.42272616	N.A.
int1	0.138851	-650.3341203	-650.1922574	N.A.
1a	0.111528	-929.5043847	-929.3898448	N.A.
TS1	0.277695	-1579.854556	-1579.573849	-252.66
int2	0.279864	-1579.883882	-1579.601006	N.A.
TS2	0.274027	-1579.840232	-1579.563193	-162.20
$MeSO_2^-$	0.018047	-588.6125196	-588.5914607	N.A.
int3	0.235379	-991.2327021	-990.9943112	N.A.
TS3	0.235035	-991.2086747	-990.9706278	-246.76
int4	0.236746	-991.2236264	-990.9838685	N.A.
TS4	0.23499	-991.2098408	-990.9718389	-377.35
int5	0.236967	-991.2470167	-991.0070378	N.A.
TS5	0.234463	-991.2027097	-990.9652348	-372.93
int6	0.234264	-991.2430347	-991.0057588	N.A.
TS6	0.234305	-991.2092943	-990.9719774	-419.64
5a	0.232644	-991.2704892	-991.0348333	N.A.
TS7	0.279805	-1579.848858	-1579.566041	-193.21

int7	0.277783	-1579.87434	-1579.593546	N.A.
TS8	0.275879	-1579.868556	-1579.589666	-337.82
Energies in ethanol				
2a	0.077173	-307.4378147	-307.3576298	N.A.
CO_3^{2-}	-0.010966	-264.0626113	-264.0705654	N.A.
HCO_3^-	0.001244	-264.5574293	-264.5531734	N.A.
1a	0.110649	-929.5049772	-929.3913163	N.A.
int8	0.06392	-306.9572968	-306.8903649	N.A.
TS9	0.200451	-1236.462463	-1236.259	-391.38
int9	0.19947	-1236.47255	-1236.270068	N.A.
TS10	0.197077	-1236.460716	-1236.260627	-303.41
TS10b	0.15297	-647.7757022	-647.6197203	-1899.30
int10	0.192543	-1236.500366	-1236.304811	N.A.
TS11	0.19095	-1236.49538	-1236.301418	-614.12
$MeSO_2H$	0.029224	-589.0880479	-589.055812	N.A.
int11	0.145705	-647.4343557	-647.2856388	N.A.
$MeSO_2^-$	0.018272	-588.6290134	-588.6077295	N.A.
3a	0.157722	-647.905991	-647.7452571	N.A.
TS12	0.200862	-1236.46604	-1236.262166	-377.88
int12	0.200891	-1236.490162	-1236.286259	N.A.
TS13	0.195766	-1236.4476	-1236.248822	-1755.65
int13	0.201423	-1236.522237	-1236.317802	N.A.
TS14	0.199124	-1236.49308	-1236.290944	-163.64
int14	0.160304	-647.8657077	-647.7023918	N.A.
TS15	0.157724	-647.8052703	-647.6445344	-642.01

TS16	0.198234	-1236.45099	-1236.249745	-226.21
int15	0.157796	-647.8285187	-647.6677108	N.A.
TS17	0.153689	-647.7294266	-647.5727257	-415.66
int16	0.15967	-647.8528325	-647.6901505	N.A.
TS18	0.157972	-647.8136869	-647.652703	-326.39
int17	0.159613	-647.8803507	-647.7177258	N.A.
int18	0.213642	-1236.99956	-1236.782906	N.A.
int19	0.172718	-648.3221448	-648.3191329	N.A.
TS19	0.171034	-647.7254833	-647.5514374	-726.45
int20	0.171867	-648.277722	-648.1028431	N.A.
TS20	0.15297	-647.7757022	-647.6197203	-1899.30
int21	0.157798	-647.8285182	-647.6677083	N.A.
TS21	0.154346	-647.7277093	-647.5703514	-413.14
int22	0.156013	-647.8644779	-647.705453	N.A.

Cartesian coordinates of calculated stationary points (in angstrom)

4a

C	1.45326400	-0.81286100	-0.22519100
C	1.31194400	0.56654400	-0.09180300
C	2.38754400	1.39986500	0.21829500
C	3.63665400	0.81637300	0.38487900
C	3.79011000	-0.57100800	0.24585400
C	2.70786400	-1.39502800	-0.05663300
C	0.13420000	-1.48781700	-0.52497100
C	0.86052000	-0.33278900	-0.72442800
C	0.09723400	0.95106900	-0.31077400
H	2.24190800	2.47153800	0.31919400
H	4.49946600	1.43061900	0.62181300
H	4.77402500	-1.01121200	0.37862600
H	2.84225900	-2.46820500	-0.15669500
H	0.19891200	-2.12755600	-1.40888900
O	0.58911700	2.05021300	-0.19270600
H	0.17279400	-2.11413200	0.31865600
H	1.14233600	-0.20583700	-1.77396800
C	2.11467100	-0.44071500	0.11164500
O	2.17652700	-0.98693700	1.18903900
O	3.14293400	0.18285300	-0.46417300
C	4.35044600	0.20594900	0.30493900
H	4.69295800	-0.81063600	0.50932600
H	5.08141800	0.73546800	-0.30415100
H	4.19069600	0.73343500	1.24793000

HCO_3^- in DMF

C	0.00000000	0.15636600	0.00000000
O	1.21716600	0.43479900	0.00000000
O	-0.28637800	-1.22892000	0.00000000
O	-1.00456300	0.88204600	0.00000000
H	0.59020700	-1.64159500	0.00000000

CO_2

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16279700
O	0.00000000	0.00000000	-1.16279700

H_2O

O	0.00000000	0.00000000	0.11976300
H	0.00000000	0.76112300	-0.47905200
H	0.00000000	-0.76112300	-0.47905200

Int1

C	1.31143700	-0.86366600	-0.00032300
C	1.43942100	0.52642500	-0.00012800
C	2.68799500	1.13875900	0.00032400
C	3.82697400	0.33310300	0.00060000

C	3.70470300	-1.06078400	0.00038400
C	2.44609400	-1.66923300	-0.00009300
C	-0.15169200	-1.24207700	-0.00065900
C	-0.85091900	0.10054500	-0.00057400
C	0.07882100	1.17751100	-0.00033100
H	2.75965300	2.22361600	0.00041600
H	4.81525200	0.78456900	0.00100900
H	4.59952700	-1.67698200	0.00062000
H	2.36175700	-2.75367800	-0.00026900
H	-0.39207600	-1.86294100	0.87512800
O	-0.06531100	2.41232000	-0.00020800
C	-2.26698700	0.24233500	-0.00031300
O	-2.89399300	-0.99064400	-0.00047500
O	-2.94348000	1.26605600	0.00012900
C	-4.30834300	-0.93820100	0.00107500
H	-4.65281000	-1.97423100	0.00151800
H	-4.69015000	-0.42380200	0.88858300
H	-4.69215200	-0.42397800	-0.88566200
H	-0.39174900	-1.86272500	-0.87667900

1a in DMF

N	0.03597000	-1.17231400	1.23417700
N	1.22257100	-0.97560400	1.03865600
S	1.86153600	0.03403800	-0.36146500
C	-1.05900600	-0.51720900	0.57563700
C	-1.98742500	-1.31489400	-0.08888500
C	-1.26891400	0.84711100	0.76750400
C	-3.11264100	-0.71233400	-0.64223100
H	-1.81253100	-2.38187800	-0.18341400
C	-2.41620300	1.42819500	0.23690000
H	-0.55828500	1.43411900	1.34137800
C	-3.33016300	0.65569700	-0.47825600
H	-3.82933600	-1.31708500	-1.18856100
H	-2.59340700	2.48894900	0.38310400
H	-4.21952000	1.11684600	-0.89560500
O	0.85742400	0.45546800	-1.33260900
O	2.96622500	-0.81052400	-0.80256600
C	2.49792100	1.42918400	0.53202200
H	3.10955200	1.05973400	1.35734900
H	3.11298400	2.00085400	-0.16886300
H	1.66555400	2.03523100	0.89348600

TS1

C	1.46393600	-1.31805200	-1.23545500
C	1.97951500	-1.34737900	0.06074600
C	3.34642500	-1.33121500	0.31141400
C	4.21422200	-1.27707600	-0.77926000
C	3.70611000	-1.24658300	-2.08284300
C	2.32922700	-1.26776000	-2.32297400
C	-0.05022800	-1.29728200	-1.19587300
C	-0.35468600	-1.09267900	0.26083400
C	0.85650800	-1.31551900	1.04467500

H	3.71713100	-1.34439500	1.33304700
H	5.28842300	-1.25290700	-0.62145100
H	4.39475900	-1.20157400	-2.92182600
H	1.94826500	-1.23548400	-3.34055200
H	-0.48463000	-2.22335200	-1.59013500
O	0.98521200	-1.44270900	2.26008300
C	-1.63912700	-1.49741100	0.85654700
O	-2.25158100	-2.46330800	0.13927600
O	-2.10237300	-1.08112200	1.90027600
C	-3.56670500	-2.78649000	0.57107700
H	-3.95088600	-3.51325600	-0.14572500
H	-3.55644600	-3.22316000	1.57362100
H	-4.19415600	-1.89207400	0.57135200
H	-0.46137700	-0.47066700	-1.80177200
N	-0.59756900	1.04110300	0.34001600
N	-1.07041800	1.45919800	-0.80570700
S	-2.73822000	1.31329300	-0.84730200
C	0.75980900	1.46387100	0.51212900
C	1.25005200	1.48051100	1.82088200
C	1.57680600	1.88588400	-0.54373900
C	2.55524700	1.89610900	2.06960000
H	0.59956400	1.15110400	2.62334400
C	2.88114200	2.29627400	-0.28766900
H	1.18342100	1.88422600	-1.55434700
C	3.37631700	2.30141100	1.01779000
H	2.93018300	1.90648000	3.08877700
H	3.51473800	2.61441600	-1.11065100
H	4.39436000	2.62425900	1.21390200
O	-3.15146000	-0.08435000	-1.03735200
O	-3.19065800	2.28278700	-1.84919300
C	-3.32174800	1.82313600	0.75835400
H	-2.97602200	2.83894800	0.95805600
H	-4.41318700	1.79275900	0.71978800
H	-2.93676100	1.12100500	1.49910900

Int2

C	2.70636200	-0.37087400	-0.38720100
C	2.40904000	-0.74846000	0.92022500
C	3.38565300	-0.82366700	1.91319200
C	4.69418200	-0.50610200	1.57059900
C	5.00364500	-0.12420600	0.25730300
C	4.02055800	-0.05517800	-0.72830900
C	1.48563400	-0.37128000	-1.27299300
C	0.30864100	-0.77486800	-0.34570300
C	0.96360500	-1.02847200	1.04343400
H	3.11892300	-1.12091100	2.92351900
H	5.48141600	-0.55095300	2.31668600
H	6.03071800	0.12292100	0.00444600
H	4.27656300	0.24188400	-1.74152900
H	1.61162800	-1.08109700	-2.09700700
O	0.37053900	-1.35994700	2.04463800
C	-0.31637200	-2.06781800	-0.86388200

O	-0.76493200	-1.92247700	-2.11705300
O	-0.35815100	-3.11261500	-0.26073200
C	-1.38337400	-3.08263600	-2.68141000
H	-1.71461500	-2.78805100	-3.67619400
H	-0.66660400	-3.90401000	-2.74834500
H	-2.23735100	-3.39396700	-2.07406000
H	1.28693200	0.61392200	-1.70411000
N	-0.68192800	0.32169800	-0.23813600
N	-0.00781800	1.45814200	0.33694900
S	-0.18971900	2.73185300	-0.62412700
C	-1.88813200	-0.01082100	0.46905000
C	-2.88415400	-0.74612400	-0.18819600
C	-2.14246000	0.45054200	1.76689400
C	-4.08287100	-1.05218000	0.45351000
H	-2.72984600	-1.04704700	-1.21868400
C	-3.34625000	0.15248400	2.39775500
H	-1.38535300	1.04515800	2.26216100
C	-4.32175000	-0.60766500	1.75153000
H	-4.84087800	-1.62084900	-0.07779300
H	-3.52240300	0.51502100	3.40687600
H	-5.26032200	-0.83502700	2.24768700
O	0.20973100	2.53137200	-2.03693700
O	0.45086900	3.87048200	0.05983600
C	-1.94263400	3.10641700	-0.71513500
H	-2.32123600	3.29945500	0.29062600
H	-2.07586600	3.98927400	-1.34499900
H	-2.46836200	2.25666900	-1.15695600

TS2

C	-2.19057700	0.61340500	-0.97272000
C	-2.23870700	0.42485100	0.40655000
C	-3.29939700	-0.23308700	1.02386400
C	-4.32813600	-0.71343500	0.22073000
C	-4.28447600	-0.53105300	-1.16845400
C	-3.21944400	0.13204900	-1.77745400
C	-0.94383200	1.36504100	-1.38352700
C	-0.06033300	1.35454400	-0.11676400
C	-1.03427400	1.01627500	1.03491000
H	-3.30287100	-0.37500000	2.10027100
H	-5.16719100	-1.23915900	0.66581700
H	-5.09387600	-0.91708800	-1.78125500
H	-3.19376000	0.26494800	-2.85536200
H	-1.19994700	2.39889700	-1.64484200
O	-0.83196400	1.22317200	2.20648400
C	0.61116000	2.70669900	0.06301600
O	1.71068100	2.81683800	-0.68738600
O	0.15491100	3.60991900	0.72092800
C	2.36564700	4.08632400	-0.62016600
H	3.23993700	4.00372200	-1.26438000
H	1.70426900	4.87856600	-0.97863700
H	2.67074200	4.30430200	0.40573200
H	-0.44167500	0.92918500	-2.25021500

N	1.01959700	0.30208800	-0.08990200
N	1.85450900	0.31757300	0.84961500
S	1.01567100	-1.35436100	2.26424900
C	1.10273500	-0.67946200	-1.15652600
C	0.11658900	-1.64698200	-1.34721800
C	2.24444200	-0.65972000	-1.95663500
C	0.27859500	-2.59070000	-2.36112000
H	-0.73091100	-1.67890000	-0.67293300
C	2.40019900	-1.60971200	-2.96251600
H	2.99958000	0.09996400	-1.77726100
C	1.41423900	-2.57468100	-3.16964500
H	-0.48338200	-3.35017100	-2.51052600
H	3.28839300	-1.59320900	-3.58702600
H	1.53382500	-3.31505000	-3.95483700
O	-0.29273200	-1.75617200	1.62133200
O	1.05310500	-1.51364900	3.76504000
C	2.13332900	-2.67713400	1.70373000
H	3.14084100	-2.49344700	2.08726100
H	1.75750700	-3.63023800	2.09006800
H	2.15048800	-2.69536800	0.61062100

$MeSO_2^-$ in DMF

S	-0.22132000	0.00012000	-0.38554500
O	-0.71146200	-1.26696800	0.29525300
O	-0.70809700	1.26860900	0.29515800
C	1.54153600	-0.00162500	0.12215100
H	2.04740100	0.89403700	-0.25149000
H	1.55356700	-0.00297700	1.21779100
H	2.04740300	-0.89635100	-0.25378200

Int3

C	-1.69963800	-0.78577700	-0.85470000
C	-1.92915800	-0.78797200	0.52160200
C	-2.95088000	-1.53913600	1.10428800
C	-3.76440400	-2.29043100	0.26666100
C	-3.54457100	-2.28846200	-1.11845600
C	-2.51512400	-1.54348500	-1.69060700
C	-0.51803100	0.07795400	-1.23916900
C	-0.14022000	0.79309000	0.07428900
C	-0.93504000	0.06779400	1.19506000
H	-3.10127000	-1.52535900	2.17962700
H	-4.57444000	-2.88217500	0.68049900
H	-4.19048500	-2.88234100	-1.75822100
H	-2.35366100	-1.55566100	-2.76433900
H	-0.77204500	0.79053100	-2.02746400
O	-0.71860100	0.19852700	2.37480300
C	-0.58028300	2.26083900	0.04808300
O	0.01394500	2.90907000	-0.94884100
O	-1.39147400	2.74258200	0.79758400
C	-0.27514800	4.31066700	-1.02300300
H	0.29126100	4.68476800	-1.87409400
H	-1.34393100	4.47195700	-1.17686800

H	0.04539100	4.80641100	-0.10395700
H	0.30821000	-0.53348900	-1.61449200
N	1.32948500	0.83613600	0.46311600
N	1.78518600	1.80072800	1.04181100
C	2.14868000	-0.35206700	0.16291400
C	1.66697400	-1.64257900	0.35316300
C	3.45268000	-0.11968800	-0.26121200
C	2.51779000	-2.72074200	0.11247400
H	0.65315100	-1.82930600	0.69395100
C	4.28889400	-1.20251300	-0.50944800
H	3.79354000	0.90281900	-0.38692800
C	3.82326700	-2.50405100	-0.32127000
H	2.15327800	-3.73088300	0.26817900
H	5.30466100	-1.02914800	-0.85011300
H	4.47796000	-3.34825300	-0.51264700

TS3

C	1.95672300	-0.59936700	0.92678000
C	2.18690200	-0.17929400	-0.38746400
C	3.31109600	-0.61445400	-1.08938600
C	4.19295700	-1.50588500	-0.48531600
C	3.95061900	-1.95320900	0.81538200
C	2.83553300	-1.50423100	1.52011200
C	0.74328500	0.00488400	1.61624900
C	0.01292200	0.75576600	0.55141400
C	1.21852800	0.79370400	-1.04382500
H	3.48367800	-0.25847500	-2.10109000
H	5.06676600	-1.85499400	-1.02673000
H	4.64091300	-2.64714900	1.28557900
H	2.65892500	-1.83929600	2.53892100
H	1.04329800	0.71061500	2.39801500
O	1.55652500	1.78752900	-1.67120900
C	-0.41443300	2.13657000	0.66015100
O	-1.30126200	2.47899700	-0.29274600
O	0.02329200	2.91475600	1.48580600
C	-1.62240300	3.86966000	-0.34833300
H	-2.33243600	3.97692400	-1.16755600
H	-2.07750100	4.19923200	0.58826400
H	-0.72584600	4.46162500	-0.54567100
H	0.13653300	-0.77631200	2.09218300
N	-0.62811100	-0.06165100	-0.44603100
N	-0.00680500	0.01960100	-1.52635000
C	-1.76927900	-0.89786900	-0.25951400
C	-2.63392100	-0.60386100	0.79273000
C	-1.98706200	-1.96443400	-1.13148000
C	-3.75569400	-1.40563900	0.97120600
H	-2.43729400	0.24029200	1.44624100
C	-3.11777800	-2.74848200	-0.94314400
H	-1.27520700	-2.17483100	-1.92260400
C	-3.99809000	-2.47094100	0.10476300
H	-4.44293600	-1.19296800	1.78284200
H	-3.30651900	-3.58530700	-1.60699600

H	-4.87583800	-3.09277800	0.24850800

Int4

C	-1.05299900	-1.23285900	-0.91633600
C	-1.46067900	-0.99612800	0.42232300
C	-2.26819900	-1.96541200	1.03964400
C	-2.63814200	-3.13820500	0.39541600
C	-2.21398100	-3.37069200	-0.91053200
C	-1.43010300	-2.41956700	-1.55088300
C	-0.21834000	-0.23796300	-1.73132400
C	-0.02337000	0.88933400	-0.78180800
C	-1.14878100	0.17327800	1.39559700
H	-2.60108800	-1.78045500	2.05475100
H	-3.25538200	-3.86604100	0.91255200
H	-2.49980900	-4.27939300	-1.43146000
H	-1.11107200	-2.58021100	-2.57755200
H	-0.74829000	0.07916600	-2.63051500
O	-1.97634900	0.46830900	2.23885300
C	-1.08916200	1.92885400	-0.72313800
O	-0.78522600	2.96485700	0.05790500
O	-2.07888300	1.86665800	-1.42054200
C	-1.78903500	3.98342600	0.13088600
H	-1.40959500	4.72026000	0.83702400
H	-1.94231000	4.44088400	-0.84888500
H	-2.72961600	3.56143800	0.49192200
H	0.72412400	-0.70687600	-2.02771400
N	0.72890000	0.63488700	0.29350300
N	0.14491200	0.70629100	1.47956700
C	2.07143800	0.15924100	0.20895500
C	2.90506000	0.65663100	-0.79240700
C	2.50991600	-0.78465800	1.13579700
C	4.20763800	0.17860900	-0.87363200
H	2.53809000	1.41926800	-1.47282100
C	3.82048300	-1.24077500	1.05077500
H	1.82342800	-1.15760200	1.88809100
C	4.66519300	-0.76447200	0.04754800
H	4.87142200	0.55627300	-1.64416900
H	4.17914100	-1.97833100	1.76100800
H	5.68631000	-1.12706400	-0.01473800

TS4

C	0.73022000	-1.34093800	-1.00365200
C	0.75984600	-1.60940800	0.37644500
C	1.88200700	-2.24618800	0.92126000
C	2.96915400	-2.58464100	0.12575600
C	2.94181700	-2.30092300	-1.23915900
C	1.82741300	-1.68329600	-1.79577500
C	-0.49028600	-0.72359900	-1.64930000
C	-1.25448100	0.01349300	-0.60623000
C	-0.33754500	-1.28739200	1.37925600
H	1.88785000	-2.46548600	1.98403500
H	3.83507500	-3.06682600	0.56807700

H	3.78669400	-2.56056900	-1.86952700
H	1.79660600	-1.46593700	-2.85988100
H	-1.14305000	-1.48292900	-2.08982700
O	-0.55998000	-2.06435500	2.29310000
C	-2.74594400	-0.18346800	-0.50525800
O	-3.36693900	0.86560200	0.01404700
O	-3.28491100	-1.17725800	-0.93378400
C	-4.79011300	0.72944000	0.12980600
H	-5.13742400	1.65765900	0.57976400
H	-5.23816200	0.59293300	-0.85673400
H	-5.03811400	-0.12022900	0.76924700
H	-0.19491100	-0.04062300	-2.45655900
N	-0.64781300	0.76495600	0.30883500
N	-1.00810600	-0.05379000	1.39902700
C	0.47381800	1.60162200	0.23317500
C	0.62413000	2.42850100	-0.88438500
C	1.39494100	1.62805500	1.28196300
C	1.72634200	3.27148800	-0.95614100
H	-0.12544000	2.41866800	-1.67077000
C	2.47634500	2.50080100	1.20504800
H	1.26667500	0.96750200	2.13342300
C	2.65204200	3.31523800	0.08763200
H	1.85232900	3.91075300	-1.82418200
H	3.19444800	2.52909100	2.01852500
H	3.50526400	3.98321300	0.02982000

Int5

C	-1.77921700	-0.38031600	-0.74014000
C	-1.83364100	-1.06803000	0.48113100
C	-2.91052500	-1.90000000	0.79426800
C	-3.96153600	-2.03019100	-0.10445400
C	-3.92107100	-1.34041200	-1.31810200
C	-2.83710000	-0.52552900	-1.63641400
C	-0.55621500	0.44560200	-1.08463500
C	0.03572600	1.05585000	0.17129100
C	-0.68457400	-0.95492200	1.41696800
H	-2.91313000	-2.42829500	1.74284400
H	-4.80915700	-2.66393500	0.13495100
H	-4.74084000	-1.43946400	-2.02303600
H	-2.80917200	0.00017300	-2.58673800
H	-0.82246700	1.23687600	-1.78591600
O	-0.35033200	-1.80338700	2.21410800
C	-0.11806400	2.55626600	0.38481400
O	-0.08769400	3.21184700	-0.77309600
O	-0.20613500	3.07613800	1.46699200
C	-0.16632400	4.64085300	-0.67144600
H	-0.14385300	5.01081700	-1.69477300
H	-1.09537800	4.93374400	-0.17864500
H	0.68605800	5.02454500	-0.10738300
H	0.18728600	-0.18580100	-1.58595700
N	1.27445600	0.58200600	0.82616700
N	-0.03993100	0.30105900	1.37786100

C	2.08312400	-0.43346700	0.20742100
C	3.41804400	-0.03955100	0.06268700
C	1.68532400	-1.69818100	-0.23829500
C	4.34413000	-0.88633600	-0.53374400
H	3.71081300	0.93981000	0.42775100
C	2.62544900	-2.54678800	-0.82359800
H	0.66719200	-2.05452000	-0.14671500
C	3.94978700	-2.14845400	-0.97625300
H	5.37493500	-0.56402100	-0.64216300
H	2.30827100	-3.52793700	-1.16250500
H	4.67117000	-2.81860100	-1.43295000

TS5

C	-2.08878900	0.27351600	-0.75667800
C	-2.30333100	-0.37303800	0.47318400
C	-3.55998400	-0.88327400	0.80272900
C	-4.61884200	-0.74077100	-0.08432300
C	-4.41244300	-0.10174900	-1.30784500
C	-3.15677300	0.39856600	-1.64322600
C	-0.72417100	0.83015000	-1.12636100
C	0.05772400	1.05754800	0.10551300
C	-1.16336700	-0.62410300	1.39548800
H	-3.68909700	-1.38957000	1.75420300
H	-5.59972600	-1.12745200	0.17153500
H	-5.23623800	0.01048500	-2.00585900
H	-3.00289200	0.89712100	-2.59577600
H	-0.80659800	1.73976800	-1.72521100
O	-1.11797700	-1.47075800	2.25970300
C	0.88843800	2.28567000	0.34304100
O	1.52936500	2.61678600	-0.77490200
O	0.90985500	2.90564900	1.37692300
C	2.31732800	3.81428700	-0.69943600
H	2.74515000	3.94813200	-1.69117000
H	1.68667300	4.66602300	-0.43747100
H	3.10809700	3.69712600	0.04432200
H	-0.16614500	0.08906400	-1.73577200
N	1.30630500	-0.06479300	1.32435400
N	-0.06407500	0.19031800	1.11108900
C	1.83915100	-0.99422200	0.42687500
C	3.24819600	-1.05654000	0.40627300
C	1.11620200	-1.90996900	-0.36530500
C	3.90699200	-1.98871800	-0.37918700
H	3.80080400	-0.35449800	1.02372700
C	1.79388600	-2.83350300	-1.15933200
H	0.03084100	-1.93219400	-0.35254000
C	3.18490500	-2.88297000	-1.17545400
H	4.99272800	-2.01703400	-0.37697100
H	1.21854000	-3.53205700	-1.75984400
H	3.70158300	-3.61228000	-1.79080600

Int6

C	2.67964800	0.68969500	0.23782400

C	2.72959100	-0.67328600	-0.05322800
C	3.95029400	-1.36731000	-0.04185300
C	5.11941700	-0.69354400	0.26233300
C	5.07391200	0.67385600	0.56134600
C	3.86647300	1.35804500	0.55075200
C	1.37827600	1.42312200	0.20948500
C	0.20927300	0.62187500	-0.26554400
C	1.51569700	-1.44957600	-0.33728200
H	3.95776800	-2.42773800	-0.26982100
H	6.06637700	-1.22272000	0.27123800
H	5.98997400	1.20505200	0.80078500
H	3.83331300	2.41969700	0.77884700
H	1.47697300	2.31165000	-0.42443800
O	1.48424700	-2.62390300	-0.56165900
C	-0.98506900	1.36810600	-0.72893500
O	-1.11568300	2.51710200	-0.05802800
O	-1.71081100	1.02685800	-1.63498900
C	-2.20626300	3.34513200	-0.47763200
H	-2.17324100	4.22504800	0.16278900
H	-2.08765900	3.63285000	-1.52434100
H	-3.15205600	2.81378500	-0.34830200
H	1.15544300	1.80990300	1.21593400
N	-0.81003700	-1.52380000	-0.46187900
N	0.20430000	-0.70815300	-0.31832900
C	-2.05750400	-1.14730900	0.03702000
C	-3.17676600	-1.69974600	-0.60272400
C	-2.26425900	-0.38301800	1.20415500
C	-4.46022200	-1.49272300	-0.10597700
H	-3.01599700	-2.29348100	-1.49763200
C	-3.54805400	-0.19423900	1.69973700
H	-1.42080600	0.05082200	1.73487700
C	-4.65802000	-0.73663600	1.04703500
H	-5.30952500	-1.92725300	-0.62547900
H	-3.68298500	0.38403900	2.60951600
H	-5.65798800	-0.57309300	1.43582300

TS6

C	2.24931100	-1.13256400	-0.56624800
C	1.30716300	-1.44407900	0.40646600
C	1.23555500	-2.70533200	0.99127400
C	2.12598900	-3.68438700	0.55787500
C	3.06251800	-3.38965900	-0.43630600
C	3.12922300	-2.11666400	-1.00402100
C	2.22655500	0.30968000	-1.00951100
C	1.03931100	0.99511600	-0.37016300
C	0.39074600	-0.34025200	0.77849000
H	0.49381900	-2.91154100	1.75712800
H	2.08950600	-4.67927700	0.98985400
H	3.75374200	-4.15905900	-0.76644800
H	3.87001700	-1.89051000	-1.76563900
H	2.16909700	0.38473000	-2.10196700
O	-0.27110300	-0.19201600	1.77498900

C	1.08648200	2.40544600	0.09143200
O	2.31334000	2.92537900	-0.05769600
O	0.17131700	2.99230700	0.62232800
C	2.48216600	4.24128900	0.47914600
H	3.51686700	4.51275300	0.27553900
H	1.80193500	4.94227100	-0.00943000
H	2.29352200	4.24055600	1.55502900
H	3.14070700	0.81848400	-0.69599600
N	-1.27533300	1.00627500	-0.71842000
N	-0.19318900	0.37690300	-0.56533500
C	-2.44083100	0.26787000	-0.45677900
C	-3.63305900	0.99856400	-0.56042600
C	-2.48120800	-1.09412500	-0.11241800
C	-4.85358400	0.38291900	-0.31775100
H	-3.57294600	2.04895600	-0.82820200
C	-3.70871600	-1.70139000	0.12235100
H	-1.57128800	-1.68214300	-0.06232200
C	-4.89307100	-0.96873700	0.02683200
H	-5.77318400	0.95367300	-0.39717600
H	-3.74220000	-2.75494000	0.38138300
H	-5.84567000	-1.45373000	0.21611500

5a

C	-2.48199800	-0.91544200	-0.66004500
C	-2.65174000	-0.54684500	0.67339300
C	-3.81525100	-0.83810100	1.38631500
C	-4.83214800	-1.51258000	0.72337300
C	-4.67366500	-1.88064300	-0.62060500
C	-3.50500000	-1.58931500	-1.32207900
C	-1.12077500	-0.53210900	-1.19002600
C	-0.52492800	0.37056500	-0.08953200
C	-1.46053200	0.17598800	1.14763200
H	-3.91600300	-0.53475400	2.42424900
H	-5.75534600	-1.75281900	1.24078000
H	-5.48046000	-2.40411400	-1.12500600
H	-3.39654100	-1.88393600	-2.36173300
H	-1.17810100	-0.03407800	-2.16044500
O	-1.21712300	0.58617500	2.25679100
C	-0.70225800	1.84377100	-0.47388400
O	0.37884300	2.57743400	-0.24621800
O	-1.74161100	2.26837100	-0.91889100
C	0.24896600	3.97033500	-0.57090700
H	1.20659900	4.42080700	-0.31646900
H	0.03977600	4.09076000	-1.63568600
H	-0.55366700	4.42117900	0.01573000
H	-0.49053100	-1.41829000	-1.30865700
N	0.85784700	0.12649700	0.33618100
N	1.54896200	-0.40344000	-0.54300800
C	2.91120200	-0.63413200	-0.17553400
C	3.65209700	-1.39006600	-1.08272800
C	3.50222300	-0.14045600	0.99219900
C	4.98980500	-1.67330300	-0.81857000

H	3.16424600	-1.75040000	-1.98343500
C	4.83826600	-0.42156700	1.24639200
H	2.91331700	0.45685600	1.67957900
C	5.58218100	-1.18914100	0.34545400
H	5.56711500	-2.26624300	-1.52067700
H	5.30640000	-0.03986700	2.14837400
H	6.62599300	-1.40409100	0.55263300

TS7

C	-0.92262400	-1.63379700	-1.05270900
C	-1.31839000	-1.64056100	0.28305100
C	-2.64664400	-1.84886000	0.65741200
C	-3.59099500	-2.03371800	-0.34442200
C	-3.20182100	-2.01410800	-1.69372900
C	-1.87065100	-1.82158500	-2.05788400
C	0.55880600	-1.38268200	-1.17336500
C	0.96666200	-0.98084400	0.23108400
C	-0.15881300	-1.31023600	1.15525900
H	-2.92644400	-1.83683800	1.70758500
H	-4.63647200	-2.18171400	-0.09039800
H	-3.95396500	-2.15130600	-2.46559300
H	-1.58270800	-1.80768000	-3.10593800
H	0.76982800	-0.59563800	-1.90457500
O	-0.16869100	-1.30680400	2.37673700
C	2.32781200	-1.29174500	0.71410400
O	3.17394300	-1.52687900	-0.31564000
O	2.67926000	-1.36662600	1.87158700
C	4.53641400	-1.67523600	0.06169000
H	5.09870700	-1.76522800	-0.86838200
H	4.86852400	-0.79886100	0.62274400
H	4.67982900	-2.57244500	0.67038200
H	1.08731800	-2.28832900	-1.49254300
N	-0.24908100	1.31015500	-0.67089300
N	0.70692400	0.99483400	0.18593200
S	2.19180700	1.56853900	-0.47912400
C	-1.49320400	1.43463900	-0.05138400
C	-2.61457200	1.54442800	-0.89722000
C	-1.70798600	1.45913300	1.34163300
C	-3.89801800	1.64156200	-0.37518400
H	-2.44879300	1.52793300	-1.97140000
C	-2.99608100	1.55978300	1.85454800
H	-0.85732500	1.36792000	2.00735300
C	-4.10288100	1.64163100	1.00687700
H	-4.74686200	1.70888800	-1.05056800
H	-3.13994100	1.56742000	2.93212000
H	-5.10651700	1.70943300	1.41513100
O	2.39782600	1.20134500	-1.88081700
O	3.24868700	1.26099600	0.48386000
C	1.87903800	3.32162800	-0.40334000
H	1.60469100	3.58797600	0.61865800

Int7

C	-2.41797600	0.89219100	-0.86916900
C	-1.95151300	1.52350700	0.28133100
C	-2.46826100	2.74057800	0.72558200
C	-3.48114100	3.33109400	-0.01980500
C	-3.96096100	2.70187500	-1.17726200
C	-3.43941100	1.48364100	-1.60957200
C	-1.67613900	-0.39105900	-1.15238400
C	-0.73166400	-0.59805800	0.06005800
C	-0.91307900	0.69810700	0.92699500
H	-2.08461200	3.20420400	1.62974100
H	-3.90766700	4.27896200	0.29276800
H	-4.75539900	3.17439400	-1.74756200
H	-3.82125700	1.00866400	-2.50891400
H	-1.06755000	-0.27674600	-2.05515800
O	-0.34806400	0.90336100	1.97473300
C	-1.13760200	-1.73606700	0.99033700
O	-2.46880700	-1.80015200	1.09772700
O	-0.38086700	-2.42806300	1.62599400
C	-2.96357800	-2.77188100	2.02533100
H	-4.04818200	-2.67664900	2.00580100
H	-2.66530400	-3.77627300	1.71702100
H	-2.58207800	-2.56932900	3.02843800
H	-2.35112800	-1.23522400	-1.30444800
N	1.09045400	0.58883200	-0.84228200
N	0.68654800	-0.65328200	-0.26031900
S	1.12136100	-2.02657700	-1.18672700
C	2.16989500	1.10391500	-0.19986900
C	2.71372100	2.31722700	-0.71993200
C	2.82099400	0.58067600	0.95464300
C	3.80957400	2.93809600	-0.14487800
H	2.23676300	2.74595400	-1.59859800
C	3.92307200	1.21734100	1.51579800
H	2.42344700	-0.31886700	1.41072500
C	4.44230100	2.39856600	0.98295700
H	4.18410700	3.86018500	-0.58510400
H	4.38403400	0.77936400	2.39955300
H	5.30521300	2.88402800	1.42754200
O	1.81276200	-1.62720400	-2.41042000
O	-0.05383100	-2.89962000	-1.30771000
C	2.30814000	-2.83402000	-0.13918500
H	1.82198700	-3.05010800	0.81224100
H	2.61973500	-3.75302900	-0.64217800
H	3.15932500	-2.16408500	-0.00449000

TS8

C	-2.36563800	-1.03593200	0.86766400
C	-2.29311100	-1.44488200	-0.46162300
C	-3.02292700	-2.52855800	-0.95182300
C	-3.84470400	-3.21455600	-0.06723600
C	-3.92609800	-2.81117700	1.27371700
C	-3.19439600	-1.72559600	1.75109500
C	-1.47970700	0.15275400	1.14738800

C	-0.81133900	0.49563200	-0.20562400
C	-1.38075600	-0.56227900	-1.21103100
H	-2.94467800	-2.81768400	-1.99590400
H	-4.42842500	-4.06319700	-0.40938400
H	-4.57441100	-3.35728600	1.95282000
H	-3.26924700	-1.42567500	2.79250900
H	-0.70072300	-0.11475000	1.86830200
O	-1.11976800	-0.59510300	-2.39059200
C	-1.19699600	1.85037500	-0.78160600
O	-2.50058000	2.08620600	-0.59792800
O	-0.46538900	2.57903200	-1.40515000
C	-2.98693200	3.30772700	-1.16243700
H	-4.05057400	3.33953700	-0.93071500
H	-2.47488900	4.16196000	-0.71433200
H	-2.83443900	3.31618400	-2.24387500
H	-2.04207200	0.99718000	1.54913600
N	0.97814800	-0.84472800	0.24444400
N	0.64896000	0.34297500	-0.25757500
S	1.22858000	1.82219200	1.10728800
C	2.26646300	-1.21788800	-0.09454200
C	2.74113900	-2.44181100	0.42931900
C	3.14495000	-0.48943700	-0.92986700
C	4.01532100	-2.90871000	0.14093100
H	2.07407200	-3.01125100	1.07167300
C	4.42295100	-0.96505500	-1.20920700
H	2.80014000	0.43899600	-1.37189900
C	4.87692400	-2.17328200	-0.67955200
H	4.34452300	-3.85544000	0.56214000
H	5.07368100	-0.38179900	-1.85678100
H	5.87612400	-2.53543700	-0.90048100
O	2.05526300	1.13364200	2.12627500
O	0.12824800	2.69420500	1.61067800
C	2.32400900	2.90379800	0.18220300
H	1.78222800	3.24903700	-0.69911100
H	2.58938700	3.74453900	0.82954800
H	3.21516100	2.34169000	-0.10121600

2a

C	1.12446600	1.21938300	-0.00000700
C	-0.26848900	1.19793500	-0.00000600
C	-0.93840500	-0.02660600	-0.00000500
C	-0.21727000	-1.22261500	0.00001000
C	1.17321500	-1.18664200	-0.00001500
C	1.85331600	0.03174600	0.00000400
H	1.63995200	2.17538300	-0.00001800
H	-0.84070700	2.12225400	0.00001900
H	-0.75884600	-2.16365300	0.00003300
H	1.72871500	-2.11999100	0.00003400
H	2.93837000	0.05419400	0.00005400
O	-2.29817700	-0.11552400	-0.00002800
H	-2.68305900	0.77680000	0.00021500

CO_3^{2-}

C	0.00000000	0.00131700	0.00000000
O	-0.72423900	-1.07191600	0.00000000
O	-0.56667200	1.16410200	0.00000000
O	1.29091100	-0.09317300	0.00000000

HCO_3^- in ethanol

C	0.00000000	0.14312800	0.00000000
O	1.20528800	0.47295000	0.00000000
O	-1.02081400	0.85587500	0.00000000
O	-0.26022800	-1.22791000	0.00000000
H	0.60603600	-1.66608700	0.00000000

1a in ethanol

N	0.04262000	-1.17378700	1.25916200
N	1.22580200	-0.97482900	1.05537500
S	1.84308600	0.03570500	-0.35819400
C	-1.05329300	-0.52264100	0.59792700
C	-1.95935500	-1.31567000	-0.10095200
C	-1.27259400	0.83777000	0.80500100
C	-3.07364100	-0.70931500	-0.67178400
H	-1.77574500	-2.37975600	-0.20987800
C	-2.40826300	1.42201400	0.25244900
H	-0.57925200	1.41933200	1.40511400
C	-3.30061300	0.65555800	-0.49512700
H	-3.77350700	-1.30909700	-1.24478500
H	-2.59269300	2.48021300	0.40797100
H	-4.18080800	1.11898800	-0.92914200
O	0.83407400	0.41716600	-1.34517200
O	2.96262000	-0.79899400	-0.79160300
C	2.46450300	1.46263900	0.49025400
H	3.08499400	1.12439000	1.32258800
H	3.06914900	2.01916600	-0.23192400
H	1.62551100	2.06829100	0.83698600

Int8

C	-1.09929200	1.19845700	0.00005200
C	0.28902400	1.20605600	0.00002700
C	1.06455400	0.00001600	-0.00024400
C	0.28902000	-1.20605100	0.00002600
C	-1.09927800	-1.19847200	0.00005600
C	-1.82088500	0.00000000	-0.00006000
H	-1.63395200	2.14717500	0.00009100
H	0.83155900	2.14997400	0.00011100
H	0.83160700	-2.14993900	0.00010700
H	-1.63395100	-2.14718200	0.00008500
H	-2.90655400	-0.00001500	-0.00010100
O	2.34655400	-0.00000600	0.00007100

Int9

C	2.37687100	0.34035900	-0.62455700
C	3.18161900	-0.69475500	-0.88699300

C	3.18801200	-1.89748300	-0.03506600
C	2.22964700	-1.93102700	1.08598200
C	1.43751600	-0.88876700	1.35644900
C	1.48442600	0.39601100	0.58511900
H	2.36872700	1.21325000	-1.27345000
H	3.84933500	-0.70449200	-1.74389300
H	2.20012400	-2.84393500	1.67384700
H	0.72961400	-0.92201100	2.18099000
O	3.94668100	-2.83786800	-0.25650100
N	-0.44923400	0.02666100	-0.81178300
N	0.09836800	0.79029300	0.26593500
S	-0.07804700	2.43355200	-0.01368500
C	-1.52819300	-0.69578500	-0.40109800
C	-2.15961000	-1.51717800	-1.38193200
C	-2.11003200	-0.72878200	0.89802600
C	-3.26121300	-2.30137800	-1.08666400
H	-1.74143500	-1.51188600	-2.38598200
C	-3.21806900	-1.52428700	1.17613400
H	-1.67819900	-0.11834100	1.68426600
C	-3.81459700	-2.32260200	0.20051100
H	-3.70121200	-2.90953900	-1.87450200
H	-3.62459200	-1.51548100	2.18592900
H	-4.67900400	-2.93780800	0.42910300
O	0.37493500	2.85723100	-1.34823800
O	0.52979700	3.13844100	1.12642200
C	-1.83923600	2.62359200	0.04329700
H	-2.19811500	2.32270800	1.02781500
H	-2.03926200	3.68342700	-0.13367300
H	-2.28412800	2.01537900	-0.74468800
H	1.88880300	1.16327700	1.26541300

TS10

C	-2.24512400	0.35418200	0.77719400
C	-3.28099400	-0.44698900	1.05000500
C	-3.76048400	-1.44061800	0.07299000
C	-3.00716600	-1.55633800	-1.19019700
C	-1.98369600	-0.74152900	-1.46606200
C	-1.56418000	0.37907100	-0.56183500
H	-1.87948100	1.06025900	1.51951900
H	-3.79625400	-0.41981900	2.00608400
H	-3.31887400	-2.34162300	-1.87285400
H	-1.42307900	-0.83804700	-2.39318600
O	-4.72900100	-2.15949300	0.30778100
N	0.32197300	-0.49553200	0.42920800
N	-0.08640600	0.36519300	-0.50246000
S	0.28797400	2.28296500	0.09979700
C	1.60735500	-0.97191900	0.19970300
C	2.18264000	-1.75794800	1.22166500
C	2.37085800	-0.77961100	-0.97443400
C	3.44420300	-2.32053300	1.08163800
H	1.60366200	-1.91284200	2.12851500
C	3.63574900	-1.34403400	-1.10363400

