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Supplementary Information

Computational Design of an Intramolecular Photocyclization Reaction with State-Selective Reactivity: A Strategy for Indole Synthesis

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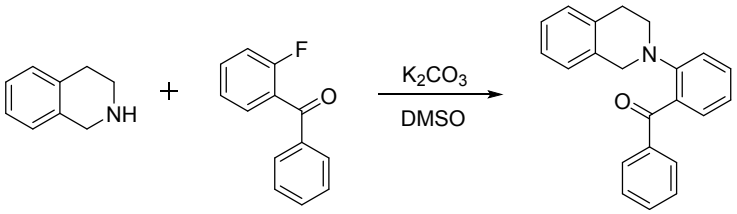
1. General Information

^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker AVANCE 400 and 500 spectrometer. Chemical shifts of protons were reported in parts per million downfield from tetramethylsilane and were referenced to residual protium in the NMR solvent ($CDCl_3$: δ 7.26), (DMSO-d6: δ 2.50). Chemical shifts of carbon were referenced to the carbon resonances of the solvent ($CDCl_3$: δ 77.0), (DMSO-d6: δ 39.5). Peaks were labeled as singlet (s), doublet (d), triplet (t), quartet (q) and multiplet (m). Melting points were measured on a WRS-2A melting point apparatus and were uncorrected. All products were further characterized by HRMS (high resolution mass spectra). Copies of their ^{1}H NMR and ^{13}C NMR spectra were provided.

2. General Procedures

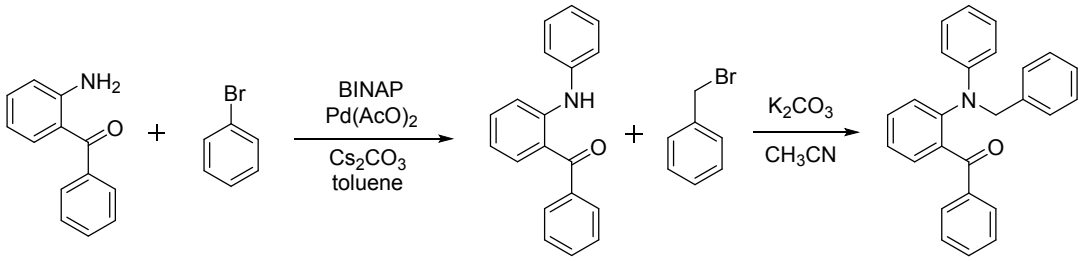
(I) Typical procedure for the preparation of substrates 1a - 1r, 1aa - 1ad, 1af - 1ar.



1a

The compound was synthesized according to a known procedure.[1] To a solution of potassium carbonate (0.83 g, 6.0 mmol) in dimethyl sulfoxide (10 mL), 1,2,3,4-tetrahydroisoquinoline (0.8 g, 6.0 mmol) and 1-(2-fluorophenyl)ethanone (0.69 g, 5 mmol) were added. The reaction mixture was stirred at 120 °C for 12 h. After completion of the reaction as shown by TLC, water (30 mL) was used to dilute the reaction. The organic layer was extracted with ethyl acetate (20 mL × 3), the combined organic layer was washed with saturated NH_4Cl (20 mL), dried with anhydrous sodium sulfate and concentrated in vacuum. The crude production was purified by flash chromatography to give a yellow oil 1a (0.94 g, yield: 60%).

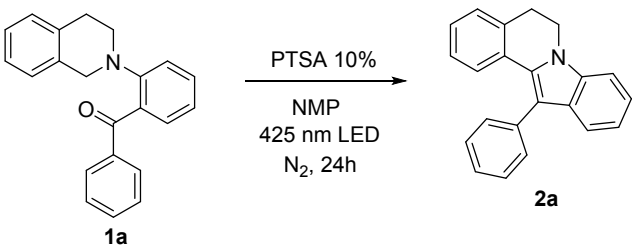
(II) Typical procedure for the preparation of substrates 1ae.



1ae

The compound was synthesized according to the similar procedures.[2-3] To a solution of Phenyl bromide (2 mmol) in toluene (5 mL) was added 1-(2-Aminophenyl)-ethanone (2.2 mmol), Cs_2CO_3 (2.8 mmol) BINAP (0.16 mmol), and $Pd(OAc)_2$ (0.10 mmol) at room temperature. The reaction mixture was allowed to stir at 120 °C for 15h. After completion of the reaction as shown by TLC, the mixture was allowed to cool to room temperature, and the crude production was purified by flash chromatography, giving a yellow solid (437 mg, yield: 80%). Then the product was added to a solution of potassium carbonate (276 mg, 2.0 mmol) and Benzylation bromide (341 mg, 2.0 mmol) in Acetonitrile (10 mL), The reaction mixture was stirred at 60 °C for 12 h. After completion of the reaction as shown by TLC, the potassium carbonate was filter out and the solvent was concentrated in vacuum. The crude production was purified by flash chromatography, giving a yellow oil **1ae** (465 mg, yield: 80%).

(III) Typical procedure for Photocyclization of 2a.



1a **2a**

(2-(3,4-dihydroisoquinolin-2(1H)-yl)phenyl)(phenyl)methanone **1a** (93.9 mg, 0.3 mmol), PTSA (5.7 mg, 0.03 mmol) were added to 20 mL quartz tube containing 3 mL NMP, the reaction mixture was stirred at room temperature under irradiation of 425nm LED in nitrogen atmosphere condition. After completion of the reaction as shown by TLC, water (3 mL) was used to dilute the reaction. The organic layer was extracted with ethyl acetate (5 mL × 3). The combined organic layer was washed with saturated NH_4Cl (5 mL), dried with anhydrous sodium sulfate and concentrated in vacuum. The crude product was purified by flash chromatography to give a white solid **2a** (75.2 mg, yield: 85%).

3. Computational Method

All the geometry optimization and vibration frequency calculation were carried out in Gaussian09 package[4], and meanwhile, the density-functional theory (DFT)[5] and time-dependent density-functional theory (TD-DFT)[6] were employed for the ground state as well as triplet state molecules calculation, and the singlet state molecules calculation, respectively. For geometry optimization, the ground state molecules (i.e., S0, B, C, TS3, TS3-3, D and product states) and singlet state molecules (i.e., S1 and TS1' states) were performed at the restricted B3LYP method[7] with 6-31+G(d, p) basis set[8], while the remaining ground state molecules (i.e., A' and TS2 states) and triplet state molecules (i.e., T1, TS1, A, TS2' and B' states) at the unrestricted B3LYP method[7] with 6-31+G(d, p) basis set[8]. The vibration frequency calculations were carried out at the same computational method and basis set to make sure that the optimized structures were true energy minima, and meanwhile, obtain the absolute free energy of optimized molecules. The reaction coordinate driving flexible scan method as well as the following restricted geometry optimization and vibration frequency were employed for the free energy profile from A state to B' state and B state to A' state at the same computational method and basis set. Both the reaction coordinates of A state to B' state and B state to A' state were the distance of C1 atom and C2 atom (see Figure 1). All the above calculations considered the solvation effect provided by the PCM solvent continuum models[9].

Based on the optimized structure of S0/S1/T1 states, the ESP charges and HOMO/LUMO/SOMO-1/SOMO orbits of S0/S1/T1 states were further calculated in Gaussian09 package[4]. The calculation theory (DFT[5] or TD-DFT[6]), calculation method (RB3LYP or UB3LYP)[7] and basis set were similar to that of the above computation. Meanwhile, the UV spectrum of optimized S0 state were also further calculated with the TD-DFT[6] at the restricted B3LYP method[7] with 6-31+G(d, p) basis set[8] in Gaussian09 package[4]. The final ESP charge surface, molecular orbital contours and UV spectrum were plotted using the GaussView software package[10]. The solvation effect provided by the PCM solvent continuum models[9] were also considered in these computations.

Besides the above computation, the Dalton2016[11] and MOMAP-v1.0 (Molecular Materials Property Prediction)[12-14] packages were also employed to calculate the rate of intersystem crossing (from S1 state to T1 state). The output files of geometry optimization and vibration frequency calculation of S0/S1/T1 states carried out in Gaussian 09 package[4] were first utilized by Dalton package[11] to obtain the spin orbital coupling constant (H_{so}) which in the following calculation could be adopted by MOMAP package[12-14] to finally calculate the rate of intersystem crossing (from S1 to T1 state).

4. References

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5. Figure S1-S9 & Table S1-S5 (1a/1j/1ae/1aj)

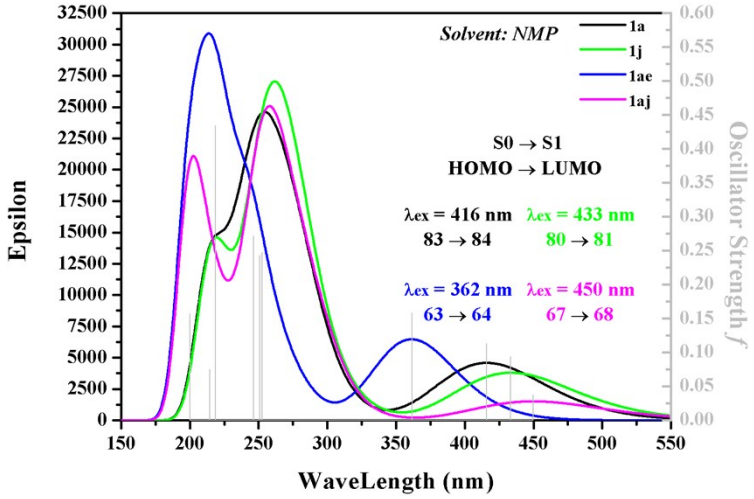

Figure S1. The UV absorption spectrums of **1a/1j/1ae/1aj** in NMP solvent, generated by quantum calculation. Under the visible light (about 350 nm to 450 nm), a distinct absorption peak matched to the S0→S1 transition which further corresponding to the HOMO→LUMO transition. Although the absorption under ultraviolet region was stronger, considered the complexity of its corresponding multiple orbital transitions, we deemed that the photocyclization reaction was hardly to occur based on it. Therefore, only the HOMO→LUMO transition and its corresponding S0→S1 transition were researched in this work.

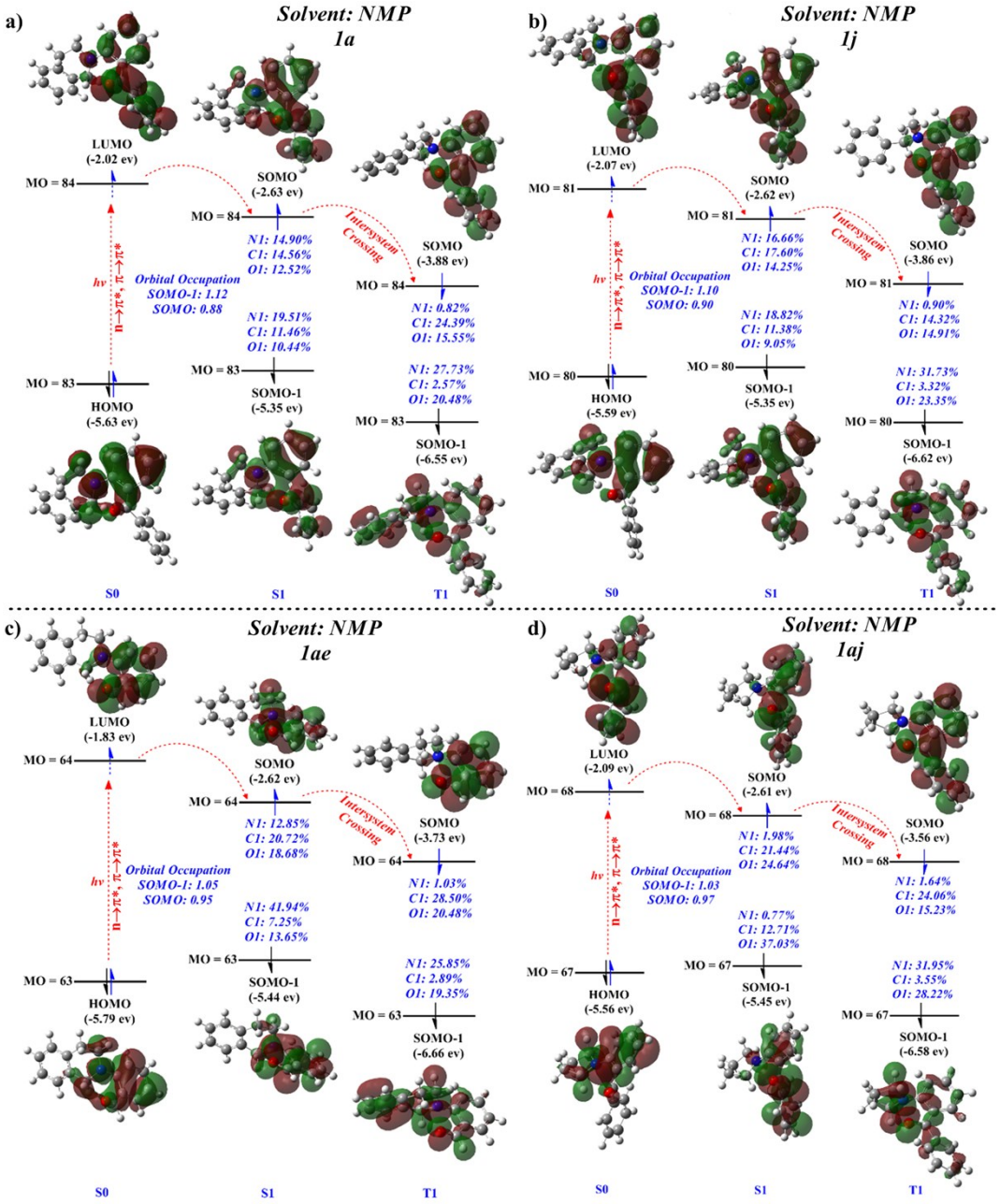

Figure S2. The frontier molecular orbital and corresponding single electron distribution of **1a/1j/1ae/1aj** (NMP solvent) in S0, S1 and T1 states. N1, C1 and O1 atom referred to **Scheme 2.** For HOMO orbits of S0 state, the electrons mainly distributed on the B rings (referred to **Scheme 2**) and the tertiary amines, while for LUMO orbits, they mostly distributed on the carbonyls and the R^1 group (referred to **Scheme 2**). It indicated that the HOMO→LUMO transitions were the processes of n→π*/π→π* transition. Meanwhile, the SOMO orbital energy gaps between S1 and T1 states for **1a/1j/1ae/1aj** were -1.25, -1.24, -1.11 and 0.95 eV, respectively. It indicated that the spontaneity of ISC from **1a** to **1aj** were tapering. And less and less S1 states would transferred to T1 states from **1a** to **1aj**. The orbital energies in Hartree were shown in **Table S3**. The single electron distribution probabilities of N1, C1 and O1 atoms were also shown in **Table 1**, and graphed in **Figure S5**.

Table S1. The relative free energies (***kcal/mol***) of key structures during the photocyclization reactions of **1a/1j/1ae/1aj** in NMP solvent. The corresponding absolute free energies referred to **Table S2** and **S11**.

Solvent	*1a/1j/1ae/1aj*			*TS2'*	*B'*	*2a/2j/2ae/2aj*			*Barrier of [1,6]-H Shift*
	S1	*TS1'*	*A'*	*TS2*	*B*	*C*	*TS3*	*D*	*ΔE(TS1' – S1)*
	T1	*TS1*	*A*						*ΔE(TS1 – T1)*
NMP	1a(0.00)			72.88	66.05		-35.53		/
	65.42	/	/	/	-0.21	2.54	25.61	-16.19	9.43
	46.57	56.00	32.04						
NMP	1j(0.00)			75.76	66.10		-31.72		/
	64.37	/	/	/	-2.08	-0.15	26.13	-19.63	9.38
	48.63	58.01	39.08						
NMP	1ae(0.00)			75.56	61.72		-37.79		15.96
	60.82	76.78	34.82	37.28	-5.05	-2.65	22.00	-15.14	8.96
	47.86	56.82	32.94						
NMP	1aj(0.00)			81.95	68.01		-28.64		12.31
	57.58	69.89	43.78	45.76	1.69	5.88	29.55	-15.36	7.18
	48.44	55.62	47.79						

Table S2. The absolute free energies (***Hartree***) of key structures during the photocyclization reactions of **1a/1j/1ae/1aj** in NMP solvent.

Solvent (Molecule)	*1a/1j/1ae/1aj*			*TS2'*	*B'*	*2a/2j/2ae/2aj*
	S1	*TS1'*	*A'*	*TS2*	*B*	*TS3-3*
	T1	*TS1*	*A*	*C*	*TS3*	*D*
NMP (1a)		-979.524818		-979.408679	-979.419567	-903.142912
	-979.420568	/	/	/	-979.525152	-979.359315
	-979.450609	-979.435581	-979.473751	-979.943151	-979.906389	-903.53447
NMP (1j)		-941.420212		-941.299485	-941.314868	-865.032233
	-941.317625	/	/	/	-941.423524	/
	-941.342709	-941.327761	-941.357935	-941.842825	-941.800946	-865.435356
NMP (1ae)		-748.526616		-748.406200	-748.428265	-672.148313
	-748.429686	-748.404256	-748.471122	-748.467199	-748.534668	/
	-748.450339	-748.436063	-748.474128	-748.953217	-748.913942	-672.534595
NMP (1aj)		-787.821987		-787.691384	-787.713602	-711.4291
	-787.730219	-787.710605	-787.752214	-787.749057	-787.819301	/
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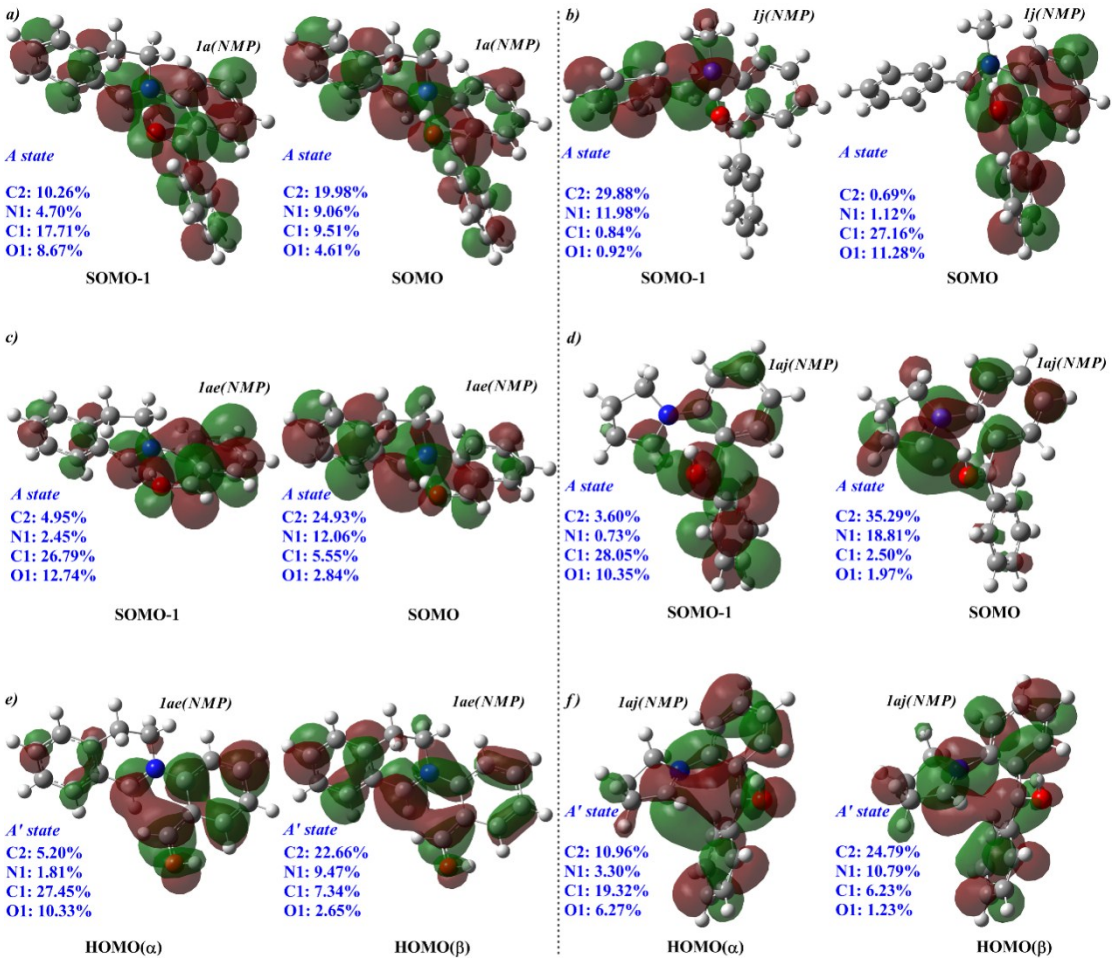


Figure S3. The frontier molecular orbital and corresponding single electron distribution of **1a/1j/1ae/1aj** (NMP solvent) in A state and A' state. C2, N1, C1 and O1 atom referred to **Scheme 2**. For A and A' states, the distribution probabilities of key atoms (C2, N1, C1 and O1) among **1a/1j/1ae/1aj** were apparent different, but in relative terms, more single electrons of SOMO-1/SOMO orbitals were distributed on the C1 and C2 atoms, to some extent indicating the form of C1-C2 diradical molecules. Meanwhile, between the A sates of **1a** and **1j**, both the C1 and C2 atoms had the similar total distribution probabilities (**Figure S4a**), determining the similar radical-radical coupling reactions between them (**Figure 1a-b**). However, the different total distribution probabilities among **1ae**, **1aj**, as well as **1a** and **1j** (**Figure S4a**), especially the different total probabilities of A' states of **1ae** and **1aj** (**Figure S4b**), yet determining the different radical-radical coupling reactions among them (**Figure 1**). The single electron distribution probabilities of C1 and C2 atoms were graphed in **Figure S4**.

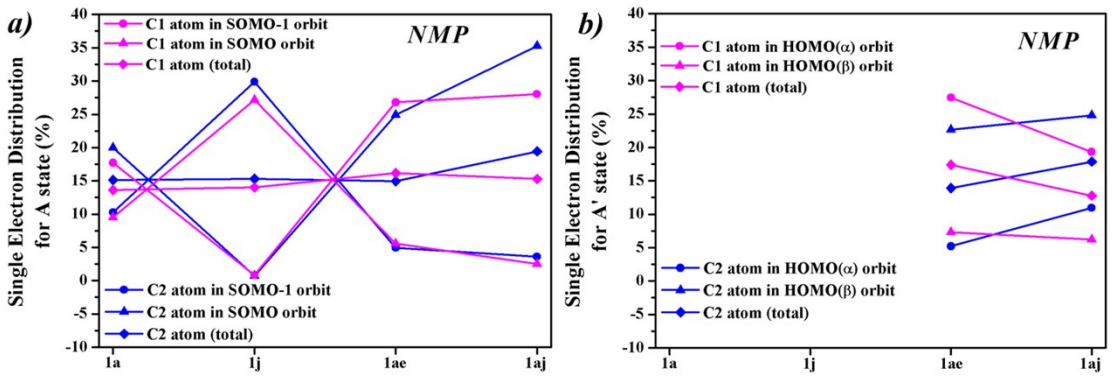


Figure S4. The characteristic of single electron distribution of A/A' state for **1a/1j/1ae/1aj** in NMP solvent. C2 and C1 atom referred to **Scheme 2**. Detailed description presented in **Figure S3**.

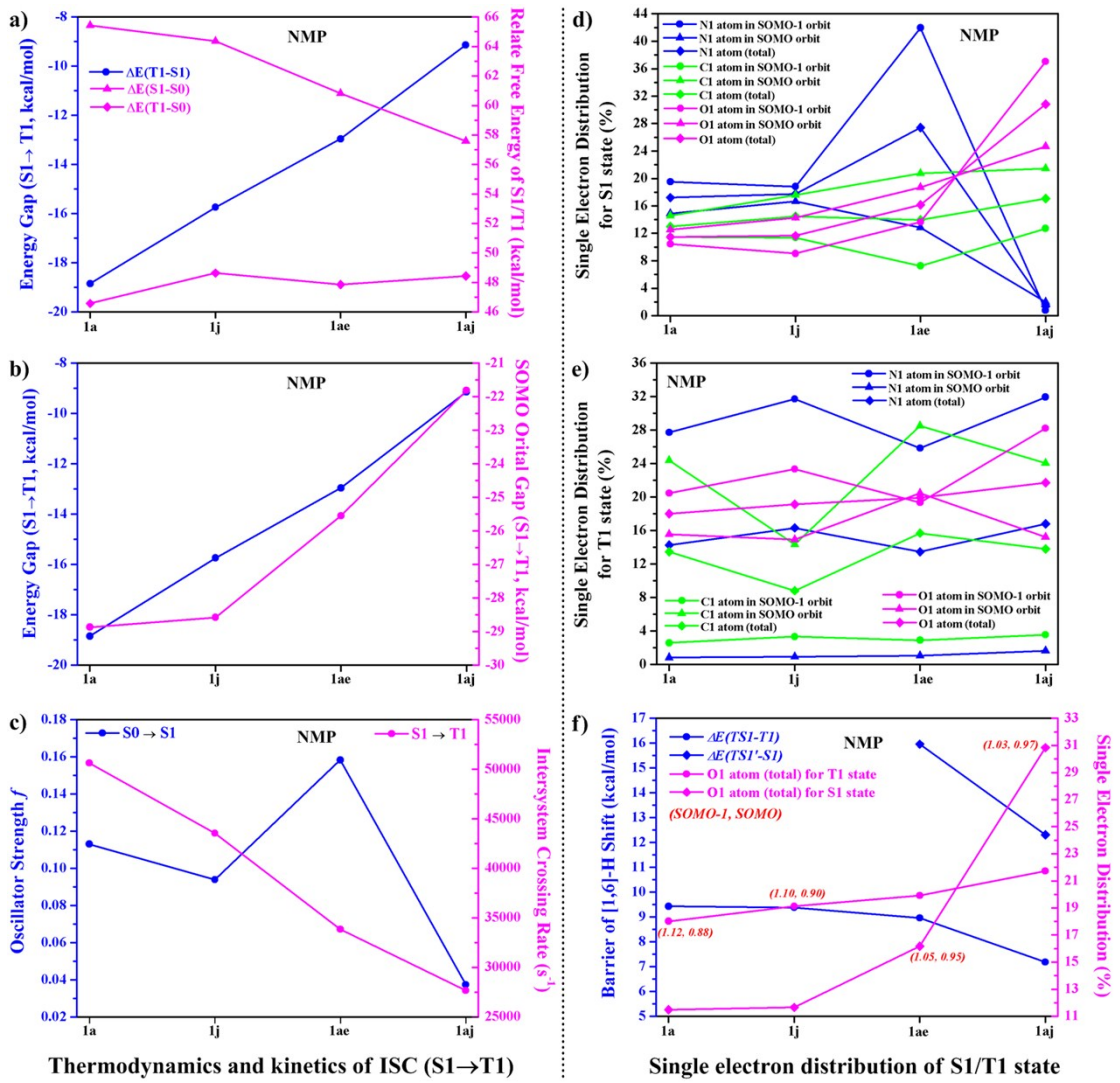


Figure S5. The thermodynamics and kinetics properties of ISC (S1→T1), as well as the characteristic of single electron distribution in S1/T1 states for **1a/1j/1ae/1aj** in NMP solvent. (a-b) The thermodynamics property of ISC (S1→T1). (c) The kinetics property of ISC (S1→T1). (d) The detailed single Electron distribution of frontier molecular orbitals in S1 state. (e) The detailed single Electron distribution of frontier molecular orbitals in T1 state. (f) The relationship between the barrier of [1, 6]-H Shift and single electron distribution on O1 atom. N1, C1 and O1 atom referred to **Scheme 2**.

Table S3. The detailed frontier molecular orbitals energy in S0, S1 and T1 for **1a/1j/1ae/1aj** in NMP solvent. Orbital energy unit: Hartree. 1Hartree = 627.5 kcal/mol.

Molecule	*Solvent*	*S0*	*S1*	*T1*
		LUMO	***SOMO***	***SOMO***
		HOMO	***SOMO-1***	***SOMO-1***
1a	***NMP***	-0.07435	-0.09657	-0.14257
		-0.20694	-0.19644	-0.24067
1j	***NMP***	-0.07606	-0.09646	-0.14201
		-0.20539	-0.19673	-0.24342
1ae	***NMP***	-0.06741	-0.09625	-0.13697
		-0.21294	-0.19992	-0.24462
1aj	***NMP***	-0.07689	-0.09599	-0.13075
		-0.20437	-0.20020	-0.24165

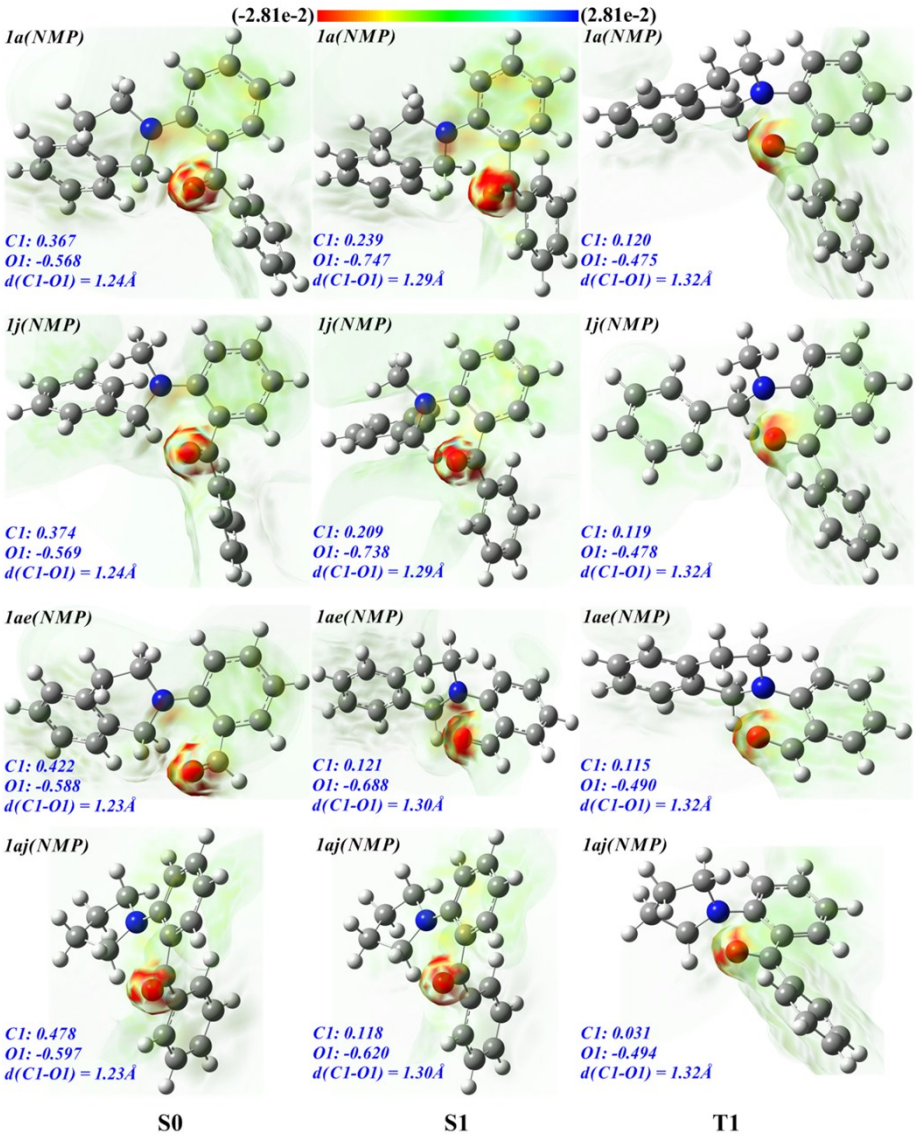


Figure S6. The ESP charge surface of **1a/1j/1ae/1aj** (NMP solvent) in S0, S1 and T1 states. C1 and O1 atom referred to **Scheme 2.** Charge unit: e. From S0 to T1 states, along with the C1-O1 bond gradually drew out, the positive charge on C1 atom gradually decreased, while the negative charge on O1 atom firstly increased in S1 state, and then in T1 state, decreased to lower than that in S0 state. It indicated that the S0→S1 transition converted the C-O double bond to single bond, but this change was more like heterolysis rather than homolysis due to the inductive effect of O1 atom become more advantageous than its conjugation effect. Inversely, the following S1→T1 crossing was more closed to homolysis by reason of the negative charge on O1 atom drop dramatically. Therefore, the T1 state appeared to more suitable for the following [1, 6]-H shift than S1 state. Meanwhile, from **1a** to **1aj**, the negative charge on O1 atoms in S1 states were also gradually decreased, even tended to close to the level of corresponding T1 states. It reminded us that the S1 state from **1a** to **1aj** may increasingly suitable for the [1, 6]-H shift. Therefore, **1a/1j/1ae/1aj** were very likely to have different 'state reactivity'.

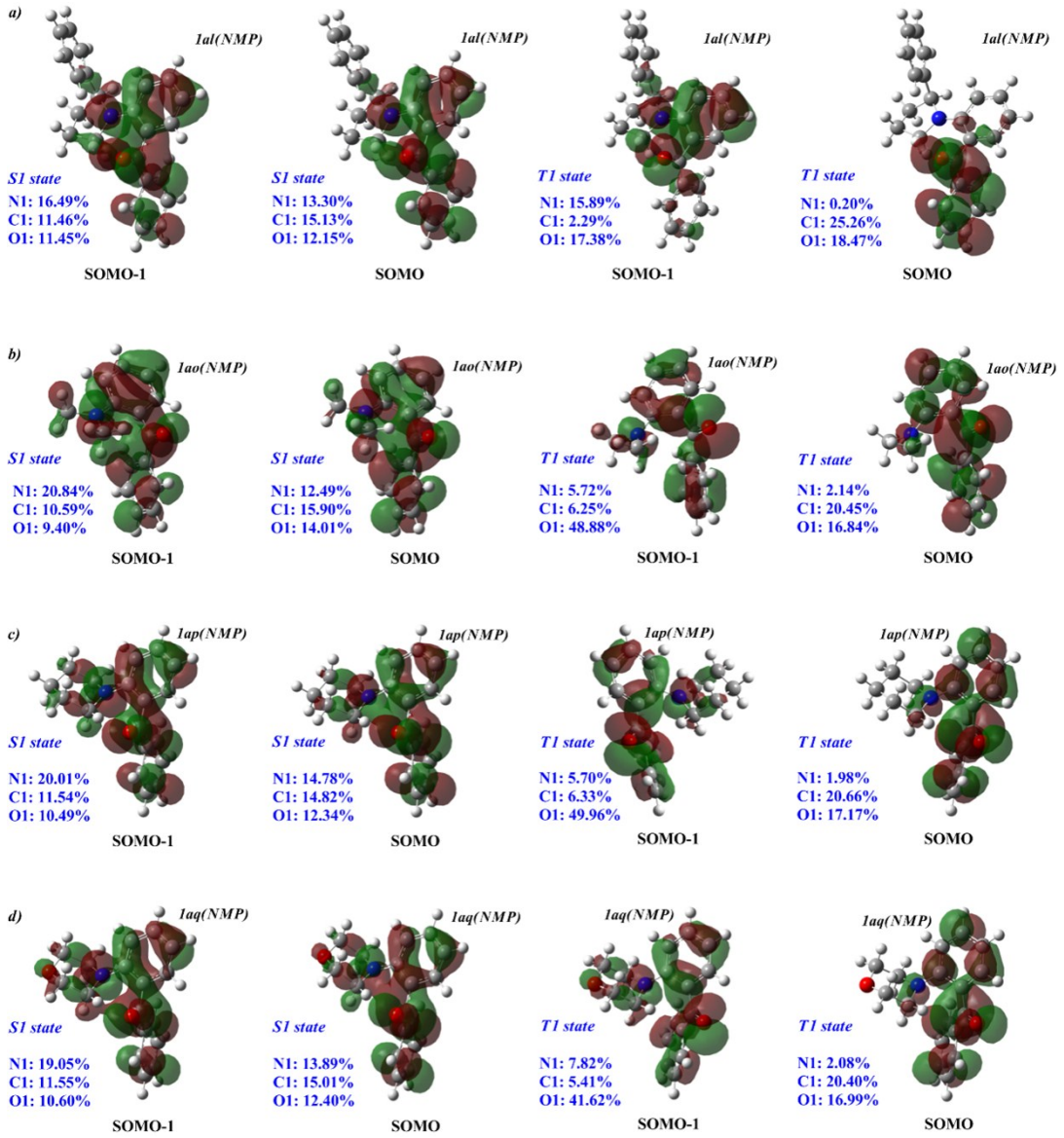


Figure S7. The frontier molecular orbital and corresponding single electron distribution of **1al/1ao/1ap/1aq** (NMP solvent) in S1 and T1. N1, C1 and O1 atom referred to **Scheme 2**. For **1al**, the higher single electron distribution probability on O1 atom for T1 state compared to that for S1 state (17.93% *vs* 11.80%, **Table 1**), as well as the strong spontaneity (-16.03 kcal/mol, **Table 1**) and fast k_{ISC} ($4.80 * 10^4$ s^{-1}, **Table 1**) of ISC, indicated that its 'state reactivity' was more likely to TSR and therefore, a high yield of 77% were obtained with no doubt accorded to the proposed hypothesis of 'state-selective reactivity'. For **1ao**, **1ap** and **1aq**, the low single electron distribution for S1 states (11.71%, 11.42% and 11.50%, respectively. **Table 1** and **Table S4**), as well as the decrease of ISC in thermodynamics (-8.84, -10.20 and -10.07 kcal/mol, respectively. **Table 1** and **Table S4**) and kinetics ($6.13*10^3$ s^{-1} for **1ao**, **Table 1**), determined that neither of TSR nor SSR was suitable for them, although their single electron distribution for T1 states up to 32.86%, 33.57% and 29.31%, respectively. Thus, the photocyclization reaction could not occur on them three accorded to the proposed hypothesis of 'state-selective reactivity'.

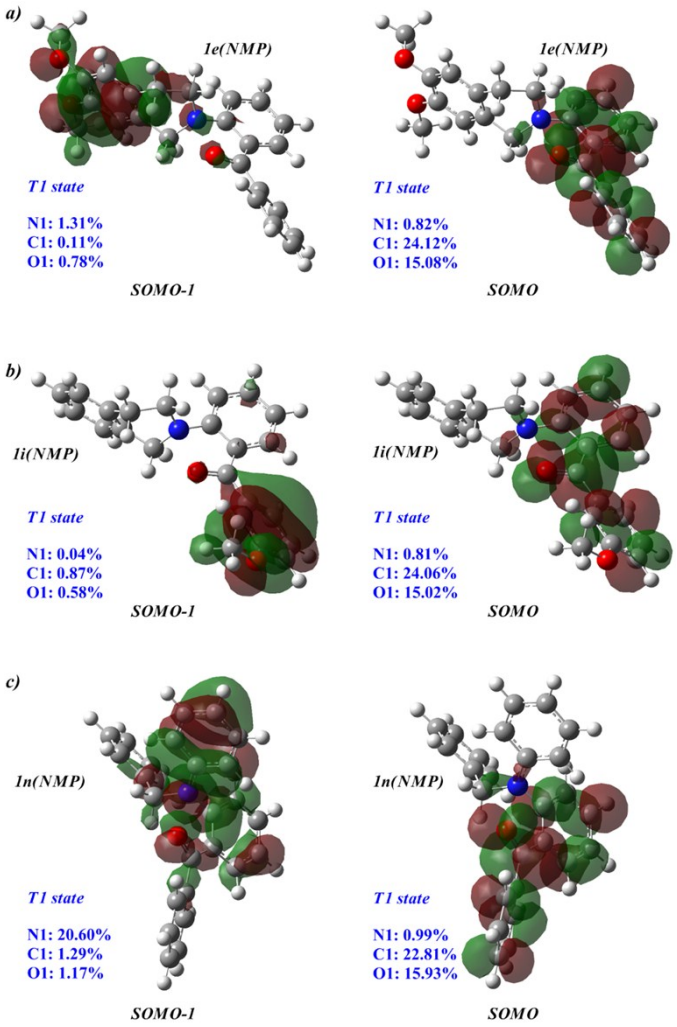


Figure S8. The frontier molecular orbital and corresponding single electron distribution of **1e/1i/1n** (NMP solvent) in T1. N1, C1 and O1 atom referred to **Scheme 2**. For **1e/1i/1n**, due to the methoxyl group substituted on the A ring (**1e**, **Scheme 3**) and the phenyl of R^1 group (**1i**, **Scheme 3**), as well as the phenyl substituted on the N1 atom (**1n**, **Scheme 3**), their single electrons of SOMO-1 orbitals for T1 state were all transferred to these substitutions, and almost no single electron distributed on the key N1, C1 and O1 atoms. Therefore, we considered that the three substrates may occur the [1, 6]-H shift only depended on the single electron of SOMO orbital. It was different from other substrates relying on both the single electrons of SOMO-1 and SOMO orbitals. Therefore, the 15.08%, 15.02% and 15.93% distribution probability of O1 atom for **1e/1i/1n** in turn, were enough to support them to occur the [1, 6]-H shift based on the T1 state. Meanwhile, their excellent spontaneity (-22.32, -19.50, -16.66 kcal/mol for **1e/1i/1n**, respectively. **Table S4**) and fast k_{ISC} ($5.31 * 10^4$ s^{-1} for **1e**, **Table S4**) of ISC, as well as the nonsupport of total single electron distribution on O1 atom for their S1 state (11.44%, 11.40% and 13.03% for **1e/1i/1n**, respectively. **Table S4**), further indicated the TSR for them. As a result, high yields (91%, 83% and 83% for **1e/1i/1n**, respectively. **Scheme 3**) were obtained for them with no doubt accorded to the proposed hypothesis of 'state-selective

reactivity'.

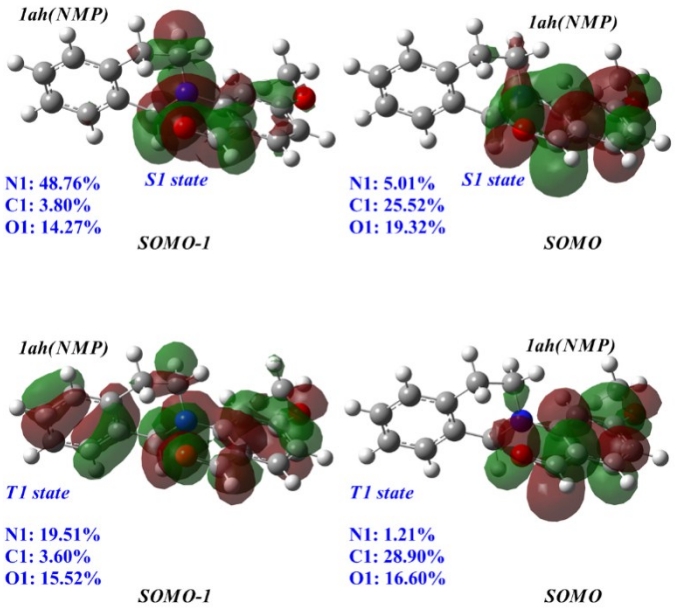


Figure S9. The frontier molecular orbital and corresponding single electron distribution of **1ah** (NMP solvent) in first single excited state (S1) and first triplet excited state (T1). N1, C1 and O1 atom referred to **Scheme 2**. For **1ah**, the closed total single electron distribution probabilities of O1 atom for S1 and T1 state (16.80 vs 16.06, **Table S4**), as well as the acceptable spontaneity (-13.51 kcal/mol, **Table S4**) of ISC, indicated that its 'state reactivity' was likely to adopt both the TSR and SSR. Therefore, a moderate yield of 71% (**Scheme 3**) were obtained also with no doubt accorded to the proposed hypothesis of 'state-selective reactivity'.

Table S4. The thermodynamics and kinetics properties of ISC (S1→T1) for **1e/1i/1n/1ah/1ap/1aq** (NMP solvent), as well as their single electron distribution of frontier molecular orbitals (SOMO-1/SOMO) for S1 and T1 states. N1, C1 and O1 atoms referred to **Scheme 2**.

/	*ISC (S1→T1)*		*Single Electron Distribution (%)*[c]				*Reactivity*
	Energy Gap[a]	k_{ISC}[b]	*SOMO-1/SOMO(S1/T1)*			*Total*	
			N1	*C1*	*O1*	*O1*	
1e	-22.32	$5.31*10^4$	19.61	11.42	10.40	11.44	TSR
			14.89	14.54	12.47		
			1.31	0.11	0.78	15.08	
			0.82	24.12	15.08		
1i	-19.50	/	19.55	11.42	10.38	11.40	
			14.99	14.41	12.41		
			0.04	0.87	0.58	15.02	
			0.81	24.06	15.02		
1n	-16.66	/	18.53	10.99	11.38	13.03	
			14.62	12.84	14.68		
			20.60	1.29	1.17	15.93	
			0.99	22.81	15.93		
1ah	-13.51	/	48.76	3.80	14.27	16.80	TSR/SSR
			5.01	25.52	19.32		
			19.51	3.60	15.52	16.06	
			1.21	28.90	16.60		
1ap	-10.20	/	20.01	11.54	10.49	11.42	/
			14.78	14.82	12.34		
			5.70	6.33	49.96	33.57	
			1.98	20.66	17.17		
1aq	-10.07	/	19.05	11.55	10.60	11.50	
			13.89	15.01	12.40		
			7.82	5.41	41.62	29.31	
			2.08	20.40	16.99		

[a] Energy Gap, energy gap between S1 and T1 states, kcal/mol; [b] k_{ISC}, rate constant of ISC; [c] For each molecule, from top to bottom were single electron distribution of SOMO-1 for S1 state, SOMO for S1 state, SOMO-1 for T1 state and SOMO for T1 state, respectively.

Table S5. The absolute (*Hartree*) and relative (***kcal/mol***) free energies of **1e/1i/1n/1ah/1al/1ao/1ap/1aq** (NMP solvent) in S0, S1 and T1 states.

Molecule	***S0***	***S1***	***T1***	***Energy Gap (S1→T1)***
1e	-1208.520688 (0.0)	-1208.408995 (70.09)	-1208.444560 (47.77)	-22.32
1i	-1094.026784 (0.0)	-1093.919503 (67.32)	-1093.950576 (47.82)	-19.50
1n	-1133.121685 (0.0)	-1133.020705 (63.36)	-1133.047256 (46.70)	-16.66
1ah	-863.031468 (0.0)	-862.927047 (65.52)	-862.948577 (52.01)	-13.51
1al	-1018.811272 (0.0)	-1018.705536 (66.35)	-1018.731078 (50.32)	-16.03
1ao	-710.428419 (0.0)	-710.330841 (61.23)	-710.344936 (52.39)	-8.84
1ap	-827.111225 (0.0)	-827.013862 (61.10)	-827.030110 (50.90)	-10.20
1aq	-863.026962 (0.0)	-862.928115 (62.03)	-862.944161 (51.96)	-10.07

6. Figure S10-S12 & Table S6-S12 (Reaction Condition Optimization)

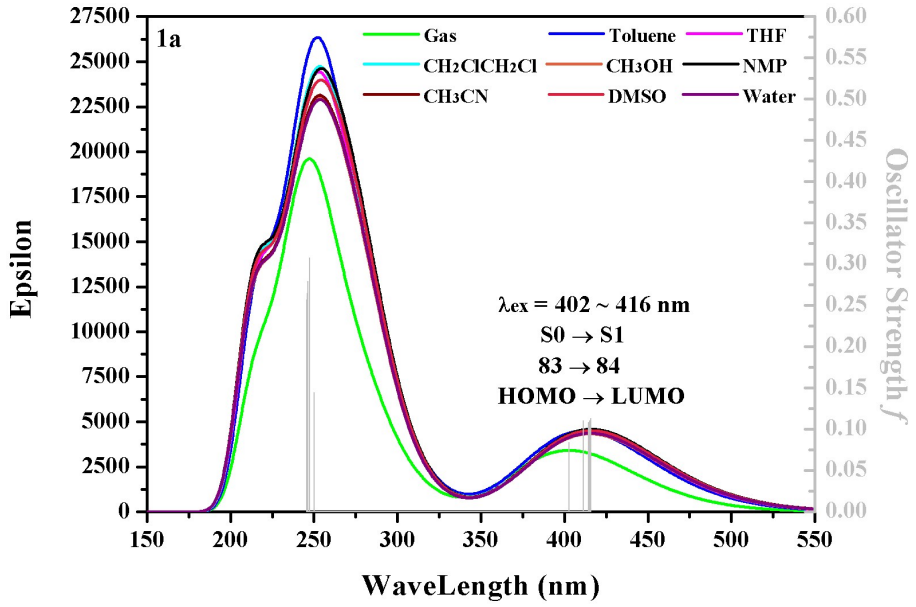


Figure S10. The UV absorption spectrums of **1a** in different solvents, generated by quantum calculation. Under the visible light (about 400 nm to 430 nm), a distinct absorption peak matched to the S0→S1 transition which further corresponding to the HOMO→LUMO transition. Although the absorption under ultraviolet region was stronger, considered the complexity of its corresponding multiple orbital transitions, we deemed that the photocyclization reaction was hardly to occur based on it. Therefore, only the HOMO→LUMO transition and its corresponding S0→S1 transition were researched in this work.

Table S6. The relative free energies (***kcal/mol***) of key structures during the photocyclization reactions of **1a** in different solvents. The corresponding absolute free energies referred to **Table S7** and **S11**.

Solvent	*1a*			*TS2'*	*B'*	*2a*			*Barrier of [1, 6]-H Shift*
	S1	*TS1'*	*A'*	*TS2*	*B*	*TS3-3*			
						C-2	*TS3-2*	*D-2*	
	T1	*TS1*	*A*			*C-1*	*TS3-1*	*D-1*	
						C	*TS3*	*D*	*ΔE(TS1 – T1)*
Gas		0.00		72.73	66.39		-32.53		
	66.53	/	/	/	-1.23		106.45		
						116.59	138.27	98.34	11.59
	47.88	59.47	31.62			110.12	131.80	91.87	
						88.68	110.37	70.44	
Toluene		0.00		73.02	66.07		-34.04		
	65.70	/	/	/	-0.72		105.57		
						61.50	83.47	42.45	11.36
	47.00	58.36	31.85			59.02	81.00	39.97	
						39.73	61.71	20.68	
THF		0.00		73.06	66.10		-35.10		
	65.63	/	/	/	-0.35		104.59		
						33.46	56.06	14.53	9.93
	46.89	56.82	32.14			31.61	54.22	12.68	
						13.12	35.73	-5.80	
CH_2Cl CH_2Cl		0.00		73.00	66.10		-35.24		
	65.58	/	/	/	-0.30		104.38		
						29.68	52.43	10.82	9.72
	46.83	56.55	32.18			27.97	50.37	9.12	
						9.62	32.37	-9.24	
CH_3OH		0.00		72.88	66.04		-35.53		
	65.42	/	/	/	-0.21		103.86		
						22.18	45.24	3.45	9.43
	46.57	56.00	32.05			20.93	43.99	2.20	
						2.58	25.64	-16.15	
NMP		0.00		72.88	66.05		-35.53		
	65.42	/	/	/	-0.21		103.85		
						22.14	45.21	3.41	9.43
	46.57	56.00	32.04			20.89	43.96	2.16	
						2.54	25.61	-16.19	
CH_3CN		0.00		72.87	66.05		-35.54		
	65.39	/	/	/	-0.21		103.83		
						21.92	45.00	3.20	9.43
	46.55	55.98	31.91			20.65	43.73	1.93	
						2.30	25.38	-16.42	
DMSO		0.00		72.86	66.06		-35.57		
	65.31	/	/	/	-0.20		103.75		
						21.28	44.38	2.56	9.43
	46.49	55.92	32.40			19.95	43.06	1.24	
						1.75	24.85	-16.97	
Water		0.00		72.84	66.08		-35.60		
	65.19	/	/	/	-0.19		103.63		
						20.44	43.57	1.72	9.43
	46.39	55.82	32.44			19.05	42.19	0.34	
						0.94	24.07	-17.78	

Table S7. The absolute free energies (***Hartree***) of key structures during the photocyclization reactions of **1a** in different solvents.

Solvent (Molecule)	*1a*			*TS2'*	*B'*	*2a*
	S1	*TS1'*	*A'*	*TS2*	*B*	*TS3-3*
	T1	*TS1*	*A*	*C*	*TS3*	*D*
Gas (1a)		-979.513487		-979.397575	-979.407692	-903.134931
	-979.407452	/	/	/	-979.515453	-979.343851
	-979.437178	-979.41872	-979.463107	-979.875852	-979.841296	-903.474519
Toluene (1a)		-979.51849		-979.402124	-979.413195	-903.138377
	-979.413775	/	/	/	-979.519645	-979.350251
	-979.443582	-979.425483	-979.467732	-979.913289	-979.878271	-903.509299
THF (1a)		-979.5227		-979.40627	-979.417366	-903.141396
	-979.418119	/	/	/	-979.523265	-979.356026
	-979.44798	-979.432157	-979.471482	-979.934441	-979.898412	-903.527367
CH_2Cl CH_2Cl (1a)		-979.523382		-979.407048	-979.418042	-903.141885
	-979.418866	/	/	/	-979.523865	-979.357035
	-979.448751	-979.433256	-979.472104	-979.937375	-979.90111	-903.529762
CH_3OH (1a)		-979.52481		-979.40867	-979.41956	-903.142906
	-979.420553	/	/	/	-979.525144	-979.359301
	-979.450595	-979.43557	-979.473736	-979.943121	-979.906361	-903.534445
NMP (1a)		-979.524818		-979.408679	-979.419567	-903.142912
	-979.420568	/	/	/	-979.525152	-979.359315
	-979.450609	-979.435581	-979.473751	-979.943151	-979.906389	-903.53447
CH_3CN (1a)		-979.524869		-979.408735	-979.419607	-903.142948
	-979.420659	/	/	/	-979.525198	-979.359406
	-979.450687	-979.435662	-979.474024	-979.943352	-979.906569	-903.53463
DMSO (1a)		-979.525018		-979.408906	-979.419741	-903.143056
	-979.420937	/	/	/	-979.525336	-979.359679
	-979.450935	-979.435909	-979.473383	-979.943915	-979.907095	-903.535099
Water (1a)		-979.525214		-979.409129	-979.419915	-903.143197
	-979.421324	/	/	/	-979.525517	-979.360068
	-979.45129	-979.436227	-979.473522	-979.944643	-979.907778	-903.535705

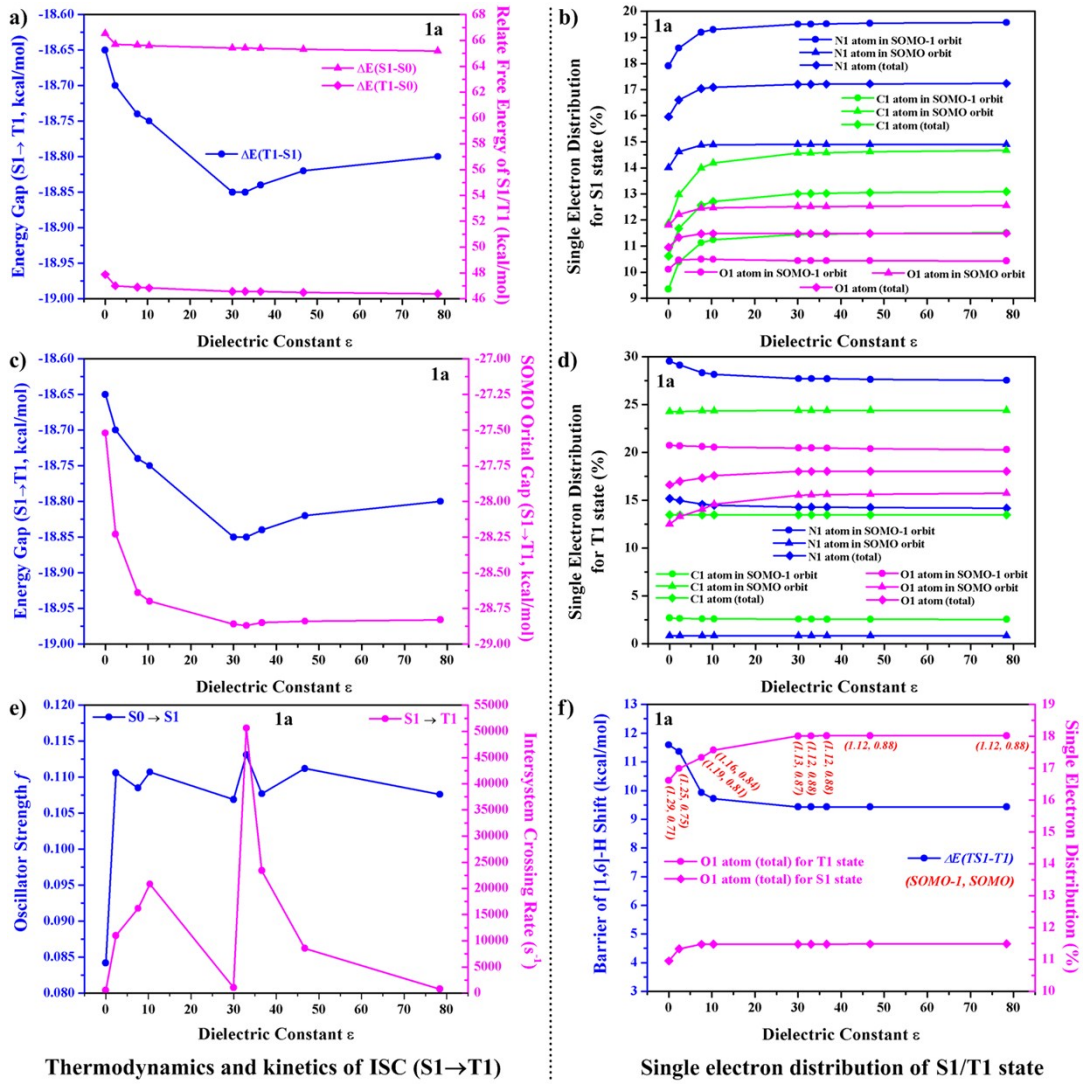


Figure S11. The thermodynamics and kinetics properties of ISC (S1→T1), as well as the characteristic of single electron distribution in S1/T1 states for compound **1a** in different solvents. N1, C1 and O1 atom referred to **Scheme 2**. Nine solvents with increasing dielectric constants, i.e., gas (ε = 0), Toluene (ε = 2.38), THF (ε = 7.58), CH_2ClCH_2Cl (ε = 10.36), CH_3OH (ε = 32.63), NMP (ε = 33.00), CH3CN (ε = 36.64), DMSO (ε = 46.7) and Water (ε = 78.39) were considered to screen the optimal solvent for the photocyclization reaction. In both the thermodynamics and kinetics of ISC, the NMP solvent could provide strongest spontaneity (**Table S8**) and fastest k_{ISC} (**Table S8**) of ISC. Meanwhile, the single electron distribution analysis (**Table S8**) revealed that when the dielectric constants increased to a certain degree (about 10 ~ 20), the total distribution probabilities on O1 atom almost did not increase any more (the corresponding barrier of [1, 6]-H shift also did not decrease any more. **Table S6**). Combined the analysis of ISC and single electron distribution, we considered that the NMP was a suitable solvent for the photocyclization reaction. The oscillator strength and SOMO orbital energy gap (**Table S9**) also supported the NMP solvent. Moreover, the NMP solvent was also recognized by the following experimental verification (**Table S12**).

Table S8. The thermodynamics and kinetics property of ISC (S1→T1) for **1a** in different solvents, as well as their single electron distribution of frontier molecular orbitals (SOMO-1/SOMO) for S1 and T1 states. N1, C1 and O1 atom referred to **Scheme 2**.

Solvent	*Orbital Occupation*	*ISC (S1→T1)*		*Single Electron Distribution (%)*[d]			
	(SOMO-1, SOMO)	*Energy Gap*[a] *SOMO Gap*[b]	k_{ISC}[c]	*SOMO-1/SOMO(S1/T1)*			*Total*
				N1	*C1*	*O1*	*O1*
Gas	(1.29, 0.71)	-18.65 -27.52	5.65×10^{2}	17.91	9.35	10.11	10.96
				14.01	11.88	11.80	
				29.54	2.69	20.74	16.62
				0.83	24.28	12.49	
Toluene	(1.25, 0.75)	-18.70 -28.23	1.10×10^{4}	18.59	10.39	10.46	11.34
				14.62	12.97	12.21	
				29.13	2.64	20.69	17.00
				0.83	24.30	13.30	
THF	(1.19, 0.81)	-18.74 -28.64	1.62×10^{4}	19.20	11.13	10.50	11.48
				14.87	14.00	12.45	
				28.33	2.60	20.62	17.34
				0.82	24.35	14.06	
CH_2Cl CH_2Cl	(1.16, 0.84)	-18.75 -28.70	2.08×10^{4}	19.30	11.24	10.49	11.48
				14.88	14.18	12.47	
				28.16	2.59	20.55	17.57
				0.82	24.36	14.59	
CH_3OH	(1.13, 0.87)	-18.85 -28.86	1.05×10^{3}	19.51	11.45	10.44	11.48
				14.90	14.56	12.52	
				27.73	2.57	20.48	18.01
				0.82	24.39	15.54	
NMP	(0.12, 0.88)	-18.85 -28.87	5.06×10^{4}	19.51	11.46	10.44	11.48
				14.90	14.56	12.52	
				27.73	2.57	20.48	18.02
				0.82	24.39	15.55	
CH_3CN	(0.12, 0.88)	-18.84 -28.85	2.34×10^{4}	19.52	11.46	10.44	11.48
				14.90	14.58	12.52	
				27.71	2.56	20.46	18.02
				0.82	24.39	15.58	
DMSO	(0.12, 0.88)	-18.82 -28.84	8.55×10^{3}	19.54	11.48	10.44	11.49
				14.90	14.62	12.53	
				27.64	2.56	20.40	18.02
				0.82	24.40	15.64	
Water	(0.12, 0.88)	-18.80 -28.83	7.77×10^{2}	19.57	11.51	10.43	11.49
				14.90	14.67	12.55	
				27.55	2.55	20.30	18.02
				0.82	24.40	15.74	

[a] Energy Gap, energy gap between S1 and T1 states, kcal/mol; [b] SOMO Gap, energy gap between the SOMO orbital of S1 and T1 states, kcal/mol; [c] k_{ISC}, rate constant of ISC; [d] For each solvent, from top to bottom were single electron distribution of SOMO-1 for S1 state, SOMO for S1 state, SOMO-1 for T1 state and SOMO for T1 state, respectively.

Table S9. The detailed frontier molecular orbitals energy in S0, S1 and T1 for **1a** in different solvents. Orbital energy unit: Hartree. 1Hartree = 627.5 kcal/mol.