H	1.95165600	-0.19191500	-1.78430700
C	4.18940900	-2.11797800	-0.08274600
H	3.85334000	-2.92059100	1.89064400
H	4.19620100	-1.17990400	-2.02109300
H	5.17733000	-2.55457500	-0.19184300
O	0.18452300	2.45688200	1.57825300
O	-0.40771300	3.30309900	-0.73910300
C	2.03456100	2.43436700	-0.26918800
H	2.18730000	2.27513100	-1.33758400
H	2.33341200	3.44790500	0.01458300
H	2.58631900	1.69766300	0.31630400
H	-1.84935400	1.31865200	-1.06480300

TS10b

C	1.44598300	0.42602900	-1.24154400
C	2.63522300	-0.22008900	-1.24422900
C	3.32320900	-0.56685800	0.00002500
C	2.63476600	-0.22115900	1.24432600
C	1.44553000	0.42496300	1.24176800
C	0.89640300	0.92467700	0.00023000
H	0.92091300	0.65060100	-2.16745100
H	3.11336500	-0.51823800	-2.17252300
H	3.11255600	-0.52013200	2.17253600
H	0.92011900	0.64870200	2.16768300
O	4.42058200	-1.14587900	-0.00001800
N	-0.52850200	1.29161800	0.00008000
N	-0.64963900	2.52400000	0.00014600
C	-1.61204100	0.34021200	-0.00004500
C	-1.31571300	-1.02074900	-0.00046600
C	-2.92314900	0.81319800	0.00028900
C	-2.36951300	-1.93130300	-0.00055200
H	-0.28749500	-1.36832900	-0.00074600
C	-3.96121600	-0.10881800	0.00019600
H	-3.11113600	1.88127700	0.00063600
C	-3.68623600	-1.47822100	-0.00021700
H	-2.15566300	-2.99487800	-0.00087200
H	-4.98820900	0.24115700	0.00045800
H	-4.50331900	-2.19276200	-0.00026800
H	0.78172300	2.33900200	0.00043000

Int10

C	2.06519700	0.27878600	-0.55602300
C	3.21202600	-0.18156300	-1.06782500
C	4.06350900	-1.13228800	-0.32902100
C	3.59063200	-1.56842500	0.99961100
C	2.45452100	-1.09831400	1.52272600
C	1.60358500	-0.08069500	0.82197200
H	1.44735000	0.98938500	-1.10187600
H	3.56590600	0.12092800	-2.04944300
H	4.20870200	-2.29197500	1.52324000
H	2.10313100	-1.43123000	2.49624300
O	5.11727100	-1.55121700	-0.79966900

N	-0.31102800	-0.82252700	-0.16021600
N	0.20397000	-0.54455900	0.93022300
S	-0.44946600	2.69158500	0.15062400
C	-1.66672400	-1.27793000	-0.07680600
C	-2.18303500	-1.83637500	-1.24475400
C	-2.46330800	-1.15189200	1.06547300
C	-3.49725400	-2.29735700	-1.26977400
H	-1.54324200	-1.90431400	-2.11968900
C	-3.77653400	-1.60411900	1.03035100
H	-2.05158500	-0.69379500	1.95839300
C	-4.29368800	-2.18069700	-0.13294300
H	-3.89922400	-2.73880000	-2.17625400
H	-4.40374100	-1.50337500	1.91082100
H	-5.32144100	-2.53016000	-0.15205600
O	0.36750000	3.09231200	-1.08207500
O	-0.95124300	3.91796700	0.90828900
C	-1.97869100	2.11755600	-0.64645600
H	-2.70836800	1.80752700	0.10759800
H	-2.37057100	2.96483200	-1.21971700
H	-1.75938200	1.28403900	-1.31966400
H	1.62369300	0.83857500	1.43081600

TS11

C	-1.78912000	-0.71034600	1.03868400
C	-3.06408100	-1.09732400	1.23548800
C	-3.94378800	-1.46219400	0.11813600
C	-3.35057900	-1.42639500	-1.22121400
C	-2.07323800	-1.04135800	-1.40871600
C	-1.24435500	-0.52816000	-0.31321800
H	-1.14811200	-0.44384900	1.87320800
H	-3.49119100	-1.16553400	2.23231000
H	-3.97824600	-1.74586800	-2.04802800
H	-1.62754400	-1.04132700	-2.40117300
O	-5.11996500	-1.79961700	0.30287000
N	0.87647000	-0.80438600	0.44725900
N	0.16207300	-0.70650100	-0.56534000
S	-0.56212400	2.97020600	0.19576600
C	2.27843100	-0.89296100	0.17665300
C	3.08977500	-1.09282300	1.29330600
C	2.84922700	-0.78368500	-1.09672700
C	4.47120000	-1.19143900	1.14528800
H	2.62033000	-1.16803800	2.26968300
C	4.22800000	-0.88084500	-1.23815600
H	2.21068000	-0.62570700	-1.95922100
C	5.04201100	-1.08525900	-0.12075400
H	5.09876100	-1.34893900	2.01700700
H	4.67420300	-0.79483300	-2.22441100
H	6.11866600	-1.15800500	-0.24077000
O	-1.61330500	2.14264400	-0.60640900
O	-0.17401800	2.22625300	1.46169200
C	0.89522500	2.73453900	-0.85213100
H	1.75284400	3.23449600	-0.39396800

H	1.08465200	1.65835900	-0.92149000
H	0.70647000	3.15116200	-1.84494000
H	-1.37129000	0.69626100	-0.46895400

$MeSO_2^-$ in Ethanol

S	-0.21068800	0.00000600	-0.39677900
O	-0.71396900	-1.26334800	0.30102200
O	-0.71364400	1.26352400	0.30100000
C	1.53108500	-0.00014400	0.13099700
H	2.03831800	0.89493600	-0.24022300
H	1.52920000	-0.00000300	1.22652500
H	2.03787900	-0.89558100	-0.23999400

3a

C	-1.85969100	-1.05247600	-0.00033700
C	-3.23505400	-1.21207700	-0.00011900
C	-4.07044500	-0.08585600	0.00017700
C	-3.52132200	1.19930600	0.00000500
C	-2.14318200	1.35040400	-0.00024100
C	-1.30226100	0.23343100	-0.00033900
H	-1.20782900	-1.91928800	-0.00048100
H	-3.67616500	-2.20534100	-0.00009300
H	-4.18421800	2.05835300	0.00013700
H	-1.69470000	2.33934800	-0.00030600
O	-5.42130800	-0.18482000	0.00055700
N	0.83020100	-0.48930600	-0.00023300
N	0.08564900	0.51232300	-0.00028900
C	2.22299400	-0.19407800	-0.00010900
C	3.06849500	-1.30477200	-0.00001100
C	2.75999700	1.09957300	-0.00001000
C	4.44995600	-1.13103000	0.00019200
H	2.62500400	-2.29600300	-0.00007300
C	4.13846800	1.26613200	0.00019400
H	2.09427300	1.95555200	-0.00008200
C	4.98624500	0.15458100	0.00030000
H	5.10481800	-1.99676700	0.00028200
H	4.55862600	2.26733900	0.00028300
H	6.06282800	0.29506900	0.00046800
H	-5.68831500	-1.11964400	0.00085500

TS12

C	0.40234800	-2.22516800	0.12307600
C	-0.53701600	-2.39614000	-0.83566000
C	-1.91669200	-1.95749600	-0.62025100
C	-2.24521500	-1.50096500	0.73642300
C	-1.28521800	-1.33734600	1.67365200
C	0.10315700	-1.44938200	1.30515100
H	1.42632400	-2.54948000	-0.04418100
H	-0.31527100	-2.87952700	-1.78369100
H	-3.29501300	-1.31389900	0.94693900
H	-1.53747700	-0.98102100	2.66845500
O	-2.78098100	-2.03839300	-1.50829400

N	0.42040900	0.32471000	0.60113300
N	-0.41257800	0.53629300	-0.41489700
S	-1.65345300	1.54239200	0.00449200
C	1.78537900	0.23359300	0.17747200
C	2.76409900	0.14681000	1.17604000
C	2.17796400	0.29033100	-1.16375300
C	4.11100400	0.09503500	0.83687600
H	2.45700200	0.13451800	2.21807300
C	3.53052700	0.24042600	-1.49505200
H	1.41895100	0.37940200	-1.93224600
C	4.50302100	0.13756800	-0.50237800
H	4.85889400	0.03182300	1.62211200
H	3.82436500	0.28370500	-2.54016500
H	5.55548900	0.10140400	-0.76642800
O	-1.91365400	1.66099800	1.45138500
O	-2.80443700	1.21494600	-0.85485500
C	-1.05945400	3.13923200	-0.52739500
H	-0.82941800	3.09198200	-1.59320700
H	-1.84278200	3.87743200	-0.33783100
H	-0.16175300	3.38267900	0.04524500
H	0.83027500	-1.46371600	2.11029900

Int12

C	-1.17417700	-1.76621800	-0.68793500
C	-2.44638700	-1.92982200	-1.06540100
C	-3.55487300	-1.36686500	-0.27246700
C	-3.19493800	-0.56781400	0.91246200
C	-1.91995700	-0.40012700	1.28164900
C	-0.77420000	-1.05774600	0.57677400
H	-0.35925900	-2.16883000	-1.28772700
H	-2.71927400	-2.46490500	-1.97086400
H	-4.01756600	-0.11435500	1.45811500
H	-1.65940400	0.20379000	2.14570700
O	-4.72797700	-1.54374200	-0.59487400
N	0.31716400	-0.09915200	0.34145400
N	-0.08271800	0.82909200	-0.67390100
S	-0.08722000	2.31108300	-0.07931900
C	1.59443100	-0.68297100	0.13785100
C	2.10754200	-1.59333200	1.07963000
C	2.40009700	-0.33199800	-0.95438600
C	3.37277100	-2.14472000	0.91673300
H	1.52685900	-1.85050100	1.96057800
C	3.67000900	-0.88693100	-1.10369500
H	2.01513900	0.37487600	-1.67874300
C	4.16708800	-1.79942900	-0.17740700
H	3.74496900	-2.84232000	1.66189100
H	4.27228000	-0.60140500	-1.96206000
H	5.15689500	-2.22844000	-0.29798000
O	-0.81406000	2.49198300	1.20301800
O	-0.53660900	3.19797300	-1.17634300
C	1.59383500	2.79351200	0.30518900
H	2.19276300	2.75624800	-0.60661000

H	1.58190400	3.80903300	0.70871000
H	1.99900000	2.10472000	1.05074200
H	-0.39818500	-1.82776000	1.26609000

TS13

C	-1.85715800	-0.85725800	-0.95386800
C	-3.21579900	-0.86157400	-0.93250200
C	-3.96848200	-0.15652500	0.09679300
C	-3.17907800	0.57564000	1.07873300
C	-1.82119100	0.57772100	1.04562400
C	-1.09332300	-0.24140000	0.10244900
H	-1.30688600	-1.36287700	-1.74308100
H	-3.78901600	-1.37964300	-1.69656600
H	-3.72419300	1.13200700	1.83624700
H	-1.24971400	1.14933800	1.77483600
O	-5.21631200	-0.16734500	0.12890700
N	0.33249000	-0.01402600	-0.10693800
N	0.90081200	-0.94525800	0.86101300
S	1.66365200	-2.16667200	0.06205500
C	0.83497800	1.30217400	-0.07019100
C	0.12358500	2.31620300	-0.73218800
C	2.04936700	1.61409500	0.55069000
C	0.62367600	3.61201000	-0.76733200
H	-0.81839100	2.07829100	-1.21926300
C	2.54000300	2.91820500	0.50445300
H	2.59372500	0.83810500	1.07620500
C	1.83657400	3.92500100	-0.15114300
H	0.05882400	4.38396000	-1.28217000
H	3.48297700	3.14432400	0.99442200
H	2.22430700	4.93825700	-0.18218400
O	0.83598300	-2.76689900	-1.00163500
O	2.14308900	-3.08615000	1.10625900
C	3.06966000	-1.43768600	-0.74869600
H	3.74598000	-1.03058400	0.00407100
H	3.56453900	-2.22692500	-1.32050100
H	2.71876500	-0.65336700	-1.42308300
H	-0.51141300	-1.18563200	0.90449600

Int13

C	-1.84474500	-0.19398500	-1.07853100
C	-3.22337700	-0.05679300	-1.08509700
C	-3.95522200	0.43106200	0.05010400
C	-3.14452900	0.76929100	1.18790500
C	-1.76736400	0.63637300	1.18071800
C	-1.09738700	0.14293400	0.05301100
H	-1.32458600	-0.56565800	-1.95847500
H	-3.79289900	-0.32145500	-1.97327800
H	-3.65225200	1.15063300	2.07121900
H	-1.18752600	0.92013000	2.05911300
O	-5.22518400	0.56076600	0.04930100
N	0.33671800	0.01995900	0.05375600
N	0.86572600	-1.01083100	0.84289900

S	1.12057000	-2.44874200	0.01047500
C	1.12847300	1.19503200	0.03142000
C	0.60360300	2.36370200	-0.54110300
C	2.44539700	1.20826400	0.51100200
C	1.38185400	3.51316300	-0.62598000
H	-0.41227700	2.36710800	-0.92060500
C	3.21040300	2.36881400	0.42064400
H	2.86448600	0.31663600	0.96144500
C	2.69070400	3.52957200	-0.14643400
H	0.95346000	4.40590600	-1.07273100
H	4.22697400	2.35785400	0.80369200
H	3.29247300	4.43026300	-0.21362500
O	0.02686700	-2.78191700	-0.90102300
O	1.46587300	-3.41444500	1.05418600
C	2.53746900	-2.03654800	-0.96438500
H	3.37495300	-1.82102400	-0.29983100
H	2.75519100	-2.90143100	-1.59561100
H	2.29061900	-1.17208200	-1.58526700
H	0.33302000	-1.19142000	1.70039800

TS14

C	1.54923700	-0.64269400	-0.86895900
C	2.87532600	-0.65966700	-1.23542800
C	3.94304200	-0.39186900	-0.30243500
C	3.51697100	-0.10918900	1.04472500
C	2.18852300	-0.08882600	1.40803600
C	1.18834200	-0.35342000	0.45844200
H	0.77279100	-0.82311300	-1.60752100
H	3.15068700	-0.86670000	-2.26628000
H	4.28725600	0.07600500	1.78848700
H	1.91131600	0.10017200	2.44380200
O	5.16304100	-0.41004800	-0.64186700
N	-0.18191500	-0.27335000	0.84329500
N	-0.63566700	0.67118500	1.57348900
S	-1.03431400	2.38051500	-0.13906600
C	-1.13419900	-1.25193200	0.39551800
C	-0.70485300	-2.54143200	0.08138700
C	-2.48577700	-0.91014900	0.33225900
C	-1.64333900	-3.49126000	-0.31210500
H	0.34391800	-2.80520700	0.15564700
C	-3.41029000	-1.87061000	-0.06014600
H	-2.80428500	0.09277200	0.58810600
C	-2.99426800	-3.16104200	-0.38725000
H	-1.31099900	-4.49576200	-0.55369400
H	-4.46117000	-1.60497200	-0.11571700
H	-3.72091900	-3.90542500	-0.69701200
O	-1.03842800	1.41937100	-1.29822900
O	-0.14126500	3.58107600	-0.32507100
C	-2.69861700	3.08646900	-0.16073700
H	-2.80102100	3.79233100	0.66635000
H	-2.81579400	3.60522200	-1.11731300
H	-3.43721800	2.28663800	-0.07136100

H	0.15018300	1.26549200	1.85557000

Int14

C	1.00002100	-0.76405700	-0.50670200
C	2.23510500	-1.32982200	-0.60182600
C	3.43593200	-0.64758400	-0.14915600
C	3.23138700	0.67736300	0.41949600
C	1.99862600	1.24791300	0.49513100
C	0.84860100	0.54626900	0.03310800
H	0.13290800	-1.29310500	-0.88810000
H	2.35681300	-2.31644700	-1.03838000
H	4.10365000	1.19074200	0.81269700
H	1.88740100	2.21800200	0.97253400
O	4.56810400	-1.16530900	-0.22877900
N	-0.38793000	1.16466000	0.05237600
N	-0.61133900	2.41411800	0.09380000
C	-1.59155300	0.35036800	0.05179200
C	-1.70627800	-0.70429600	0.95192400
C	-2.61199100	0.69427500	-0.82777700
C	-2.88853700	-1.43768900	0.96302700
H	-0.89751100	-0.93178000	1.63851200
C	-3.78231300	-0.05722500	-0.81208500
H	-2.47641700	1.52339500	-1.51407500
C	-3.92100600	-1.11852600	0.08184100
H	-3.00209400	-2.25641100	1.66568500
H	-4.58497400	0.18703700	-1.49990400
H	-4.83829200	-1.69856800	0.09266300
H	0.28059800	2.90622600	-0.02727600

TS15

C	-1.68003400	0.20193800	1.35714900
C	-2.95897400	-0.20213700	1.18053300
C	-3.52421400	-0.43354000	-0.15989200
C	-2.62880200	-0.22885100	-1.29182000
C	-1.35910400	0.21026900	-1.11271000
C	-0.84909000	0.45391100	0.21374300
H	-1.25993600	0.36326500	2.34562600
H	-3.61337200	-0.39339700	2.02594000
H	-3.01419500	-0.45661000	-2.28052900
H	-0.67835900	0.34170900	-1.94902600
O	-4.69492300	-0.81361200	-0.29656500
N	0.45386400	0.94092900	0.37700500
N	0.18043700	2.06618600	-0.29690000
C	1.66816400	0.25789300	0.17414900
C	1.71209500	-1.13704800	0.22999800
C	2.82138000	1.01347600	-0.03837400
C	2.93710900	-1.77564600	0.07793900
H	0.79677100	-1.70464500	0.37072900
C	4.03478100	0.35586400	-0.21430700
H	2.75825400	2.09727300	-0.04880800
C	4.09855600	-1.03547100	-0.15030300
H	2.98154400	-2.85937300	0.11976700

H	4.93631700	0.93547600	-0.38612900
H	5.04947400	-1.54274000	-0.27779700
H	-0.46841900	2.59419000	0.29536600

TS16

C	-1.90977300	-1.77941300	-0.13514000
C	-3.22287900	-1.75909300	-0.38583700
C	-4.03363100	-0.55306700	-0.13135600
C	-3.31675200	0.64635300	0.33643900
C	-1.99565100	0.63862800	0.54116600
C	-1.16405800	-0.60042900	0.41987100
H	-1.32988000	-2.67632100	-0.34139700
H	-3.74503000	-2.62173100	-0.78948100
H	-3.91404600	1.54088300	0.48774100
H	-1.48109300	1.53361900	0.87662900
O	-5.24746600	-0.54733400	-0.31606500
N	0.04248500	-0.33394600	-0.43697600
N	0.04788400	0.61517600	-1.27297600
S	0.88783300	2.31065600	0.01653700
C	1.20901900	-1.15173700	-0.20617100
C	1.22148000	-2.22872200	0.68707800
C	2.37307900	-0.83515500	-0.91555300
C	2.38948300	-2.96993100	0.86390400
H	0.34136000	-2.51008300	1.25315400
C	3.53100700	-1.58037700	-0.72911300
H	2.34158500	-0.00291600	-1.60887900
C	3.54872400	-2.65332400	0.16231500
H	2.38347500	-3.80233000	1.56140500
H	4.42670100	-1.31954800	-1.28557600
H	4.45417600	-3.23430200	0.30680800
O	1.00505000	1.61529700	1.35678900
O	0.06697700	3.58210800	0.09021200
C	2.57154800	2.93126800	-0.23998200
H	2.63250000	3.45427300	-1.19750000
H	2.79702600	3.62102800	0.57949300
H	3.26507500	2.08671100	-0.22629100
H	-0.81582900	-0.83897500	1.43574100

Int15

C	1.70570200	1.10422400	-0.95201100
C	2.64282500	0.15364500	-1.04236700
C	2.90885900	-0.77050700	0.07857200
C	2.05953300	-0.63670100	1.27966300
C	1.11377100	0.30524500	1.36560900
C	0.91836600	1.33198200	0.29832000
H	1.50547000	1.78729300	-1.77473300
H	3.23944600	0.01654000	-1.93933700
H	2.23461800	-1.34890100	2.08060600
H	0.48782800	0.39214800	2.25083900
O	3.78692000	-1.62390600	0.00875600
N	-0.56163900	1.58450300	-0.04521000

N	-0.96495000	2.70188100	-0.27802400
C	-1.44049200	0.40139600	-0.07668100
C	-0.99212300	-0.81843200	-0.57235000
C	-2.74720500	0.57098500	0.36766800
C	-1.88361200	-1.88915200	-0.62540400
H	0.02308600	-0.93624700	-0.93496700
C	-3.62263500	-0.50839200	0.32389000
H	-3.05846700	1.54247600	0.73773000
C	-3.19268700	-1.73875600	-0.17432600
H	-1.54834400	-2.84161700	-1.02329000
H	-4.64135600	-0.38901400	0.67908200
H	-3.87931200	-2.57866700	-0.21184500
H	1.20598000	2.30933000	0.70500700

TS17

C	2.13383600	1.29152800	-0.56300500
C	3.13392200	0.40674100	-0.61237900
C	3.07662400	-0.86421200	0.13733400
C	1.85849400	-1.12775900	0.93085300
C	0.83893600	-0.26592200	0.97668800
C	0.92663300	1.05421300	0.26385600
H	2.15148900	2.22236000	-1.12074000
H	4.01985000	0.57841400	-1.21589300
H	1.82761000	-2.06304100	1.48141700
H	-0.04486000	-0.45117700	1.57775700
O	3.99710000	-1.67166000	0.09948900
N	-0.34245000	1.27937200	-0.59150200
N	-0.20263700	2.39245200	0.12219300
C	-1.50316900	0.42670900	-0.31901700
C	-1.58989600	-0.75954900	-1.04264400
C	-2.50972800	0.81282500	0.55809100
C	-2.69811200	-1.58388100	-0.87076500
H	-0.79016300	-1.02609600	-1.72847300
C	-3.62088900	-0.01298800	0.71681200
H	-2.41437400	1.74711000	1.10122100
C	-3.71542400	-1.21037200	0.00809500
H	-2.77072900	-2.51385800	-1.42615300
H	-4.41535500	0.27984300	1.39661700
H	-4.58359900	-1.84948200	0.13635800
H	0.87159000	1.74244600	1.18362300

Int16

C	2.04442500	1.17928600	-0.80433700
C	3.14691600	0.42569800	-0.74904200
C	3.23018100	-0.74252100	0.15239500
C	2.04845600	-1.03774500	0.98879200
C	0.94272300	-0.28623900	0.92725800
C	0.85789100	0.88194300	0.02814800
H	1.96565500	2.04143100	-1.46084900
H	4.02143300	0.63653200	-1.35688800
H	2.12295000	-1.89347000	1.65258500
H	0.07504800	-0.50850200	1.54372700

O	4.23785300	-1.43860100	0.20505400
N	-0.42310900	1.23042100	-0.57656000
N	0.09792000	2.05005600	0.49297800
C	-1.56554400	0.41764700	-0.31501100
C	-1.65963300	-0.82325600	-0.95267800
C	-2.61379200	0.88759600	0.47433300
C	-2.80081000	-1.59678700	-0.78139400
H	-0.83536600	-1.17158100	-1.56898900
C	-3.75694400	0.10366900	0.63392400
H	-2.54836500	1.86286200	0.94848400
C	-3.85441400	-1.13738300	0.01253400
H	-2.86835900	-2.56413700	-1.26980600
H	-4.57290200	0.47254100	1.24798400
H	-4.74475800	-1.74440900	0.14205100
H	-0.35856900	1.78274900	1.37679400

TS18

C	-2.41028600	1.42187700	0.14767700
C	-3.50455100	0.64789500	0.36067900
C	-3.48834100	-0.79608500	0.10885800
C	-2.23360600	-1.35158900	-0.37473000
C	-1.13186500	-0.57319200	-0.54740700
C	-1.19189700	0.83846800	-0.31614100
H	-2.43151200	2.49488600	0.31443500
H	-4.44163700	1.07711100	0.70319500
H	-2.20693400	-2.41653900	-0.58338400
H	-0.20243100	-1.01096300	-0.90133600
O	-4.49989700	-1.49459000	0.29474900
N	0.59416100	1.12199100	0.48839600
N	-0.06788100	1.68478400	-0.54760000
C	1.76511200	0.41994800	0.22119600
C	2.48611700	0.03898600	1.37031800
C	2.27515300	0.12137900	-1.05823200
C	3.71352000	-0.59008200	1.24443400
H	2.06294300	0.26878600	2.34324700
C	3.50705200	-0.50717200	-1.16998000
H	1.71348600	0.34544400	-1.95981200
C	4.22764500	-0.86013600	-0.02643600
H	4.27170000	-0.87374900	2.13056600
H	3.90328200	-0.73829200	-2.15337800
H	5.18674900	-1.35848500	-0.12722200
H	0.37524600	1.65931900	-1.47128500

int17

C	2.18190500	1.29567800	-0.31243800
C	3.53704600	1.19418000	-0.28263300
C	4.20015900	-0.06820100	0.01508700
C	3.32576700	-1.20837100	0.28193000
C	1.97210300	-1.10198600	0.25249900
C	1.37111400	0.15448000	-0.04967200
H	1.69761100	2.24405800	-0.53743900
H	4.16785300	2.05521900	-0.48033600

H	3.80621800	-2.15435400	0.51274300
H	1.33412300	-1.95558700	0.45785800
O	5.44045800	-0.17406400	0.04689100
N	-0.82995000	-0.63049600	0.03876100
N	0.02402100	0.30276300	-0.10327800
C	-2.17784000	-0.25302100	0.04051300
C	-3.08577200	-1.27650700	-0.27003000
C	-2.65757700	1.02813600	0.36176600
C	-4.44829800	-1.01397900	-0.30616600
H	-2.69704600	-2.26493100	-0.49433500
C	-4.02496700	1.27666400	0.32477800
H	-1.98865900	1.82127700	0.68516800
C	-4.92342900	0.26530000	-0.01467500
H	-5.14169000	-1.80982200	-0.55907700
H	-4.39127000	2.26558500	0.58215700
H	-5.98909200	0.46988600	-0.03575600
H	-0.30147400	1.26107500	-0.30024400

Int18

C	-1.76263100	-0.12049300	-1.10422700
C	-3.14380000	0.02767900	-1.12338400
C	-3.81103500	0.45420400	0.02762500
C	-3.09517400	0.73421800	1.19472800
C	-1.71252500	0.59308000	1.20186700
C	-1.04447200	0.15786100	0.05692100
H	-1.23137300	-0.45268300	-1.99037800
H	-3.71879400	-0.18333600	-2.01932400
H	-3.62337900	1.06891800	2.08328900
H	-1.14695700	0.82619200	2.10105900
O	-5.16128300	0.58276600	-0.04472200
N	0.38805800	0.01849300	0.06380500
N	0.89529800	-1.02348800	0.84196800
S	1.08994500	-2.47073000	0.00601500
C	1.18890300	1.19045200	0.04102200
C	0.66615100	2.37169400	-0.50352300
C	2.51345400	1.17486900	0.49502300
C	1.45950700	3.51157500	-0.58730500
H	-0.35593900	2.39906300	-0.86530000
C	3.29276700	2.32539500	0.40508300
H	2.92735800	0.26948900	0.92236100
C	2.77727200	3.50116100	-0.13475300
H	1.03556300	4.41653600	-1.01275200
H	4.31683200	2.29487800	0.76587900
H	3.39072200	4.39382200	-0.20207200
O	-0.03368800	-2.75531300	-0.88443700
O	1.41658600	-3.44482900	1.04610300
C	2.50440900	-2.10645400	-0.98979500
H	3.35733000	-1.92004100	-0.33611200
H	2.68341100	-2.97779200	-1.62420900
H	2.27831500	-1.23320800	-1.60631500
H	0.40181900	-1.18093700	1.72710900
H	-5.50738900	0.89332100	0.80885900

Int19

C	-1.84685300	1.20018100	0.67839600
C	-3.11039900	0.64580500	0.64525500
C	-3.34278200	-0.52044100	-0.09946000
C	-2.29794400	-1.13366200	-0.80562100
C	-1.02599700	-0.59341200	-0.76169800
C	-0.81252400	0.57731300	-0.02838200
H	-1.65574600	2.07975900	1.28646700
H	-3.92829700	1.08740900	1.20354600
H	-2.49221600	-2.03120900	-1.38482600
H	-0.21843100	-1.05629300	-1.31844900
O	-4.59243500	-1.00859100	-0.08881200
N	0.48950800	1.17940900	-0.02079700
N	0.68531700	2.40715300	-0.04416000
C	1.65976700	0.33239000	0.03074100
C	1.62806800	-0.82809800	0.80218400
C	2.79262500	0.73965900	-0.67124900
C	2.78400000	-1.59682600	0.87517500
H	0.73744900	-1.10719200	1.35470800
C	3.93231700	-0.04974200	-0.59415700
H	2.76559800	1.63979900	-1.27562300
C	3.92883800	-1.21169900	0.17861900
H	2.78823500	-2.49625800	1.48111000
H	4.82161200	0.23921900	-1.14379000
H	4.82402100	-1.82257100	0.23513900
H	-0.21420300	2.89446900	-0.16803600
H	-4.64700800	-1.83314400	-0.60387600

TS19

C	1.14061500	-0.09983500	-1.01215500
C	2.40526900	-0.60577200	-1.20192800
C	3.36110400	-0.45851100	-0.18377500
C	3.03645000	0.17282400	1.05091900
C	1.77612800	0.65619900	1.25818000
C	0.81698900	0.53191300	0.21943000
H	0.36973000	-0.21853700	-1.76714700
H	2.68283700	-1.11235600	-2.11891800
H	3.79731800	0.24051000	1.82260800
H	1.49358100	1.13355400	2.19042000
O	4.57011200	-0.94663200	-0.41248100
N	-0.51685700	1.05474600	0.39709200
N	-0.18786000	1.95746400	-0.51257600
C	-1.71231300	0.31164800	0.20766300
C	-1.77871400	-1.01376000	0.63994200
C	-2.81429300	0.96521000	-0.34018000
C	-2.97919500	-1.69747600	0.50178100
H	-0.90031500	-1.49924600	1.05463800
C	-4.00443400	0.25887100	-0.48442400
H	-2.74043400	2.00939400	-0.62824100
C	-4.08985100	-1.06713800	-0.06396100
H	-3.04528800	-2.73057400	0.82688000

H	-4.86966500	0.75230000	-0.91475600
H	-5.02288100	-1.61059500	-0.17210400
H	0.49455200	2.59457700	-0.07930200
H	5.16613900	-0.79649800	0.34519600

Int20

C	0.89382300	-0.26950300	-0.94702500
C	2.01022800	-1.02254500	-1.00222200
C	3.12050700	-0.68864200	-0.15686600
C	3.08855600	0.42858500	0.73977800
C	1.97044100	1.18042500	0.79762100
C	0.81083900	0.88136700	-0.04415400
H	0.03456600	-0.48938000	-1.57309100
H	2.11005800	-1.87621900	-1.66262800
H	3.95817300	0.63140700	1.35697400
H	1.89125700	2.02812300	1.47284500
O	4.15496100	-1.45964900	-0.24896600
N	-0.47698300	1.25930100	0.57723200
N	-0.00994200	1.99314400	-0.54956100
C	-1.61544600	0.42520900	0.30914700
C	-1.77917200	-0.71594200	1.09544400
C	-2.57047800	0.79134200	-0.63440700
C	-2.90986300	-1.50492900	0.92076000
H	-1.02127000	-0.97622900	1.82898700
C	-3.70621900	-0.00275600	-0.79159700
H	-2.42686700	1.68727600	-1.22855500
C	-3.87741100	-1.14993100	-0.02161900
H	-3.03851700	-2.39801300	1.52434500
H	-4.45737400	0.28070000	-1.52237200
H	-4.76179400	-1.76566900	-0.15123400
H	0.37935300	2.86920300	-0.18611900
H	4.88636400	-1.19720500	0.34971800

TS20

C	1.44598300	0.42602900	-1.24154400
C	2.63522300	-0.22008900	-1.24422900
C	3.32320900	-0.56685800	0.00002500
C	2.63476600	-0.22115900	1.24432600
C	1.44553000	0.42496300	1.24176800
C	0.89640300	0.92467700	0.00023000
H	0.92091300	0.65060100	-2.16745100
H	3.11336500	-0.51823800	-2.17252300
H	3.11255600	-0.52013200	2.17253600
H	0.92011900	0.64870200	2.16768300
O	4.42058200	-1.14587900	-0.00001800
N	-0.52850200	1.29161800	0.00008000
N	-0.64963900	2.52400000	0.00014600
C	-1.61204100	0.34021200	-0.00004500
C	-1.31571300	-1.02074900	-0.00046600
C	-2.92314900	0.81319800	0.00028900
C	-2.36951300	-1.93130300	-0.00055200
H	-0.28749500	-1.36832900	-0.00074600

C	-3.96121600	-0.10881800	0.00019600
H	-3.11113600	1.88127700	0.00063600
C	-3.68623600	-1.47822100	-0.00021700
H	-2.15566300	-2.99487800	-0.00087200
H	-4.98820900	0.24115700	0.00045800
H	-4.50331900	-2.19276200	-0.00026800
H	0.78172300	2.33900200	0.00043000

Int21

C	-1.11398800	0.30552800	1.36556200
C	-2.05968800	-0.63647800	1.27969400
C	-2.90901100	-0.77038600	0.07861600
C	-2.64263600	0.15332900	-1.04260200
C	-1.70549400	1.10389600	-0.95235700
C	-0.91845200	1.33200700	0.29807300
H	-0.48809700	0.39260700	2.25081400
H	-2.23478600	-1.34859300	2.08070900
H	-3.23909600	0.01593500	-1.93963500
H	-1.50507000	1.78669100	-1.77525800
O	-3.78729500	-1.62357200	0.00900200
N	0.56174800	1.58449300	-0.04520000
N	0.96514400	2.70183900	-0.27787600
C	1.44051400	0.40134700	-0.07662600
C	0.99214400	-0.81850800	-0.57217600
C	2.74727800	0.57095800	0.36762700
C	1.88364700	-1.88923100	-0.62521900
H	-0.02308000	-0.93641700	-0.93473100
C	3.62270800	-0.50840600	0.32388200
H	3.05856200	1.54247600	0.73759800
C	3.19274400	-1.73881500	-0.17423600
H	1.54833000	-2.84170700	-1.02303500
H	4.64144600	-0.38899000	0.67901700
H	3.87937600	-2.57871800	-0.21175500
H	-1.20606200	2.30952200	0.70436500

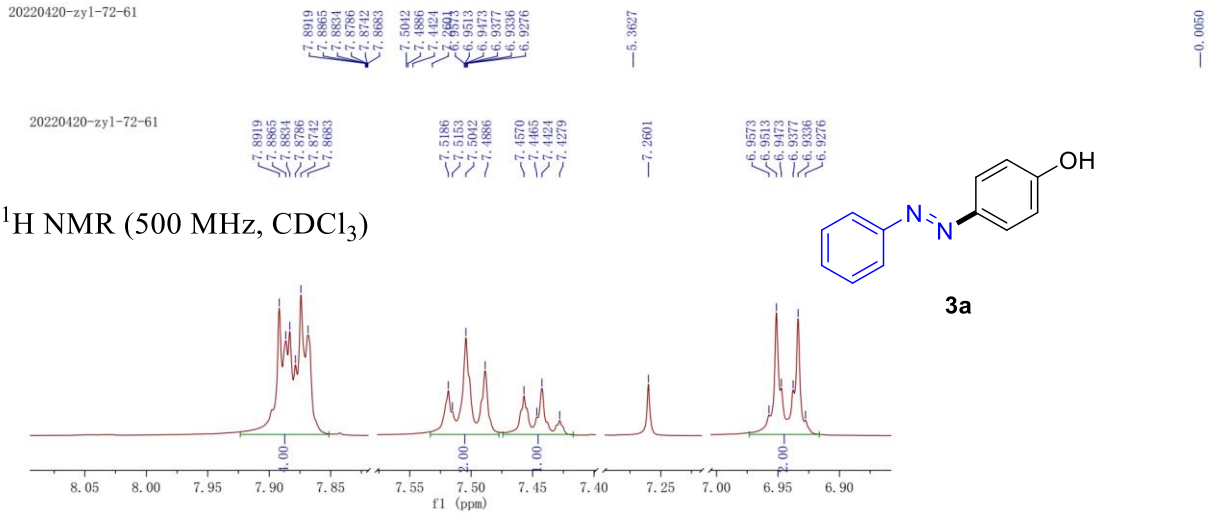
TS21

C	-0.88075100	-0.16920100	1.04681200
C	-1.83154000	-1.10339800	0.95874800
C	-3.03798300	-0.91254200	0.12917800
C	-3.15735700	0.36343500	-0.60547400
C	-2.22386200	1.31557900	-0.51445400
C	-1.03880300	1.16547500	0.36448100
H	-0.00632100	-0.30178700	1.67679200
H	-1.75546800	-2.04016800	1.50266000
H	-4.03529000	0.48335300	-1.23301500
H	-2.29696300	2.24907500	-1.06279900
O	-3.90124900	-1.77847700	0.04946900
N	0.30956400	1.18110900	-0.65242700
N	0.16868500	2.33306400	-0.05812700
C	1.50987900	0.39868000	-0.34866600
C	1.64515300	-0.80148300	-1.03960300
C	2.48413000	0.83906700	0.54268300

C	2.78242400	-1.57954200	-0.83791200
H	0.86076000	-1.10950200	-1.72560100
C	3.62119200	0.06101500	0.73397000
H	2.33599600	1.77757800	1.06705800
C	3.76935300	-1.14618000	0.04676700
H	2.90003700	-2.51820200	-1.37019200
H	4.39352700	0.39149700	1.42183900
H	4.65839500	-1.74966200	0.20301700
H	-1.04343500	1.86099700	1.23919700
C	-2.66671100	1.08723400	0.01518500
C	-4.00837900	-1.33461200	-0.39911500
H	-2.08466200	-2.26124900	-0.03547400
C	-4.02369500	1.08093400	-0.28040800
H	-2.13369000	2.01793000	0.17553900
C	-4.69648200	-0.12696100	-0.48605100
H	-4.52846900	-2.27373600	-0.55937100
H	-4.56286900	2.02053200	-0.35280900
H	-5.75759800	-0.12207700	-0.71612900
H	1.56939600	1.17046700	1.90591600

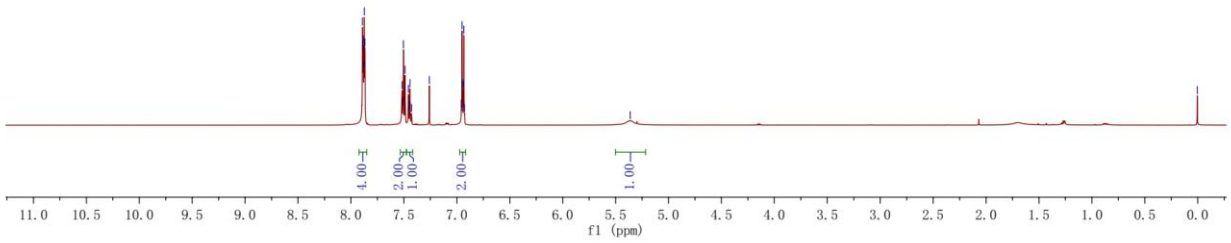
Int22

C	2.16892200	1.48070300	-0.08495200
C	3.25027200	1.02592200	-0.72442900
C	3.76789800	-0.33608300	-0.48760900
C	3.01195500	-1.18980800	0.45004400
C	1.91895000	-0.74314600	1.07652400
C	1.42961100	0.66459300	0.93495400
H	1.78398800	2.48059100	-0.26916400
H	3.78829200	1.63309700	-1.44649000
H	3.38630900	-2.19932200	0.59374600
H	1.36377300	-1.38610400	1.75353500
O	4.77584100	-0.74489600	-1.05515100
N	-0.58377700	-0.24781800	0.39554200
N	-0.01359100	0.82009400	0.65217000
C	-1.98077500	-0.12845700	0.10250500
C	-2.64650400	-1.33480000	-0.10699200

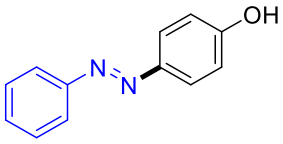


^{1}H NMR (500 MHz, $CDCl_3$)

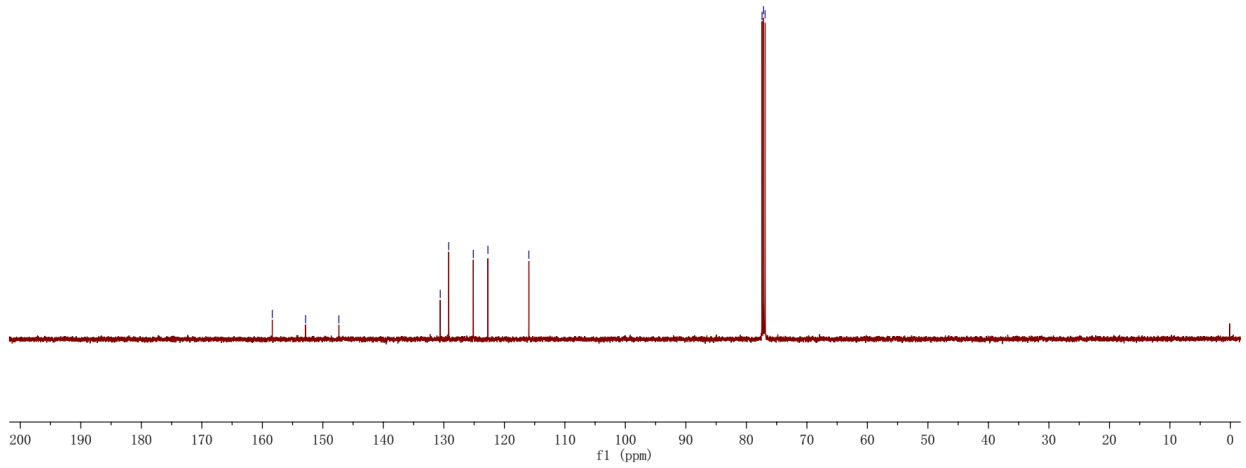
3a

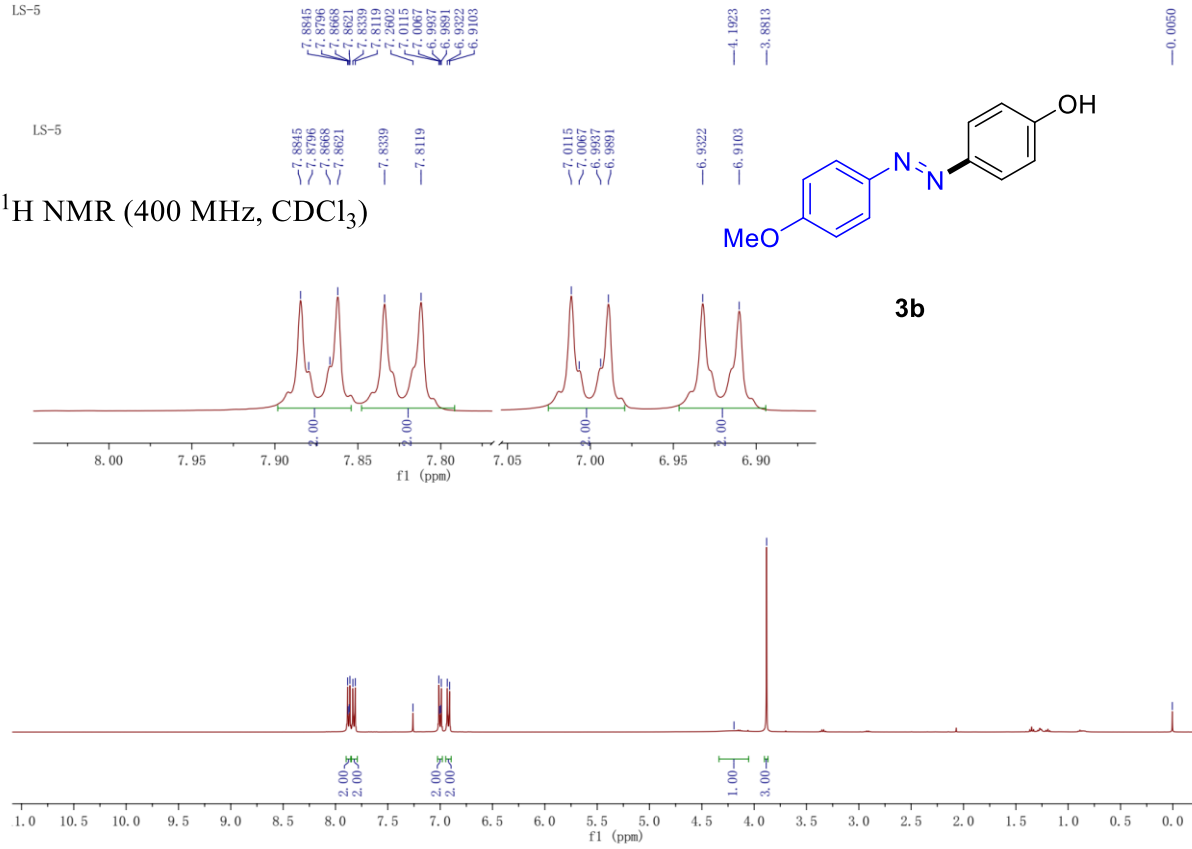


^{13}C NMR (125 MHz, $CDCl_3$)