Molecule	*Solvent*	*S0*	*S1*	*T1*
		LUMO	*SOMO*	*SOMO*
		HOMO	*SOMO-1*	*SOMO-1*
1a	*Gas*	-0.06669	-0.09244	-0.13630
		-0.20211	-0.18727	-0.23656
	Toluene	-0.06954	-0.09335	-0.13833
		-0.20344	-0.19095	-0.23751
	THF	-0.07267	-0.09532	-0.14096
		-0.20560	-0.19453	-0.23937
	CH_2Cl	-0.07320	-0.09570	-0.14144
	CH_2Cl	-0.20601	-0.19514	-0.23976
	CH_3OH	-0.07435	-0.09657	-0.14256
		-0.20693	-0.19643	-0.24067
	NMP	-0.07435	-0.09657	-0.14257
		-0.20694	-0.19644	-0.24067
	CH_3CN	-0.07440	-0.09661	-0.14258
		-0.20697	-0.19648	-0.24071
	DMSO	-0.07452	-0.09671	-0.14267
		-0.20707	-0.19662	-0.24083
	Water	-0.07468	-0.09684	-0.14279
		-0.20721	-0.19680	-0.24099

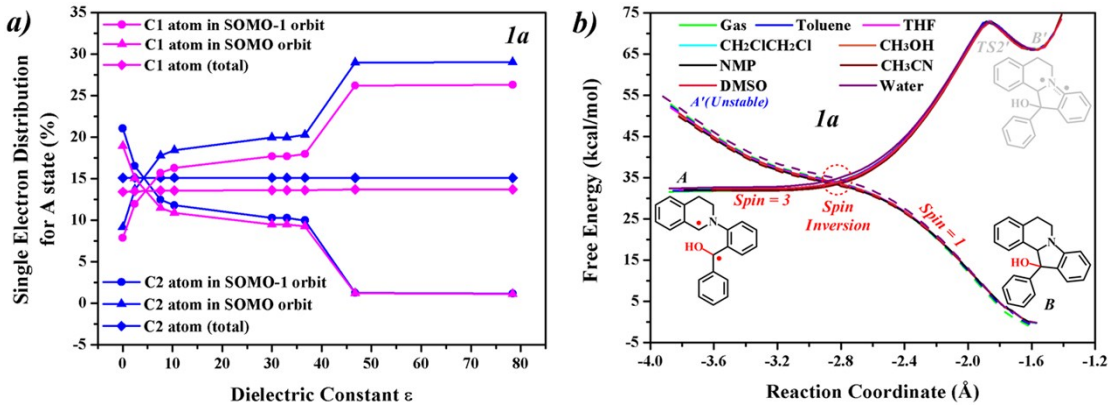


Figure S12. The characteristic of single electron distribution of A/A' state, as well as the profiles of radical-radical coupling reaction for **1a** in different solvents. C2 and C1 atom referred to **Scheme 2**. Among the A sates of **1a** in different solvents, both the C1 and C2 atoms had the similar total distribution probabilities, therefore the similar radical-radical coupling reactions were described among them. The single electron distribution probabilities of C1 and C2 atoms for **1a** in different solvents were also shown in **Table S10**.

Table S10. The detailed single electron distribution of frontier molecular orbitals in A state for **1a** in different solvents. C2, N1, C1 and O1 atoms referred to **Scheme 2.** For A state of **1a**, the distribution probabilities of key atoms (C2, N1, C1 and O1) in different solvents were apparent different, but in relative terms, more single electrons of SOMO-1/SOMO orbitals were distributed on the C1 and C2 atoms, to some extent indicating the form of C1-C2 diradical molecules.

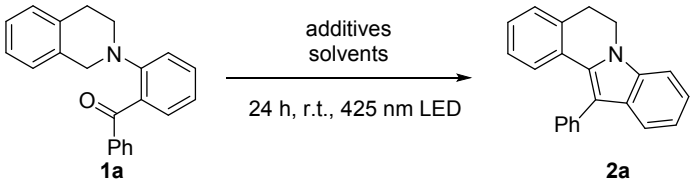
Molecule (State)	***Solvent***	***Single Electron Distribution (%)[a]***					
		SOMO-1/SOMO				***Total***	
		C2	***N1***	***C1***	***O1***	***C2***	***C1***
1a(A)	***Gas***	21.05	8.85	7.88	4.84	15.11	13.42
		9.16	4.79	18.96	8.62		
	Toluene	16.54	7.03	11.96	6.50	15.12	13.51
		13.69	6.61	15.05	6.93		
	THF	12.47	5.50	15.68	7.92	15.12	13.58
		17.77	8.20	11.47	5.42		
	CH_2Cl	11.80	5.26	16.29	8.15	15.12	13.59
	CH_2Cl	18.44	8.46	10.88	5.18		
	CH_3OH	10.27	4.70	17.70	8.67	15.12	13.61
		19.97	9.05	9.52	4.62		
	NMP	10.26	4.70	17.71	8.67	15.12	13.61
		19.98	9.06	9.51	4.61		
	CH_3CN	9.97	4.60	17.97	8.77	15.12	13.62
		20.27	9.17	9.26	4.51		
	DMSO	1.24	1.22	26.21	11.54	15.11	13.71
		28.98	12.86	1.21	1.36		
	Water	1.15	1.18	26.31	11.57	15.11	13.72
		29.06	12.91	1.12	1.33		

[a] For each solvent, from top to bottom were single electron distribution of SOMO-1 for A state and SOMO for A state, respectively.

Table S11. The absolute free energies (***Hartree***) of key structures in different solvents.

Solvent	***PTSA***	***PhCOOH***	***CH_3COOH***	***H2O***
	PTSA-noH	***$PhCOO^-$***	***CH_3COO^-***	
Gas	-895.293450	-420.771740	-229.071513	-76.430410
	-894.789755	-420.233888	-228.523349	
Toluene	-895.299125	-420.775713	-229.075282	-76.434353
	-894.841005	-420.286856	-228.582474	
THF	-895.303842	-420.778636	-229.078120	-76.437235
	-894.871186	-420.316523	-228.613062	
CH_2Cl CH_2Cl	-895.304611	-420.779070	-229.078538	-76.437661
	-894.875292	-420.320496	-228.617253	
CH_3OH	-895.306215	-420.779945	-229.079380	-76.438520
	-894.883799	-420.328287	-228.625730	
NMP	-895.306225	-420.779949	-229.079385	-76.438525
	-894.883846	-420.328329	-228.625767	
CH_3CN	-895.306316	-420.779980	-229.079414	-76.438554
	-894.884174	-420.328596	-228.626001	
DMSO	-895.306459	-420.780070	-229.079500	-76.438642
	-894.884775	-420.329378	-228.626693	
Water	-895.306686	-420.780186	-229.079613	-76.438757
	-894.885765	-420.330393	-228.627616	

Table S12. Optimization of reaction conditions. [a] Based on our computational results, the proposed photocyclization was first evaluated with no photocatalyst added in NMP solvent under Ar and room temperature. The anticipated product was acquired in 57% yield. Meanwhile, Toluene, THF and CH_2ClCH_2Cl with lower yields, as well as other solvents such as Dioxane, Methol, DMA, DMF and DMSO incompatible with the reaction, indicated that NMP solvent should be a better reaction solvent, and it was also confirmed by our computations (**Figure S11**). Considering the indole synthesis contains photocyclization and the subsequent dehydration, some additives were added to detect whether a favorable consequence could be acquired. The results display that the addition of acid or dehydrants can slightly increase the yields. More specifically, we found that the additive of PTSA in trace quantities provided a significant improvement (It also confirmed by our computations as shown in **Figure 1a**). Further increases of the PTSA loading resulted in a lower yield. It is worth mentioning that a comparative yield was acquired when NMP was replaced by DMPU which is costless and greener in industry. Some radical scavengers were added to explore the possible reaction pathway. The reaction was completely inhibited by oxygen, p-benzoquinone and DPPH (2, 2-diphenyl-1-picrylhydrazyl). Furthermore, the reaction was also carried out smoothly under sunlight, with the product obtained in 78% yield.



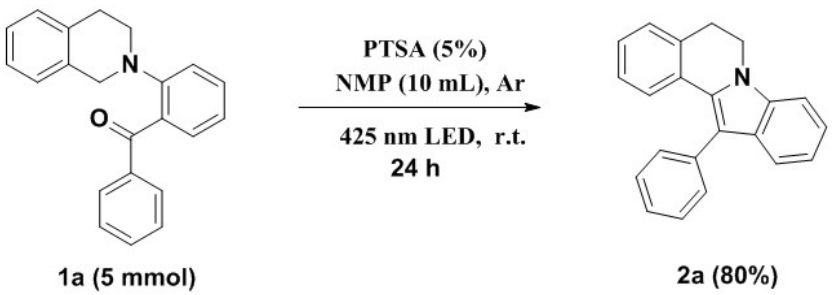
Entry	*solvent*	*additive (equiv.)*	*yield*
1	CH_3CN	-	35%
2	THF	-	25%
3	CH_2ClCH_2Cl	-	20%
4	Toluene	-	10%
5	DMF	-	-
6	DMA	-	-
7	DMSO	-	-
8	Dioxane	-	-
9	CH_3OH	-	-
10	NMP	-	57%
12	NMP	CH_3COOH (1.0)	52%
13	NMP	PhCOOH (1.0)	50%
14	NMP	PTSA (1.0)	65%
15	NMP	PTSA (0.1)	85%
16	DMPU	PTSA (0.1)	83%
17[b]	NMP	PTSA (0.1)	-
18[c]	NMP	PTSA (0.1)	-
19[d]	NMP	PTSA (0.1)	-
20[e]	NMP	PTSA (0.1)	78%

[a] Reaction condition: (2-(3,4-dihydroisoquinolin-2(1H)-yl)phenyl)(phenyl) methanone **1a** (0.2 mmol), CH_3CN (2 mL), room temperature, 425 nm, 24 h, under an argon atmosphere, isolated yield; [b] Reaction was carried out in dark; [c] Reaction was carried out under an oxygen atmosphere; [d] DPPH (0.2 mmol) was added. [e] Reaction was carried out in sunlight.

7. Table S13 and Scheme S1

Table S13. Comparison between the conventional approach and the new application. All the reagents are referred to the price of *J&K*. Synthesis of **2aa** (1G) was setting as the common task. The assessment referred to experimental expenditure, catalyst, additive, solvent, byproduct, reaction time, and environmental pollution. The difference between every indicator were listed, and the comprehensive assessment were summarized in the end.

Items	***Conventional approach***	***New application***
Catalyst	$Ir(ppy)_2(dbbpy)PF_6$ (1 mmol%, 38 mg) (470￥)	-
Additive	K_2HPO_4 (0.5eq., 410 mg) (0.7￥)	-
	Thiol (0.5eq., 179 mg) (1.31￥) (high toxic)	-
	-	PTSA (10%, 99 mg) (0.13￥)
Solvent	MeCN (medium toxic)	NMP (low toxic)
Reaction time	48 h.	24 h.
Byproduct	H_2O	H_2O
Pollution	Residual of heavy metal, high toxic additive	-
Total expenditure	475.01￥	0.13￥
Comprehensive assessment	High expenditure, mild condition, environment unfriendly	Low expenditure, simple and mild condition, environment friendly

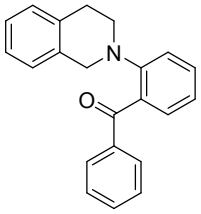


1a (5 mmol) **2a (80%)**

Scheme S1. Gram scale experiment.

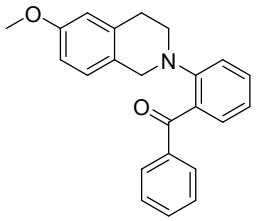
8. Characterization Data

(2-(3,4-dihydroisoquinolin-2(1H)-yl)phenyl)(phenyl)methanone (1a).



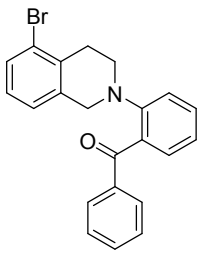
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.77 (d, J = 7.6 Hz, 2H), 7.44 – 7.36 (m, 4H), 7.32 (t, J = 7.7 Hz, 2H), 7.13 (d, J = 8.2 Hz, 1H), 7.06 (t, J = 5.1 Hz, 2H), 6.96 (t, J = 6.0 Hz, 2H), 4.15 (s, 2H), 3.24 (t, J = 5.7 Hz, 2H), 2.50 (t, J = 5.6 Hz, 2H). **^{13}C NMR** (125 MHz, CDCl3) δ 198.64, 150.77, 137.41, 134.56, 134.31, 132.84, 131.64, 130.36, 129.86, 128.65, 128.13, 128.09, 126.19, 126.12, 125.74, 121.42, 118.48, 53.39, 50.66, 28.63. **HRMS** (ESI) calculated for $C_{22}H_{20}NO$ $(M+H)^+$: 314.1539, found : 314.1542.

(2-(6-methoxy-3,4-dihydroisoquinolin-2(1H)-yl)phenyl)(phenyl)methanone (1b).



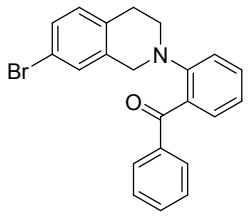
Yield: 75%, Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.81 (d, J = 7.3 Hz, 2H), 7.48 (dd, J = 15.4, 8.0 Hz, 2H), 7.43 (d, J = 7.6 Hz, 1H), 7.37 (t, J = 7.6 Hz, 2H), 7.17 (d, J = 8.1 Hz, 1H), 7.09 (t, J = 7.4 Hz, 1H), 6.93 (d, J = 8.3 Hz, 1H), 6.70 (dd, J = 8.4, 2.3 Hz, 1H), 6.54 (s, 1H), 4.14 (s, 2H), 3.76 (s, 3H), 3.26 (t, J = 5.7 Hz, 2H), 2.52 (t, J = 5.6 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 198.58, 157.85, 150.81, 137.44, 135.75, 132.77, 132.27, 131.57, 130.31, 129.83, 128.09, 127.09, 126.53, 121.35, 118.45, 113.23, 112.08, 55.23, 52.86, 50.55, 28.91. **HRMS** (ESI) calculated for $C_{23}H_{22}NO_2$ $(M+H)^+$: 344.1645, found : 344.1650.

(2-(5-bromo-3,4-dihydroisoquinolin-2(1H)-yl)phenyl)(phenyl)methanone (1c).



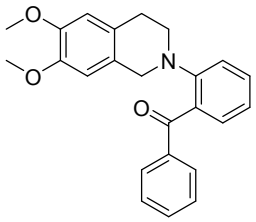
Yield: 55%, Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.86 (d, J = 7.7 Hz, 1H), 7.77 (d, J = 7.7 Hz, 2H), 7.50 – 7.42 (m, 3H), 7.36 – 7.32 (m, 2H), 7.19 – 7.12 (m, 2H), 7.00 – 6.92 (m, 2H), 4.15 (s, 2H), 3.28 (t, J = 5.9 Hz, 2H), 2.52 (t, J = 5.8 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 198.49, 150.35, 137.40, 136.85, 134.24, 132.81, 131.65, 131.50, 130.76, 129.98, 129.73, 128.15, 128.06, 126.97, 125.27, 122.01, 118.84, 53.83, 50.50, 29.64. **HRMS** (ESI) calculated for $C_{22}H_{19}NOBr$ $(M+H)^+$: 392.0645, found : 392.0641.

(2-(7-bromo-3,4-dihydroisoquinolin-2(1H)-yl)phenyl)(phenyl)methanone (1d)



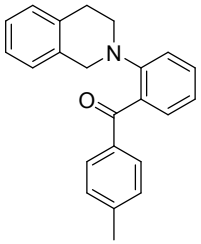
Yield: 57%, Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.78 (d, J = 7.3 Hz, 2H), 7.52 – 7.45 (m, 2H), 7.45 – 7.41 (m, 2H), 7.36 (t, J = 7.7 Hz, 2H), 7.16 – 7.11 (m, 3H), 6.86 (d, J = 8.1 Hz, 1H), 4.13 (s, 2H), 3.25 (t, J = 5.7 Hz, 2H), 2.47 (t, J = 5.7 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 198.46, 150.36, 137.36, 136.49, 133.49, 132.83, 132.69, 131.59, 130.74, 130.31, 130.25, 129.75, 129.17, 128.93, 128.11, 121.96, 118.77, 53.03, 50.45, 28.09. HRMS (ESI) calcd. for $C_{22}H_{19}NOBr$ $(M+H)^+$: 392.0645, found : 392.0647.

(2-(6,7-dimethoxy-3,4-dihydroisoquinolin-2(1H)-yl)phenyl)(phenyl)methanone (1e)



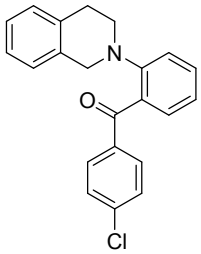
Yield: 82%, Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.79 (d, J = 7.6 Hz, 2H), 7.52 – 7.31 (m, 5H), 7.15 (d, J = 8.1 Hz, 1H), 7.08 (t, J = 7.4 Hz, 1H), 6.49 (d, J = 6.9 Hz, 2H), 4.10 (s, 2H), 3.83 (s, 3H), 3.81 (s, 3H), 3.26 (t, J = 5.7 Hz, 2H), 2.45 (t, J = 5.5 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 198.59, 150.76, 147.38, 147.25, 137.43, 132.75, 132.35, 131.54, 130.29, 129.81, 128.08, 126.43, 126.11, 121.39, 118.56, 111.37, 108.96, 55.94, 55.87, 53.10, 50.58, 28.04. HRMS (ESI) calcd. for $C_{24}H_{24}NO_3(M+H)^+$: 374.1751, found: 374.1753.

(2-(3,4-dihydroisoquinolin-2(1H)-yl)phenyl)(p-tolyl)methanone (1f).



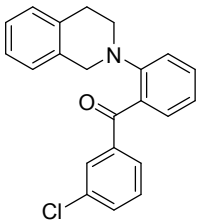
Yield: 75%, Yellow oil, **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.75 (d, J = 8.1 Hz, 2H), 7.51 – 7.44 (m, 1H), 7.41 (dd, J = 7.5, 1.2 Hz, 1H), 7.19 (d, J = 8.0 Hz, 3H), 7.15 – 7.06 (m, 3H), 7.03 (d, J = 6.0 Hz, 2H), 4.23 (s, 2H), 3.32 (t, J = 5.7 Hz, 2H), 2.61 (t, J = 5.6 Hz, 2H), 2.39 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 198.23, 150.59, 143.66, 134.85, 134.69, 134.47, 132.49, 131.34, 130.20, 130.11, 128.90, 128.66, 126.23, 126.10, 125.74, 121.26, 118.38, 53.27, 50.72, 28.71, 21.72. **HRMS** (ESI) calculated for $C_{23}H_{22}NO$ $(M+H)^+$: 328.1696, found:328.1695.

(4-chlorophenyl)(2-(3,4-dihydroisoquinolin-2(1H)-yl)phenyl)methanone (1g).



Yield: 78%, Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.74 (d, J = 8.5 Hz, 2H), 7.53 – 7.47 (m, 1H), 7.44 (dd, J = 7.5, 1.3 Hz, 1H), 7.36 – 7.31 (m, 3H), 7.20 (d, J = 8.2 Hz, 1H), 7.16 – 7.12 (m, 2H), 7.02 (dd, J = 8.7, 4.9 Hz, 2H), 4.19 (s, 2H), 3.29 (t, J = 5.8 Hz, 2H), 2.59 (t, J = 5.7 Hz, 2H). **^{13}C NMR** (125 MHz, CDCl3) δ 197.30, 150.79, 139.04, 135.89, 134.36, 134.17, 131.84, 131.15, 130.22, 129.01, 128.69, 128.39, 128.29, 126.13, 125.82, 121.80, 118.77, 53.69, 50.55, 28.61. **HRMS** (ESI) calculated for $C_{22}H_{19}NOCl$ $(M+H)^+$: 348.1150, found: 348.1148.

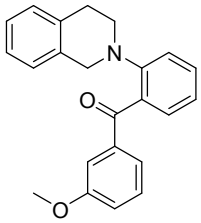
(3-chlorophenyl)(2-(3,4-dihydroisoquinolin-2(1H)-yl)phenyl)methanone (1h)



Yield: 73%, Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.79 (s, 1H), 7.67 (d, J = 7.8 Hz, 1H), 7.52 (t, J = 8.5 Hz, 1H), 7.47 (dd, J = 7.6, 1.3 Hz, 1H), 7.43 (dd, J = 8.0, 0.8 Hz, 1H), 7.27 (t, J = 7.8 Hz, 1H), 7.21 (d, J = 8.2 Hz, 1H), 7.17 – 7.09 (m, 3H), 7.02 (dd, J = 9.0, 5.6 Hz, 2H), 4.18 (s, 2H), 3.30 (t, J = 5.8 Hz, 2H), 2.61 (t, J = 5.7 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 197.11, 150.99, 139.21, 134.30, 134.26, 134.13, 132.54, 132.16, 131.84, 130.45, 129.67, 129.43, 128.69, 127.85, 126.26, 126.15,

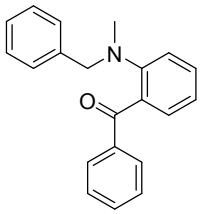
125.84, 121.87, 118.97, 53.87, 50.44, 28.60. **HRMS** (ESI) calcd. for $C_{22}H_{19}NOCl$ $(M+H)^+$: 348.1150, found: 348.1152;

(2-(3,4-dihydroisoquinolin-2(1H)-yl)phenyl)(3-methoxyphenyl)methanone (1i)



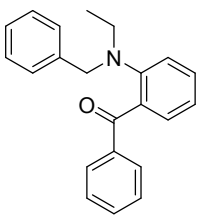
Yield: 69%, Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.52 – 7.45 (m, 1H), 7.45 – 7.39 (m, 2H), 7.34 (d, J = 7.6 Hz, 1H), 7.27 (t, J = 7.8 Hz, 1H), 7.19 (d, J = 8.2 Hz, 1H), 7.12 (dd, J = 9.9, 5.9 Hz, 3H), 7.08 – 7.02 (m, 3H), 4.22 (s, 2H), 3.78 (s, 3H), 3.31 (t, J = 5.7 Hz, 2H), 2.61 (t, J = 5.7 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 198.30, 159.56, 150.80, 139.03, 134.59, 134.41, 132.55, 131.54, 130.18, 129.06, 128.65, 126.15, 126.13, 125.73, 122.78, 121.40, 119.36, 118.69, 113.77, 55.40, 53.61, 50.52, 28.73. **HRMS** (ESI) calcd. for $C_{23}H_{22}NO_2$ $(M+H)^+$: 344.1645, found: 344.1643;

(2-(benzyl(methyl)amino)phenyl)(phenyl)methanone (1j)



Yellow oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.84 (d, J = 7.7 Hz, 2H), 7.60 (t, J = 7.4 Hz, 1H), 7.50 – 7.37 (m, 4H), 7.23 – 7.15 (m, 3H), 7.12 (d, J = 8.2 Hz, 1H), 7.05 (t, J = 7.4 Hz, 1H), 6.96 – 6.85 (m, 2H), 4.16 (s, 2H), 2.57 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 198.63, 151.58, 138.01, 137.88, 132.82, 131.61, 131.37, 130.18, 129.92, 128.34, 128.26, 127.89, 127.00, 120.67, 118.72, 59.98, 41.14. **HRMS** (ESI) calcd. for $C_{21}H_{20}NO$ $(M+H)^+$: 302.1540, found: 302.1545;

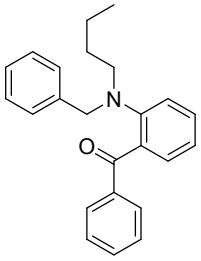
(2-(benzyl(ethyl)amino)phenyl)(phenyl)methanone (1k)



Yield: 47%, Yellow oil, **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.79 – 7.72 (m, 2H), 7.57 (t, J = 7.4 Hz, 1H), 7.46 – 7.39 (m, 3H), 7.37 (dd, J = 7.5, 1.6 Hz, 1H), 7.17 – 7.05 (m, 5H), 6.83 (dd, J = 7.4, 1.9 Hz, 2H), 4.08 (s, 2H), 2.89 (q, J = 7.1 Hz, 2H), 0.82 (t, J = 7.1 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 193.96, 147.61, 134.16, 133.01, 132.78,

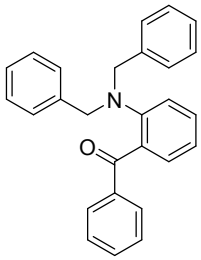
131.91, 129.76, 127.92, 127.22, 126.67, 126.44, 77.29, 77.03, 76.78, 52.50, 28.55. **HRMS** (ESI) calcd. for $C_{22}H_{22}NO$ $(M+H)^+$: 316.1700, found: 316.1701;

(2-(benzyl(butyl)amino)phenyl)(phenyl)methanone (1l)



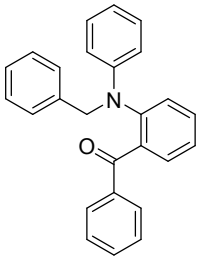
Yield: 43%, Yellow oil, **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.85 – 7.81 (m, 3H), 7.53 (d, J = 7.4 Hz, 1H), 7.44 – 7.38 (m, 4H), 7.32 (d, J = 4.5 Hz, 4H), 6.99 (d, J = 8.2 Hz, 1H), 6.90 (t, J = 7.9 Hz, 1H), 3.79 (s, 2H), 2.67 – 2.58 (m, 2H), 1.53 – 1.47 (m, 2H), 1.40 – 1.30 (m, 2H), 0.91 (t, J = 7.3 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 198.24, 151.65, 137.75, 132.69, 131.48, 130.76, 129.98, 129.09, 128.40, 128.16, 128.14, 126.90, 118.85, 116.46, 54.10, 49.20, 32.22, 20.51, 14.06. **HRMS** (ESI) calcd. for $C_{24}H_{26}NO$ $(M+H)^+$: 344.2009, found: 344.2010;

(2-(dibenzylamino)phenyl)(phenyl)methanone (1m)



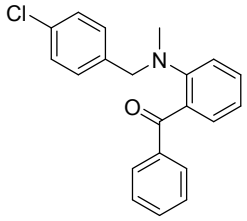
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.82 (d, J = 7.8 Hz, 2H), 7.66 (t, J = 7.3 Hz, 1H), 7.50 (t, J = 7.7 Hz, 2H), 7.42 (dd, J = 11.9, 7.6 Hz, 2H), 7.27 – 7.10 (m, 7H), 7.04 (d, J = 8.1 Hz, 1H), 6.94 – 6.82 (m, 4H), 4.08 (s, 4H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 199.20, 150.03, 138.37, 137.21, 134.48, 132.88, 130.77, 129.82, 129.64, 128.81, 128.52, 128.11, 127.08, 122.14, 121.69, 56.57. **HRMS** (ESI) calcd. for $C_{27}H_{24}NO$ $(M+H)^+$: 378.1853, found: 378.1851;

(2-(benzyl(phenyl)amino)phenyl)(phenyl)methanone (1n)



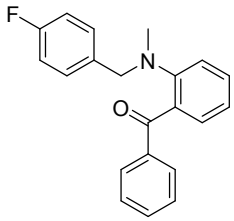
Yellow oil, **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.58 (d, J = 7.2 Hz, 2H), 7.55 – 7.48 (m, 3H), 7.41 (d, J = 8.7 Hz, 1H), 7.36 (d, J = 7.8 Hz, 2H), 7.33 (s, 1H), 7.29 (d, J = 6.3 Hz, 1H), 7.25 – 7.17 (m, 4H), 7.00 (t, J = 8.0 Hz, 2H), 6.68 (t, J = 7.3 Hz, 1H), 6.54 (d, J = 8.5 Hz, 2H), 4.76 (s, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 197.07, 147.52, 147.24, 138.52, 137.61, 136.00, 132.73, 132.15, 130.70, 129.47, 128.69, 128.45, 127.94, 127.22, 126.80, 126.77, 124.72, 119.16, 116.78, 56.88. **HRMS** (ESI) calcd. for $C_{26}H_{22}NO$ $(M+H)^+$: 364.1696, found: 364.1698;

(2-((4-chlorobenzyl)(methyl)amino)phenyl)(phenyl)methanone (1o)



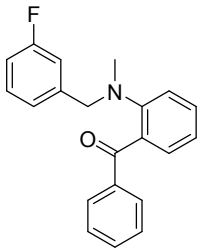
Yield: 53%, Yellow oil, **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.78 (d, J = 7.4 Hz, 2H), 7.57 (t, J = 7.4 Hz, 1H), 7.47 – 7.39 (m, 3H), 7.36 (d, J = 7.5 Hz, 1H), 7.14 – 7.01 (m, 4H), 6.79 (d, J = 8.3 Hz, 2H), 4.06 (s, 2H), 2.51 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 198.55, 151.32, 137.96, 136.43, 132.88, 132.67, 132.33, 131.31, 129.99, 129.84, 129.25, 128.36, 121.29, 118.98, 59.53, 41.23. **HRMS** (ESI) calcd. for $C_{21}H_{19}NOCl$ $(M+H)^+$: 336.1150, found: 336.1151;

(2-((4-fluorobenzyl)(methyl)amino)phenyl)(phenyl)methanone (1p)



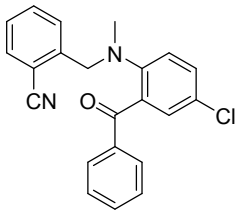
Yield: 57%, Yellow oil, **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.83 – 7.76 (m, 2H), 7.57 (t, J = 7.4 Hz, 1H), 7.45 – 7.40 (m, 3H), 7.40 – 7.34 (m, 1H), 7.14 – 7.00 (m, 2H), 6.83 (d, J = 7.1 Hz, 4H), 4.06 (s, 2H), 2.51 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 198.67, 161.88 (d, $^1J_{CF}$ = 243.4 HZ), 151.39, 137.93, 133.51 (d, $^4J_{CF}$ = 3.0 HZ), 132.89, 132.12, 131.36, 130.05, 129.87, 129.43 (d, $^3J_{CF}$ = 8.0 HZ), 128.37, 121.15, 118.91, 115.03 (d, $^2J_{CF}$ = 21.2 HZ), 59.44, 41.08. **HRMS** (ESI) calcd. for $C_{21}H_{19}NOF$ $(M+H)^+$: 320.1445, found: 320.1447;

(2-((3-fluorobenzyl)(methyl)amino)phenyl)(phenyl)methanone (1q)



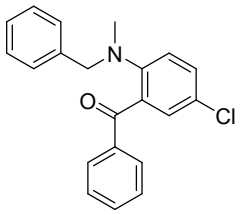
Yield: 59%, Yellow oil, **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.85 (d, J = 7.4 Hz, 2H), 7.61 (t, J = 7.4 Hz, 1H), 7.52 – 7.43 (m, 3H), 7.42 (dd, J = 7.5, 1.2 Hz, 1H), 7.15 (dd, J = 7.0, 4.4 Hz, 2H), 7.09 (t, J = 7.4 Hz, 1H), 6.88 (td, J = 8.4, 2.3 Hz, 1H), 6.75 (d, J = 7.6 Hz, 1H), 6.57 (d, J = 9.9 Hz, 1H), 4.14 (s, 2H), 2.58 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 198.61, 162.93 (d, $^1J_{CF}$ = 244.2 HZ), 151.34, 140.74 (d, $^3J_{CF}$ = 6.9 HZ), 137.91, 133.06, 132.22, 131.38, 130.05, 129.85, 129.69 (d, $^3J_{CF}$ = 8.1 HZ), 128.43, 123.41 (d, $^4J_{CF}$ = 2.8 HZ), 121.29, 118.90, 114.60 (d, $^2J_{CF}$ = 20.5 HZ), 113.93 (d, $^2J_{CF}$ = 21.1 HZ), 59.74, 41.30. **HRMS** (ESI) calcd. for $C_{21}H_{19}NOF(M+H)^+$: 320.1445, found: 320.1449;

2-(((2-benzoyl-4-chlorophenyl)(methyl)amino)methyl)benzonitrile (1r)



Yield: 62%, Yellow oil, **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.81 (d, J = 7.2 Hz, 2H), 7.62 (t, J = 7.4 Hz, 1H), 7.58 (d, J = 7.6 Hz, 1H), 7.47 (t, J = 7.7 Hz, 2H), 7.41 (dd, J = 8.7, 2.5 Hz, 1H), 7.38 – 7.28 (m, 3H), 7.12 (d, J = 8.7 Hz, 1H), 6.94 (d, J = 7.7 Hz, 1H), 4.35 (s, 2H), 2.62 (s, 3H)**. ^{13}C NMR** (100 MHz, $CDCl_3$) δ 196.64, 149.37, 141.38, 137.19, 133.74, 133.40, 132.87, 132.69, 131.13, 129.86, 129.45, 128.66, 128.58, 127.63, 127.03, 120.89, 117.35, 111.74, 57.75, 41.97. **HRMS** (ESI) calcd. for $C_{22}H_{18}N_2OCl(M+H)^+$: 361.1102, found: 361.1100;

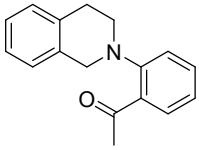
(2-(benzyl(methyl)amino)-5-chlorophenyl)(phenyl)methanone (1s)



Yield: 66%, Yellow oil, **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.85 (d, J = 7.2 Hz, 2H), 7.63 (t, J = 6.8 Hz, 1H), 7.49 (t, J = 7.7 Hz, 2H), 7.40 (d, J = 7.1 Hz, 2H), 7.24 – 7.19 (m, 3H), 7.04 (d, J = 8.5 Hz, 1H), 6.93 (dd, J = 6.4, 2.8 Hz, 2H), 4.14 (s, 2H), 2.57 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 197.01, 150.01, 137.40, 137.31, 133.23, 131.11,

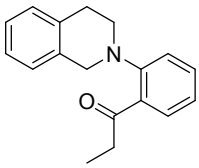
129.94, 129.68, 128.50, 128.36, 127.82, 127.69, 127.17, 125.69, 120.12, 59.93, 41.18. **HRMS** (ESI) calcd. for $C_{21}H_{19}NOCl$ $(M+H)^+$: 336.1500, found: 336.1501;

1-(2-(3,4-dihydroisoquinolin-2(1H)-yl)phenyl)ethan-1-one (1aa).



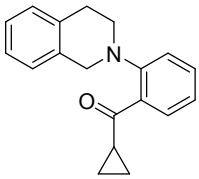
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.51 (dd, J = 7.6, 1.6 Hz, 1H), 7.47 – 7.41 (m, 1H), 7.24 – 7.16 (m, 4H), 7.15 – 7.06 (m, 2H), 4.25 (s, 2H), 3.39 (t, J = 5.9 Hz, 2H), 3.03 (t, J = 5.8 Hz, 2H), 2.65 (s, 3H). **^{13}C NMR** (100 MHz, CDCl3) δ 204.49, 151.07, 135.14, 134.36, 134.18, 132.06, 129.40, 128.93, 126.54, 126.33, 126.05, 122.39, 119.04, 55.04, 51.38, 29.32, 28.96. HRMS (ESI) calculated for $C_{17}H_{18}NO$ (M+H)+ : 252.1383, found: 252.1389.

1-(2-(3,4-dihydroisoquinolin-2(1H)-yl)phenyl)propan-1-one (1ab).



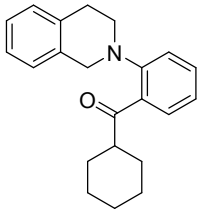
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.46–7.35 (m, 2H), 7.25–7.13 (m, 4H), 7.12–7.03 (m, 2H), 4.19 (s, 2H), 3.32 (t, J = 5.6 Hz, 2H), 3.09–2.90 (m, 4H), 1.18–0.98 (m, 3H). **^{13}C NMR** (100 MHz, CDCl3) δ 208.57, 150.53, 135.73, 134.39, 134.21, 131.42, 128.93, 128.77, 126.43, 126.28, 126.04, 122.62, 119.02, 54.79, 51.43, 34.92, 29.01, 8.84. HRMS (ESI) calculated for $C_{18}H_{20}NO$ (M+H)+ : 266.1540, found : 266.1536.

cyclopropyl(2-(3,4-dihydroisoquinolin-2(1H)-yl)phenyl)methanone (1ac).



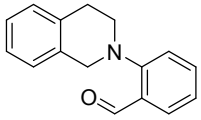
Yield: 67%, Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.46 (d, J = 7.6 Hz, 1H), 7.38 (t, J = 7.7 Hz, 1H), 7.18 – 7.08 (m, 4H), 7.08 – 7.04 (m, 1H), 7.01 (t, J = 7.5 Hz, 1H), 4.24 (s, 2H), 3.36 (t, J = 5.9 Hz, 2H), 2.97 (t, J = 5.8 Hz, 2H), 2.89 (ddd, J = 12.4, 7.9, 4.6 Hz, 1H), 1.16 (dt, J = 7.3, 3.5 Hz, 2H), 0.78 (td, J = 7.0, 3.4 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 206.58, 151.17, 134.57, 134.46, 134.27, 132.01, 129.73, 128.87, 126.47, 126.37, 126.01, 121.79, 118.33, 54.54, 51.58, 29.12, 20.34, 12.53. **HRMS** (ESI) calculated for $C_{19}H_{20}NO$ $(M+H)^+$: 278.1540, found: 278.1542.

cyclohexyl(2-(3,4-dihydroisoquinolin-2(1H)-yl)phenyl)methanone (1ad).



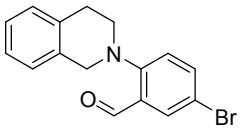
Yield: 65%, Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.45 – 7.37 (m, 1H), 7.32 – 7.27 (m, 1H), 7.22 – 7.15 (m, 4H), 7.13 – 7.04 (m, 2H), 4.20 (s, 2H), 3.36 (d, J = 5.6 Hz, 2H), 2.97 (t, J = 5.7 Hz, 2H), 1.85 – 1.65 (m, 6H), 1.43 – 1.21 (m, 3H), 1.21 – 1.07 (m, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 211.65, 150.33, 134.52, 134.16, 131.06, 128.91, 128.81, 126.34, 126.23, 125.93, 122.73, 122.65, 119.25, 55.42, 50.82, 48.93, 29.19, 29.10, 25.95, 25.84. **HRMS** (ESI) calcd. for $C_{22}H_{26}NO$ $(M+H)^+$: 320.2009, found: 320.2005.

2-(3,4-dihydroisoquinolin-2(1H)-yl)benzaldehyde (1ae).



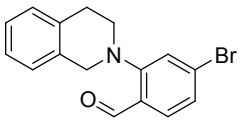
Yellow oil. **^{1}H NMR** (400 MHz, CDCl3) δ 10.38 (s, 1H), 7.90 (dd, J = 7.7, 1.6 Hz, 1H), 7.64 – 7.50 (m, 1H), 7.30 – 7.18 (m, 4H), 7.18 – 7.06 (m, 2H), 4.36 (s, 2H), 3.48 (t, J = 5.8 Hz, 2H), 3.09 (t, J = 5.7 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 190.15, 154.06, 133.78, 133.11, 132.97, 128.94, 127.86, 127.50, 125.49, 125.25, 124.99, 121.16, 117.92, 53.68, 52.39, 27.94. **HRMS** (ESI) calcd. for $C_{16}H_{16}NO$ $(M+H)^+$: 238.1227, found: 238.1222;

5-bromo-2-(3,4-dihydroisoquinolin-2(1H)-yl)benzaldehyde (1af).



Yellow oil, **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.21 (s, 1H), 7.91 (s, 1H), 7.57 (d, J = 6.2 Hz, 1H), 7.26 – 7.18 (m, 3H), 7.13 – 7.01 (m, 2H), 4.29 (s, 2H), 3.42 (t,J = 5.8 Hz 2H), 3.04 (t, J = 5.6 Hz, 2H). **^{13}C NMR** (100 MHz, CDCl3) δ 189.86, 154.01, 137.44, 134.03, 133.65, 132.48, 129.85, 129.03, 126.79, 126.36, 126.27, 121.06, 115.31, 54.70, 53.56, 28.91. **HRMS** (ESI) calculated for $C_{16}H_{15}NOBr$ $(M+H)^+$: 316.0332, found: 316.0335.

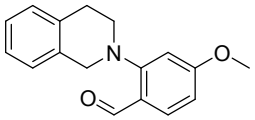
4-bromo-2-(3,4-dihydroisoquinolin-2(1H)-yl)benzaldehyde (1ag)



Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.21 (s, 1H), 7.68 (d, J = 8.3 Hz, 1H), 7.32 (s, 1H), 7.25 (d, J = 3.4 Hz, 1H), 7.23 – 7.16 (m, 3H), 7.10 (d, J = 4.6 Hz, 1H),

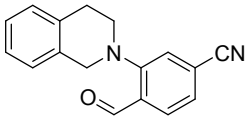
4.31 (s, 2H), 3.45 (t, J = 5.8 Hz, 2H), 3.07 (t, J = 5.7 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 190.15, 155.67, 133.97, 133.49, 131.66, 129.92, 128.99, 127.05, 126.80, 126.39, 126.26, 125.32, 122.19, 54.49, 53.44, 29.07. **HRMS** (ESI) calcd for $C_{16}H_{15}NOBr$ $(M+H)^+$: 316.0332, found: 316.0334.

2-(3,4-dihydroisoquinolin-2(1H)-yl)-4-methoxybenzaldehyde (1ah)



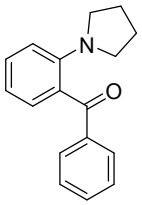
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.18 (s, 1H), 7.86 (d, J = 9.2 Hz, 1H), 7.22 (d, J = 3.5 Hz, 3H), 7.13 (s, 1H), 6.73 – 6.63 (m, 2H), 4.34 (s, 2H), 3.89 (s, 3H), 3.48 (t, J = 5.8 Hz, 2H), 3.10 (t, J = 5.7 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 189.65, 165.16, 157.08, 134.29, 134.00, 133.02, 128.97, 126.61, 126.37, 126.09, 122.29, 107.40, 104.61, 55.52, 54.51, 53.44, 29.08. **HRMS** (ESI) calcd. for $C_{17}H_{18}NO_2$ $(M+H)^+$: 268.1332, found: 268.1330;

3-(3,4-dihydroisoquinolin-2(1H)-yl)-4-formylbenzonitrile (1ai)



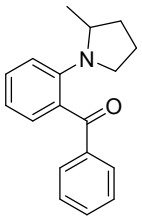
Yield: 78%, Yellow oil, **^{1}H NMR** (400 MHz, CDCl3) δ 10.31 (s, 1H), 7.91 (d, J = 7.9 Hz, 1H), 7.46 (s, 1H), 7.37 (d, J = 7.9 Hz, 1H), 7.28 – 7.19 (m, 3H), 7.15 (d, J = 4.7 Hz, 1H), 4.39 (s, 2H), 3.52 (t, J = 5.6 Hz, 2H), 3.10 (t, J = 5.6 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 189.87, 154.50, 133.77, 133.01, 130.89, 130.82, 129.04, 127.02, 126.48, 126.39, 124.81, 122.55, 118.14, 117.70, 54.31, 53.37, 28.83. **HRMS** (ESI) calcd. for $C_{17}H_{15}N_2O$ $(M+H)^+$: 263.1179, found: 263.1180;

phenyl(2-(pyrrolidin-1-yl)phenyl)methanone (1aj)



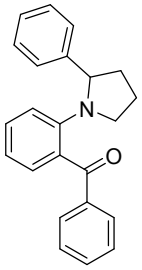
Yellow oil, **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.98 (d, J = 7.3 Hz, 2H), 7.58 (t, J = 7.3 Hz, 1H), 7.48 (t, J = 7.6 Hz, 2H), 7.42 – 7.35 (m, 1H), 7.29 (d, J = 7.5 Hz, 1H), 6.87 (d, J = 8.5 Hz, 1H), 6.71 (t, J = 7.4 Hz, 1H), 3.17 (t, J = 6.4 Hz, 4H), 1.98 – 1.83 (m, 4H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 196.76, 147.98, 138.50, 132.53, 131.54, 131.44, 130.47, 128.26, 124.04, 114.69, 113.97, 51.26, 25.92. **HRMS** (ESI) calcd. for $C_{17}H_{18}NO$ $(M+H)^+$: 252.1383, found: 252.1381;

(2-(2-methylpyrrolidin-1-yl)phenyl)(phenyl)methanone (1ak)



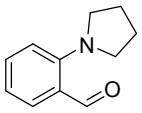
Yield: 82%, Yellow oil, **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.90 (d, J = 7.7 Hz, 2H), 7.56 (t, J = 7.3 Hz, 1H), 7.47 – 7.32 (m, 4H), 6.93 (d, J = 8.4 Hz, 1H), 6.79 (t, J = 7.3 Hz, 1H), 3.94 – 3.79 (m, 1H), 3.19 (dd, J = 16.1, 9.3 Hz, 1H), 2.87 (t, J = 8.5 Hz, 1H), 2.09 (dd, J = 9.9, 6.2 Hz, 1H), 1.73 (s, 1H), 1.61 (dt, J = 10.7, 8.1 Hz, 1H), 1.52 – 1.42 (m, 1H), 1.19 (d, J = 5.9 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 197.60, 147.45, 138.07, 132.54, 131.37, 131.28, 130.13, 128.14, 126.69, 116.24, 114.80, 54.34, 53.87, 34.25, 24.83, 19.00. **HRMS** (ESI) calcd. for $C_{18}H_{20}NO$ $(M+H)^+$: 266.1540, found: 266.1541;

phenyl(2-(2-phenylpyrrolidin-1-yl)phenyl)methanone (1al)



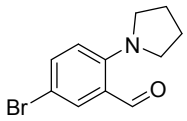
Yield: 80%, Yellow oil, **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.84 (d, J = 7.6 Hz, 2H), 7.59 (t, J = 7.3 Hz, 1H), 7.47 (t, J = 7.4 Hz, 2H), 7.31 – 7.15 (m, 7H), 6.73 (d, J = 8.5 Hz, 1H), 6.68 (t, J = 7.4 Hz, 1H), 4.81 (t, J = 7.3 Hz, 1H), 3.59 (dd, J = 15.7, 9.2 Hz, 1H), 3.13 (t, J = 8.2 Hz, 1H), 2.44 (d, J = 6.8 Hz, 1H), 2.02 – 1.71 (m, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 197.14, 147.27, 143.47, 138.43, 132.49, 131.27, 131.17, 130.32, 128.63, 128.21, 126.91, 126.38, 125.62, 115.59, 115.23, 64.19, 55.06, 37.78, 25.52. **HRMS** (ESI) calcd. for $C_{23}H_{22}NO(M+H)^+$: 328.1700, found: 328.1701;

2-(pyrrolidin-1-yl)benzaldehyde (1am)



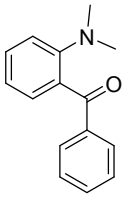
Yellow oil, **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.08 (s, 1H), 7.70 (dd, J = 7.8, 1.2 Hz, 1H), 7.43 – 7.32 (m, 1H), 6.81 (dd, J = 13.4, 7.9 Hz, 2H), 3.35 (t, J = 6.5 Hz, 4H), 2.10 – 1.87 (m, 4H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 190.13, 149.96, 134.23, 133.09, 122.97, 116.43, 114.54, 52.72, 25.97. **HRMS** (ESI) calcd. for $C_{11}H_{14}NO$ $(M+H)^+$: 176.1070, found: 176.1072;

5-bromo-2-(pyrrolidin-1-yl)benzaldehyde (1an)



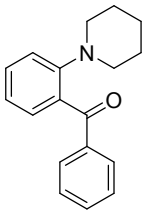
Yellow oil, **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.02 (s, 1H), 7.53 (d, J = 8.4 Hz, 1H), 6.97 (s, 1H), 6.90 (dd, J = 8.3, 1.5 Hz, 1H), 3.35 (t, J = 6.5 Hz, 4H), 2.12 – 1.83 (m, 4H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 189.13, 150.27, 134.37, 129.48, 121.68, 119.57, 117.35, 52.79, 25.98. **HRMS** (ESI) calcd. for $C_{11}H_{13}NOBr$ $(M+H)^+$: 254.0175, found: 254.0177;

(2-(dimethylamino)phenyl)(phenyl)methanone (1ao)



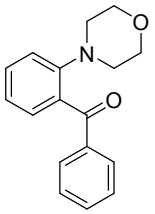
Yellow oil, **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.83 (d, J = 7.9 Hz, 2H), 7.54 (t, J = 7.3 Hz, 1H), 7.41 (dd, J = 16.6, 8.7 Hz, 3H), 7.32 (d, J = 7.6 Hz, 1H), 6.99 (d, J = 8.3 Hz, 1H), 6.90 (t, J = 7.4 Hz, 1H), 2.70 (s, 6H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 198.25, 151.66, 137.74, 132.71, 131.50, 130.75, 129.98, 129.10, 128.16, 118.87, 116.48, 43.46. **HRMS** (ESI) calcd. for $C_{15}H_{16}NO$ $(M+H)^+$: 226.1227, found: 226.1225;

phenyl(2-(piperidin-1-yl)phenyl)methanone (1ap)



Yellow oil, **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.78 (d, J = 7.3 Hz, 2H), 7.55 (t, J = 7.4 Hz, 1H), 7.50 – 7.37 (m, 4H), 7.10 (t, J = 7.3 Hz, 2H), 2.87 (s, 4H), 1.31 (s, 2H), 1.18 (s, 4H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 198.94, 137.50, 133.18, 132.57, 131.66, 130.20, 129.90, 127.86, 121.84, 118.71, 53.53, 25.55, 23.78. **HRMS** (ESI) calcd. for $C_{18}H_{20}NO$ $(M+H)^+$: 266.1540, found: 266.1542;

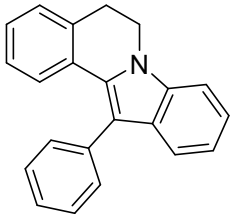
(2-morpholinophenyl)(phenyl)methanone (1aq)



Yellow oil, **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.74 (d, J = 7.1 Hz, 2H), 7.55 (t, J = 7.4 Hz, 1H), 7.50 – 7.40 (m, 4H), 7.15 (t, J = 7.0 Hz, 1H), 7.06 (d, J = 8.0 Hz, 1H), 3.34 –

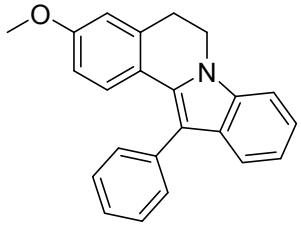
3.20 (m, 4H), 2.94 – 2.82 (m, 4H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 198.76, 150.99, 137.52, 133.47, 132.87, 131.82, 130.24, 129.75, 128.05, 122.85, 118.55, 66.52, 52.36. **HRMS** (ESI) calcd. for $C_{17}H_{18}NO_2$ $(M+H)^+$: 268.1332, found: 268.1335;

12-phenyl-5,6-dihydroindolo[2,1-a]isoquinoline (2a).



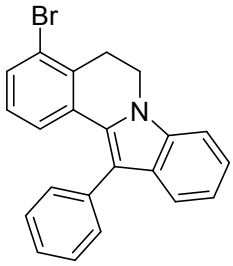
Yield: 85% (75.3 mg). White solid. m.p. 158 – 160 °C **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.56 – 7.54 (m, 3H), 7.46 (t, J = 7.5 Hz, 2H), 7.41 – 7.34 (m, 3H), 7.24 (t, J = 7.2 Hz, 2H), 7.14 (t, J = 7.1 Hz, 1H), 7.09 (t, J = 7.5 Hz, 1H), 7.02 (t, J = 7.6 Hz, 1H), 4.27 (t, J = 6.4 Hz, 2H), 3.20 (t, J = 6.3 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 135.79, 135.52, 133.58, 130.57, 130.52, 129.22, 128.79, 128.76, 128.28, 127.20, 126.74, 126.68, 126.13, 122.36, 120.04, 119.62, 113.92, 108.83, 40.30, 29.95. **HRMS** (ESI) calculated for $C_{22}H_{18}N$ $(M+H)^+$: 296.1357, found: 296.1360.

3-methoxy-12-phenyl-5,6-dihydroindolo[2,1-a]isoquinoline (2b)



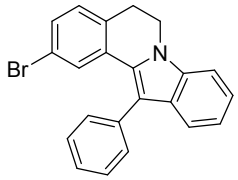
Yield: 87% (84.9 mg). White solid. m.p. 131 – 132 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.54 (t, J = 6.6 Hz, 3H), 7.46 (t, J = 7.6 Hz, 2H), 7.37 – 7.31 (m, 3H), 7.25 – 7.19 (m, 1H), 7.08 (t, J = 7.4 Hz, 1H), 6.81 (s, 1H), 6.59 (dd, J = 8.7, 2.3 Hz, 1H), 4.26 (t, J = 6.3 Hz, 2H), 3.79 (s, 3H), 3.19 (t, J = 6.3 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 158.77, 135.95, 135.35, 130.51, 128.82, 128.74, 127.49, 126.50, 122.03, 121.86, 119.91, 119.24, 113.67, 112.37, 112.30, 108.61, 55.28, 40.17, 30.23. **HRMS** (ESI) calculated for $C_{23}H_{20}NO$ $(M+H)^+$: 326.1463, found: 326.1460.

4-bromo-12-phenyl-5,6-dihydroindolo[2,1-a]isoquinoline (2c)



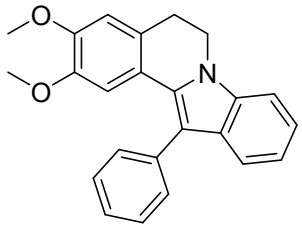
Yield: 84% (94.2 mg). Pale yellow solid. m.p. 147 – 148 °C. **^{1}H NMR** (400 MHz, DMSO) δ 7.57 (d, J = 8.2 Hz, 1H), 7.54 – 7.41 (m, 6H), 7.37 (d, J = 8.0 Hz, 1H), 7.31 – 7.22 (m, 2H), 7.07 (t, J = 7.5 Hz, 1H), 7.00 (t, J = 7.9 Hz, 1H), 4.34 (t, J = 6.3 Hz, 2H), 3.31 (t, J = 6.4 Hz, 2H). **^{13}C NMR** (100 MHz, DMSO) δ 135.56, 135.45, 133.77, 131.51, 131.20, 130.43, 129.52, 129.34, 128.52, 128.46, 127.47, 125.10, 124.37, 123.14, 120.71, 119.33, 114.16, 110.32, 40.60, 29.55. **HRMS** (ESI) calcd. for $C_{22}H_{17}NBr$ $(M+H)^+$: 374.0462, found: 374.0466.

6-bromo-12-phenyl-5,6-dihydroindolo[2,1-a]isoquinoline (2d)



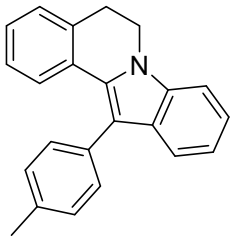
Yield: 80% (89.7 mg). Pale yellow solid. m.p. 153 – 155 °C. **^{1}H NMR** (400 MHz, CDCl3) δ 7.59 (dd, J = 7.9, 4.9 Hz, 1H), 7.56 – 7.49 (m, 4H), 7.47 – 7.41 (m, 1H), 7.39 (s, 1H), 7.33 – 7.23 (m, 3H), 7.15 (t, J = 7.9 Hz, 2H), 4.30 (t, J = 6.4 Hz, 2H), 3.19 (t, J = 6.3 Hz, 2H). **^{13}C NMR** (125 MHz, CDCl3) δ 135.60, 134.96, 132.17, 131.12, 130.31, 129.83, 129.77, 129.06, 128.91, 128.64, 128.54, 127.10, 122.83, 120.43, 120.25, 119.90, 114.92, 108.90, 40.10, 30.16. **HRMS** (ESI) calcd. for $C_{22}H_{17}NBr$ $(M+H)^+$: 374.0462, found: 374.0463.

2,3-dimethoxy-12-phenyl-5,6-dihydroindolo[2,1-a]isoquinoline (2e).



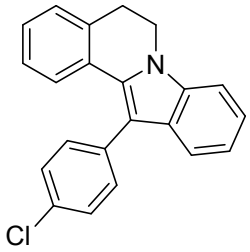
Yield: 91% (97.0 mg). White solid. m.p. 145 – 146 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.61 (d, J = 7.0 Hz, 2H), 7.57 (d, J = 7.9 Hz, 1H), 7.51 (t, J = 7.6 Hz, 2H), 7.38 (t, J = 7.3 Hz, 2H), 7.33 – 7.24 (m, 1H), 7.13 (t, J = 7.5 Hz, 1H), 6.96 (s, 1H), 6.79 (s, 1H), 4.29 (t, J = 6.4 Hz, 2H), 3.93 (s, 3H), 3.44 (s, 3H), 3.18 (t, J = 6.4 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 148.21, 147.48, 135.97, 135.46, 130.92, 130.86, 128.82, 128.70, 126.70, 126.10, 121.96, 121.62, 119.93, 119.24, 112.54, 111.10, 109.19, 108.66, 55.95, 55.23, 40.43, 29.32. **HRMS** (ESI) calculated for $C_{24}H_{22}NO$ $(M+H)^+$: 356.1568, found: 356.1570.

12-(p-tolyl)-5,6-dihydroindolo[2,1-a]isoquinoline (2f)



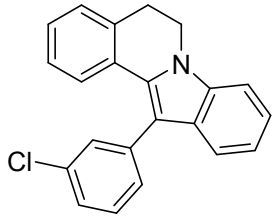
Yield: 81% (75.1 mg). White solid. m.p. 206 – 207 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.59 (d, J = 8.0 Hz, 1H), 7.48 (d, J = 7.9 Hz, 3H), 7.40 (d, J = 8.2 Hz, 1H), 7.34 – 7.28 (m, 4H), 7.19 (t, J = 7.5 Hz, 1H), 7.13 (t, J = 7.5 Hz, 1H), 7.08 (t, J = 7.6 Hz, 1H), 4.31 (t, J = 6.4 Hz, 2H), 3.25 (t, J = 6.3 Hz, 2H), 2.50 (s, 3H). **^{13}C NMR** (100MHz, $CDCl_3$) δ 136.24, 135.50, 133.52, 132.66, 130.45, 130.32, 129.54, 129.35, 128.86, 128.24, 127.10, 126.72, 126.11, 122.29, 119.93, 119.69, 113.88, 108.78, 40.30, 29.96, 21.39. HRMS (ESI) calcd. for $C_{23}H_{20}N$ $(M+H)^+$: 310.0513, found: 310.0509;

12-(4-chlorophenyl)-5,6-dihydroindolo[2,1-a]isoquinoline (2g)



Yield: 88% (87.1 mg). White solid. m.p. 230 – 231 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.55 – 7.40 (m, 5H), 7.36 (d, J = 8.2 Hz, 2H), 7.28 – 7.21 (m, 2H), 7.19 – 7.13 (m, 1H), 7.10 (t, J = 7.5 Hz, 1H), 7.05 (t, J = 7.5 Hz, 1H), 4.26 (t, J = 6.4 Hz, 2H), 3.19 (t, J = 6.3 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 135.54, 134.35, 133.65, 132.48, 131.79, 130.76, 129.03, 128.95, 128.54, 128.36, 127.41, 126.84, 126.02, 122.51, 120.24, 119.29, 112.50, 108.91, 40.29, 29.90. **HRMS** (ESI) calcd. for $C_{22}H_{17}NCl$ $(M+H)^+$: 330.0967, found : 330.0972.

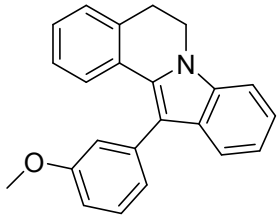
12-(3-chlorophenyl)-5,6-dihydroindolo[2,1-a]isoquinoline (2h).



Yield: 87% (86.1 mg). White solid. m.p. 150 – 151 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.69 (s, 1H), 7.66 (d, J = 8.0 Hz, 1H), 7.55 (d, J = 5.0 Hz, 1H), 7.51 – 7.45 (m, 4H), 7.40 – 7.33 (m, 2H), 7.26 (dd, J = 15.1, 7.4 Hz, 2H), 7.16 (t, J = 7.4 Hz, 1H), 4.33 (t, J = 6.4 Hz, 2H), 3.28 (t, J = 6.3 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 137.91, 135.58, 134.60, 133.75, 130.98, 130.43, 130.16, 128.87, 128.84, 128.51, 128.48,

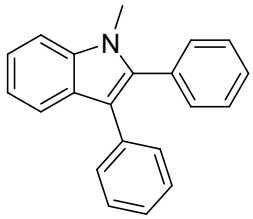
127.58, 126.96, 126.88, 126.16, 122.64, 120.42, 119.35, 112.39, 109.05, 40.34, 29.93. **HRMS** (ESI) calculated for $C_{22}H_{17}NCl$ $(M+H)^+$: 330.0967, found : 330.0970.

12-(3-methoxyphenyl)-5,6-dihydroindolo[2,1-a]isoquinoline (2i)



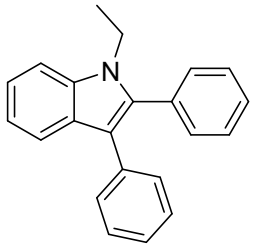
Yield: 83% (80.9 mg). White solid. m.p. 156 – 157 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.57 (d, J = 8.0 Hz, 1H), 7.44 (d, J = 7.8 Hz, 1H), 7.39 – 7.31 (m, 2H), 7.23 (td, J = 6.9, 1.0 Hz, 2H), 7.16 – 7.06 (m, 4H), 7.02 (t, J = 7.6 Hz, 1H), 6.92 (ddd, J = 8.3, 2.6, 0.8 Hz, 1H), 4.22 (t, J = 6.4 Hz, 2H), 3.79 (s, 3H), 3.16 (t, J = 6.4 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 160.01, 137.22, 135.54, 133.59, 130.66, 129.83, 129.17, 128.75, 128.31, 127.29, 126.81, 126.32, 123.04, 122.43, 120.14, 119.71, 115.64, 113.81, 112.70, 108.90, 55.37, 40.34, 29.95. HRMS (ESI) calcd. for $C_{23}H_{20}NO$ $(M+H)^+$: 326.1463, found: 326.1460.

1-methyl-2,3-diphenyl-1H-indole (2j)



Yield: 71% (60.3 mg). White solid. m.p. 138 – 139 °C. **^{1}H NMR** (400 MHz, CDCl3) δ 7.79 (d, J = 7.9 Hz, 1H), 7.39 (d, J = 8.2 Hz, 1H), 7.36 – 7.28 (m, 7H), 7.25 (t, J = 7.7 Hz, 3H), 7.20 – 7.12 (m, 2H), 3.64 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 137.81, 137.44, 135.33, 132.02, 131.24, 129.97, 128.47, 128.26, 128.11, 127.10, 125.59, 122.27, 120.29, 119.71, 115.22, 109.66, 31.00. **HRMS** (ESI) calcd. for $C_{21}H_{18}N$ $(M+H)^+$: 284.1357, found: 284.1357.

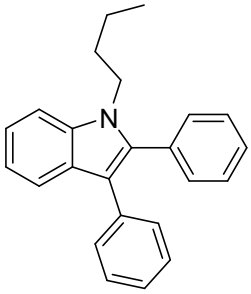
1-ethyl-2,3-diphenyl-1H-indole (2k)



Yield: 73% (65.0 mg). White solid. m.p. 134 – 135 °C. **^{1}H NMR** (400 MHz, CDCl3) δ 7.87 (d, J = 7.9 Hz, 1H), 7.50 (d, J = 8.2 Hz, 1H), 7.46 – 7.37 (m, 5H), 7.37 – 7.28 (m, 5H), 7.26 – 7.17 (m, 2H), 4.19 (q, J = 7.2 Hz, 2H), 1.34 (t, J = 7.2 Hz, 3H). **^{13}C**

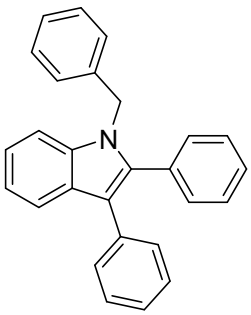
NMR (100 MHz, $CDCl_3$) δ 137.31, 136.10, 135.25, 132.28, 131.10, 129.85, 128.46, 128.14, 128.12, 127.28, 125.44, 122.06, 120.13, 119.80, 115.34, 109.83, 38.67, 15.43. **HRMS** (ESI) calcd. for $C_{22}H_{20}N$ $(M+H)^+$: 298.1513, found: 298.1518.

1-butyl-2,3-diphenyl-1H-indole (2l)



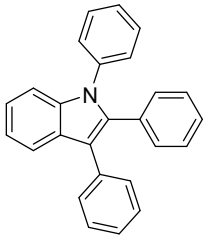
Yield: 69% (67.3 mg). White solid. m.p. 83 – 84 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.80 (d, J = 7.6 Hz, 1H), 7.43 (d, J = 8.2 Hz, 1H), 7.39 – 7.35 (m, 3H), 7.33 – 7.31 (m, 2H), 7.29 (d, J = 7.2, 2H), 7.24 (dd, J = 10.7, 4.7 Hz, 3H), 7.19 – 7.13 (m, 2H), 4.14 – 4.04 (m, 2H), 1.66 (dt, J = 15.2, 7.6 Hz, 2H), 1.23 – 1.13 (m, 2H), 0.78 (t, J = 7.4 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 137.57, 136.42, 135.27, 132.33, 131.20, 129.88, 128.41, 128.11, 128.06, 127.19, 125.41, 121.97, 120.06, 119.74, 115.23, 110.00, 43.65, 32.13, 20.06, 13.65. **HRMS** (ESI) calcd. for $C_{24}H_{24}N$ $(M+H)^+$: 326.1826, found: 326.1824.

1-benzyl-2,3-diphenyl-1H-indole (2m)



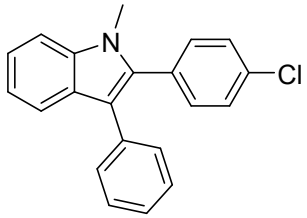
Yield: 75% (80.9 mg). White solid. m.p. 159 – 160 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.82 (dd, J = 6.2, 2.5 Hz, 1H), 7.38 – 7.31 (m, 2H), 7.31 – 7.21 (m, 11H), 7.21 – 7.15 (m, 3H), 7.01 (d, J = 6.8 Hz, 2H), 5.29 (s, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 138.15, 137.93, 137.02, 135.16, 131.83, 131.12, 129.96, 128.72, 128.44, 128.22, 128.20, 127.42, 127.21, 126.16, 125.63, 122.42, 120.47, 119.77, 115.71, 110.57, 47.65. **HRMS** (ESI) calcd. for $C_{27}H_{22}N$ $(M+H)^+$: 360.1670, found: 360.1671.

1,2,3-triphenyl-1H-indole (2n)



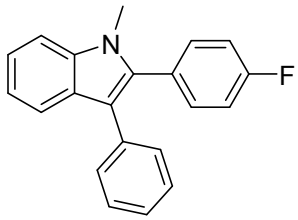
Yield: 83% (85.9 mg). White solid. m.p. 187 – 189 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.87 (dd, J = 5.8, 3.1 Hz, 1H), 7.48 – 7.41 (m, 3H), 7.41 – 7.33 (m, 5H), 7.31 – 7.28 (m, 5H), 7.23 – 7.13 (m, 5H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 138.21, 137.98, 137.11, 134.99, 131.67, 131.24, 130.29, 129.10, 128.34, 128.31, 127.94, 127.64, 127.38, 127.19, 125.98, 122.79, 120.94, 119.65, 116.79, 110.70. **HRMS** (ESI) calcd. for $C_{26}H_{20}N$ $(M+H)^+$: 346.1513, found: 346.1515.

2-(4-chlorophenyl)-1-methyl-3-phenyl-1H-indole (2o)



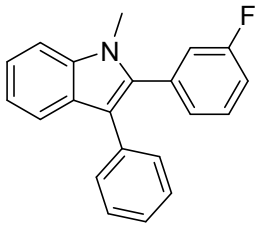
Yield: 72% (68.6 mg). White solid. m.p. 157 – 158 °C. **^{1}H NMR** (400 MHz, CDCl3) δ 7.83 (d, J = 7.9 Hz, 1H), 7.52 – 7.29 (m, 10H), 7.28 – 7.20 (m, 2H), 3.72 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 137.51, 136.34, 134.92, 134.20, 132.44, 130.43, 129.93, 128.77, 128.35, 127.00, 125.79, 122.51, 120.39, 119.74, 115.67, 109.65, 31.00. **HRMS** (ESI) calcd. for $C_{21}H_{17}NCl$ $(M+H)^+$: 318.0967, found: 318.0969.

2-(4-fluorophenyl)-1-methyl-3-phenyl-1H-indole (2p)



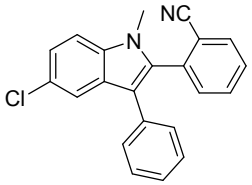
Yield: 70% (63.2 mg). White solid. m.p. 143 – 145 °C. **^{1}H NMR** (400 MHz, CDCl3) δ 7.78 (d, J = 8.0 Hz, 1H), 7.40 (d, J = 8.2 Hz, 1H), 7.32 – 7.24 (m, 7H), 7.19 (t, J = 7.3 Hz, 2H), 7.07 (t, J = 8.7 Hz, 2H), 3.66 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 162.60 (d, $^{1}J_{CF}$ = 246.5 HZ), 137.32, 136.60, 135.04, 132.90 (d, $^{3}J_{CF}$ = 8.1 HZ), 129.87, 129.20, 128.39, 128.29, 126.92, 125.67, 122.36, 120.32, 119.67, 115.60 (d, $^{2}J_{CF}$ = 21.4 HZ), 109.61, 30.92. **HRMS** (ESI) calcd. for $C_{21}H_{17}NF$ $(M+H)^+$: 302.1263, found: 302.1260.

2-(3-fluorophenyl)-1-methyl-3-phenyl-1H-indole (2q)



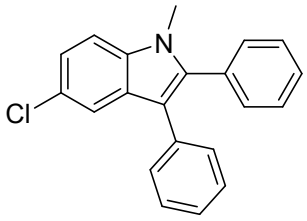
Yield: 69% (62.3 mg). White solid. m.p. 124 – 125 °C. **^{1}H NMR** (400 MHz, CDCl3) δ 7.77 (d, J = 7.9 Hz, 1H), 7.40 (d, J = 8.2 Hz, 1H), 7.38 – 7.22 (m, 6H), 7.23 – 7.13 (m, 2H), 7.09 (d, J = 7.7 Hz, 1H), 7.05 (t, J = 9.0 Hz, 2H), 3.66 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 162.60 (d, $^{1}J_{CF}$ = 245.4 HZ), 137.49, 136.20, 134.86, 134.14 (d, $^{3}J_{CF}$ = 8.1 HZ), 130.01 (d, $^{3}J_{CF}$ = 8.7 HZ), 129.91, 128.83, 127.06 (d, $^{4}J_{CF}$ = 2.8 HZ), 126.98, 125.85, 122.58, 120.41, 119.83, 118.03 (d, $^{2}J_{CF}$ = 21.5 HZ), 115.78, 115.12 (d, $^{2}J_{CF}$ = 20.9 HZ), 109.68, 31.02. **HRMS** (ESI) calcd. for $C_{21}H_{17}NF$ $(M+H)^+$: 302.1263, found: 302.1265.

4-(5-chloro-1-methyl-3-phenyl-1H-indol-2-yl)benzonitrile (2r)



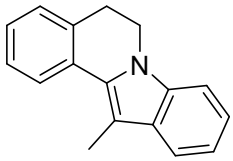
Yield: 77% (79.2 mg). White solid. m.p. 161 – 162 °C. **^{1}H NMR** (400 MHz, CDCl3) δ 7.77 – 7.69 (m, 2H), 7.59 (td, J = 7.7, 1.1 Hz, 1H), 7.49 (td, J = 7.7, 1.0 Hz, 1H), 7.40 (d, J = 7.7 Hz, 1H), 7.33 (d, J = 8.7 Hz, 1H), 7.30 – 7.24 (m, 3H), 7.24 – 7.17 (m, 3H), 3.63 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 136.10, 135.54, 134.31, 133.73, 133.36, 132.83, 132.70, 129.67, 129.15, 128.52, 127.79, 126.38, 123.33, 119.44, 117.46, 117.42, 114.87, 110.94, 31.09. **HRMS** (ESI) calcd. for $C_{22}H_{16}N_2Cl$ $(M+H)^+$: 343.0920, found: 343.0921.

5-chloro-1-methyl-2,3-diphenyl-1H-indole (2s)



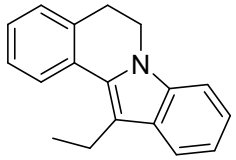
Yield: 70% (66.7 mg). White solid. m.p. 130 – 131 °C. **^{1}H NMR** (400 MHz, CDCl3) δ 7.77 (d, J = 1.9 Hz, 1H), 7.45 – 7.39 (m, 3H), 7.38 – 7.32 (m, 3H), 7.31 (s, 1H), 7.30 – 7.25 (m, 4H), 7.25 – 7.19 (m, 1H), 3.69 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 138.96, 135.76, 134.56, 131.43, 131.06, 129.77, 128.49, 128.34, 128.32, 128.04, 125.98, 125.85, 122.38, 119.02, 114.87, 110.63, 31.13. **HRMS** (ESI) calcd. for $C_{21}H_{17}NCl$ $(M+H)^+$: 318.0967, found: 318.0965.

12-methyl-5,6-dihydroindolo[2,1-a]isoquinoline (2aa)



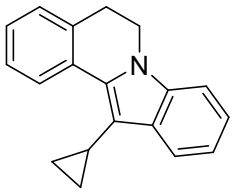
Yield: 82% (57.3 mg). White solid. m.p. 149 – 151 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.83 (d, J = 7.8 Hz, 1H), 7.60 (d, J = 7.5 Hz, 1H), 7.32 (t, J = 7.5 Hz, 1H), 7.25 (t, J = 6.7 Hz, 2H), 7.19 (t, J = 7.3 Hz, 2H), 7.10 (t, J = 7.4 Hz, 1H), 4.16 (t, J = 6.3 Hz, 2H), 3.07 (t, J = 6.3 Hz, 2H), 2.61 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 135.37, 133.55, 130.75, 130.38, 129.46, 128.43, 127.16, 126.65, 125.62, 121.99, 119.08, 118.93, 108.66, 107.23, 40.15, 30.28, 10.86. **HRMS** (ESI) calcd. for $C_{17}H_{16}N$ $(M+H)^+$: 234.1200, found: 234.1207;

12-ethyl-5,6-dihydroindolo[2,1-a]isoquinoline (2ab)



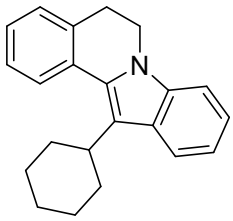
Yield: 84% (61.5 mg). White solid. m.p. 135 – 137 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.80 (d, J = 7.8 Hz, 1H), 7.64 (d, J = 7.9 Hz, 1H), 7.35 (t, J = 7.5 Hz, 1H), 7.29 (t, J = 7.1 Hz, 2H), 7.24 – 7.19 (m, 2H), 7.10 (t, J = 7.4 Hz, 1H), 4.21 (t, J = 6.3 Hz, 2H), 3.16 – 3.02 (m, 4H), 1.39 (t, J = 7.5 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 135.40, 133.68, 130.17, 130.07, 128.56, 128.43, 127.25, 126.70, 125.36, 121.96, 119.01, 118.88, 114.29, 108.70, 40.09, 30.23, 18.40, 15.22. **HRMS** (ESI) calculated for $C_{18}H_{18}N$ $(M+H)^+$: 248.1357, found : 248.1356.

12-cyclopropyl-5,6-dihydroindolo[2,1-a]isoquinoline (2ac)



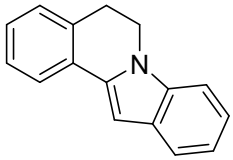
Yield: 74% (57.5 mg). White solid. m.p. 175 – 177 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.30 (d, J = 7.9 Hz, 1H), 7.84 (d, J = 7.9 Hz, 1H), 7.40 – 7.32 (m, 1H), 7.28 (d, J = 8.2 Hz, 1H), 7.26 – 7.23 (m, 1H), 7.22 (dd, J = 4.2, 1.0 Hz, 1H), 7.19 (dd, J = 8.1, 1.1 Hz, 1H), 7.14 – 7.04 (m, 1H), 4.19 (t, J = 6.4 Hz, 2H), 3.11 (t, J = 6.4 Hz, 2H), 2.11 – 2.05 (m, 1H), 1.14 – 1.03 (m, 2H), 0.75 – 0.60 (m, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 135.15, 133.29, 132.79, 129.58, 128.05, 126.89, 126.81, 121.83, 119.92, 119.17, 113.07, 108.73, 40.13, 29.98, 7.76, 6.73. **HRMS** (ESI) calcd. for $C_{19}H_{18}N$ $(M+H)^+$: 260.1357, found: 260.1357.

12-cyclohexyl-5,6-dihydroindolo[2,1-a]isoquinoline (2ad)



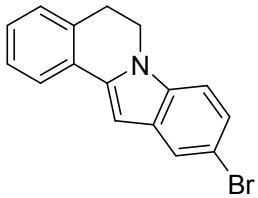
Yield: 78% (70.5 mg). White solid. m.p. 187 – 189 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.89 (d, J = 8.1 Hz, 1H), 7.70 (d, J = 7.8 Hz, 1H), 7.37 (d, J = 7.5 Hz, 1H), 7.30 (d, J = 7.8 Hz, 2H), 7.24 (t, J = 7.4 Hz, 1H), 7.18 (t, J = 7.6 Hz, 1H), 7.05 (t, J = 7.5 Hz, 1H), 4.16 (t, J = 6.0 Hz, 2H), 3.35 (t, J = 12.2 Hz, 1H), 3.08 (t, J = 6.0 Hz, 2H), 2.27 – 2.07 (m, 2H), 1.93 (t, J = 11.8 Hz, 4H), 1.84 (s, 1H), 1.51 – 1.38 (m, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 135.84, 134.63, 130.39, 129.89, 128.33, 127.19, 127.17, 126.76, 126.08, 121.64, 121.49, 118.43, 117.91, 108.91, 40.11, 37.28, 33.09, 30.57, 27.37, 26.46. **HRMS** (ESI) calculated for $C_{22}H_{24}N$ $(M+H)^+$: 302.1826, found : 302.1822.

5,6-dihydroindolo[2,1-a]isoquinoline (2ae)



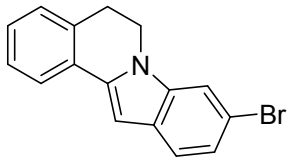
Yield: 72% (47.4 mg). White solid. m.p. 168 – 169 °C. **^{1}H NMR** (400 MHz, CDCl3) δ 7.76 (d, J = 7.6 Hz, 1H), 7.63 (d, J = 7.9 Hz, 1H), 7.32 (t, J = 8.0 Hz, 1H), 7.28 (d, J = 5.7 Hz, 1H), 7.26 – 7.17 (m, 3H), 7.10 (t, J = 7.4 Hz, 1H), 6.87 (s, 1H), 4.26 (t, J = 6.5 Hz, 2H), 3.19 (t, J = 6.5 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 136.66, 135.62, 132.17, 129.03, 128.80, 128.31, 127.42, 127.26, 124.39, 121.68, 120.75, 119.88, 108.96, 96.44, 40.11, 29.18. **HRMS** (ESI) calculated for $C_{16}H_{14}N$ $(M+H)^+$: 220.1044, found : 220.1042.

10-bromo-5,6-dihydroindolo[2,1-a]isoquinoline (2af)



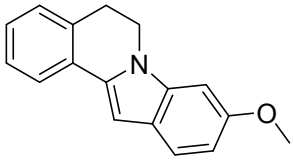
Yield: 73% (65.3 mg). Pale yellow solid. m.p. 176 – 178 °C. **^{1}H NMR** (400 MHz, CDCl3) δ 7.73 (s, 2H), 7.35 – 7.23 (m, 4H), 7.18 (d, J = 8.6 Hz, 1H), 6.78 (s, 1H), 4.21 (t, J = 6.4 Hz, 2H), 3.19 (t, J = 6.5 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 136.72, 135.33, 132.15, 130.42, 128.49, 128.38, 127.90, 127.38, 124.54, 124.40, 123.07, 113.02, 110.38, 95.89, 40.25, 29.00. **HRMS** (ESI) calcd. for $C_{16}H_{13}NBr$ $(M+H)^+$: 298.0149, found: 298.0151.

9-bromo-5,6-dihydroindolo[2,1-a]isoquinoline (2ag)



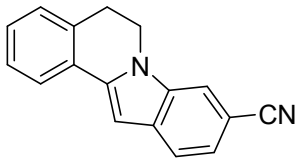
Yield: 75% (67.1 mg). Pale yellow solid. m.p. 150 – 151 °C. **^{1}H NMR** (400 MHz, CDCl3) δ 7.73 (s, 2H), 7.37 – 7.21 (m, 4H), 7.17 (d, J = 8.5 Hz, 1H), 6.78 (s, 1H), 4.20 (t, J = 5.9 Hz, 2H), 3.18 (t, J = 6.2 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 137.49, 136.29, 132.09, 128.58, 128.37, 127.77, 127.64, 127.37, 124.45, 123.12, 121.86, 115.13, 112.07, 96.55, 40.24, 29.03. **HRMS** (ESI) calcd. for $C_{16}H_{13}NBr$ $(M+H)^+$: 298.0149, found: 298.0150.

9-methoxy-5,6-dihydroindolo[2,1-a]isoquinoline (2ah)



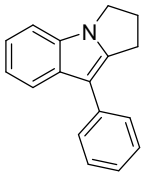
Yield: 71% (53.0 mg). White solid. m.p. 168 – 170 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.75 (d, J = 7.6 Hz, 1H), 7.55 (d, J = 8.5 Hz, 1H), 7.37 – 7.30 (m, 1H), 7.30 – 7.26 (m, 1H), 7.24 (d, J = 7.1 Hz, 1H), 6.89 – 6.76 (m, 3H), 4.23 (t, J = 6.5 Hz, 2H), 3.93 (s, 3H), 3.22 (t, J = 6.4 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 156.41, 137.44, 134.78, 131.66, 129.27, 128.26, 127.21, 126.91, 123.89, 123.15, 121.37, 109.87, 96.41, 92.69, 55.76, 40.15, 29.20. **HRMS** (ESI) calcd. for $C_{17}H_{16}NO$ $(M+H)^+$: 250.1151, found: 250.1150.

5,6-dihydroindolo[2,1-a]isoquinoline-9-carbonitrile (2ai)



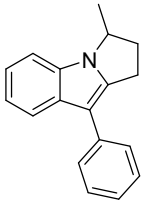
Yield: 76% (55.6 mg). White solid. m.p. 189 – 190 °C. **^{1}H NMR** (400 MHz, CDCl3) δ 7.76 (d, J = 7.3 Hz, 1H), 7.70 – 7.59 (m, 2H), 7.35 – 7.30 (m, 4H), 6.89 (s, 1H), 4.26 (t, J = 6.6 Hz, 2H), 3.22 (t, J = 6.6 Hz, 2H). **^{13}C NMR** (100 MHz, CDCl3) δ 139.33, 135.50, 132.49, 131.94, 128.71, 128.48, 127.81, 127.54, 124.93, 122.83, 121.23, 120.89, 113.72, 103.61, 97.14, 40.36, 28.80. HRMS (ESI) calcd. for $C_{17}H_{13}N_2$ $(M+H)^+$: 245.0996, found: 245.0994.

9-phenyl-2,3-dihydro-1H-pyrrolo[1,2-a]indole (2aj)



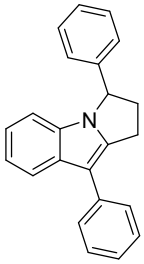
Yield: 56% (39.1 mg). White solid. m.p. 109 – 111 °C. **^{1}H NMR** (400 MHz, CDCl3) δ 7.92 (d, J = 7.9 Hz, 1H), 7.66 (d, J = 7.8 Hz, 2H), 7.47 (t, J = 7.7 Hz, 2H), 7.30 (dd, J = 13.0, 5.5 Hz, 2H), 7.20 (dt, J = 16.0, 5.3 Hz, 2H), 4.16 (t, J = 7.0 Hz, 2H), 3.24 (t, J = 7.4 Hz, 2H), 2.78 – 2.62 (m, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 142.11, 136.31, 132.95, 130.60, 128.68, 127.37, 124.94, 120.78, 119.73, 119.54, 109.63, 107.84, 43.77, 27.70, 24.83. **HRMS** (ESI) calcd. for $C_{17}H_{16}N$ $(M+H)^+$: 234.1200, found: 234.1202.

3-methyl-9-phenyl-2,3-dihydro-1H-pyrrolo[1,2-a]indole (2ak)



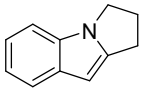
Yield: 75% (55.6 mg). Colourless oil. **^{1}H NMR** (400 MHz, CDCl3) δ 7.93 (d, J = 7.1 Hz, 1H), 7.67 (d, J = 7.1 Hz, 2H), 7.48 (t, J = 7.7 Hz, 2H), 7.40 (d, J = 7.2 Hz, 1H), 7.28 (d, J = 6.5 Hz, 1H), 7.20 (tt, J = 12.9, 3.5 Hz, 2H), 4.76 – 4.60 (m, 1H), 3.29 (ddd, J = 15.8, 8.5, 7.1 Hz, 1H), 3.17 (ddd, J = 16.3, 8.9, 5.0 Hz, 1H), 2.95 – 2.77 (m, 1H), 2.30 (ddd, J = 13.0, 8.9, 4.7 Hz, 1H), 1.61 (d, J = 6.4 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 141.77, 136.30, 132.35, 130.89, 128.66, 127.45, 124.93, 120.63, 119.61, 109.70, 107.57, 52.68, 36.10, 23.77, 20.34. **HRMS** (ESI) calcd. for $C_{18}H_{18}N$ $(M+H)^+$: 248.1357, found: 248.1358.

3,9-diphenyl-2,3-dihydro-1H-pyrrolo[1,2-a]indole (2al)



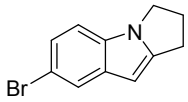
Yield: 77% (71.4 mg). White solid. m.p. 150 – 151 °C. **^{1}H NMR** (400 MHz, CDCl3) δ 7.90 (d, J = 8.0 Hz, 1H), 7.68 (d, J = 7.5 Hz, 2H), 7.46 (t, J = 7.7 Hz, 2H), 7.36 – 7.28 (m, 3H), 7.24 (d, J = 5.4 Hz, 1H), 7.15 (d, J = 6.5 Hz, 2H), 7.10 (t, J = 7.6 Hz, 1H), 6.99 (t, J = 7.5 Hz, 1H), 6.80 (d, J = 8.1 Hz, 1H), 5.46 (dd, J = 7.6, 5.5 Hz, 1H), 3.42 – 3.28 (m, 1H), 3.25 – 3.15 (m, 1H), 3.13 – 2.98 (m, 1H), 2.53 (ddd, J = 18.5, 8.6, 5.6 Hz, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 142.33, 141.13, 136.18, 132.69, 131.04, 128.93, 128.75, 127.88, 127.50, 126.26, 125.11, 120.80, 119.91, 119.55, 110.49, 108.05, 60.85, 38.93, 24.14. **HRMS** (ESI) calcd. for $C_{23}H_{20}N$ $(M+H)^+$: 310.1513, found: 310.1512.

2,3-dihydro-1H-pyrrolo[1,2-a]indole (2am)



Yield: 47% (22.1 mg). White solid. m.p. 77 – 78 °C. **^{1}H NMR** (400 MHz, CDCl3) δ 7.57 (d, J = 7.8 Hz, 1H), 7.27 (d, J = 8.0 Hz, 1H), 7.14 (t, J = 7.0 Hz, 1H), 7.08 (t, J = 7.0 Hz, 1H), 6.19 (s, 1H), 4.09 (t, J = 7.0 Hz, 2H), 3.05 (t, J = 7.4 Hz, 2H), 2.71 – 2.55 (m, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 144.61, 133.30, 132.70, 120.33, 120.14, 119.13, 109.41, 92.31, 43.62, 27.88, 24.32. **HRMS** (ESI) calcd. for $C_{11}H_{12}N$ $(M+H)^+$: 158.0887, found: 158.0885.

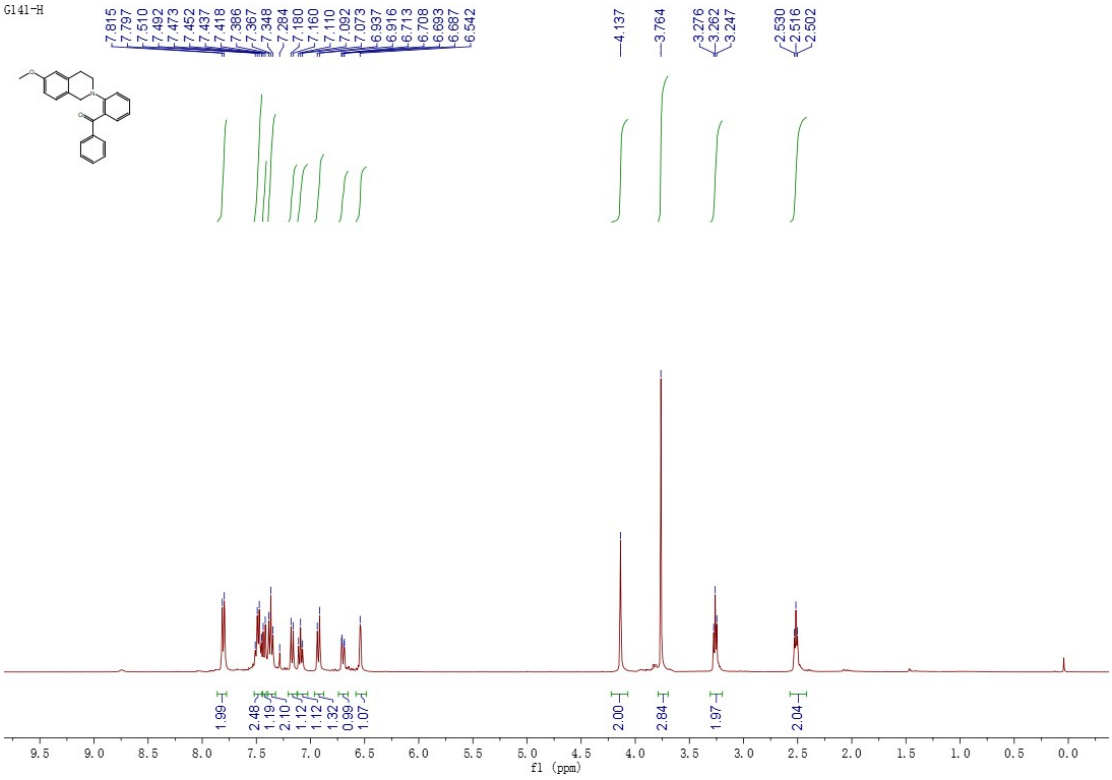
7-bromo-2,3-dihydro-1H-pyrrolo[1,2-a]indole (2an)

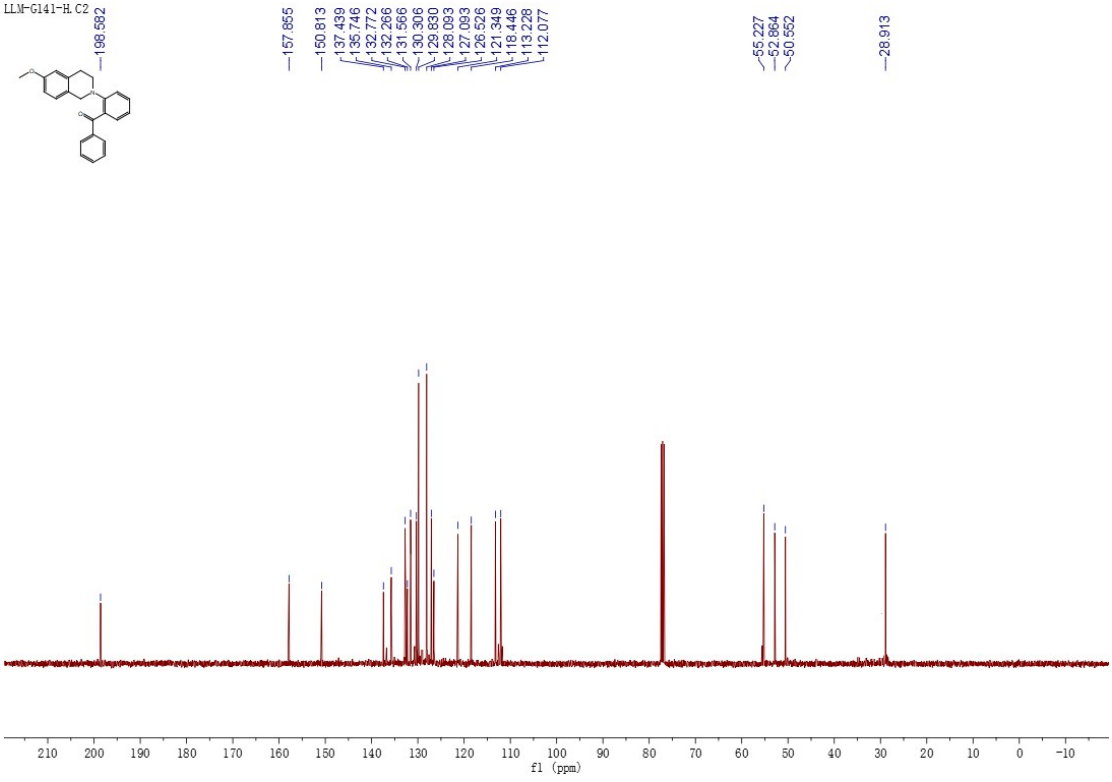


Yield: 45% (31.8 mg). Pale white solid. m.p. 88 – 89 °C. **^{1}H NMR** (400 MHz, CDCl3) δ 7.64 (s, 1H), 7.17 (d, J = 8.5 Hz, 1H), 7.07 (d, J = 8.5 Hz, 1H), 6.09 (s, 1H), 4.02 (t, J = 6.9 Hz, 2H), 3.00 (t, J = 7.4 Hz, 2H), 2.71 – 2.52 (m, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 145.99, 134.87, 131.33, 122.84, 122.71, 112.38, 110.71, 92.14, 43.81, 27.79, 24.39. **HRMS** (ESI) calcd. for $C_{11}H_{11}NBr$ $(M+H)^+$: 235.9993, found: 235.9996.

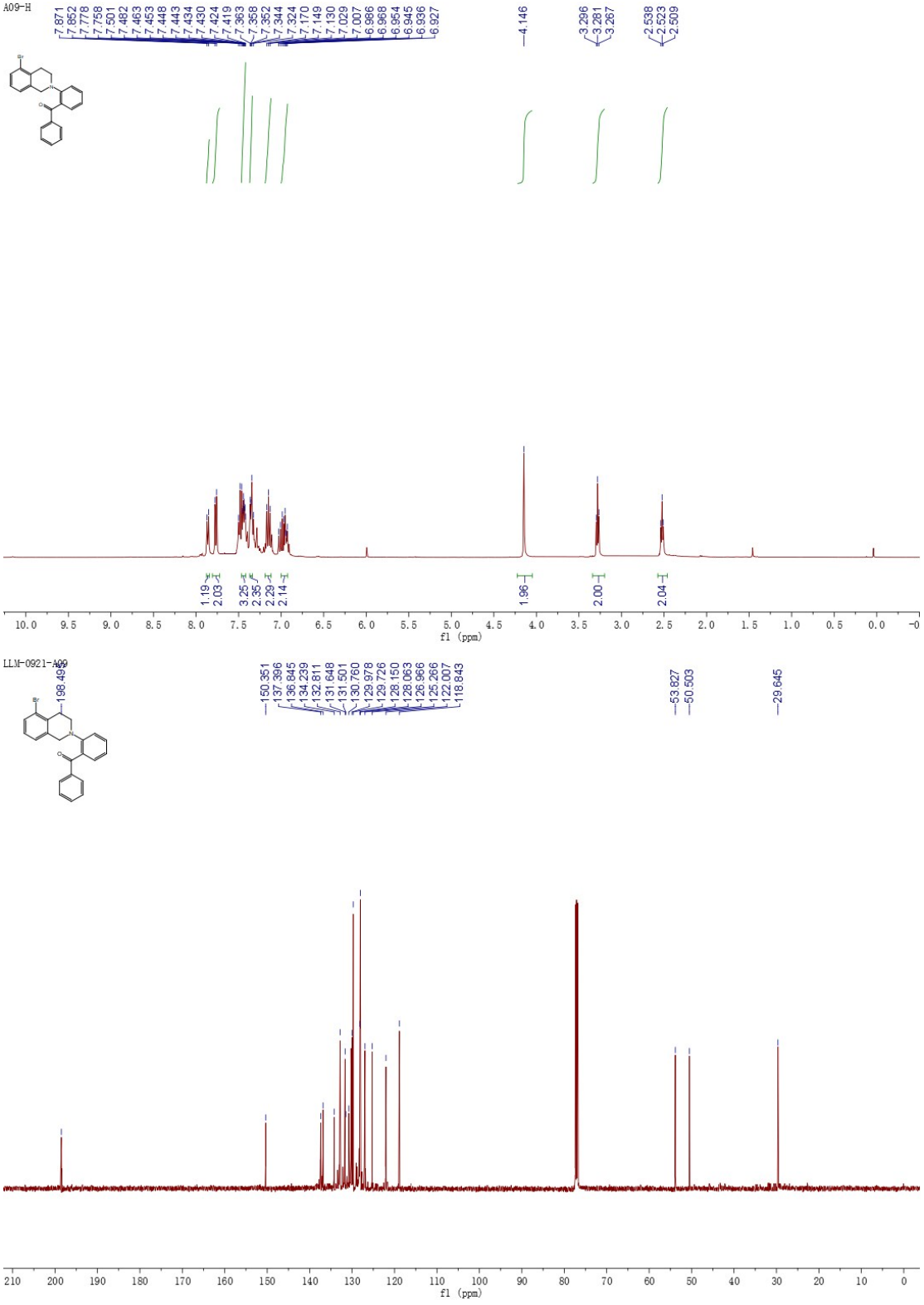
9. ^{1}H and ^{13}C NMR Spectra

NMR of 1b

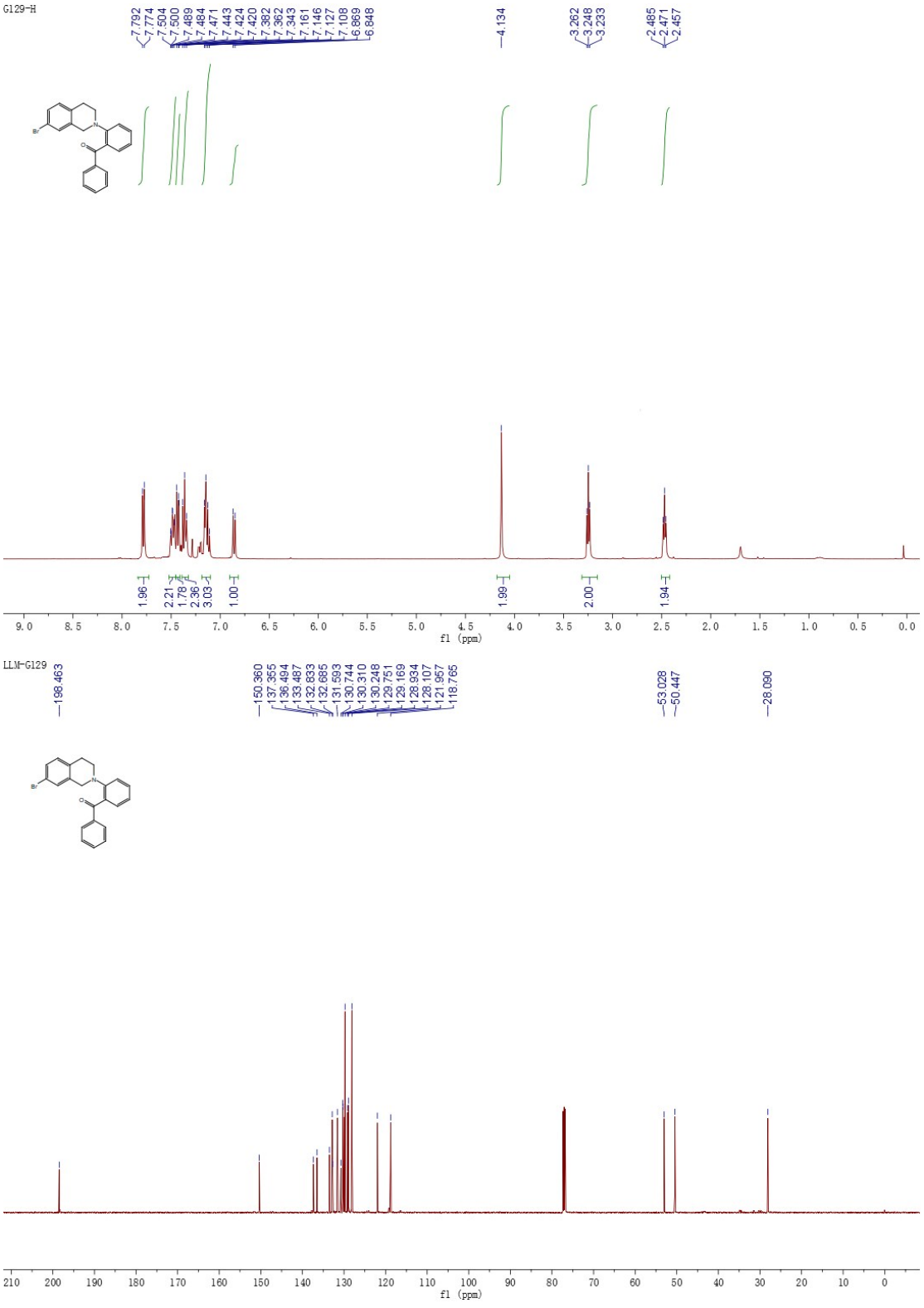




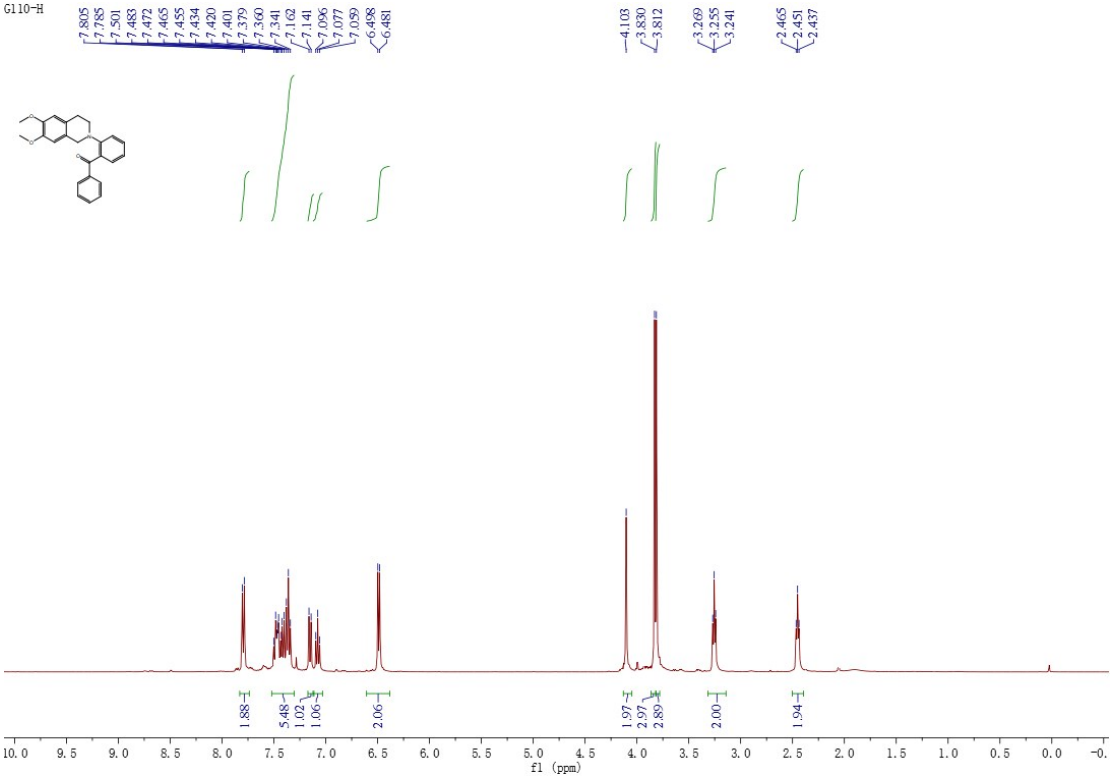
NMR of 1c

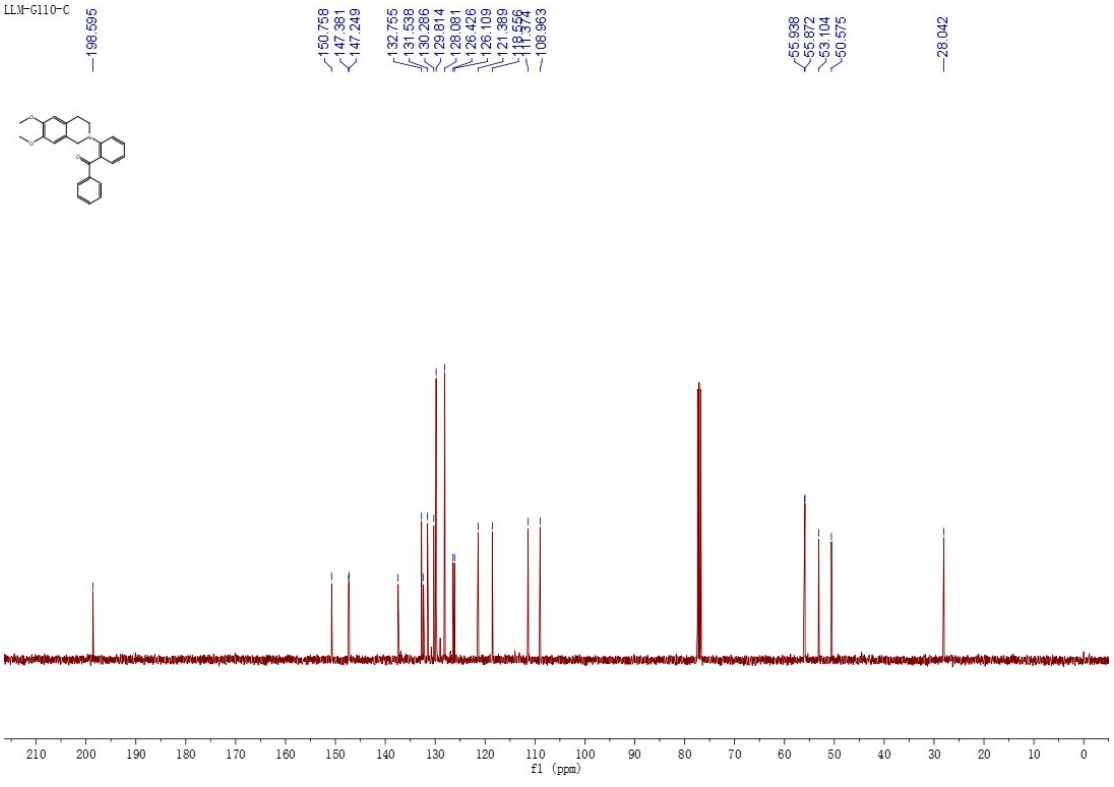

A09-H
7.871
7.852
7.778
7.758
7.501
7.482
7.463
7.453
7.448
7.443
7.434
7.430
7.424
7.419
7.363
7.358
7.352
7.344
7.324
7.170
7.149
7.130
7.029
7.007
6.986
6.968
6.954
6.945
6.936
6.927
4.146
3.296
3.281
3.267
2.538
2.523
2.509
1.19
2.03
3.25
2.35
2.29
2.14
1.96
2.00
2.04
f1 (ppm)
LLM-0921-A09
198.499
150.351
137.396
136.845
134.239
132.811
131.648
131.501
130.760
129.978
129.726
128.150
128.063
126.966
125.266
122.007
118.843
53.827
50.503
29.645
f1 (ppm)

NMR of 1d

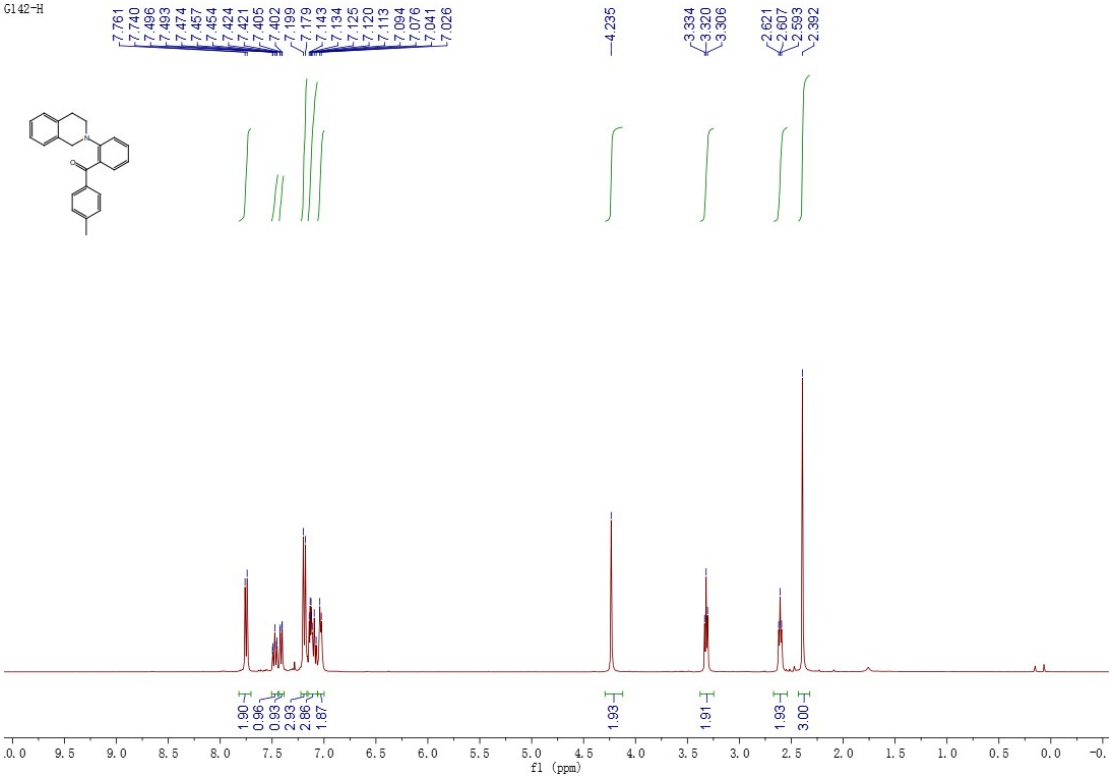

G129-H
7.792
7.774
7.504
7.500
7.489
7.484
7.471
7.443
7.424
7.420
7.382
7.362
7.343
7.161
7.146
7.127
7.108
6.869
6.848
4.134
3.262
3.248
3.233
2.485
2.471
2.457
1.96
2.21
1.78
2.36
3.03
1.00
1.99
2.00
1.94
f1 (ppm)
LLM-G129
198.463
150.360
137.355
136.494
133.487
132.833
132.685
131.593
130.744
130.310
130.248
129.751
129.169
128.934
128.107
121.957
118.765
53.028
50.447
28.090
f1 (ppm)

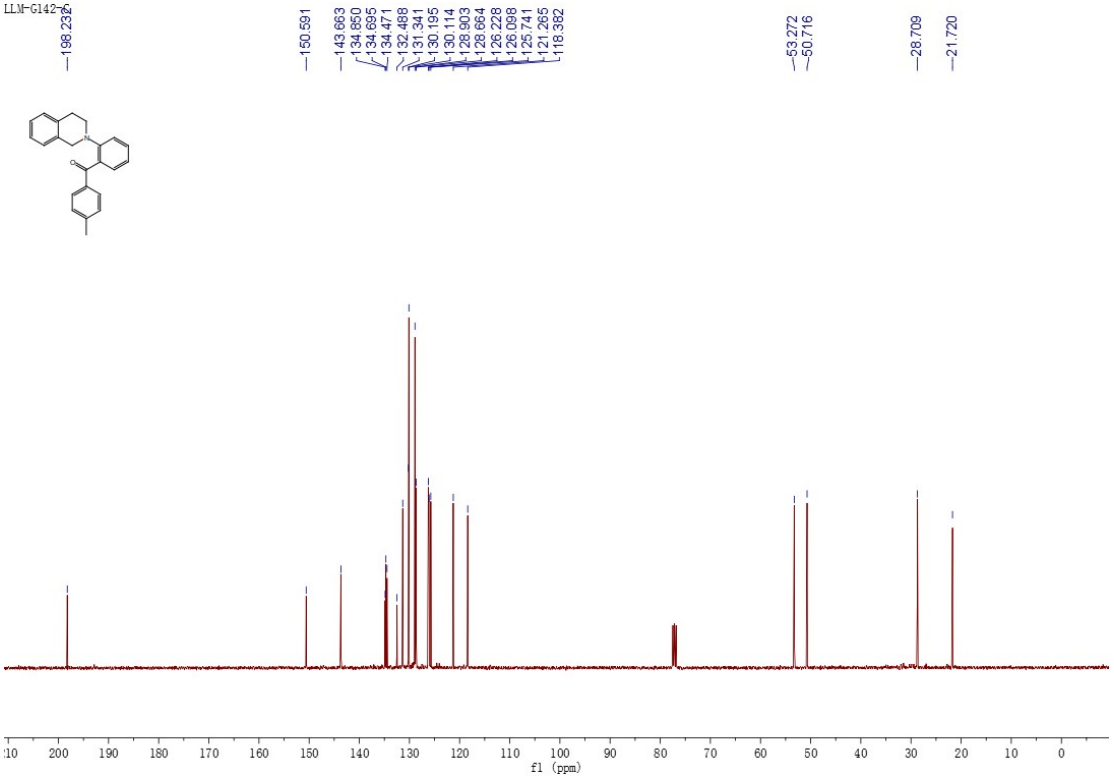
NMR of 1e


G110-H
7.805
7.785
7.501
7.483
7.472
7.465
7.455
7.434
7.420
7.401
7.379
7.360
7.341
7.162
7.141
7.096
7.077
7.059
6.498
6.481
4.103
3.830
3.812
3.269
3.255
3.241
2.465
2.451
2.437
1.88
5.48
1.02
1.06
2.06
1.97
2.97
2.89
2.00
1.94
f1 (ppm)

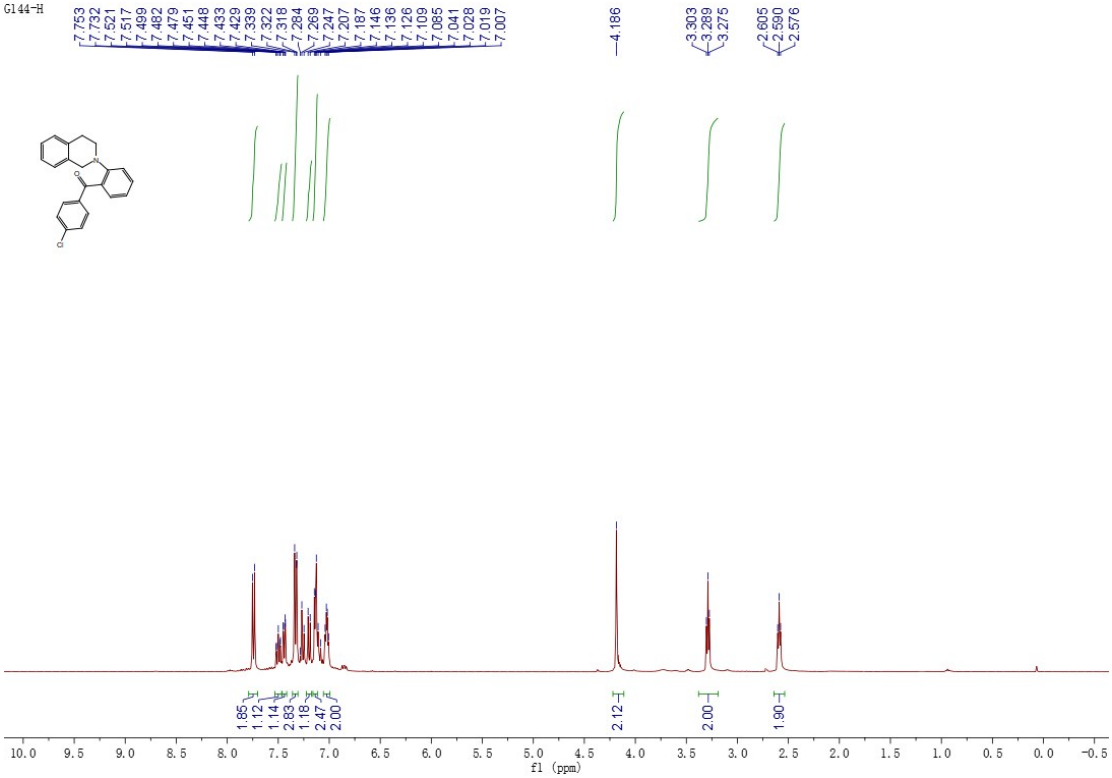

LLM-G110-C
198.595
150.758
147.381
147.249
132.755
131.538
130.286
129.814
128.081
126.426
126.109
121.389
118.556
117.374
108.963
55.938
55.872
53.104
50.575
28.042
f1 (ppm)

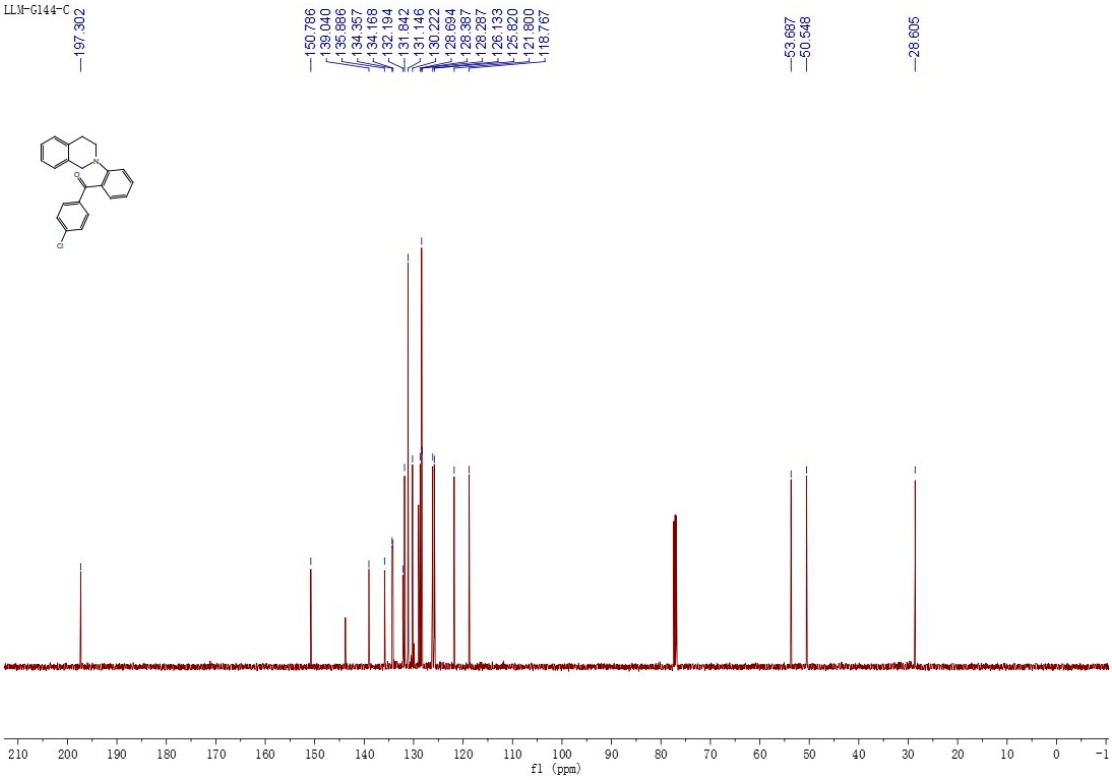
NMR of 1f


G142-H
7.761
7.740
7.496
7.493
7.474
7.457
7.454
7.424
7.421
7.405
7.402
7.199
7.179
7.143
7.134
7.125
7.120
7.113
7.094
7.076
7.041
7.026
4.235
3.334
3.320
3.306
2.621
2.607
2.593
2.392
1.90
0.96
0.93
2.93
2.86
1.87
1.93
1.91
1.93
3.00
f1 (ppm)

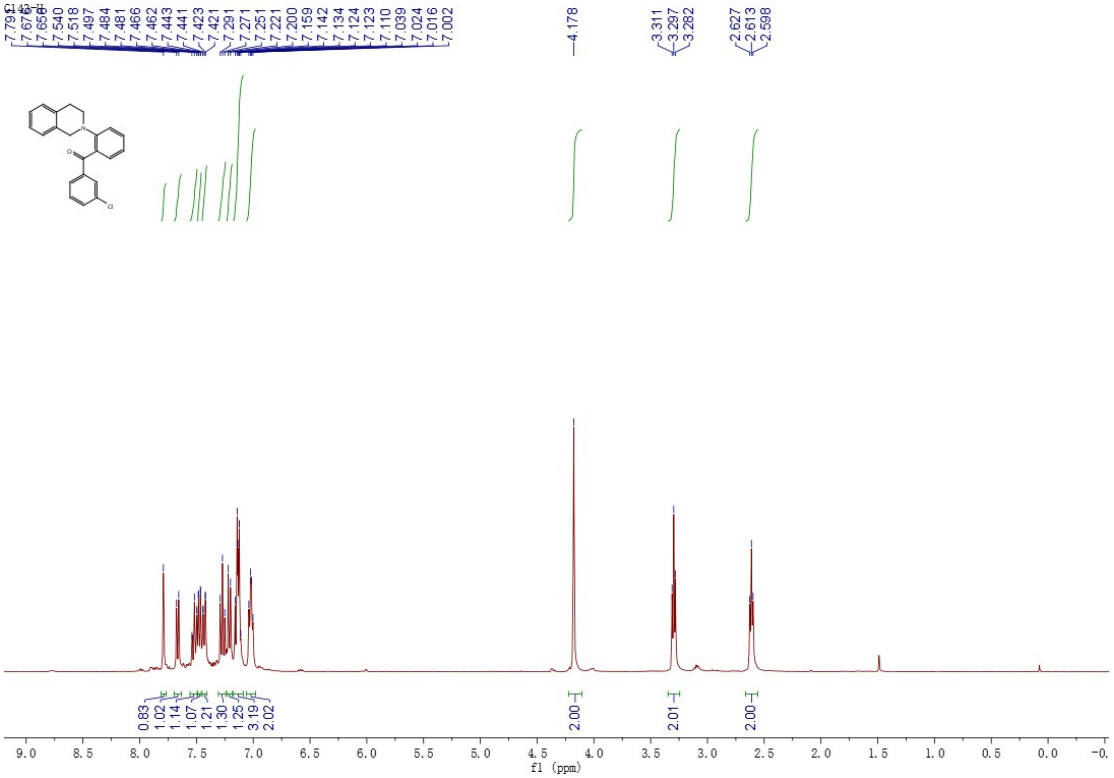

LLM-G142-C
198.232
150.591
143.663
134.850
134.695
134.471
132.488
131.341
130.195
130.114
128.903
128.664
126.228
126.098
125.741
121.265
118.382
53.272
50.716
28.709
21.720
f1 (ppm)

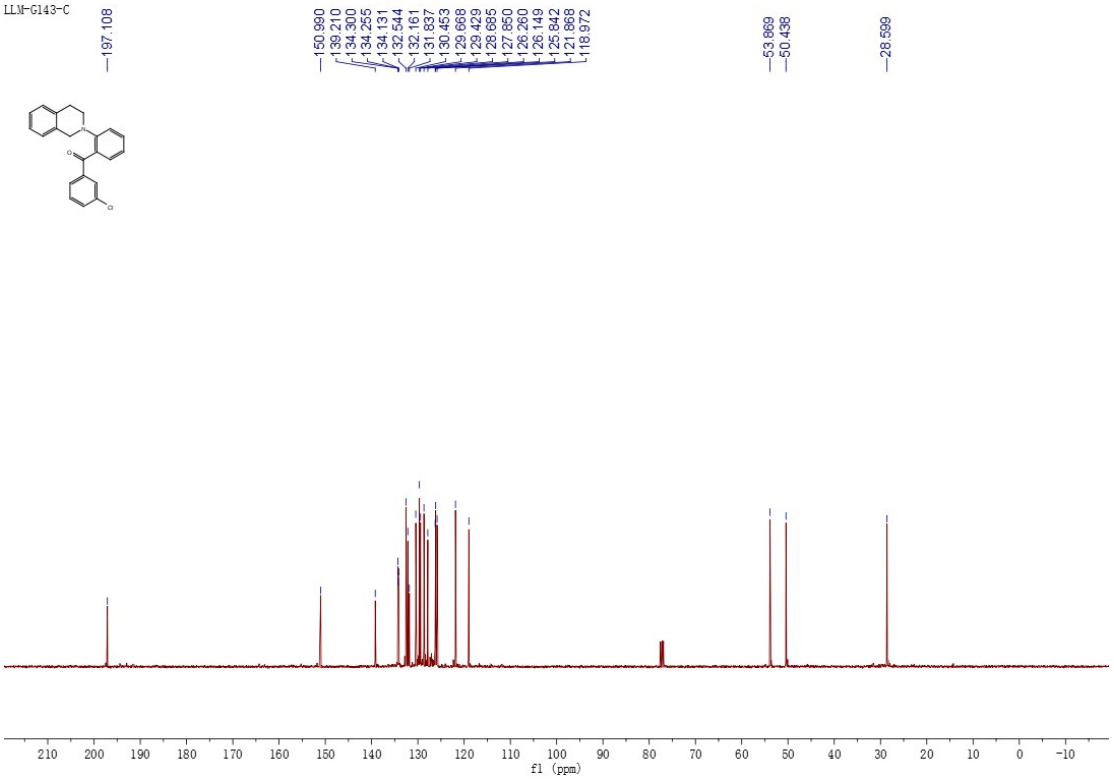
NMR of 1g


G144-H
7.753
7.732
7.521
7.517
7.499
7.482
7.479
7.451
7.448
7.433
7.429
7.339
7.322
7.318
7.284
7.269
7.247
7.207
7.187
7.146
7.136
7.126
7.109
7.085
7.041
7.028
7.019
7.007
4.186
3.303
3.289
3.275
2.605
2.590
2.576
1.85
1.12
1.14
2.83
1.18
2.47
2.00
2.12
2.00
1.90
f1 (ppm)

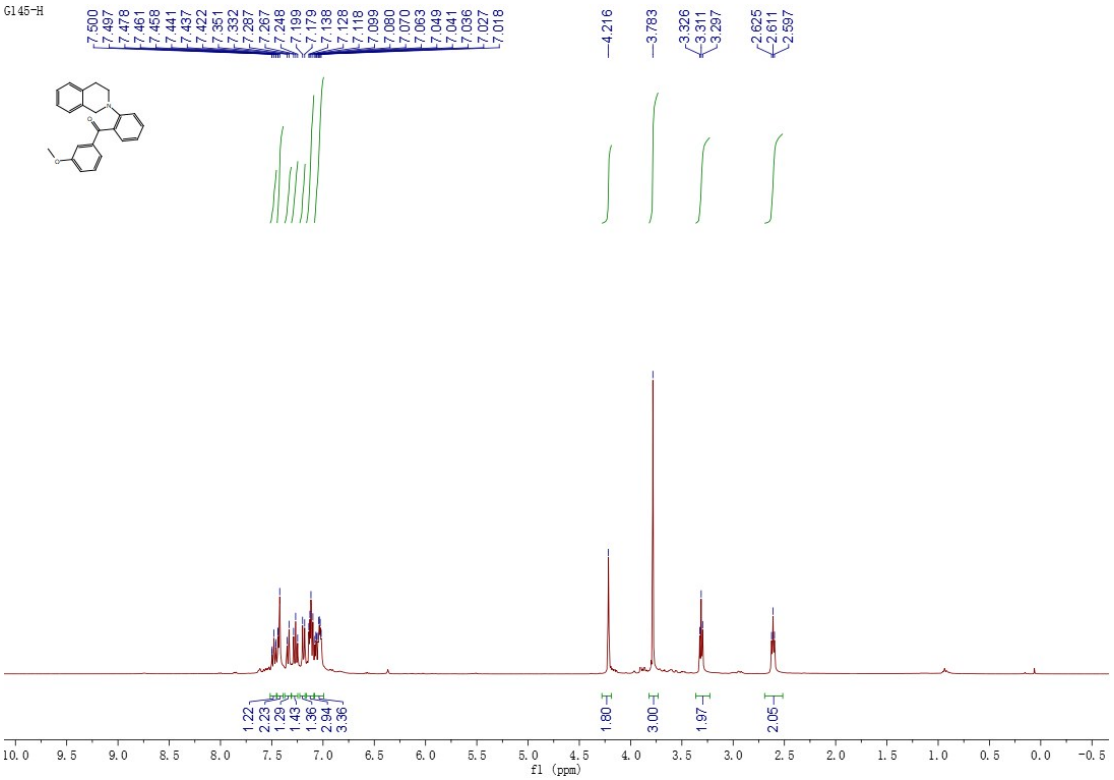

LLM-G144-C
197.302
150.786
139.040
135.886
134.357
134.168
132.194
131.842
131.146
130.222
128.694
128.387
128.287
126.133
125.820
121.800
118.767
53.687
50.548
28.605
f1 (ppm)