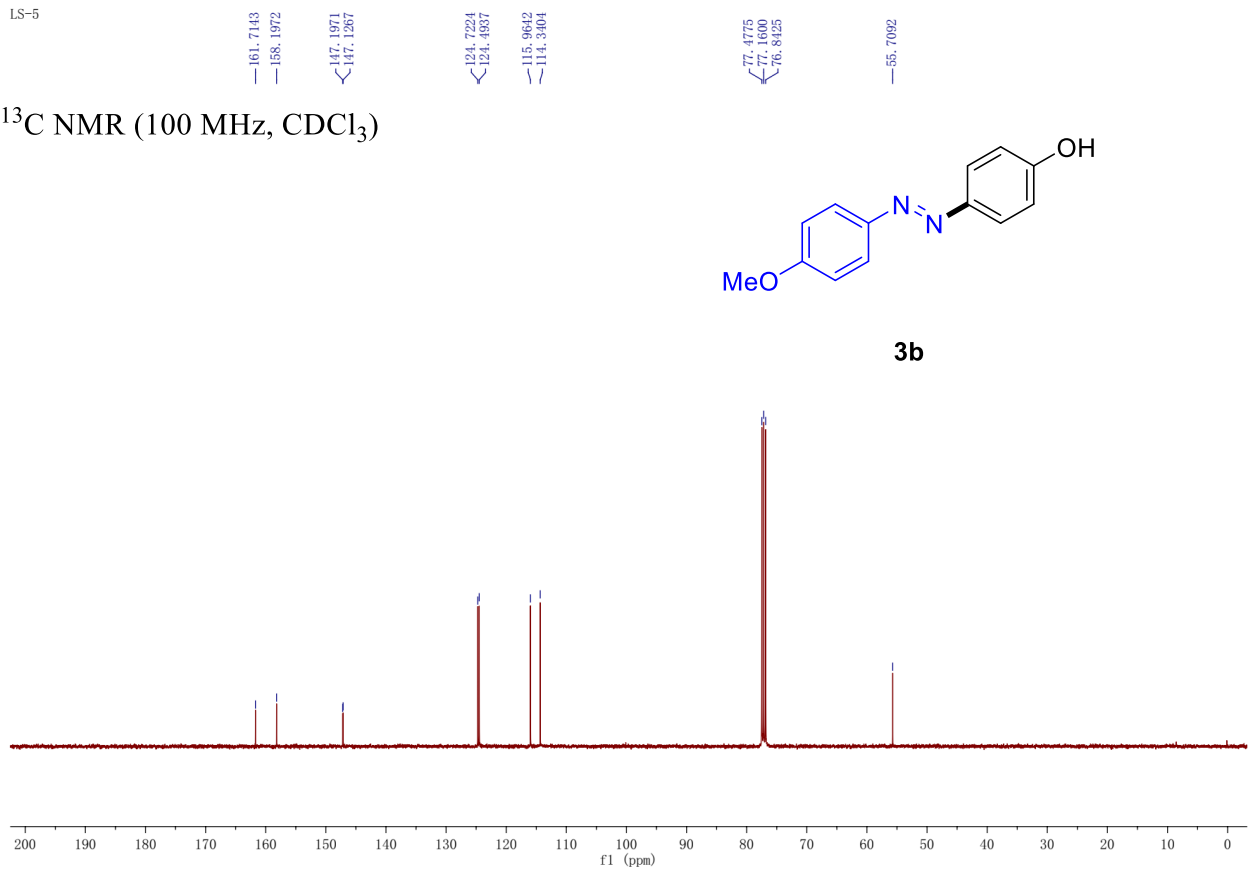
3a





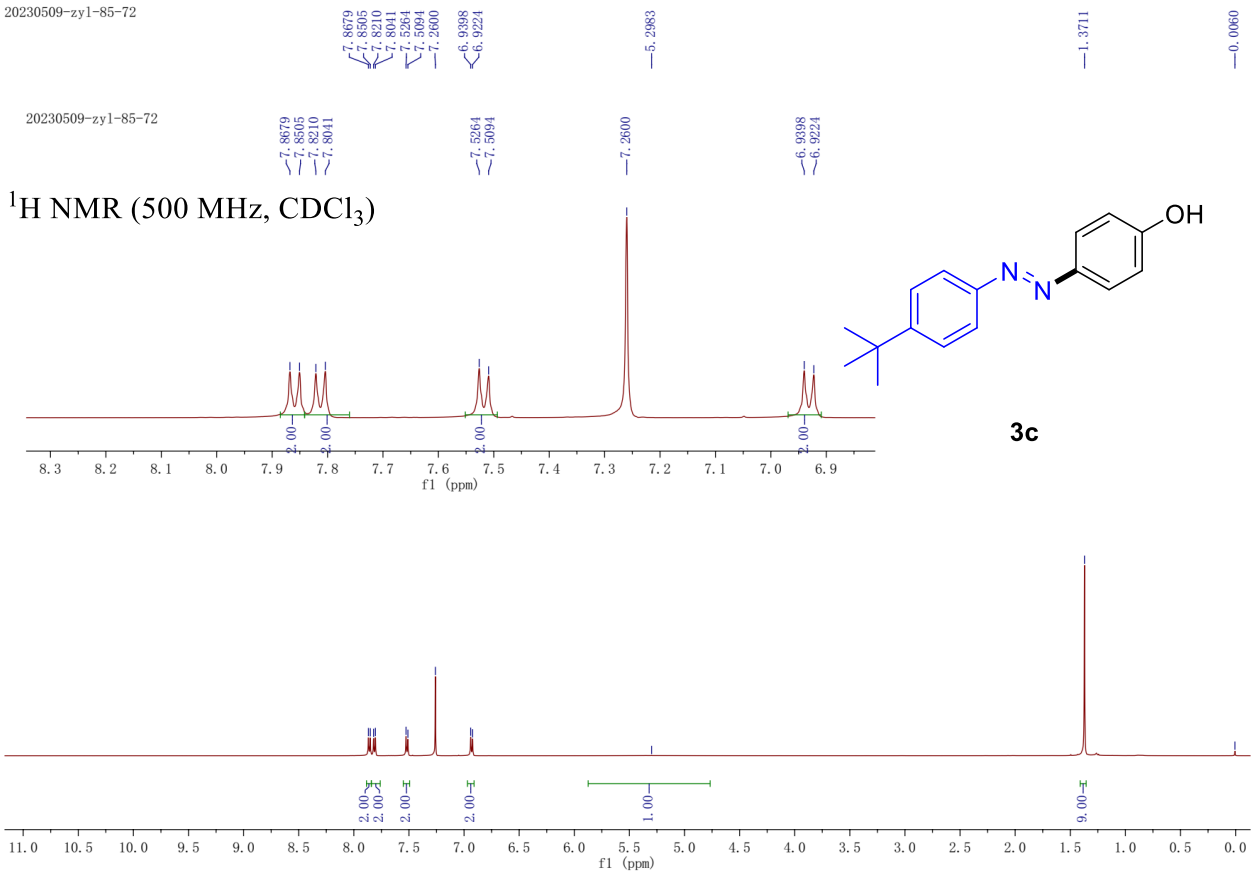
^{1}H NMR (400 MHz, $CDCl_3$)

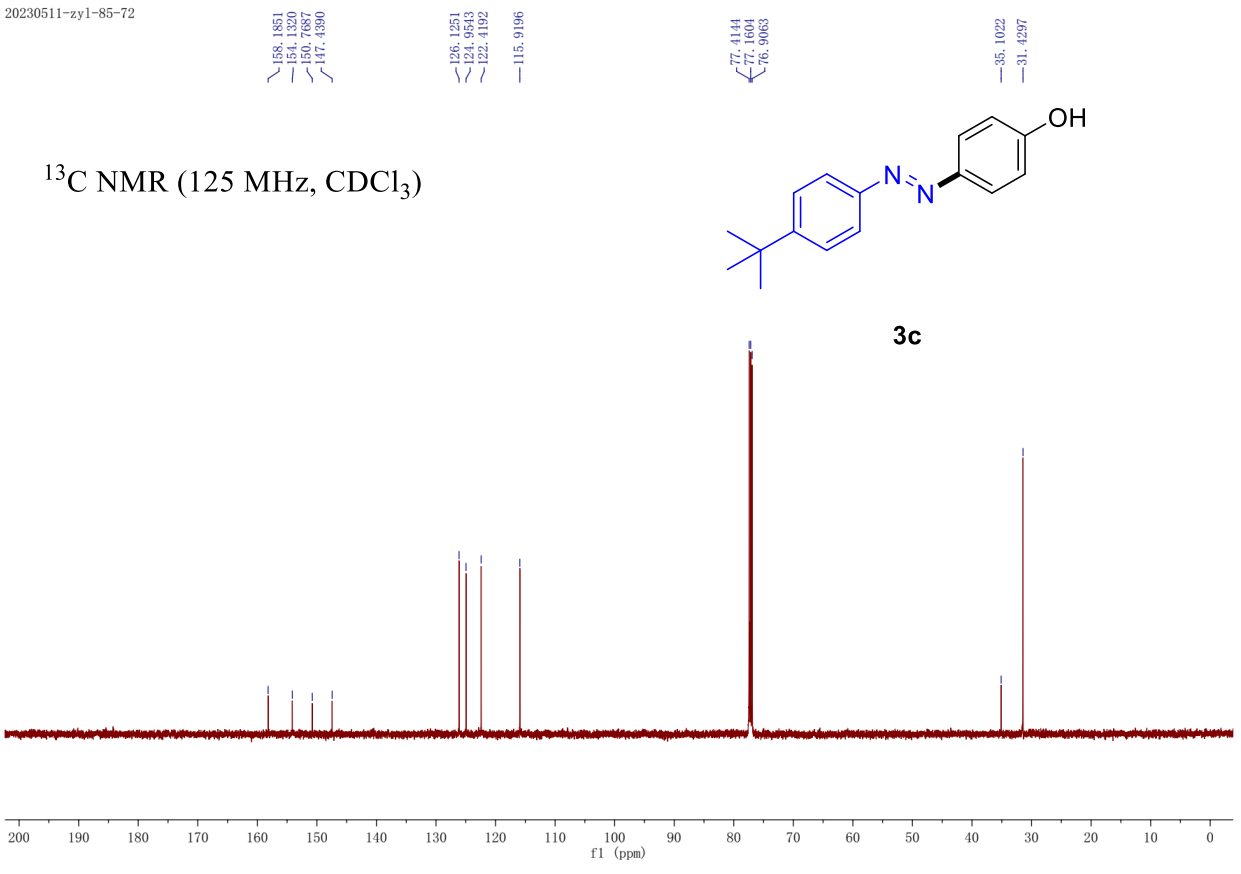
3b



^{13}C NMR (100 MHz, $CDCl_3$)

3b


20230509-zyl-85-72
7.8679
7.8505
7.8210
7.8041
7.5264
7.5094
7.2600
6.9398
6.9224
5.2983
1.3711
0.0060
20230509-zyl-85-72
7.8679
7.8505
7.8210
7.8041
7.5264
7.5094
7.2600
6.9398
6.9224
1H NMR (500 MHz, CDCl3)
OH
N
N
3c
2.00
2.00
2.00
2.00
2.00
8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9
f1 (ppm)
2.00
2.00
2.00
2.00
1.00
9.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


20230511-zyl-85-72
158.1851
154.1320
150.7687
147.4390
126.1251
124.9543
122.4192
115.9196
77.4144
77.1604
76.9063
35.1022
31.4297
13C NMR (125 MHz, CDCl3)
OH
N
N
3c
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

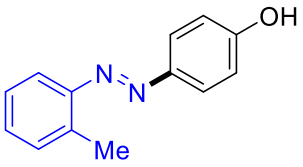
20230515-zyl-85-82

7.8761
7.8585
7.3228
7.3202
7.3178
7.3118
6.9422
6.9246
4.1297
2.6880

20230515-zyl-85-82

7.8761
7.8585
7.5878
7.5720
7.3228
7.3202
7.3178
7.3118
7.2604
7.2533
7.2493
7.2439
7.2370
7.2270
6.9422
6.9246

^{1}H NMR (500 MHz, $CDCl_3$)

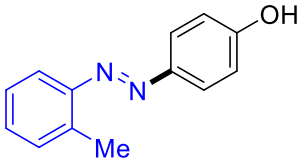


3d

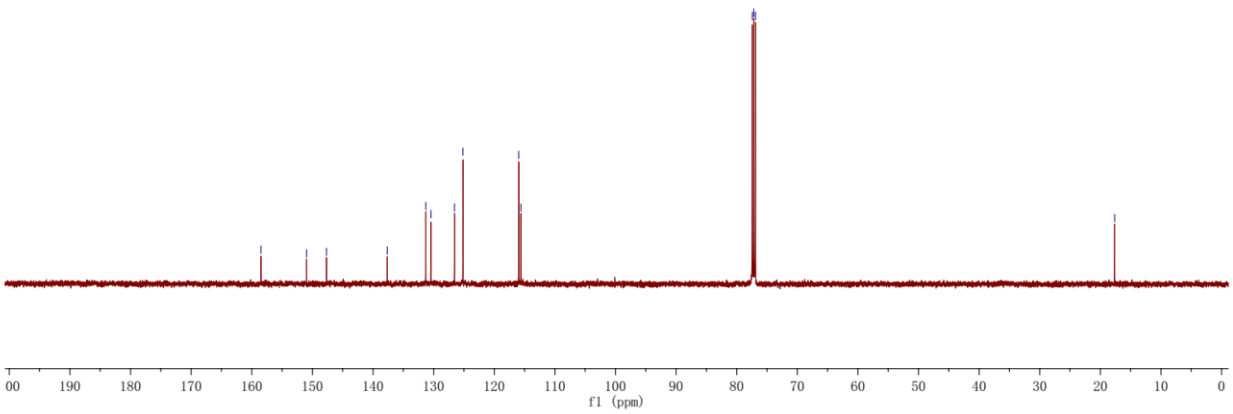
20230517-zyl-85-82

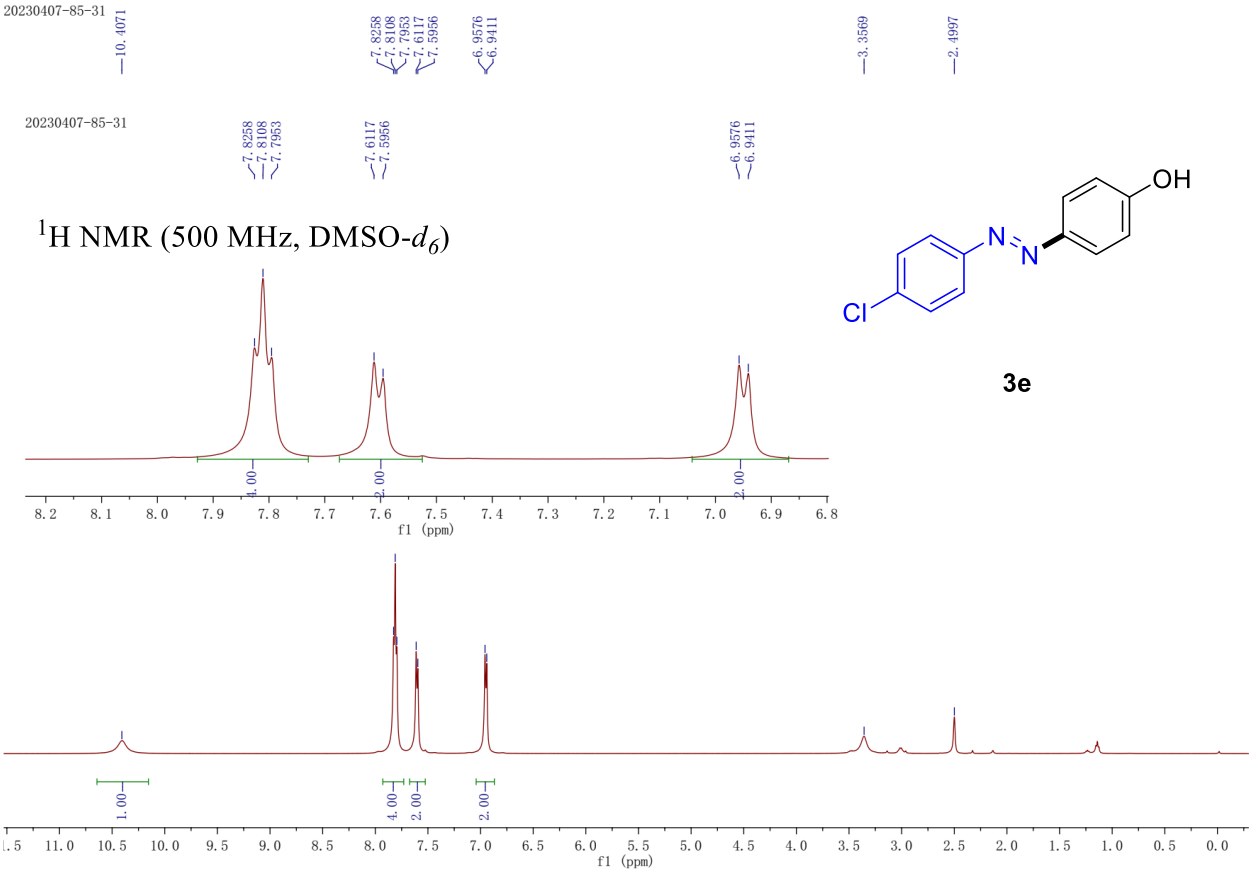
158.4744
150.9539
147.6676
137.6369
131.2950
130.4550
126.5528
125.1605
115.9553
115.5750
77.4142
77.1603
76.9064
17.6450

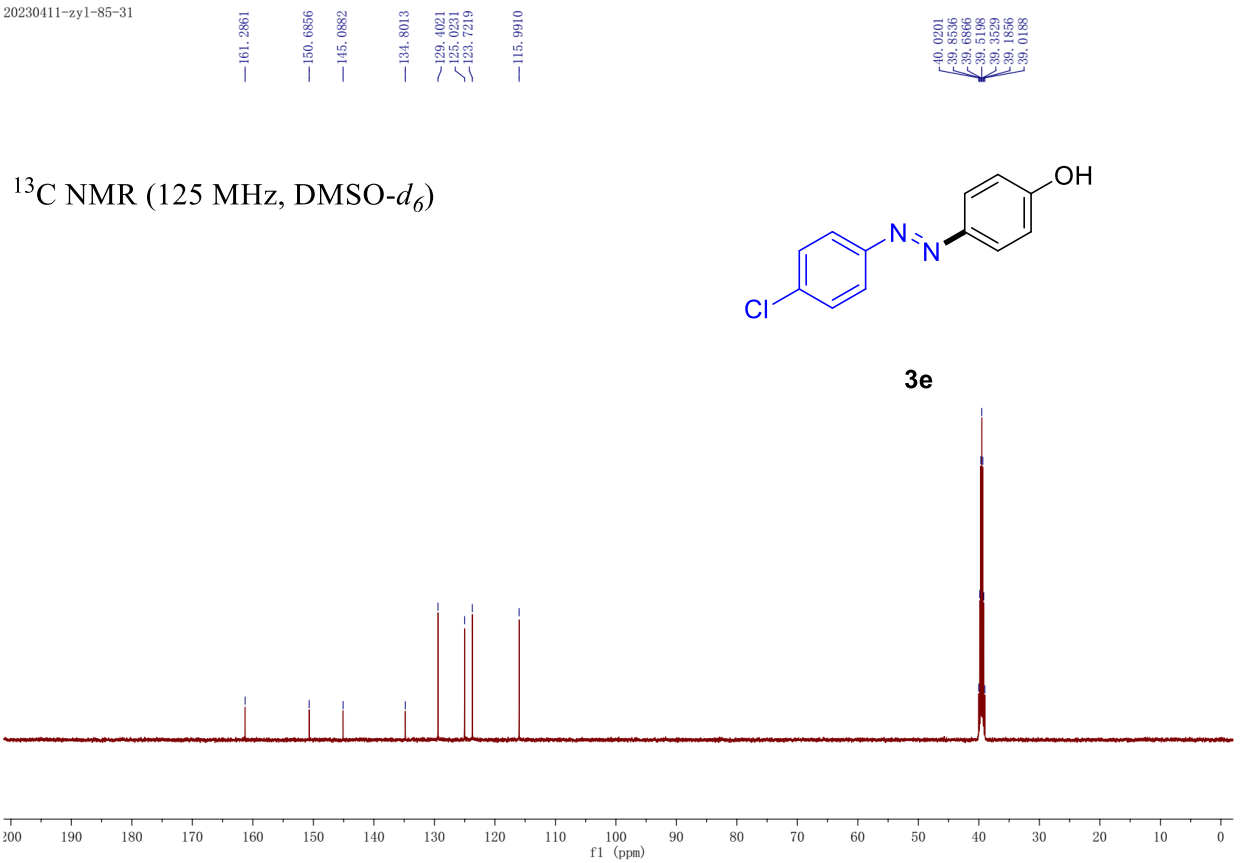
^{13}C NMR (125 MHz, $CDCl_3$)

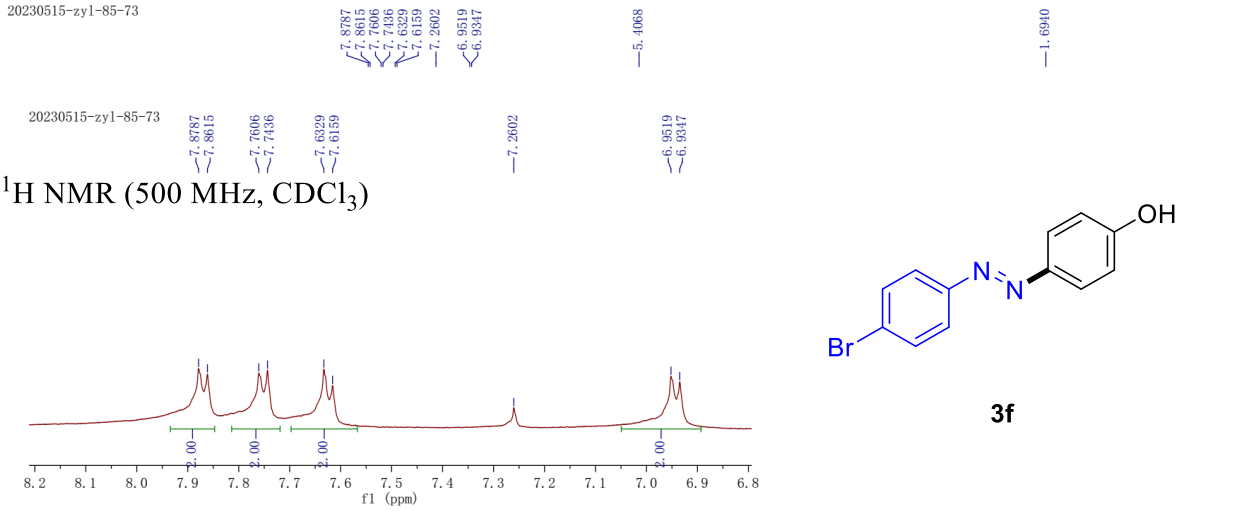


3d



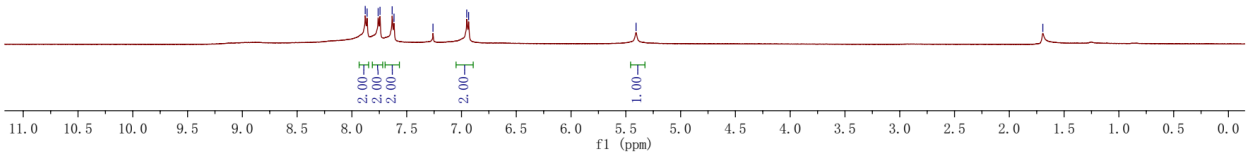

20230407-85-31
10.4071
7.8258
7.8108
7.7953
7.6117
7.5956
6.9576
6.9411
3.3569
2.4997
20230407-85-31
7.8258
7.8108
7.7953
7.6117
7.5956
6.9576
6.9411
1H NMR (500 MHz, DMSO-d6)
OH
N
N
Cl
3e
4.00
2.00
2.00
f1 (ppm)
1.00
4.00
2.00
2.00
f1 (ppm)

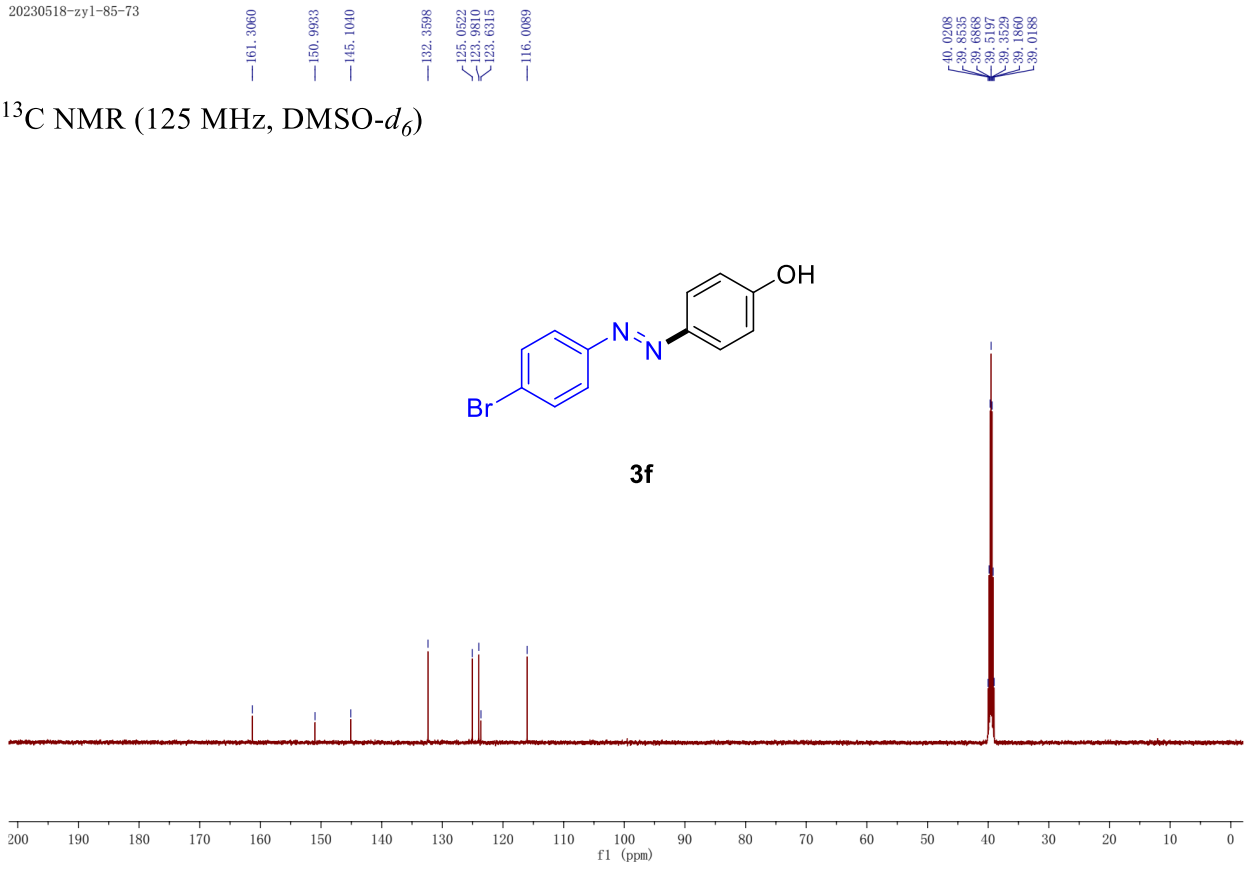

20230411-zyl-85-31
161.2861
150.6856
145.0882
134.8013
129.4021
125.0231
123.7219
115.9910
40.0201
39.8536
39.6866
39.5198
39.3529
39.1856
39.0188
13C NMR (125 MHz, DMSO-d6)
OH
N
N
Cl
3e
f1 (ppm)



^{1}H NMR (500 MHz, $CDCl_3$)

3f





^{13}C NMR (125 MHz, DMSO-d_6)

3f

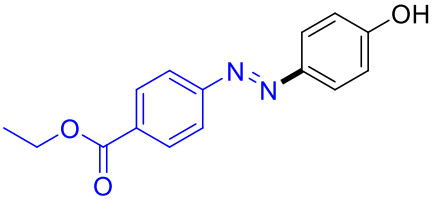
LS-2-7

8.1881
8.1672
7.9161
7.9089
7.8943
7.8876
7.2604
6.9884
6.9667
6.2277
4.4510
4.4332
4.4154
4.3976
1.4485
1.4307
1.4129
0.0000

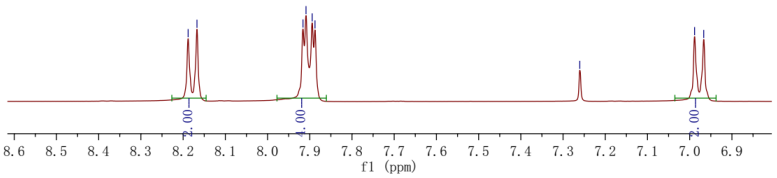
LS-2-7

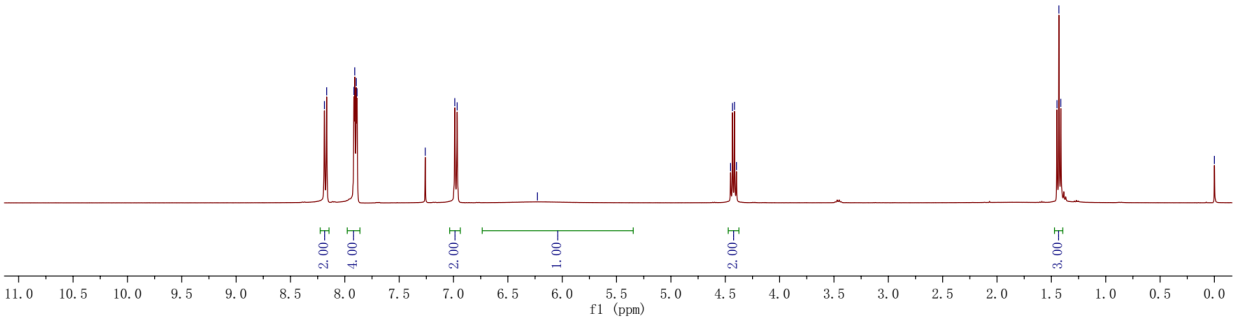
8.1881
8.1672
7.9161
7.9089
7.8943
7.8876
7.2604
6.9884
6.9667

^{1}H NMR (400 MHz, $CDCl_3$)



3g

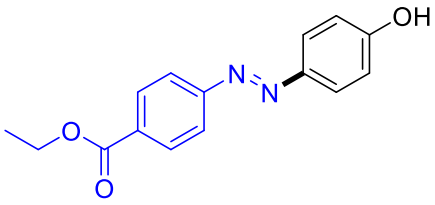




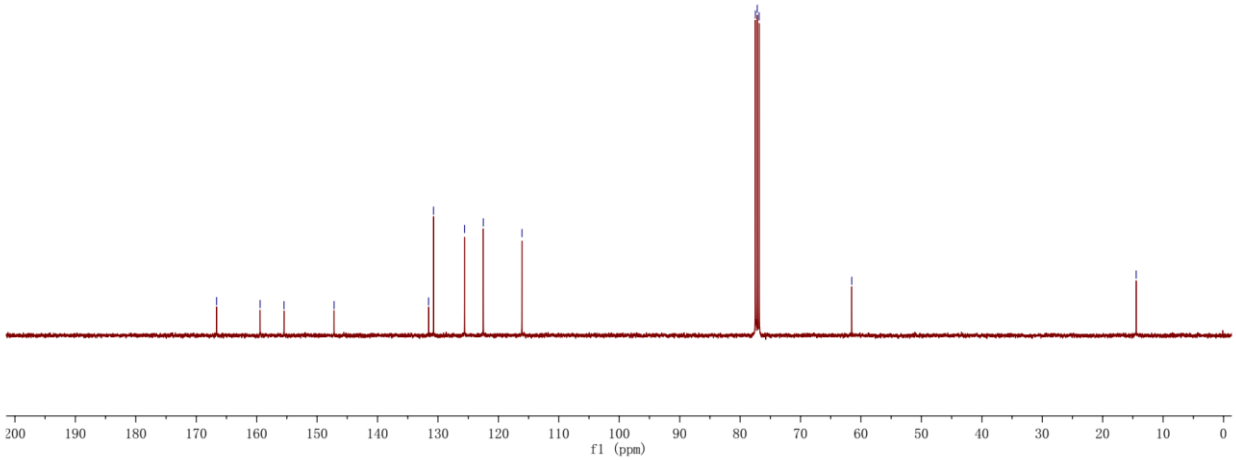
LS-2-7

166.6469
159.4298
155.4696
147.1860
131.5465
130.7257
125.5840
122.4970
116.1088
77.4777
77.1601
76.8426
61.5291
14.4569

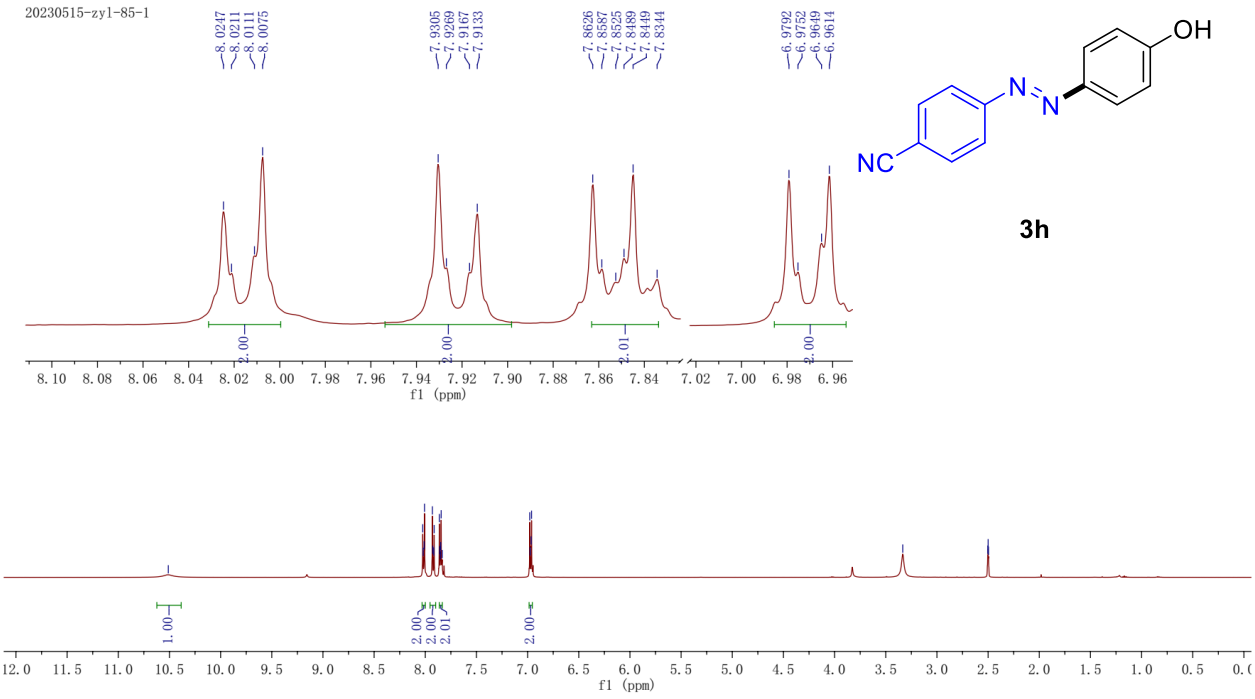
^{13}C NMR (100 MHz, $CDCl_3$)

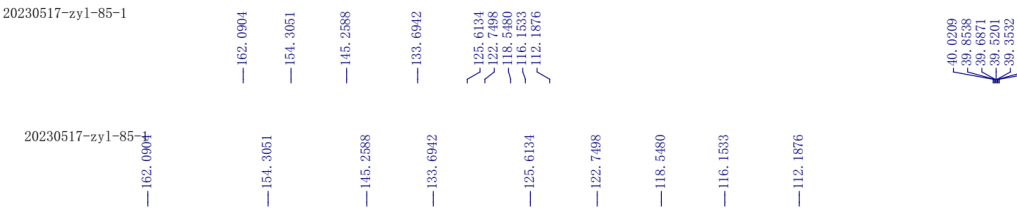


3g

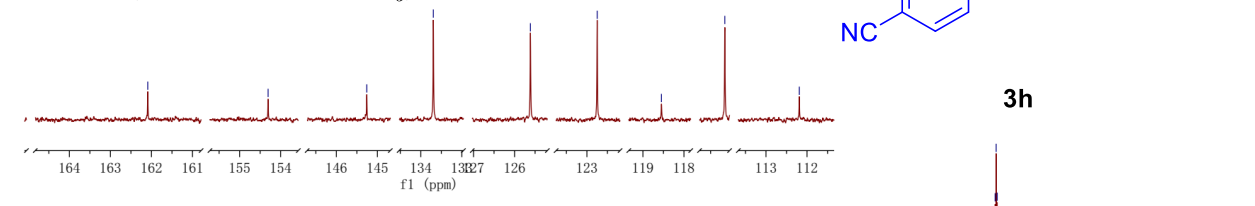


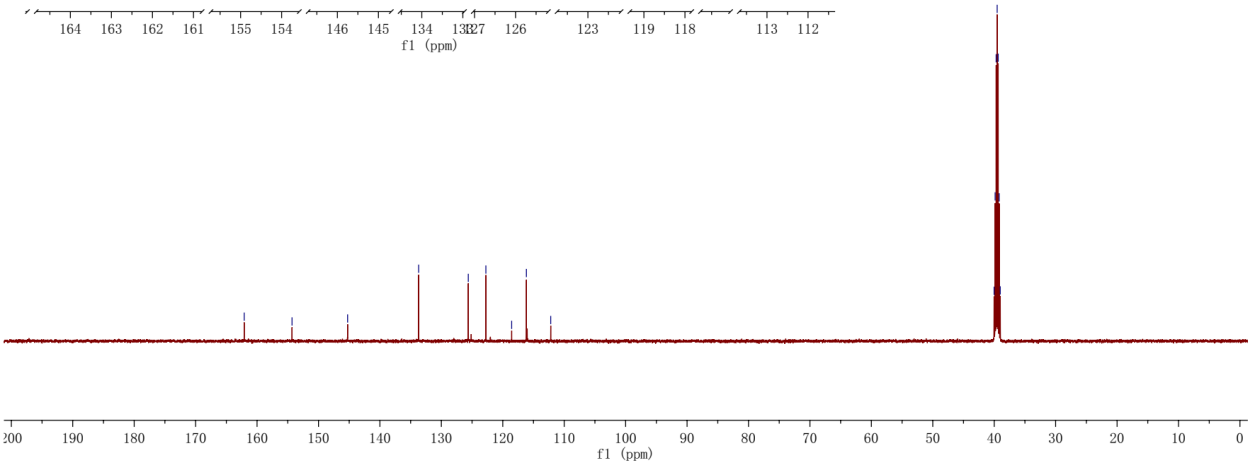
^{1}H NMR (500 MHz, DMSO-d_6)

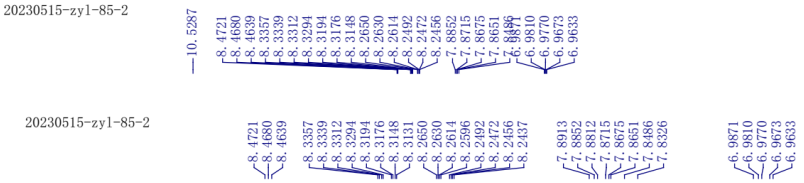




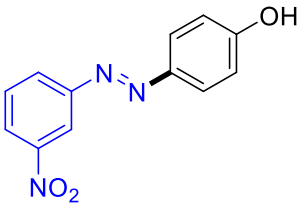
^{13}C NMR (125 MHz, DMSO-d_6)



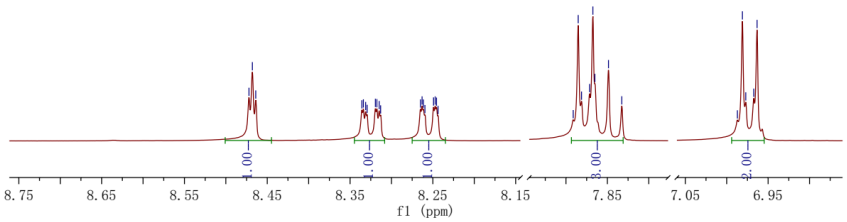


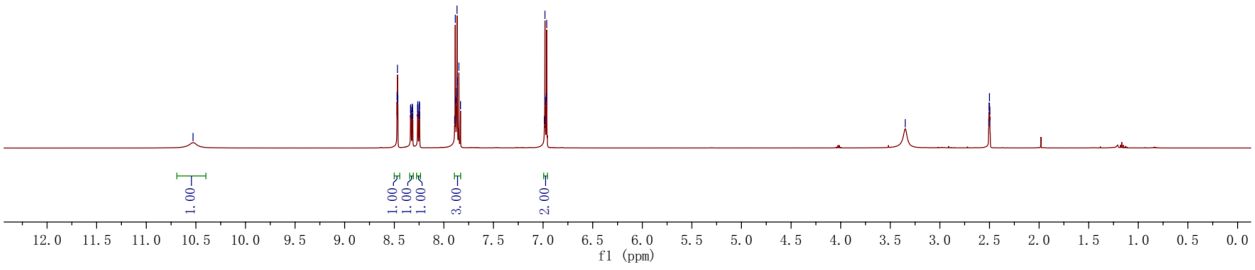


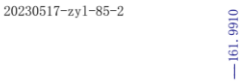
^{1}H NMR (500 MHz, DMSO-d_6)