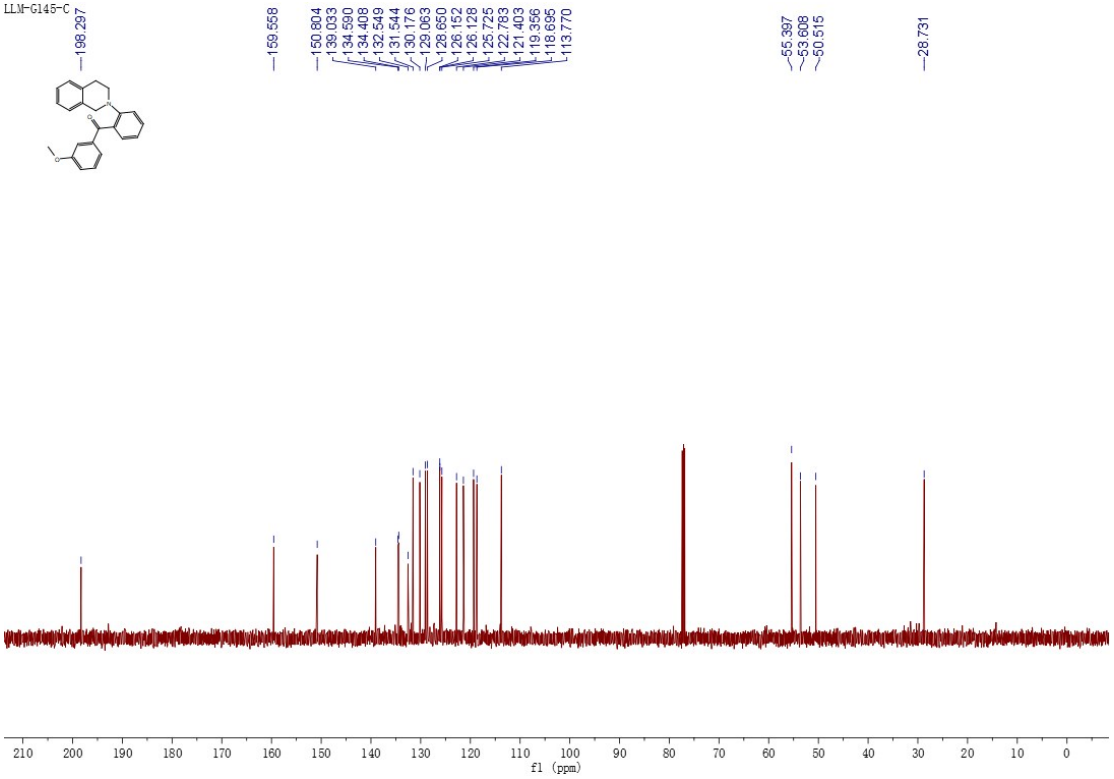
NMR of 1h


LLM-G143-H
7.914
7.678
7.656
7.540
7.518
7.497
7.484
7.481
7.466
7.462
7.443
7.441
7.423
7.421
7.291
7.271
7.251
7.221
7.200
7.159
7.142
7.134
7.124
7.123
7.110
7.039
7.024
7.016
7.002
4.178
3.311
3.297
3.282
2.627
2.613
2.598
0.83
1.02
1.14
1.07
1.21
1.30
1.25
3.19
2.02
2.00
2.01
2.00
f1 (ppm)

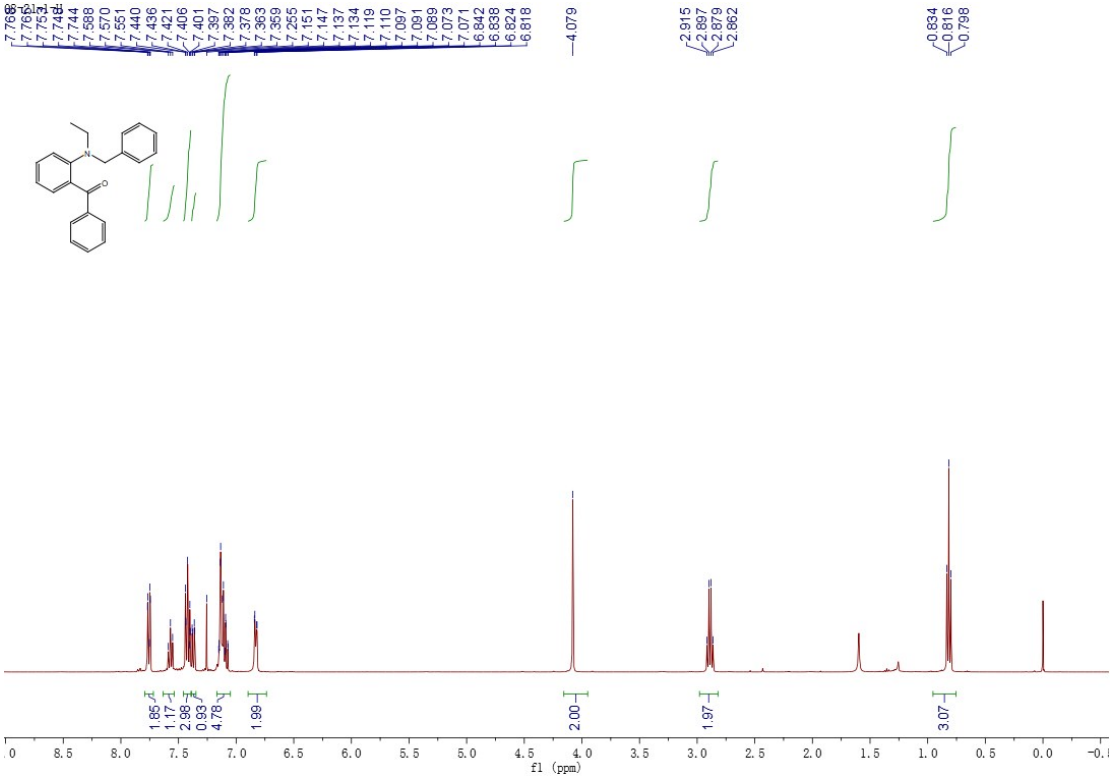

LLM-G143-C
197.108
150.990
139.210
134.300
134.255
134.131
132.544
132.161
131.837
130.453
129.668
129.429
128.685
127.850
126.260
126.149
125.842
121.868
118.972
53.869
50.438
28.599
f1 (ppm)

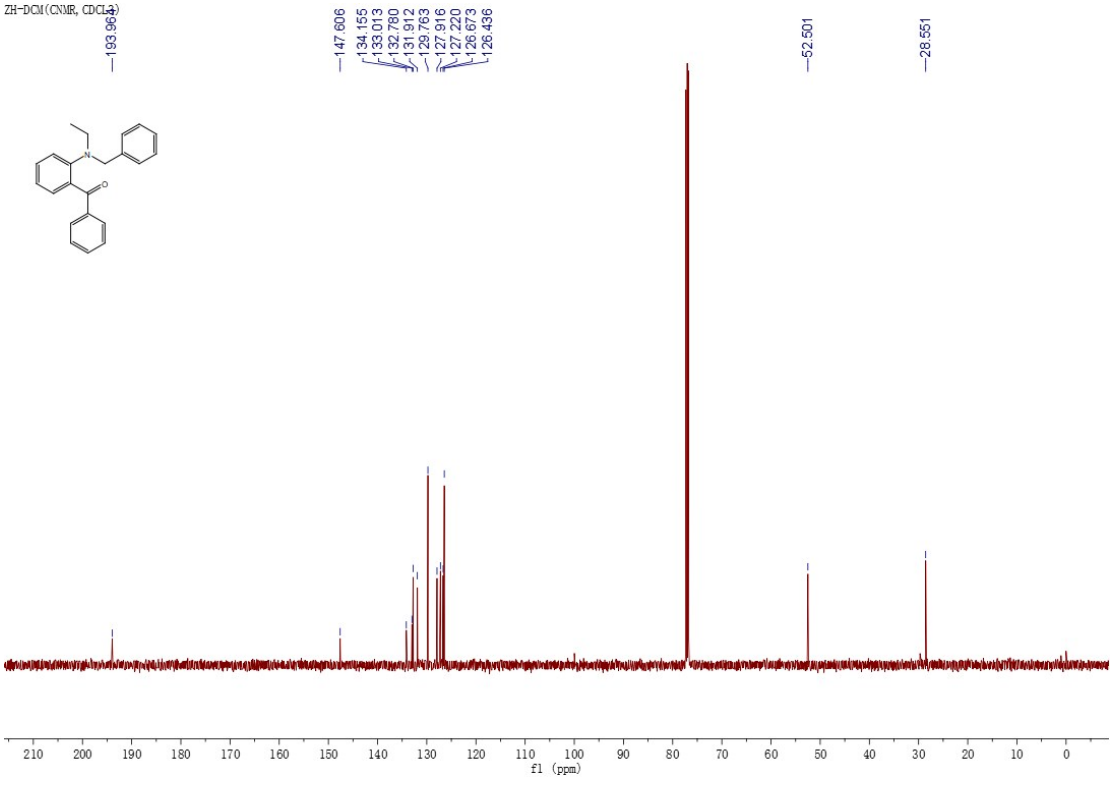
NMR of 1i


G145-H
7.500
7.497
7.478
7.461
7.458
7.441
7.437
7.422
7.351
7.332
7.287
7.267
7.248
7.199
7.179
7.138
7.128
7.118
7.099
7.080
7.070
7.063
7.049
7.041
7.036
7.027
7.018
4.216
3.783
3.326
3.311
3.297
2.625
2.611
2.597
1.22
2.23
1.29
1.43
1.36
2.94
3.36
1.80
3.00
1.97
2.05
f1 (ppm)

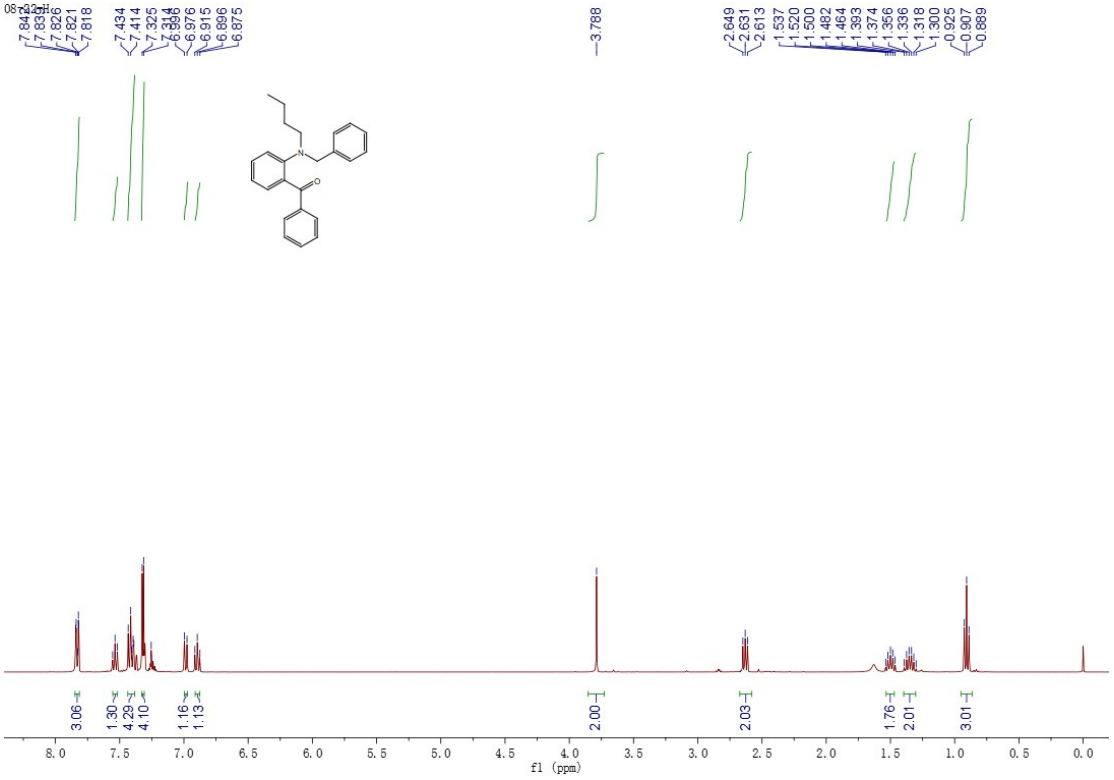

LLM-G145-C
198.297
159.558
150.804
139.033
134.590
134.408
132.549
131.544
130.176
129.063
128.650
126.152
126.128
125.725
122.783
121.403
119.396
118.695
113.770
55.397
53.608
50.515
28.731
f1 (ppm)

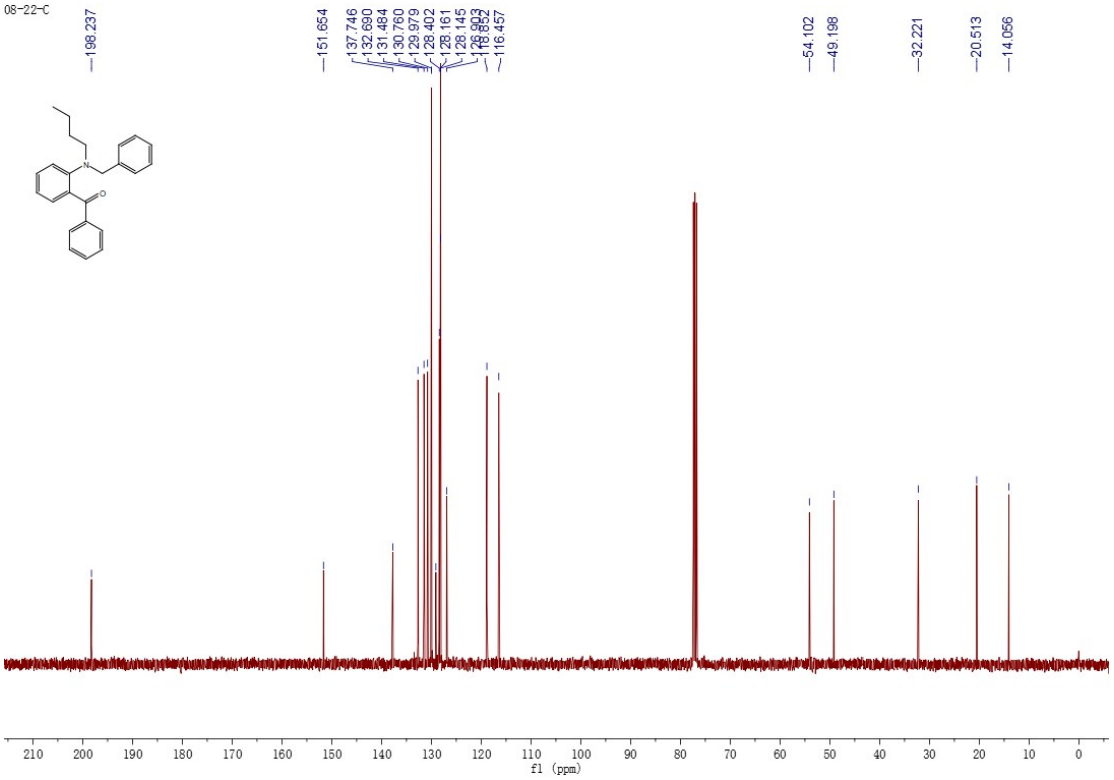
NMR of 1k


7.768
7.762
7.752
7.744
7.588
7.570
7.551
7.440
7.436
7.421
7.406
7.401
7.397
7.382
7.378
7.363
7.359
7.255
7.151
7.147
7.137
7.134
7.119
7.110
7.097
7.091
7.089
7.073
7.071
6.842
6.838
6.824
6.818
4.079
2.915
2.897
2.879
2.862
0.834
0.816
0.798
1.85
1.17
2.98
0.93
4.78
1.99
2.00
1.97
3.07
f1 (ppm)

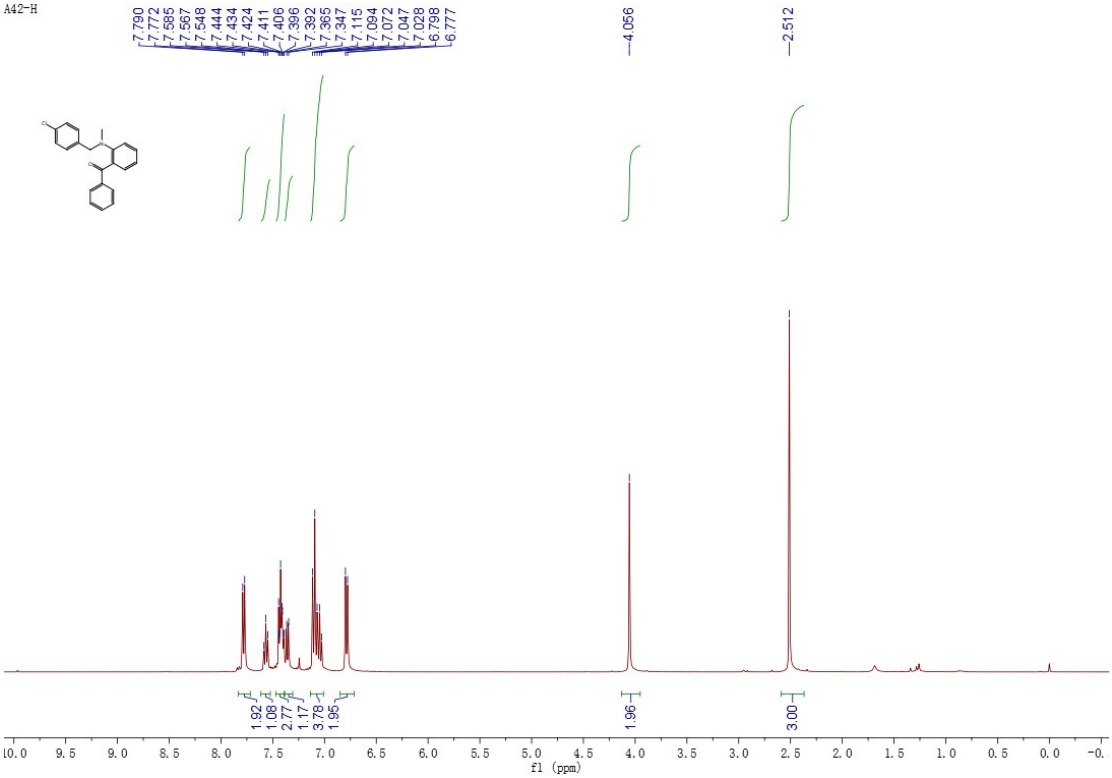

ZH-DCM(CNMR, CDCl3)
193.963
147.606
134.155
133.013
132.780
131.912
129.763
127.916
127.220
126.673
126.436
52.501
28.551
f1 (ppm)

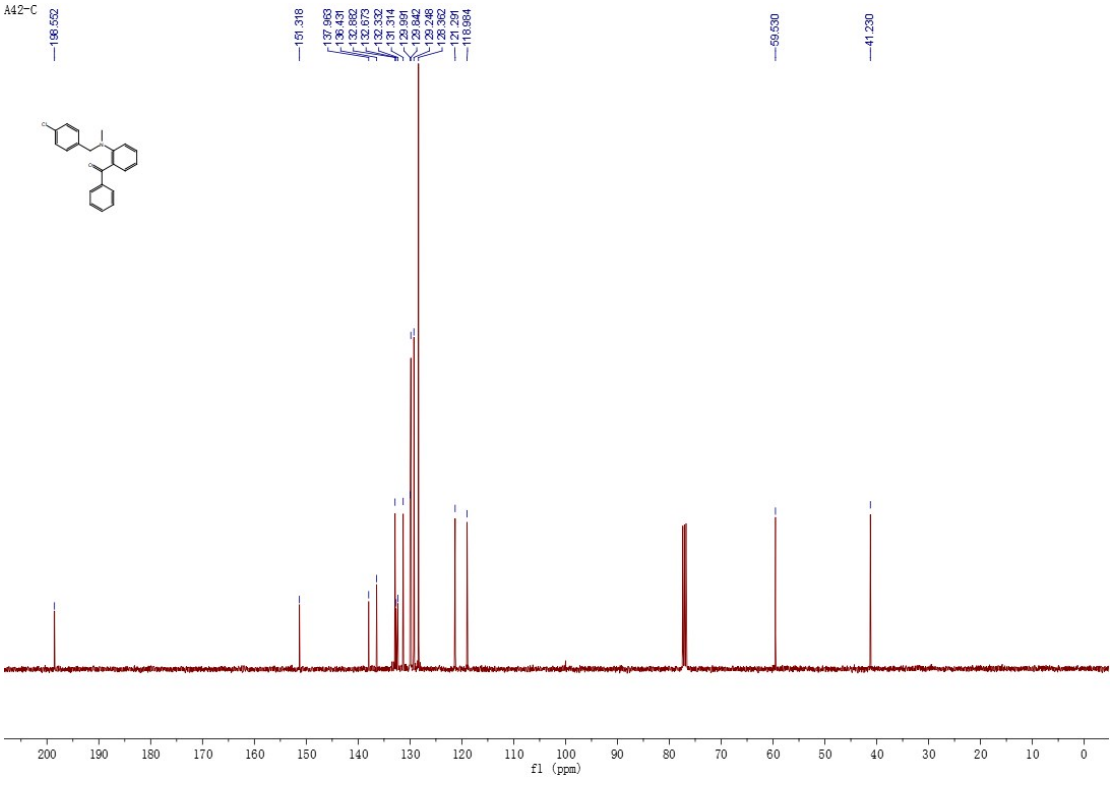
NMR of 1l


08-22-H
7.842
7.838
7.826
7.821
7.818
7.434
7.414
7.325
7.314
6.976
6.915
6.896
6.875
3.788
2.649
2.631
2.613
1.537
1.520
1.500
1.482
1.464
1.393
1.374
1.356
1.336
1.318
1.300
0.925
0.907
0.889
3.06
1.30
4.29
4.10
1.16
1.13
2.00
2.03
1.76
2.01
3.01
f1 (ppm)

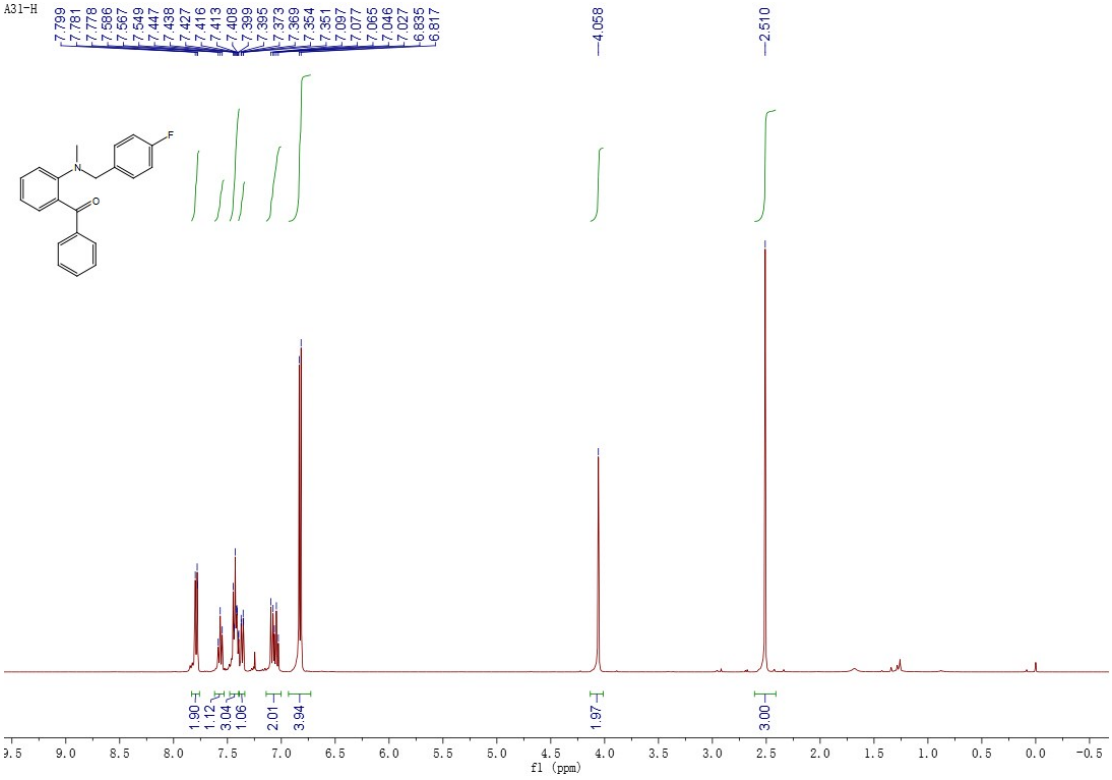

08-22-C
198.237
151.654
137.746
132.690
131.484
130.760
129.979
128.402
128.161
128.145
126.903
118.852
116.457
54.102
49.198
32.221
20.513
14.056
f1 (ppm)

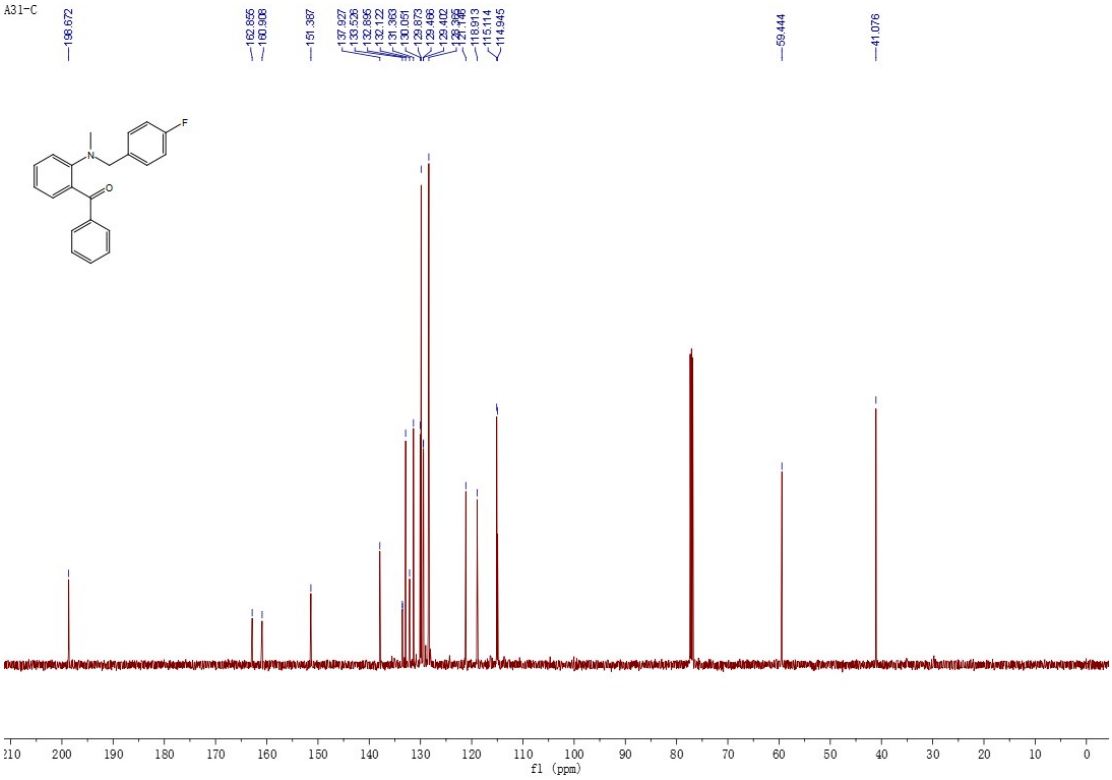
NMR of 1o


A42-H
7.790
7.772
7.585
7.567
7.548
7.444
7.434
7.424
7.411
7.406
7.396
7.392
7.365
7.347
7.115
7.094
7.072
7.047
7.028
6.798
6.777
4.056
2.512
1.92
1.08
2.77
1.17
3.78
1.95
1.96
3.00
f1 (ppm)

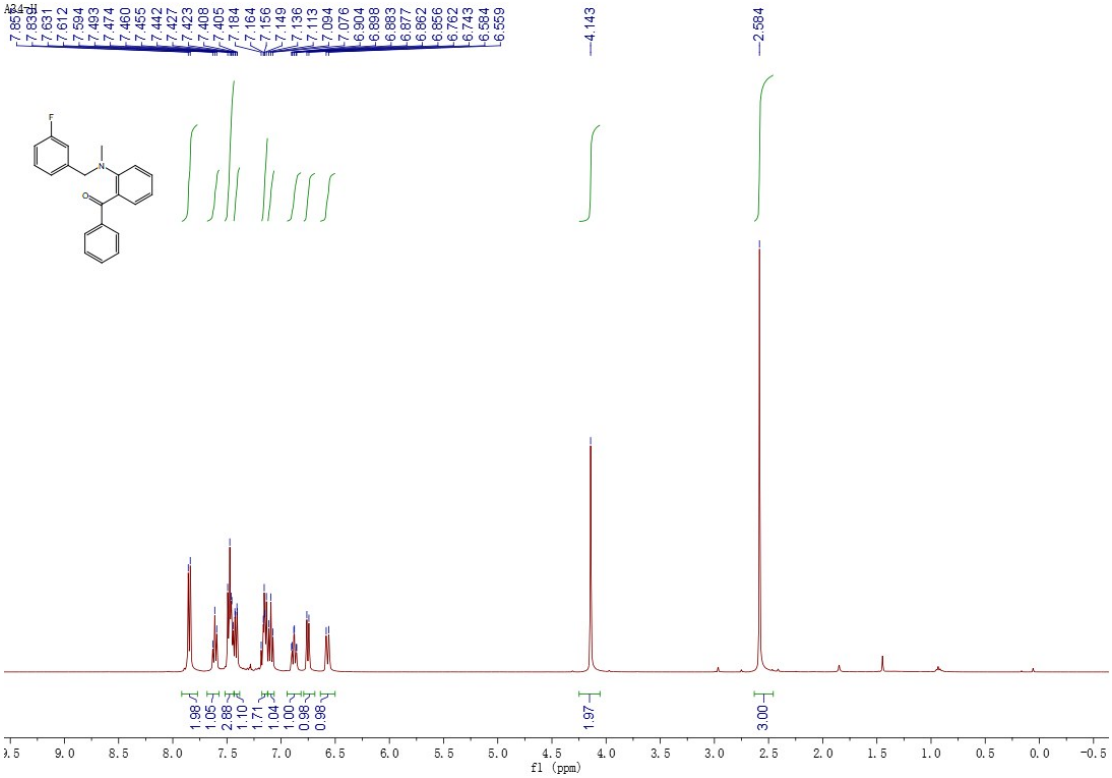

A42-C
196.552
151.318
137.963
136.431
132.892
132.573
132.332
131.314
129.991
129.842
129.248
128.362
121.291
118.984
59.530
41.230
f1 (ppm)

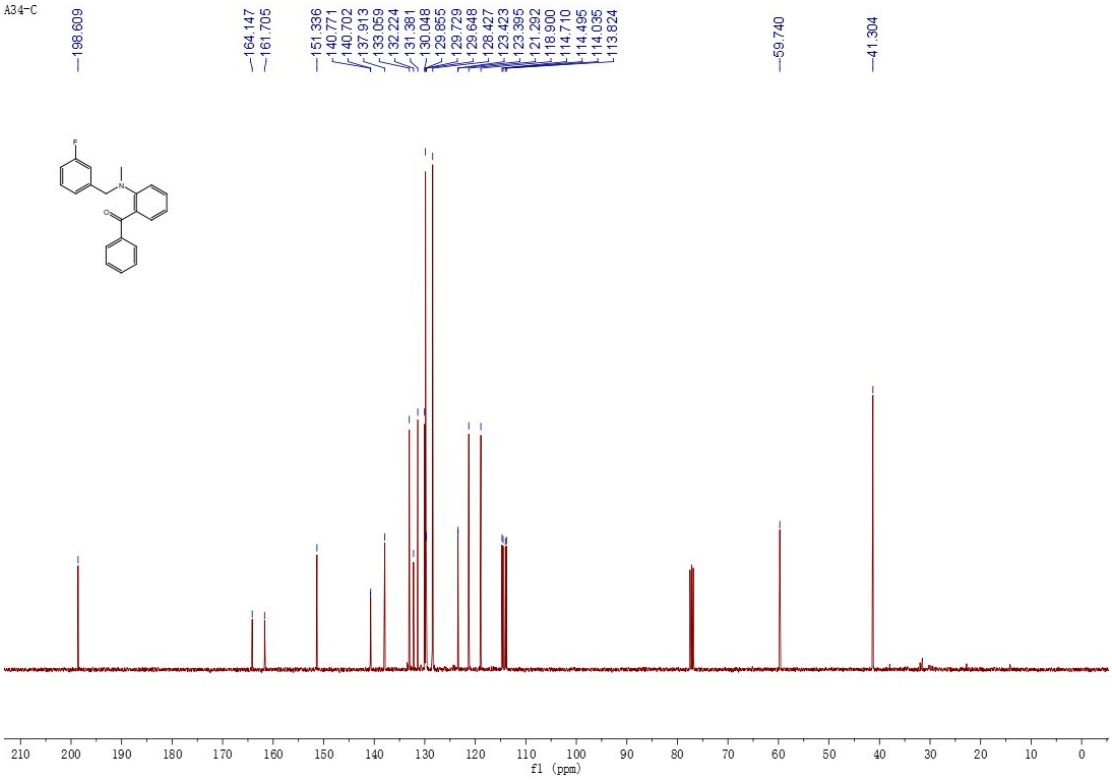
NMR of 1p


A31-H
7.799
7.781
7.778
7.586
7.567
7.549
7.447
7.438
7.427
7.416
7.413
7.408
7.399
7.395
7.373
7.369
7.354
7.351
7.097
7.077
7.065
7.046
7.027
6.835
6.817
4.058
2.510
1.90
1.12
3.04
1.06
2.01
3.94
1.97
3.00
f1 (ppm)

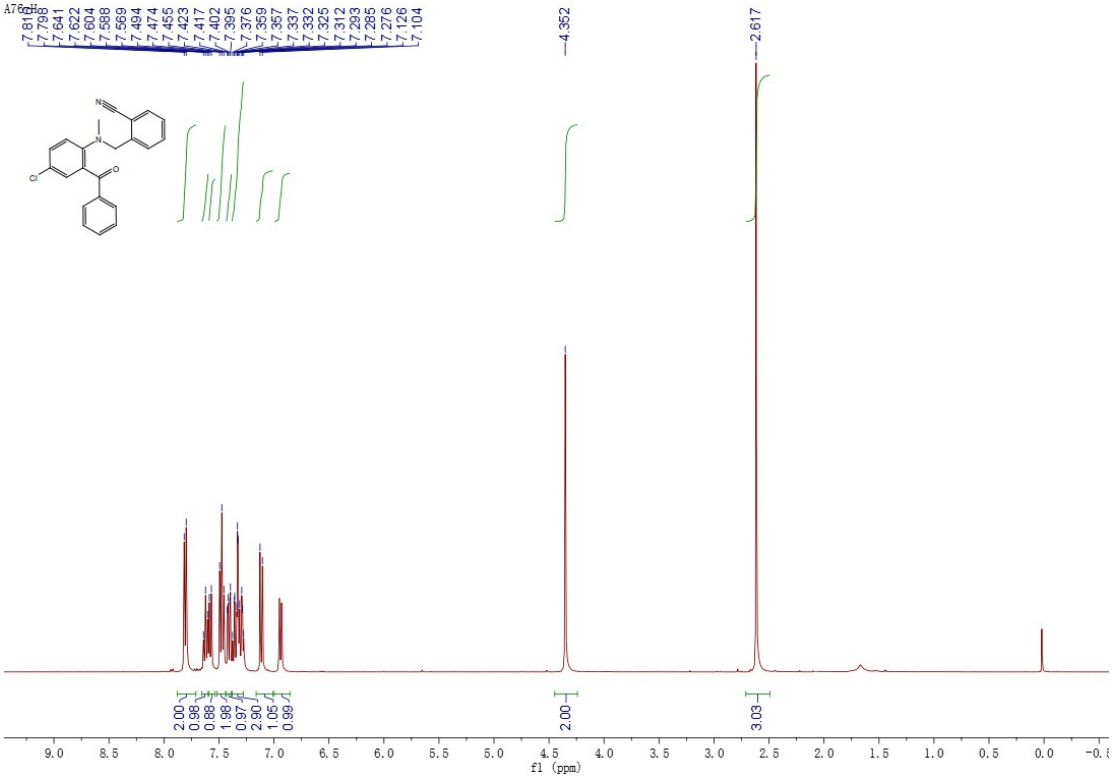

A31-C
196.672
162.855
160.908
151.387
137.927
133.526
132.956
132.722
131.363
130.051
129.873
129.466
129.402
118.913
115.114
114.945
59.444
41.076
f1 (ppm)

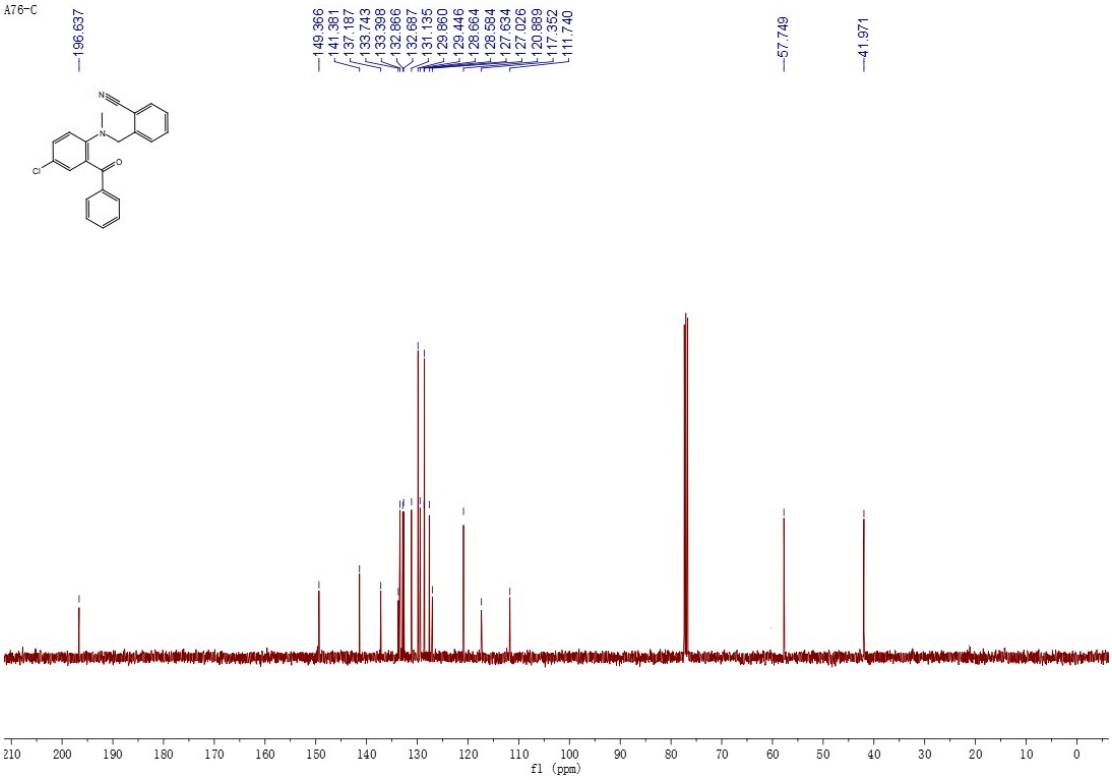
NMR of 1q


A34-H
7.854
7.839
7.631
7.612
7.594
7.493
7.474
7.460
7.455
7.442
7.427
7.423
7.408
7.405
7.184
7.164
7.156
7.149
7.136
7.113
7.094
7.076
6.904
6.898
6.883
6.877
6.862
6.856
6.762
6.743
6.584
6.559
4.143
2.584
1.98
1.05
2.88
1.10
1.71
1.04
1.00
0.98
0.98
1.97
3.00
f1 (ppm)

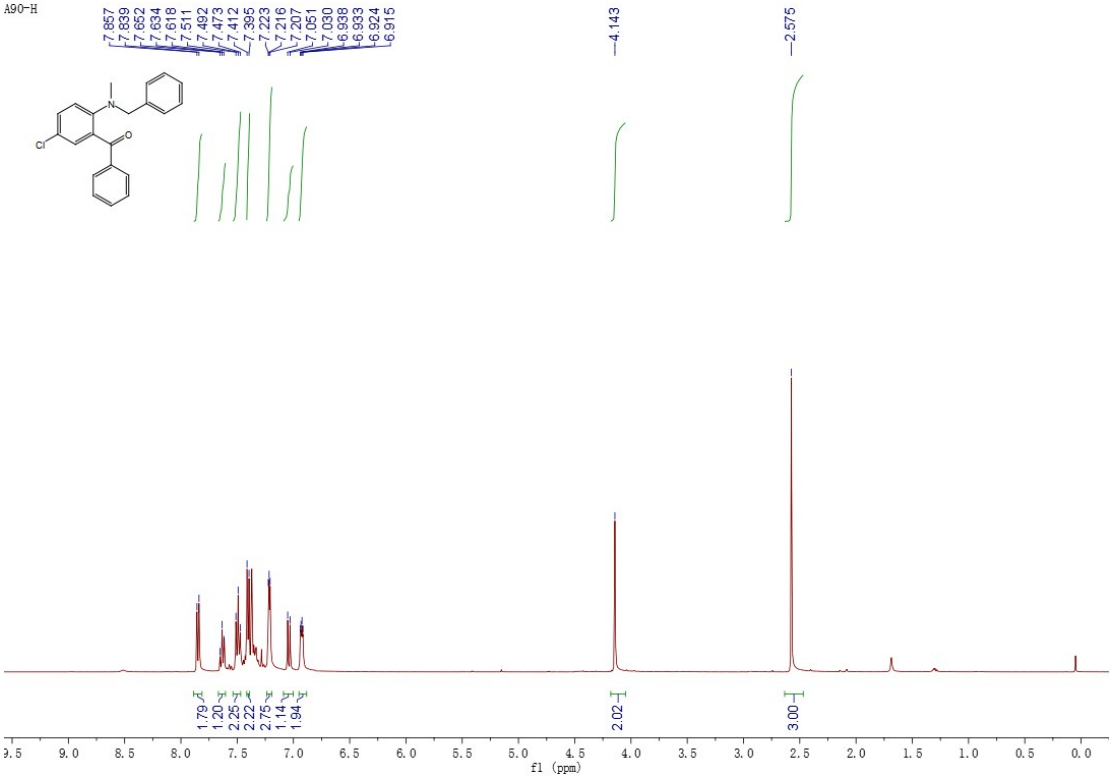

A34-C
198.609
164.147
161.705
151.336
140.771
140.702
137.913
133.059
132.224
131.381
130.048
129.855
129.729
129.648
128.427
123.423
123.395
121.292
118.900
114.710
114.495
114.035
113.824
59.740
41.304
f1 (ppm)

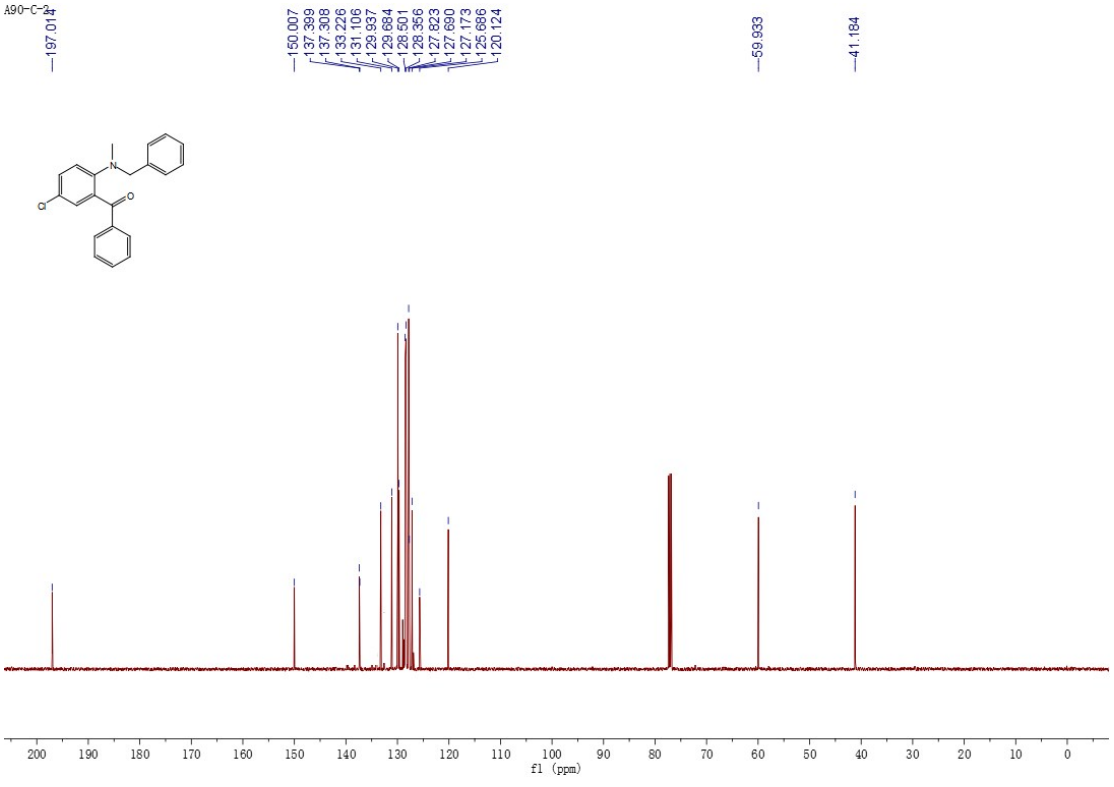
NMR of 1r


A76-H
7.816
7.798
7.641
7.622
7.604
7.588
7.569
7.494
7.474
7.455
7.423
7.417
7.402
7.395
7.376
7.359
7.357
7.337
7.332
7.325
7.312
7.293
7.285
7.276
7.126
7.104
4.352
2.617
2.00
0.98
0.88
1.98
0.97
2.90
1.05
0.99
2.00
3.03
f1 (ppm)

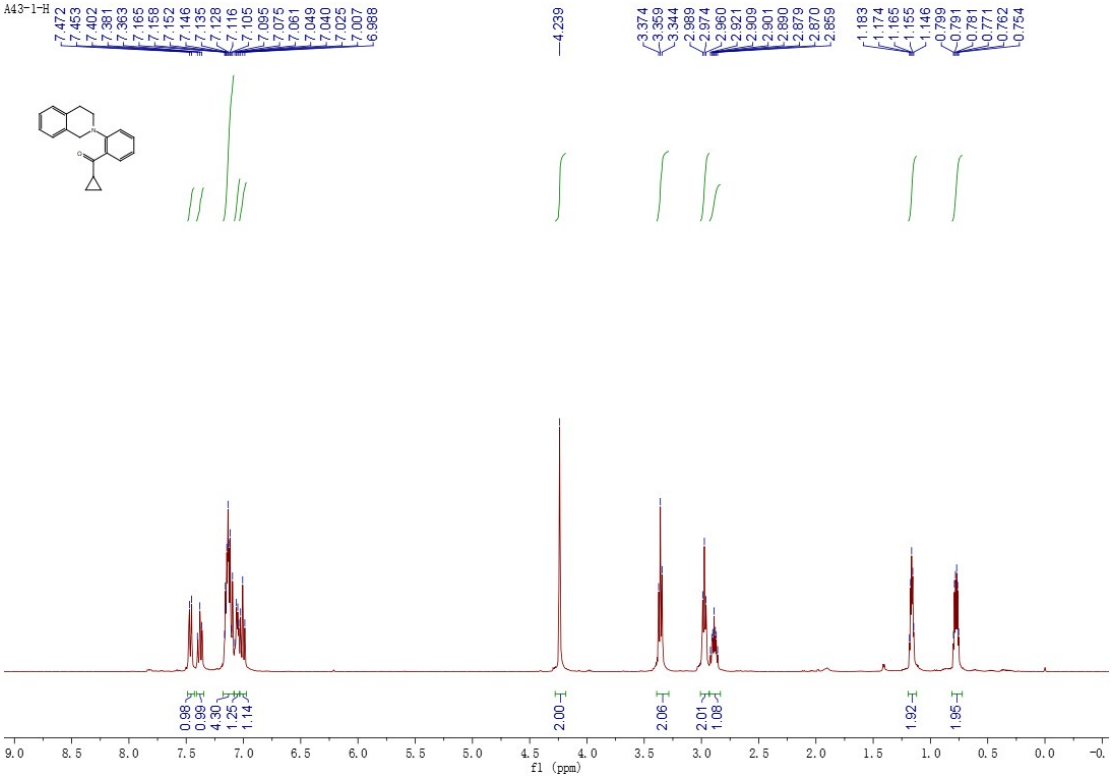

A76-C
196.637
149.366
141.381
137.187
133.743
133.398
132.866
132.687
131.135
129.860
129.446
128.664
128.584
127.634
127.026
120.889
117.352
111.740
57.749
41.971
f1 (ppm)

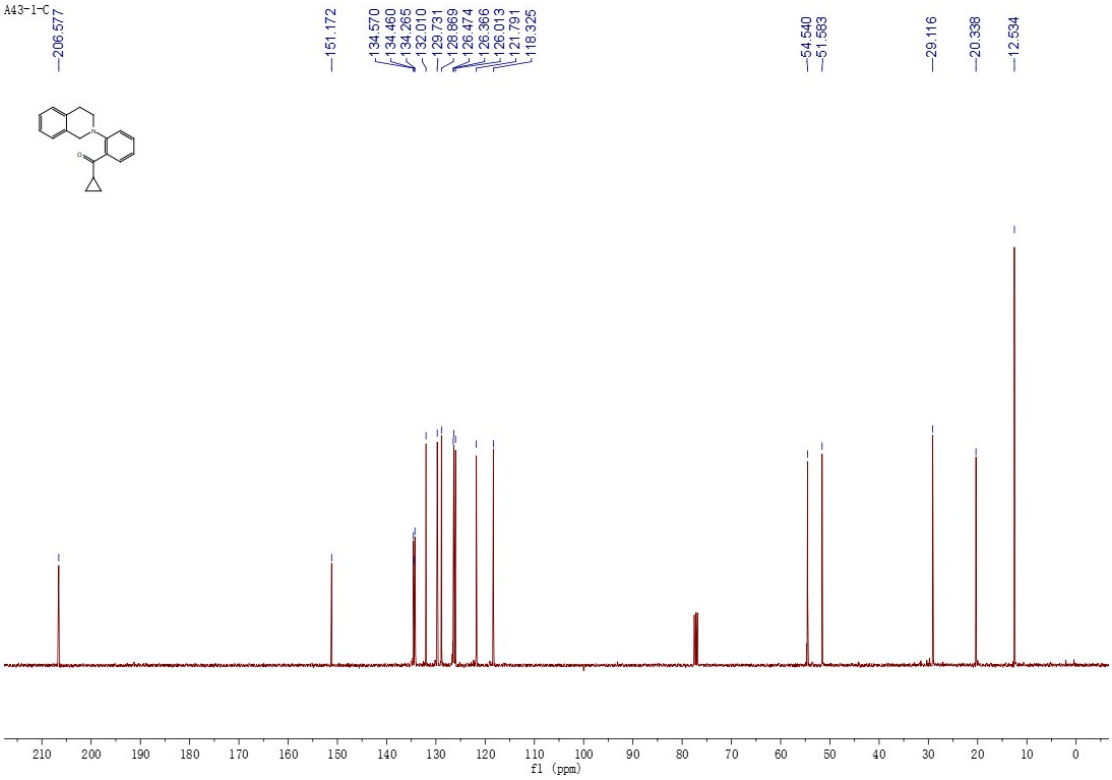
NMR of 1s


A90-H
7.857
7.839
7.652
7.634
7.618
7.511
7.492
7.473
7.412
7.395
7.223
7.216
7.207
7.051
7.030
6.938
6.933
6.924
6.915
4.143
2.575
1.79
1.20
2.25
2.22
2.75
1.14
1.94
2.02
3.00
f1 (ppm)

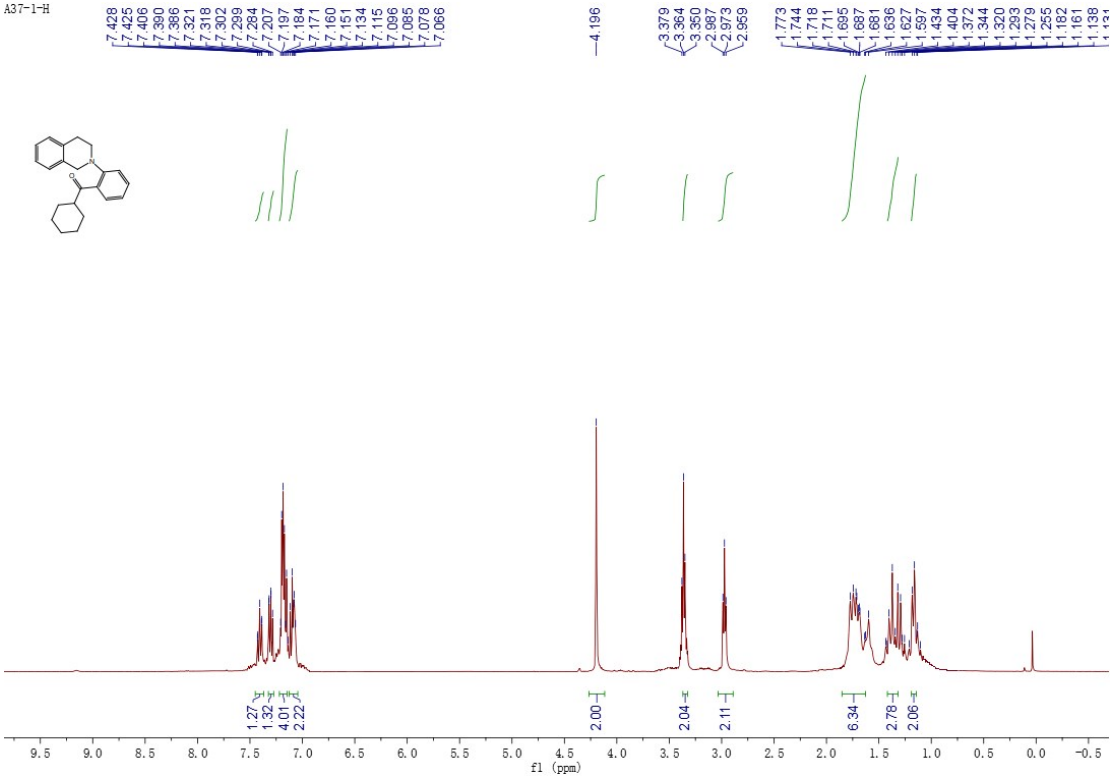

A90-C-2
197.014
150.007
137.399
137.308
133.226
131.106
129.937
129.684
128.501
128.356
127.823
127.690
127.173
125.686
120.124
59.933
41.184
f1 (ppm)

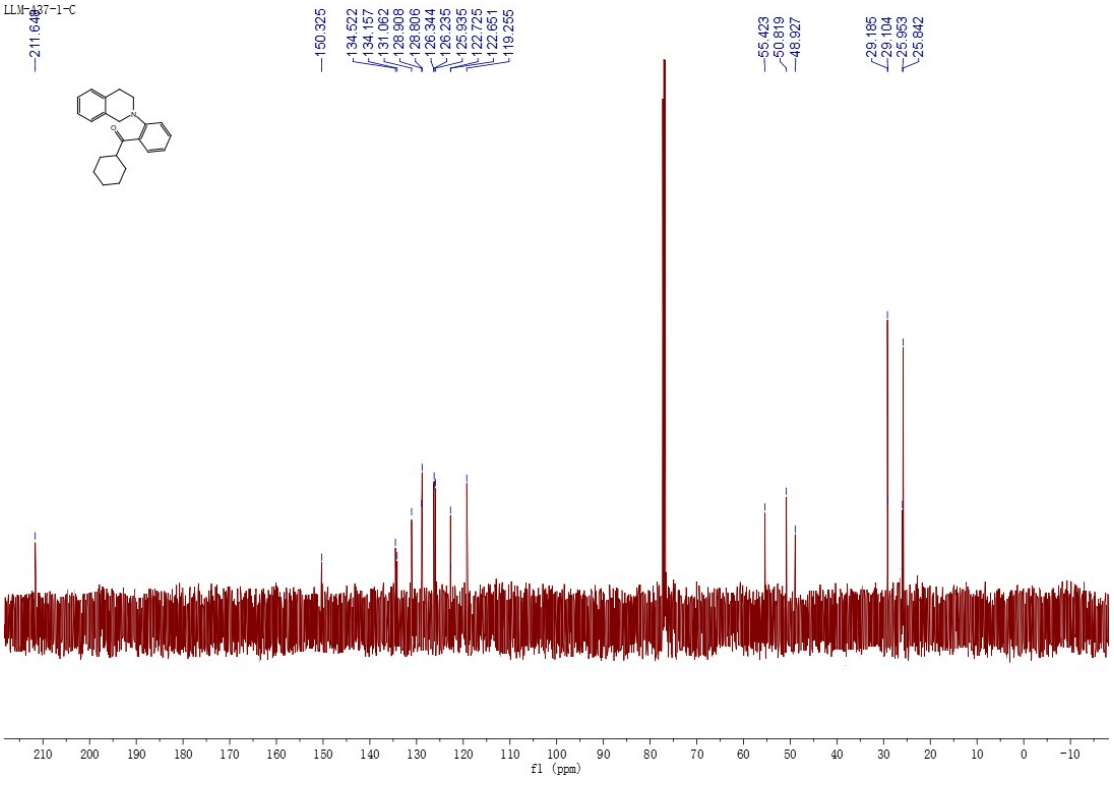
NMR of 1ac


A43-1-H
7.472
7.453
7.402
7.381
7.363
7.165
7.158
7.152
7.146
7.135
7.128
7.116
7.105
7.095
7.075
7.061
7.049
7.040
7.025
7.007
6.988
4.239
3.374
3.359
3.344
2.989
2.974
2.960
2.921
2.909
2.901
2.890
2.879
2.870
2.859
1.183
1.174
1.165
1.155
1.146
0.799
0.791
0.781
0.771
0.762
0.754
0.98
0.99
4.30
1.25
1.14
2.00
2.06
2.01
1.08
1.92
1.95
f1 (ppm)

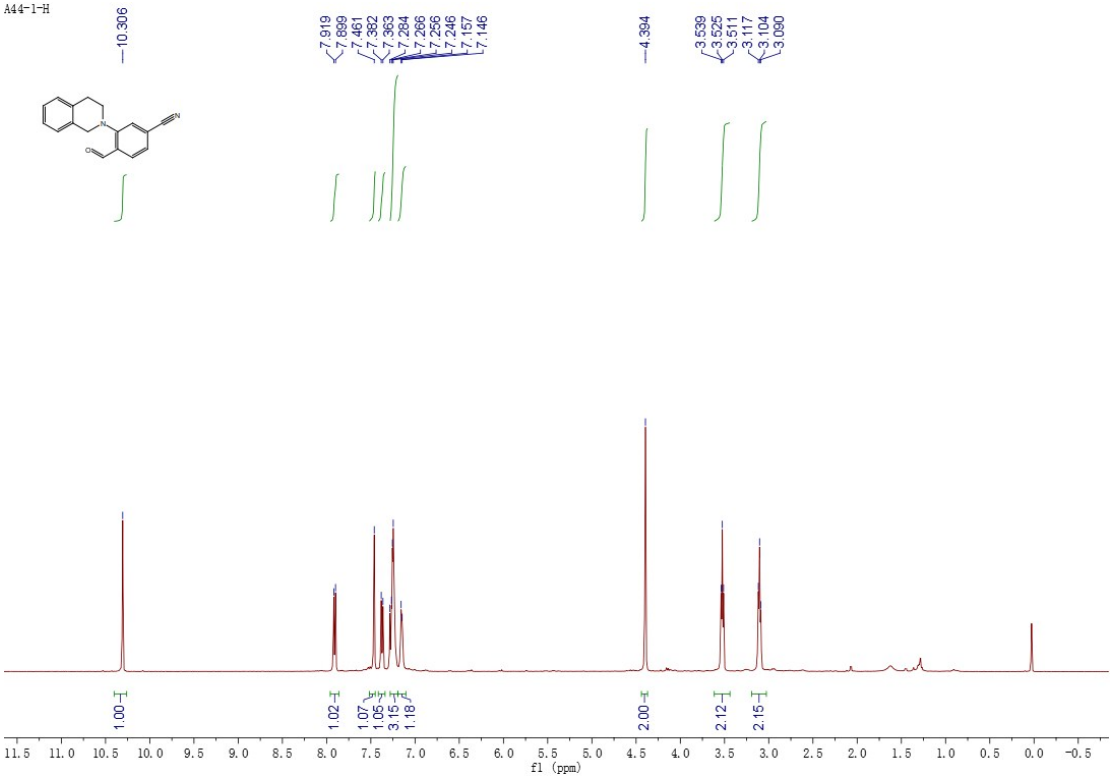

A43-1-C
206.577
151.172
134.570
134.460
134.265
132.010
129.731
128.869
126.474
126.366
126.013
121.791
118.325
54.540
51.583
29.116
20.338
12.534
f1 (ppm)

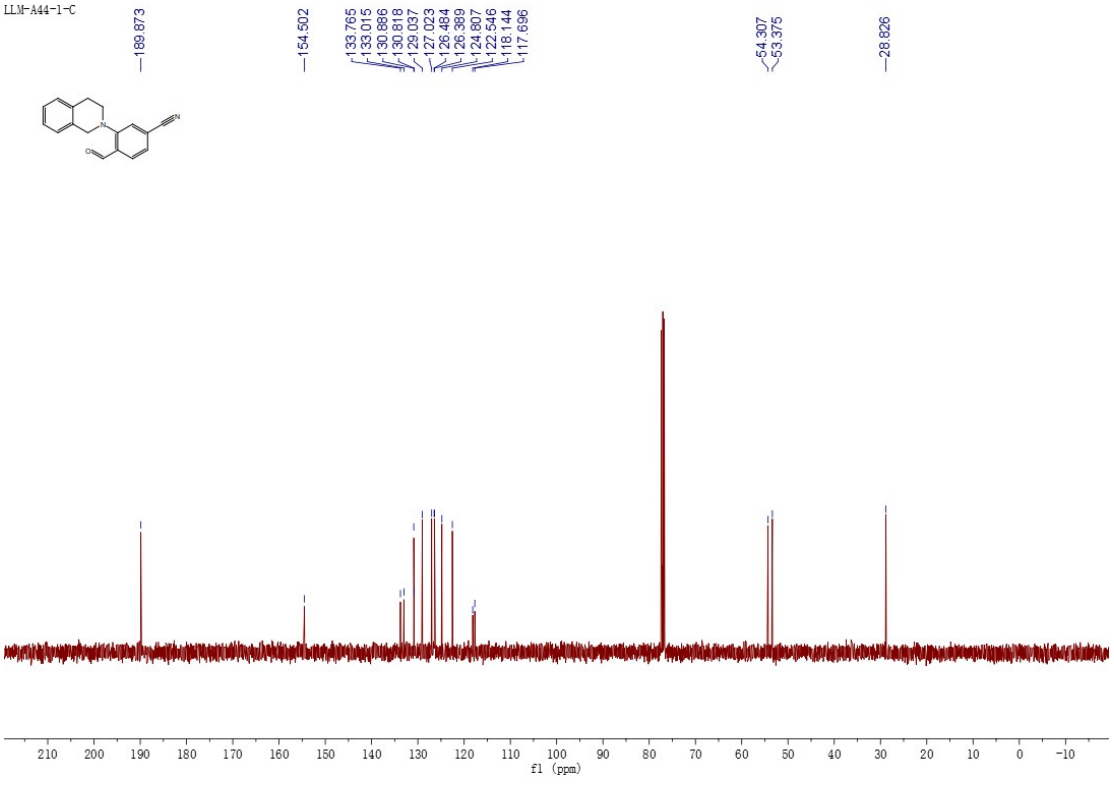
NMR of 1ad


A37-1-H
7.428
7.425
7.406
7.390
7.386
7.321
7.318
7.302
7.299
7.284
7.207
7.197
7.184
7.171
7.160
7.151
7.134
7.115
7.096
7.085
7.078
7.066
4.196
3.379
3.364
3.350
2.987
2.973
2.959
1.773
1.744
1.718
1.711
1.695
1.687
1.681
1.636
1.627
1.597
1.434
1.404
1.372
1.344
1.320
1.293
1.279
1.255
1.182
1.161
1.138
1.27
1.32
4.01
2.22
2.00
2.04
2.11
6.34
2.78
2.06
f1 (ppm)