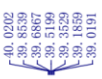


3i

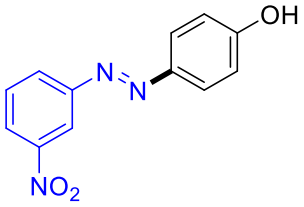




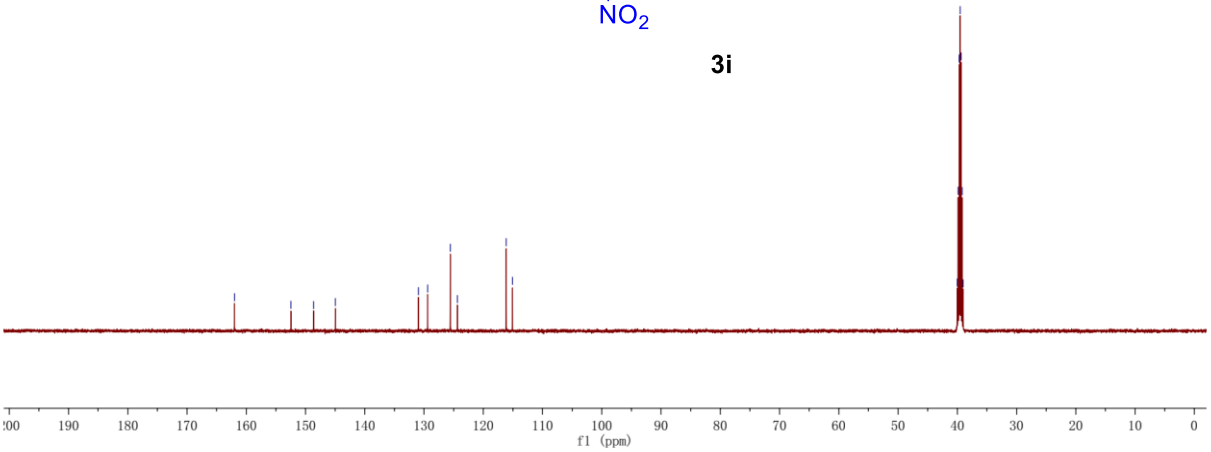




^{13}C NMR (125 MHz, DMSO-d_6)



3i

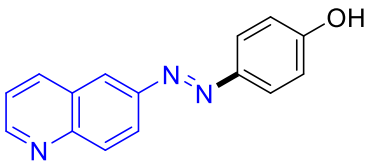


20230515-zy1-85-74

10.3838
8.9641
8.9609
8.9558
8.9526
8.5559
8.4857
8.4817
8.1942
8.1899
8.1292
8.1111
7.8862
7.8686
7.6280
7.6196
6.9927
6.9751
3.3444
2.5039
2.5005
2.4970

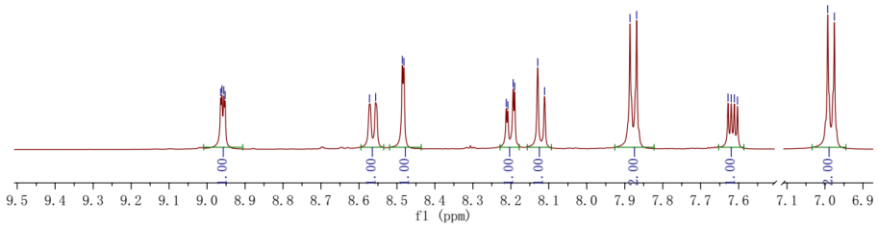
20230515-zy1-85-74

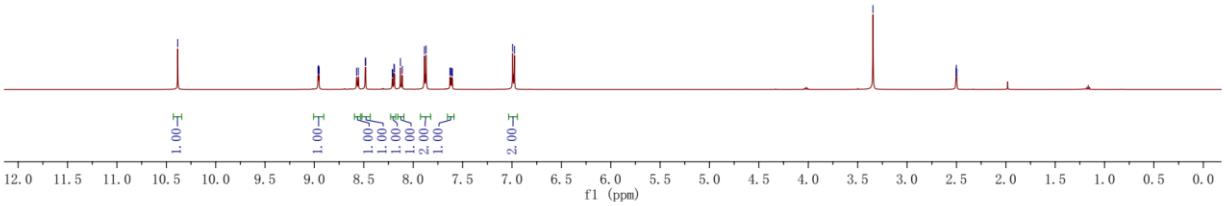
8.9641
8.9609
8.9558
8.9526
8.5724
8.5559
8.4857
8.4817
8.2123
8.2080
8.1942
8.1899
8.1292
8.1111
7.8862
7.8686
7.6280
7.6196
7.6115
7.6031
6.9927
6.9751



3j

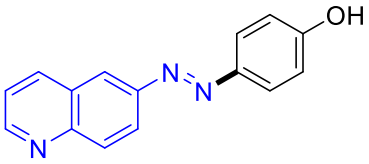
^{1}H NMR (500 MHz, DMSO-d_6)





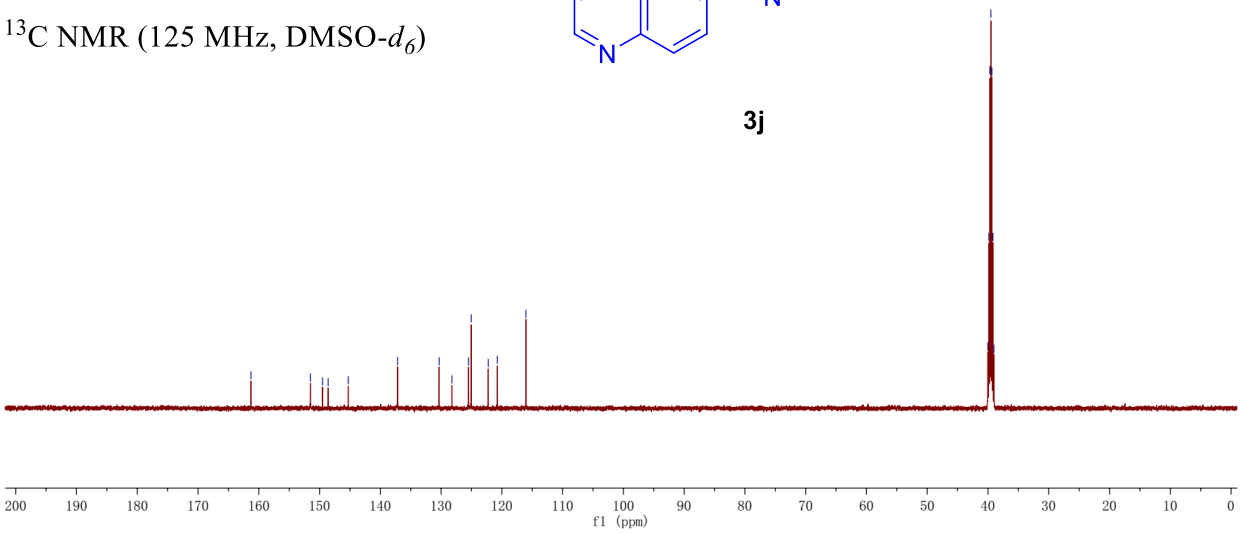
20230517-zy1-85-74

161.2868
151.5216
149.5038
148.5815
145.2898
137.1780
130.3250
128.2180
125.4753
125.0366
122.2416
120.7382
116.0421
40.0205
39.8533
39.6864
39.5196
39.3525
39.1856
39.0202



3j

^{13}C NMR (125 MHz, DMSO-d_6)

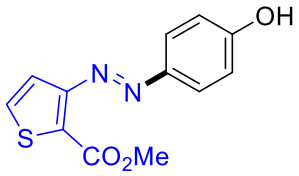


20230518-zyl-85-83

10.4340
7.9044
7.8936
7.8285
7.8224
7.8184
7.8087
7.8047
7.7987
7.3956
7.3848
6.9751
6.9691
6.9651
6.9553
6.9514
6.9452
3.8750
3.3304
2.5036
2.5001
2.4965
2.4931

20230518-zyl-85-83

^{1}H NMR (500 MHz, DMSO-d_6)

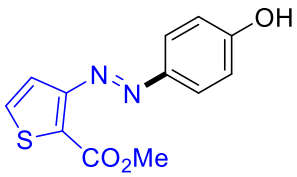


3k

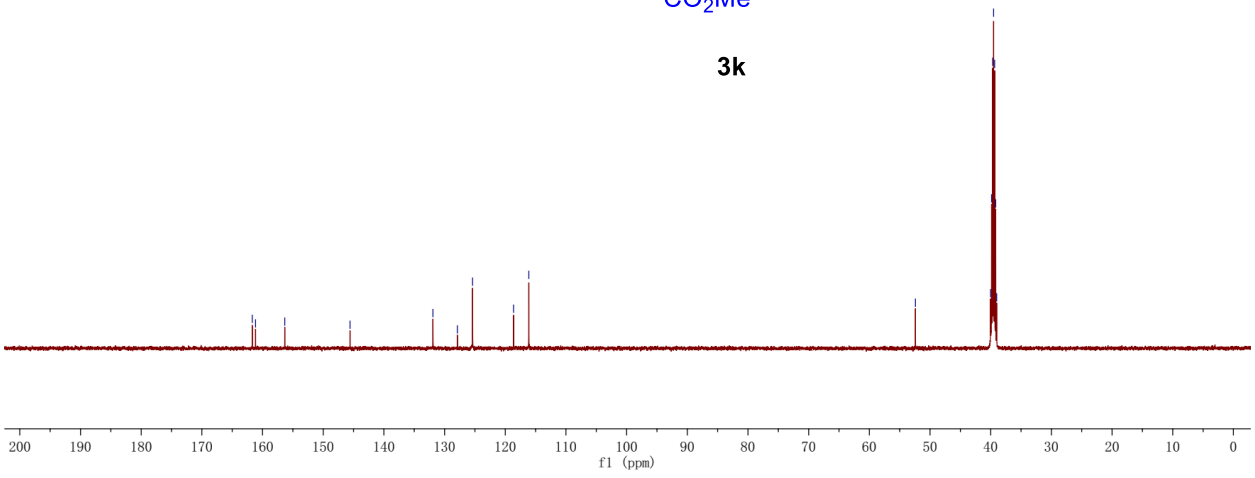
20230519-zyl-85-83

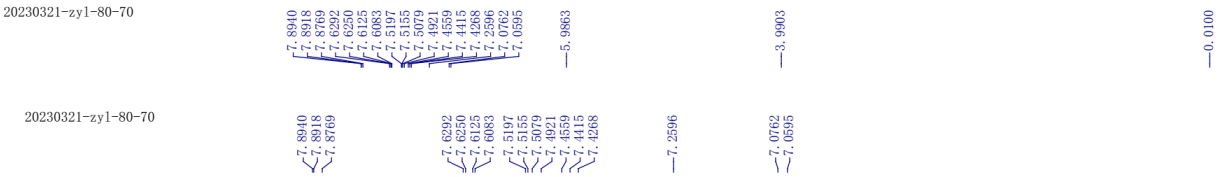
161.6925
161.1487
156.3313
145.5817
131.9187
127.8937
125.3850
118.6330
116.1158
52.4028
40.0205
39.8534
39.6865
39.5196
39.3528
39.1857
39.0187

^{13}C NMR (125 MHz, DMSO-d_6)

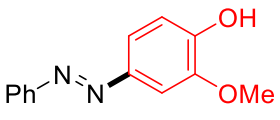


3k

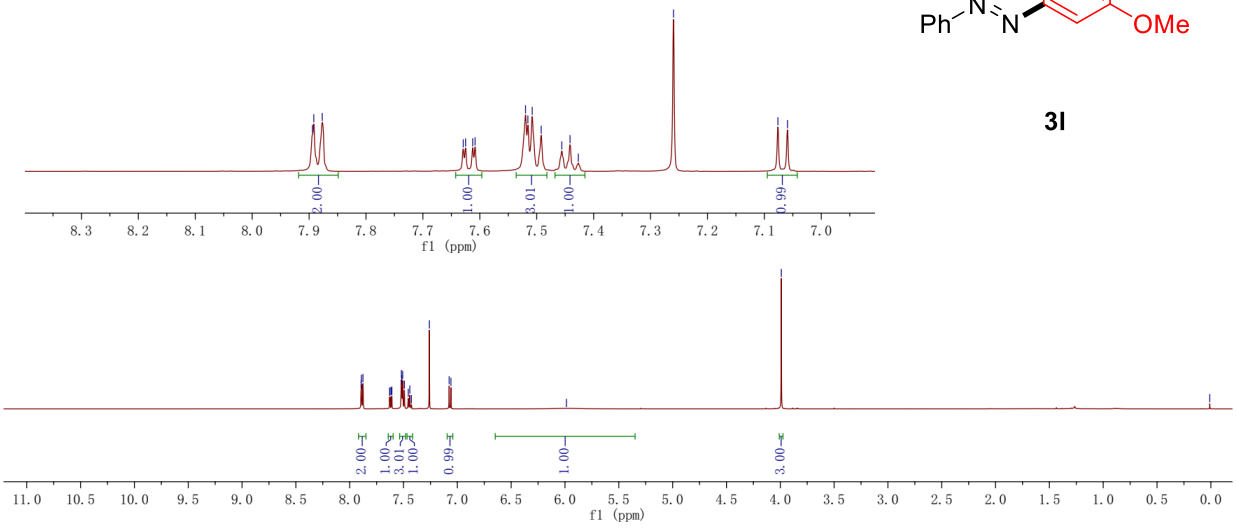




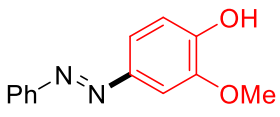
^{1}H NMR (500 MHz, $CDCl_3$)



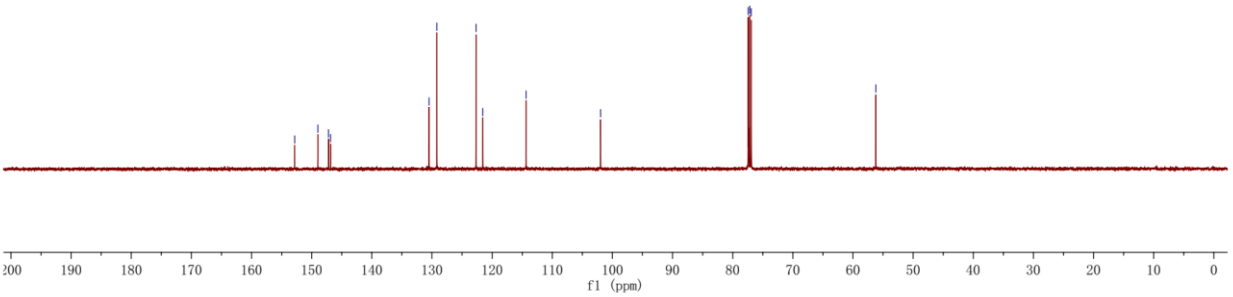
3l

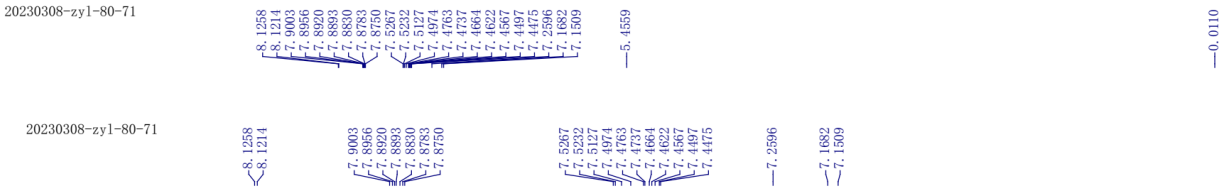


^{13}C NMR (125 MHz, $CDCl_3$)



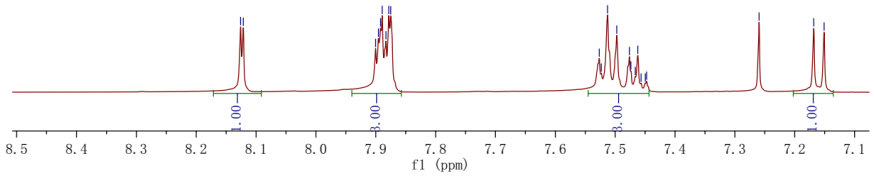
3l

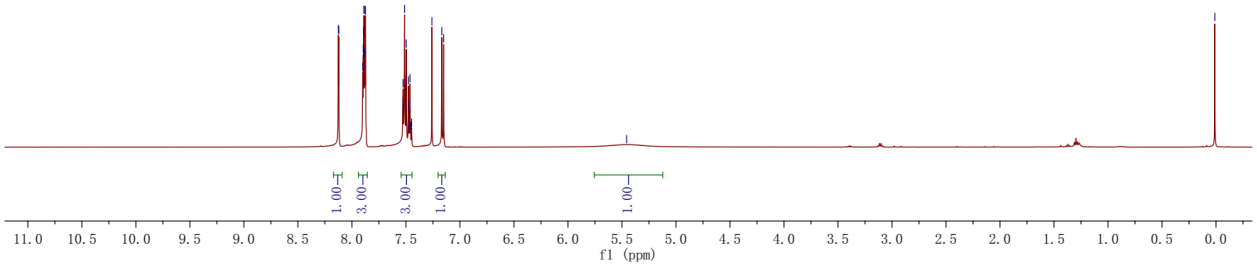




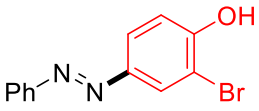
^{1}H NMR (500 MHz, $CDCl_3$)

3m

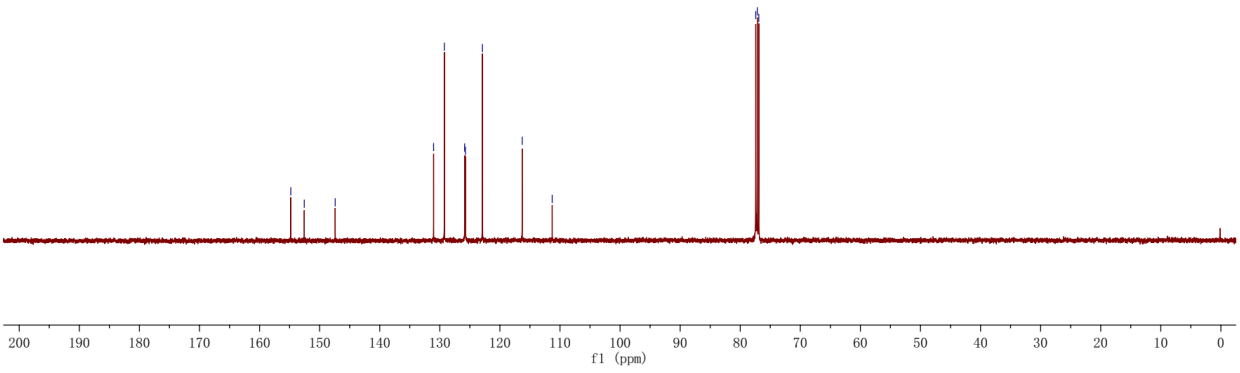


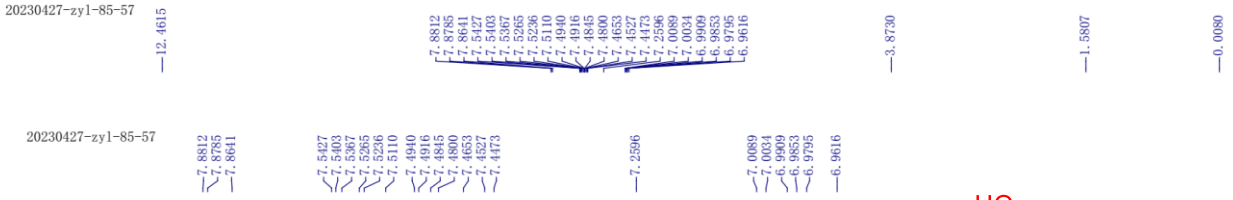


^{13}C NMR (125 MHz, $CDCl_3$)

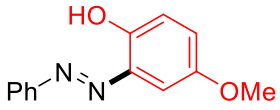


3m

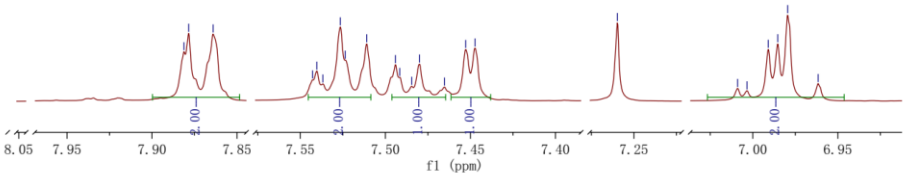


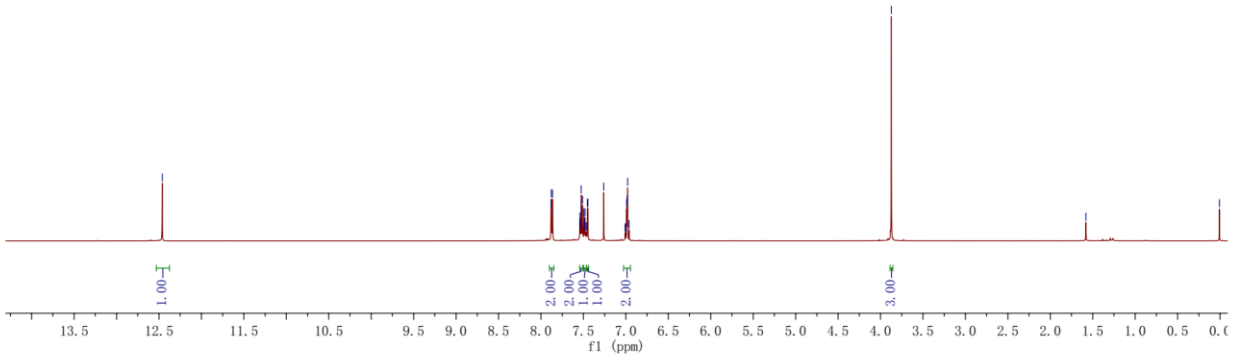


^{1}H NMR (500 MHz, $CDCl_3$)

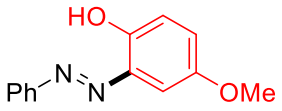


3n

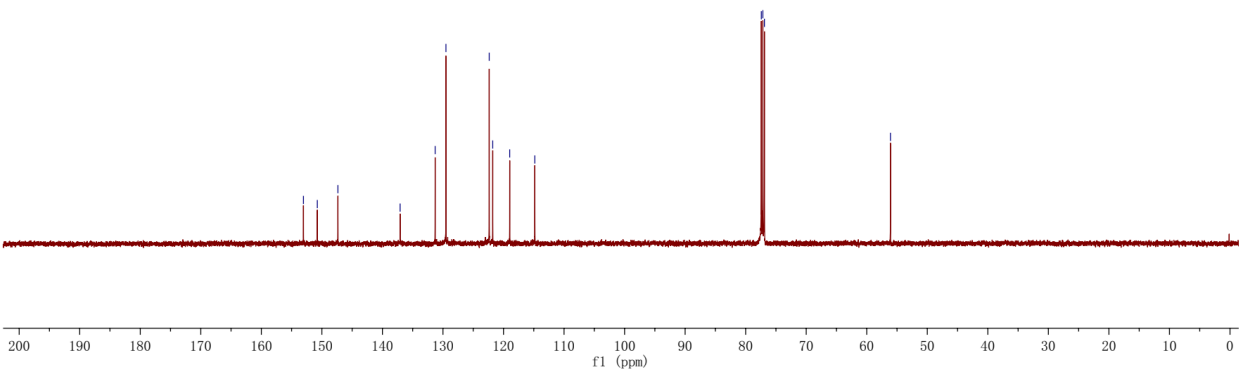




^{13}C NMR (125 MHz, $CDCl_3$)



3n



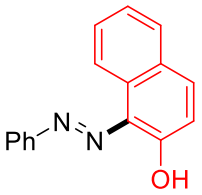
ZYL-80-122-H-20221121-ZYL

8.5494 8.5332 7.7289 7.7136 7.7031 7.6835 7.5708 7.5411 7.4882 7.4727 7.4640 7.4572 6.8552 6.8457 6.8366 1.6484 0.0160

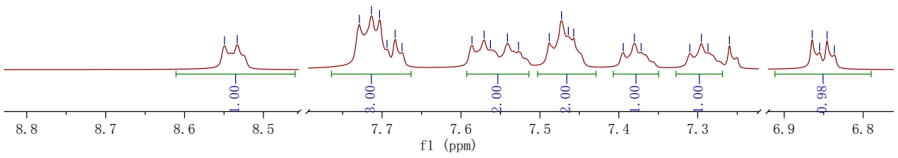
ZYL-80-122-H-20221121-ZYL

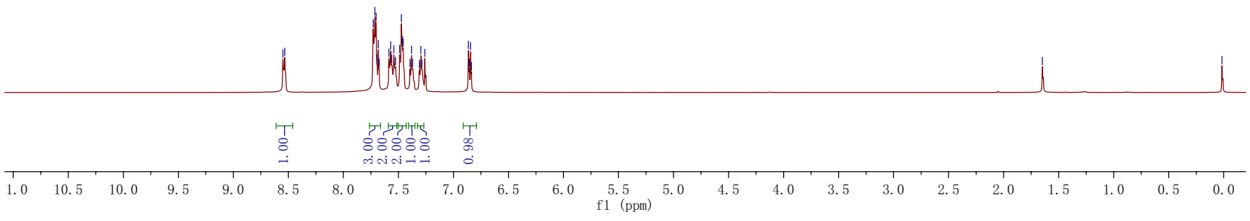
8.5494 8.5332 7.7289 7.7136 7.7031 7.6937 7.6835 7.6748 7.5861 7.5708 7.5626 7.5411 7.5271 7.4882 7.4727 7.4640 7.4572 7.3944 7.3802 7.3718 7.3100 7.2955 7.2871 7.2598 6.8645 6.8552 6.8457 6.8366

^{1}H NMR (500 MHz, $CDCl_3$)



3o

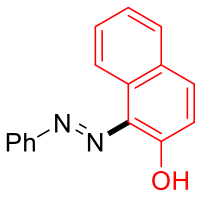




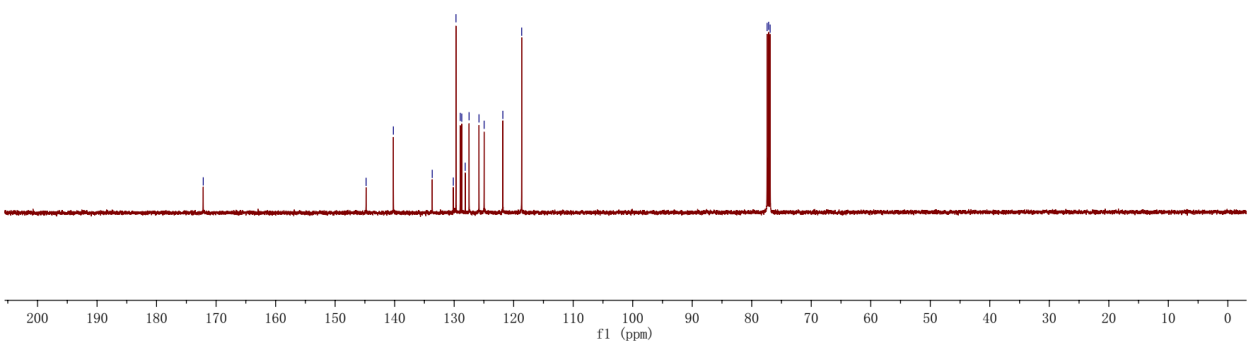
ZYL-80-122-C-20221130-ZYL

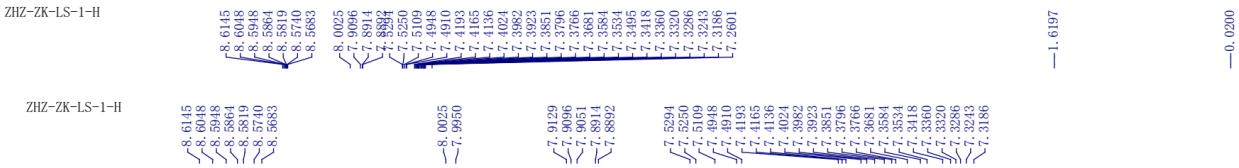
172.1651 144.7966 140.2111 133.6843 130.1427 129.6898 128.9665 128.7221 128.1424 127.4927 125.8242 124.9622 121.8188 118.6517 77.4144 77.1602 76.9062

^{13}C NMR (125 MHz, $CDCl_3$)

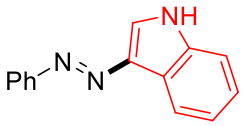


3o

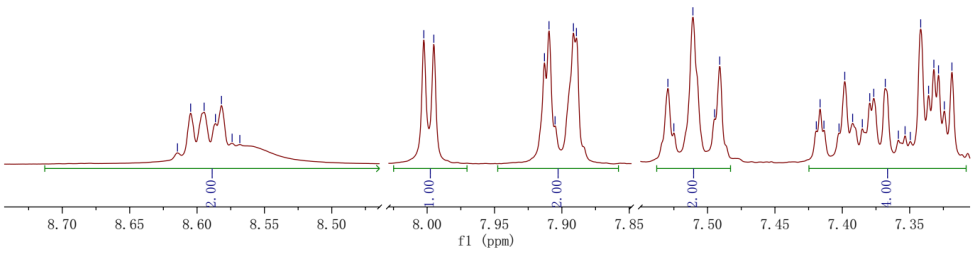


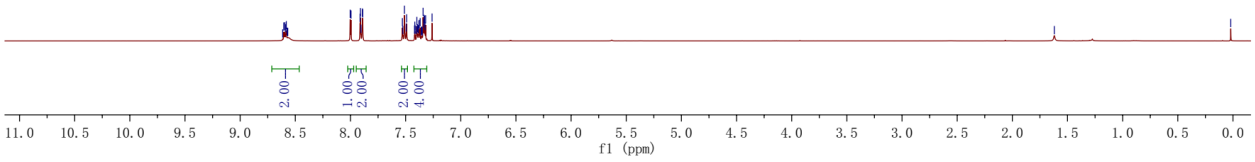


^{1}H NMR (400 MHz, $CDCl_3$)

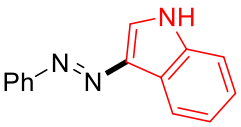


3p

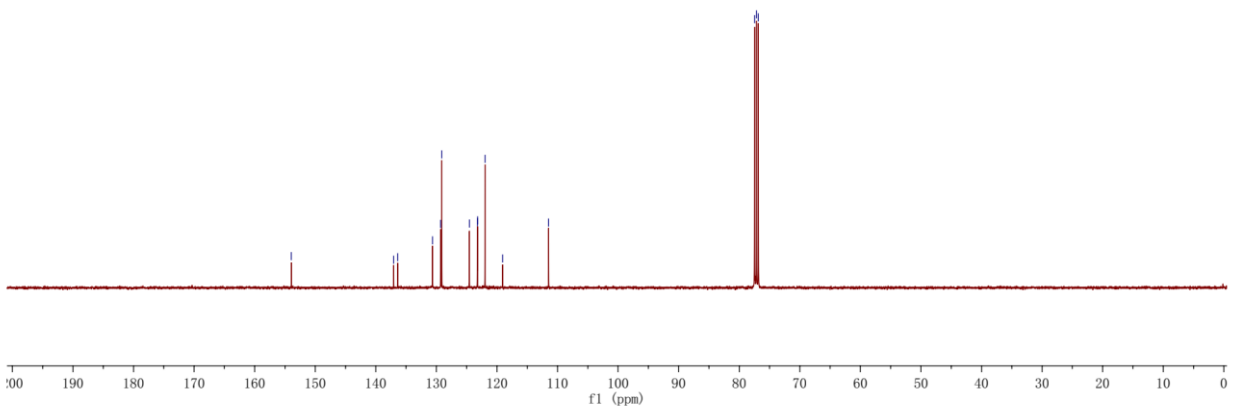


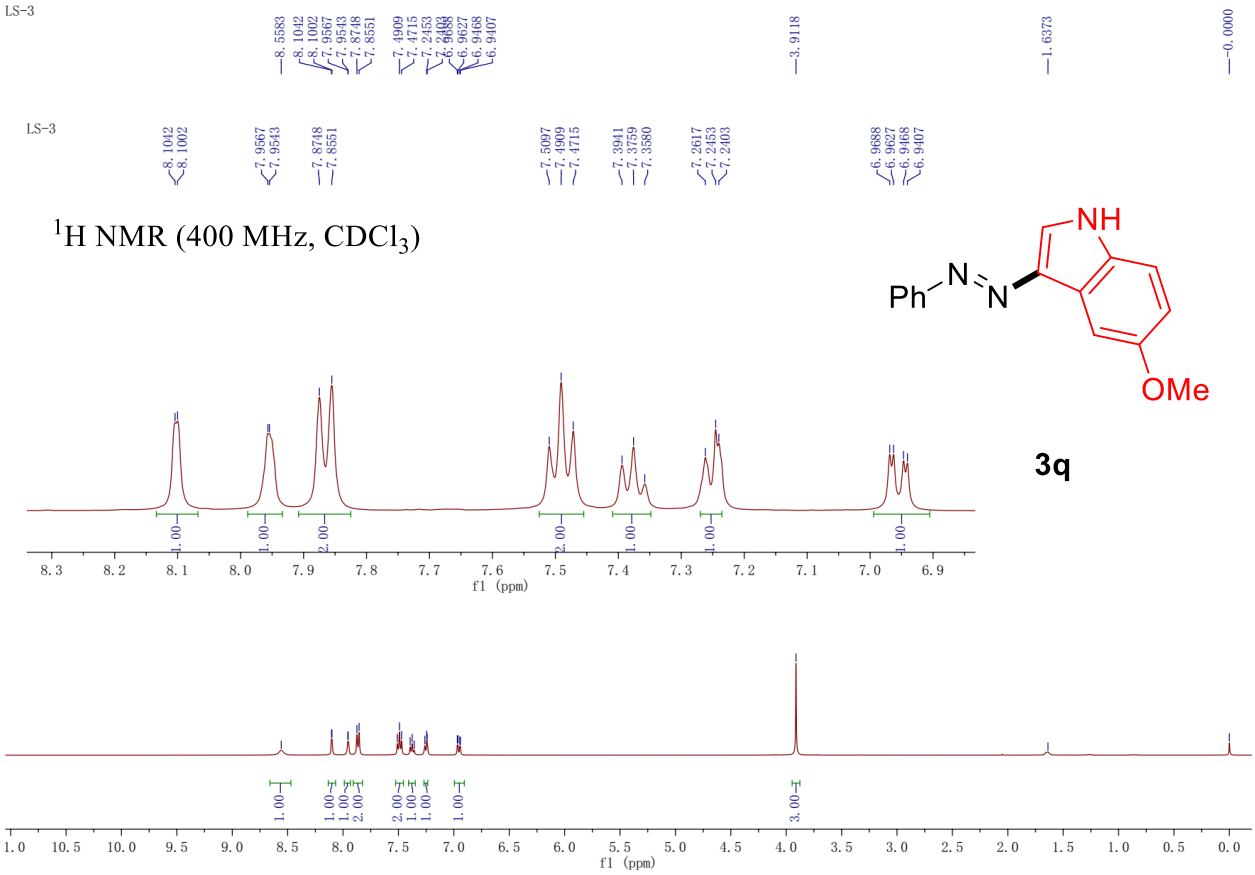


^{13}C NMR (100 MHz, $CDCl_3$)



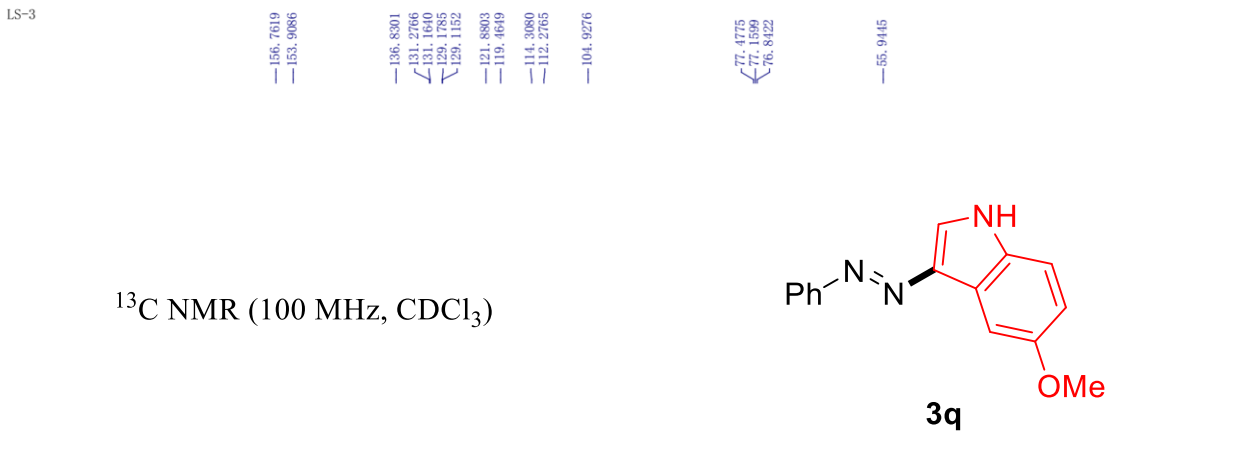
3p





^{1}H NMR (400 MHz, $CDCl_3$)

3q



^{13}C NMR (100 MHz, $CDCl_3$)

3q

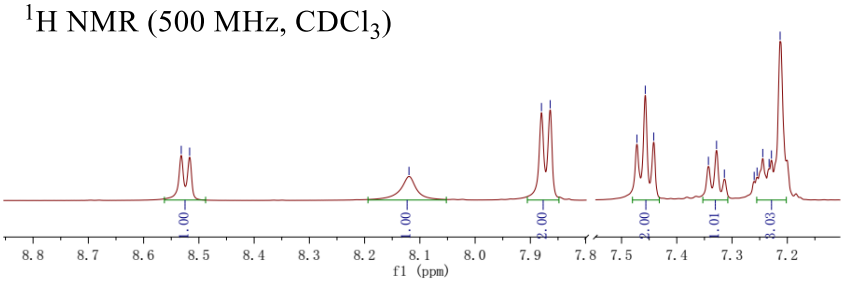
20230309-zyl-80-69

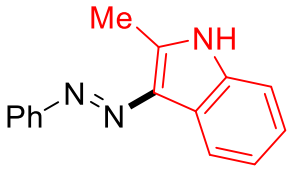
8.5319 8.5167 8.1197 7.8799 7.8641 7.4722 7.4570 7.4418 7.3428 7.3281 7.3139 7.2600 7.2547 7.2444 7.2329 7.2287 7.2130 2.7375 0.0100

20230309-zyl-80-69

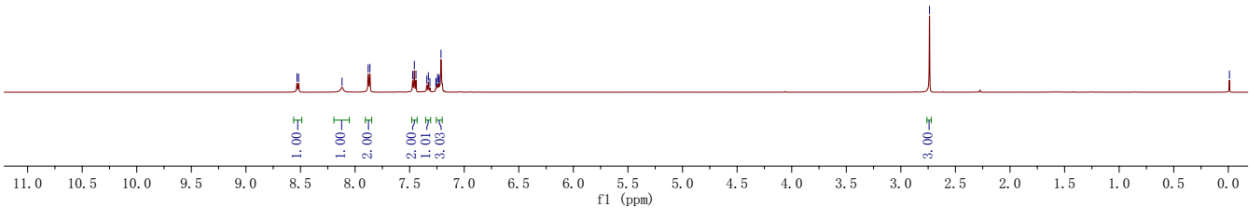
8.5319 8.5167 8.1197 7.8799 7.8641 7.4722 7.4570 7.4418 7.3428 7.3281 7.3139 7.2600 7.2547 7.2444 7.2329 7.2287 7.2130

^{1}H NMR (500 MHz, $CDCl_3$)





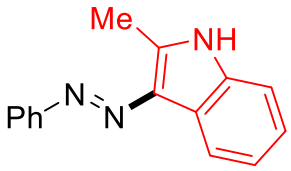
3r



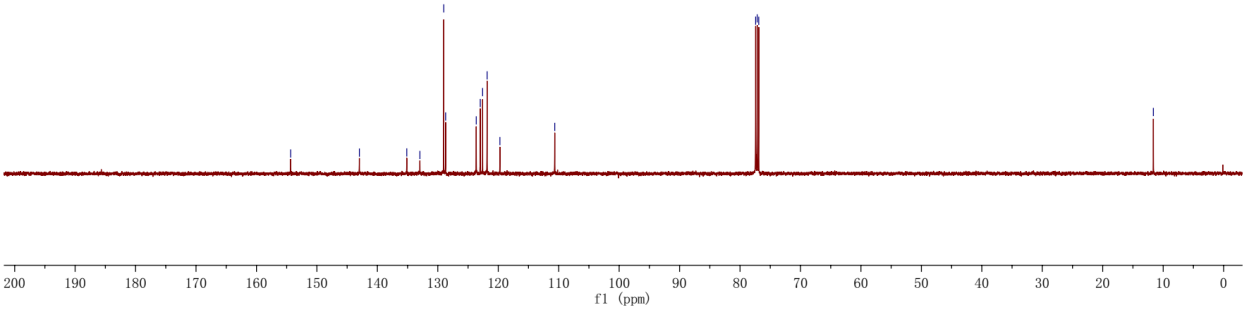
20230310-zyl-80-69

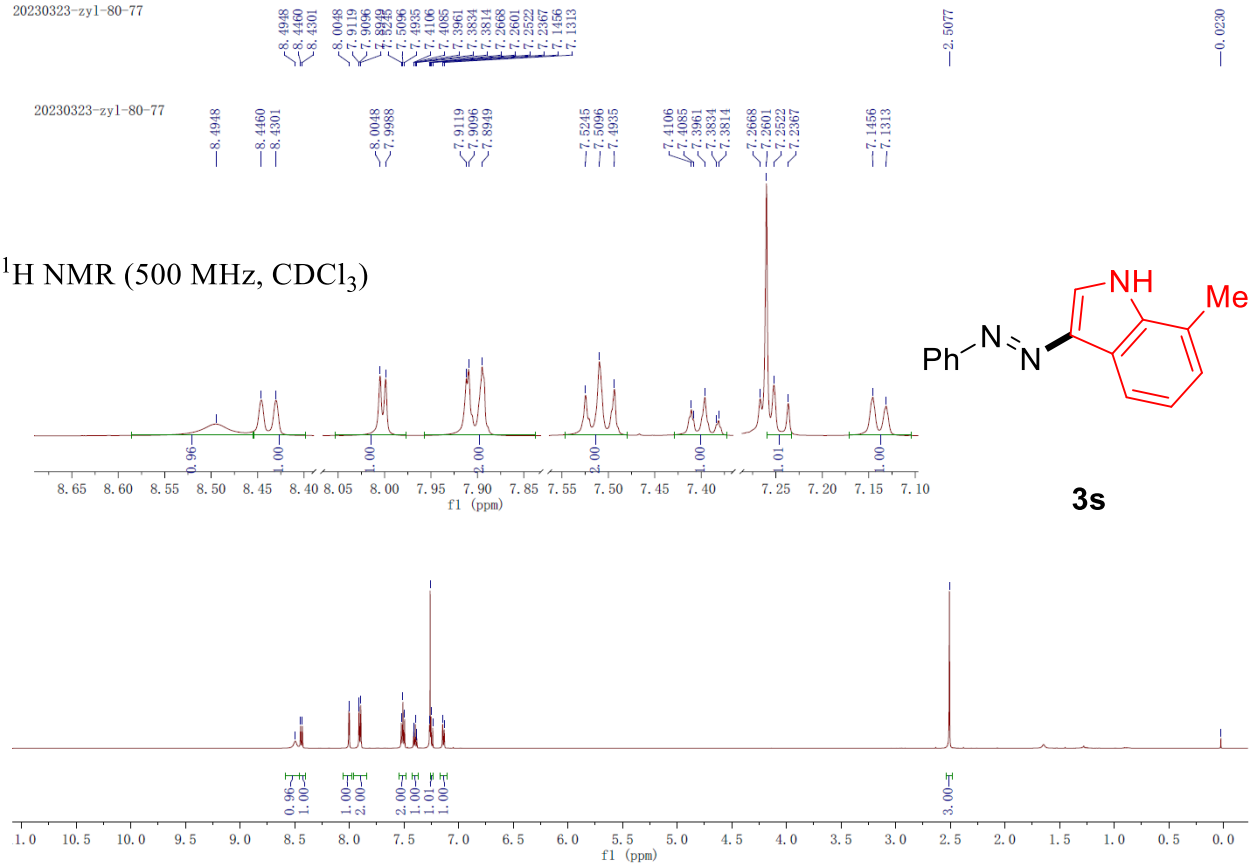
154.3387 142.9769 135.1314 132.9621 129.0155 128.7041 123.6427 122.9759 122.5847 121.8426 119.7234 110.6463 77.4141 77.1602 76.9061 11.6242