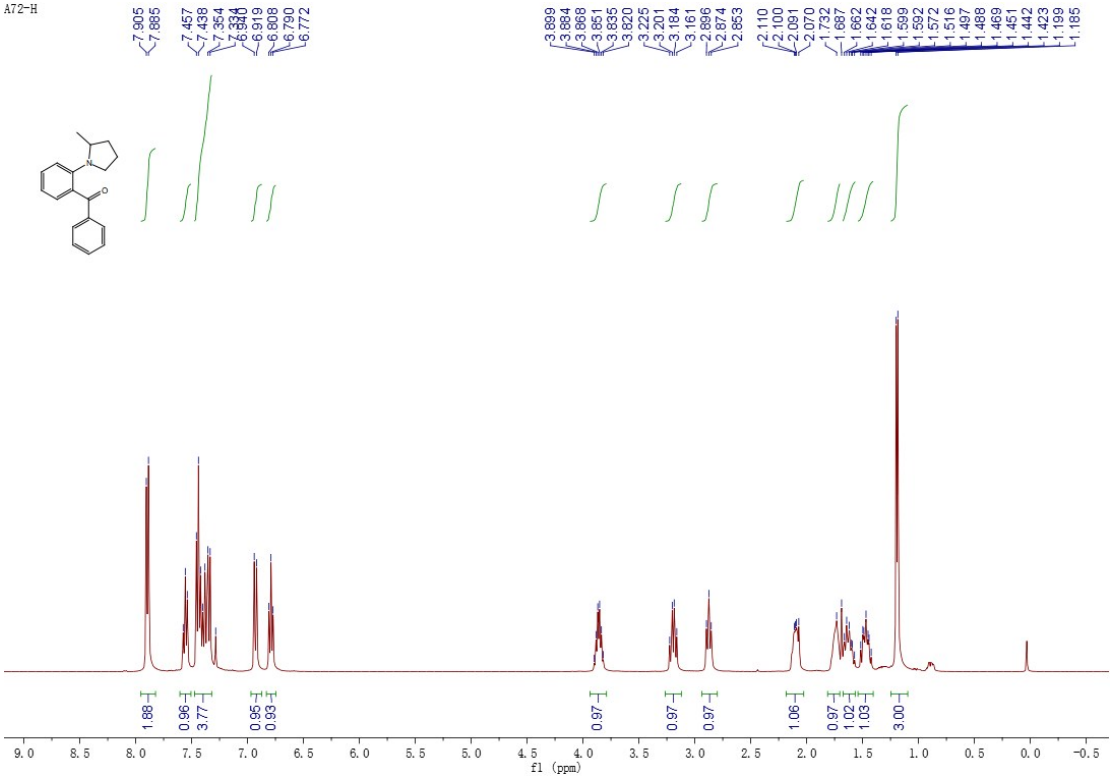

LLM-A37-1-C
211.648
150.325
134.522
134.157
131.062
128.908
128.806
126.344
126.235
125.935
122.725
122.651
119.255
55.423
50.819
48.927
29.185
29.104
25.953
25.842
f1 (ppm)

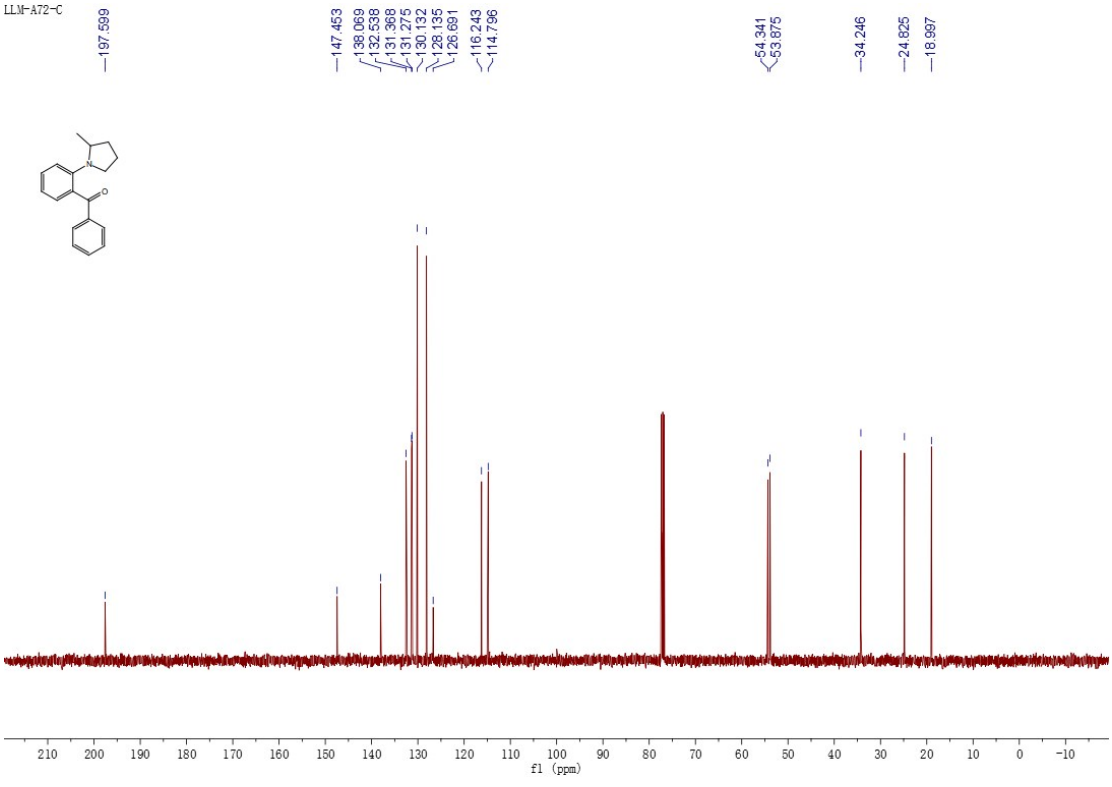
NMR of 1ai


A44-1-H
10.306
7.919
7.899
7.461
7.382
7.363
7.284
7.266
7.256
7.246
7.157
7.146
4.394
3.539
3.525
3.511
3.117
3.104
3.090
1.00
1.02
1.07
1.05
3.15
1.18
2.00
2.12
2.15
f1 (ppm)

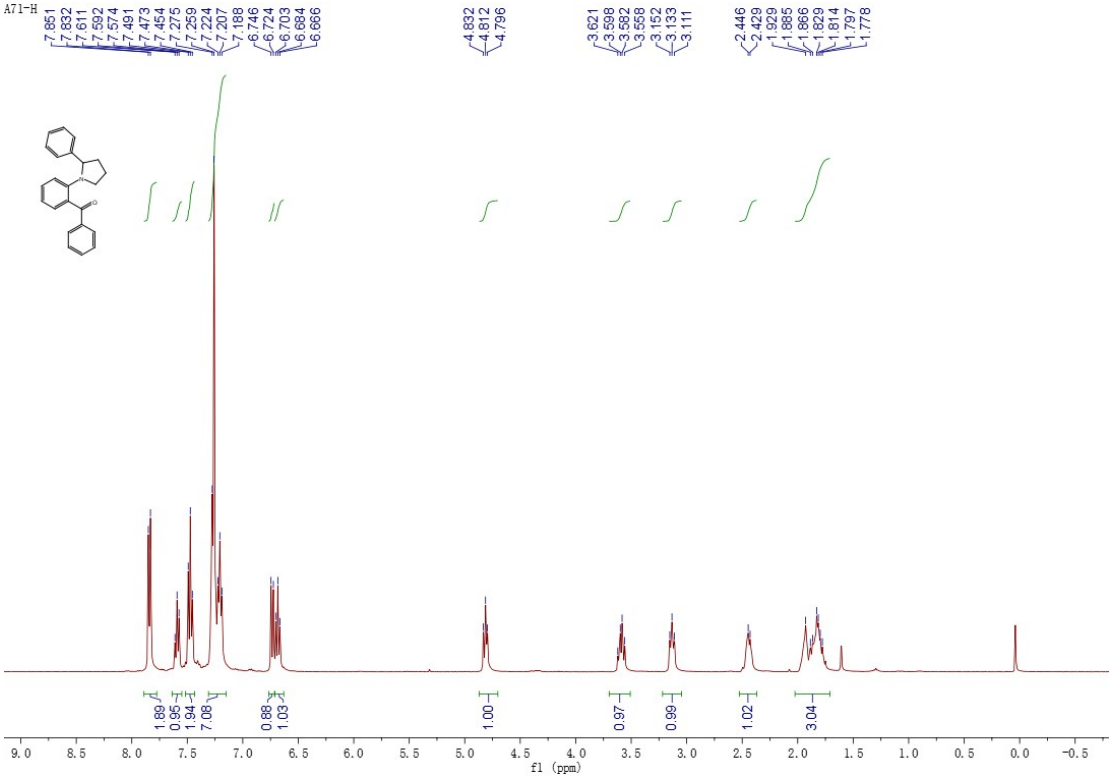

LLM-A44-1-C
189.873
154.502
133.765
133.015
130.886
130.818
129.037
127.023
126.484
126.389
124.807
122.546
118.144
117.696
54.307
53.375
28.826
f1 (ppm)

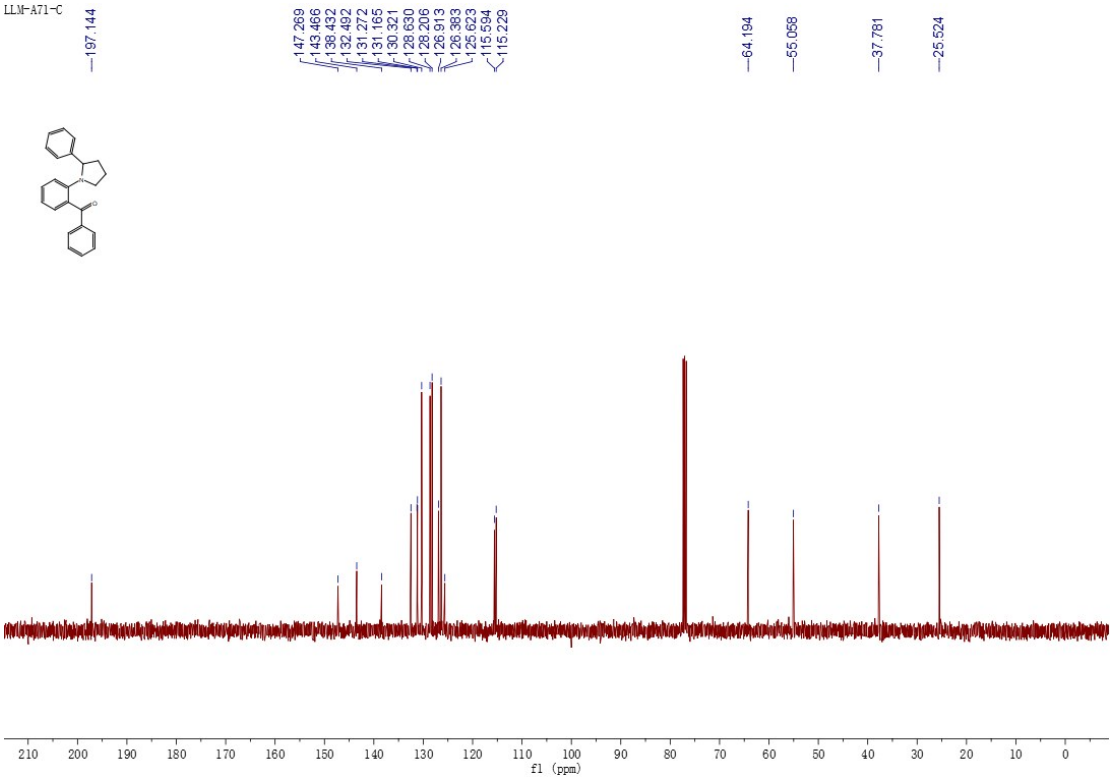
NMR of 1ak


A72-H
7.905
7.885
7.457
7.438
7.354
6.919
6.808
6.790
6.772
3.899
3.884
3.868
3.851
3.835
3.820
3.225
3.201
3.184
3.161
2.896
2.874
2.853
2.110
2.100
2.091
2.070
1.732
1.687
1.662
1.642
1.618
1.599
1.592
1.572
1.516
1.497
1.488
1.469
1.451
1.442
1.423
1.199
1.185
1.88
0.96
3.77
0.95
0.93
0.97
0.97
0.97
1.06
0.97
1.02
1.03
3.00
f1 (ppm)

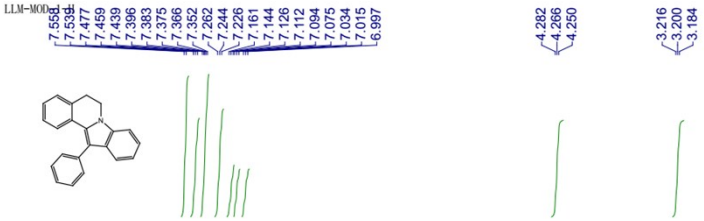

LLM-A72-C
197.599
147.453
138.069
132.538
131.368
131.275
130.132
128.135
126.691
116.243
114.796
54.341
53.875
34.246
24.825
18.997
f1 (ppm)

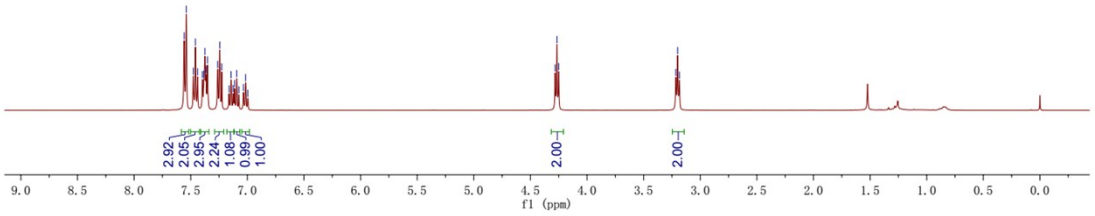
NMR of 1al

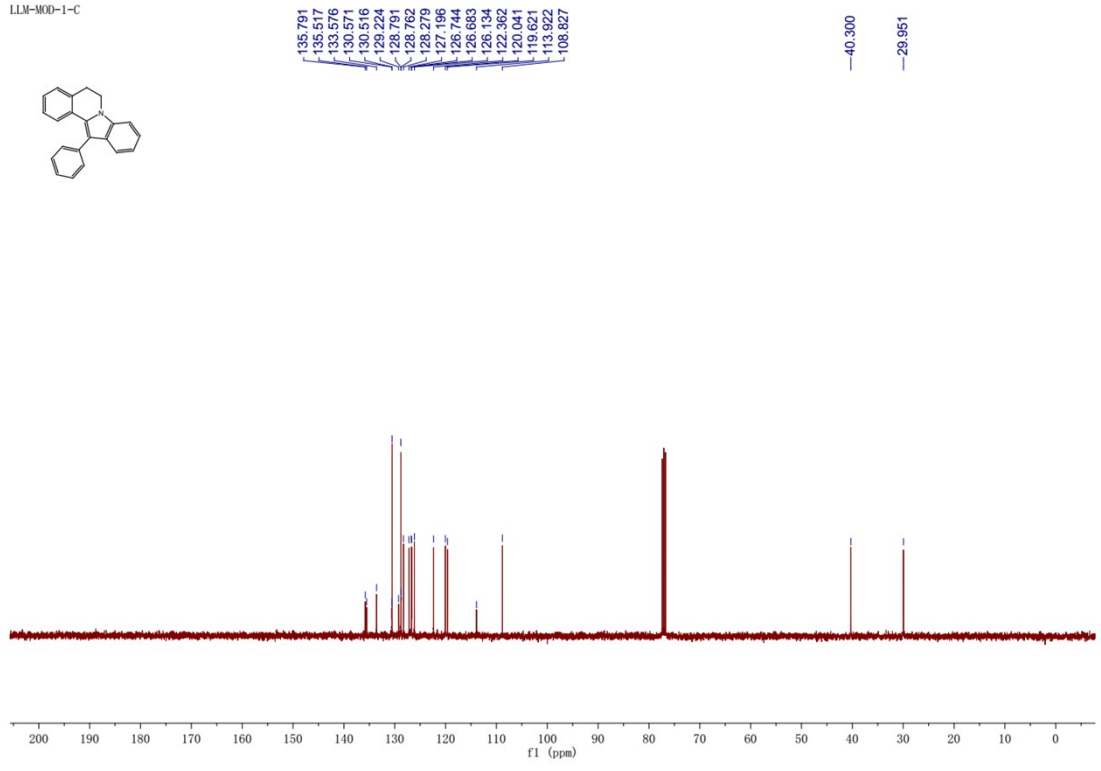

A71-H
7.851
7.832
7.611
7.592
7.574
7.491
7.473
7.454
7.275
7.259
7.224
7.207
7.188
6.746
6.724
6.703
6.684
6.666
4.832
4.812
4.796
3.621
3.598
3.582
3.558
3.152
3.133
3.111
2.446
2.429
1.929
1.885
1.866
1.829
1.814
1.797
1.778
1.89
0.95
1.94
7.08
0.88
1.03
1.00
0.97
0.99
1.02
3.04
f1 (ppm)


LLM-A71-C
197.144
147.269
143.466
138.432
132.492
131.272
131.165
130.321
128.630
128.206
126.913
126.383
125.623
115.594
115.229
64.194
55.058
37.781
25.524
f1 (ppm)

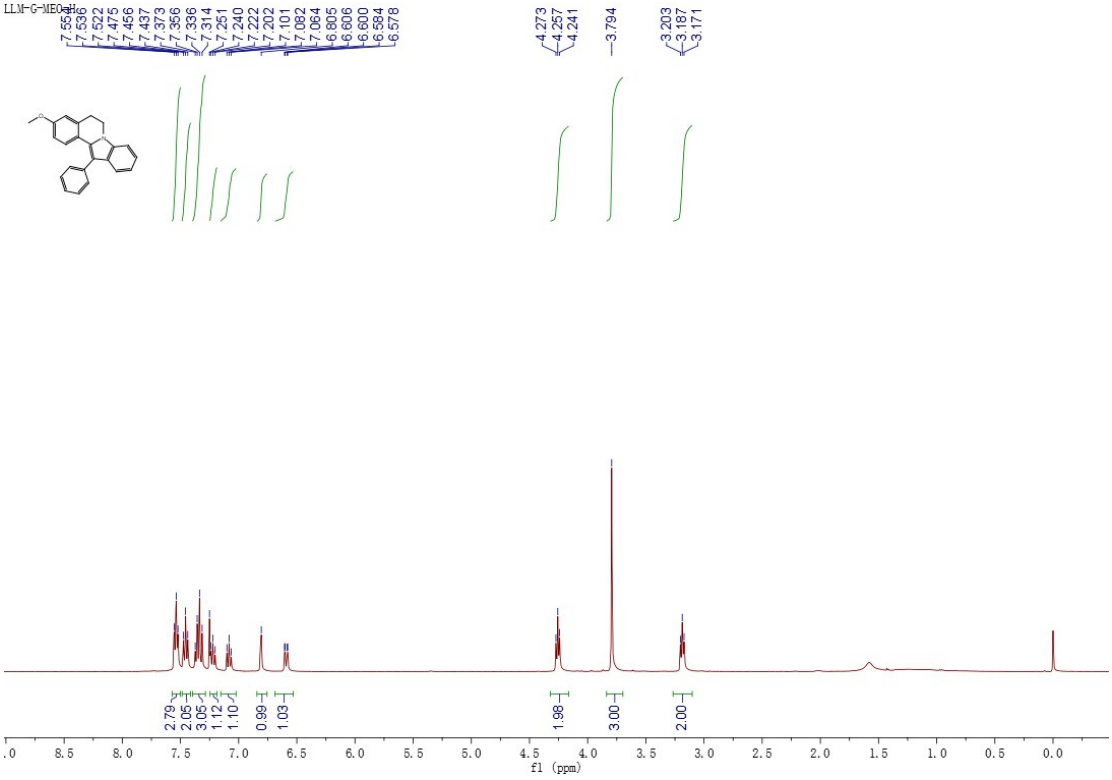
NMR of 2a

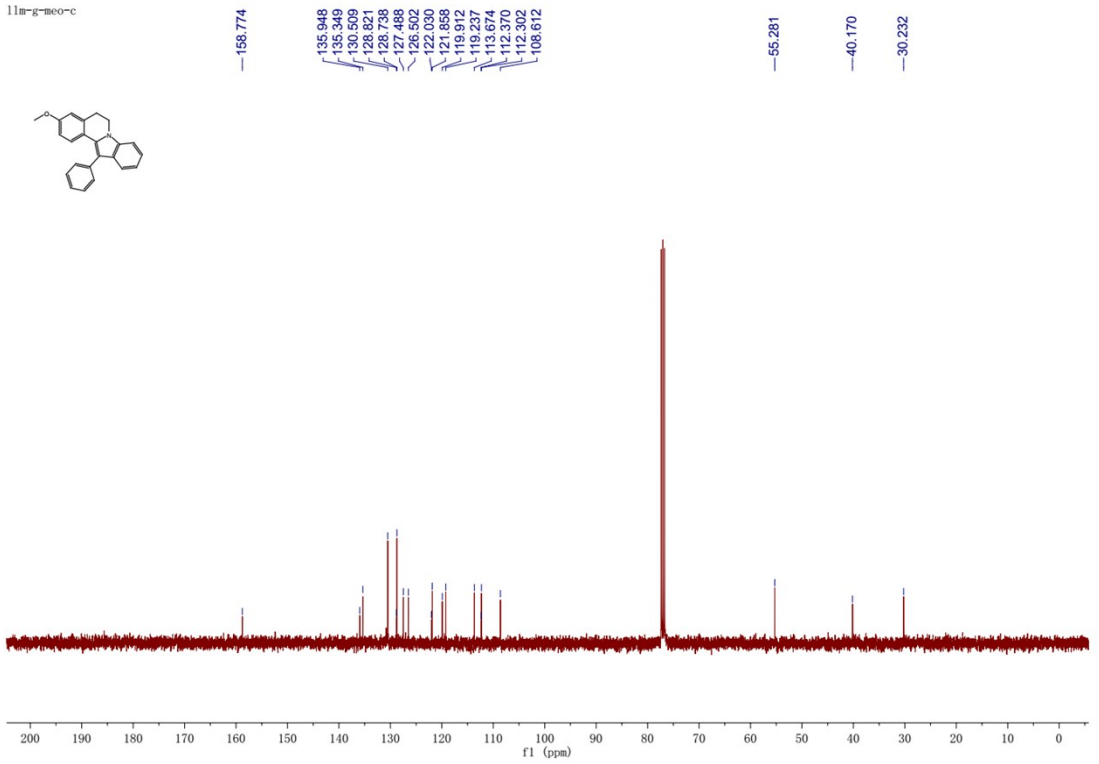

LLM-MOD
7.558
7.539
7.477
7.459
7.439
7.396
7.383
7.375
7.366
7.352
7.262
7.244
7.226
7.161
7.144
7.126
7.112
7.094
7.075
7.034
7.015
6.997
4.282
4.266
4.250
3.216
3.200
3.184


2.92
2.05
2.95
2.24
1.08
0.99
1.00
2.00
2.00
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)

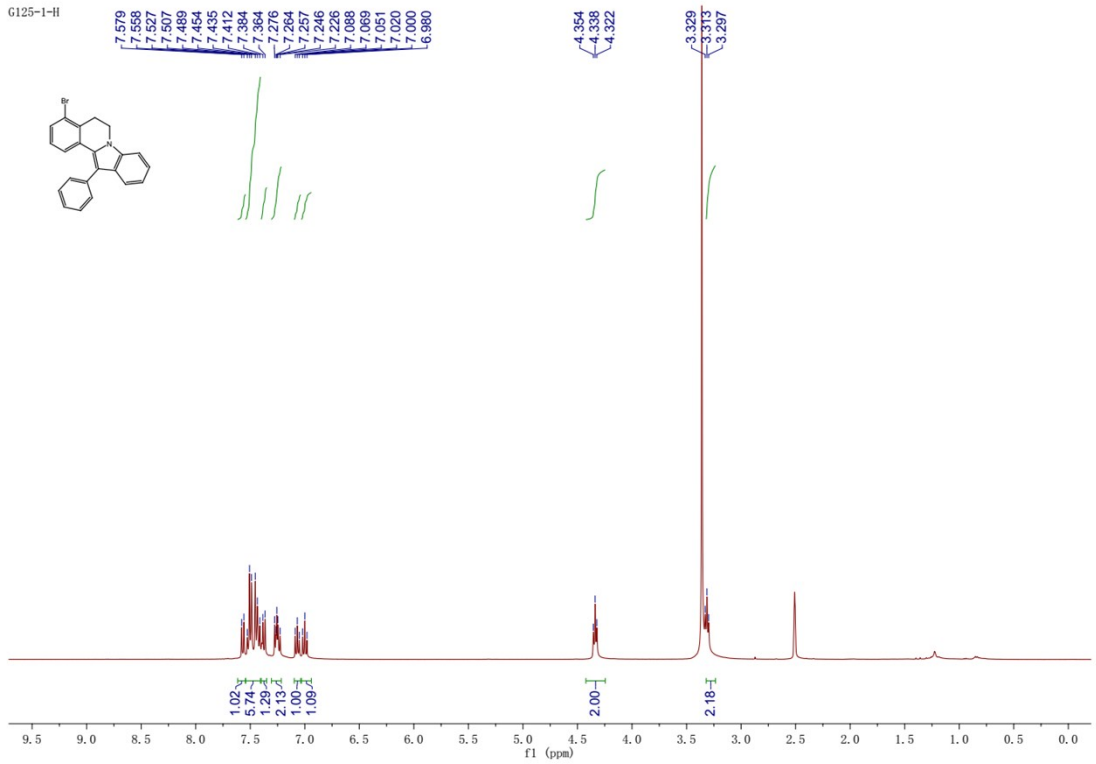

LLM-MOD-1-C
135.791
135.517
133.576
130.571
130.516
129.224
128.791
128.762
128.279
127.196
126.744
126.683
126.134
122.362
120.041
119.621
113.922
108.827
40.300
29.951
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

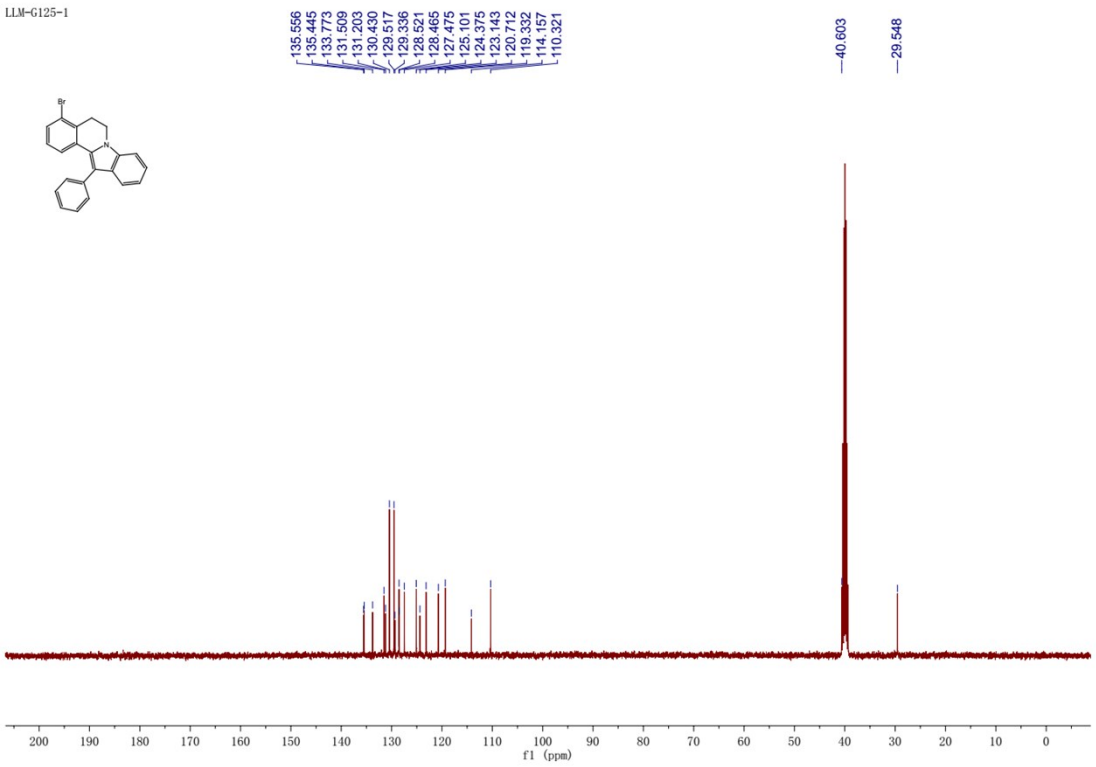
NMR of 2b


LLM-G-MEO-H
7.550
7.536
7.522
7.475
7.456
7.437
7.373
7.356
7.336
7.314
7.251
7.240
7.222
7.202
7.101
7.082
7.064
6.805
6.606
6.600
6.584
6.578
4.273
4.257
4.241
3.794
3.203
3.187
3.171
2.79
2.05
3.05
1.12
1.10
0.99
1.03
1.98
3.00
2.00
f1 (ppm)

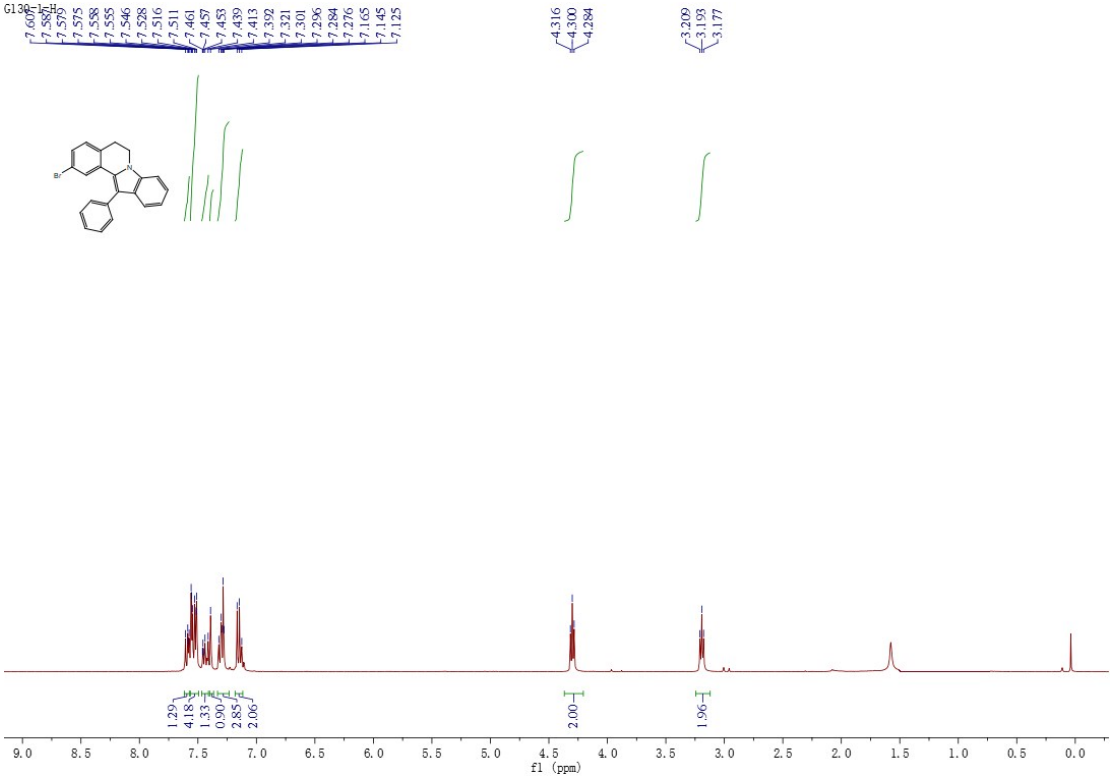

llm-g-meo-c
158.774
135.948
135.349
130.509
128.821
128.738
127.488
126.502
122.030
121.858
119.912
119.237
113.674
112.370
112.302
108.612
55.281
40.170
30.232
f1 (ppm)

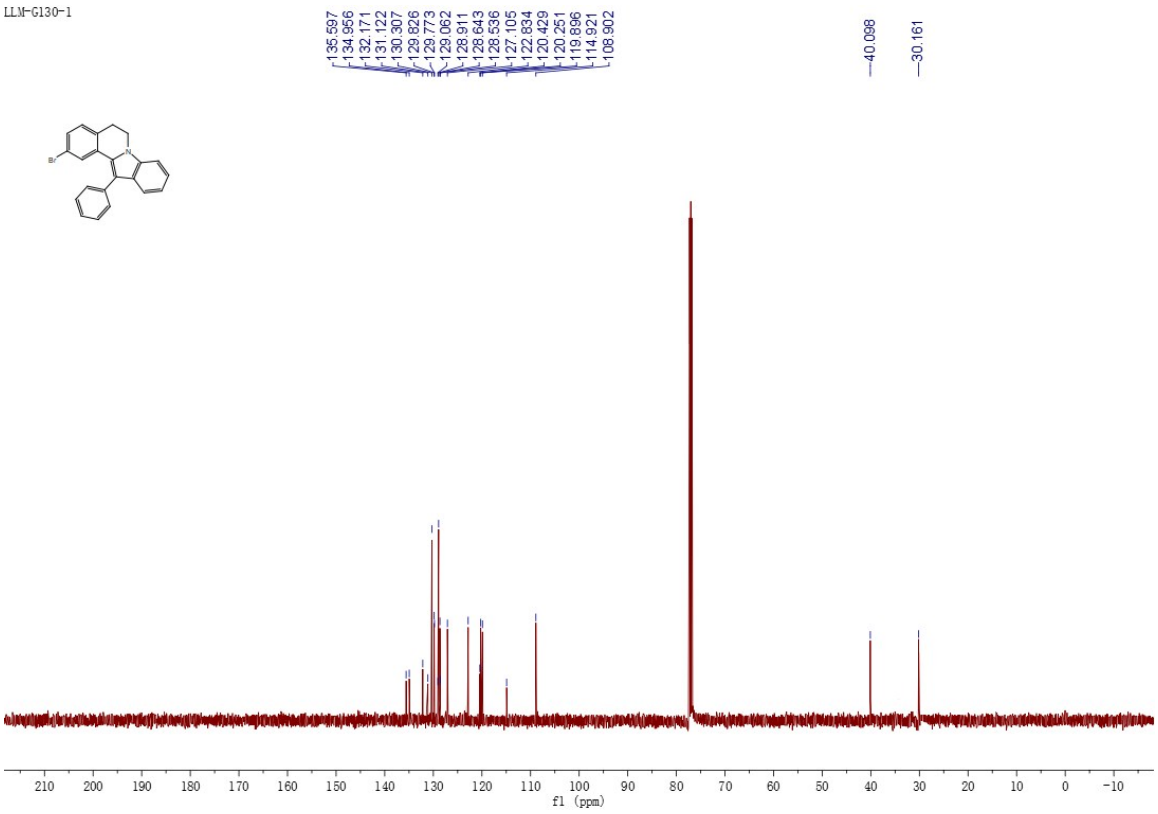
NMR of 2c


G125-1-H
7.579
7.558
7.527
7.507
7.489
7.454
7.435
7.412
7.384
7.364
7.276
7.264
7.257
7.246
7.226
7.088
7.069
7.051
7.020
7.000
6.980
4.354
4.338
4.322
3.329
3.313
3.297
1.02
5.74
1.29
2.13
1.00
1.09
2.00
2.18
f1 (ppm)

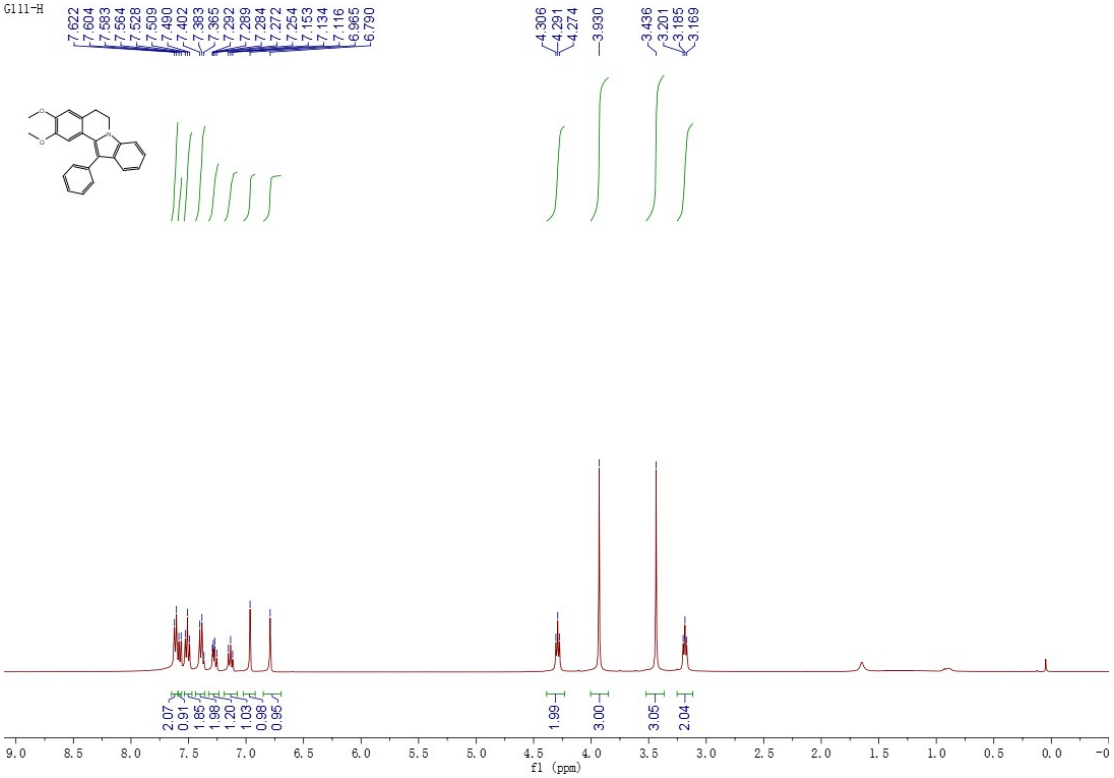

LLM-G125-1
135.556
135.445
133.773
131.509
131.203
130.430
129.517
129.336
128.521
128.465
127.475
125.101
124.375
123.143
120.712
119.332
114.157
110.321
40.603
29.548
f1 (ppm)

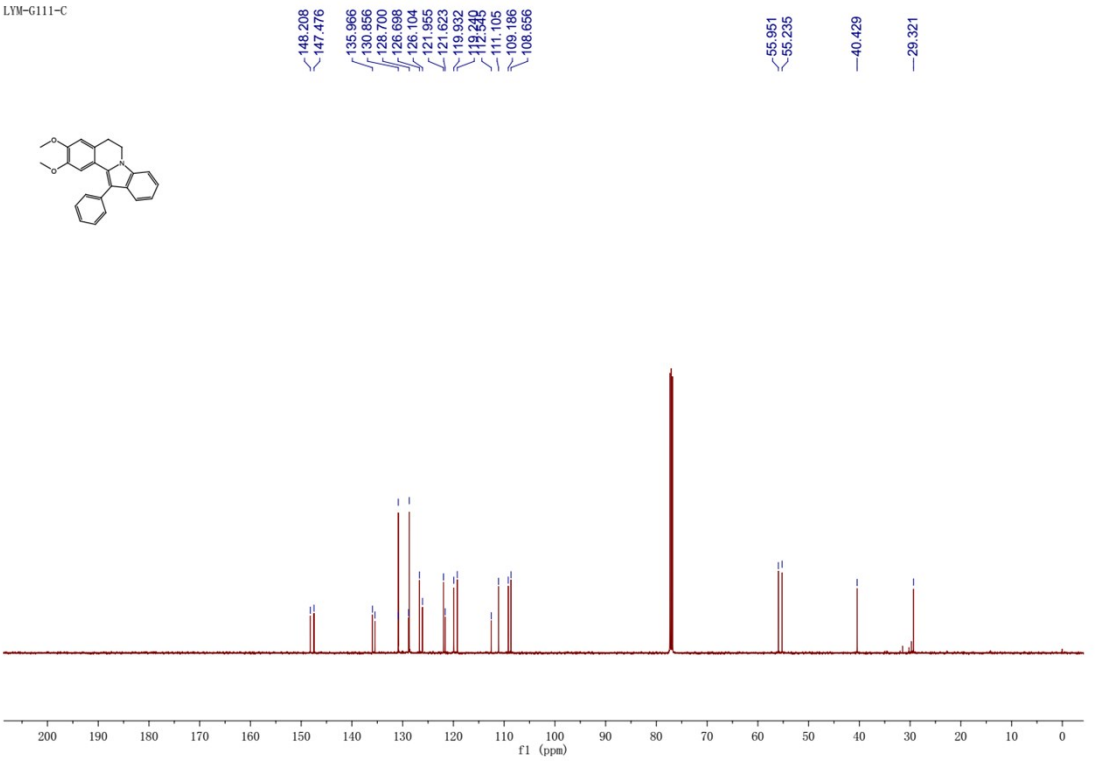
NMR of 2d


G130-1-H
7.606
7.582
7.579
7.575
7.558
7.555
7.546
7.528
7.516
7.511
7.461
7.457
7.453
7.439
7.413
7.392
7.321
7.301
7.296
7.284
7.276
7.165
7.145
7.125
4.316
4.300
4.284
3.209
3.193
3.177
1.29
4.18
1.33
0.90
2.85
2.06
2.00
1.96
f1 (ppm)

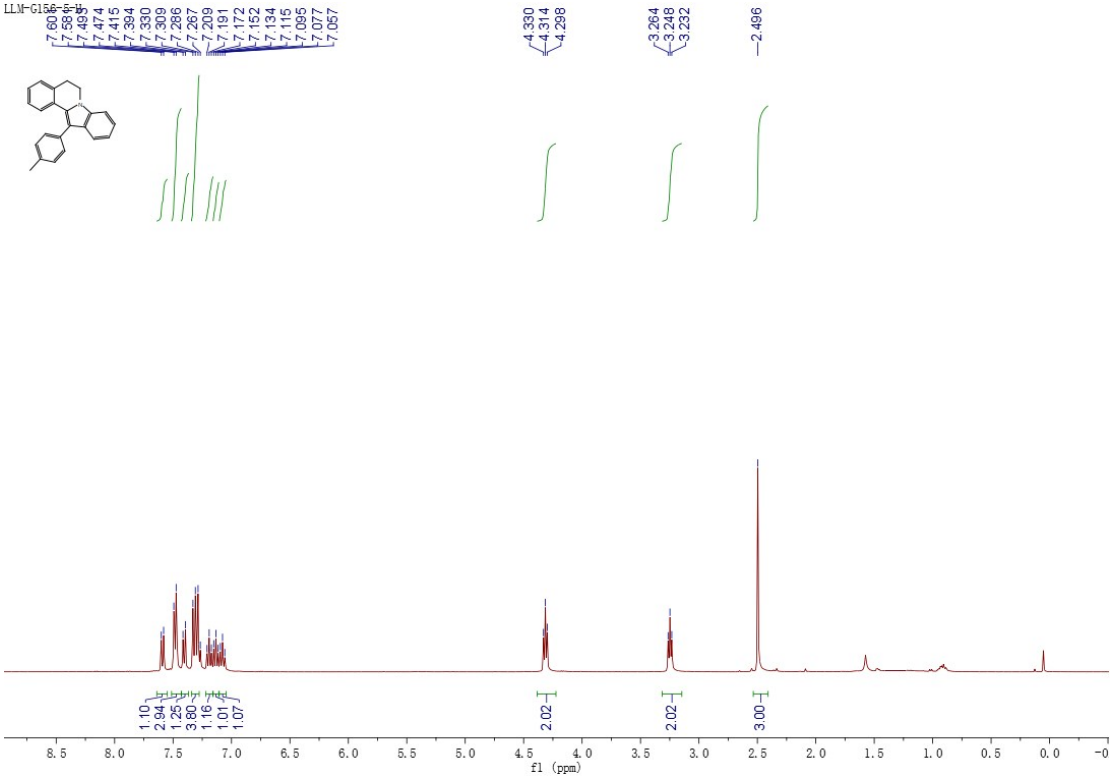

LLM-G130-1
135.597
134.956
132.171
131.122
130.307
129.826
129.773
129.062
128.911
128.643
128.536
127.105
122.834
120.429
120.251
119.896
114.921
108.902
40.098
30.161
f1 (ppm)

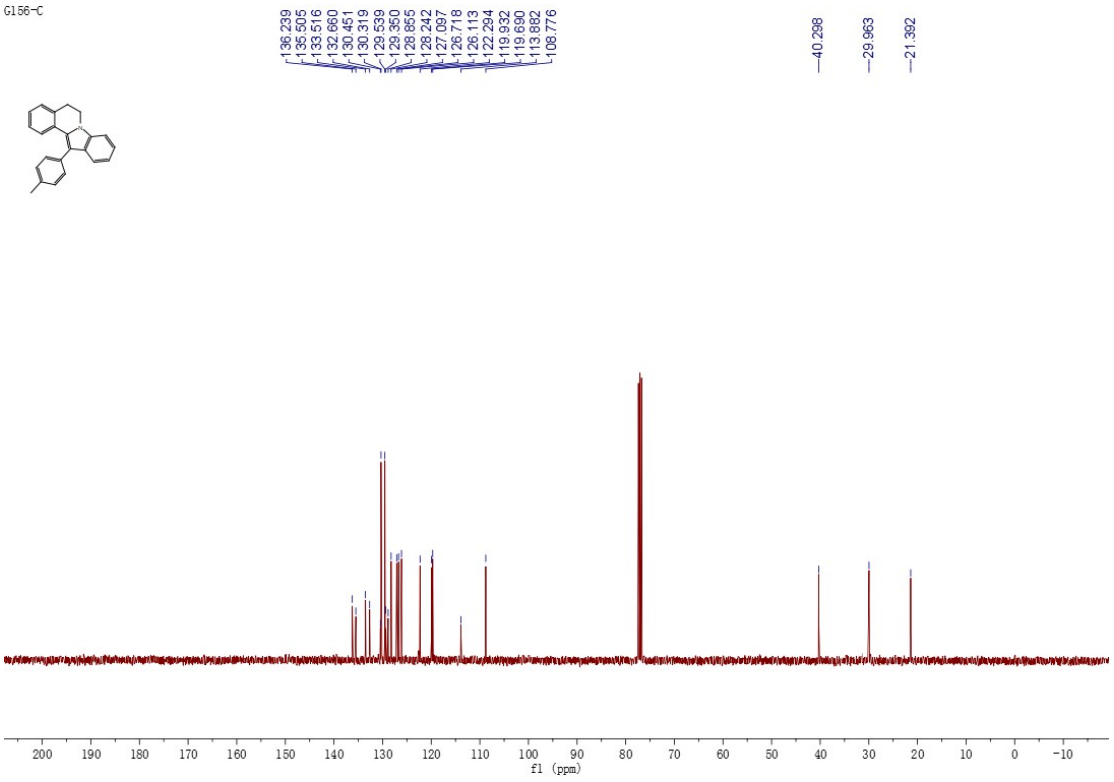
NMR of 2e


G111-H
7.622
7.604
7.583
7.564
7.528
7.509
7.490
7.402
7.383
7.385
7.292
7.289
7.284
7.272
7.254
7.153
7.134
7.116
6.965
6.790
4.306
4.291
4.274
3.930
3.436
3.201
3.185
3.169
2.07
0.91
1.85
1.98
1.20
1.03
0.98
0.95
1.99
3.00
3.05
2.04
f1 (ppm)

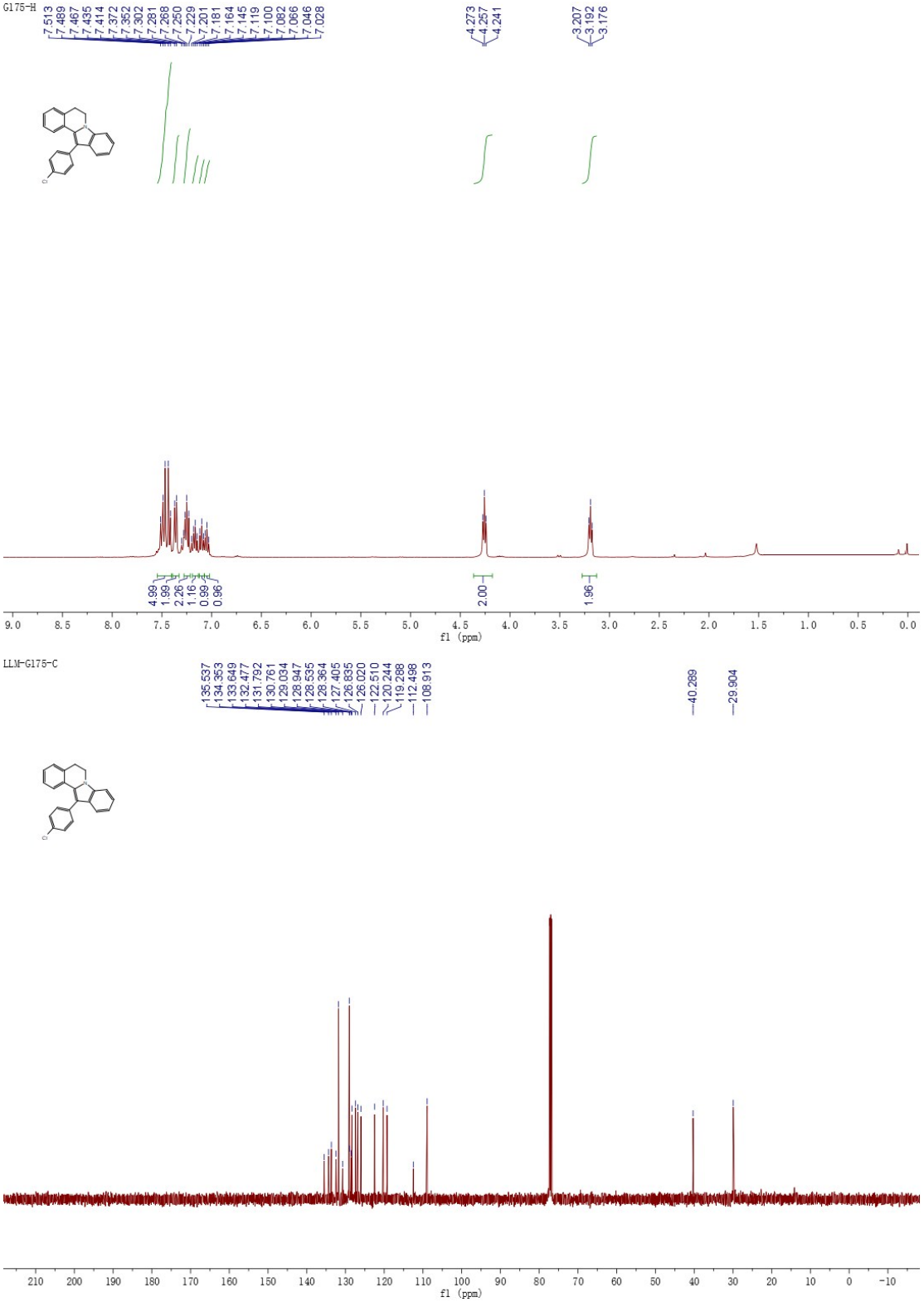

LYM-G111-C
148.208
147.476
135.966
130.856
128.700
126.698
126.104
121.955
121.623
119.932
112.845
111.105
109.186
108.656
55.951
55.235
40.429
29.321
f1 (ppm)

NMR of 2f

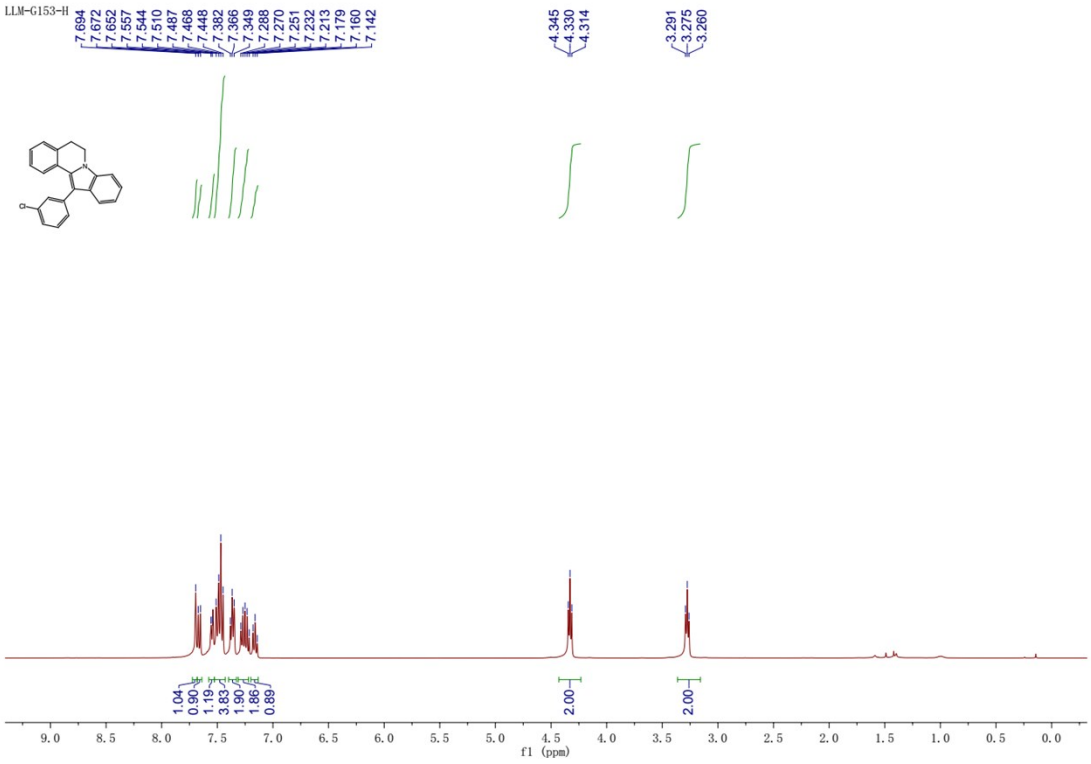

LLM-G156-S-H
7.606
7.589
7.495
7.474
7.415
7.394
7.330
7.309
7.286
7.267
7.209
7.191
7.172
7.152
7.134
7.115
7.095
7.077
7.057
4.330
4.314
4.298
3.264
3.248
3.232
2.496
1.10
2.94
1.25
3.80
1.16
1.01
1.07
2.02
2.02
3.00
f1 (ppm)

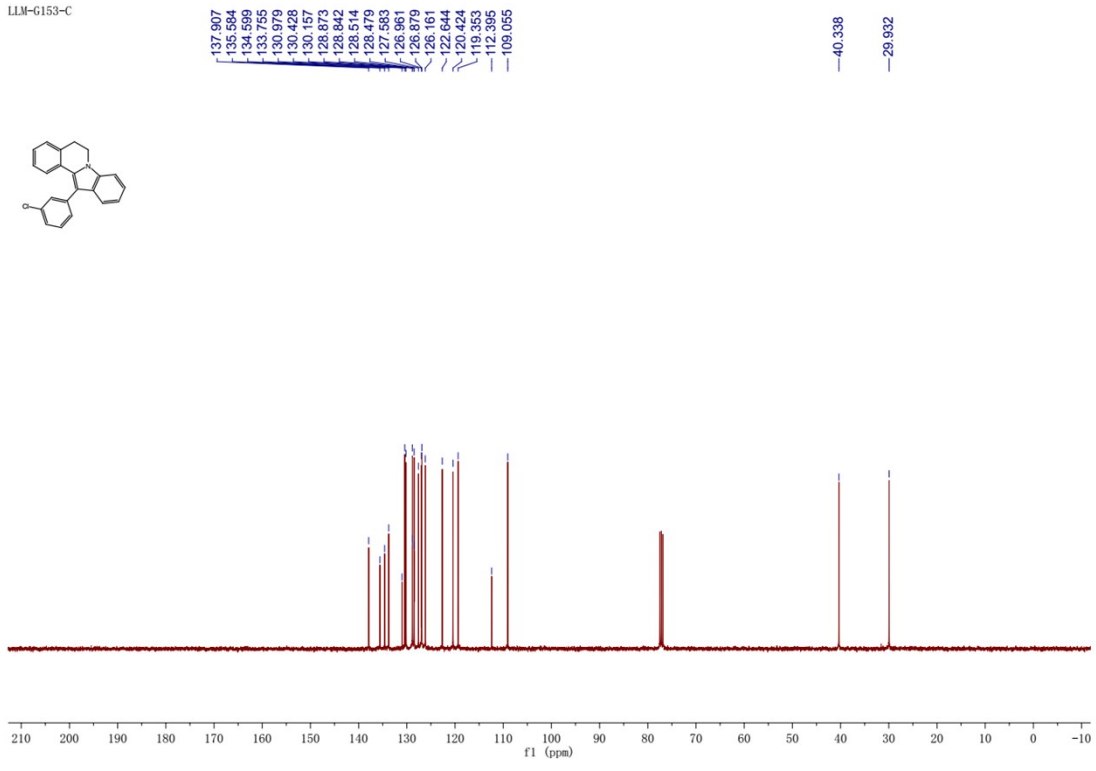

G156-C
136.239
135.505
133.516
132.660
130.451
130.319
129.539
129.350
128.855
128.242
127.097
126.718
126.113
122.294
119.932
119.690
113.882
108.776
40.298
29.963
21.392
f1 (ppm)

NMR of 2g

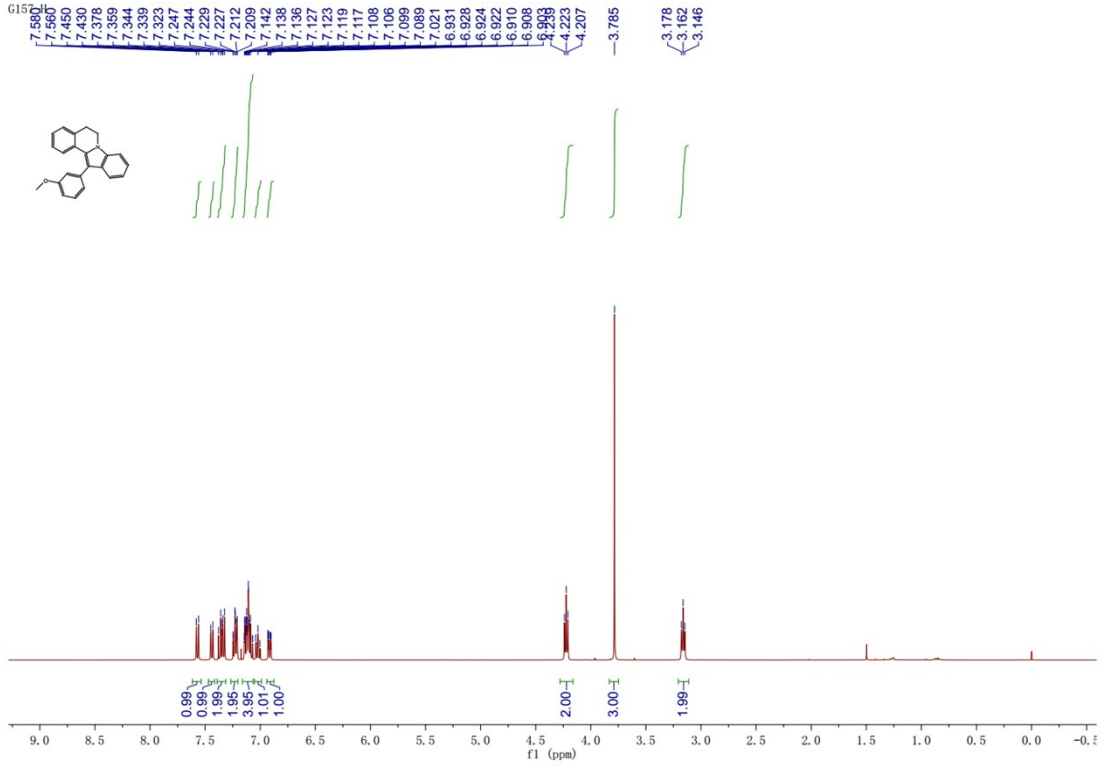

G175-H
7.513
7.489
7.467
7.435
7.414
7.372
7.352
7.302
7.281
7.268
7.250
7.229
7.201
7.181
7.164
7.145
7.119
7.100
7.082
7.066
7.046
7.028
4.273
4.257
4.241
3.207
3.192
3.176
4.99
1.99
2.26
1.16
0.99
0.96
2.00
1.96
f1 (ppm)
LLM-G175-C
135.537
134.353
133.649
132.477
131.792
130.761
129.034
128.947
128.535
128.364
127.405
126.835
126.020
122.510
120.244
119.288
112.498
108.913
40.289
29.904
f1 (ppm)

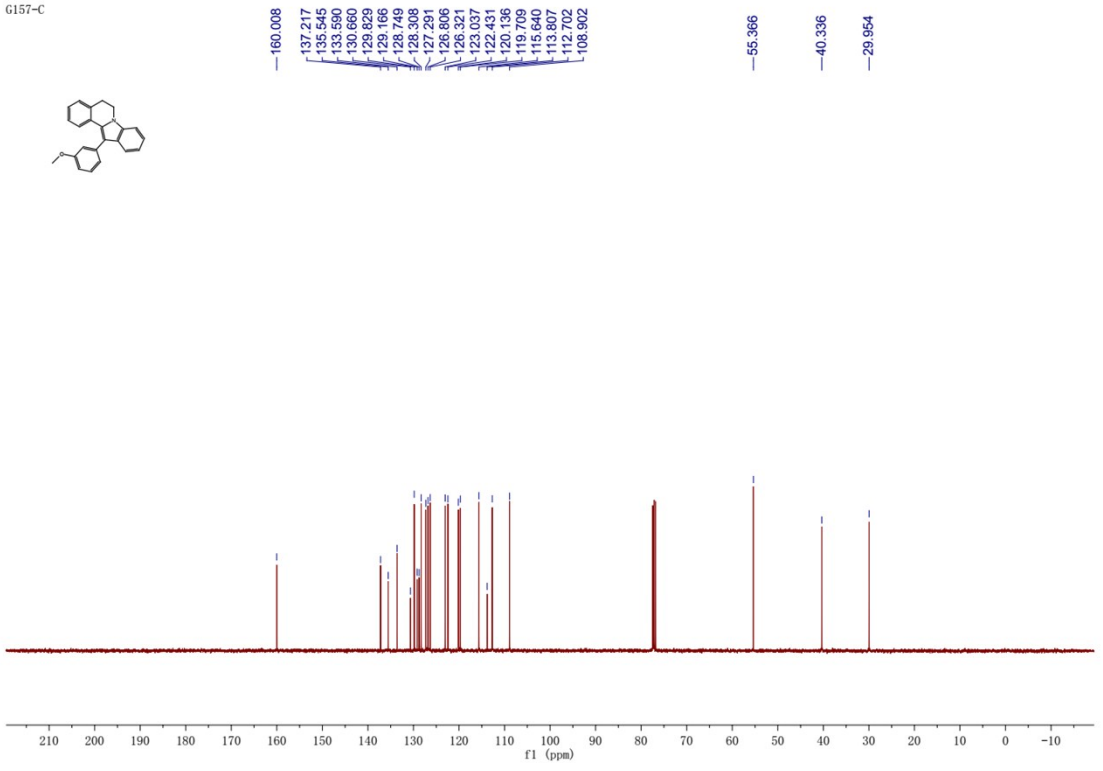
NMR of 2h


LLM-G153-H
7.694
7.672
7.652
7.557
7.544
7.510
7.487
7.468
7.448
7.382
7.366
7.349
7.288
7.270
7.251
7.232
7.213
7.179
7.160
7.142
4.345
4.330
4.314
3.291
3.275
3.260
1.04
0.90
1.19
3.83
1.90
1.86
0.89
2.00
2.00
f1 (ppm)