^{13}C NMR (125 MHz, $CDCl_3$)



3r



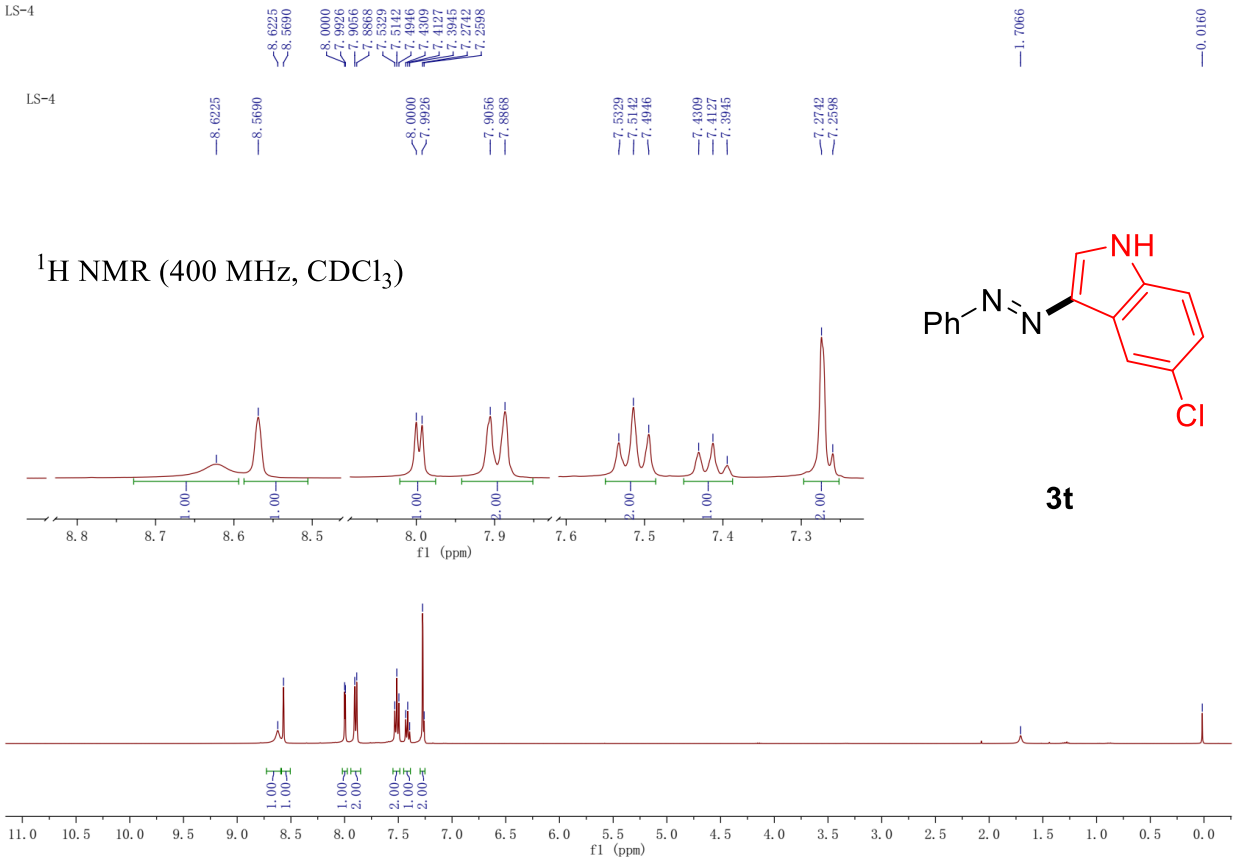


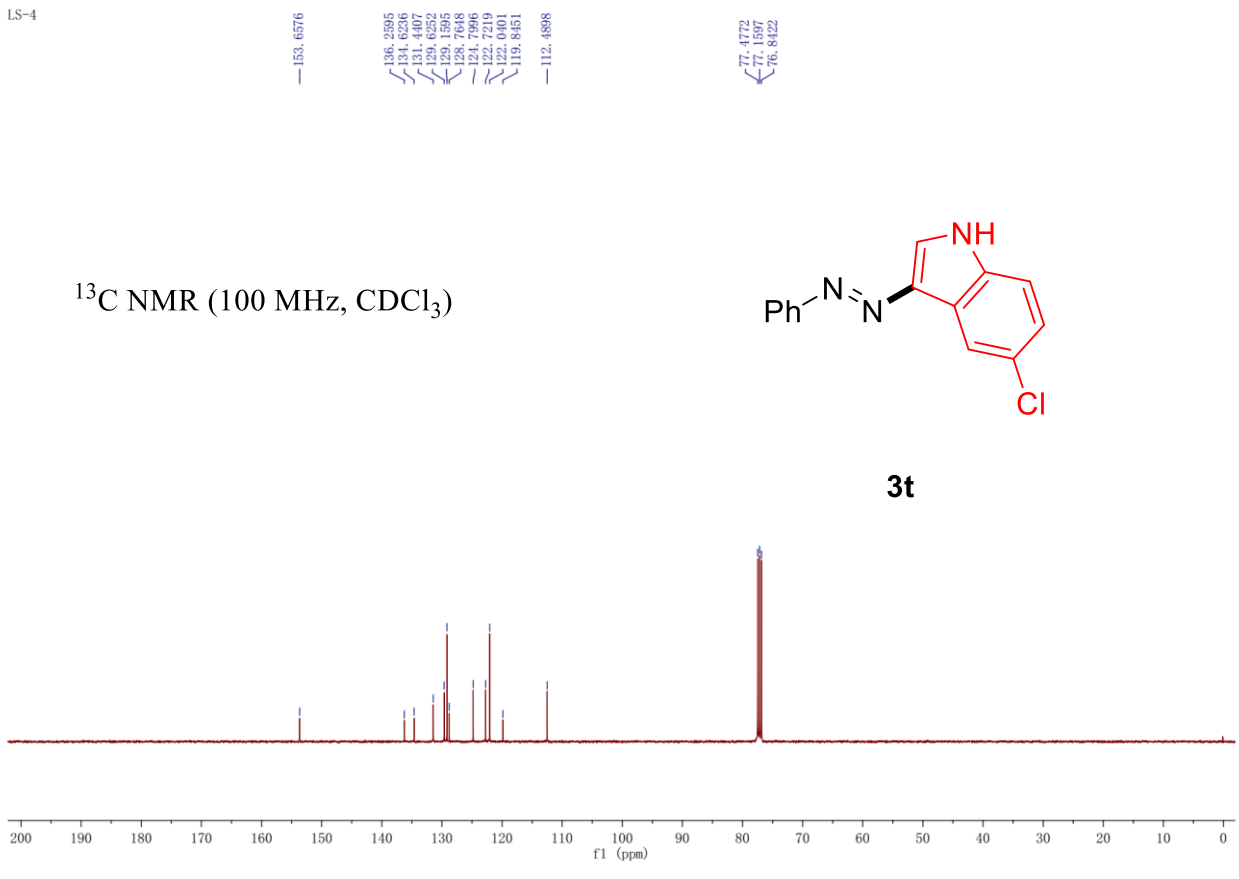
^{1}H NMR (500 MHz, $CDCl_3$)

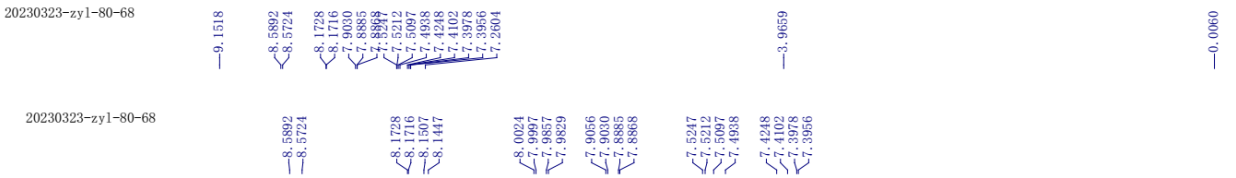
3s

^{13}C NMR (125 MHz, $CDCl_3$)

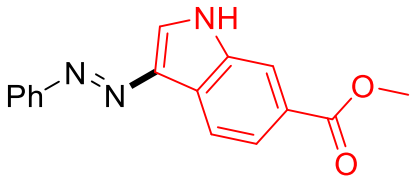
3s


LS-4
8.6225
8.5690
8.0000
7.9926
7.9056
7.8868
7.5329
7.5142
7.4946
7.4309
7.4127
7.3945
7.2742
7.2598
1.7066
0.0160
LS-4
8.6225
8.5690
8.0000
7.9926
7.9056
7.8868
7.5329
7.5142
7.4946
7.4309
7.4127
7.3945
7.2742
7.2598
1H NMR (400 MHz, CDCl3)
NH
Ph
N
N
Cl
3t
1.00
1.00
1.00
2.00
2.00
1.00
2.00
8.8
8.7
8.6
8.5
8.0
7.9
7.6
7.5
7.4
7.3
f1 (ppm)
1.00
1.00
1.00
2.00
2.00
1.00
2.00
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

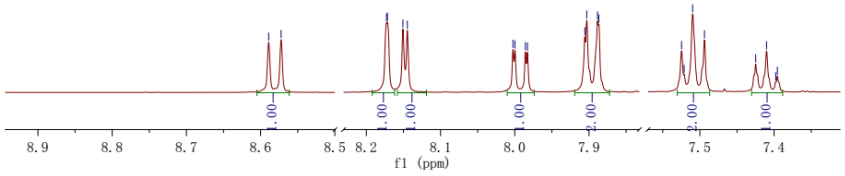

LS-4
153.6576
136.2595
134.6236
131.4407
129.6252
129.1395
128.7648
124.7996
122.7219
122.0401
119.8451
112.4898
77.4772
77.1597
76.8422
13C NMR (100 MHz, CDCl3)
NH
Ph
N
N
Cl
3t
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

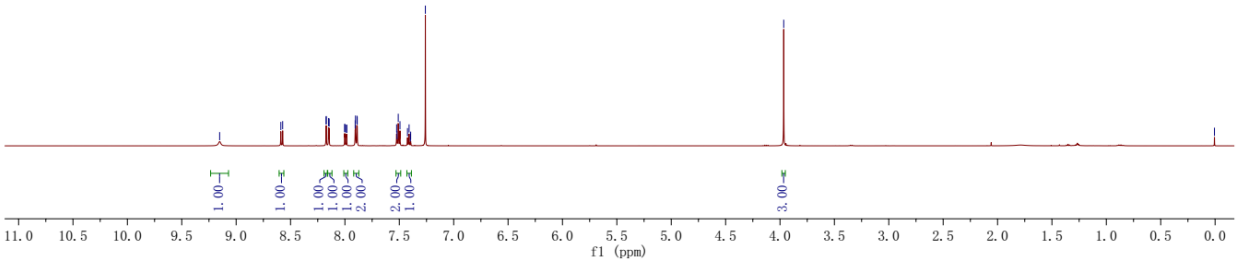


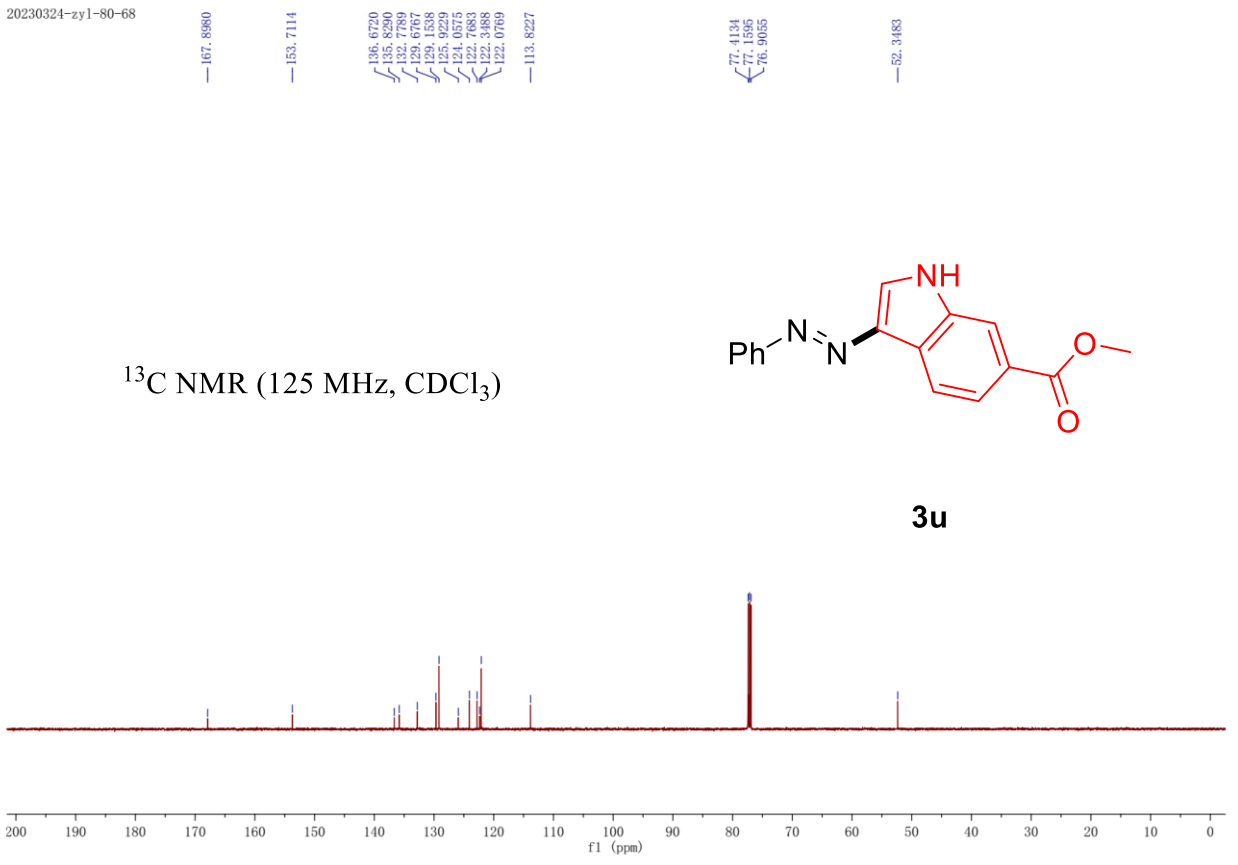
^{1}H NMR (500 MHz, $CDCl_3$)



3u

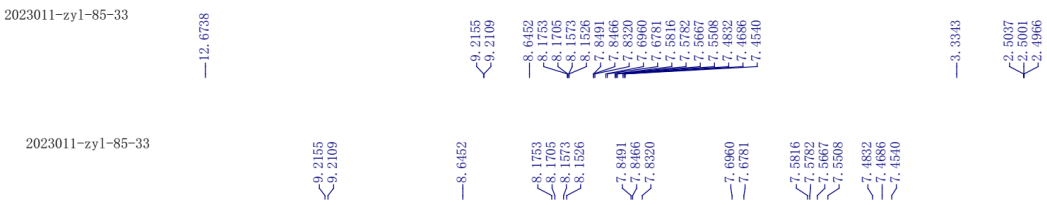




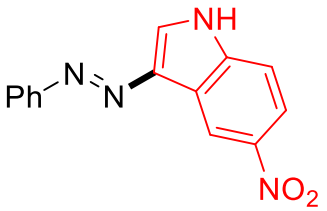


^{13}C NMR (125 MHz, $CDCl_3$)

3u



^{1}H NMR (500 MHz, DMSO-d_6)



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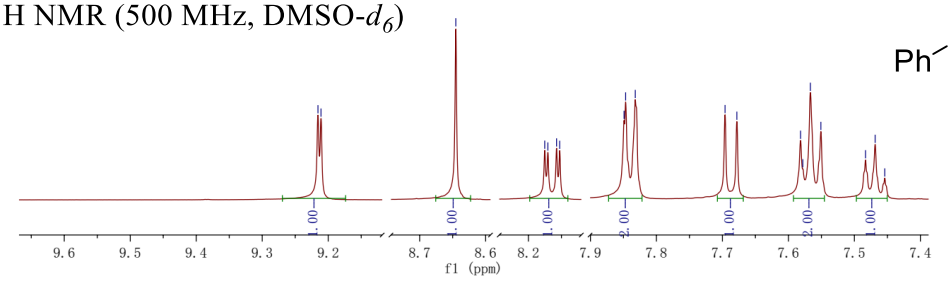
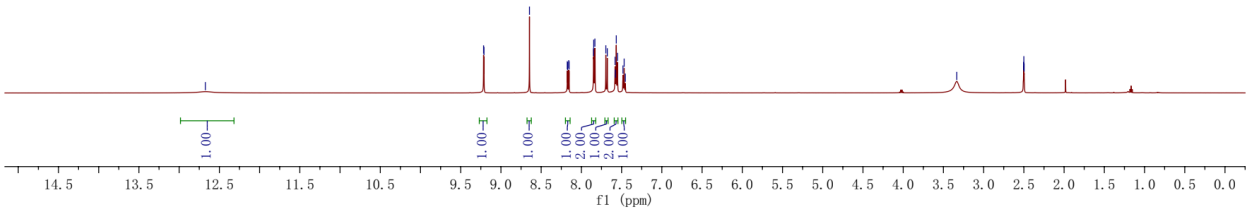
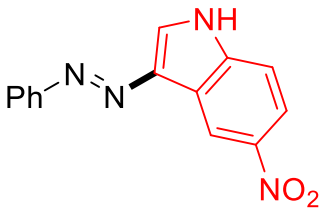
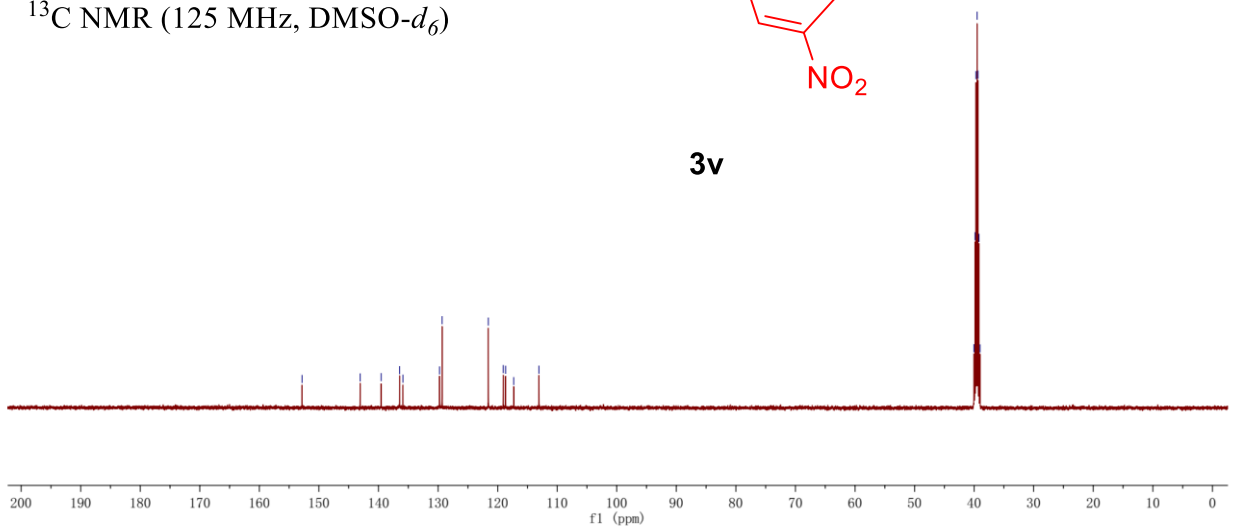


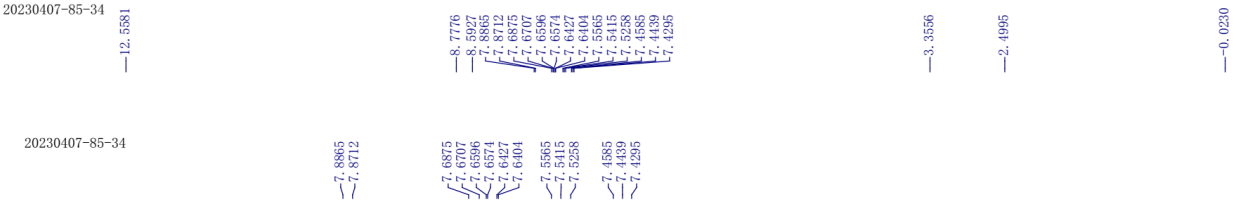


^{13}C NMR (125 MHz, DMSO-d_6)

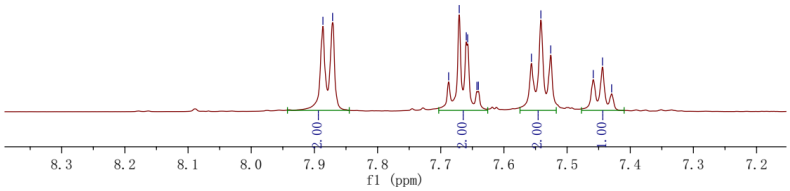


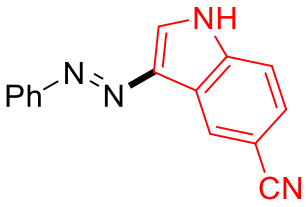
3v



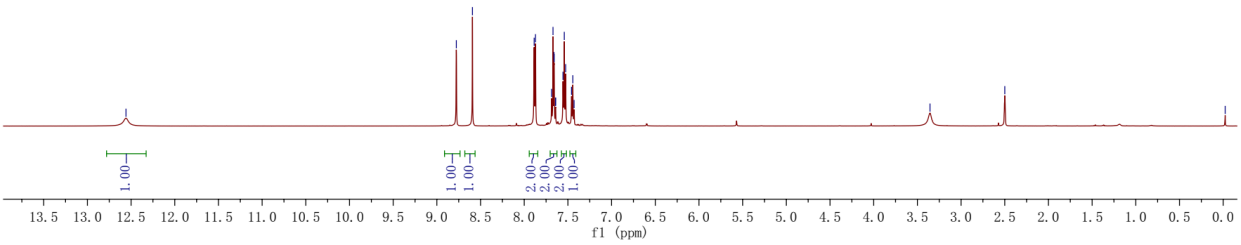


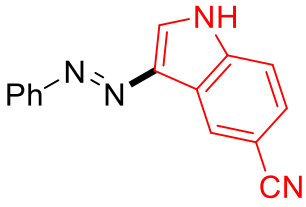
^{1}H NMR (500 MHz, DMSO-d_6)





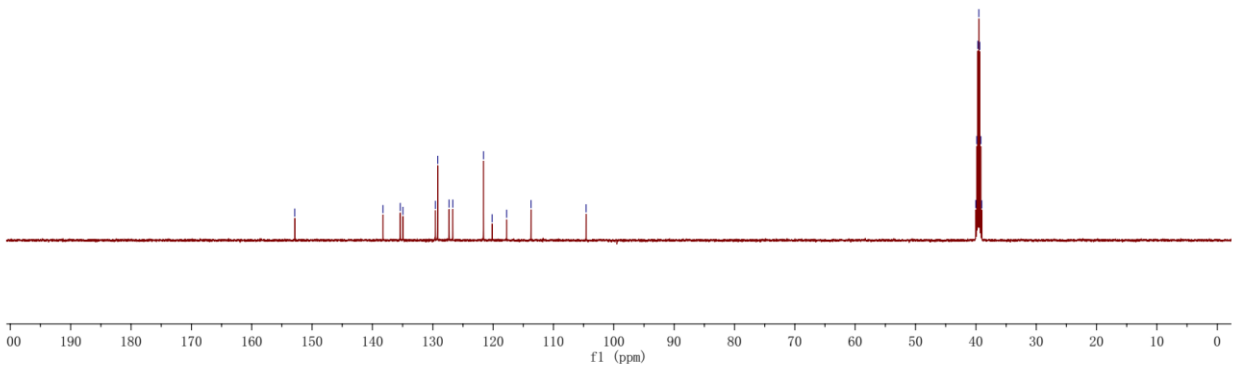
3w

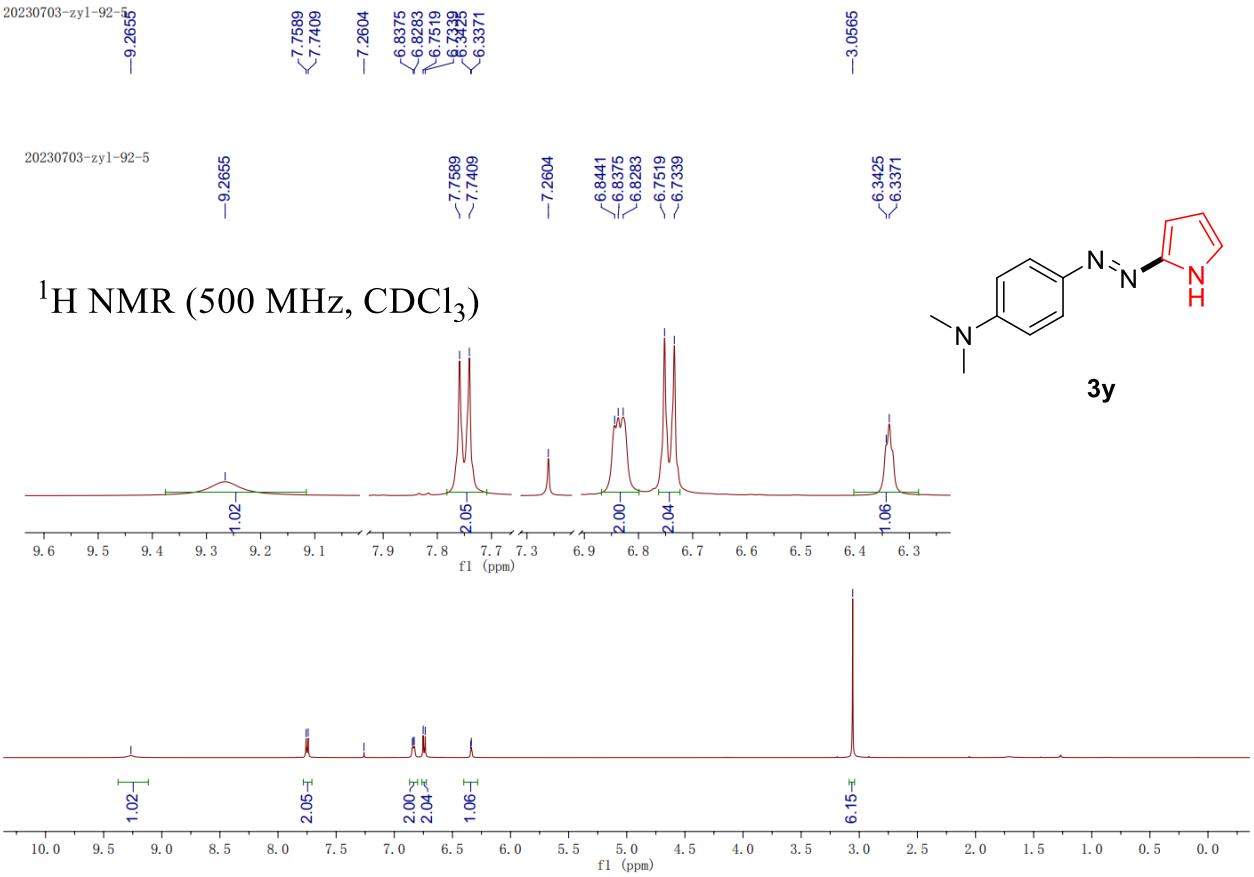


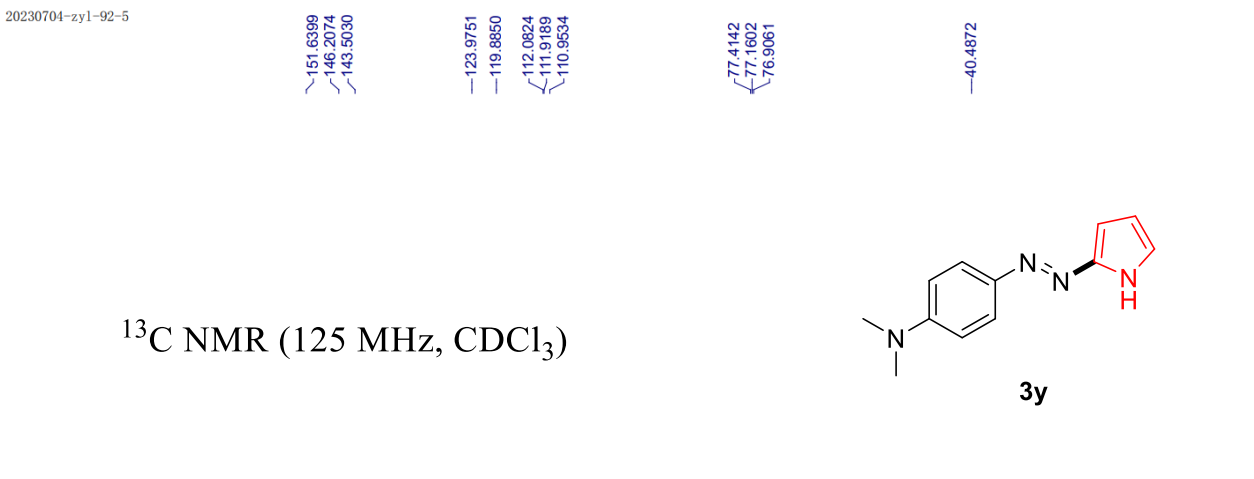


^{13}C NMR (125 MHz, DMSO-d_6)

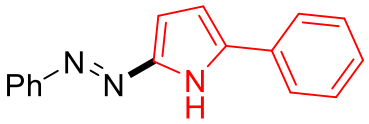
3w

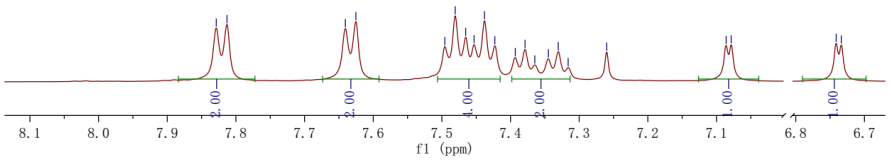



20230703-zyl-92-5
9.2655
7.7589
7.7409
7.2604
6.8375
6.8283
6.7519
6.3425
6.3371
3.0565
20230703-zyl-92-5
9.2655
7.7589
7.7409
7.2604
6.8441
6.8375
6.8283
6.7519
6.7339
6.3425
6.3371
1H NMR (500 MHz, CDCl3)
1.02
2.05
2.00
2.04
1.06
6.15
f1 (ppm)
3y

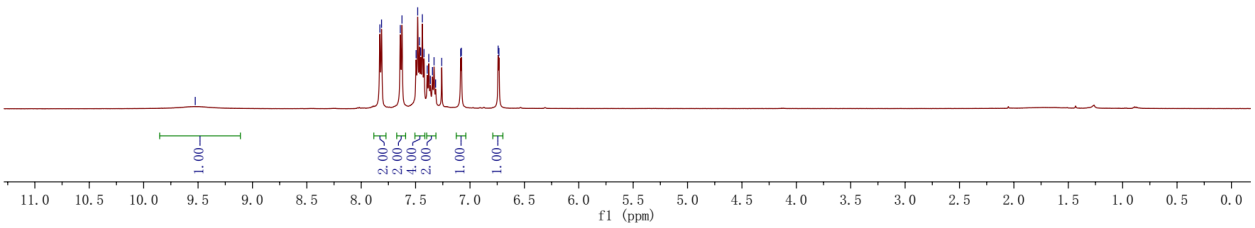

20230704-zyl-92-5
151.6399
146.2074
143.5030
123.9751
119.8850
112.0824
111.9189
110.9534
77.4142
77.1602
76.9061
40.4872
13C NMR (125 MHz, CDCl3)
3y
f1 (ppm)

^{1}H NMR (500 MHz, $CDCl_3$)

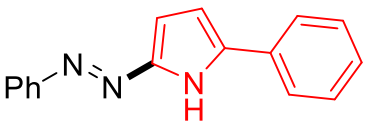




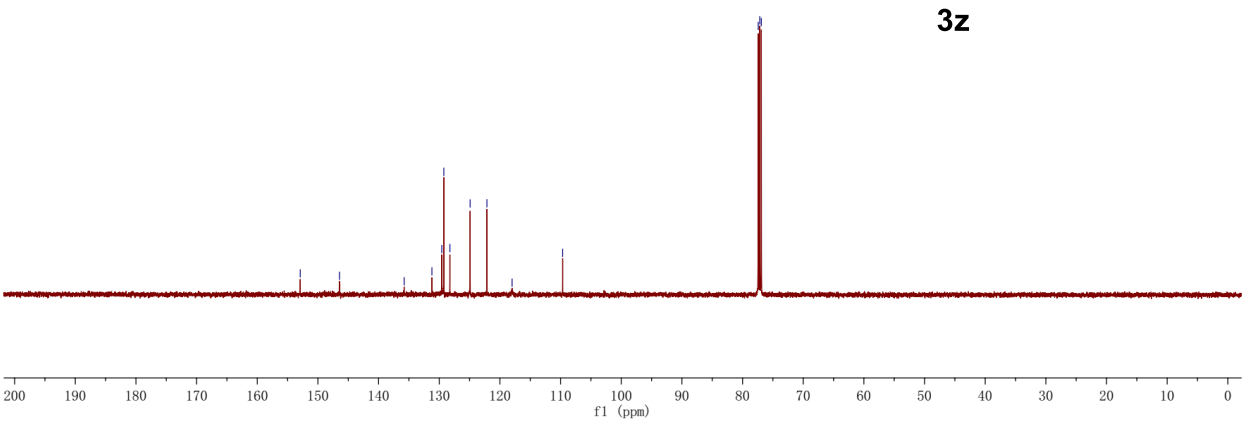
3z



^{13}C NMR (125 MHz, $CDCl_3$)



3z



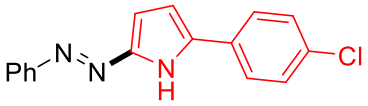
20230522-zy1-85-105

9.4899
7.8238
7.8087
7.5520
7.5351
7.4960
7.4810
7.4651
7.4034
7.3867
7.3718
7.2605
7.0751
7.0672
6.7085
6.7006

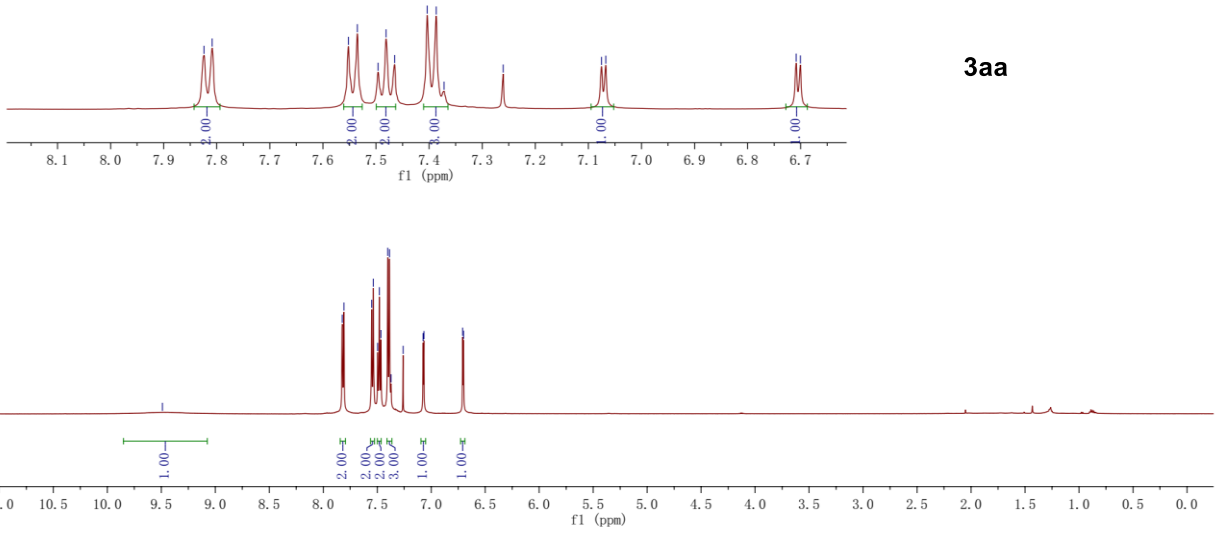
20230522-zy1-85-105

7.8238
7.8087
7.5520
7.5351
7.4960
7.4810
7.4651
7.4034
7.3867
7.3718
7.2605
7.0751
7.0672
6.7085
6.7006

^{1}H NMR (500 MHz, $CDCl_3$)



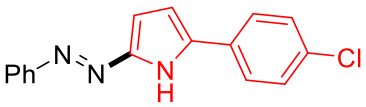
3aa



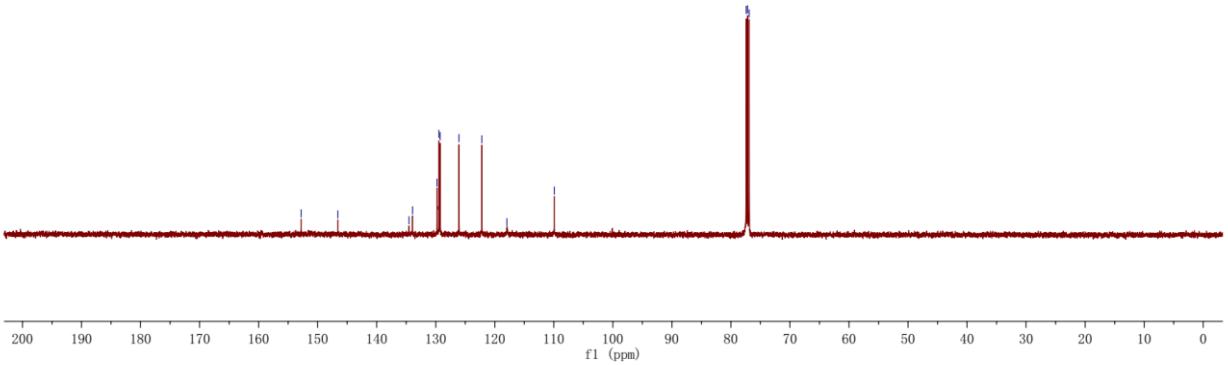
20230523-zy1-85-105

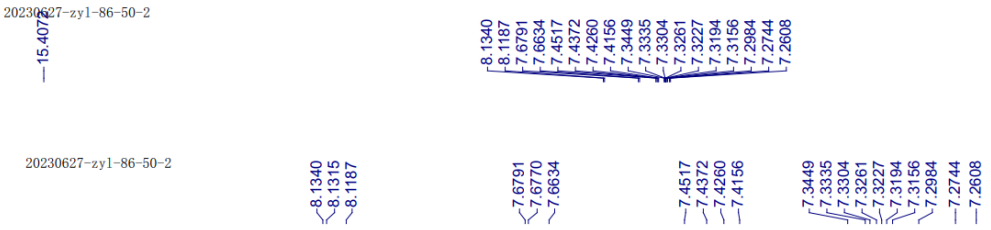
152.8097
146.5837
134.5182
133.9270
129.7741
129.4463
129.2599
126.0553
122.1863
117.9441
109.9133
77.4141
77.1601
76.9060

^{13}C NMR (125 MHz, $CDCl_3$)

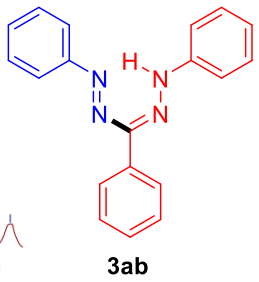


3aa

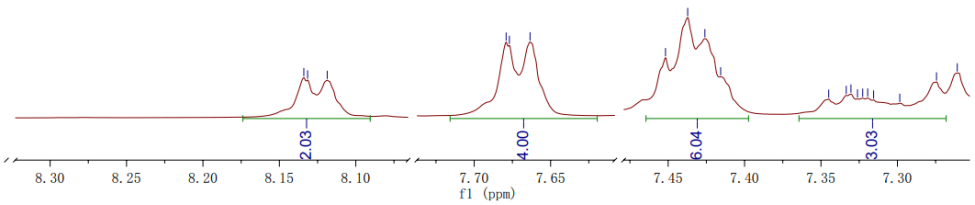


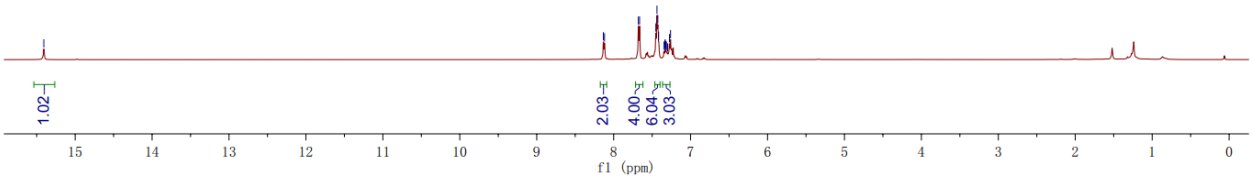


^{1}H NMR (500 MHz, $CDCl_3$)