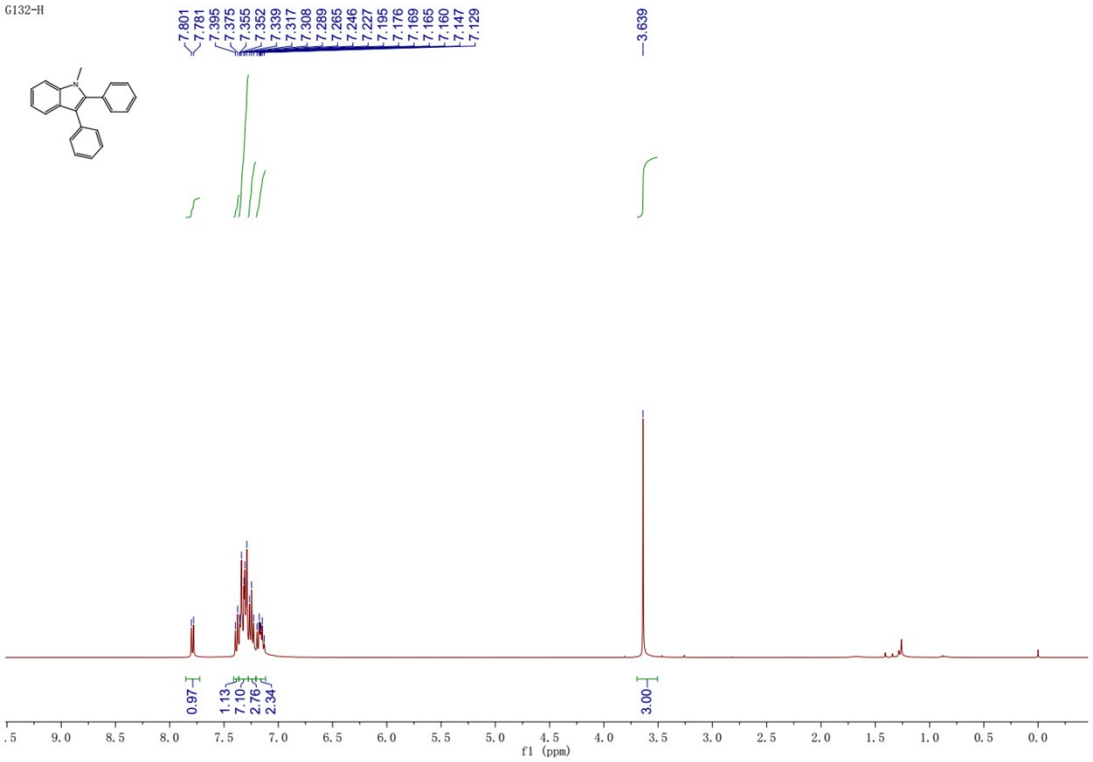

LLM-G153-C
137.907
135.584
134.599
133.755
130.979
130.428
130.157
128.873
128.842
128.514
128.479
127.583
126.961
126.879
126.161
122.644
120.424
119.353
112.395
109.055
40.338
29.932
f1 (ppm)

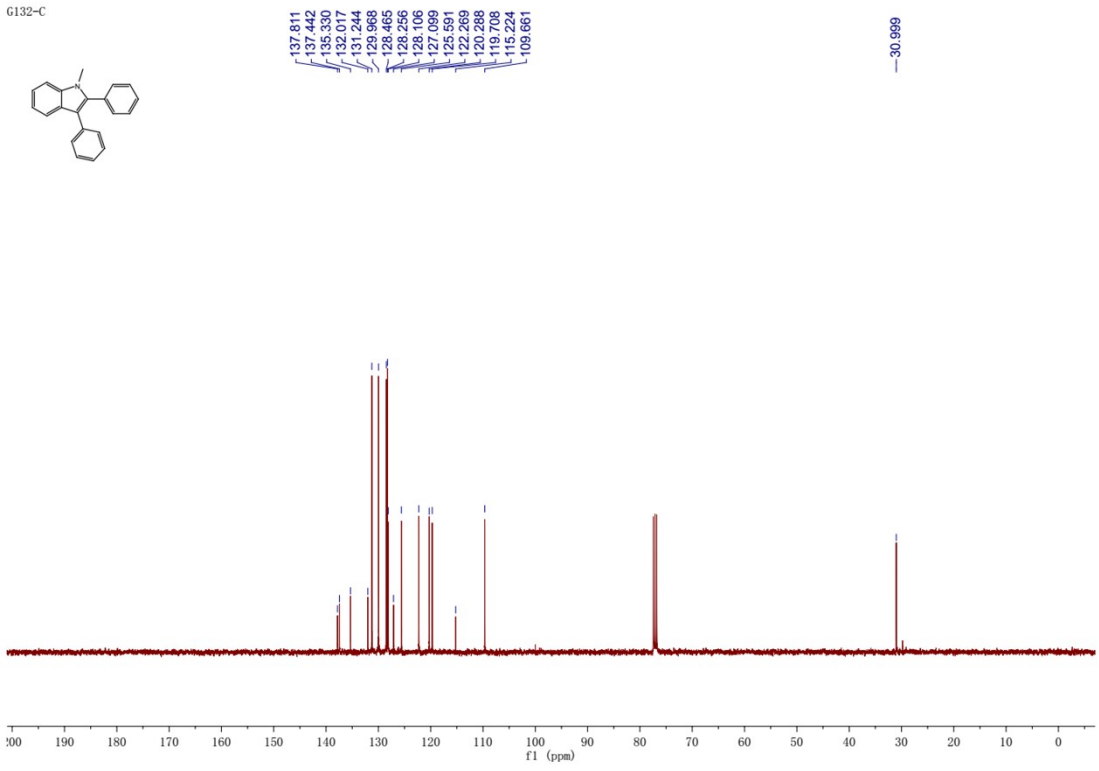
NMR of 2i


G157-H
7.590
7.560
7.450
7.430
7.378
7.359
7.344
7.339
7.323
7.247
7.244
7.229
7.227
7.212
7.209
7.142
7.138
7.136
7.127
7.123
7.119
7.117
7.108
7.106
7.099
7.089
7.021
6.931
6.928
6.924
6.922
6.910
6.908
4.223
4.207
3.785
3.178
3.162
3.146
0.99
0.99
1.99
1.95
3.95
1.01
1.00
2.00
3.00
1.99
f1 (ppm)

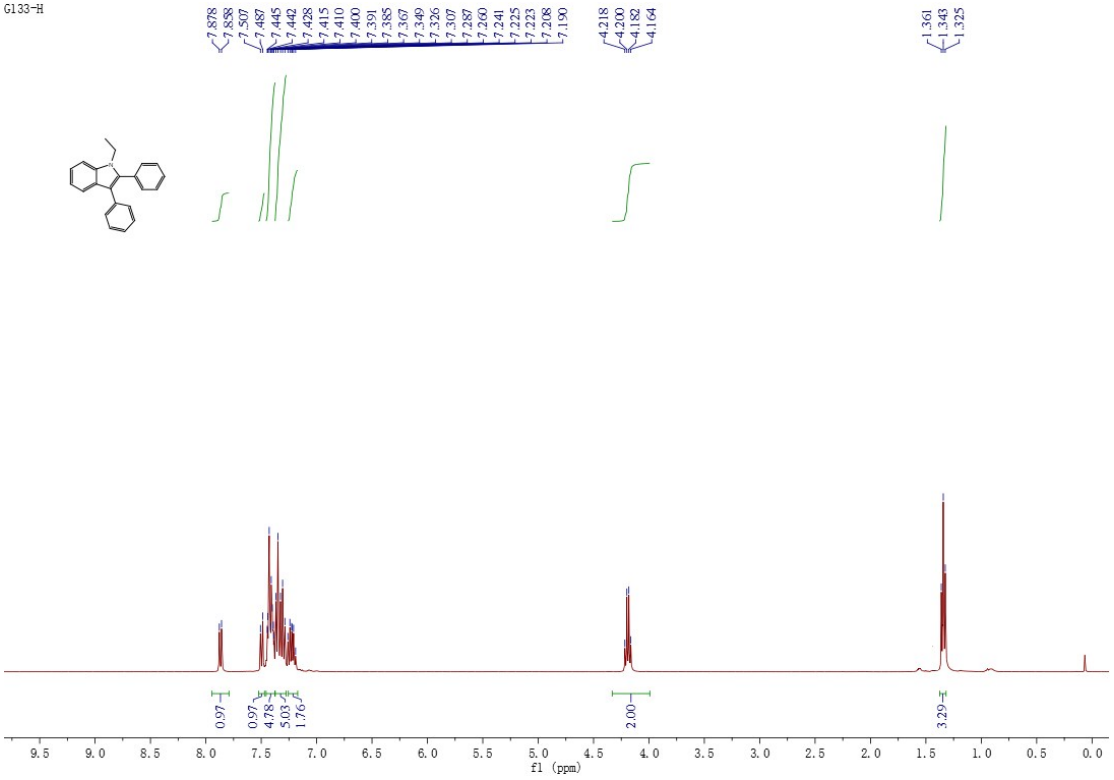

G157-C
160.008
137.217
135.545
133.590
130.660
129.829
129.166
128.749
128.308
127.291
126.806
126.321
123.037
122.431
120.136
119.709
115.640
113.807
112.702
108.902
55.366
40.336
29.954
f1 (ppm)

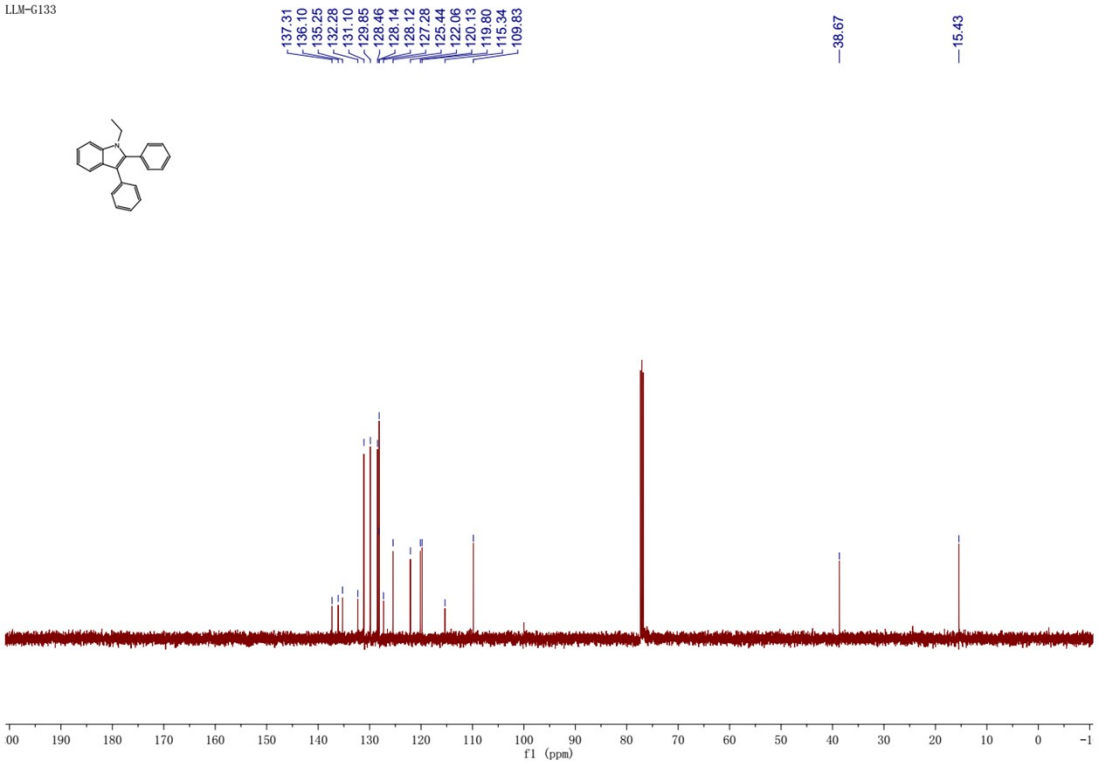
NMR of 2j


G132-H
7.801
7.781
7.395
7.375
7.355
7.352
7.339
7.317
7.308
7.289
7.265
7.246
7.227
7.195
7.176
7.169
7.165
7.160
7.147
7.129
3.639
0.97
1.13
7.10
2.76
2.34
3.00
f1 (ppm)

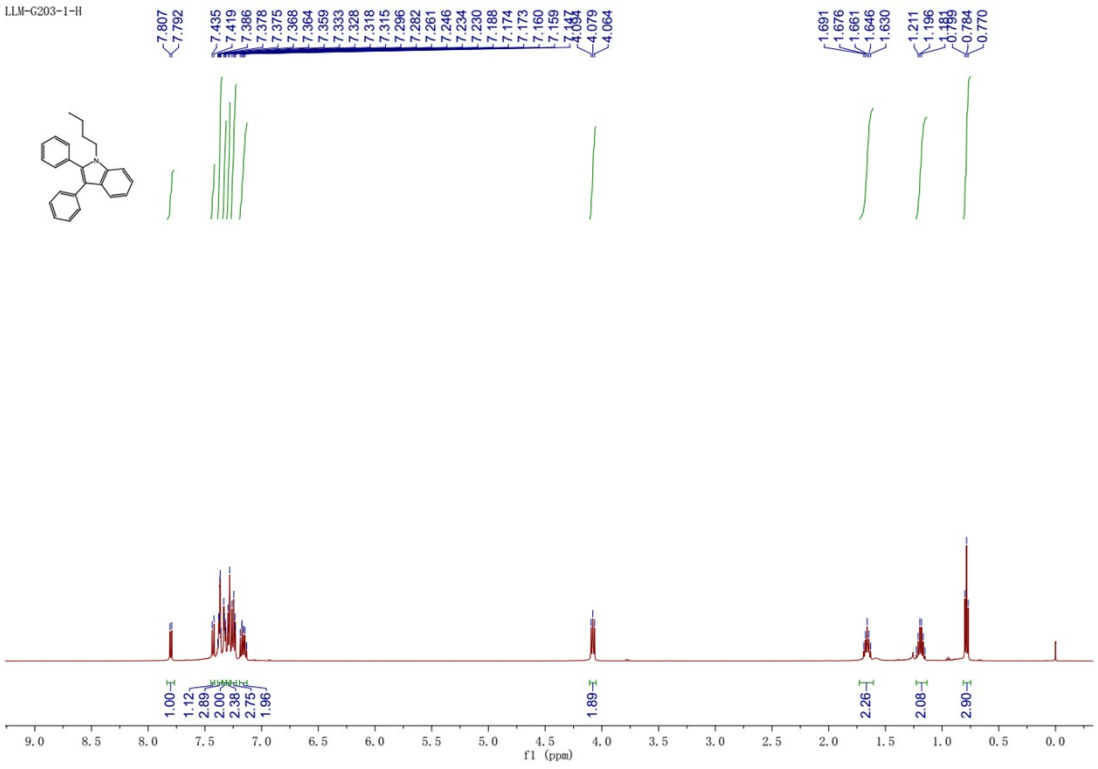

G132-C
137.811
137.442
135.330
132.017
131.244
129.968
128.465
128.256
128.106
127.099
125.591
122.269
120.288
119.708
115.224
109.661
30.999
f1 (ppm)

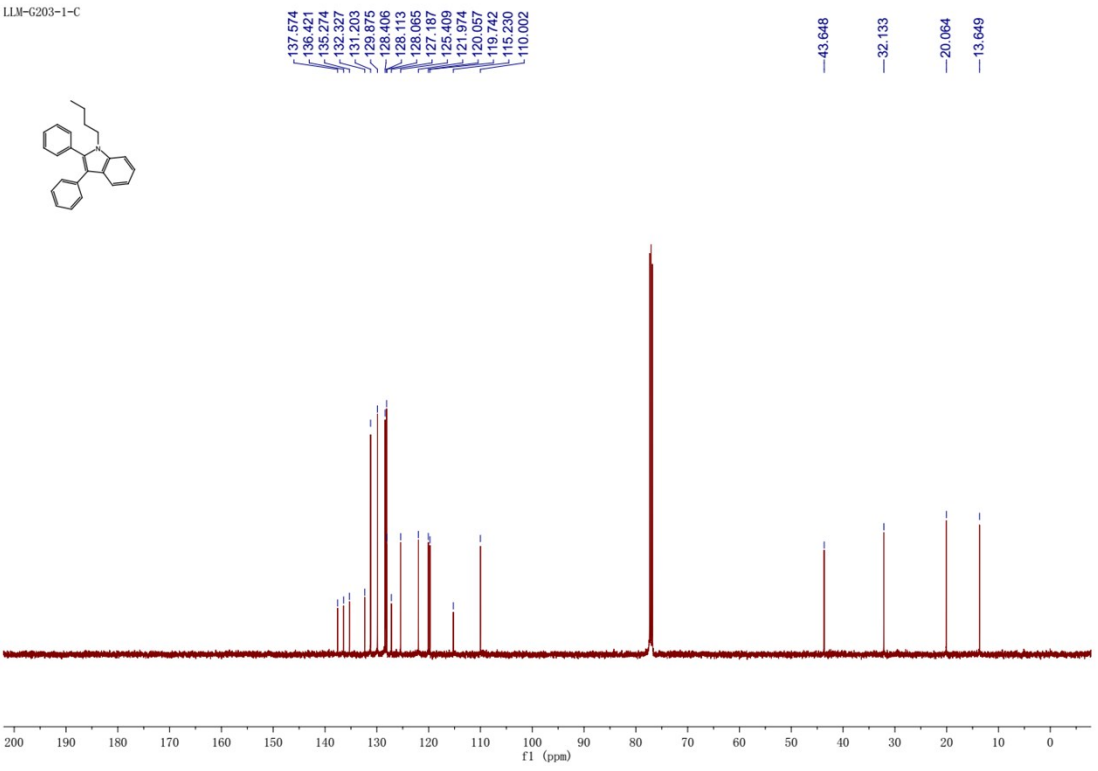
NMR of 2k


G133-H
7.878
7.858
7.507
7.487
7.445
7.442
7.428
7.415
7.410
7.400
7.391
7.385
7.367
7.349
7.326
7.307
7.287
7.260
7.241
7.225
7.223
7.208
7.190
4.218
4.200
4.182
4.164
1.361
1.343
1.325
0.97
0.97
4.78
5.03
1.76
2.00
3.29
f1 (ppm)

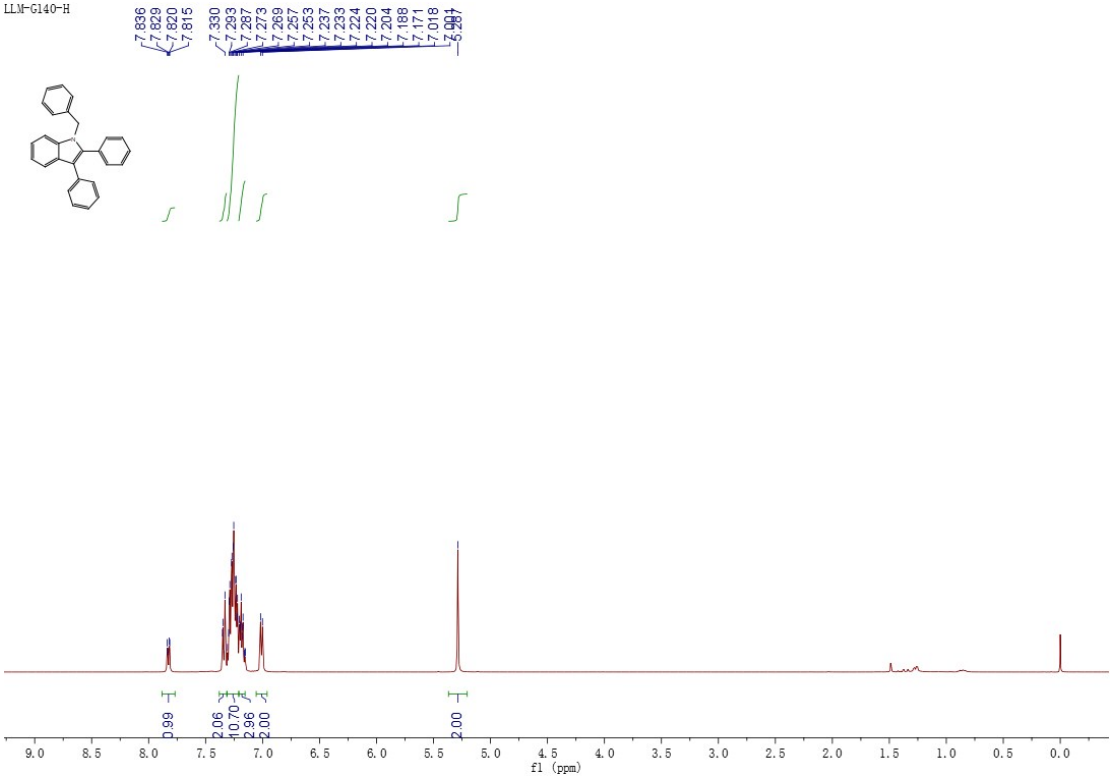

LLM-G133
137.31
136.10
135.25
132.28
131.10
129.85
128.46
128.14
128.12
127.28
125.44
122.06
120.13
119.80
115.34
109.83
38.67
15.43
f1 (ppm)

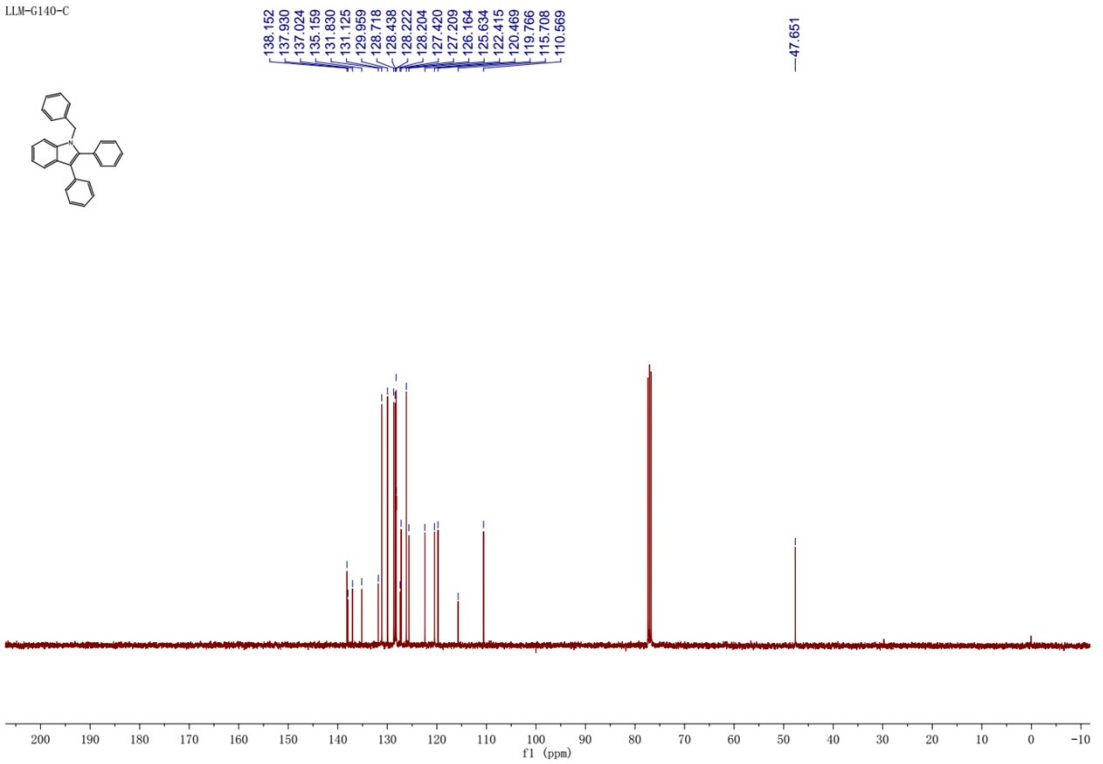
NMR of 2l


LLM-G203-1-H
7.807
7.792
7.435
7.419
7.386
7.378
7.375
7.368
7.364
7.359
7.333
7.328
7.318
7.315
7.296
7.282
7.261
7.246
7.234
7.230
7.188
7.174
7.173
7.160
7.159
4.079
4.064
1.691
1.676
1.661
1.646
1.630
1.211
1.196
0.784
0.770
1.00
1.12
2.89
2.00
2.38
2.75
1.96
1.89
2.26
2.08
2.90
f1 (ppm)

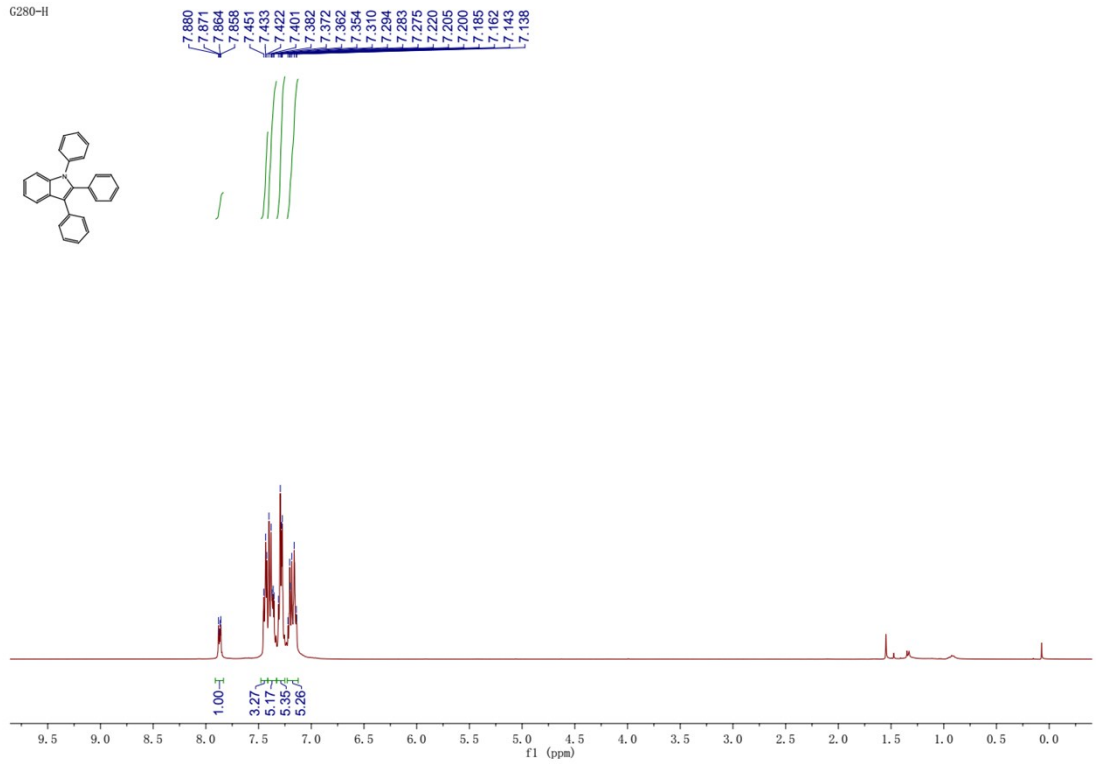

LLM-G203-1-C
137.574
136.421
135.274
132.327
131.203
129.875
128.406
128.113
128.065
127.187
125.409
121.974
120.057
119.742
115.230
110.002
43.648
32.133
20.064
13.649
f1 (ppm)

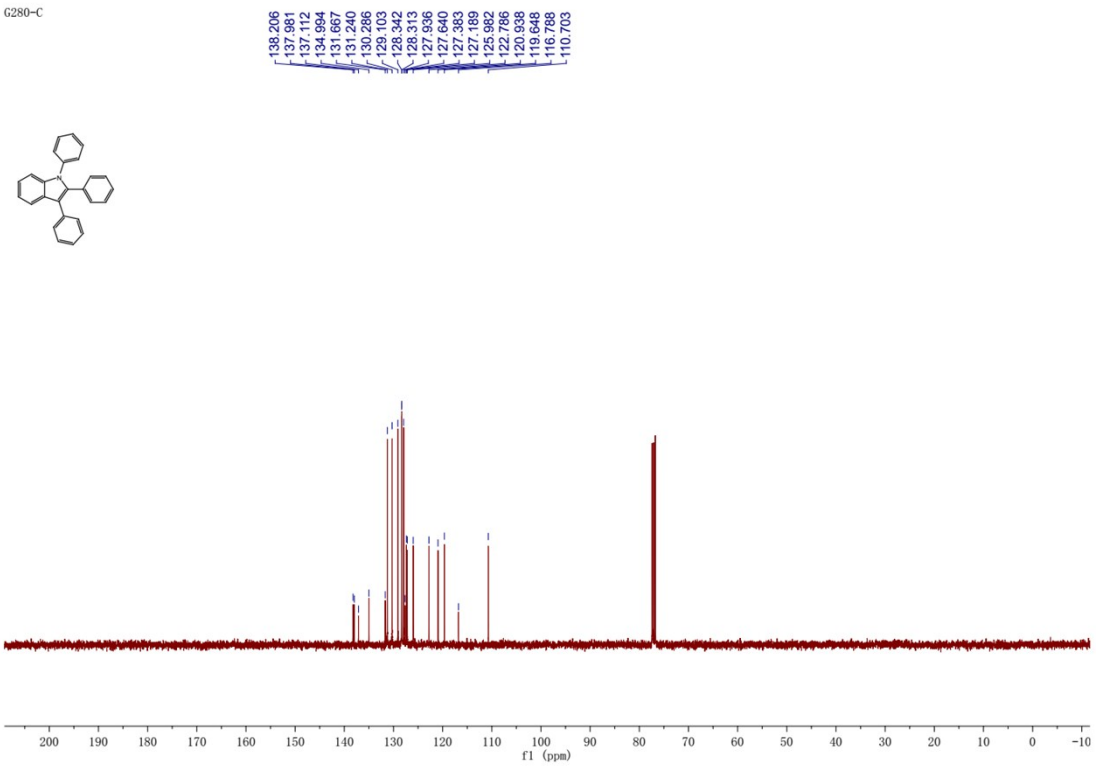
NMR of 2m


LLM-G140-H
7.836
7.829
7.820
7.815
7.330
7.293
7.287
7.273
7.269
7.257
7.253
7.237
7.233
7.224
7.220
7.204
7.188
7.171
7.018
5.287
0.99
2.06
10.70
2.96
2.00
2.00
f1 (ppm)

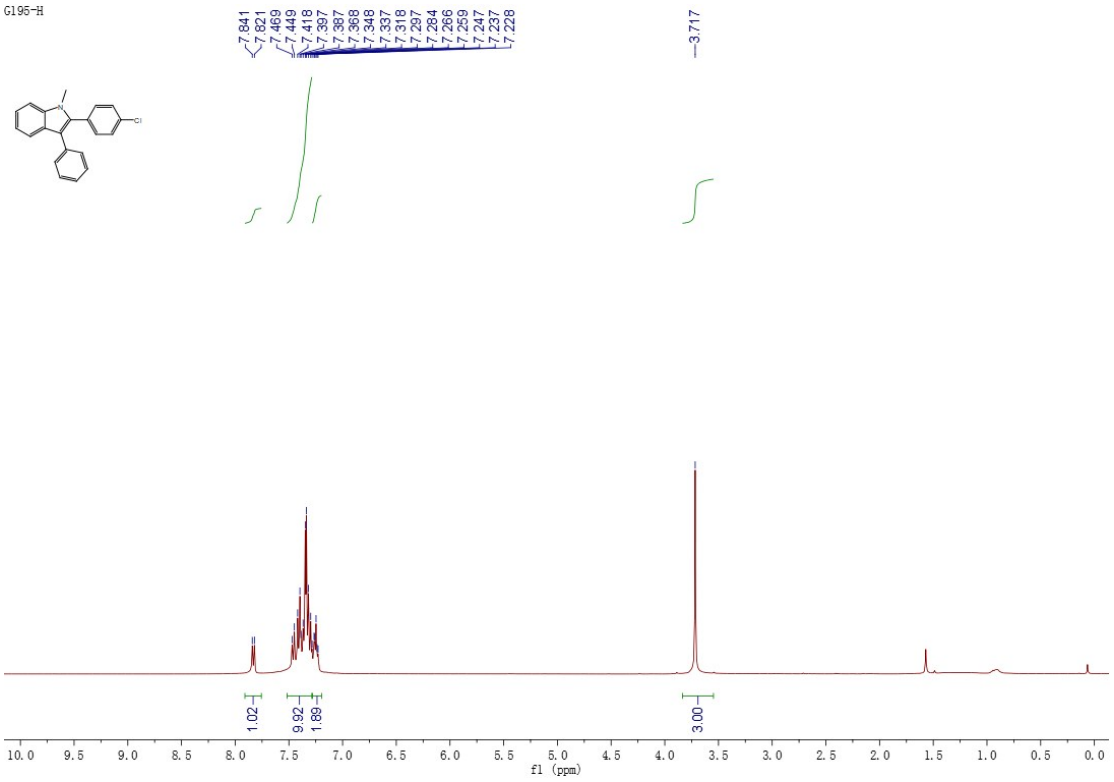

LLM-G140-C
138.152
137.930
137.024
135.159
131.830
131.125
129.959
128.718
128.438
128.222
128.204
127.420
127.209
126.164
125.634
122.415
120.469
119.766
115.708
110.569
47.651
f1 (ppm)

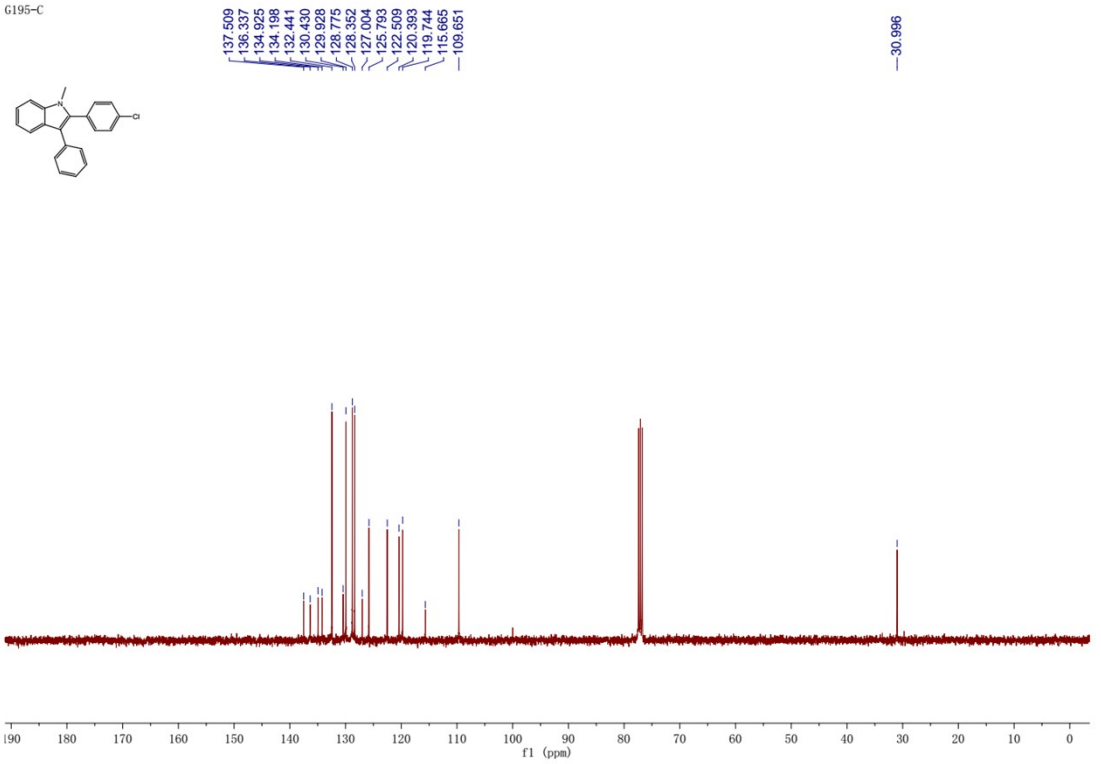
NMR of 2n


G280-H
7.880
7.871
7.864
7.858
7.451
7.433
7.422
7.401
7.382
7.372
7.362
7.354
7.310
7.294
7.283
7.275
7.220
7.205
7.200
7.185
7.162
7.143
7.138
1.00
3.27
5.17
5.35
5.26
f1 (ppm)

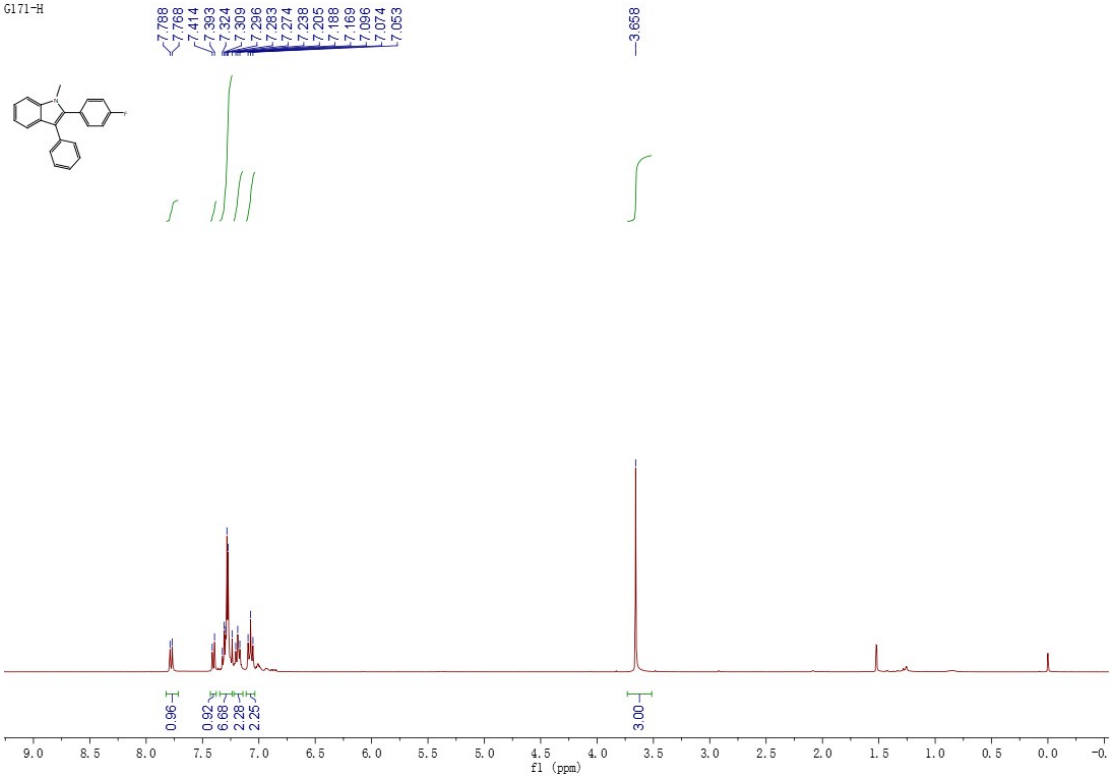

G280-C
138.206
137.981
137.112
134.994
131.667
131.240
130.286
129.103
128.342
128.313
127.936
127.640
127.383
127.189
125.982
122.786
120.938
119.648
116.788
110.703
f1 (ppm)

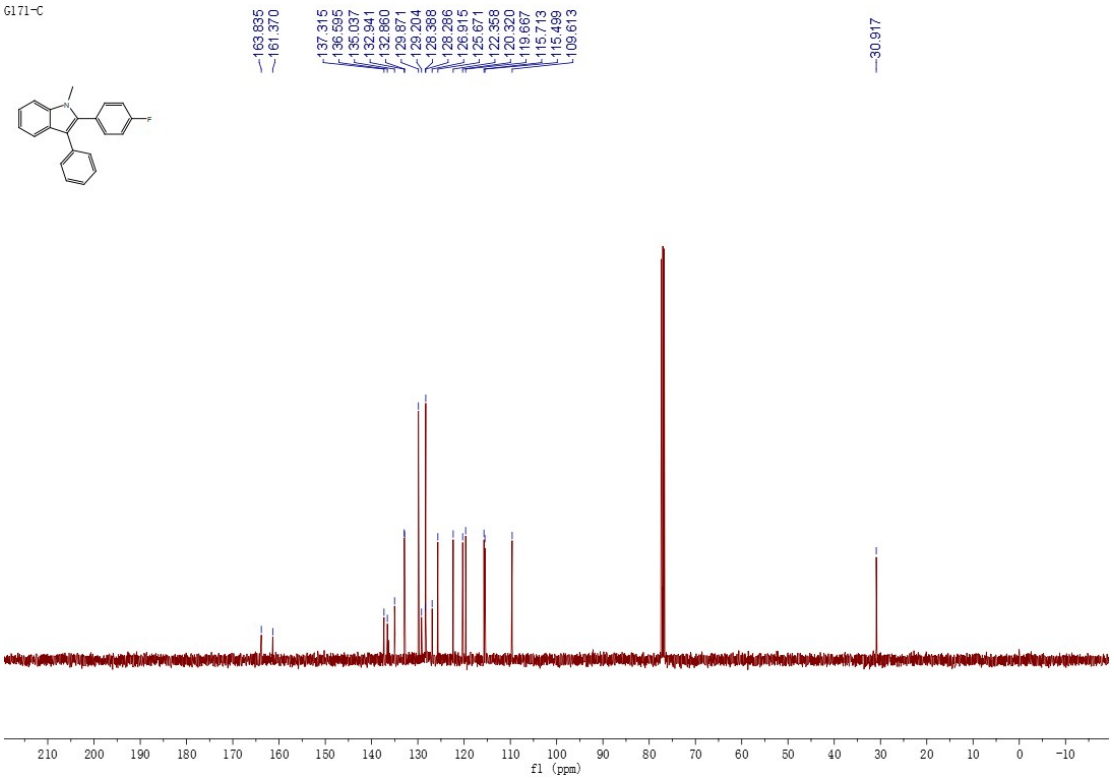
NMR of 2o


G195-H
7.841
7.821
7.469
7.449
7.418
7.397
7.387
7.368
7.348
7.337
7.318
7.297
7.284
7.266
7.259
7.247
7.237
7.228
3.717
1.02
9.92
1.89
3.00
f1 (ppm)

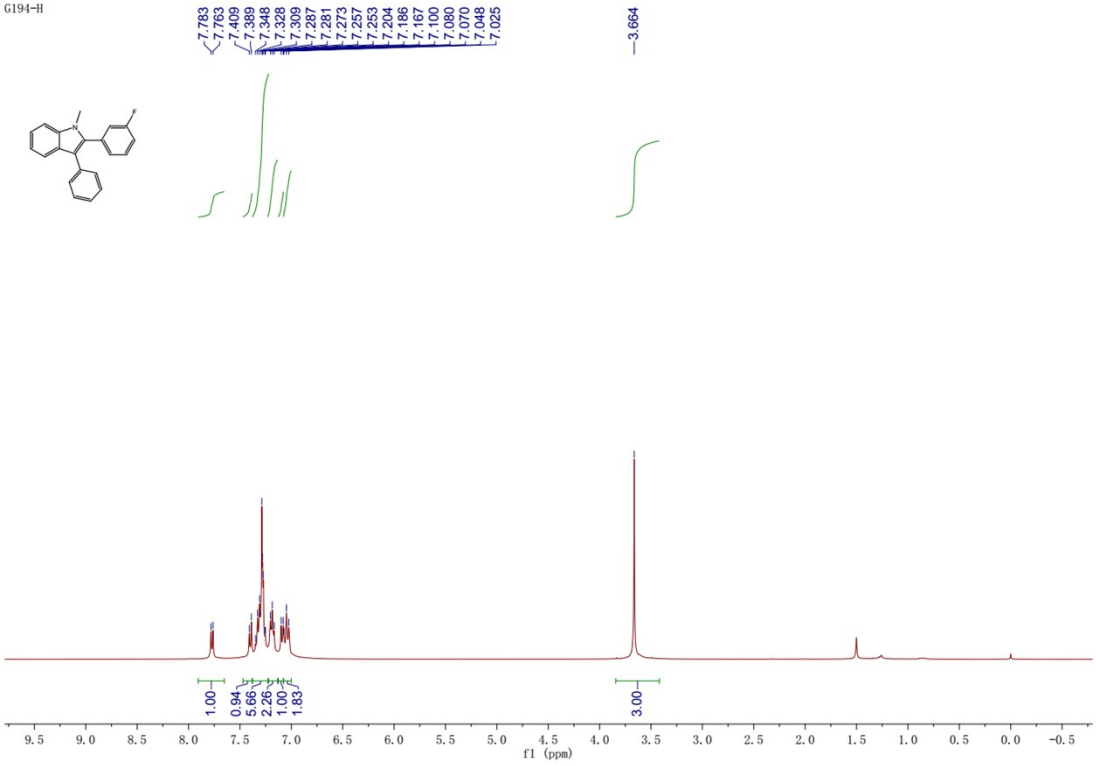

G195-C
137.509
136.337
134.925
134.198
132.441
130.430
129.928
128.775
128.352
127.004
125.793
122.509
120.393
119.744
115.665
109.651
30.996
f1 (ppm)

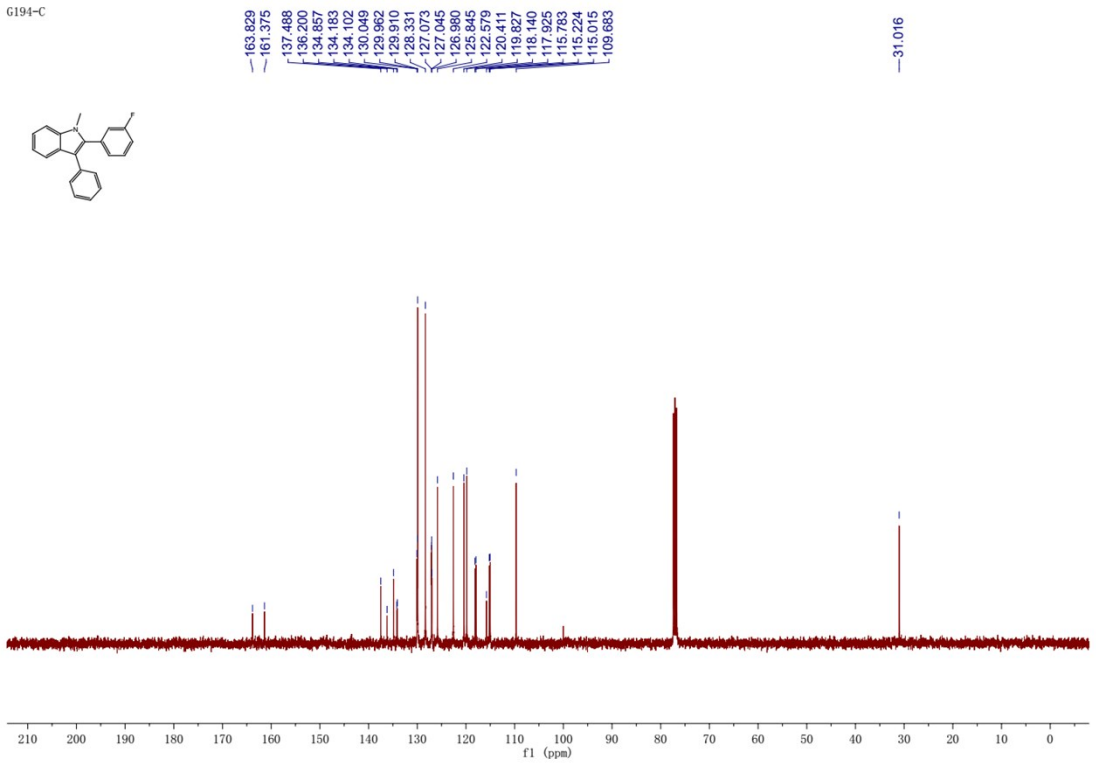
NMR of 2p


G171-H
7.788
7.768
7.414
7.393
7.324
7.309
7.296
7.283
7.274
7.238
7.205
7.188
7.169
7.096
7.074
7.053
3.658
0.96
0.92
6.68
2.28
2.25
3.00
f1 (ppm)

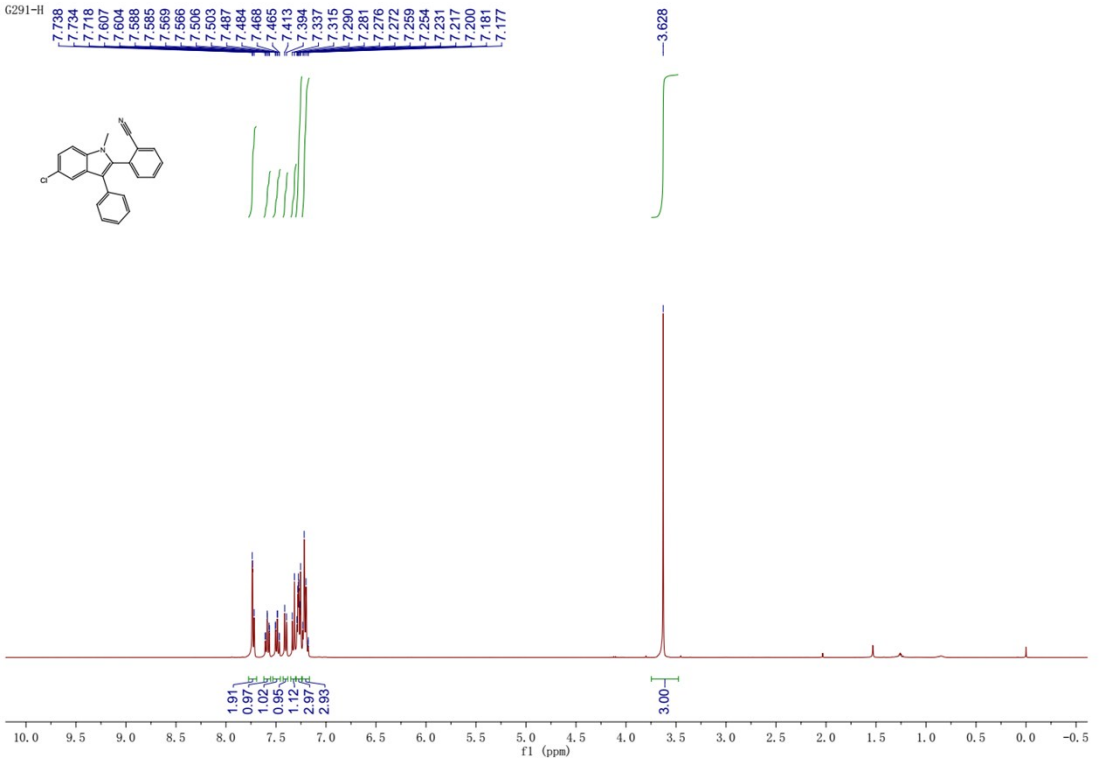

G171-C
163.835
161.370
137.315
136.595
135.037
132.941
132.860
129.871
129.204
128.388
128.286
126.915
125.671
122.358
120.320
119.667
115.713
115.499
109.613
30.917
f1 (ppm)

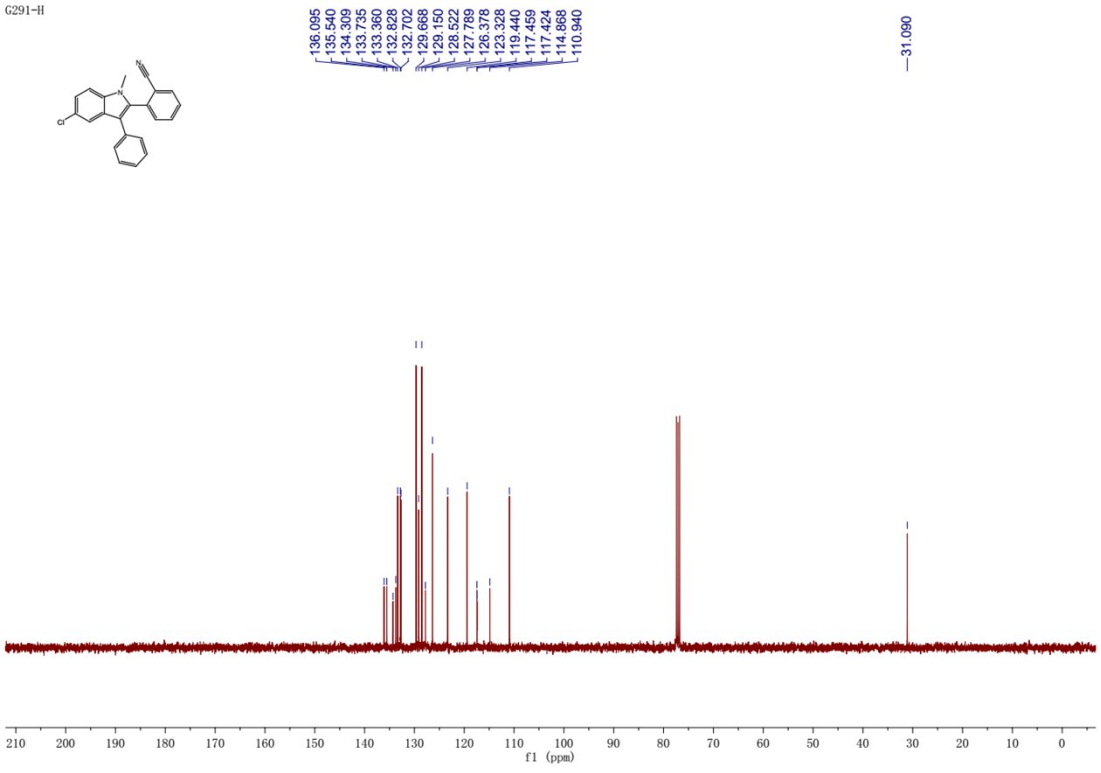
NMR of 2q


G194-H
7.783
7.763
7.409
7.389
7.348
7.328
7.309
7.287
7.281
7.273
7.257
7.253
7.204
7.186
7.167
7.100
7.080
7.070
7.048
7.025
3.664
1.00
0.94
5.66
2.26
1.00
1.83
3.00
f1 (ppm)

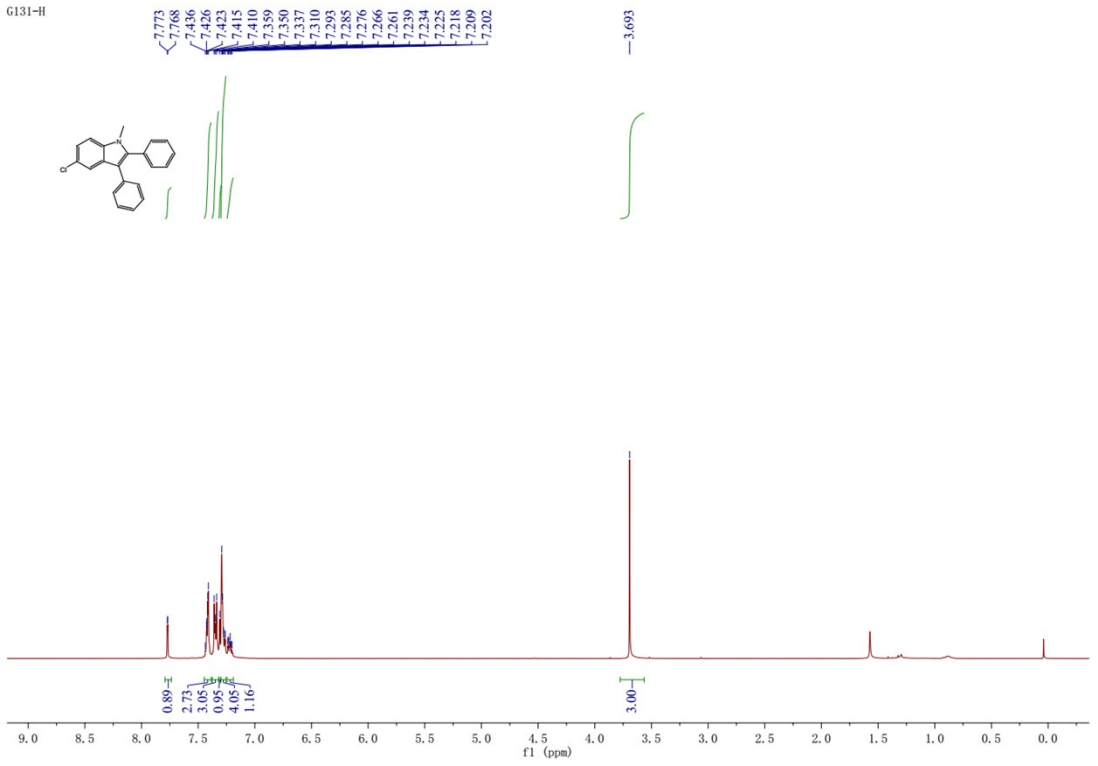

G194-C
163.829
161.375
137.488
136.200
134.857
134.183
134.102
130.049
129.962
129.910
128.331
127.073
127.045
126.980
125.845
122.579
120.411
119.827
118.140
117.925
115.783
115.224
115.015
109.683
31.016
f1 (ppm)

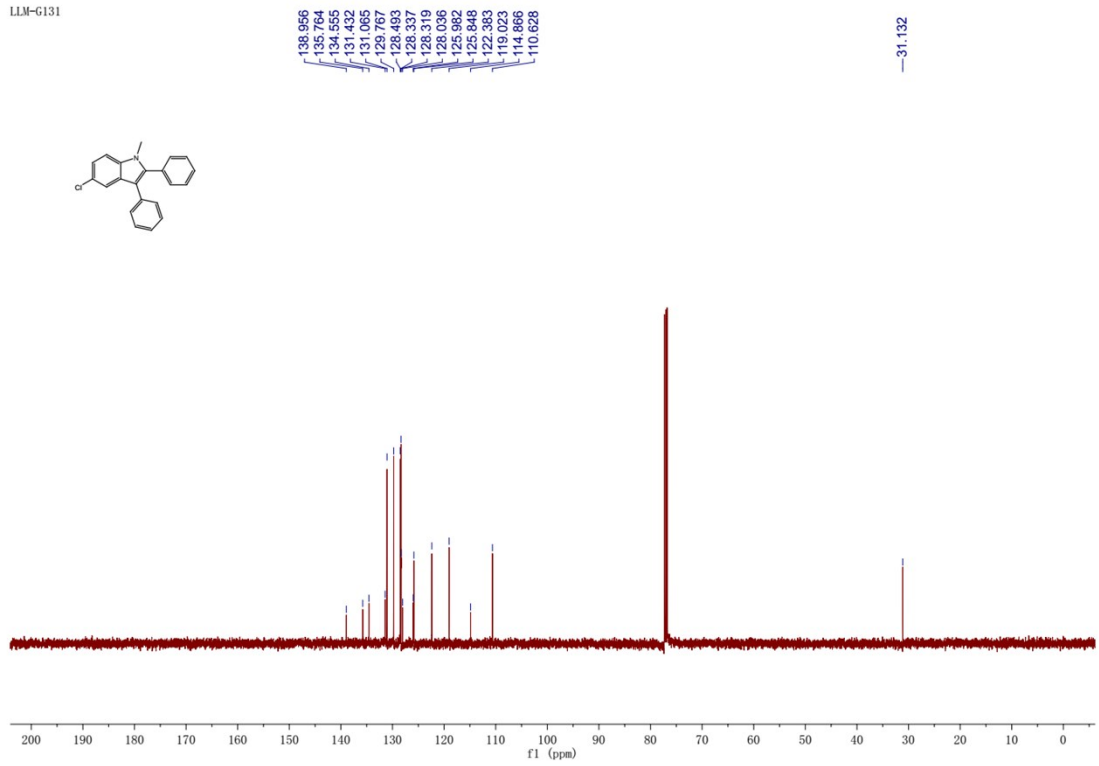
NMR of 2r


G291-H
7.738
7.734
7.718
7.607
7.604
7.588
7.585
7.569
7.566
7.506
7.503
7.487
7.484
7.468
7.465
7.413
7.394
7.337
7.315
7.290
7.281
7.276
7.272
7.259
7.254
7.231
7.217
7.200
7.181
7.177
3.628
1.91
0.97
1.02
0.95
1.12
2.97
2.93
3.00
f1 (ppm)

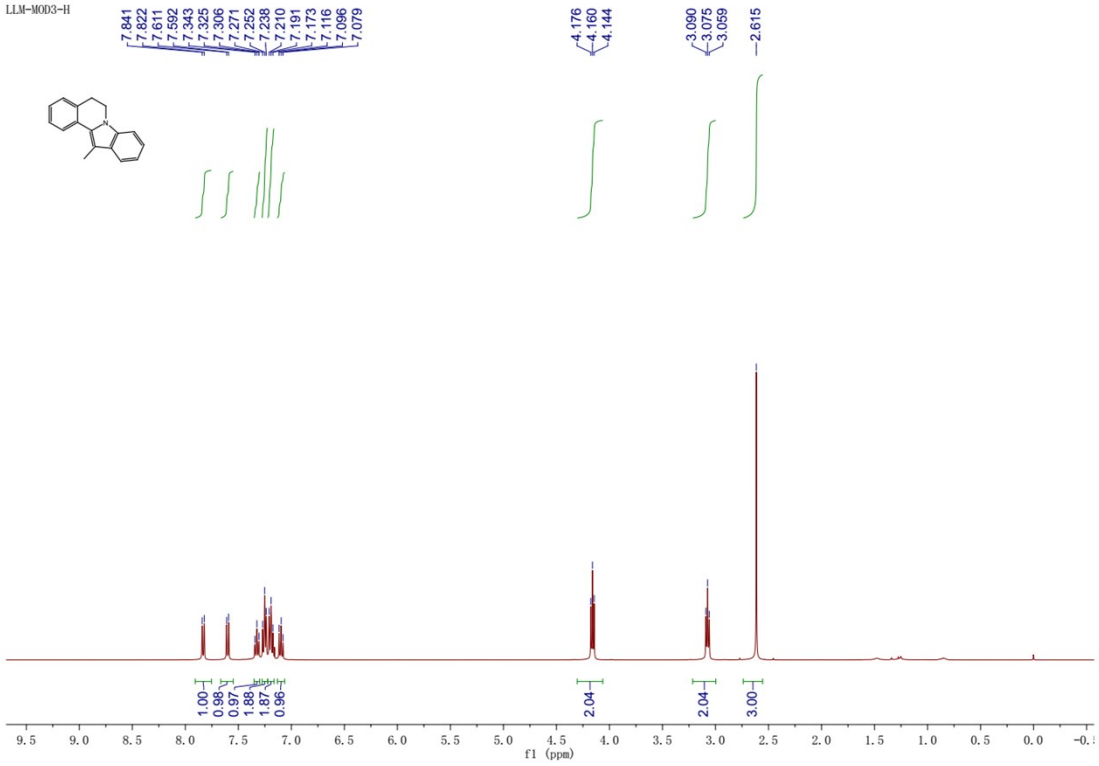

G291-H
136.095
135.540
134.309
133.735
133.360
132.828
132.702
129.668
129.150
128.522
127.789
126.378
123.328
119.440
117.459
117.424
114.868
110.940
31.090
f1 (ppm)

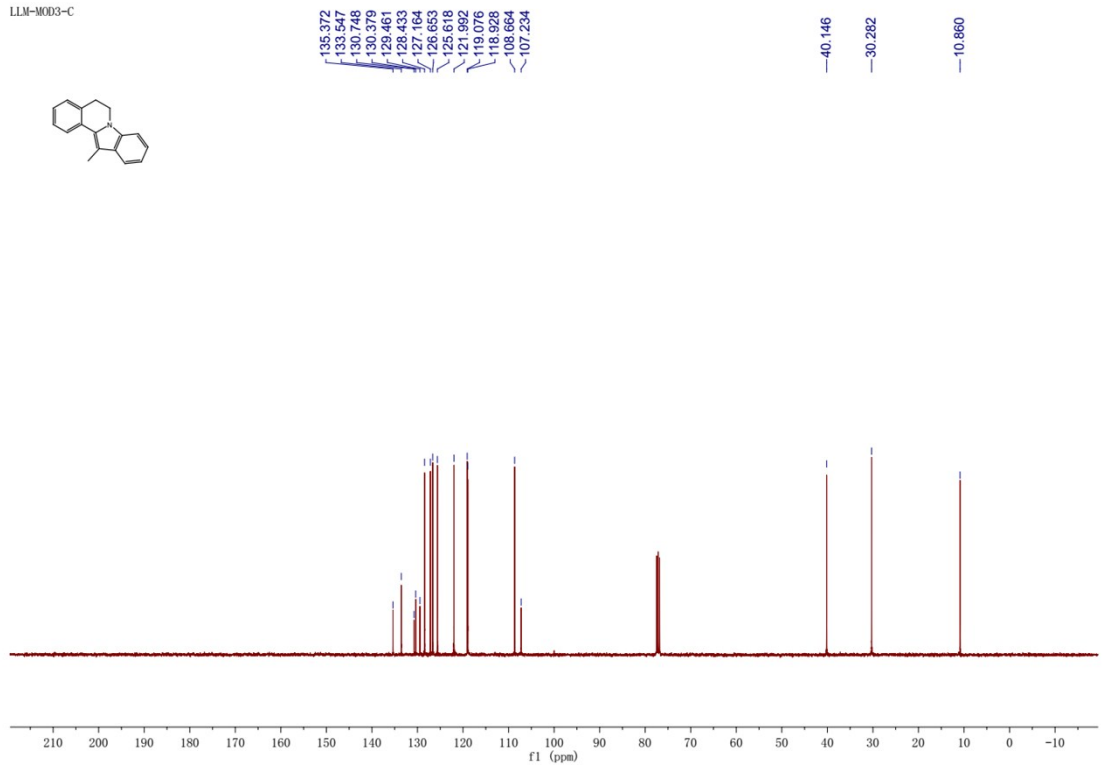
NMR of 2s


G131-H
7.773
7.768
7.436
7.426
7.423
7.415
7.410
7.359
7.350
7.337
7.310
7.293
7.285
7.276
7.266
7.261
7.239
7.234
7.225
7.218
7.209
7.202
3.693
0.89
2.73
3.05
0.95
4.05
1.16
3.00
f1 (ppm)

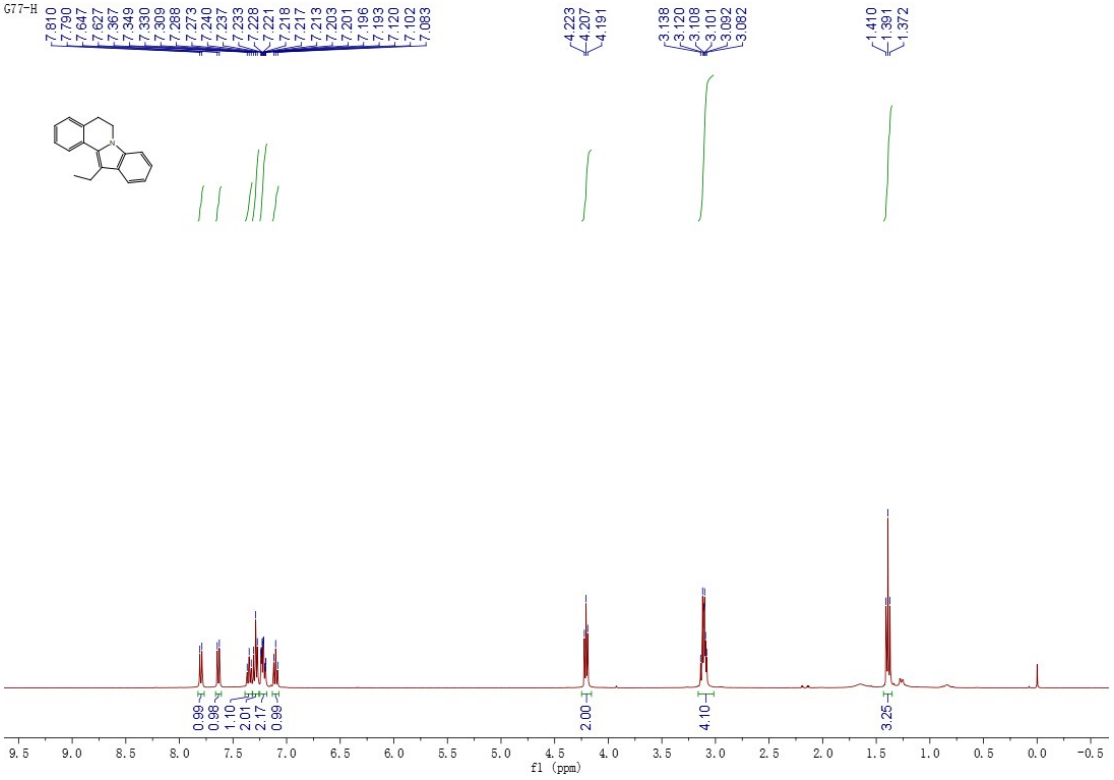

LLM-G131
138.956
135.764
134.555
131.432
131.065
129.767
128.493
128.337
128.319
128.036
125.982
125.848
122.383
119.023
114.866
110.628
31.132
f1 (ppm)

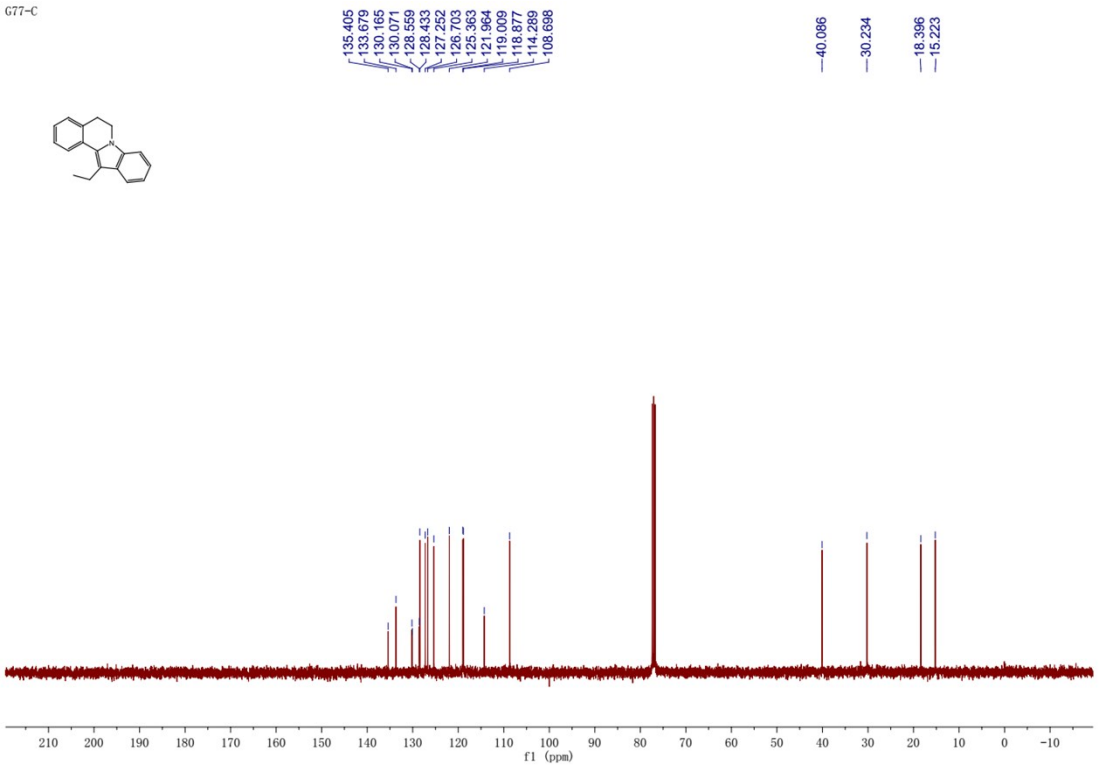
NMR of 2aa


LLM-MOD3-H
7.841
7.822
7.611
7.592
7.343
7.325
7.306
7.271
7.252
7.238
7.210
7.191
7.173
7.116
7.096
7.079
4.176
4.160
4.144
3.090
3.075
3.059
2.615
1.00
0.98
0.97
1.88
1.87
0.96
2.04
2.04
3.00
f1 (ppm)

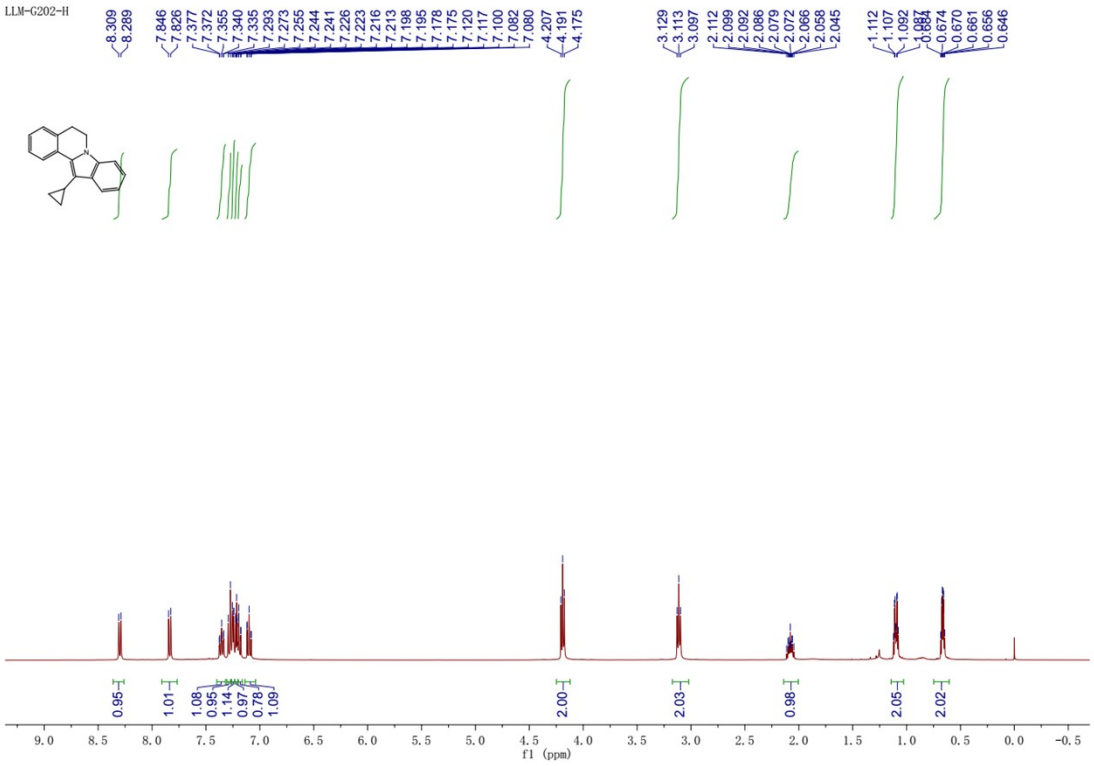

LLM-MOD3-C
135.372
133.547
130.748
130.379
129.461
128.433
127.164
126.653
125.618
121.992
119.076
118.928
108.664
107.234
40.146
30.282
10.860
f1 (ppm)

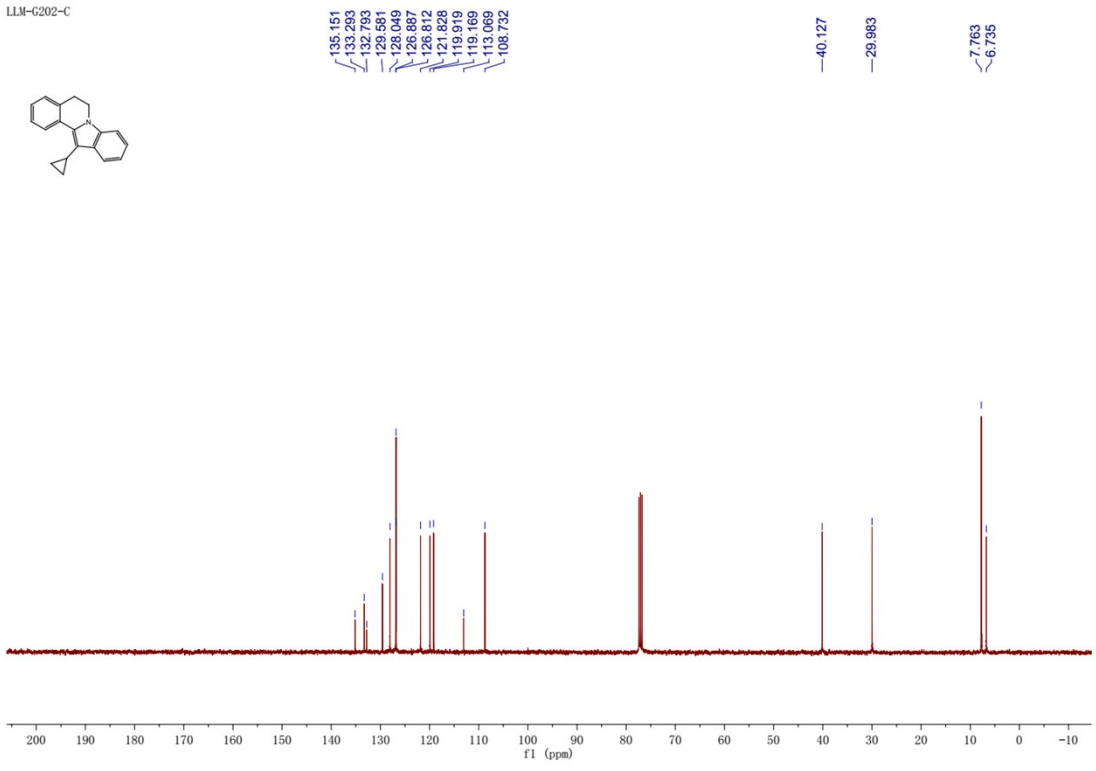
NMR of 2ab


G77-H
7.810
7.790
7.647
7.627
7.367
7.349
7.330
7.309
7.288
7.273
7.240
7.237
7.233
7.228
7.221
7.218
7.217
7.213
7.203
7.201
7.196
7.193
7.120
7.102
7.083
4.223
4.207
4.191
3.138
3.120
3.108
3.101
3.092
3.082
1.410
1.391
1.372
0.99
0.98
1.10
2.01
2.17
0.99
2.00
4.10
3.25
f1 (ppm)

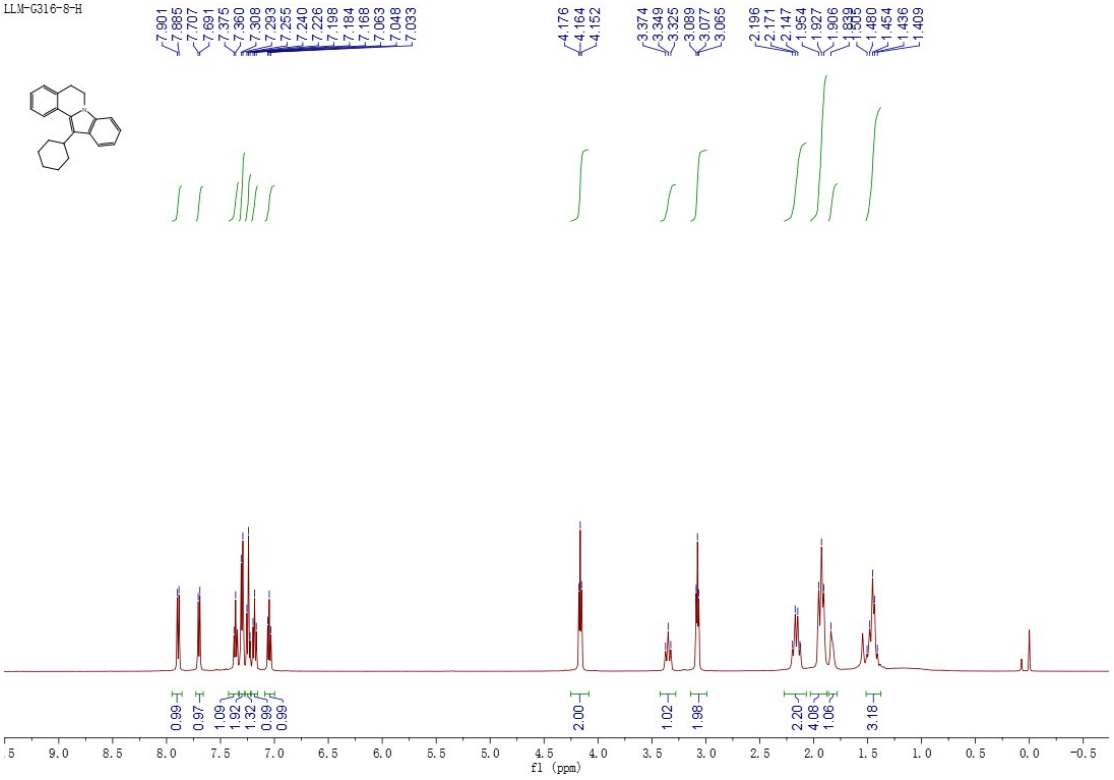

G77-C
135.405
133.679
130.165
130.071
128.559
128.433
127.252
126.703
125.363
121.964
119.009
118.877
114.289
108.698
40.086
30.234
18.396
15.223
f1 (ppm)

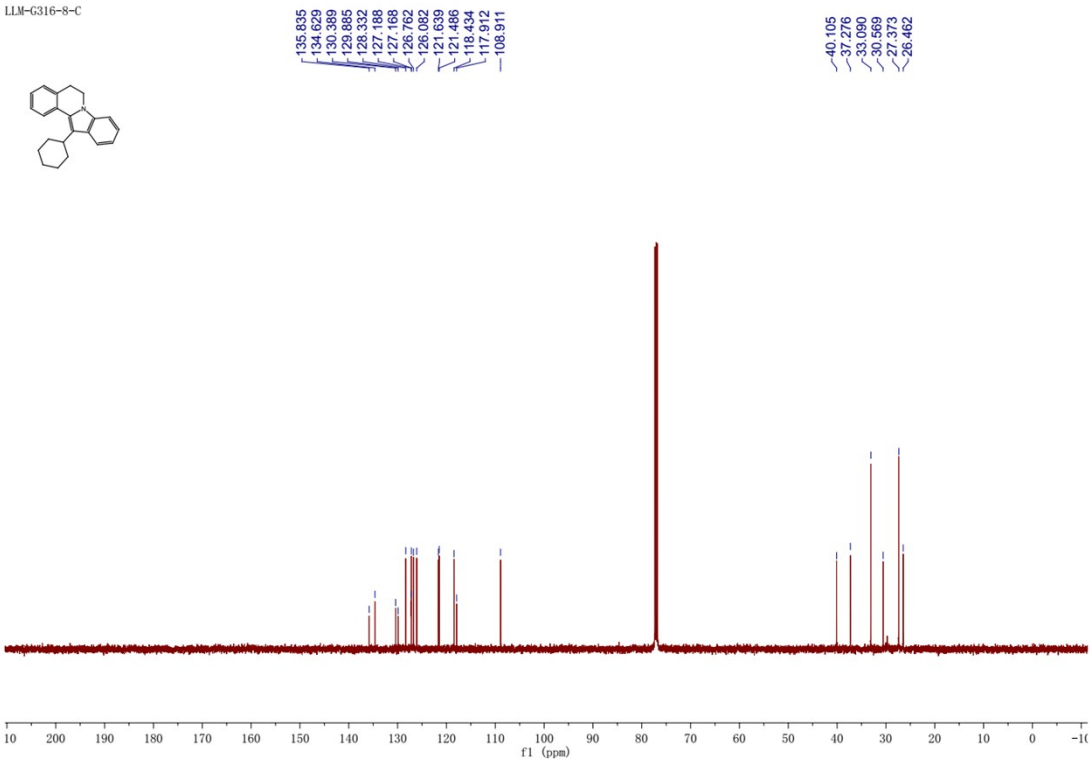
NMR of 2ac


LLM-G202-H
8.309
8.289
7.846
7.826
7.377
7.372
7.355
7.340
7.335
7.293
7.273
7.255
7.244
7.241
7.226
7.223
7.216
7.213
7.198
7.195
7.178
7.175
7.120
7.117
7.100
7.082
7.080
4.207
4.191
4.175
3.129
3.113
3.097
2.112
2.099
2.092
2.086
2.079
2.072
2.066
2.058
2.045
1.112
1.107
1.092
0.674
0.670
0.661
0.656
0.646
0.95
1.01
1.08
0.95
1.14
0.97
0.78
1.09
2.00
2.03
0.98
2.05
2.02
f1 (ppm)

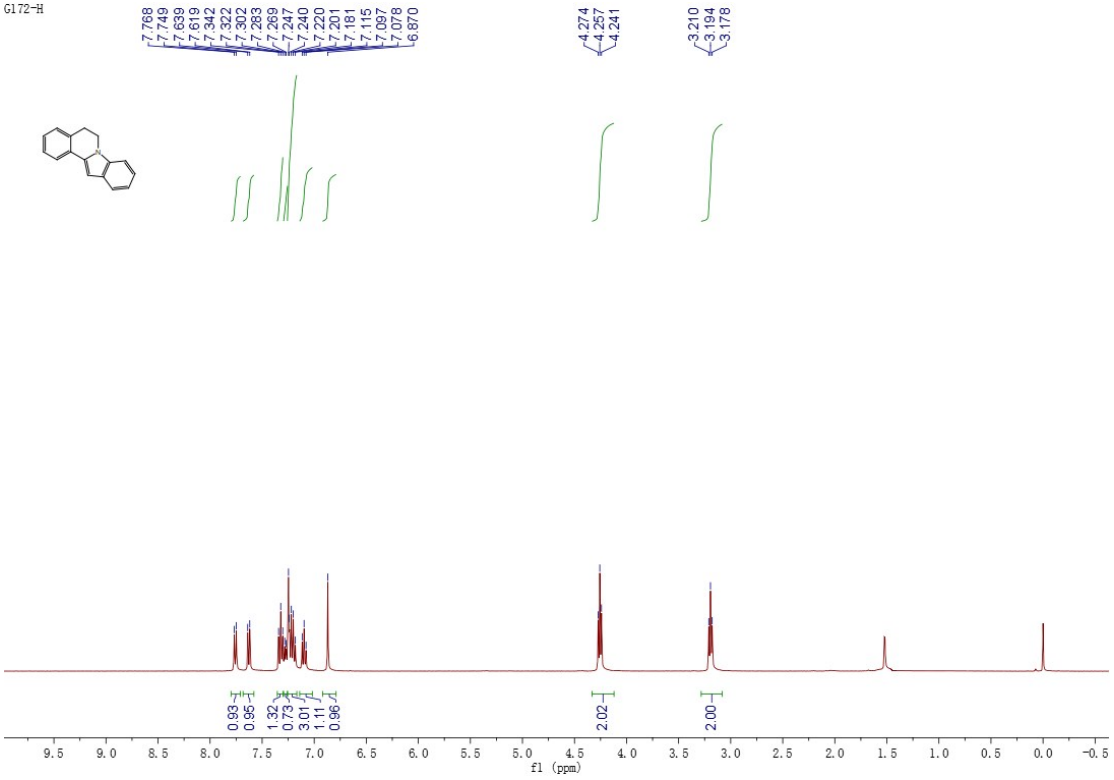

LLM-G202-C
135.151
133.293
132.793
129.581
128.049
126.887
126.812
121.828
119.919
119.169
113.069
108.732
40.127
29.983
7.763
6.735
f1 (ppm)

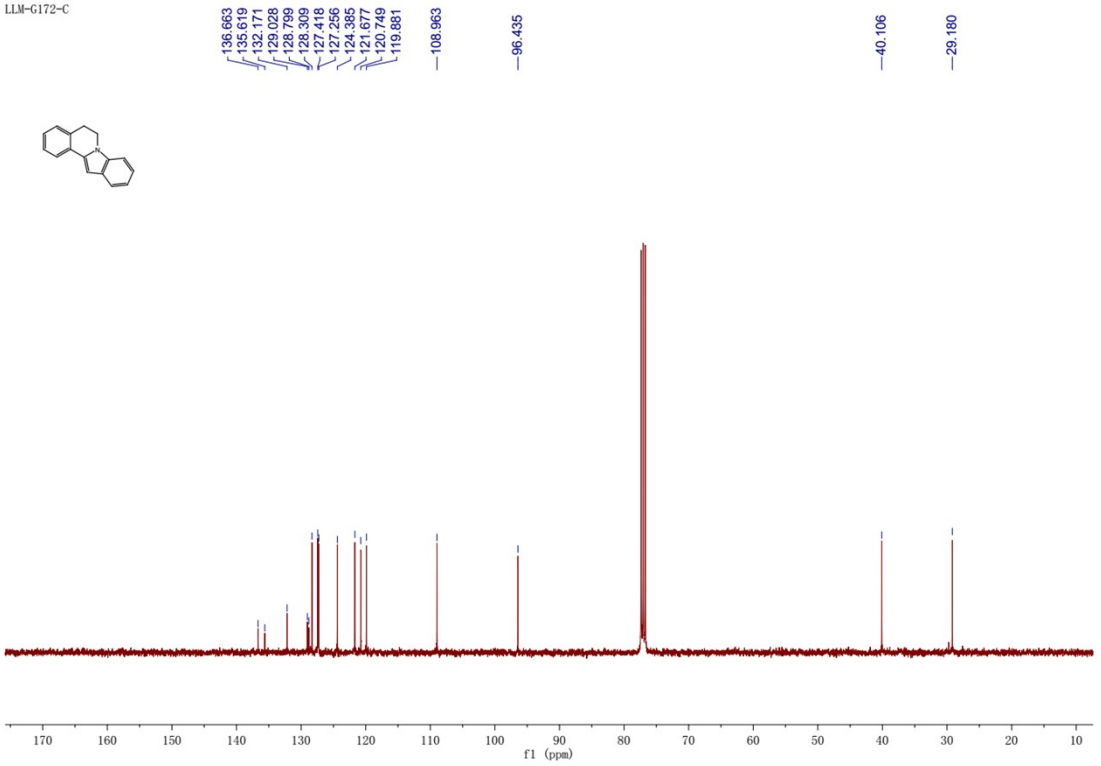
NMR of 2ad


LLM-G316-8-H
7.901
7.885
7.707
7.691
7.375
7.360
7.308
7.293
7.255
7.240
7.226
7.198
7.184
7.168
7.063
7.048
7.033
4.176
4.164
4.152
3.374
3.349
3.325
3.089
3.077
3.065
2.196
2.171
2.147
1.954
1.927
1.906
1.480
1.454
1.436
1.409
0.99
0.97
1.09
1.92
1.32
0.99
0.99
2.00
1.02
1.98
2.20
4.08
1.06
3.18
f1 (ppm)

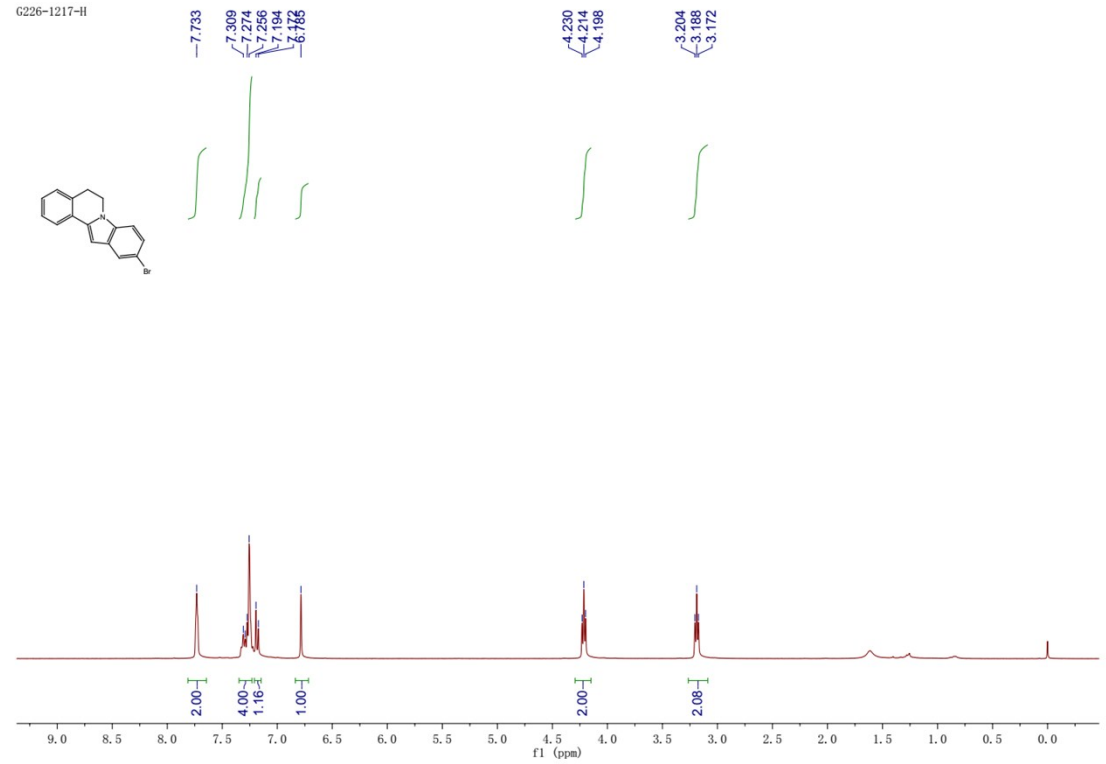

LLM-G316-8-C
135.835
134.629
130.389
129.885
128.332
127.188
127.168
126.762
126.082
121.639
121.486
118.434
117.912
108.911
40.105
37.276
33.090
30.569
27.373
26.462
f1 (ppm)

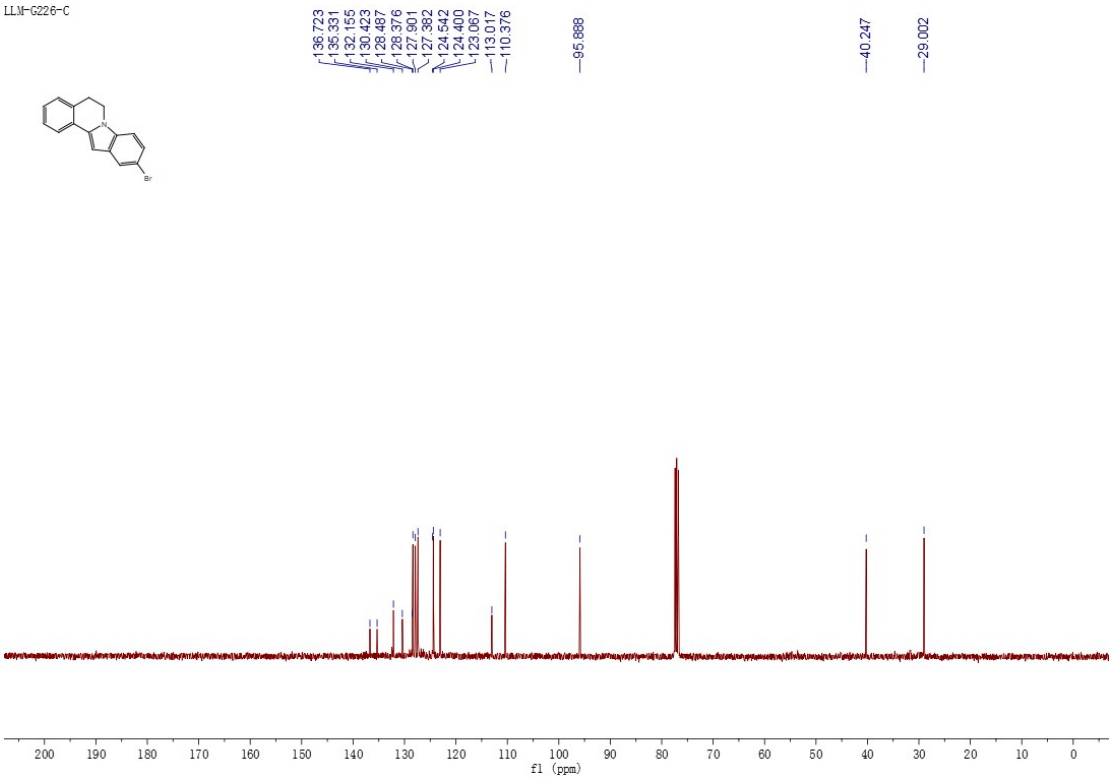
NMR of 2ae


G172-H
7.768
7.749
7.639
7.619
7.342
7.322
7.302
7.283
7.269
7.247
7.240
7.220
7.201
7.181
7.115
7.097
7.078
6.870
4.274
4.257
4.241
3.210
3.194
3.178
0.93
0.95
1.32
0.73
3.01
1.11
0.96
2.02
2.00
f1 (ppm)

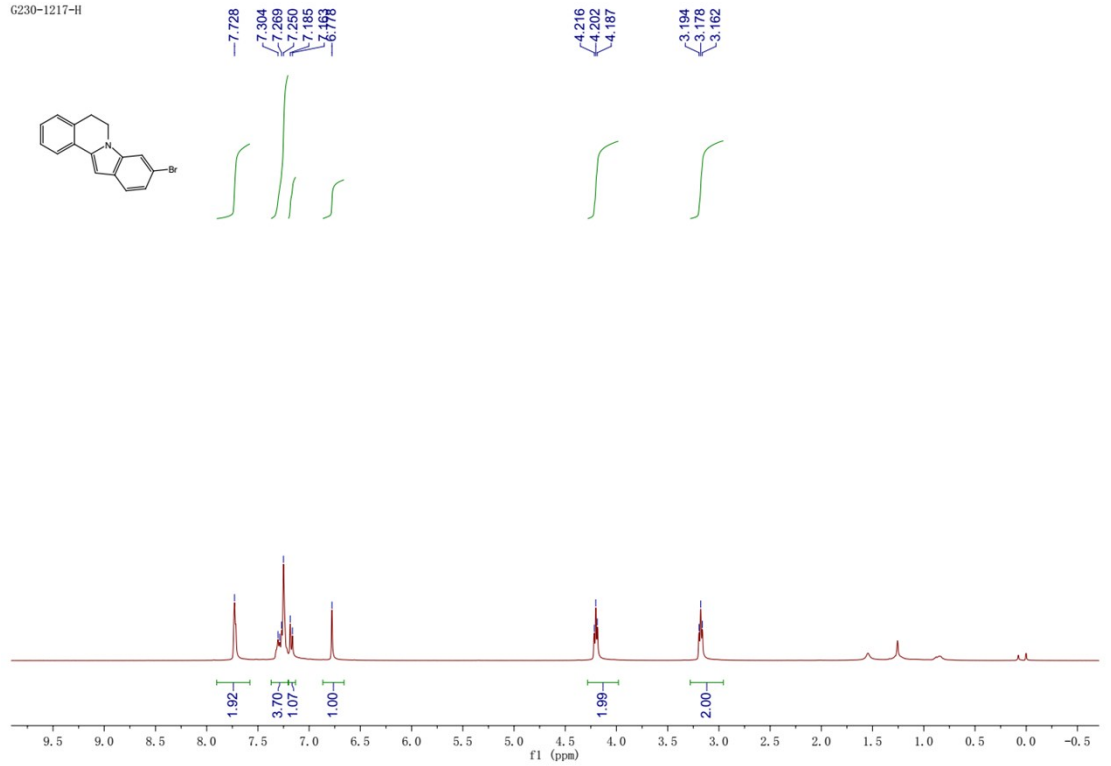

LLM-G172-C
136.663
135.619
132.171
129.028
128.799
128.309
127.418
127.256
124.385
121.677
120.749
119.881
108.963
96.435
40.106
29.180
f1 (ppm)

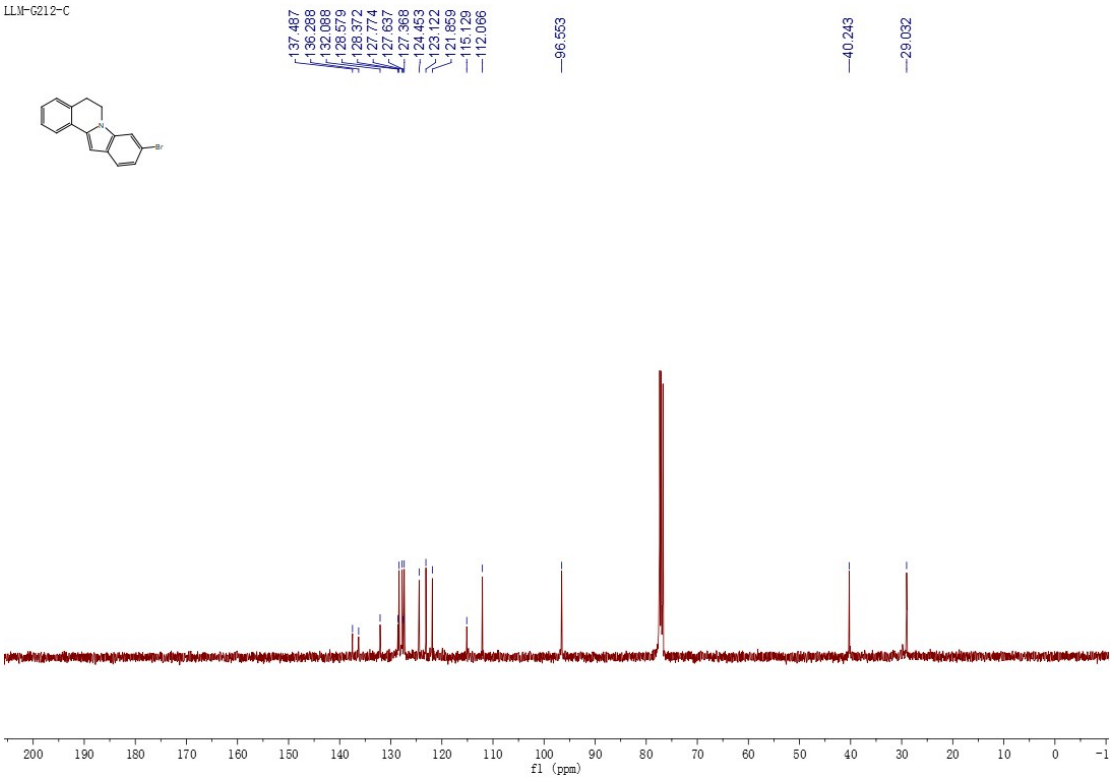
NMR of 2af


G226-1217-H
7.733
7.309
7.274
7.256
7.194
7.172
6.785
4.230
4.214
4.198
3.204
3.188
3.172
2.00
4.00
1.16
1.00
2.00
2.08
f1 (ppm)

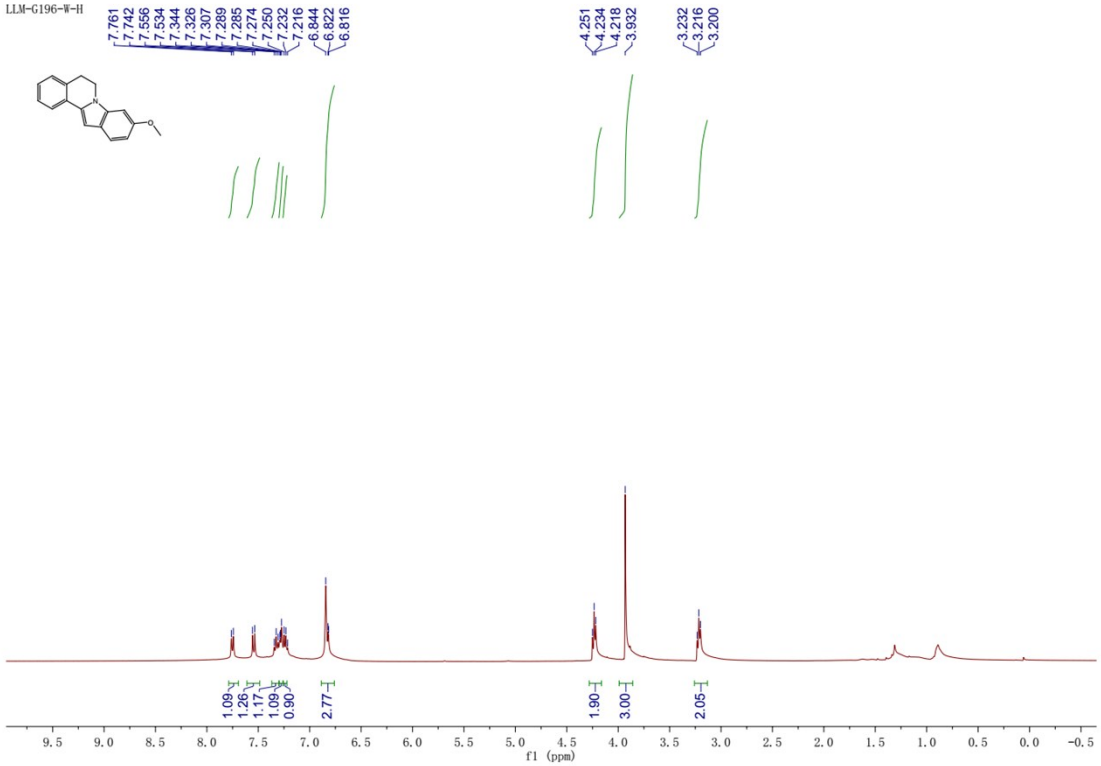

LLM-G226-C
136.723
135.331
132.155
130.423
128.487
128.376
127.901
127.382
124.542
124.400
123.067
113.017
110.376
95.888
40.247
29.002
f1 (ppm)

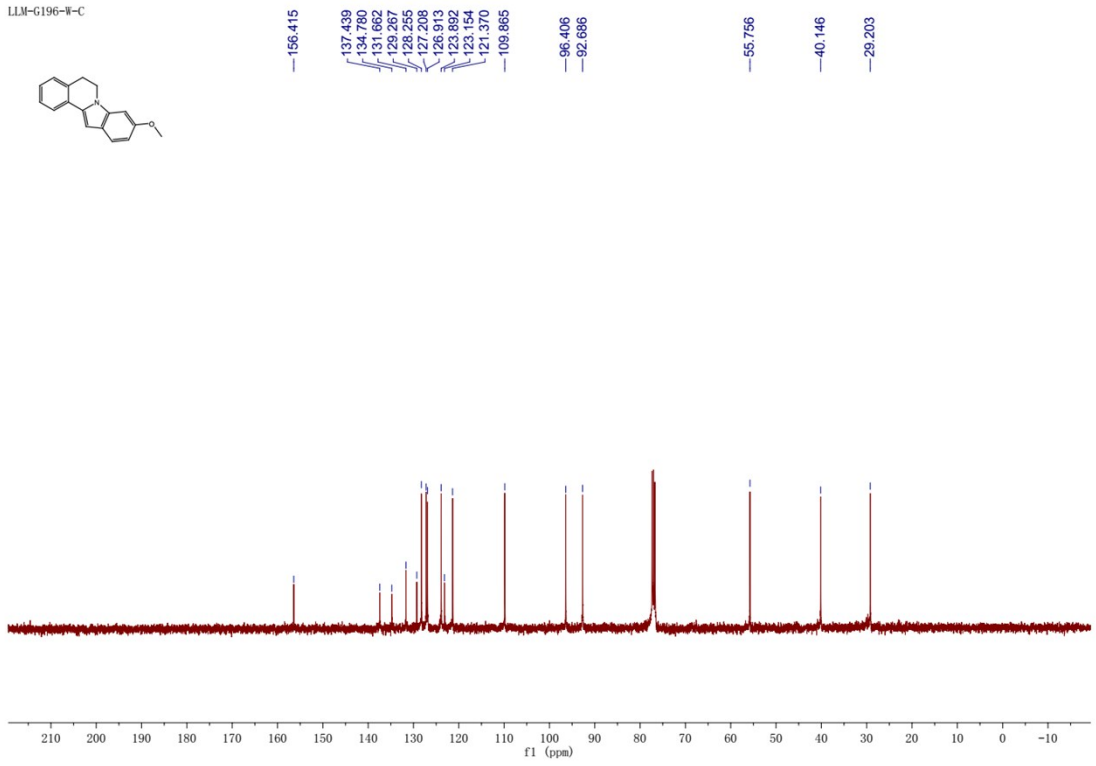
NMR of 2ag


G230-1217-H
7.728
7.304
7.269
7.250
7.185
4.216
4.202
4.187
3.194
3.178
3.162
1.92
3.70
1.07
1.00
1.99
2.00
f1 (ppm)

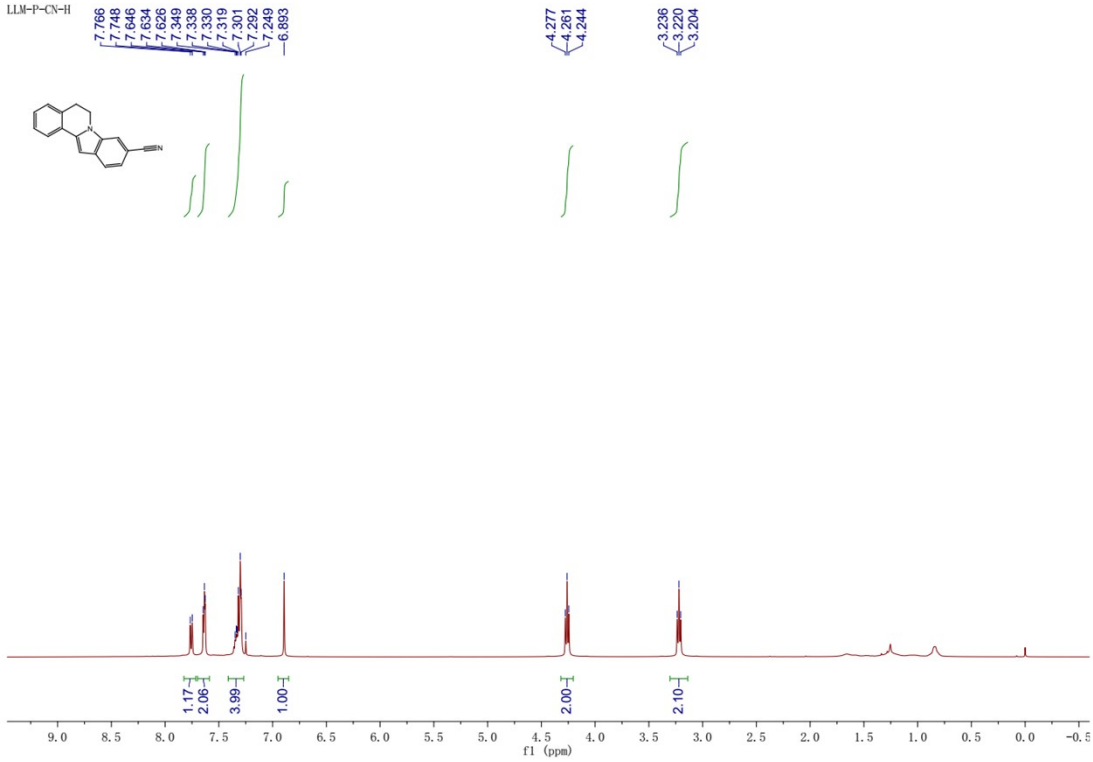

LLM-G212-C
137.487
136.288
132.088
128.579
128.372
127.774
127.637
127.368
124.453
123.122
121.859
115.129
112.066
96.553
40.243
29.032
f1 (ppm)

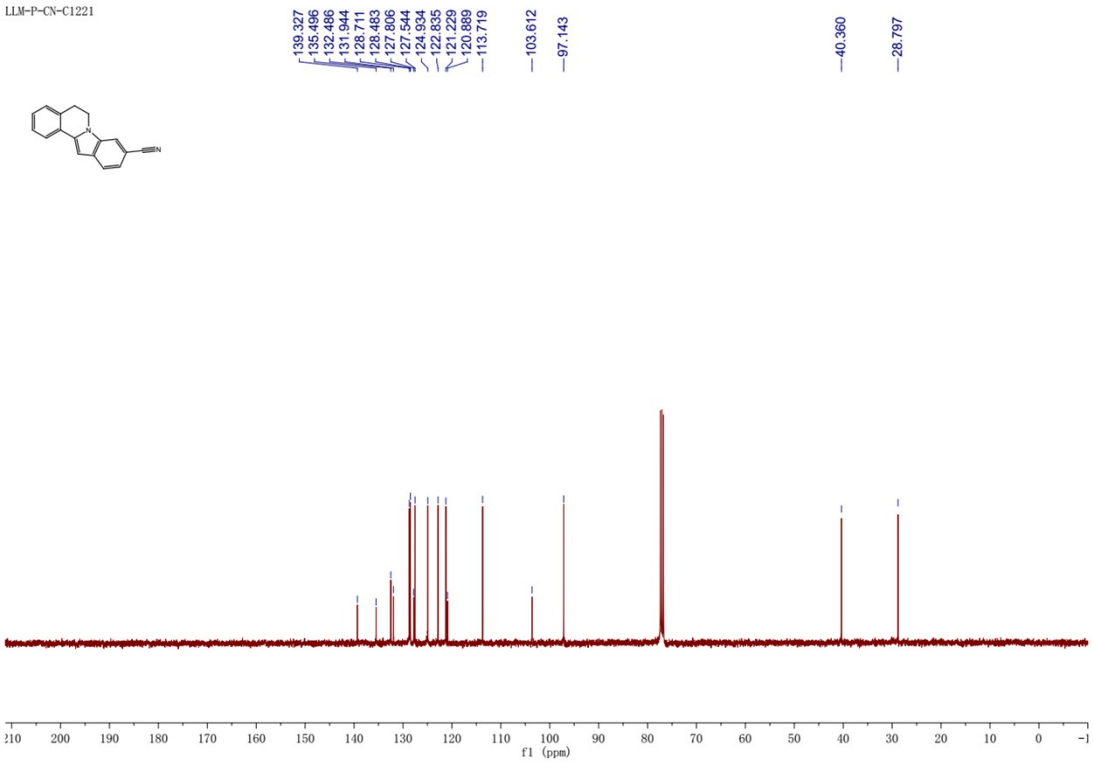
NMR of 2ah


LLM-G196-W-H
7.761
7.742
7.556
7.534
7.344
7.326
7.307
7.289
7.285
7.274
7.250
7.232
7.216
6.844
6.822
6.816
4.251
4.234
4.218
3.932
3.232
3.216
3.200
1.09
1.26
1.17
1.09
0.90
2.77
1.90
3.00
2.05
f1 (ppm)


LLM-G196-W-C
156.415
137.439
134.780
131.662
129.267
128.255
127.208
126.913
123.892
123.154
121.370
109.865
96.406
92.686
55.756
40.146
29.203
f1 (ppm)

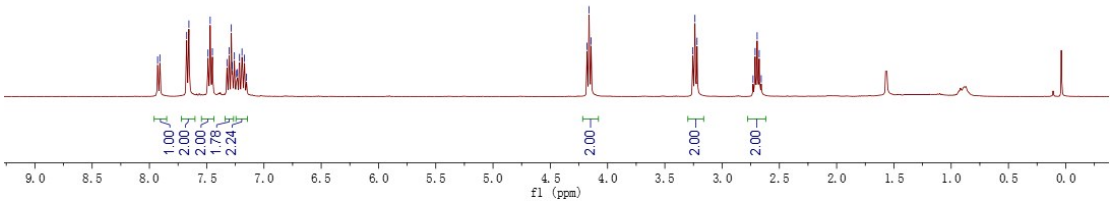
NMR of 2ai

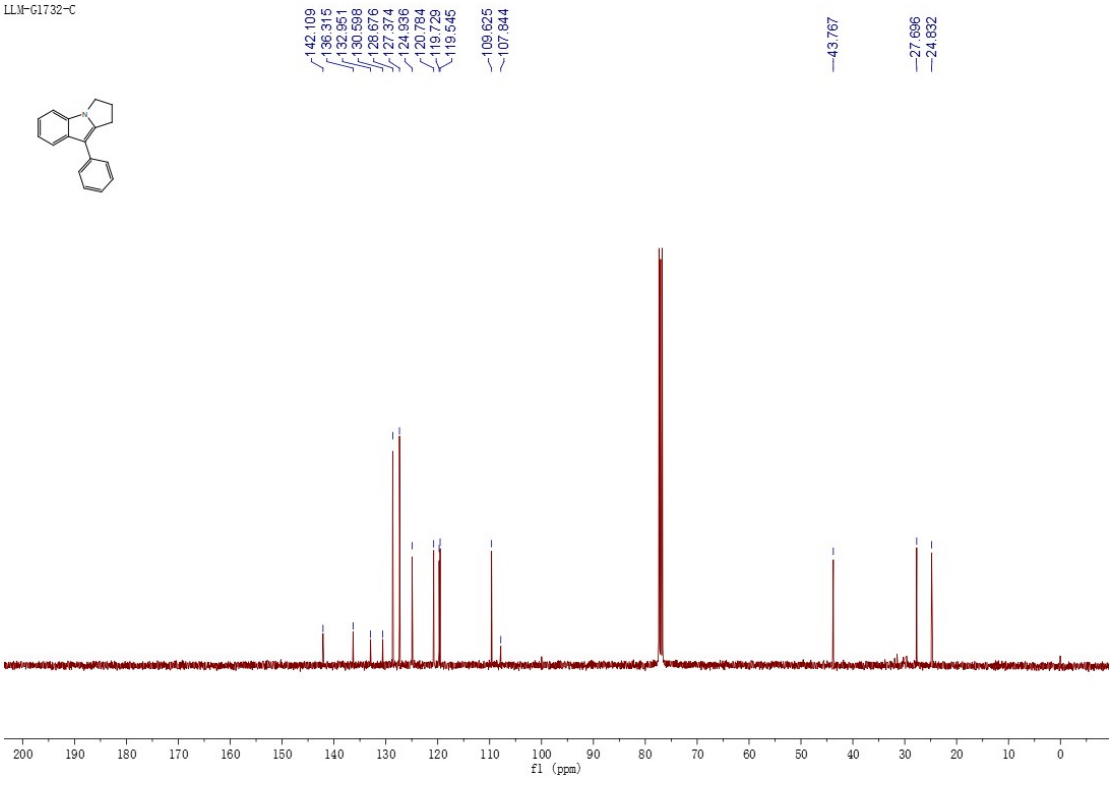

LLM-P-CN-H
7.766
7.748
7.646
7.634
7.626
7.349
7.338
7.330
7.319
7.301
7.292
7.249
6.893
4.277
4.261
4.244
3.236
3.220
3.204
1.17
2.06
3.99
1.00
2.00
2.10
f1 (ppm)


LLM-P-CN-C1221
139.327
135.496
132.486
131.944
128.711
128.483
127.806
127.544
124.934
122.835
121.229
120.889
113.719
103.612
97.143
40.360
28.797
f1 (ppm)

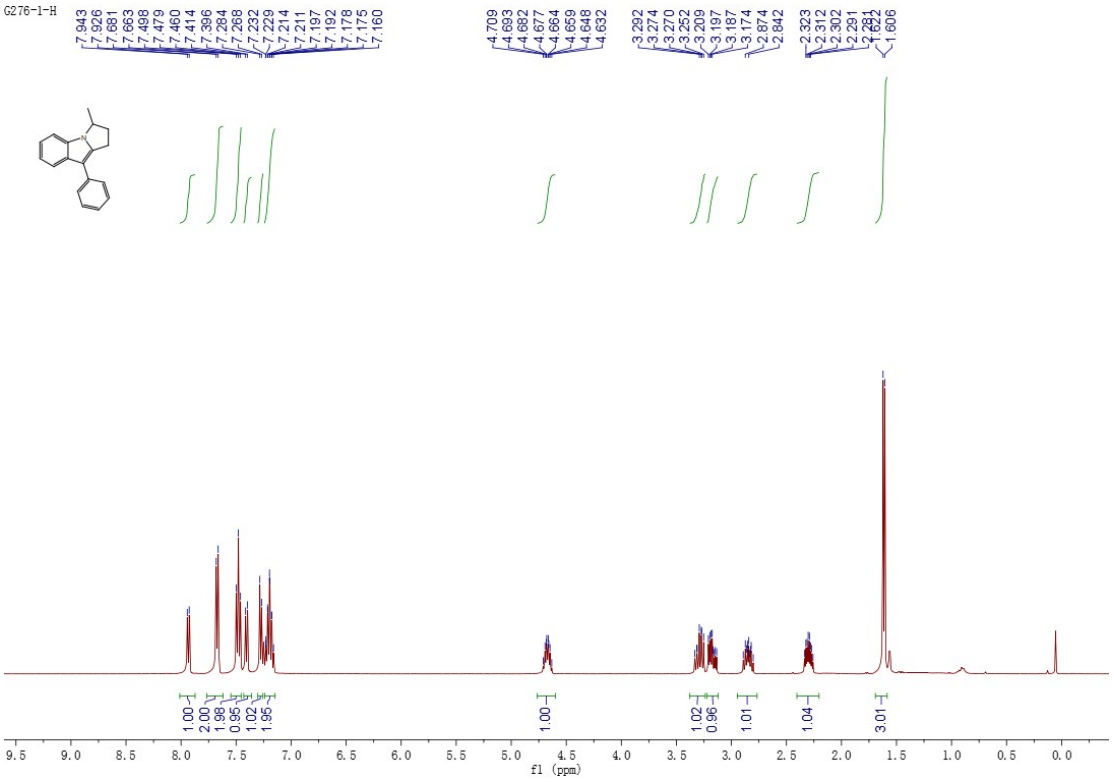
NMR of 2aj

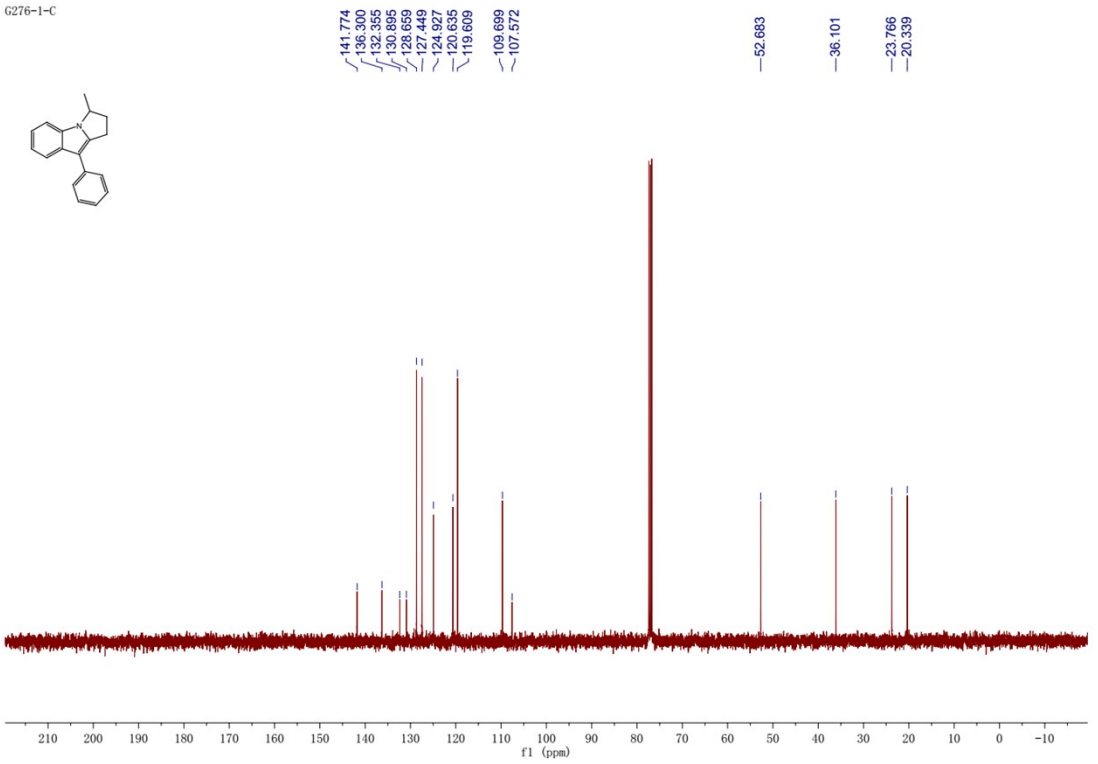

LLM-G178-1-H
7.928
7.906
7.675
7.655
7.488
7.469
7.450
7.323
7.304
7.285
7.277
7.258
7.239
7.231
7.213
7.192
7.170
7.152
4.179
4.161
4.144
3.256
3.237
3.219
2.730
2.712
2.694
2.676
2.658


1.00
2.00
2.00
1.78
2.24
2.00
2.00
2.00
f1 (ppm)

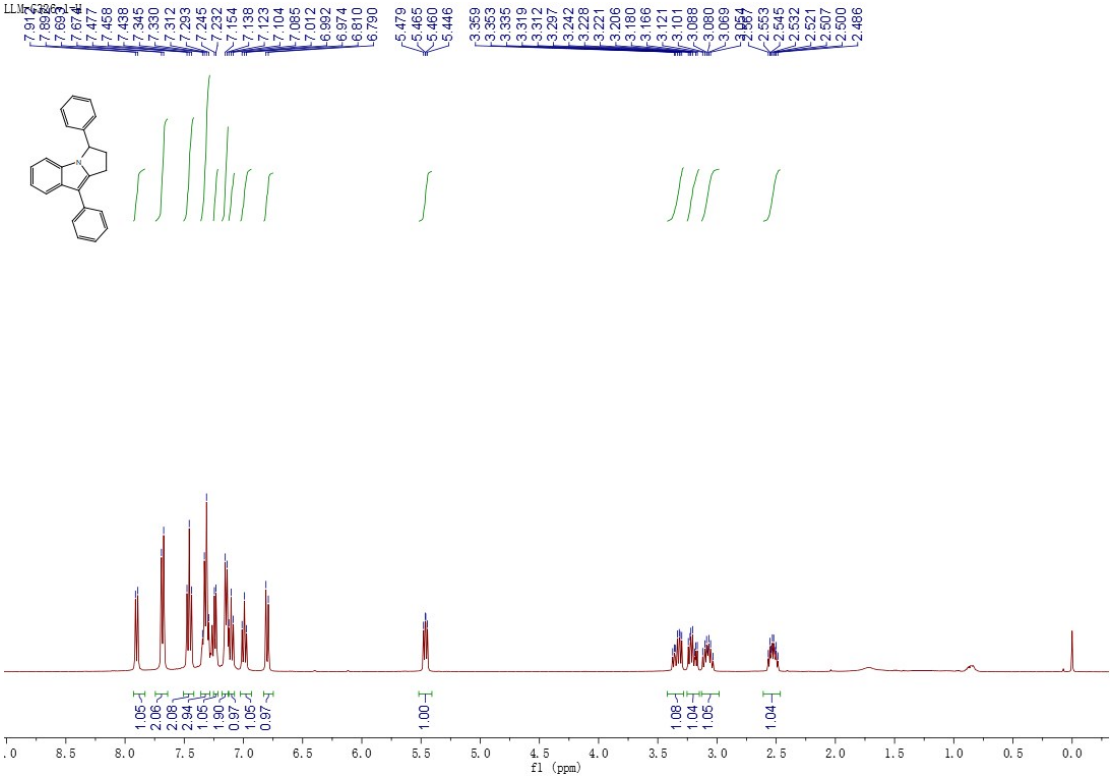

LLM-G1732-C
142.109
136.315
132.951
130.598
128.676
127.374
124.936
120.784
119.729
119.545
109.625
107.844
43.767
27.696
24.832
f1 (ppm)