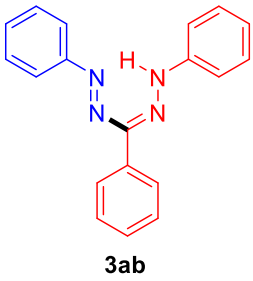


3ab

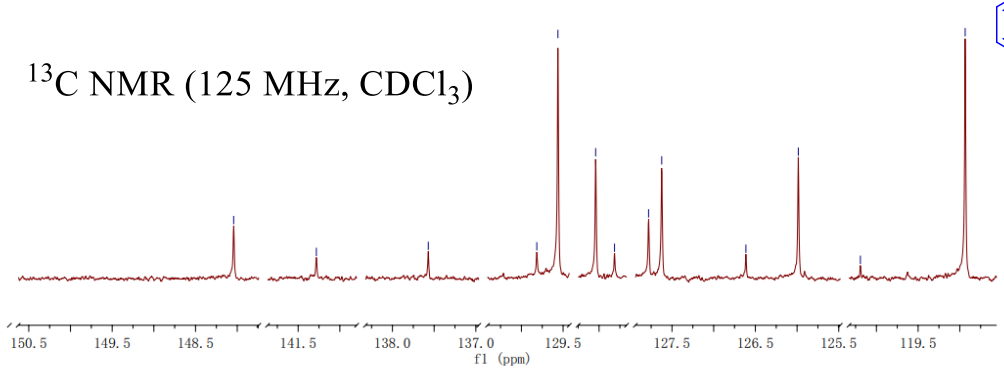


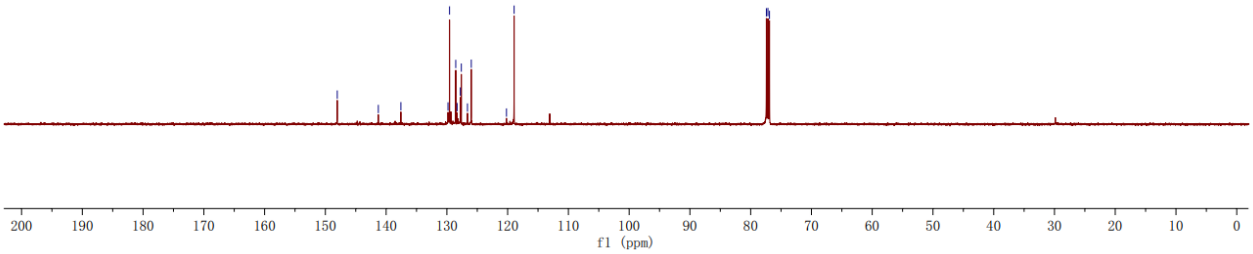


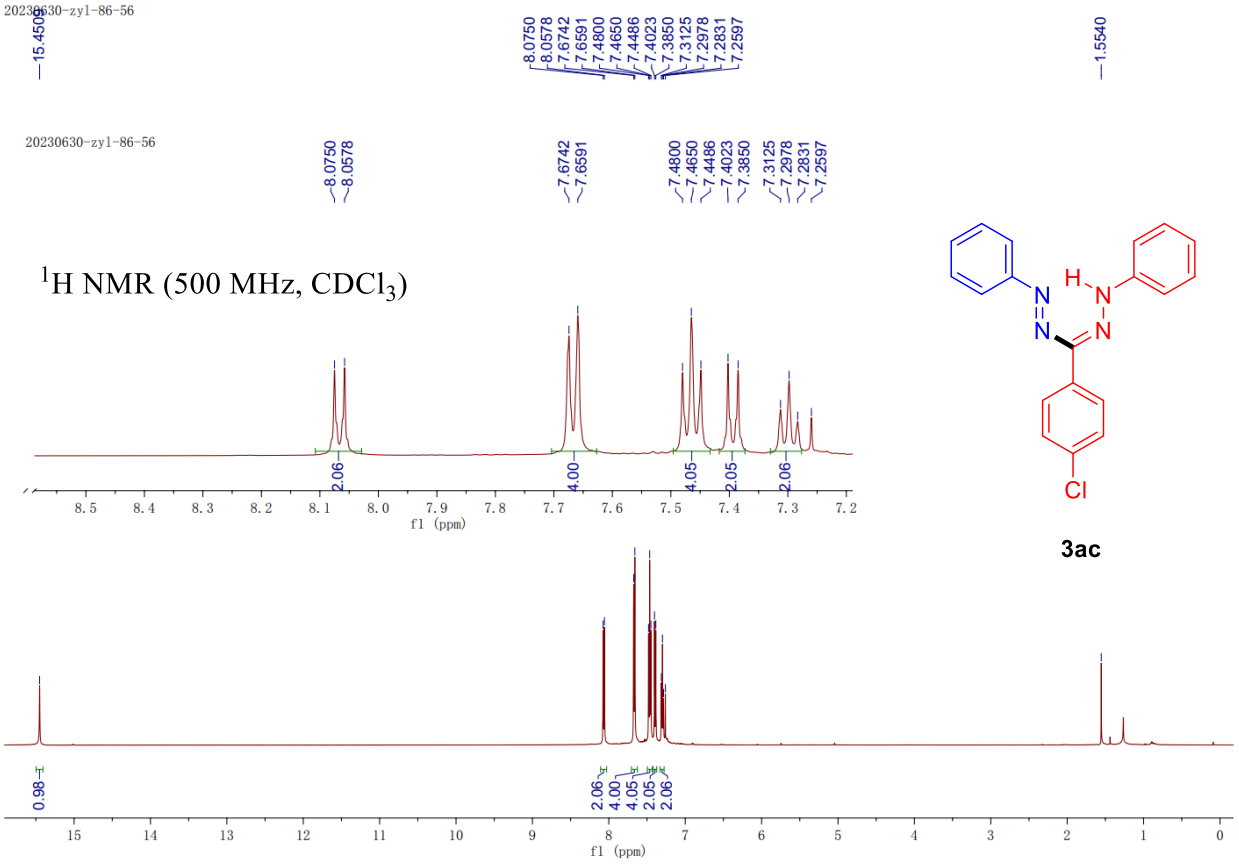
^{13}C NMR (125 MHz, $CDCl_3$)

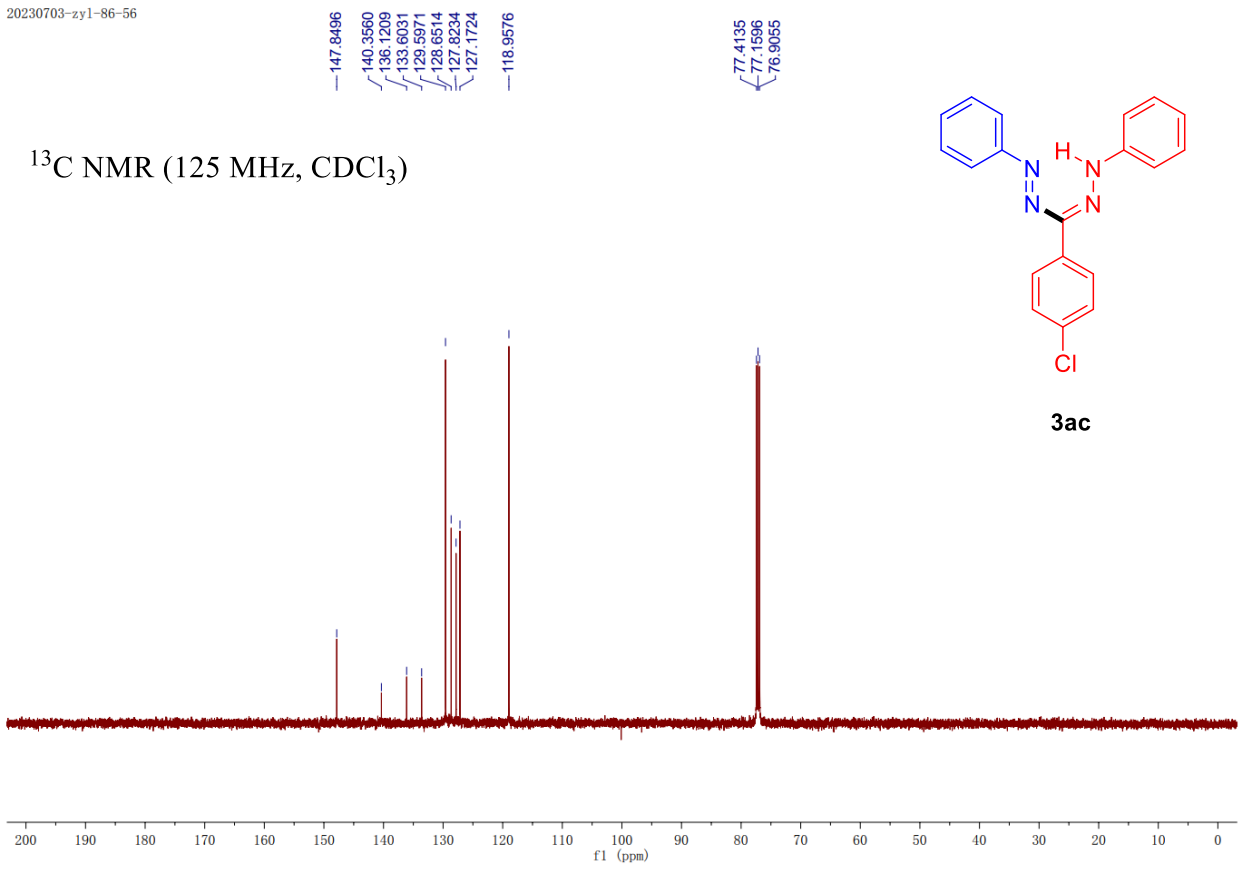


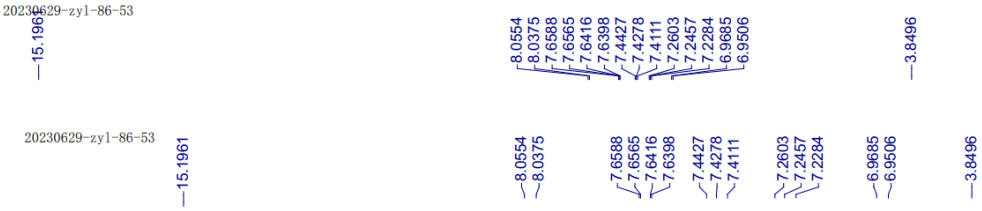
3ab



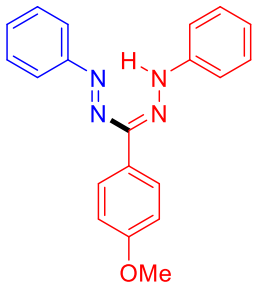



20230630-zyl-86-56
15.4506
8.0750
8.0578
7.6742
7.6591
7.4800
7.4650
7.4486
7.4023
7.3850
7.3125
7.2978
7.2831
7.2597
1.5540
20230630-zyl-86-56
8.0750
8.0578
7.6742
7.6591
7.4800
7.4650
7.4486
7.4023
7.3850
7.3125
7.2978
7.2831
7.2597
1H NMR (500 MHz, CDCl3)
2.06
4.00
4.05
2.05
2.06
f1 (ppm)
0.98
2.06
4.00
4.05
2.05
2.06
f1 (ppm)
H
N
N
N
N
Cl
3ac

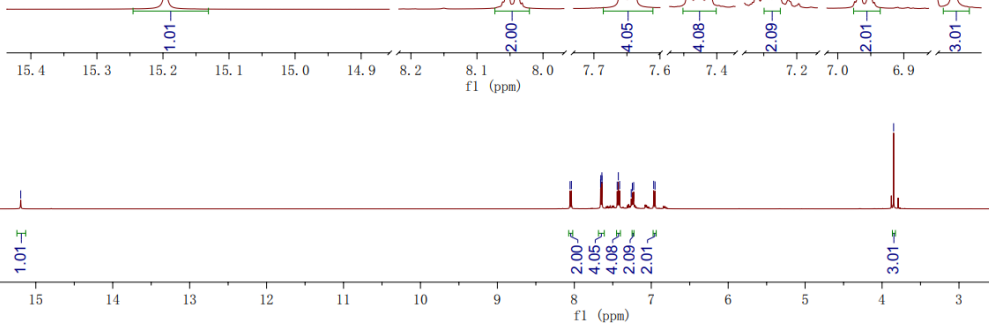

20230703-zyl-86-56
147.8496
140.3560
136.1209
133.6031
129.5971
128.6514
127.8234
127.1724
118.9576
77.4135
77.1596
76.9055
13C NMR (125 MHz, CDCl3)
f1 (ppm)
H
N
N
N
N
Cl
3ac

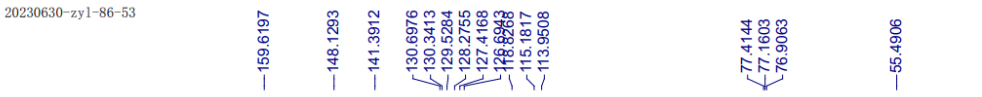


^{1}H NMR (500 MHz, $CDCl_3$)

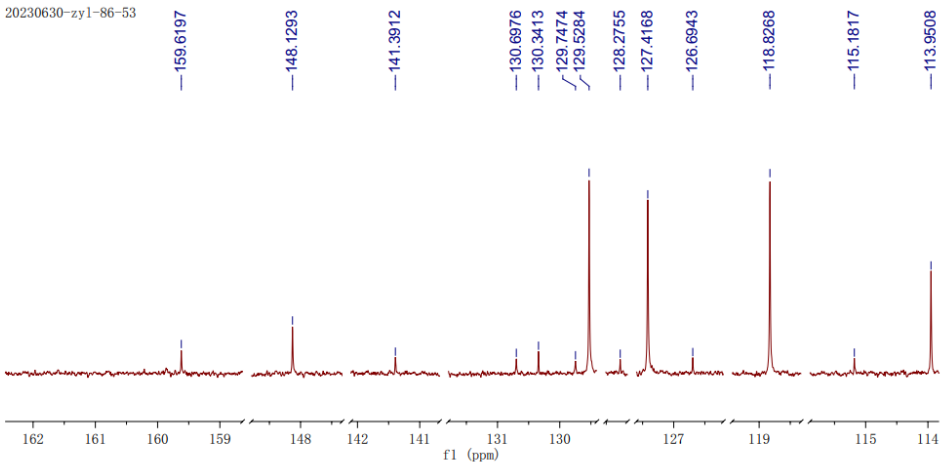


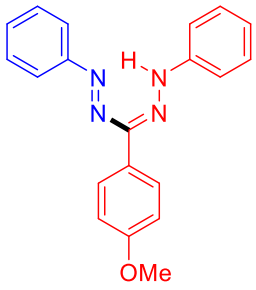
3ad



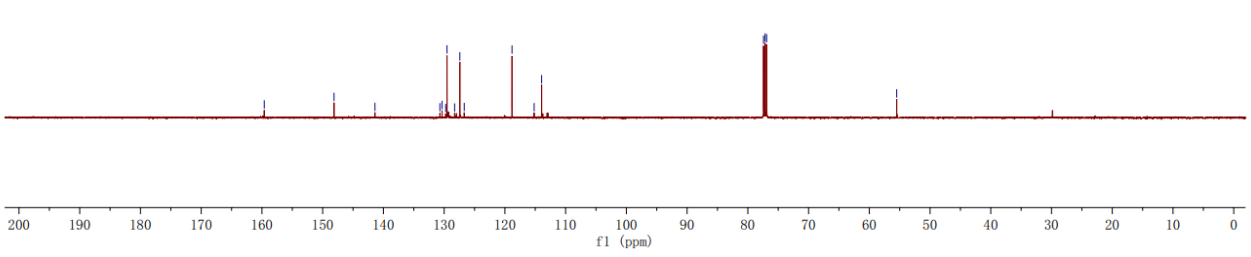


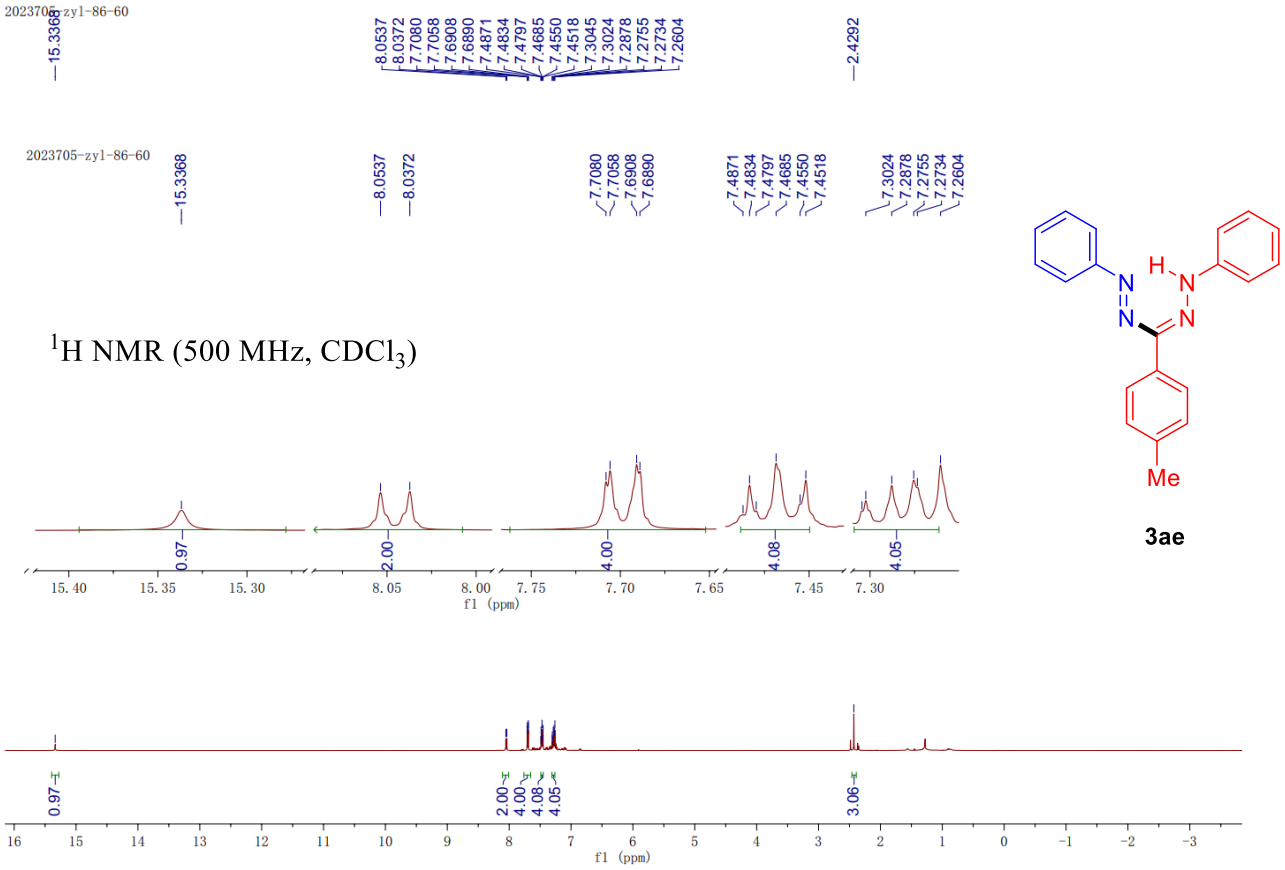
^{13}C NMR (125 MHz, $CDCl_3$)

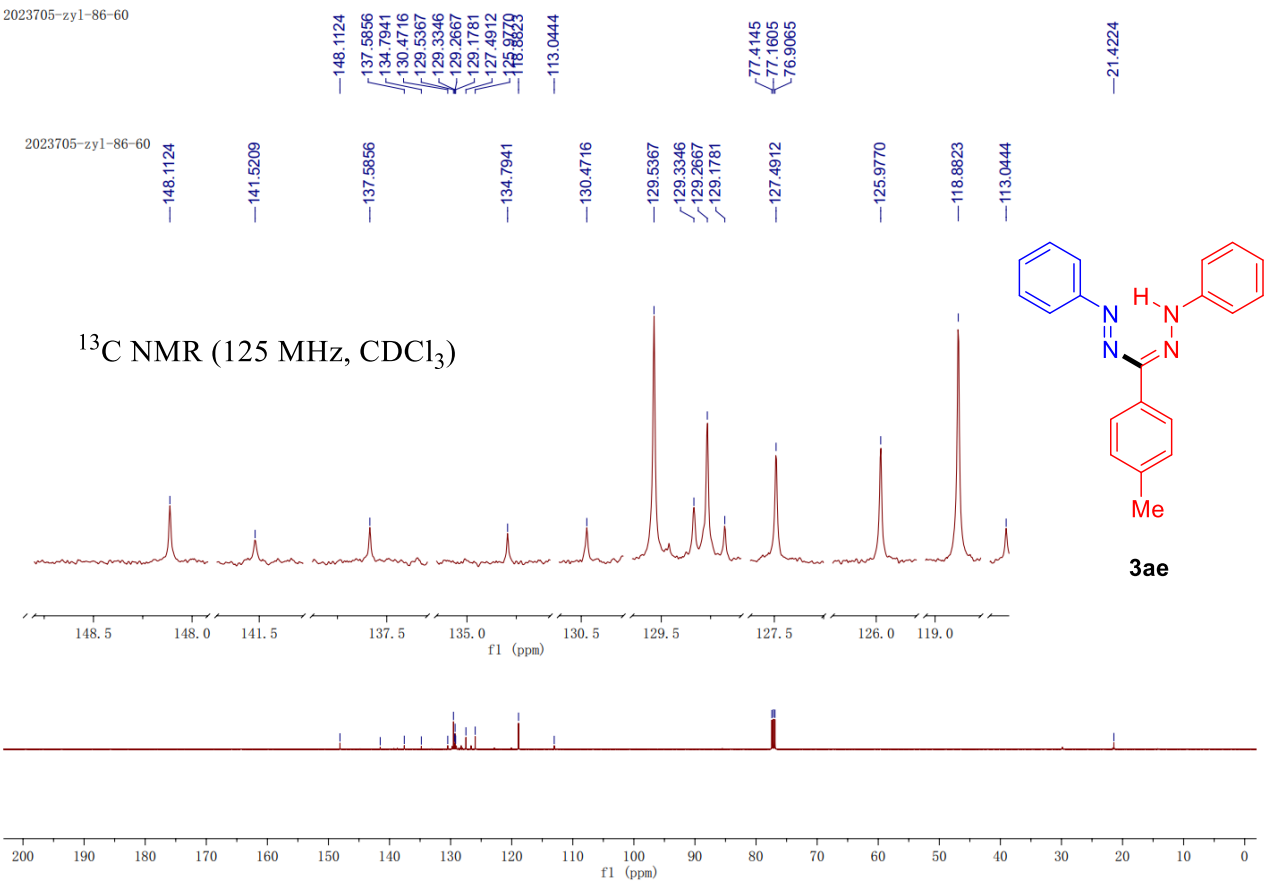


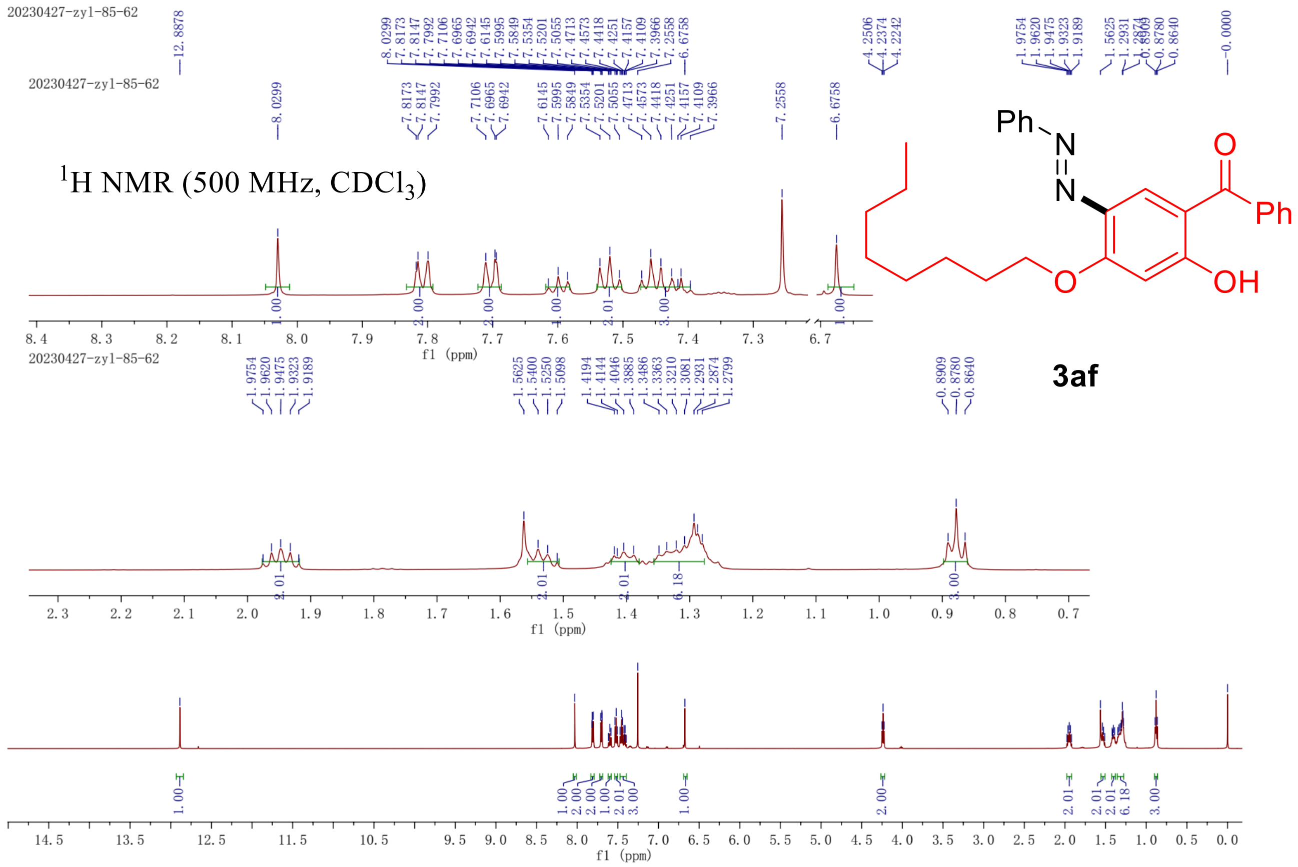


3ad



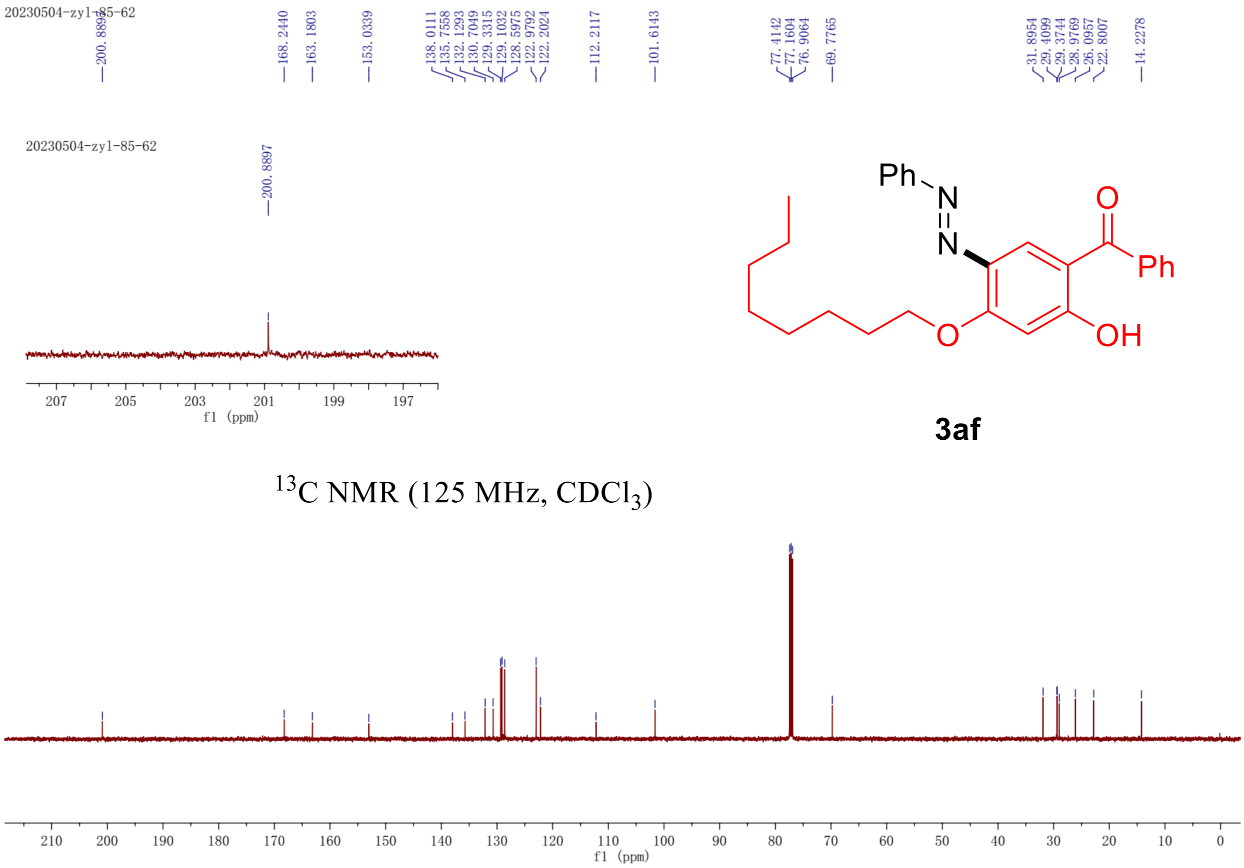

2023705-zyl-86-60
15.3368
8.0537
8.0372
7.7080
7.7058
7.6908
7.6890
7.4871
7.4834
7.4797
7.4685
7.4550
7.4518
7.3045
7.3024
7.2878
7.2755
7.2734
7.2604
2.4292
2023705-zyl-86-60
15.3368
8.0537
8.0372
7.7080
7.7058
7.6908
7.6890
7.4871
7.4834
7.4797
7.4685
7.4550
7.4518
7.3024
7.2878
7.2755
7.2734
7.2604
1H NMR (500 MHz, CDCl3)
0.97
2.00
4.00
4.08
4.05
15.40
15.35
15.30
8.05
8.00
7.75
7.70
7.65
7.45
7.30
f1 (ppm)
0.97
2.00
4.00
4.08
4.05
3.06
f1 (ppm)
Me
3ae


2023705-zyl-86-60
148.1124
137.5856
134.7941
130.4716
129.5367
129.3346
129.2667
129.1781
127.4912
125.9770
118.8823
113.0444
77.4145
77.1605
76.9065
21.4224
2023705-zyl-86-60
148.1124
141.5209
137.5856
134.7941
130.4716
129.5367
129.3346
129.2667
129.1781
127.4912
125.9770
118.8823
113.0444
13C NMR (125 MHz, CDCl3)
148.5
148.0
141.5
137.5
135.0
130.5
129.5
127.5
126.0
119.0
f1 (ppm)
f1 (ppm)
Me
3ae



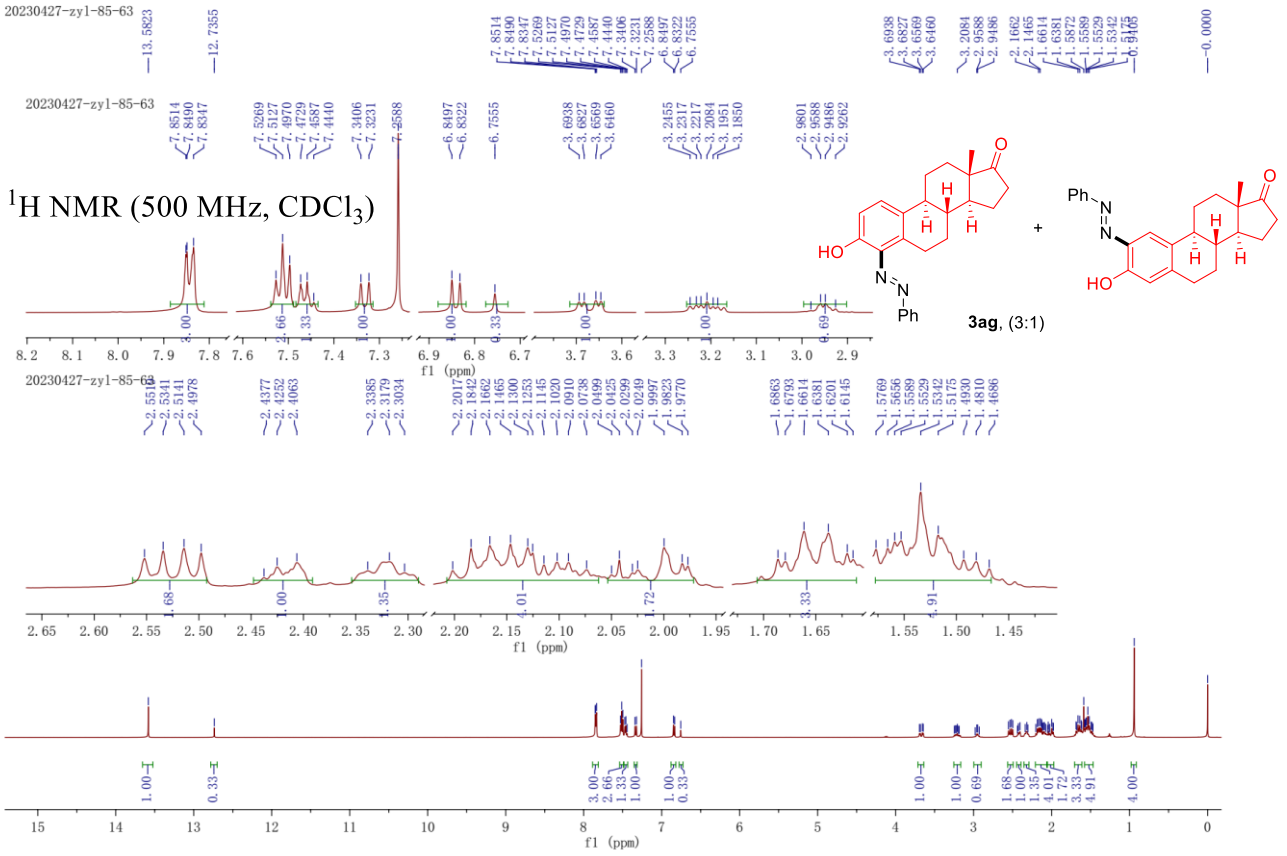
^{1}H NMR (500 MHz, $CDCl_3$)

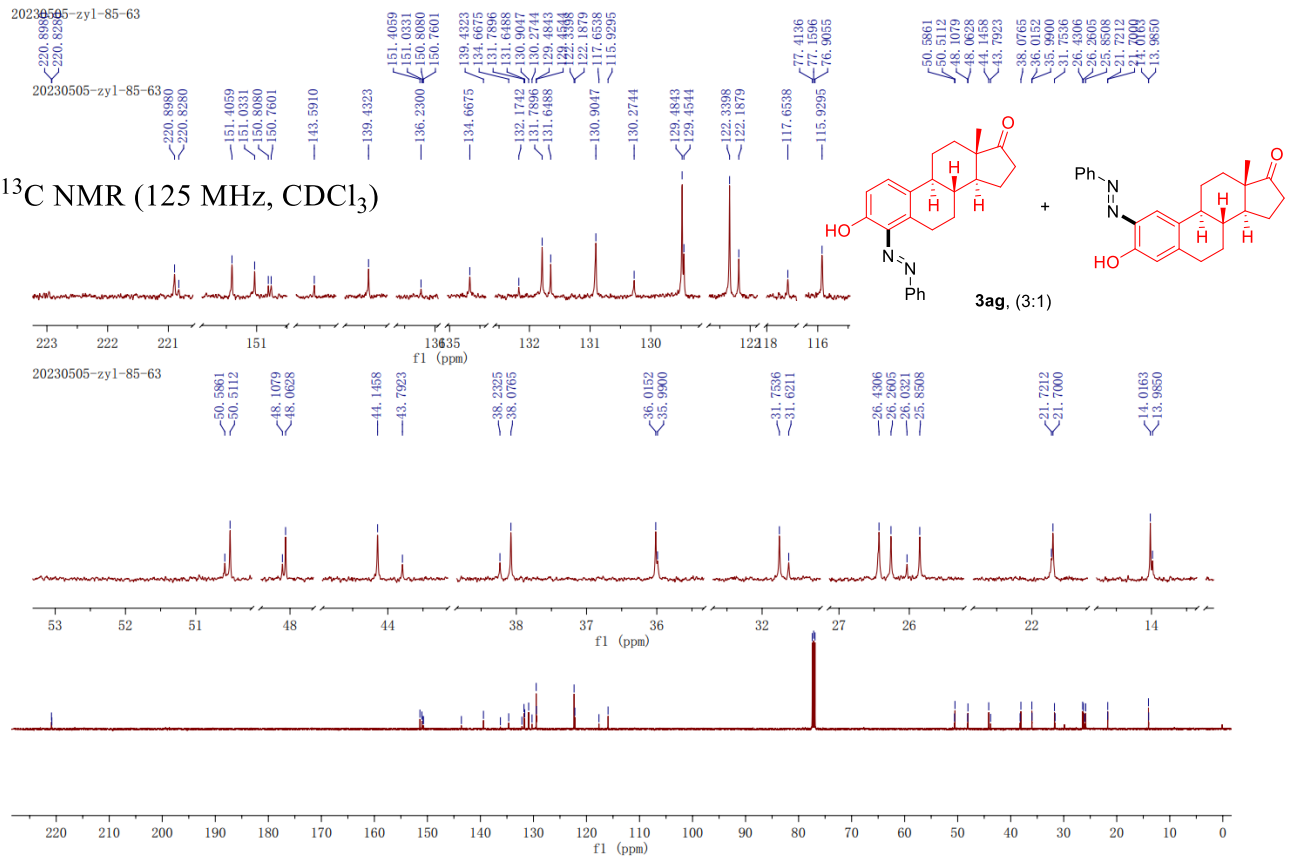
3af

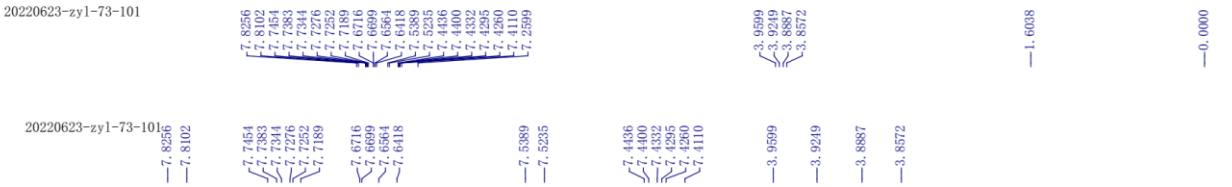


3af

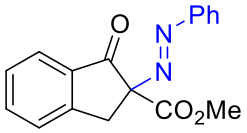
^{13}C NMR (125 MHz, $CDCl_3$)


20230427-zyl-85-63
^{1}H NMR (500 MHz, $CDCl_3$)
3ag, (3:1)

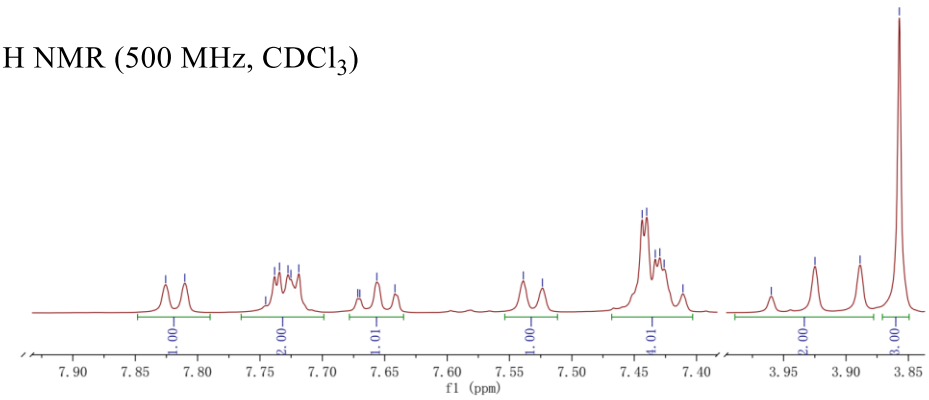

20230505-zyl-85-63
^{13}C NMR (125 MHz, $CDCl_3$)
3ag, (3:1)

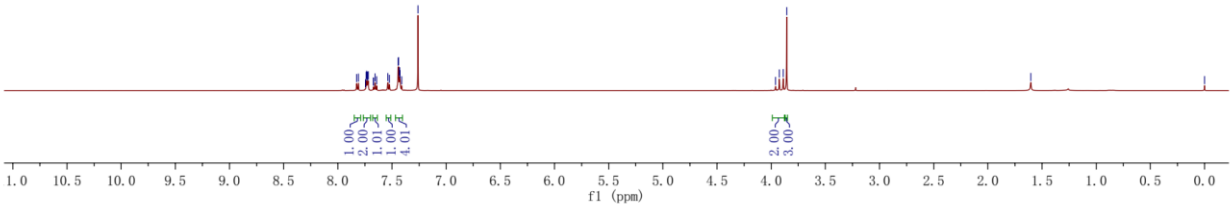


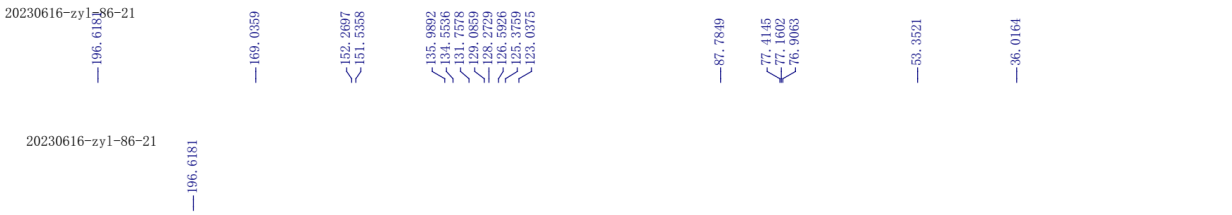
^{1}H NMR (500 MHz, $CDCl_3$)



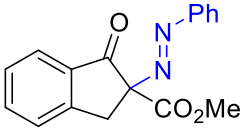
5a



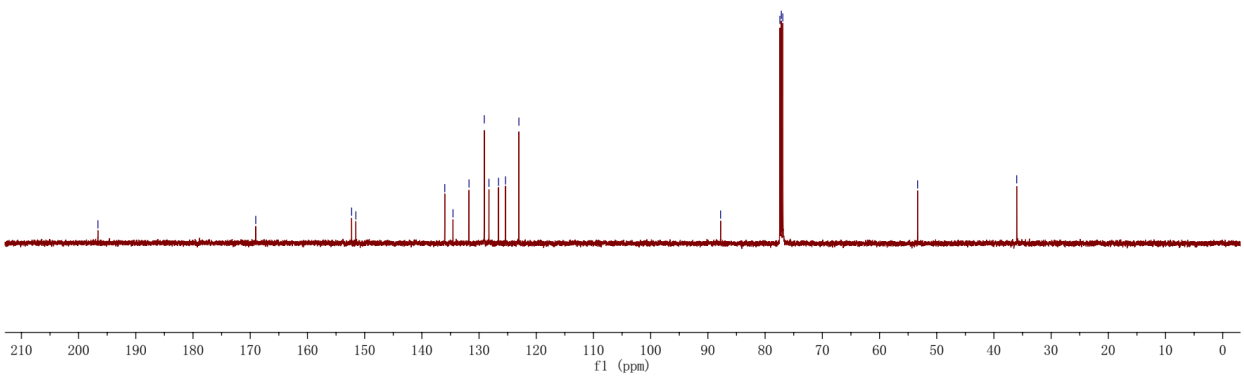


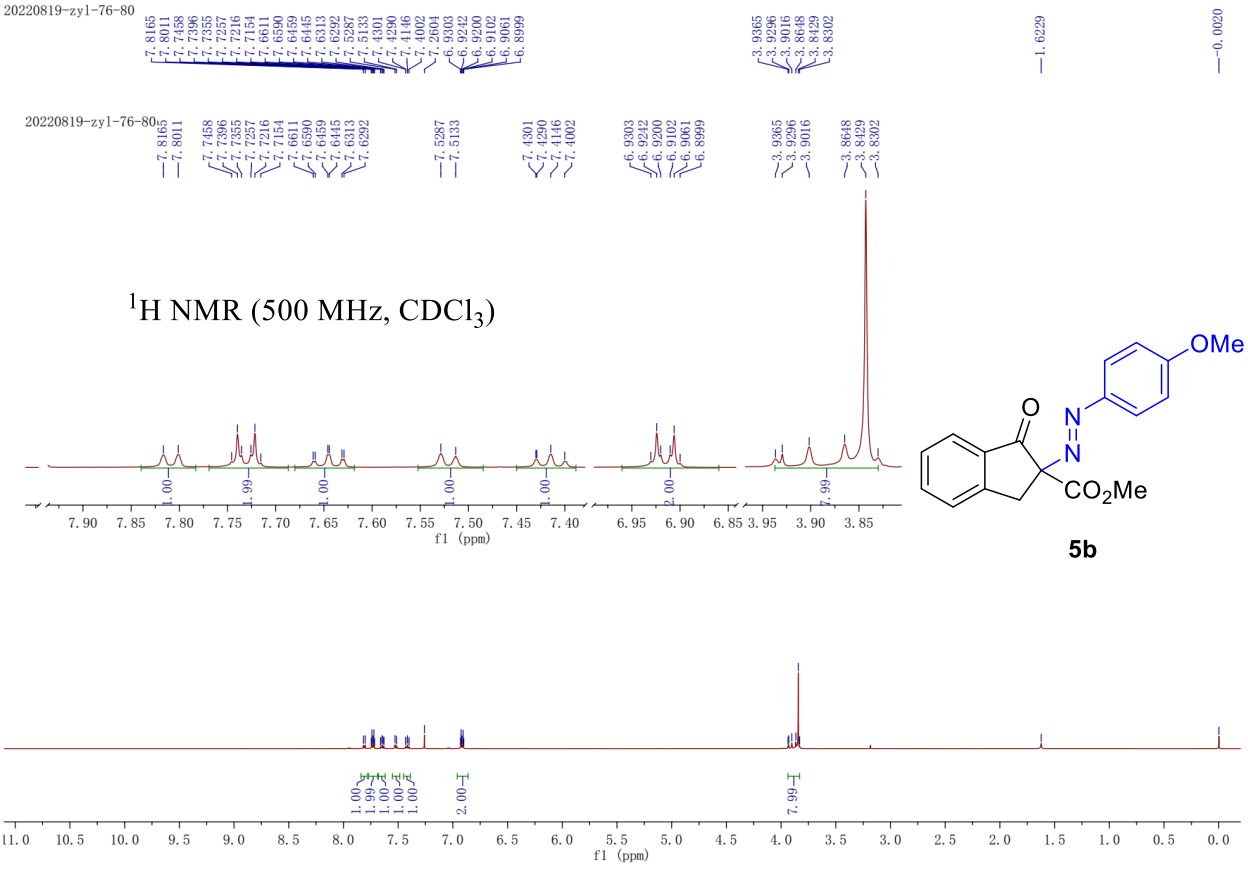


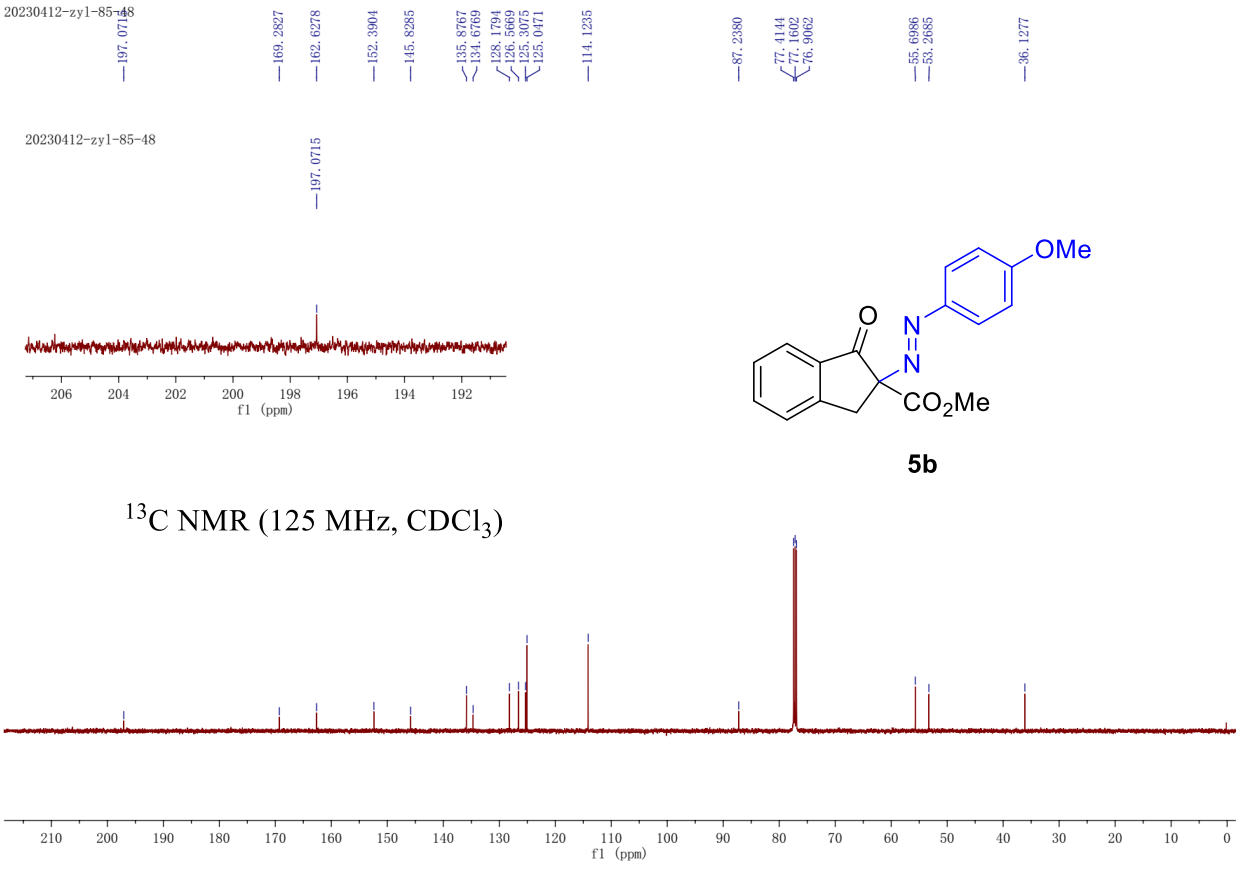
^{13}C NMR (125 MHz, $CDCl_3$)

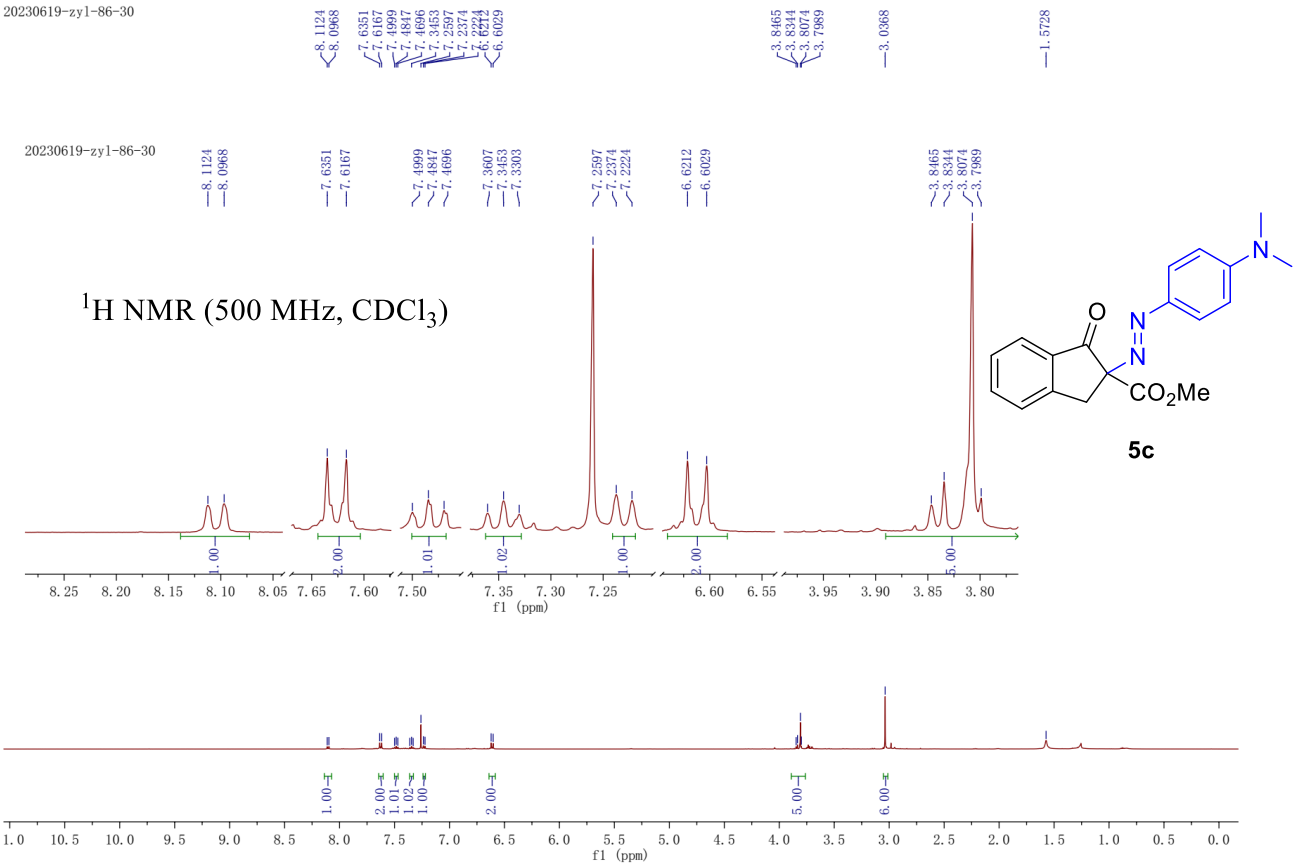


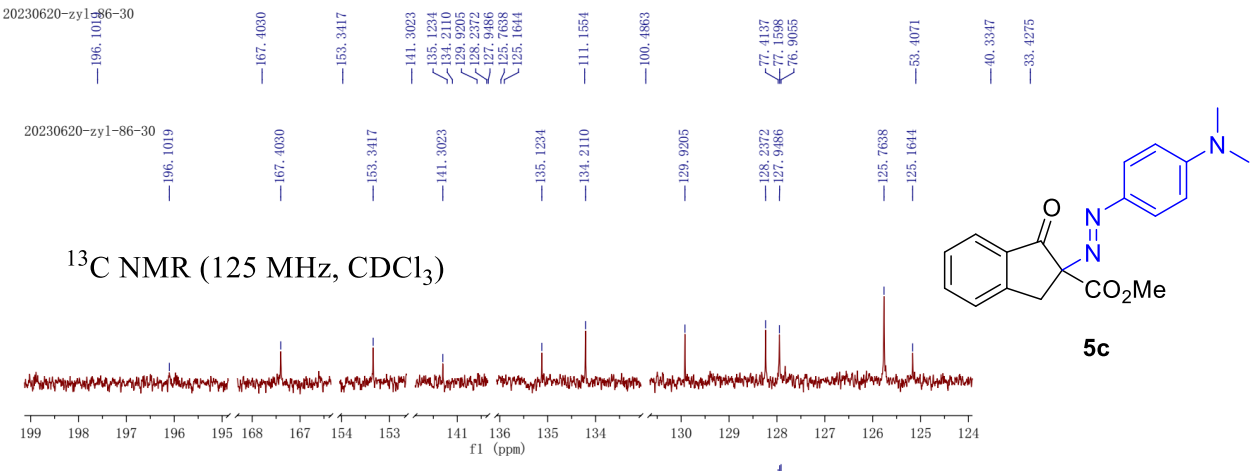
5a



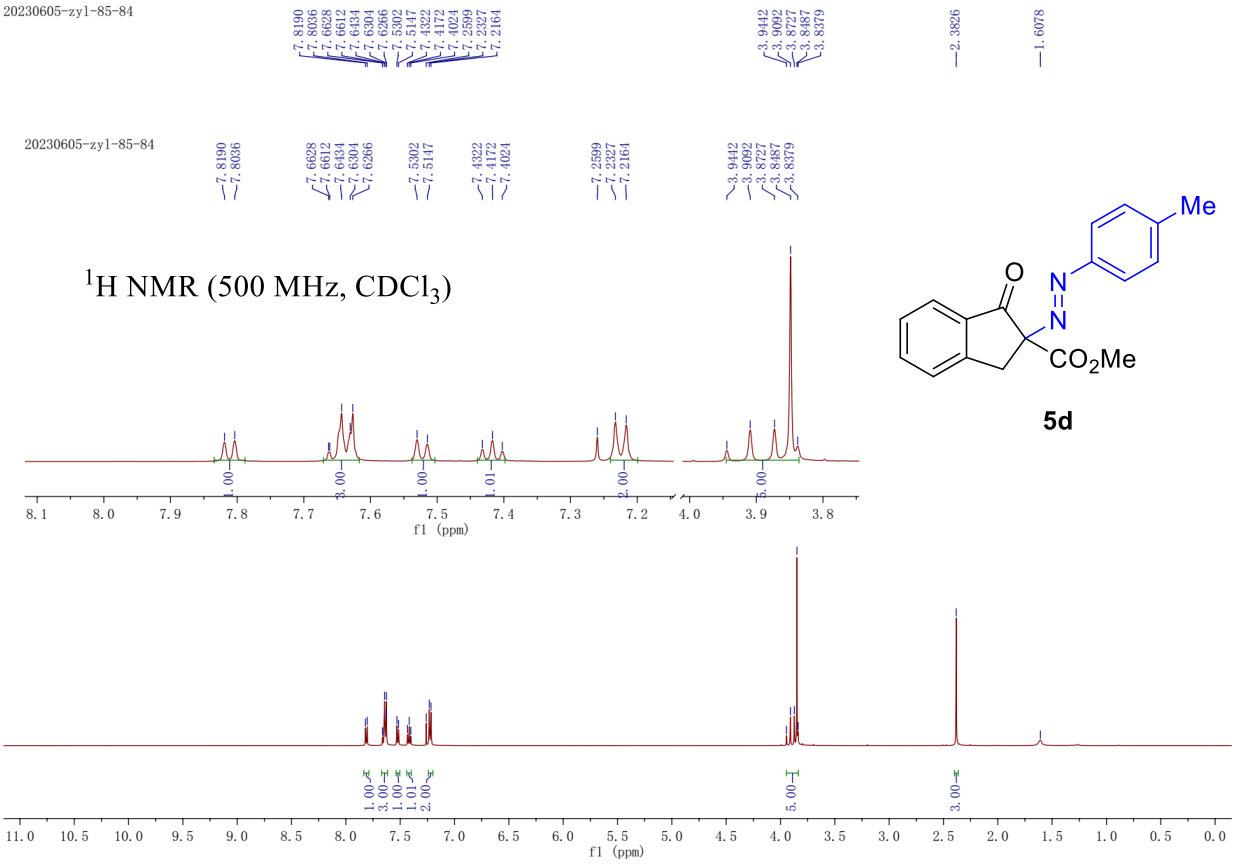

20220819-zyl-76-80
^{1}H NMR (500 MHz, CDCl$_3$)
OMe
O
N
N
CO$_2$Me
5b

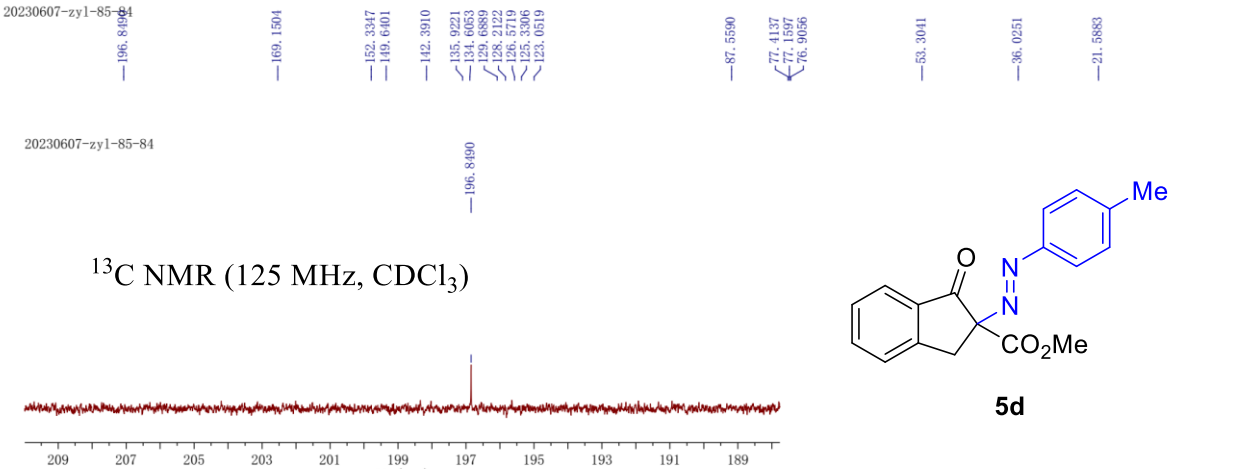

20230412-zyl-85-48
^{13}C NMR (125 MHz, CDCl$_3$)
OMe
O
N
N
CO$_2$Me
5b

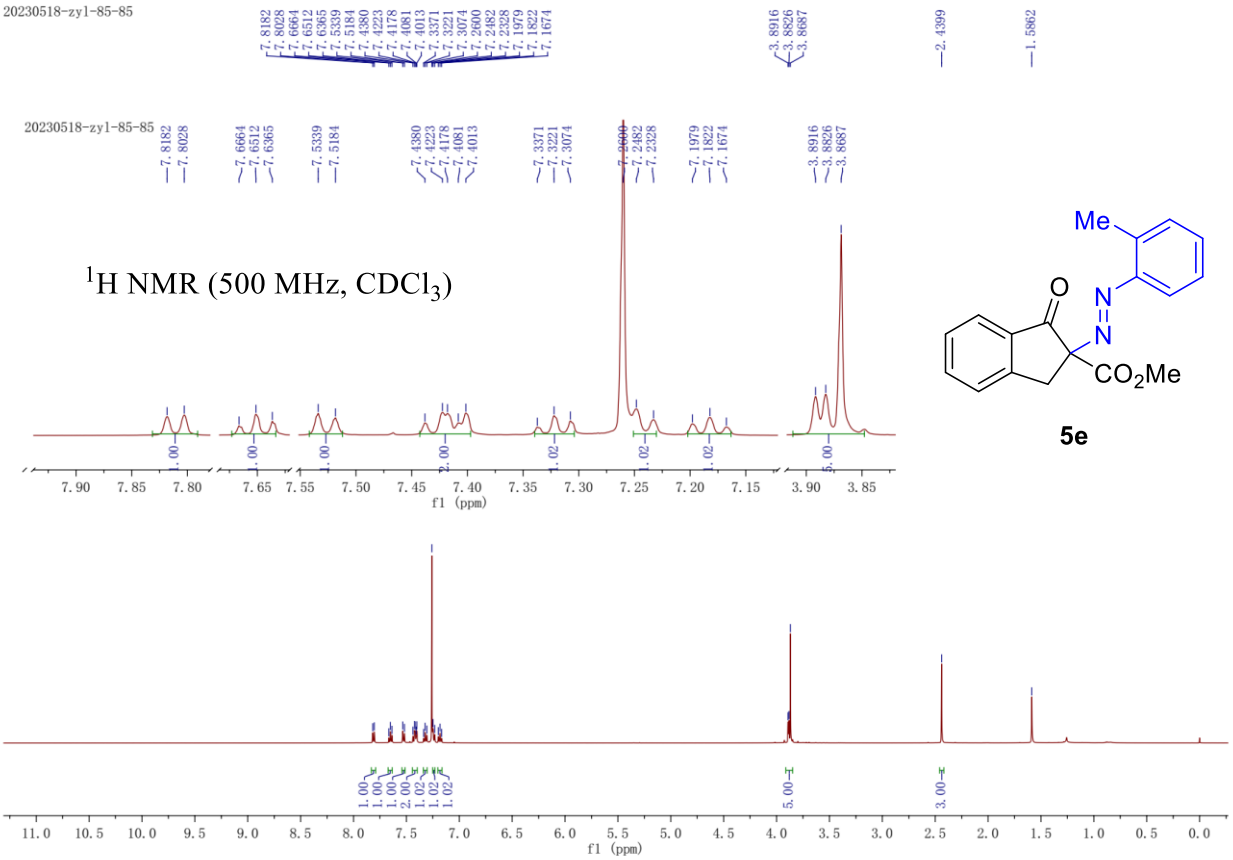

20230619-zyl-86-30
8.1124
8.0968
7.6351
7.6167
7.4999
7.4847
7.4696
7.3453
7.2597
7.2374
7.2224
6.6212
6.6029
3.8465
3.8344
3.8074
3.7989
3.0368
1.5728
20230619-zyl-86-30
^{1}H NMR (500 MHz, $CDCl_3$)
O
N
N
CO_2Me
N
5c
1.00
2.00
1.01
1.02
1.00
2.00
5.00
f1 (ppm)

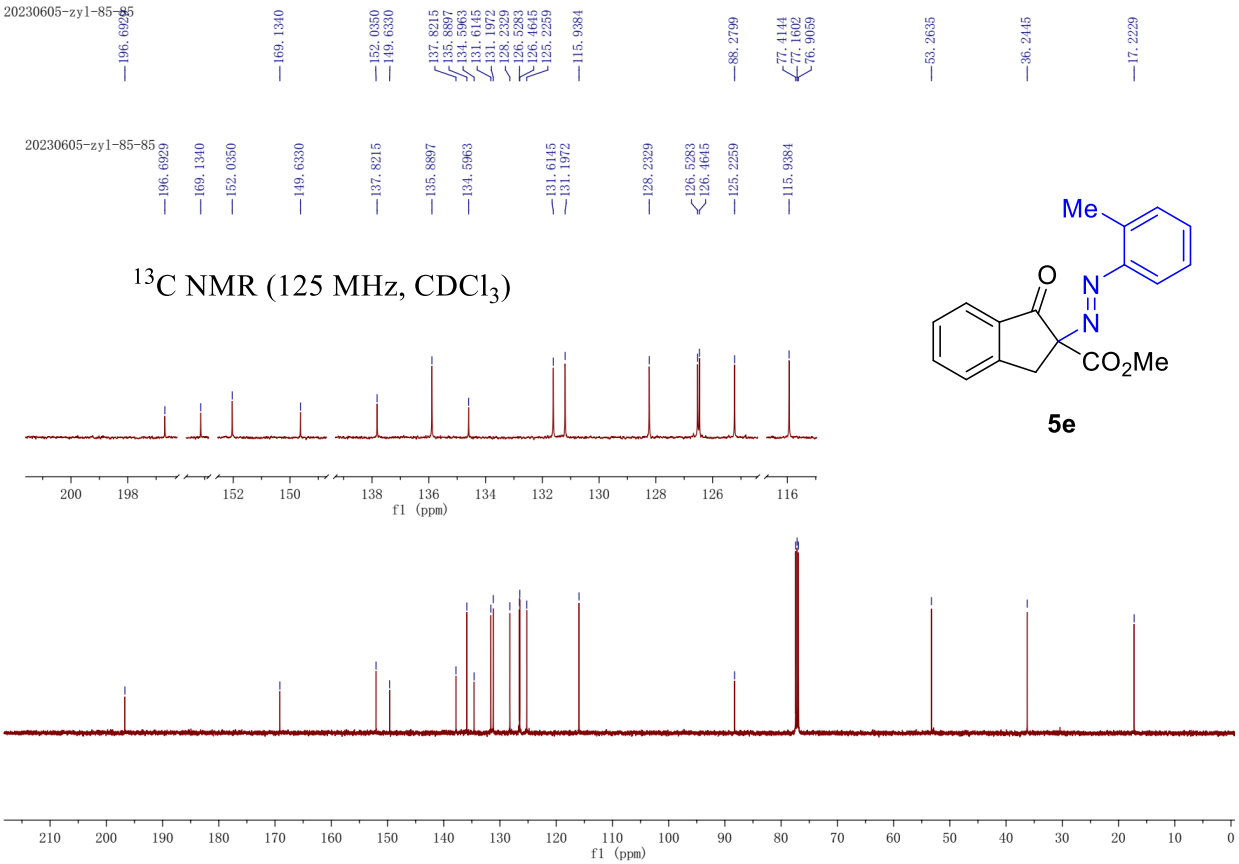

1.00
2.00
1.01
1.02
1.00
2.00
5.00
6.00
f1 (ppm)

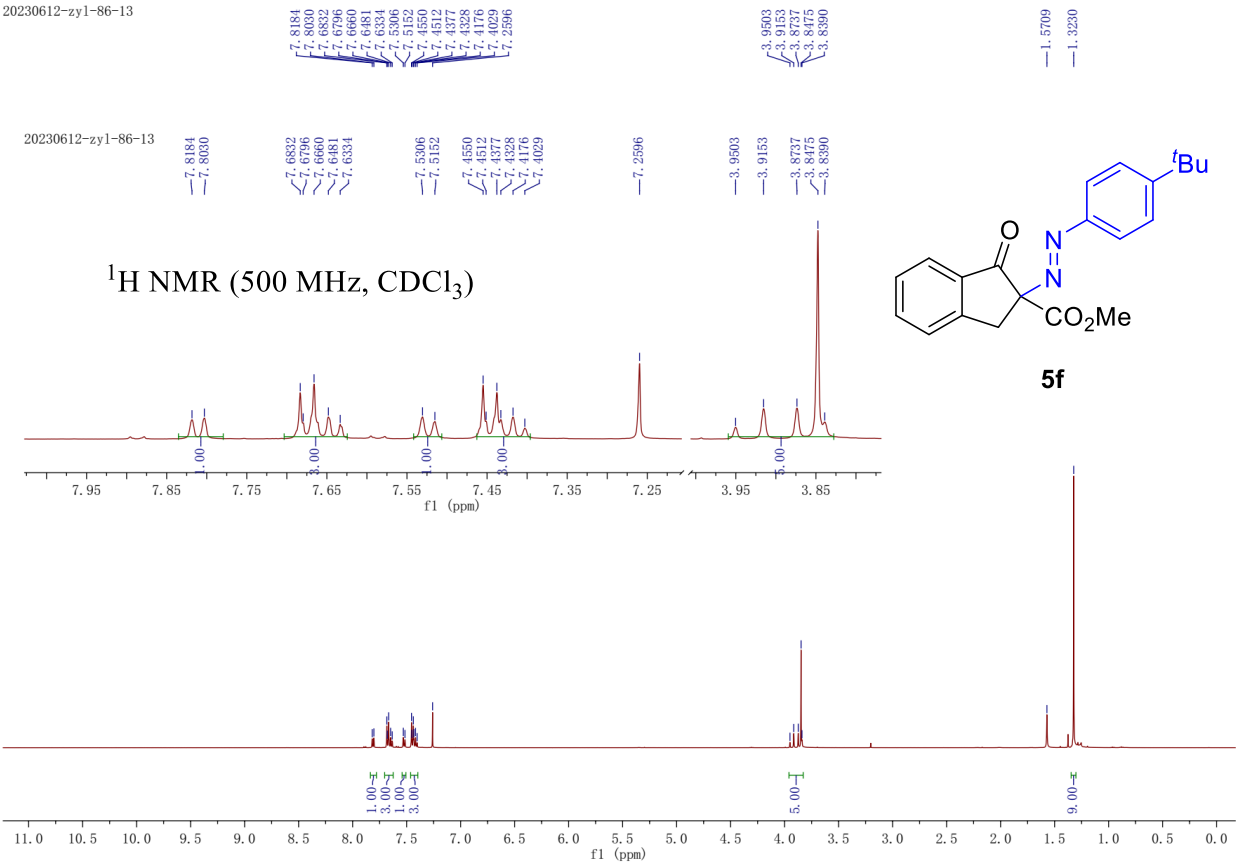
20230620-zyl-86-30
196.1019
167.4030
153.3417
141.3023
135.1234
134.2110
129.9205
128.2372
127.9486
125.7638
125.1644
111.1554
100.4863
77.4137
77.1598
76.9055
53.4071
40.3347
33.4275
20230620-zyl-86-30
^{13}C NMR (125 MHz, $CDCl_3$)
O
N
N
CO_2Me
N
5c
f1 (ppm)

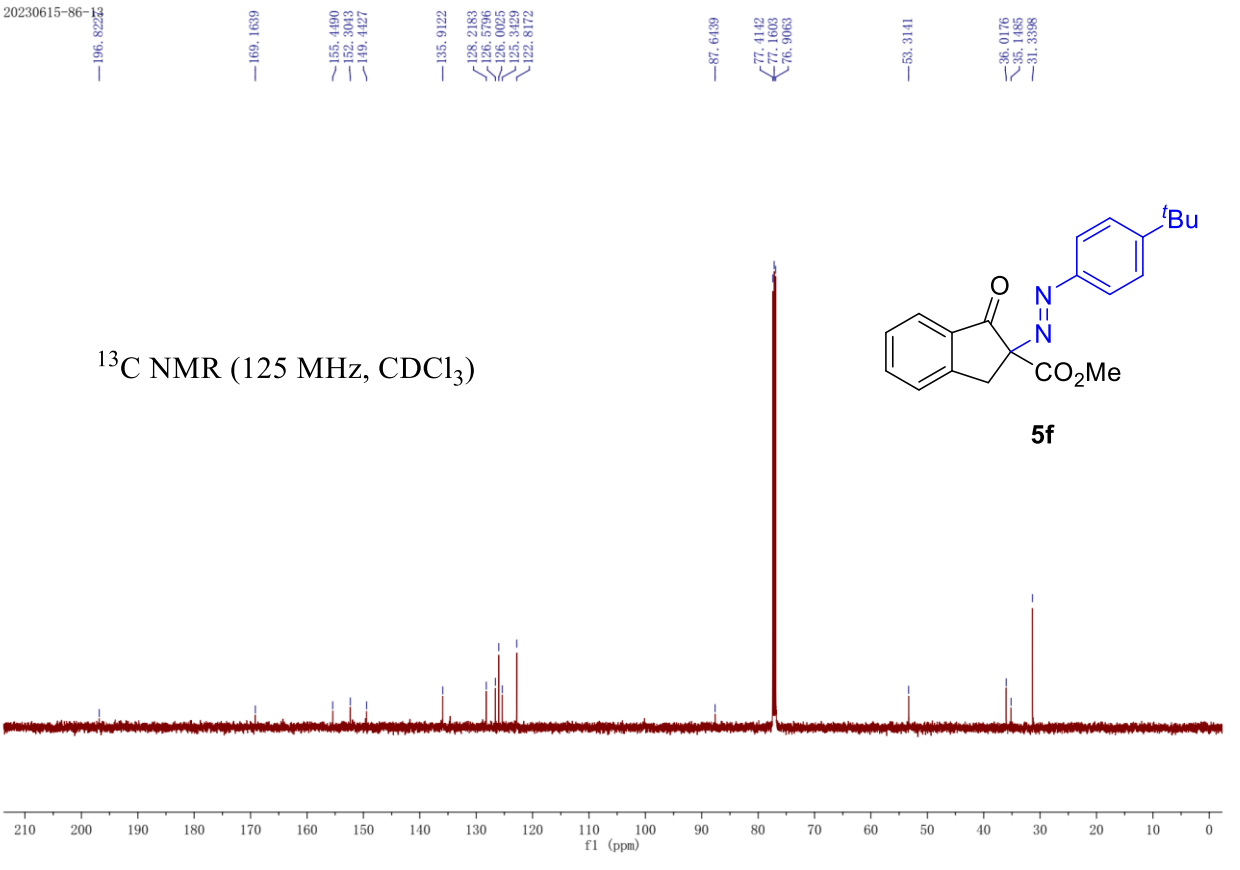

20230605-zy1-85-84
7.8190
7.8036
7.6628
7.6612
7.6434
7.6304
7.6266
7.5302
7.5147
7.4322
7.4172
7.4024
7.2599
7.2327
7.2164
3.9442
3.9092
3.8727
3.8487
3.8379
2.3826
1.6078
20230605-zy1-85-84
1H NMR (500 MHz, CDCl3)
Me
O
N
N
CO2Me
5d
f1 (ppm)

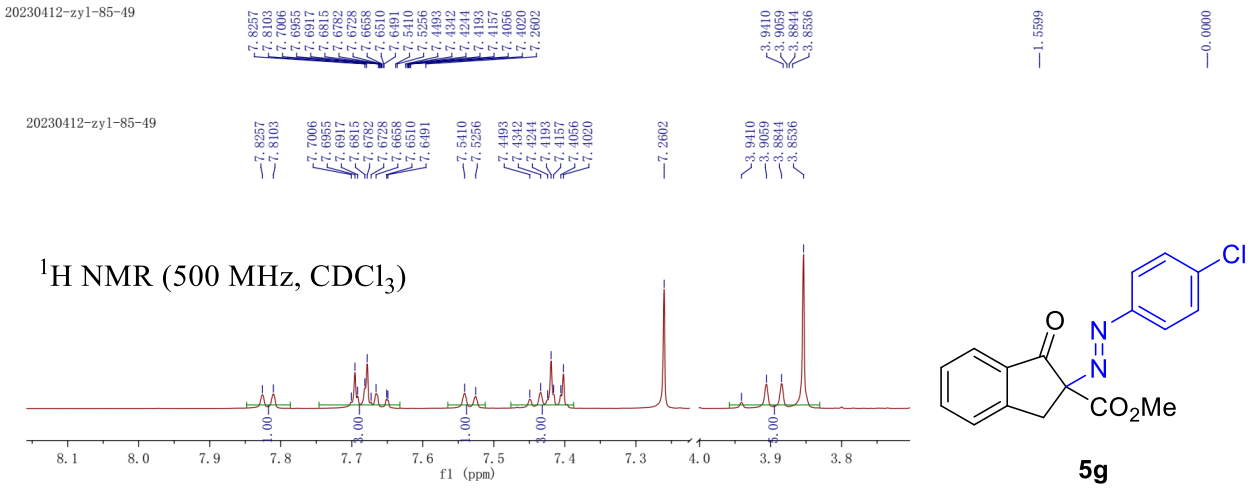

20230607-zy1-85-84
196.8490
169.1504
152.3347
149.6401
142.3910
135.9221
134.6053
129.6889
128.2122
126.5719
125.3306
123.0519
87.5590
77.4137
77.1597
76.9056
53.3041
36.0251
21.5883
20230607-zy1-85-84
196.8490
13C NMR (125 MHz, CDCl3)
Me
O
N
N
CO2Me
5d
f1 (ppm)

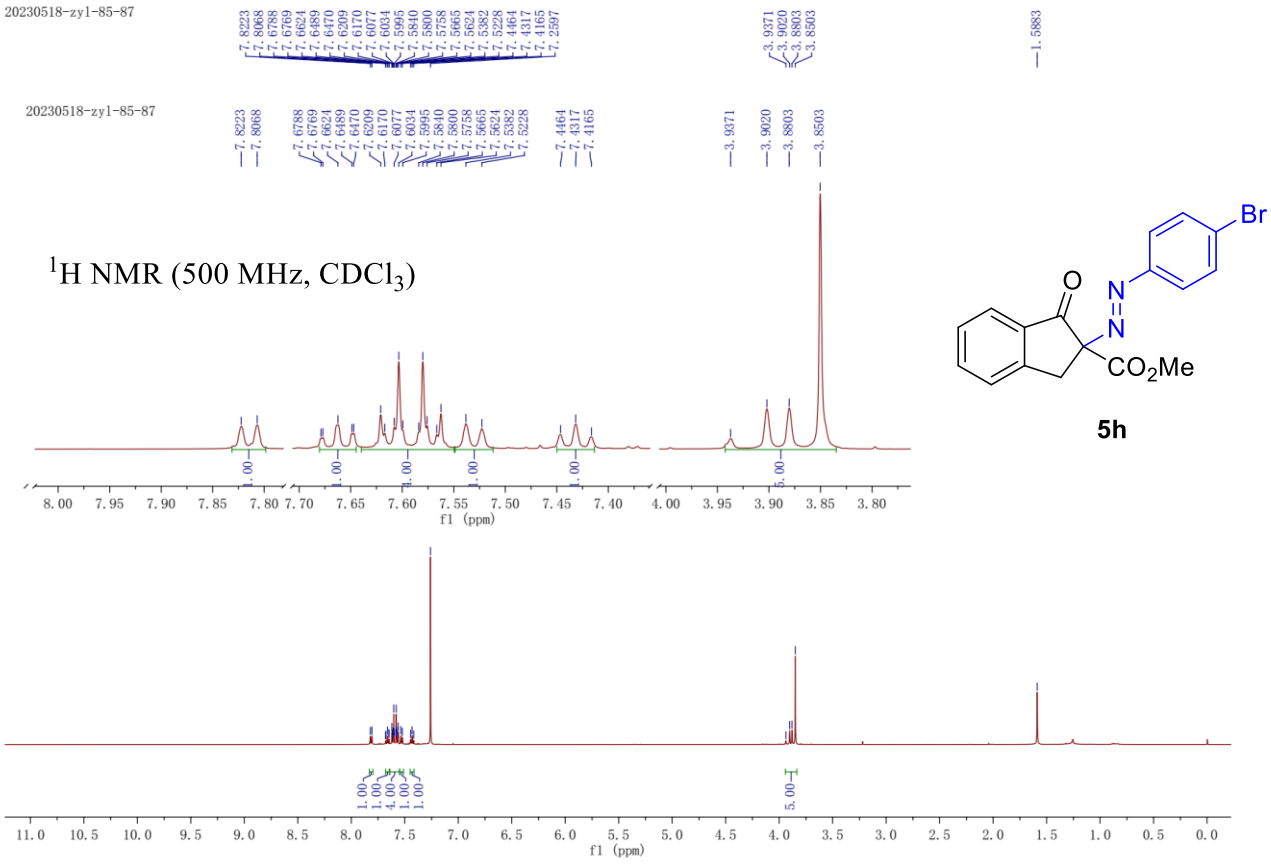

20230518-zy1-85-85
^{1}H NMR (500 MHz, $CDCl_3$)
Me
O
N
N
CO_2Me
5e
f1 (ppm)

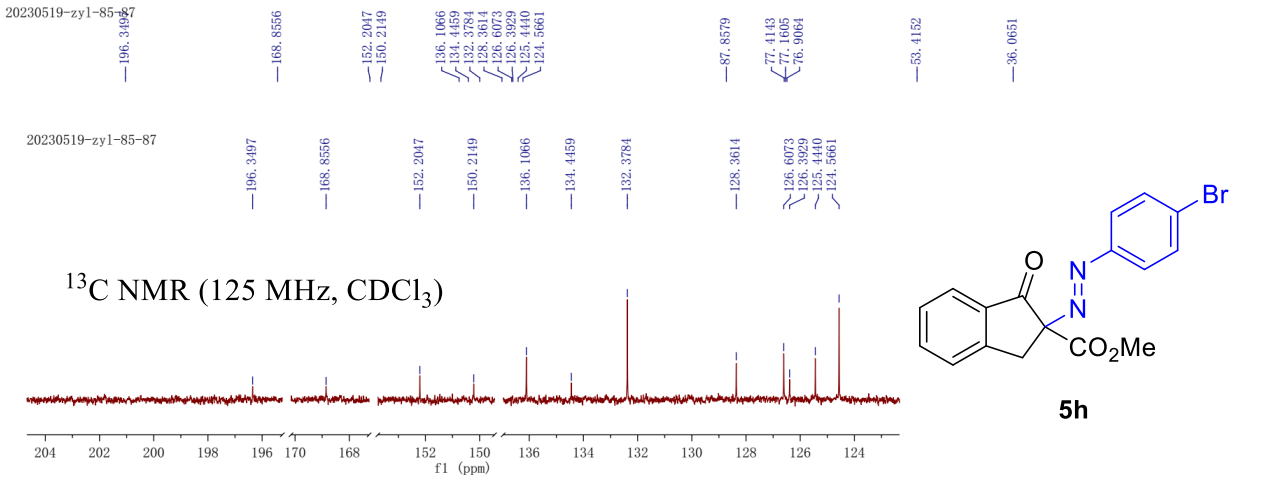

20230605-zy1-85-85
^{13}C NMR (125 MHz, $CDCl_3$)
Me
O
N
N
CO_2Me
5e
f1 (ppm)


20230612-zy1-86-13
7.8184
7.8030
7.6832
7.6796
7.6660
7.6481
7.6334
7.5306
7.5152
7.4550
7.4512
7.4377
7.4328
7.4176
7.4029
7.2596
3.9503
3.9153
3.8737
3.8475
3.8390
1.5709
1.3230
20230612-zy1-86-13
^{1}H NMR (500 MHz, $CDCl_3$)
tBu
O
N
N
CO2Me
5f
1.00
3.00
1.00
3.00
1.00
3.00
5.00
9.00
f1 (ppm)

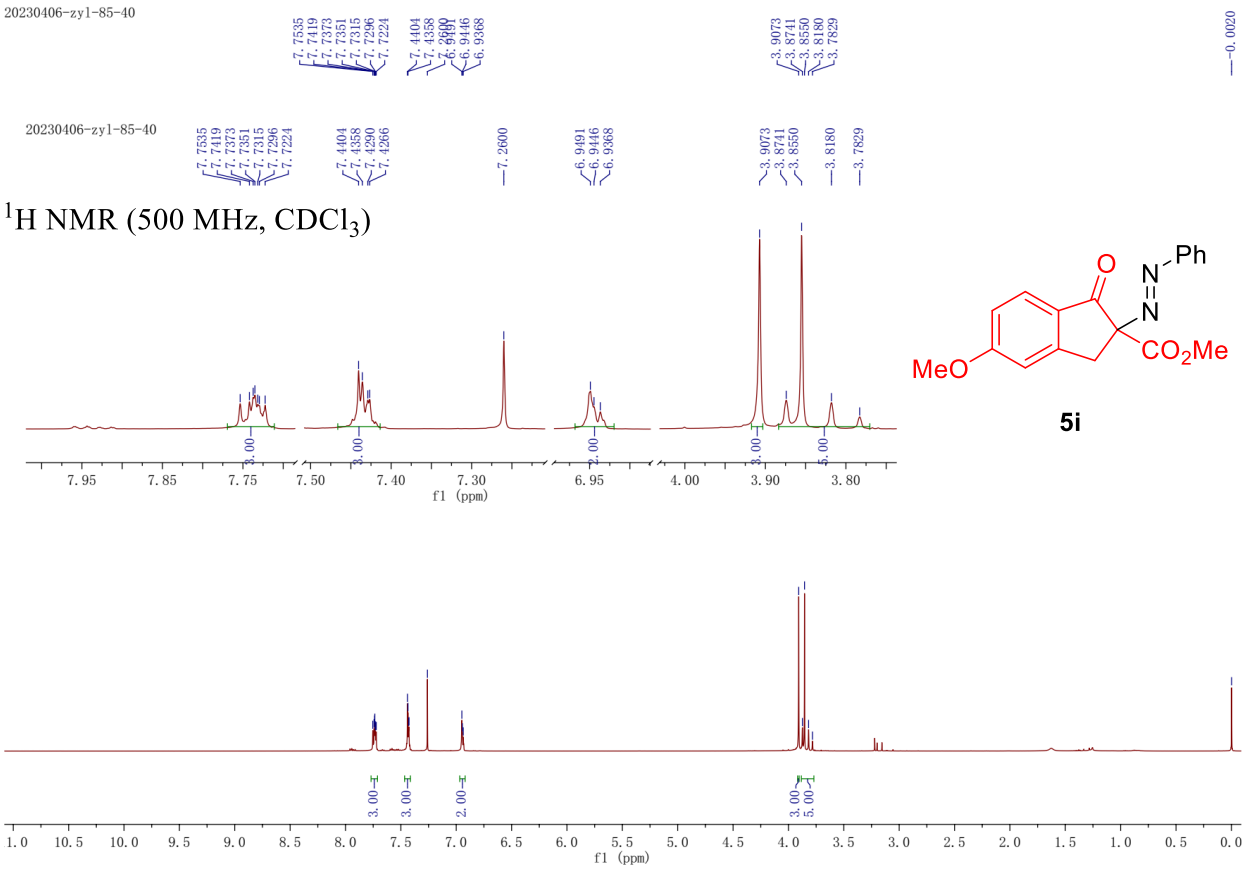

20230615-86-13
196.8224
169.1639
155.4900
152.3043
149.4427
135.9122
128.2183
126.5796
126.0025
125.3429
122.8172
87.6439
77.4142
77.1603
76.9063
53.3141
36.0176
35.1485
31.3398
^{13}C NMR (125 MHz, $CDCl_3$)
tBu
O
N
N
CO2Me
5f
f1 (ppm)

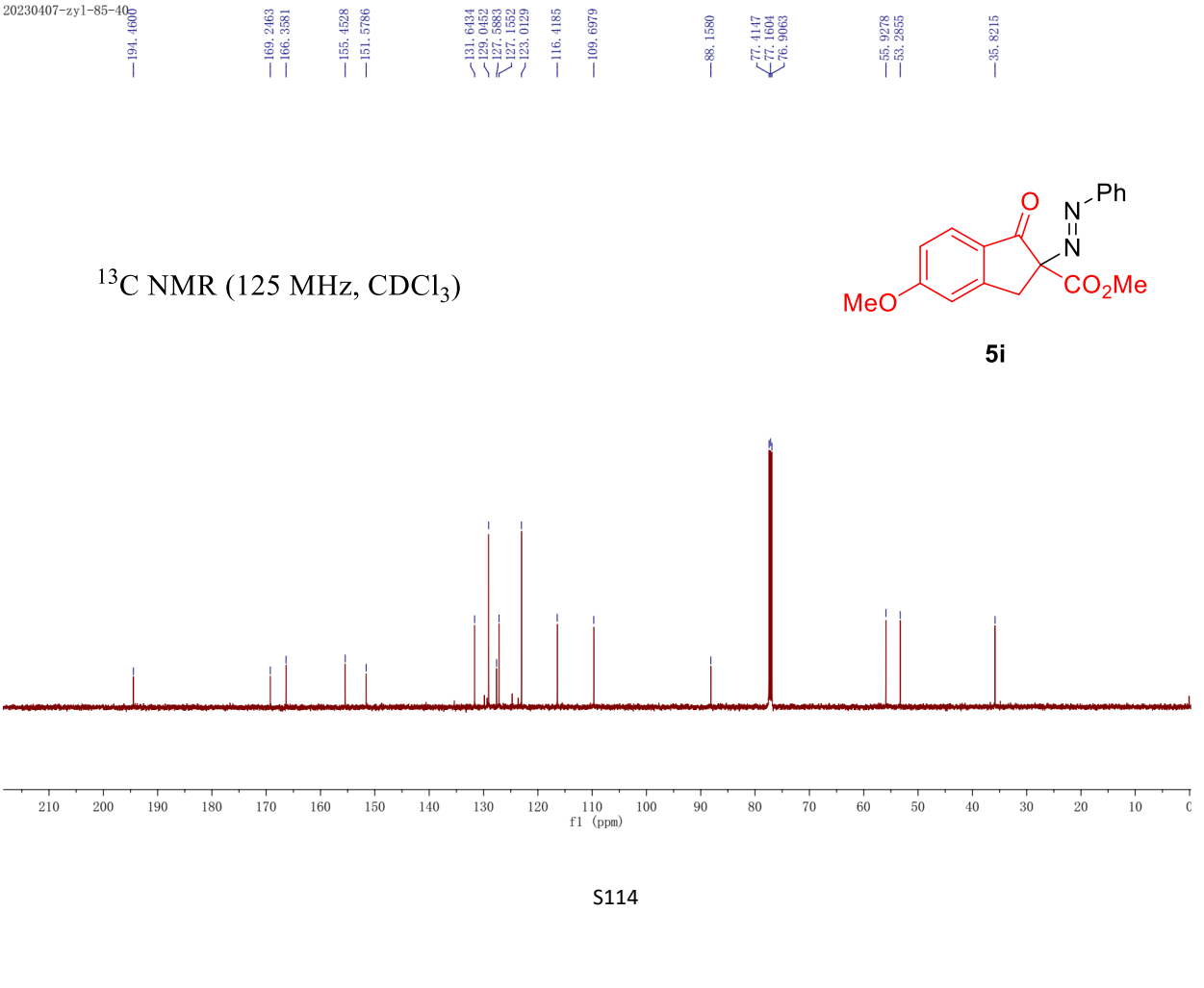

20230412-zyl-85-49
7.8257
7.8103
7.7006
7.6955
7.6917
7.6815
7.6782
7.6728
7.6658
7.6510
7.6491
7.5410
7.5256
7.4493
7.4342
7.4244
7.4193
7.4157
7.4056
7.4020
7.2602
3.9410
3.9059
3.8844
3.8536
1.5599
0.0000
20230412-zyl-85-49
1H NMR (500 MHz, CDCl3)
1.00
3.00
1.00
3.00
1.00
3.00
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
4.0
3.9
3.8
f1 (ppm)
Cl
O
N
N
CO2Me
5g
1.00
3.00
1.00
3.00
5.00
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
20230414-zyl-85-49
196.3337
168.8512
152.1696
149.8304
137.8519
136.0600
134.4419
129.3446
128.3239
126.5822
125.3853
124.3315
87.7862
77.4141
77.1599
76.9057
53.3528
36.0630
20230414-zyl-85-49
196.3337
13C NMR (125 MHz, CDCl3)
201
200
199
198
197
196
195
194
193
192
f1 (ppm)
Cl
O
N
N
CO2Me
5g
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

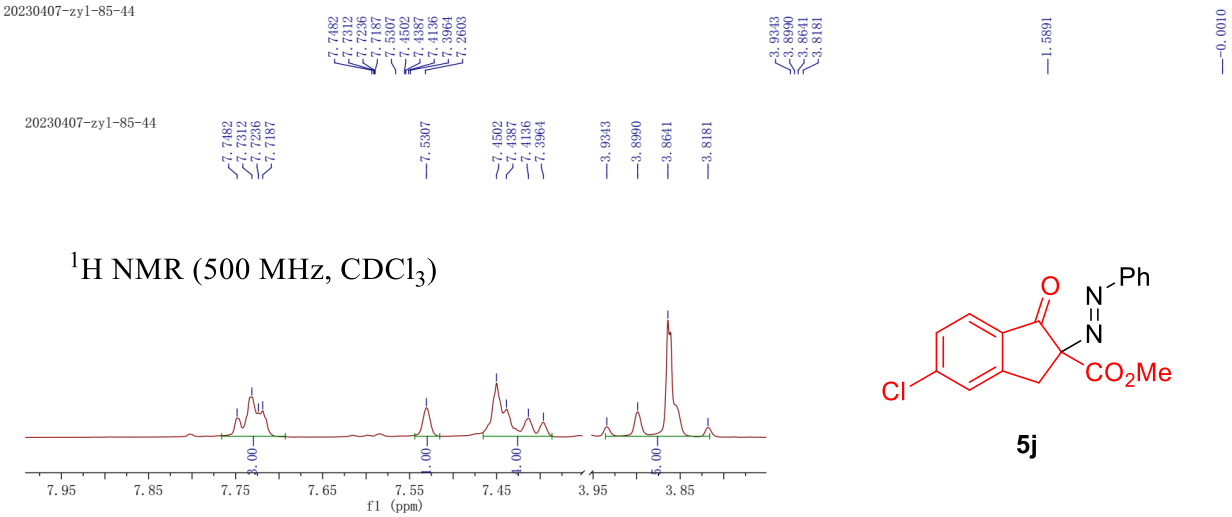

20230518-zyl-85-87
7.8223
7.8068
7.6788
7.6769
7.6624
7.6489
7.6470
7.6209
7.6170
7.6077
7.6034
7.5995
7.5840
7.5800
7.5758
7.5665
7.5624
7.5382
7.5228
7.4464
7.4317
7.4165
7.2597
3.9371
3.9020
3.8803
3.8503
1.5883
20230518-zyl-85-87
^{1}H NMR (500 MHz, $CDCl_3$)
Br
O
N
N
CO_2Me
5h
f1 (ppm)


1.00
1.00
4.00
1.00
1.00
5.00
f1 (ppm)

20230519-zyl-85-87
196.3497
168.8556
152.2047
150.2149
136.1066
134.4459
132.3784
128.3614
126.6073
126.3929
125.4440
124.5661
87.8579
77.4143
77.1605
76.9064
53.4152
36.0651
20230519-zyl-85-87
^{13}C NMR (125 MHz, $CDCl_3$)
Br
O
N
N
CO_2Me
5h
f1 (ppm)

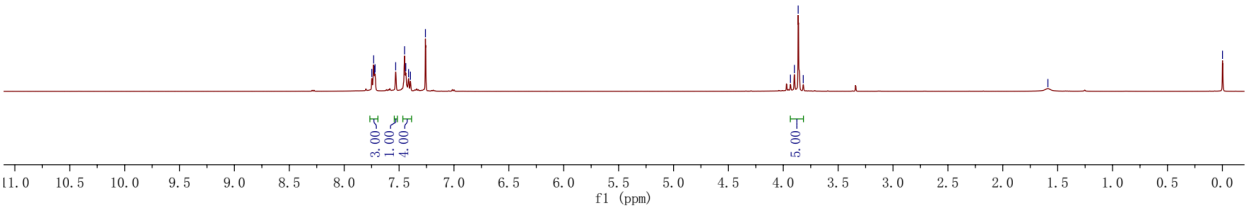

20230406-zyl-85-40
7.535
7.419
7.373
7.351
7.315
7.296
7.224
7.404
7.358
7.290
7.266
7.2600
6.9491
6.9446
6.9368
3.9073
3.8741
3.8550
3.8180
3.7829
-0.0020
20230406-zyl-85-40
1H NMR (500 MHz, CDCl3)
Ph
N
N
O
MeO
CO2Me
5i
3.00
3.00
2.00
3.00
5.00
7.95
7.85
7.75
7.50
7.40
7.30
6.95
4.00
3.90
3.80
f1 (ppm)
3.00
3.00
2.00
3.00
5.00
f1 (ppm)

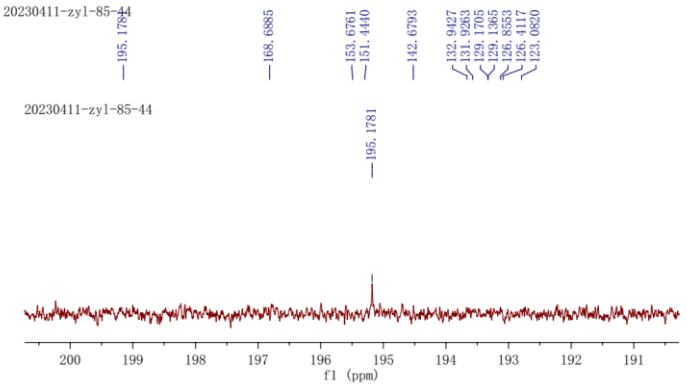

20230407-zyl-85-40
194.4600
169.2463
166.3581
155.4528
151.5786
131.6434
129.0452
127.5883
127.1552
123.0129
116.4185
109.6979
88.1580
77.4147
77.1604
76.9063
55.9278
53.2855
35.8215
13C NMR (125 MHz, CDCl3)
Ph
N
N
O
MeO
CO2Me
5i
f1 (ppm)

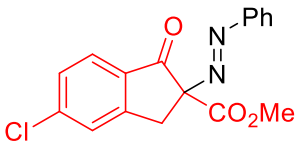


^{1}H NMR (500 MHz, $CDCl_3$)

5j

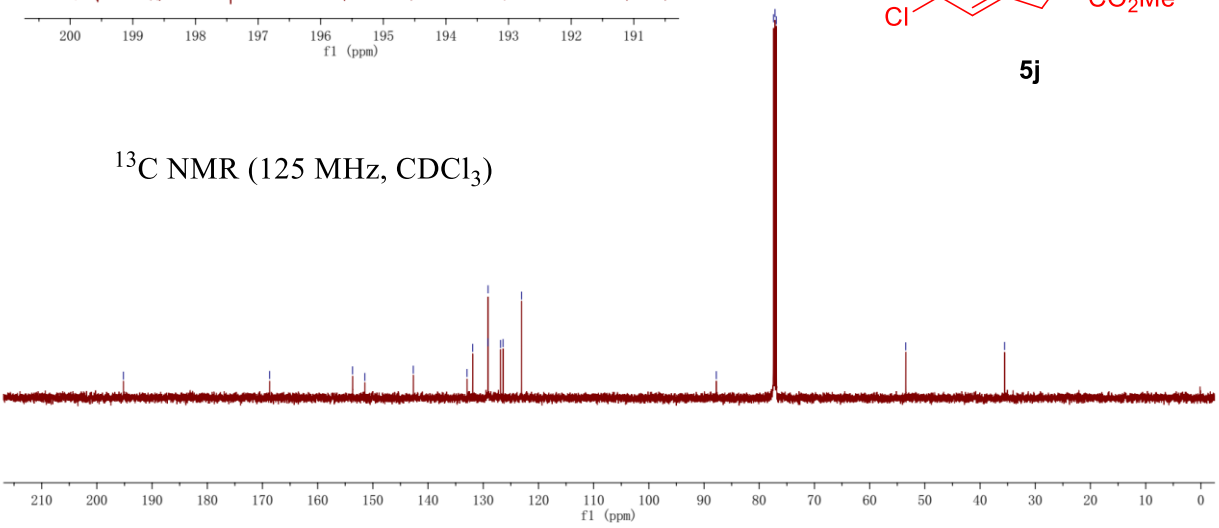






5j

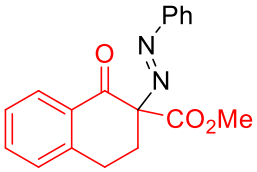
^{13}C NMR (125 MHz, $CDCl_3$)



20230407-zyl-85-42

20230407-zyl-85-42

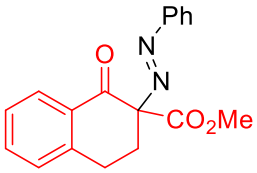
^{1}H NMR (500 MHz, $CDCl_3$)



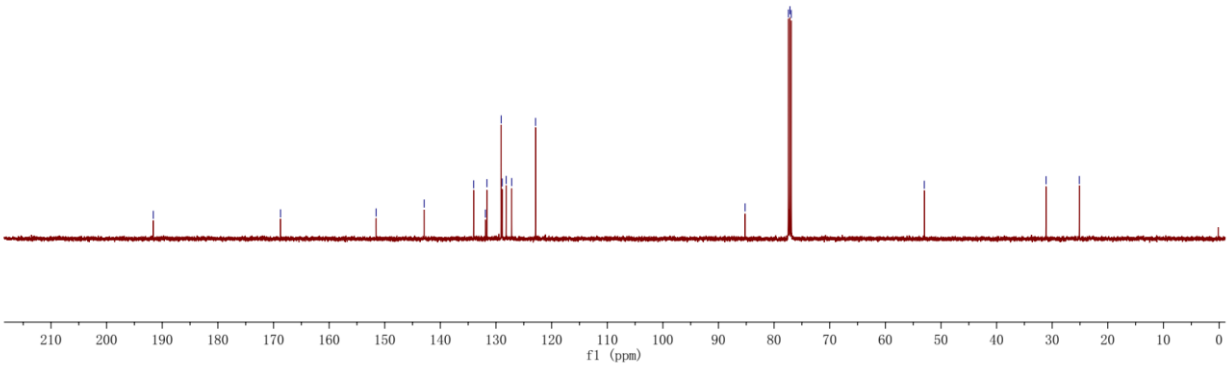
5k

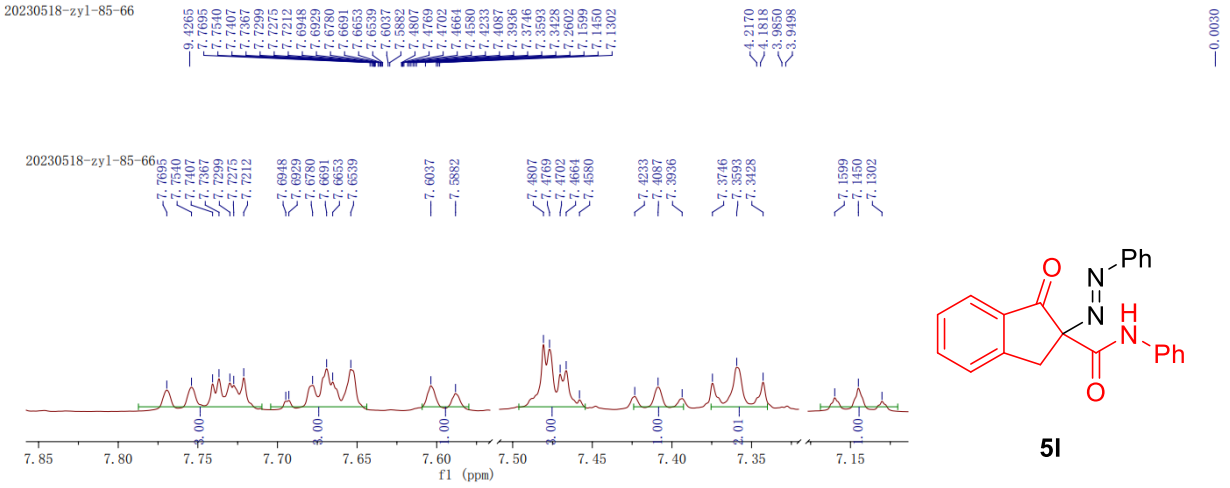
20230411-zyl-85-42

^{13}C NMR (125 MHz, $CDCl_3$)

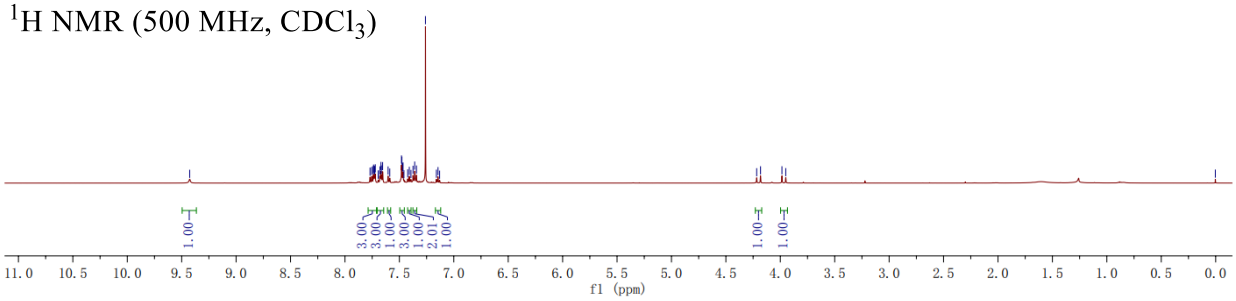


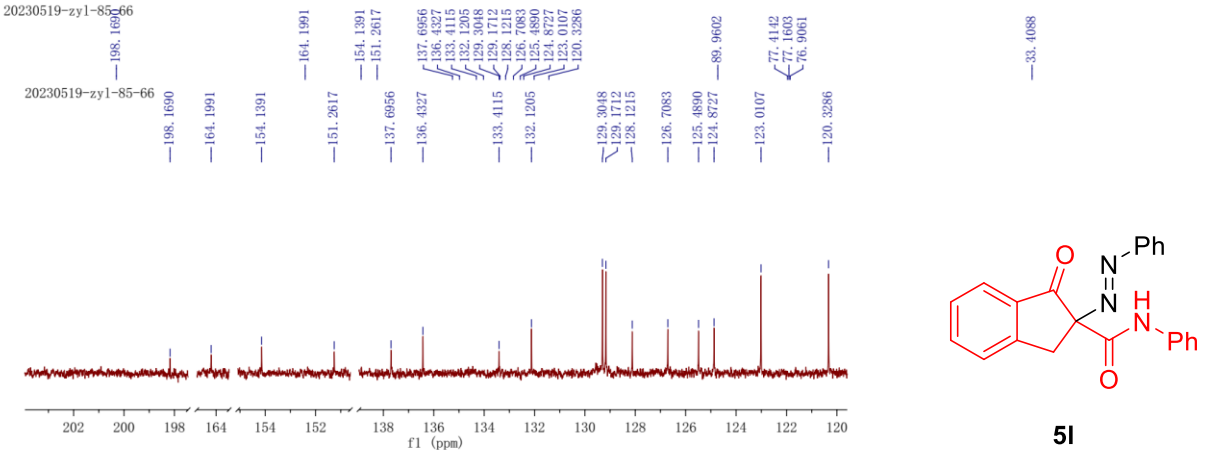
5k



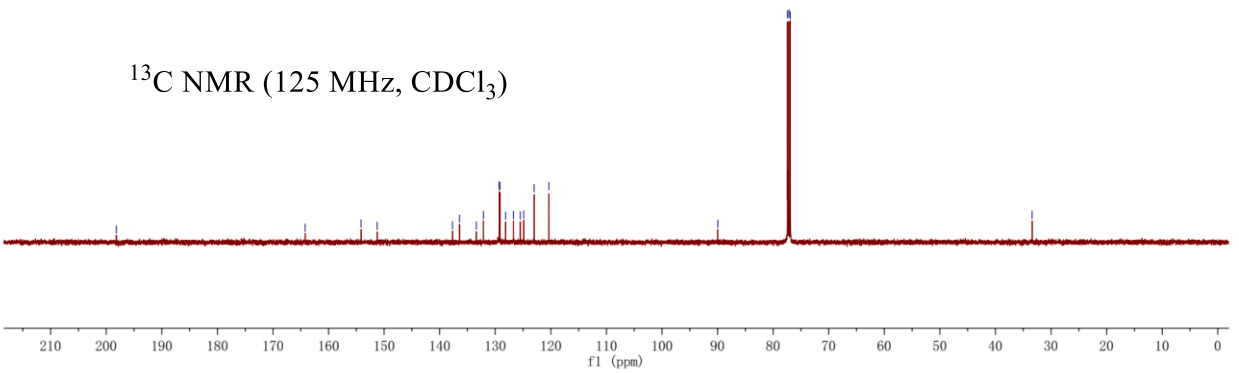


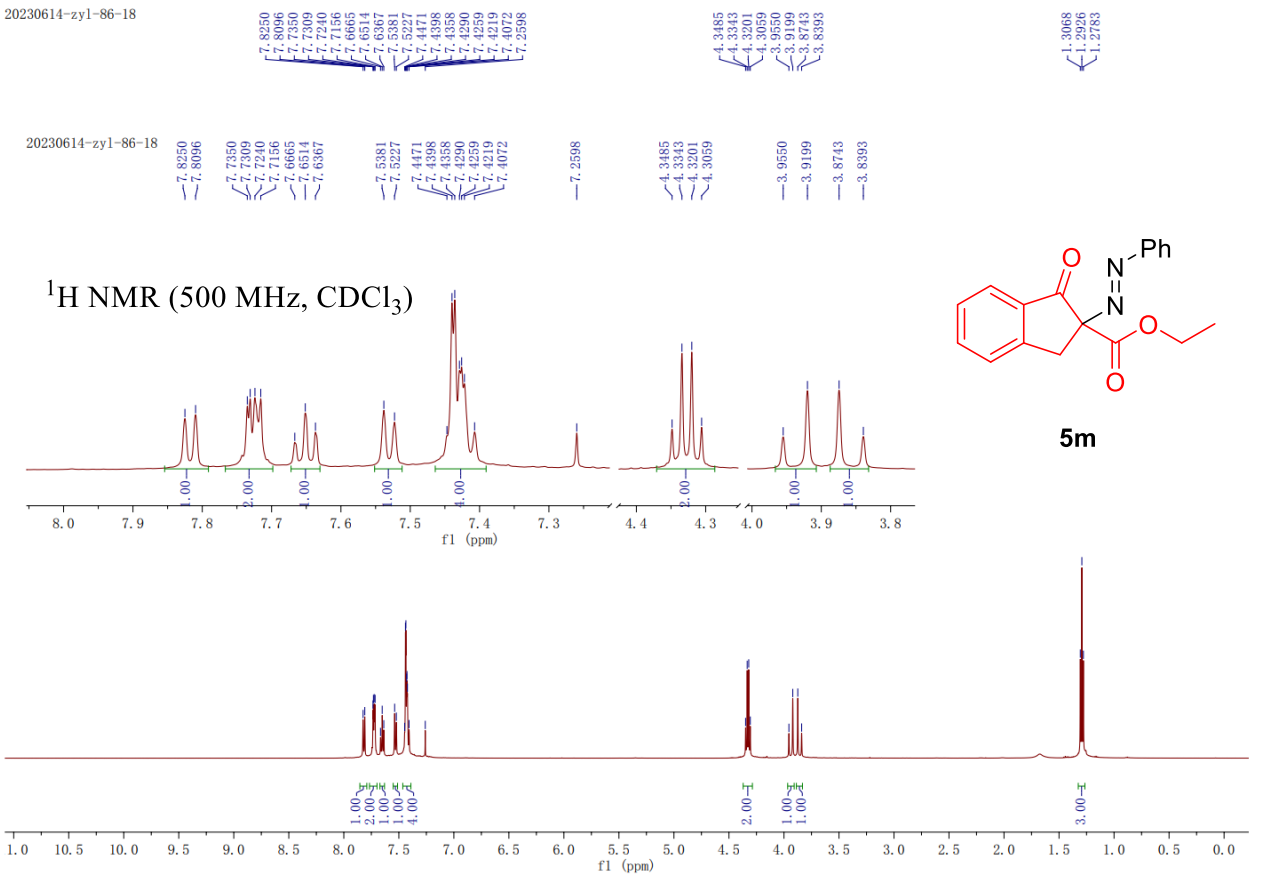
^{1}H NMR (500 MHz, $CDCl_3$)





^{13}C NMR (125 MHz, $CDCl_3$)

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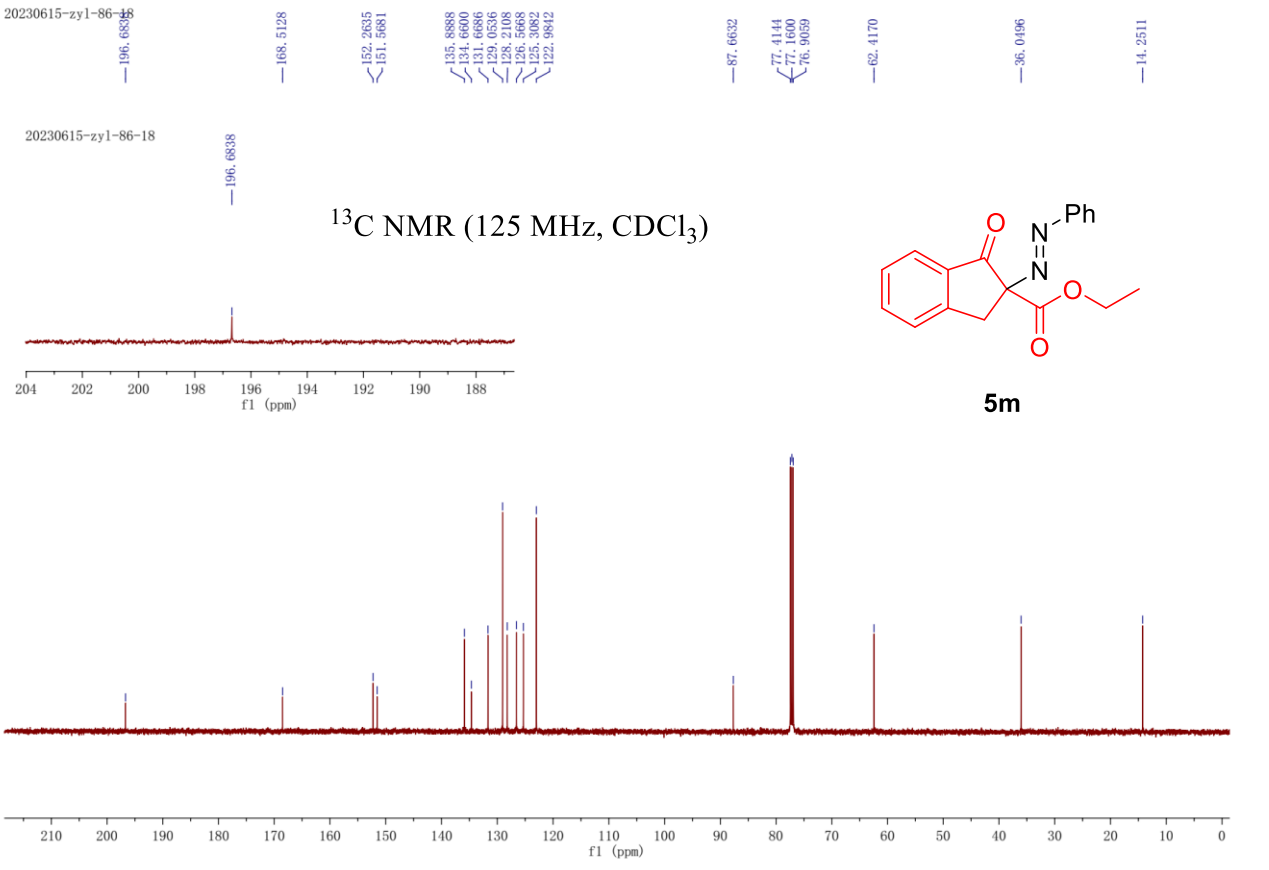
5m
f1 (ppm)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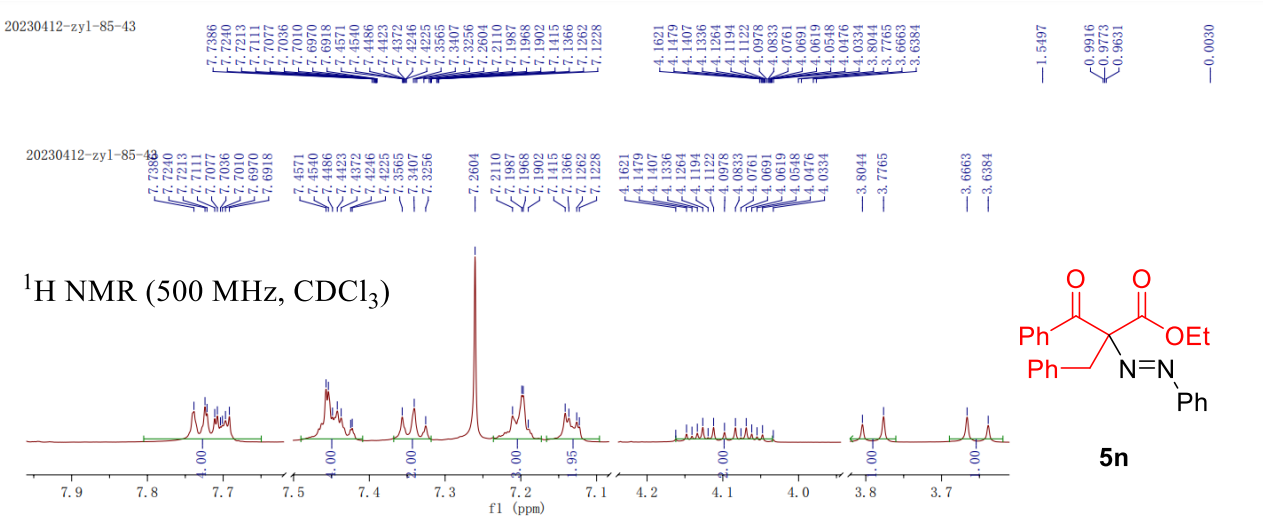
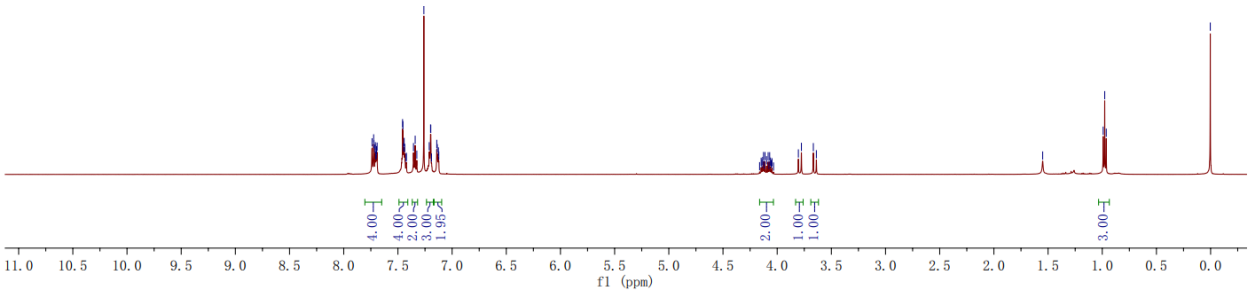
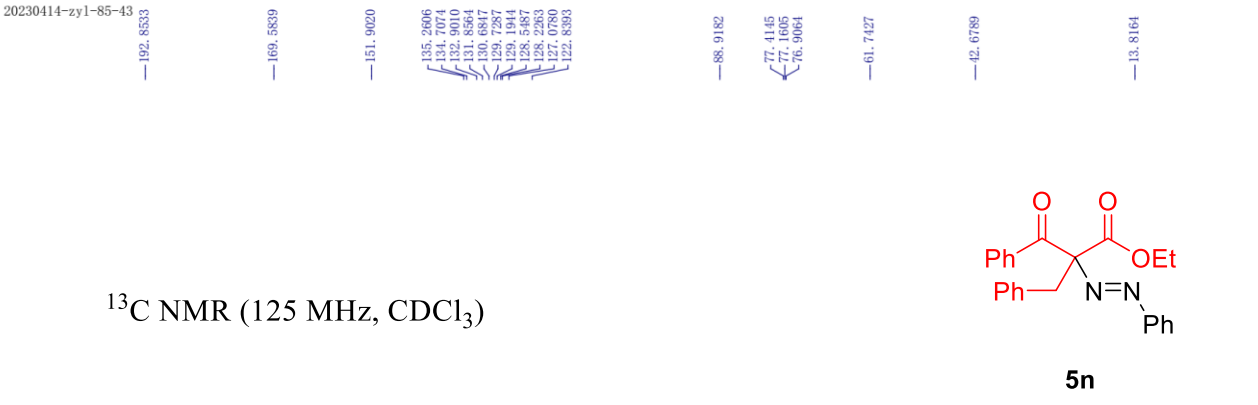
^{13}C NMR (125 MHz, $CDCl_3$)
5m
f1 (ppm)


20230412-zyl-85-43
20230412-zyl-85-43
1H NMR (500 MHz, CDCl3)
Ph
O
O
OEt
Ph
N=N
Ph
5n
f1 (ppm)


f1 (ppm)


20230414-zyl-85-43
13C NMR (125 MHz, CDCl3)
Ph
O
O
OEt
Ph
N=N
Ph
5n
f1 (ppm)

20230612-zy1-86-12

7.7481 7.7437 7.7360 7.7286 7.4863 7.4816 7.4748 7.4728 7.2595 7.2459 7.2352 7.2275 7.2184 7.2131 7.1975

4.2819 4.2747 4.2676 4.2604 4.2535 4.2462 4.2393 4.2319 4.2250 4.2178 4.2108 4.2035 3.5808

1.2342 1.2199 1.2054

20230612-zy1-86-12

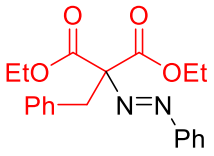
7.7481 7.7437 7.7360 7.7286

7.4863 7.4816 7.4748 7.4728

7.2595 7.2459 7.2352 7.2275 7.2184 7.2131 7.1975

4.2819 4.2747 4.2676 4.2604 4.2535 4.2462 4.2393 4.2319 4.2250 4.2178 4.2108 4.2035

^{1}H NMR (500 MHz, $CDCl_3$)



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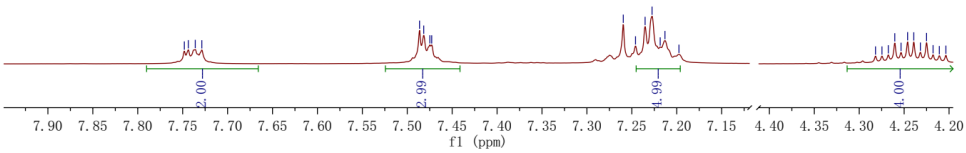
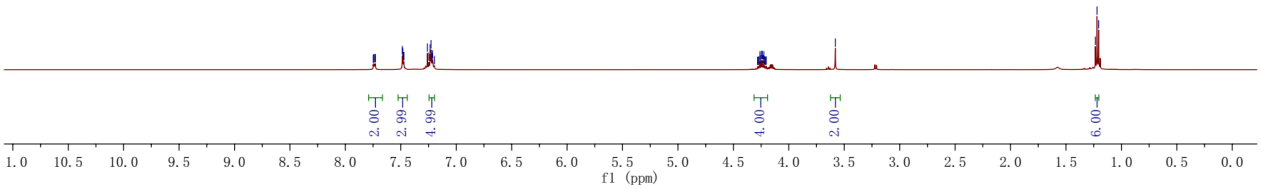




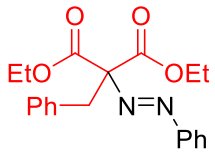
20230615-zy1-86-12

167.9985 151.5909 134.9908 131.7750 130.7812 129.1771 128.2037 127.1456 123.0288 86.0588 77.4139 77.1597 76.9057 61.9139 41.7035 14.1506

20230615-zy1-86-12

134.9908 131.7750 130.7812 129.1771 128.2037 127.1456 123.0288

^{13}C NMR (125 MHz, $CDCl_3$)



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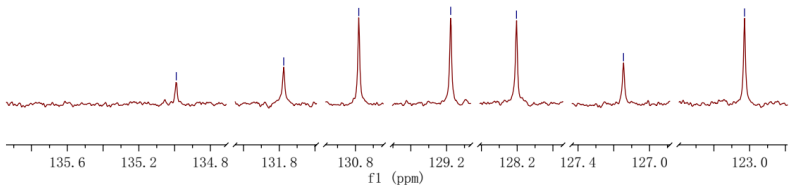

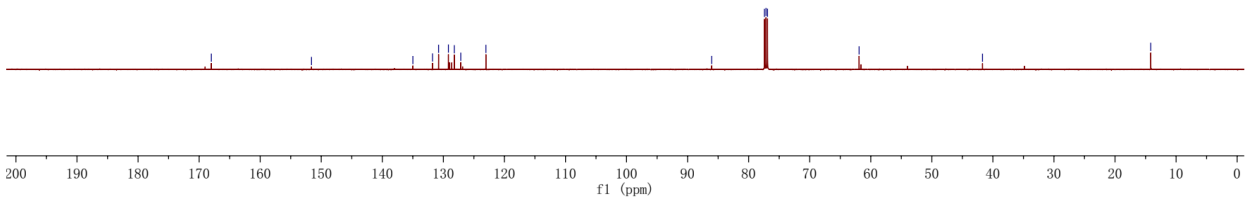

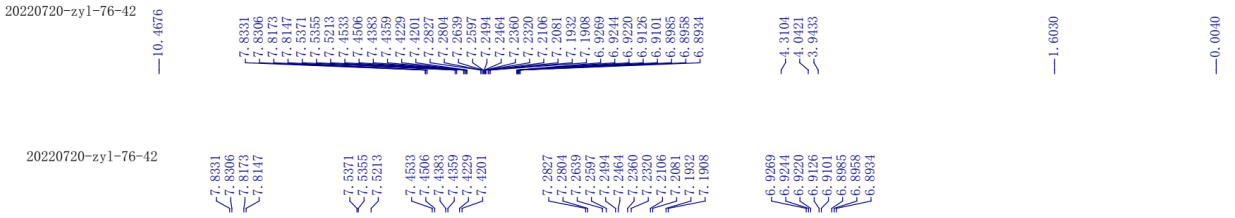

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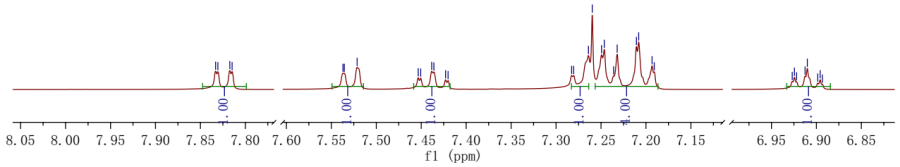
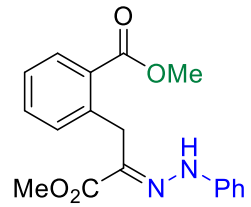
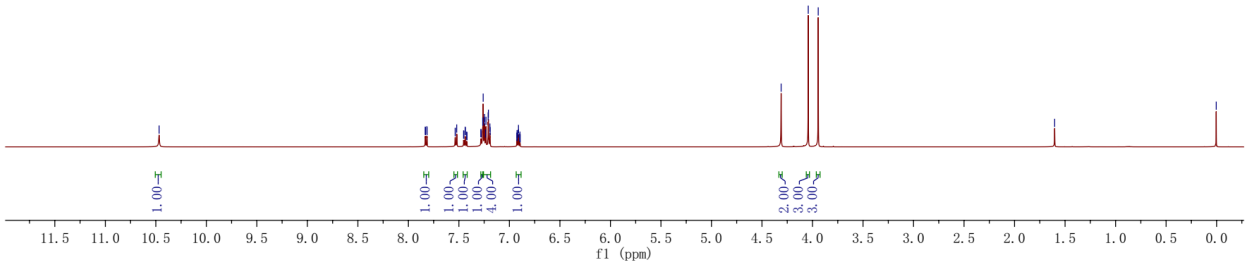
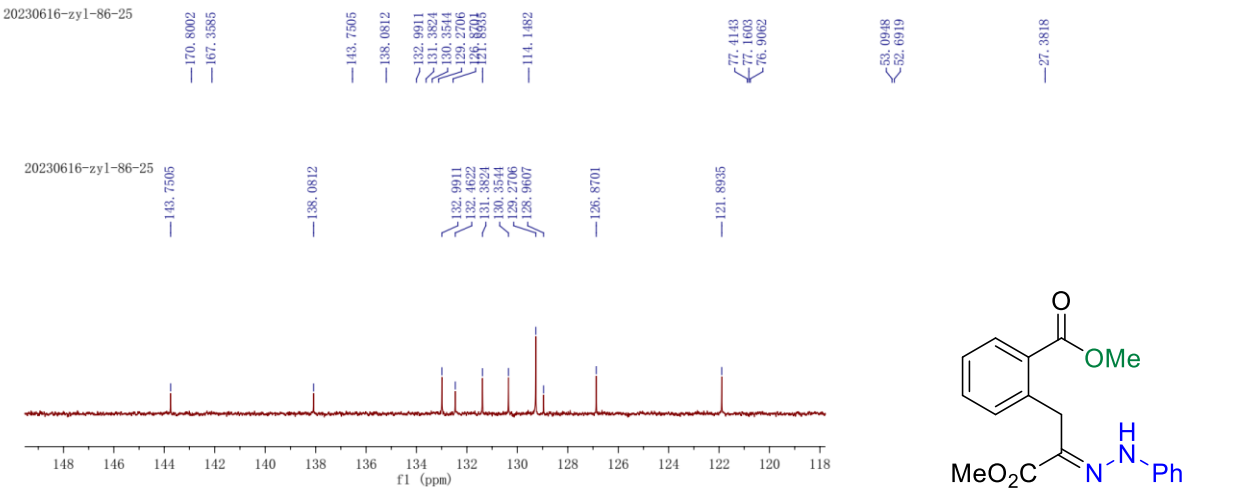




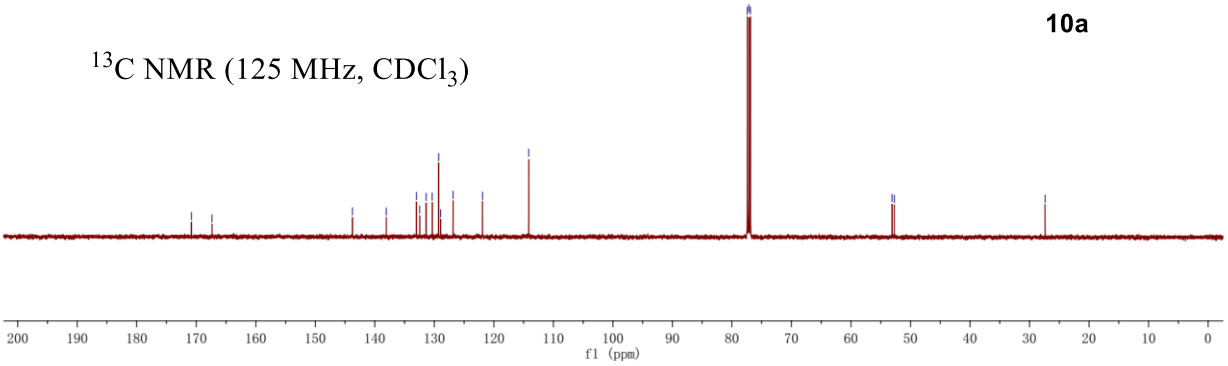
10a





10a

^{13}C NMR (125 MHz, $CDCl_3$)



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