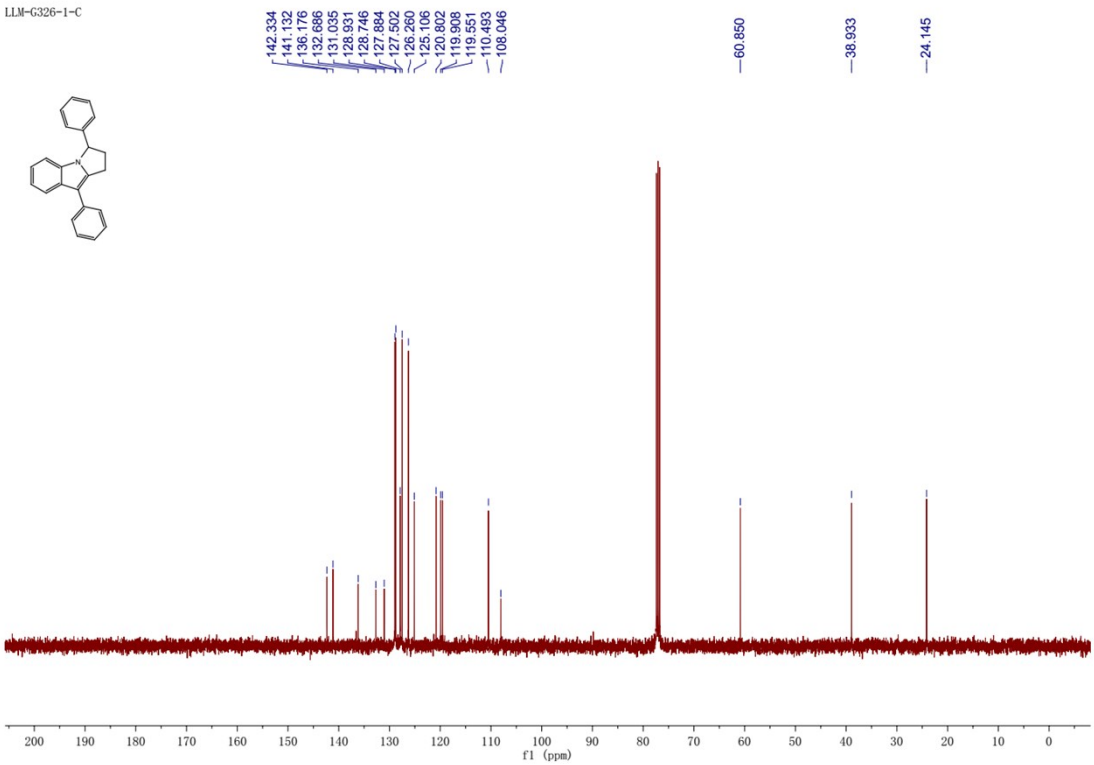
NMR of 2ak


G276-1-H
7.943
7.926
7.681
7.663
7.498
7.479
7.460
7.414
7.396
7.284
7.268
7.232
7.229
7.214
7.211
7.197
7.192
7.178
7.175
7.160
4.709
4.693
4.682
4.677
4.664
4.659
4.648
4.632
3.292
3.274
3.270
3.252
3.209
3.197
3.187
3.174
2.874
2.842
2.323
2.312
2.302
2.291
2.281
1.622
1.606
1.00
2.00
1.98
0.95
1.02
1.95
1.00
1.02
0.96
1.01
1.04
3.01
f1 (ppm)

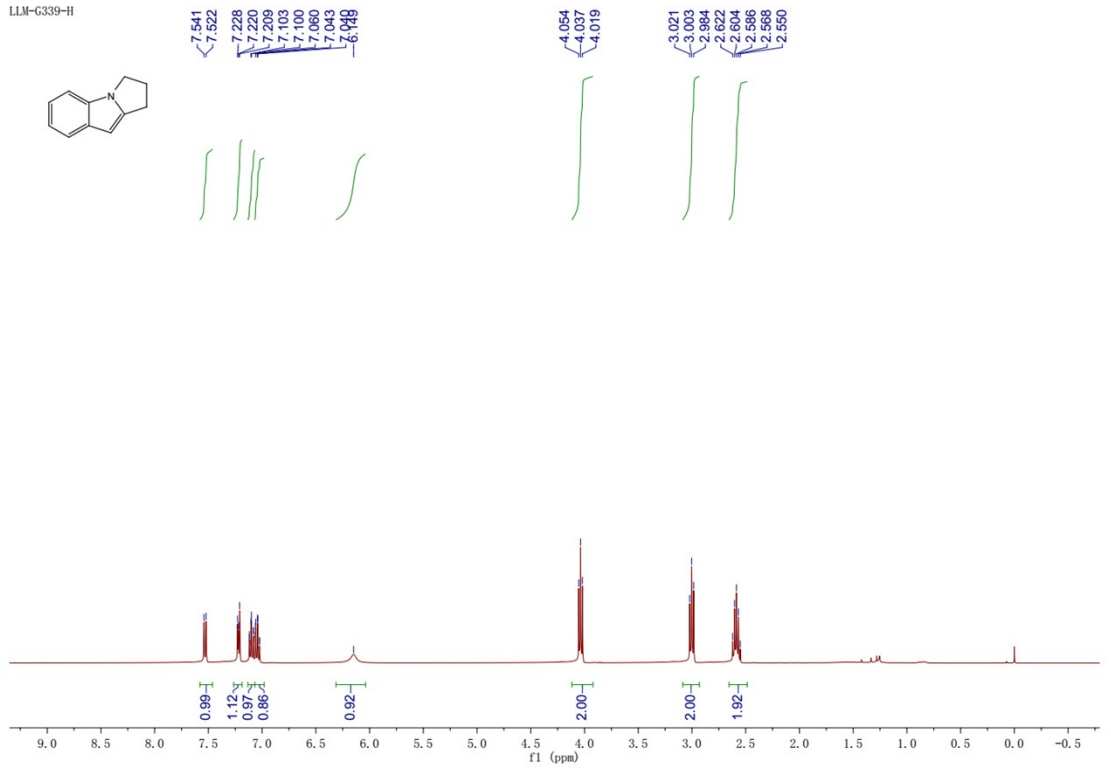

G276-1-C
141.774
136.300
132.355
130.895
128.659
127.449
124.927
120.635
119.609
109.699
107.572
52.683
36.101
23.766
20.339
f1 (ppm)

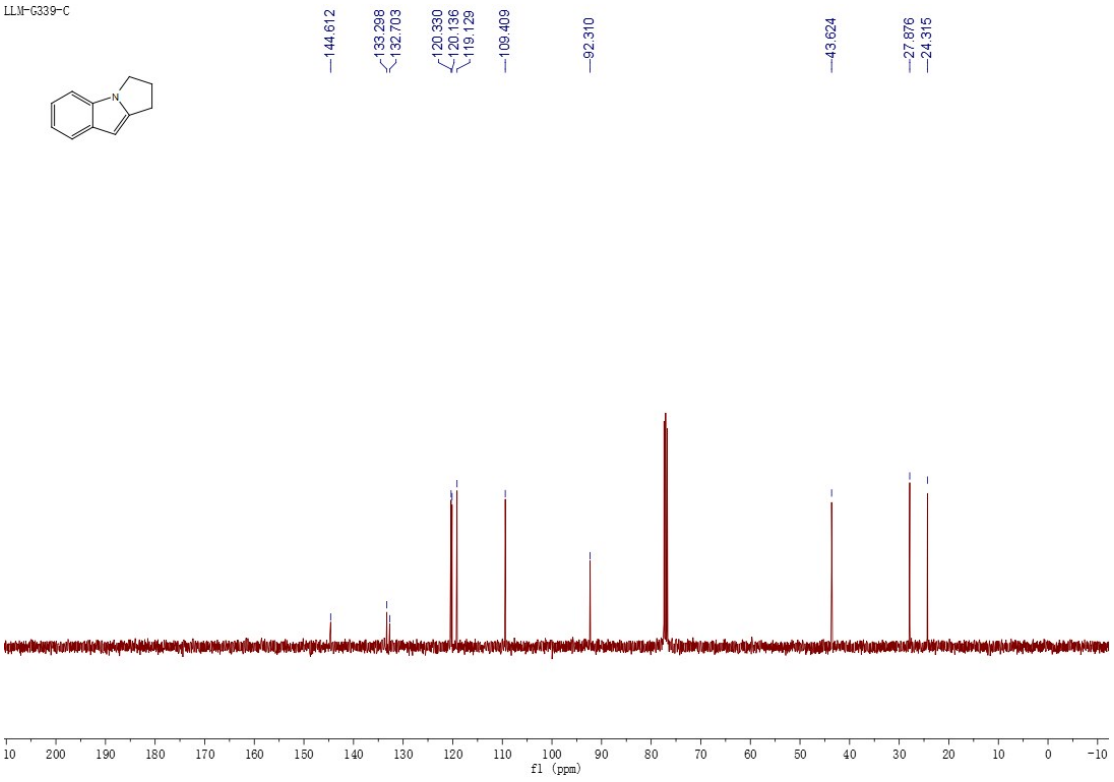
NMR of 2al


7.914
7.893
7.691
7.674
7.477
7.458
7.438
7.345
7.330
7.312
7.293
7.245
7.232
7.154
7.138
7.123
7.104
7.085
7.012
6.992
6.974
6.810
6.790
5.479
5.465
5.460
5.446
3.359
3.353
3.335
3.319
3.312
3.297
3.242
3.228
3.221
3.206
3.180
3.166
3.121
3.101
3.088
3.080
3.069
2.553
2.545
2.532
2.521
2.507
2.500
2.486
1.05
2.06
2.08
2.94
1.05
1.90
0.97
1.05
0.97
1.00
1.08
1.04
1.05
1.04
f1 (ppm)

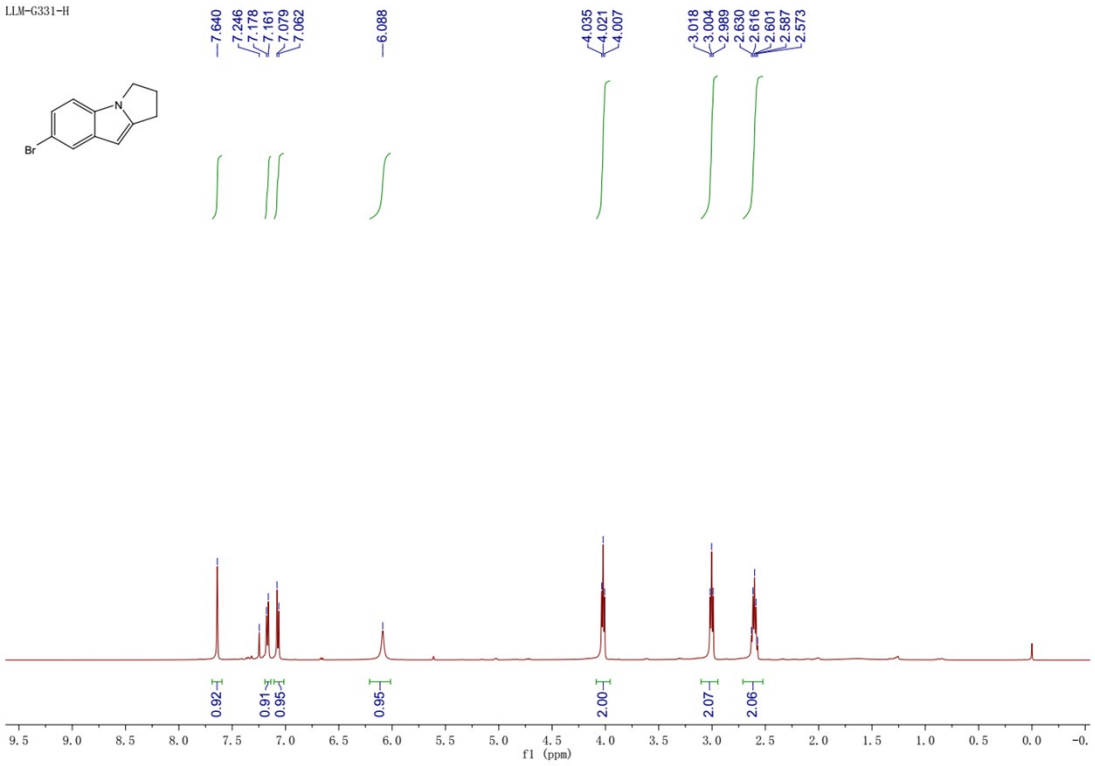

LLM-G326-1-C
142.334
141.132
136.176
132.686
131.035
128.931
128.746
127.884
127.502
126.260
125.106
120.802
119.908
119.551
110.493
108.046
60.850
38.933
24.145
f1 (ppm)

NMR of 2am


LLM-G339-H
7.541
7.522
7.228
7.220
7.209
7.103
7.100
7.060
7.043
7.040
6.149
4.054
4.037
4.019
3.021
3.003
2.984
2.622
2.604
2.586
2.568
2.550
0.99
1.12
0.97
0.86
0.92
2.00
2.00
1.92
f1 (ppm)


LLM-G339-C
144.612
133.298
132.703
120.330
120.136
119.129
109.409
92.310
43.624
27.876
24.315
f1 (ppm)

NMR of 2an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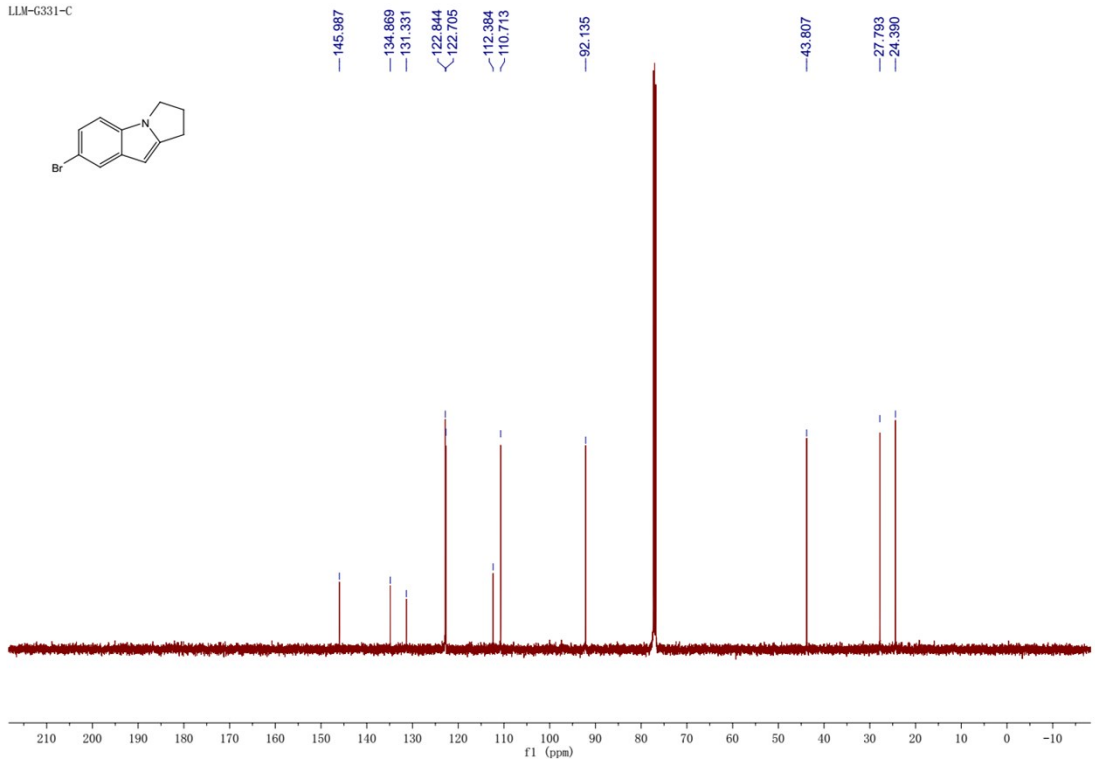
7.640
7.246
7.178
7.161
7.079
7.062
6.088
4.035
4.021
4.007
3.018
3.004
2.989
2.630
2.616
2.601
2.587
2.573
Br
0.92
0.91
0.95
0.95
2.00
2.07
2.06
f1 (ppm)


LLM-G331-C
145.987
134.869
131.331
122.844
122.705
112.384
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92.135
43.807
27.793
24.390
Br
f1 (ppm)

10. Molecular Coordinates

1a (S0, NMP)

Number	Atomic Number	X	Y	Z
1	6	-3.672239	-0.417092	0.408486
2	6	-4.906030	-0.987061	0.078252
3	6	-4.962098	-2.133717	-0.721474
4	6	-3.781012	-2.705319	-1.205695
5	6	-2.545671	-2.131265	-0.886815
6	6	-2.487375	-0.991798	-0.077060
7	6	-3.509163	0.830550	1.236610
8	6	-1.170181	-0.388906	0.358557
9	7	-1.189776	1.082781	0.385033
10	6	-2.483181	1.756879	0.574715
11	6	2.078942	3.377202	-1.032505
12	6	0.779056	3.896938	-0.997710
13	6	-0.278519	3.146060	-0.499346
14	6	-0.091969	1.828323	-0.000183
15	6	1.253770	1.330441	0.041552
16	6	1.679330	0.169213	0.874325
17	8	1.189646	-0.023145	1.994099
18	6	2.293663	2.105190	-0.516199
19	6	4.730888	-2.562428	-0.461282
20	6	3.940607	-1.899720	-1.405428
21	6	2.967537	-0.988578	-0.987887
22	6	2.764040	-0.744031	0.380934
23	6	3.553630	-1.426616	1.322665
24	6	4.537024	-2.322200	0.904762
25	1	-5.823384	-0.533615	0.445585
26	1	-5.923250	-2.573336	-0.972167
27	1	-3.820548	-3.589793	-1.834890
28	1	-1.627805	-2.572552	-1.267510
29	1	-3.170322	0.577402	2.250984
30	1	-4.456930	1.367323	1.338593
31	1	-0.379603	-0.712661	-0.324708
32	1	-0.900739	-0.780193	1.350178
33	1	-2.327496	2.641958	1.200340
34	1	-2.891707	2.097724	-0.388824
35	1	2.904313	3.958604	-1.429809
36	1	0.579163	4.893765	-1.381216
37	1	-1.271011	3.575340	-0.532250
38	1	3.304783	1.712891	-0.479837
39	1	5.493085	-3.264241	-0.786933

40	1	4.081257	-2.090789	-2.465014
41	1	2.354808	-0.479840	-1.724958
42	1	3.389156	-1.240775	2.378988
43	1	5.151200	-2.833895	1.639777

1a (S1, NMP)

Number	Atomic Number	X	Y	Z
1	6	-3.418481	-0.011390	0.395547
2	6	-4.702644	-0.526230	0.193694
3	6	-4.876221	-1.731391	-0.493905
4	6	-3.765513	-2.416582	-0.997084
5	6	-2.480576	-1.898649	-0.808952
6	6	-2.307407	-0.700902	-0.107601
7	6	-3.128800	1.290916	1.093496
8	6	-0.921619	-0.172095	0.185043
9	7	-0.834646	1.303012	0.119649
10	6	-2.079769	2.079771	0.304175
11	6	2.685694	3.383380	-0.771358
12	6	1.430474	3.949729	-1.046861
13	6	0.282106	3.253107	-0.728459
14	6	0.348347	1.950785	-0.146424
15	6	1.635577	1.373222	0.157711
16	6	1.833192	0.140377	1.009598
17	8	1.592481	0.330352	2.264191
18	6	2.765117	2.126211	-0.164716
19	6	3.214456	-3.571203	-0.639914
20	6	2.963765	-2.472482	-1.480812
21	6	2.524492	-1.257769	-0.965554
22	6	2.312241	-1.079449	0.440029
23	6	2.566594	-2.214087	1.277306
24	6	3.006923	-3.417729	0.745282
25	1	-5.565025	0.015946	0.572490
26	1	-5.875425	-2.129123	-0.644651
27	1	-3.898111	-3.347525	-1.539947
28	1	-1.616996	-2.427368	-1.203341
29	1	-2.761736	1.117504	2.113621
30	1	-4.025711	1.910563	1.175054
31	1	-0.200641	-0.590596	-0.515310
32	1	-0.609672	-0.470246	1.194552
33	1	-1.824971	3.004728	0.821411
34	1	-2.483900	2.331232	-0.684330
35	1	3.593424	3.921596	-1.023650

36	1	1.357072	4.921260	-1.522848
37	1	-0.678463	3.679227	-0.985457
38	1	3.738838	1.714095	0.080075
39	1	3.559427	-4.515650	-1.048451
40	1	3.115980	-2.568062	-2.553511
41	1	2.349148	-0.429602	-1.646199
42	1	2.408147	-2.110402	2.345731
43	1	3.193599	-4.256699	1.412252

1a (T1, NMP)

Number	Atomic Number	X	Y	Z
1	6	3.272987	-0.567468	-0.630061
2	6	4.357872	-1.441393	-0.804636
3	6	5.031614	-1.982440	0.290217
4	6	4.625746	-1.649368	1.588077
5	6	3.551789	-0.779164	1.772621
6	6	2.870276	-0.236569	0.672830
7	6	2.530322	-0.009452	-1.823901
8	6	1.727151	0.722020	0.936710
9	7	0.993013	1.112614	-0.267615
10	6	1.785361	1.282256	-1.488735
11	6	-2.448611	3.481624	0.270794
12	6	-1.190861	4.104370	0.220681
13	6	-0.047788	3.315276	0.039615
14	6	-0.166457	1.932906	-0.074184
15	6	-1.429143	1.271971	-0.005790
16	6	-1.416747	-0.156506	-0.207270
17	8	-0.280502	-0.706762	-0.579627
18	6	-2.572236	2.101519	0.158900
19	6	-4.712564	-2.904095	0.149045
20	6	-4.681420	-1.750488	0.942563
21	6	-3.627763	-0.842237	0.838312
22	6	-2.569042	-1.057205	-0.076650
23	6	-2.602884	-2.243519	-0.851213
24	6	-3.659888	-3.144870	-0.743871
25	1	4.673871	-1.695863	-1.813426
26	1	5.869390	-2.655794	0.134223
27	1	5.142971	-2.063378	2.448521
28	1	3.236011	-0.517267	2.779803
29	1	1.802765	-0.746612	-2.181680
30	1	3.225799	0.188873	-2.645969
31	1	2.114338	1.639122	1.410846

32	1	1.006225	0.284822	1.633506
33	1	1.105686	1.568155	-2.292548
34	1	2.499713	2.106297	-1.334634
35	1	-3.344897	4.085072	0.384011
36	1	-1.100556	5.181837	0.310824
37	1	0.933886	3.777662	-0.010204
38	1	-3.561479	1.661309	0.155937
39	1	-5.535896	-3.607222	0.232697
40	1	-5.476106	-1.562703	1.659617
41	1	-3.607929	0.015171	1.501274
42	1	-1.792226	-2.437272	-1.545771
43	1	-3.664924	-4.039418	-1.361032

1a (TS1, NMP)

Number	Atomic Number	X	Y	Z
1	6	-3.669171	-0.219064	0.328132
2	6	-4.913278	-0.854208	0.353993
3	6	-5.094409	-2.086995	-0.282512
4	6	-4.025767	-2.687050	-0.958625
5	6	-2.782242	-2.054580	-0.996714
6	6	-2.596705	-0.818576	-0.356247
7	6	-3.396581	1.102621	0.999863
8	6	-1.251220	-0.184478	-0.332198
9	7	-1.195671	1.224359	-0.146255
10	6	-2.442436	1.953321	0.156496
11	6	2.392474	3.440691	-0.132105
12	6	1.186398	4.029431	-0.511513
13	6	0.030110	3.253713	-0.498209
14	6	0.045477	1.888950	-0.137658
15	6	1.293128	1.245489	0.200360
16	6	1.486231	-0.155523	0.663560
17	8	0.585936	-0.695259	1.472004
18	6	2.422715	2.090457	0.225444
19	6	4.865466	-2.612740	-0.356843
20	6	4.622249	-1.430953	-1.075798
21	6	3.547471	-0.607837	-0.756812
22	6	2.651979	-0.934374	0.305542
23	6	2.903374	-2.154684	1.001998
24	6	3.988413	-2.963631	0.681561
25	1	-5.744137	-0.382700	0.872646
26	1	-6.065185	-2.572889	-0.255953
27	1	-4.162618	-3.640904	-1.459094

28	1	-1.952712	-2.516368	-1.525786
29	1	-2.957199	0.944414	1.994062
30	1	-4.320609	1.669924	1.145624
31	1	-0.617871	-0.488948	-1.172702
32	1	-0.610242	-0.579803	0.601545
33	1	-2.189030	2.868899	0.688044
34	1	-2.924858	2.221507	-0.793772
35	1	3.308822	4.022573	-0.104288
36	1	1.136339	5.071625	-0.807975
37	1	-0.903470	3.707280	-0.808247
38	1	3.362235	1.668973	0.563357
39	1	5.709492	-3.248289	-0.607457
40	1	5.275179	-1.154470	-1.899816
41	1	3.376909	0.281254	-1.353576
42	1	2.225092	-2.440325	1.798128
43	1	4.154020	-3.880085	1.242737

1a (A, NMP)

Number	Atomic Number	X	Y	Z
1	6	3.678112	-0.687147	-0.614762
2	6	4.944832	-1.259207	-0.693698
3	6	5.689194	-1.543771	0.461622
4	6	5.147807	-1.247337	1.725164
5	6	3.890456	-0.669414	1.831359
6	6	3.126413	-0.367512	0.666503
7	6	2.827475	-0.417731	-1.835036
8	6	1.850448	0.232982	0.766786
9	7	1.091674	0.563150	-0.370079
10	6	1.886501	0.768124	-1.612657
11	6	-1.966210	3.471661	0.152330
12	6	-0.616923	3.851668	0.181311
13	6	0.360340	2.867554	0.017820
14	6	0.019924	1.526205	-0.156364
15	6	-1.348825	1.101527	-0.130969
16	6	-1.753951	-0.276898	-0.278422
17	8	-0.854527	-1.194571	-0.733621
18	6	-2.319643	2.139005	-0.001012
19	6	-5.598768	-2.055346	0.422170
20	6	-5.200916	-0.943388	1.174328
21	6	-3.961984	-0.343152	0.954766
22	6	-3.078103	-0.836518	-0.035696
23	6	-3.486019	-1.980321	-0.767183

24	6	-4.727807	-2.571545	-0.545500
25	1	5.359964	-1.492520	-1.671771
26	1	6.675603	-1.989627	0.378166
27	1	5.716701	-1.467675	2.624215
28	1	3.476812	-0.434841	2.808877
29	1	2.232004	-1.309370	-2.079270
30	1	3.455281	-0.213537	-2.708702
31	1	1.377448	0.413589	1.724472
32	1	0.034124	-0.749598	-0.733578
33	1	1.185079	0.873494	-2.443258
34	1	2.465459	1.698407	-1.533029
35	1	-2.746902	4.221734	0.239086
36	1	-0.332181	4.890385	0.314097
37	1	1.411225	3.141818	0.024259
38	1	-3.369895	1.884342	-0.058673
39	1	-6.565717	-2.518149	0.595013
40	1	-5.852966	-0.548983	1.948593
41	1	-3.662315	0.486605	1.584613
42	1	-2.820389	-2.389502	-1.518941
43	1	-5.018974	-3.438686	-1.131813

1a (TS2', NMP)

Number	Atomic Number	X	Y	Z
1	6	2.732670	-1.182302	0.176957
2	6	4.077417	-0.882237	0.395857
3	6	4.620166	0.348074	-0.004737
4	6	3.805396	1.279579	-0.660476
5	6	2.462271	0.989316	-0.896182
6	6	1.900627	-0.233731	-0.468358
7	6	2.136104	-2.515300	0.570923
8	6	0.470177	-0.492346	-0.678218
9	7	0.048347	-1.845511	-0.501484
10	6	1.032878	-2.924562	-0.413245
11	6	-4.037266	-1.659576	0.088684
12	6	-3.472595	-2.969729	-0.161664
13	6	-2.099864	-3.110589	-0.334828
14	6	-1.287606	-1.973486	-0.205143
15	6	-1.834887	-0.671321	0.185814
16	6	-0.761054	0.272943	0.505622
17	8	-0.066589	-0.018732	1.729011
18	6	-3.239362	-0.537923	0.242786
19	6	-1.306076	4.479646	-0.252911

20	6	-1.797997	3.523544	-1.150260
21	6	-1.621858	2.162966	-0.897582
22	6	-0.965134	1.721503	0.273295
23	6	-0.458025	2.694941	1.157960
24	6	-0.630704	4.055332	0.899387
25	1	4.714306	-1.622081	0.875634
26	1	5.668405	0.565872	0.177145
27	1	4.218533	2.228299	-0.991806
28	1	1.833450	1.711380	-1.410263
29	1	1.708805	-2.459936	1.580080
30	1	2.905465	-3.294110	0.584298
31	1	0.082235	-0.050935	-1.601800
32	1	-0.733060	-0.259090	2.388953
33	1	0.524894	-3.830325	-0.081470
34	1	1.456469	-3.103325	-1.409115
35	1	-5.115151	-1.562811	0.182475
36	1	-4.127714	-3.829362	-0.249353
37	1	-1.674481	-4.070456	-0.614035
38	1	-3.687714	0.425802	0.466644
39	1	-1.440701	5.538778	-0.452019
40	1	-2.314458	3.839215	-2.052642
41	1	-1.998660	1.433964	-1.609330
42	1	0.062428	2.371225	2.052100
43	1	-0.240433	4.787872	1.600729

1a (B', NMP)

Number	Atomic Number	X	Y	Z
1	6	-2.984308	0.436957	0.038918
2	6	-4.215962	-0.161409	0.345493
3	6	-4.362789	-1.548705	0.353760
4	6	-3.271538	-2.360985	0.027535
5	6	-2.045760	-1.777016	-0.291439
6	6	-1.883295	-0.383394	-0.267010
7	6	-2.852965	1.944993	0.001226
8	6	-0.528101	0.201606	-0.620112
9	7	-0.541212	1.675113	-0.674892
10	6	-1.772684	2.375464	-0.998807
11	6	3.192166	2.789444	0.669406
12	6	2.347111	3.865896	0.172241
13	6	1.042640	3.562200	-0.306577
14	6	0.638402	2.234691	-0.298674
15	6	1.506972	1.130008	0.162682

16	6	0.675206	-0.094163	0.361383
17	8	0.082168	-0.118589	1.697588
18	6	2.806938	1.467403	0.677242
19	6	2.781984	-3.794319	-0.513596
20	6	2.796115	-2.732648	-1.425769
21	6	2.114804	-1.549266	-1.134409
22	6	1.403966	-1.404640	0.069116
23	6	1.394093	-2.472897	0.974762
24	6	2.080388	-3.658844	0.686651
25	1	-0.240547	-0.176476	-1.611484
26	1	-5.069006	0.473795	0.571174
27	1	-5.324400	-1.992311	0.594836
28	1	-3.376377	-3.441801	0.012635
29	1	-1.204320	-2.409366	-0.557469
30	1	-2.590281	2.334799	0.993213
31	1	-3.807554	2.401364	-0.279781
32	1	0.763090	0.178464	2.318601
33	1	-1.592070	3.449232	-0.953165
34	1	-2.072994	2.118250	-2.022456
35	1	4.176259	3.049688	1.053812
36	1	2.708985	4.886853	0.188294
37	1	0.399017	4.345085	-0.694538
38	1	3.470378	0.696649	1.058019
39	1	3.314162	-4.714427	-0.737018
40	1	3.340995	-2.823903	-2.361054
41	1	2.145029	-0.725373	-1.842762
42	1	0.846788	-2.374713	1.905192
43	1	2.063692	-4.475158	1.403341

1a (B, NMP)

Number	Atomic Number	X	Y	Z
1	6	-3.050134	-0.612110	0.129065
2	6	-4.328928	-0.058182	-0.045684
3	6	-4.509002	1.312638	-0.227591
4	6	-3.396017	2.160013	-0.227130
5	6	-2.120270	1.625050	-0.049406
6	6	-1.929421	0.243882	0.115557
7	6	-2.912952	-2.114019	0.316731
8	6	-0.547763	-0.323395	0.378315
9	7	-0.525863	-1.782657	0.201132
10	6	-1.558222	-2.521799	0.903887
11	6	3.532963	-2.486956	-0.429942

12	6	2.751070	-3.576053	-0.025047
13	6	1.380079	-3.439930	0.234452
14	6	0.802714	-2.174710	0.072680
15	6	1.587586	-1.073425	-0.323561
16	6	0.674753	0.141990	-0.500419
17	8	0.296091	0.266100	-1.882191
18	6	2.942749	-1.221640	-0.583060
19	6	2.479502	3.894122	0.744401
20	6	2.386757	2.820107	1.636384
21	6	1.808384	1.616162	1.229589
22	6	1.301045	1.463484	-0.071486
23	6	1.406542	2.541795	-0.961035
24	6	1.990731	3.747383	-0.555609
25	1	-0.277749	-0.095298	1.425603
26	1	-5.193588	-0.717712	-0.033174
27	1	-5.508166	1.717666	-0.360221
28	1	-3.520066	3.230720	-0.361019
29	1	-1.261695	2.287537	-0.043076
30	1	-3.035630	-2.607904	-0.656258
31	1	-3.721068	-2.481622	0.958957
32	1	-0.102433	-0.573534	-2.154746
33	1	-1.396064	-3.593465	0.768112
34	1	-1.522333	-2.312477	1.987252
35	1	4.593950	-2.618983	-0.617813
36	1	3.214715	-4.550734	0.100218
37	1	0.793671	-4.295533	0.552775
38	1	3.540880	-0.368163	-0.890852
39	1	2.931447	4.830201	1.059187
40	1	2.769713	2.915888	2.648325
41	1	1.763955	0.788616	1.931390
42	1	1.028829	2.437361	-1.970790
43	1	2.060953	4.570787	-1.260824

1a (C, NMP)

Number	Atomic Number	X	Y	Z
1	6	-3.029427	-0.704541	0.252673
2	6	-4.333486	-0.202050	0.133462
3	6	-4.566292	1.139377	-0.164851
4	6	-3.485045	2.005356	-0.353043
5	6	-2.182235	1.522134	-0.242427
6	6	-1.943373	0.171982	0.052531
7	6	-2.847061	-2.187290	0.547329

8	6	-0.536525	-0.344317	0.263845
9	7	-0.491631	-1.842741	-0.032800
10	6	-1.413725	-2.597898	0.884992
11	6	3.679633	-2.274628	-0.281767
12	6	2.947018	-3.430415	0.011495
13	6	1.550316	-3.388246	0.129116
14	6	0.954512	-2.151987	-0.050476
15	6	1.655779	-0.986184	-0.341591
16	6	0.687107	0.183529	-0.546078
17	8	0.255648	0.209439	-1.911585
18	6	3.041467	-1.039900	-0.460715
19	6	2.252111	3.993465	0.826919
20	6	2.232085	2.888134	1.684129
21	6	1.728793	1.664267	1.239623
22	6	1.227705	1.529685	-0.065093
23	6	1.253761	2.639342	-0.919009
24	6	1.764866	3.863702	-0.475263
25	1	-0.271027	-0.275397	1.323437
26	1	-5.173318	-0.875811	0.281280
27	1	-5.584453	1.507281	-0.247276
28	1	-3.653018	3.052343	-0.585152
29	1	-1.349374	2.199387	-0.384952
30	1	-3.190784	-2.766692	-0.318836
31	1	-3.486943	-2.484328	1.383663
32	1	-0.838947	-1.962241	-0.994639
33	1	1.030113	0.209598	-2.493617
34	1	-1.257741	-3.664719	0.727110
35	1	-1.121143	-2.339609	1.904392
36	1	4.760058	-2.333758	-0.363855
37	1	3.461915	-4.374632	0.153449
38	1	0.981441	-4.283364	0.352988
39	1	3.616985	-0.145408	-0.675554
40	1	2.646787	4.944476	1.171536
41	1	2.613211	2.974996	2.697099
42	1	1.740595	0.813435	1.915073
43	1	0.866603	2.553029	-1.928146
44	1	1.777376	4.713995	-1.150526

1a (TS3, NMP)

Number	Atomic Number	X	Y	Z
1	6	2.637627	-1.488909	0.006611
2	6	4.026329	-1.298023	0.079609

3	6	4.603260	-0.058801	-0.193149
4	6	3.791690	1.017674	-0.565990
5	6	2.411193	0.845280	-0.647613
6	6	1.823159	-0.392520	-0.341057
7	6	2.059344	-2.863331	0.296997
8	6	0.328404	-0.572866	-0.495331
9	7	-0.138784	-1.878581	0.078001
10	6	0.660292	-3.057238	-0.286328
11	6	-4.247933	-1.142529	-0.117014
12	6	-3.847051	-2.473408	-0.271722
13	6	-2.491214	-2.842259	-0.244348
14	6	-1.566910	-1.824451	-0.072529
15	6	-1.956835	-0.481300	0.074121
16	6	-0.685776	0.314163	0.309306
17	8	-0.221662	-0.113752	1.728798
18	6	-3.298788	-0.125392	0.069598
19	6	-0.679642	4.591893	-0.165263
20	6	-1.283730	3.767684	-1.119691
21	6	-1.295153	2.382743	-0.946059
22	6	-0.687420	1.807329	0.182052
23	6	-0.077688	2.636000	1.134397
24	6	-0.080467	4.022472	0.960906
25	1	0.039855	-0.503407	-1.552129
26	1	4.659387	-2.140501	0.345774
27	1	5.680511	0.063110	-0.131725
28	1	4.230731	1.982596	-0.799709
29	1	1.787557	1.676726	-0.957130
30	1	2.016353	-3.020787	1.382707
31	1	2.724466	-3.635069	-0.102220
32	1	-0.065883	-1.173381	1.409063
33	1	-0.944087	-0.041618	2.380880
34	1	0.184688	-3.943249	0.138501
35	1	0.686123	-3.166654	-1.377940
36	1	-5.303268	-0.892350	-0.142895
37	1	-4.597760	-3.243765	-0.417170
38	1	-2.193623	-3.878578	-0.357312
39	1	-3.608069	0.906862	0.195151
40	1	-0.677947	5.669307	-0.298434
41	1	-1.753102	4.200052	-1.997765
42	1	-1.771961	1.754699	-1.691801
43	1	0.403562	2.206710	2.005468
44	1	0.391096	4.654108	1.707272

1a (D, NMP)

Number	Atomic Number	X	Y	Z
1	6	2.344246	-1.626866	-0.197664
2	6	2.730813	-2.827279	-0.815559
3	6	1.821308	-3.858555	-1.038649
4	6	0.494496	-3.707282	-0.627146
5	6	0.091536	-2.523696	-0.010252
6	6	0.998522	-1.474216	0.194630
7	6	3.386493	-0.550536	0.030458
8	6	0.534121	-0.184502	0.912206
9	7	1.595417	0.819641	0.900642
10	6	2.969566	0.401547	1.154551
11	6	-0.205220	4.084815	-0.855183
12	6	1.191640	4.172132	-0.531596
13	6	1.889997	3.137662	0.044553
14	6	1.175658	1.939823	0.305215
15	6	-0.222283	1.811415	-0.060079
16	6	-0.647478	0.543894	0.304960
17	6	-0.910138	2.936357	-0.621647
18	6	-4.633894	-0.966059	0.062445
19	6	-3.876494	-1.175456	1.220181
20	6	-2.567522	-0.704563	1.296102
21	6	-2.001246	0.008659	0.216877
22	6	-2.777355	0.218172	-0.943169
23	6	-4.078180	-0.275384	-1.019731
24	1	0.303224	-0.428921	1.961175
25	1	3.767532	-2.947846	-1.118156
26	1	2.147261	-4.776564	-1.518057
27	1	-0.225150	-4.505635	-0.779131
28	1	-0.937370	-2.426391	0.313130
29	1	3.535737	0.028013	-0.890034
30	1	4.349600	-1.007175	0.278389
31	1	3.611498	1.280655	1.205531
32	1	2.999084	-0.097429	2.127419
33	1	-0.697836	4.952753	-1.279139
34	1	1.709967	5.103632	-0.737225
35	1	2.937990	3.240204	0.297412
36	1	-1.968401	2.874526	-0.844775
37	1	-5.650483	-1.342023	0.003121
38	1	-4.304981	-1.706036	2.064411
39	1	-1.997526	-0.860047	2.206503
40	1	-2.343313	0.724967	-1.798226
41	1	-4.656268	-0.124682	-1.925857

1a (TS3-3, NMP)

Number	Atomic Number	X	Y	Z
1	6	2.821950	-0.366665	0.748347
2	6	4.183419	-0.497918	0.427979
3	6	4.619960	-1.133002	-0.731251
4	6	3.654621	-1.666209	-1.590893
5	6	2.301253	-1.569270	-1.277476
6	6	1.821406	-0.911311	-0.111998
7	6	2.499280	0.395376	2.024413
8	6	0.361943	-0.900979	0.325632
9	7	0.159069	0.193147	1.318140
10	6	1.049823	0.199751	2.469340
11	6	-0.395295	3.349799	-1.406618
12	6	-0.013727	3.681288	-0.101518
13	6	0.183609	2.699361	0.881532
14	6	0.000248	1.357541	0.532206
15	6	-0.435096	1.027218	-0.787381
16	6	-0.728896	-0.437221	-0.636659
17	8	-0.498287	-1.525324	-1.683875
18	6	-0.631595	2.006856	-1.748791
19	6	-4.840784	-1.180163	0.574903
20	6	-3.795825	-1.867877	1.200521
21	6	-2.470675	-1.623555	0.832537
22	6	-2.169949	-0.673924	-0.156499
23	6	-3.224219	0.017664	-0.773821
24	6	-4.551133	-0.239861	-0.417587
25	1	-0.178585	-2.098750	-0.722139
26	1	4.914574	-0.075922	1.115197
27	1	5.679525	-1.215099	-0.955441
28	1	3.951280	-2.171156	-2.506759
29	1	1.608154	-2.026396	-1.970374
30	1	2.686300	1.464117	1.854230
31	1	3.184300	0.092687	2.826014
32	1	-1.343975	-1.848272	-2.049802
33	1	0.740741	0.976653	3.176075
34	1	0.923650	-0.764378	2.972213
35	1	-0.522317	4.129183	-2.151414
36	1	0.151966	4.723394	0.157935
37	1	0.501298	2.983029	1.879757
38	1	-0.956676	1.743142	-2.751359
39	1	-5.870745	-1.374075	0.859935
40	1	-4.011291	-2.595911	1.977340

41	1	-1.659872	-2.159444	1.312150
42	1	-3.013431	0.765764	-1.530851
43	1	-5.353999	0.300604	-0.910188

1a (2a, NMP)

Number	Atomic Number	X	Y	Z
1	6	2.788896	-1.151942	0.211715
2	6	4.149697	-0.843352	0.118132
3	6	4.574371	0.415562	-0.314726
4	6	3.624880	1.377277	-0.676135
5	6	2.264491	1.083166	-0.593168
6	6	1.825785	-0.173011	-0.133927
7	6	2.315512	-2.510670	0.677905
8	6	0.403657	-0.528752	-0.046294
9	7	0.072039	-1.882080	-0.022268
10	6	1.068436	-2.946688	-0.093692
11	6	-4.056110	-1.717472	-0.012773
12	6	-3.475907	-3.006236	-0.033292
13	6	-2.093253	-3.175584	-0.044544
14	6	-1.297199	-2.020369	-0.040162
15	6	-1.861223	-0.712204	-0.039435
16	6	-0.768016	0.227345	-0.032544
17	6	-3.263201	-0.573836	-0.012026
18	6	-1.304751	4.489202	0.270308
19	6	-1.893243	3.775223	-0.778024
20	6	-1.706537	2.393581	-0.880765
21	6	-0.926907	1.695999	0.060639
22	6	-0.349841	2.427333	1.116172
23	6	-0.531602	3.808257	1.217437
24	1	4.883245	-1.600415	0.383825
25	1	5.635059	0.638887	-0.381598
26	1	3.942702	2.352580	-1.032983
27	1	1.538014	1.827956	-0.895259
28	1	2.073313	-2.475658	1.749259
29	1	3.105041	-3.256892	0.550137
30	1	0.641325	-3.852405	0.341739
31	1	1.316521	-3.157818	-1.142750
32	1	-5.137988	-1.621612	0.001655
33	1	-4.118969	-3.881500	-0.038669
34	1	-1.655947	-4.168815	-0.057113
35	1	-3.718781	0.411835	0.004684
36	1	-1.448753	5.562745	0.350769

37	1	-2.495219	4.292922	-1.519649
38	1	-2.157727	1.849475	-1.705576
39	1	0.242050	1.904724	1.862067
40	1	-0.075768	4.351573	2.040542

1j (S0, NMP)

Number	Atomic Number	X	Y	Z
1	6	-3.411628	-1.800181	0.848240
2	6	-4.580994	-2.308072	0.269896
3	6	-4.969862	-1.889184	-1.004987
4	6	-4.181884	-0.962403	-1.699104
5	6	-3.013912	-0.462147	-1.120156
6	6	-2.615592	-0.875197	0.161265
7	6	-1.321822	-0.361276	0.775787
8	7	-1.250090	1.098856	0.846386
9	6	-2.426271	1.781943	1.376764
10	6	1.789051	3.360318	-1.045676
11	6	0.503884	3.881569	-0.851785
12	6	-0.478564	3.135426	-0.210125
13	6	-0.220136	1.830564	0.281167
14	6	1.114131	1.328033	0.148942
15	6	1.631222	0.158826	0.923197
16	8	1.303180	-0.019660	2.101343
17	6	2.072135	2.092471	-0.548483
18	6	4.404709	-2.627947	-0.835764
19	6	3.500815	-1.946425	-1.656290
20	6	2.615645	-1.018208	-1.102923
21	6	2.614744	-0.776010	0.281329
22	6	3.516894	-1.477789	1.099938
23	6	4.413089	-2.389722	0.544458
24	1	-5.186441	-3.024961	0.817244
25	1	-5.878255	-2.278737	-1.455334
26	1	-4.476826	-0.632852	-2.691403
27	1	-2.406435	0.257064	-1.663810
28	1	-0.492014	-0.710759	0.158193
29	1	-1.181929	-0.803848	1.770732
30	1	-2.127015	2.693918	1.899679
31	1	-3.163059	2.043776	0.604982
32	1	2.554609	3.935882	-1.555478
33	1	0.254544	4.871477	-1.224015
34	1	-1.475182	3.550552	-0.122482
35	1	3.079159	1.698832	-0.643355

36	1	5.098645	-3.342808	-1.268134
37	1	3.485081	-2.135778	-2.725342
38	1	1.915186	-0.493819	-1.744705
39	1	3.508880	-1.292851	2.169123
40	1	5.116302	-2.915846	1.183125
41	1	-3.117293	-2.125919	1.842915
42	1	-2.916702	1.124447	2.098476

1j (S1, NMP)

Number	Atomic Number	X	Y	Z
1	6	-3.286949	-1.467734	1.017026
2	6	-4.327781	-2.074409	0.306141
3	6	-4.349969	-2.015439	-1.089778
4	6	-3.323549	-1.353329	-1.773432
5	6	-2.280899	-0.754374	-1.063939
6	6	-2.254665	-0.807427	0.338383
7	6	-1.105200	-0.179621	1.114534
8	7	-1.085031	1.283943	0.938478
9	6	-2.253179	1.988252	1.476517
10	6	1.660106	3.430144	-1.376179
11	6	0.335477	3.875300	-1.242865
12	6	-0.549230	3.156271	-0.463103
13	6	-0.148314	1.950081	0.185691
14	6	1.219750	1.498109	0.066722
15	6	1.817933	0.403915	0.920335
16	8	1.886278	0.697074	2.173674
17	6	2.079691	2.273216	-0.709626
18	6	3.319856	-3.250405	-0.760858
19	6	2.676428	-2.306116	-1.581846
20	6	2.188292	-1.114166	-1.060345
21	6	2.319936	-0.801856	0.331405
22	6	2.972804	-1.779880	1.150233
23	6	3.456693	-2.964019	0.610925
24	1	-5.118595	-2.588709	0.844056
25	1	-5.159000	-2.483268	-1.642763
26	1	-3.332196	-1.308088	-2.858393
27	1	-1.484104	-0.250462	-1.604535
28	1	-0.152282	-0.582417	0.781258
29	1	-1.213902	-0.384649	2.182108
30	1	-1.972552	2.992398	1.789829
31	1	-3.058345	2.040646	0.736657
32	1	2.362290	3.985335	-1.989400

33	1	-0.000844	4.767879	-1.758538
34	1	-1.579942	3.480048	-0.398920
35	1	3.117223	1.964199	-0.784967
36	1	3.700952	-4.178165	-1.175444
37	1	2.556570	-2.507066	-2.643945
38	1	1.696050	-0.410870	-1.725111
39	1	3.083370	-1.572975	2.209521
40	1	3.949991	-3.681777	1.262852
41	1	-3.275665	-1.515049	2.102616
42	1	-2.617421	1.429722	2.338739

1j (T1, NMP)

Number	Atomic Number	X	Y	Z
1	6	-2.653582	-1.652539	-0.390075
2	6	-3.648406	-2.616799	-0.212481
3	6	-4.995953	-2.240498	-0.171056
4	6	-5.343061	-0.893716	-0.307914
5	6	-4.345494	0.070927	-0.484032
6	6	-2.993149	-0.296909	-0.523620
7	6	-1.927239	0.752506	-0.754396
8	7	-1.116331	1.101404	0.434743
9	6	-1.793824	1.260803	1.717461
10	6	2.242594	3.545284	-0.289906
11	6	0.974515	4.138865	-0.181041
12	6	-0.138645	3.324476	0.062693
13	6	0.017419	1.945932	0.177838
14	6	1.289952	1.314258	0.049017
15	6	1.320490	-0.112189	0.259992
16	8	0.212121	-0.684181	0.680274
17	6	2.404051	2.169430	-0.176014
18	6	4.667914	-2.784046	-0.185658
19	6	4.579513	-1.641572	-0.990838
20	6	3.508396	-0.757601	-0.858607
21	6	2.489160	-0.986350	0.096999
22	6	2.580445	-2.161808	0.883438
23	6	3.654498	-3.038806	0.747960
24	1	-3.372598	-3.662561	-0.110914
25	1	-5.768453	-2.992123	-0.036773
26	1	-6.386298	-0.592736	-0.281287
27	1	-4.622300	1.116260	-0.595256
28	1	-2.396330	1.679261	-1.115657
29	1	-1.217946	0.427052	-1.519655

30	1	-2.396826	0.375993	1.923874
31	1	-1.043478	1.386394	2.497675
32	1	3.117705	4.168571	-0.451207
33	1	0.854249	5.213294	-0.272670
34	1	-1.126553	3.765097	0.162488
35	1	3.402406	1.752806	-0.219957
36	1	5.504682	-3.468077	-0.291327
37	1	5.342677	-1.443624	-1.738752
38	1	3.443156	0.090426	-1.530606
39	1	1.800888	-2.366595	1.609712
40	1	3.703800	-3.925163	1.374915
41	1	-1.607456	-1.939937	-0.411462
42	1	-2.451535	2.141387	1.702899

1j (TS1, NMP)

Number	Atomic Number	X	Y	Z
1	6	3.466415	-0.801202	-0.990374
2	6	4.720623	-1.415142	-0.992585
3	6	5.309316	-1.814689	0.212175
4	6	4.634151	-1.600241	1.417689
5	6	3.380129	-0.982781	1.418833
6	6	2.785547	-0.563922	0.217123
7	6	1.413649	0.039205	0.230156
8	7	1.251993	1.435234	0.013953
9	6	2.394024	2.306952	-0.273635
10	6	-2.532293	3.322186	-0.031759
11	6	-1.375745	4.034761	0.276860
12	6	-0.154099	3.364492	0.279812
13	6	-0.050692	1.984259	0.008270
14	6	-1.244252	1.217607	-0.262966
15	6	-1.334292	-0.219161	-0.638225
16	8	-0.397409	-0.740582	-1.432808
17	6	-2.446337	1.955977	-0.308011
18	6	-4.496700	-2.884323	0.531144
19	6	-4.345009	-1.653333	1.189604
20	6	-3.343104	-0.762677	0.819286
21	6	-2.431086	-1.068701	-0.235134
22	6	-2.587258	-2.338169	-0.868803
23	6	-3.601552	-3.214541	-0.498227
24	1	5.232680	-1.590385	-1.934140
25	1	6.282453	-2.296701	0.209914
26	1	5.081066	-1.913837	2.356559

27	1	2.858822	-0.821176	2.358548
28	1	0.834671	-0.266561	1.108822
29	1	0.727223	-0.435999	-0.677957
30	1	3.250855	1.700662	-0.551406
31	1	2.152455	2.989665	-1.089728
32	1	-3.497567	3.817841	-0.070197
33	1	-1.410221	5.095085	0.503663
34	1	0.738469	3.926023	0.523526
35	1	-3.350126	1.433093	-0.597222
36	1	-5.284547	-3.572757	0.821662
37	1	-5.011782	-1.390595	2.006891
38	1	-3.239479	0.164667	1.371271
39	1	-1.892659	-2.609384	-1.655620
40	1	-3.696175	-4.167885	-1.012223
41	1	3.007893	-0.510593	-1.931892
42	1	2.662672	2.887522	0.616918

1j (A, NMP)

Number	Atomic Number	X	Y	Z
1	6	3.256371	-0.684412	-0.808090
2	6	4.260174	-1.647391	-0.853119
3	6	4.765275	-2.216766	0.324573
4	6	4.235518	-1.813889	1.561760
5	6	3.233062	-0.855319	1.620180
6	6	2.714823	-0.248465	0.436538
7	6	1.683251	0.720011	0.578262
8	7	1.167000	1.530953	-0.455569
9	6	2.124271	2.410395	-1.168328
10	6	-2.585051	3.252181	0.565293
11	6	-1.432326	4.045076	0.556528
12	6	-0.208587	3.470126	0.204311
13	6	-0.115204	2.119062	-0.139403
14	6	-1.283693	1.292440	-0.149544
15	6	-1.268004	-0.081877	-0.627463
16	8	-0.340463	-0.435768	-1.567950
17	6	-2.508712	1.908679	0.215967
18	6	-3.969643	-3.261430	0.348579
19	6	-3.832776	-2.168597	1.215731
20	6	-2.966666	-1.122292	0.910197
21	6	-2.203770	-1.129763	-0.287350
22	6	-2.338877	-2.256785	-1.142132
23	6	-3.210043	-3.296527	-0.828222

24	1	4.648269	-1.965233	-1.816934
25	1	5.549912	-2.965694	0.280053
26	1	4.609858	-2.254199	2.481769
27	1	2.831436	-0.551476	2.583395
28	1	1.200214	0.826508	1.545553
29	1	0.365129	0.249367	-1.556020
30	1	1.610403	2.889760	-2.003444
31	1	2.543380	3.178113	-0.506941
32	1	-3.547654	3.685367	0.820075
33	1	-1.479612	5.096188	0.823225
34	1	0.686598	4.081380	0.216621
35	1	-3.421852	1.327828	0.166263
36	1	-4.647739	-4.074097	0.590832
37	1	-4.395704	-2.138393	2.144486
38	1	-2.851017	-0.310550	1.619414
39	1	-1.758562	-2.297007	-2.056706
40	1	-3.299520	-4.140424	-1.506846
41	1	2.866901	-0.289515	-1.740013
42	1	2.947911	1.814817	-1.557824

1j (TS2', NMP)

Number	Atomic Number	X	Y	Z
1	6	2.121649	-1.949687	0.714636
2	6	3.483516	-2.155960	0.924329
3	6	4.434808	-1.542133	0.096183
4	6	3.999635	-0.720380	-0.953335
5	6	2.638355	-0.519871	-1.173003
6	6	1.665158	-1.134975	-0.349409
7	6	0.249994	-0.846125	-0.582419
8	7	-0.714606	-1.888936	-0.358038
9	6	-0.484610	-3.292204	-0.686219
10	6	-4.328954	0.063316	0.108216
11	6	-4.380224	-1.369423	-0.106058
12	6	-3.195608	-2.091103	-0.237879
13	6	-1.976201	-1.416543	-0.081518
14	6	-1.918312	0.002761	0.281088
15	6	-0.556301	0.426571	0.595718
16	8	-0.047958	0.006351	1.854273
17	6	-3.131303	0.734185	0.271802
18	6	0.782375	4.396533	-0.406706
19	6	-0.066161	3.690868	-1.269076
20	6	-0.501426	2.408752	-0.934899

21	6	-0.115213	1.806476	0.281393
22	6	0.749314	2.520955	1.134252
23	6	1.189617	3.801408	0.793235
24	1	3.807803	-2.790562	1.744730
25	1	5.495463	-1.698800	0.268311
26	1	4.724846	-0.238468	-1.603384
27	1	2.313465	0.115076	-1.993527
28	1	0.070497	-0.319444	-1.524144
29	1	-0.657504	-0.642477	2.231878
30	1	-0.904805	-3.932968	0.094247
31	1	-0.968750	-3.533891	-1.640780
32	1	-5.261192	0.618319	0.164598
33	1	-5.339749	-1.864986	-0.202949
34	1	-3.218492	-3.144648	-0.499318
35	1	-3.122391	1.804068	0.457928
36	1	1.124398	5.393386	-0.668997
37	1	-0.383911	4.137956	-2.206878
38	1	-1.149337	1.869242	-1.619562
39	1	1.061134	2.070641	2.069270
40	1	1.848856	4.338482	1.469700
41	1	1.402132	-2.411518	1.383200
42	1	0.582794	-3.478200	-0.774233

1j (B', NMP)

Number	Atomic Number	X	Y	Z
1	6	2.358789	-1.614899	0.730311
2	6	3.720515	-1.709803	1.022204
3	6	4.641994	-0.885429	0.365740
4	6	4.192404	0.026816	-0.592545
5	6	2.828865	0.110919	-0.892178
6	6	1.897436	-0.701431	-0.230238
7	6	0.428151	-0.559106	-0.564999
8	7	-0.288820	-1.853415	-0.671121
9	6	0.207480	-2.945740	-1.492462
10	6	-4.091030	-0.997308	0.683291
11	6	-3.885381	-2.343084	0.145659
12	6	-2.604043	-2.700804	-0.354673
13	6	-1.579629	-1.771805	-0.248705
14	6	-1.770307	-0.427693	0.337390
15	6	-0.456973	0.261767	0.459042
16	8	0.130007	0.036966	1.778909
17	6	-3.085930	-0.062607	0.776010

18	6	-0.496455	4.500475	-0.516996
19	6	-1.184047	3.579828	-1.316425
20	6	-1.171264	2.222025	-0.991327
21	6	-0.471128	1.757371	0.134558
22	6	0.217296	2.685480	0.926303
23	6	0.203338	4.047888	0.603888
24	1	0.350677	-0.051830	-1.535901
25	1	4.062791	-2.424689	1.764977
26	1	5.700886	-0.958890	0.596011
27	1	4.899455	0.665680	-1.113639
28	1	2.487379	0.812194	-1.649219
29	1	-0.581494	0.148161	2.426206
30	1	-0.047241	-3.901689	-1.027616
31	1	-0.245005	-2.907110	-2.491805
32	1	-5.089686	-0.729298	1.021258
33	1	-4.717754	-3.034304	0.092869
34	1	-2.438304	-3.666874	-0.820729
35	1	-3.283052	0.928123	1.174547
36	1	-0.508931	5.557622	-0.766117
37	1	-1.734359	3.919083	-2.189440
38	1	-1.716814	1.517119	-1.613109
39	1	0.762445	2.338097	1.796362
40	1	0.740854	4.752824	1.231986
41	1	1.649314	-2.249459	1.250948
42	1	1.290054	-2.873735	-1.584106

1j (B, NMP)

Number	Atomic Number	X	Y	Z
1	6	-2.222830	-1.935575	-0.644741
2	6	-3.581530	-2.107977	-0.922096
3	6	-4.533147	-1.270550	-0.330227
4	6	-4.115781	-0.265828	0.547928
5	6	-2.756035	-0.100555	0.828233
6	6	-1.793129	-0.926651	0.229963
7	6	-0.327281	-0.694961	0.522246
8	7	0.491728	-1.923886	0.511347
9	6	0.258548	-2.888470	1.578776
10	6	4.222407	-0.461042	-0.683580
11	6	4.183308	-1.727124	-0.084673
12	6	2.981287	-2.288423	0.364597
13	6	1.801080	-1.551533	0.194073
14	6	1.840570	-0.270848	-0.385378

15	6	0.421718	0.264168	-0.500753
16	8	-0.057206	0.086351	-1.844273
17	6	3.037198	0.273503	-0.836589
18	6	-0.126078	4.441134	0.558907
19	6	0.651542	3.600369	1.362913
20	6	0.831673	2.261397	1.010554
21	6	0.237845	1.734858	-0.148430
22	6	-0.538851	2.584263	-0.948036
23	6	-0.718919	3.927159	-0.596586
24	1	-0.239784	-0.220025	1.512211
25	1	-3.896656	-2.897608	-1.598420
26	1	-5.589344	-1.405813	-0.544534
27	1	-4.846638	0.383824	1.020987
28	1	-2.440825	0.675079	1.521262
29	1	0.145278	-0.818256	-2.121937
30	1	0.597380	-2.514500	2.558670
31	1	-0.808890	-3.108846	1.638352
32	1	5.167944	-0.045839	-1.018214
33	1	5.105105	-2.288177	0.042393
34	1	2.975509	-3.268871	0.828699
35	1	3.055414	1.262157	-1.287265
36	1	-0.265206	5.483549	0.830407
37	1	1.122730	3.986860	2.262123
38	1	1.445604	1.624698	1.641017
39	1	-1.001275	2.194680	-1.846778
40	1	-1.324614	4.569035	-1.230168
41	1	-1.489525	-2.597340	-1.095922
42	1	0.781764	-3.822097	1.359255

1j (C, NMP)

Number	Atomic Number	X	Y	Z
1	6	2.279192	-1.530414	1.027808
2	6	3.652158	-1.734910	1.177816
3	6	4.538674	-1.350196	0.166677
4	6	4.045998	-0.765902	-1.002685
5	6	2.671530	-0.572563	-1.160137
6	6	1.775032	-0.947011	-0.146956
7	6	0.304322	-0.706607	-0.375722
8	7	-0.543825	-1.997556	-0.282869
9	6	-0.339073	-2.932325	-1.439960
10	6	-4.303445	-0.220929	0.406538
11	6	-4.298732	-1.551338	-0.028681

12	6	-3.094812	-2.218996	-0.288178
13	6	-1.927617	-1.496664	-0.094475
14	6	-1.902746	-0.175468	0.335750
15	6	-0.467587	0.292818	0.545025
16	8	-0.075480	-0.010141	1.888039
17	6	-3.105647	0.478954	0.593391
18	6	0.416494	4.391364	-0.569771
19	6	-0.438772	3.616830	-1.360531
20	6	-0.733015	2.301772	-0.995278
21	6	-0.175032	1.742122	0.165275
22	6	0.686326	2.520634	0.948866
23	6	0.977288	3.839310	0.584341
24	1	0.150182	-0.370738	-1.402714
25	1	4.028859	-2.189435	2.088897
26	1	5.605904	-1.507857	0.289553
27	1	4.725693	-0.466849	-1.794507
28	1	2.293762	-0.126669	-2.075919
29	1	-0.262128	-2.494425	0.570535
30	1	-0.676987	0.436756	2.502194
31	1	-0.897673	-3.848185	-1.254796
32	1	-0.693741	-2.441914	-2.345250
33	1	-5.248932	0.276613	0.596584
34	1	-5.236949	-2.076817	-0.171792
35	1	-3.093061	-3.249312	-0.624474
36	1	-3.114388	1.512486	0.923915
37	1	0.642093	5.415448	-0.851716
38	1	-0.881592	4.036017	-2.259030
39	1	-1.403970	1.717041	-1.618212
40	1	1.130627	2.095155	1.841595
41	1	1.644655	4.431255	1.203615
42	1	1.610620	-1.812380	1.833668
43	1	0.724428	-3.155072	-1.511041

1j (TS3, NMP)

Number	Atomic Number	X	Y	Z
1	6	1.996837	-1.905391	0.807905
2	6	3.356455	-2.218411	0.871662
3	6	4.209724	-1.880501	-0.182894
4	6	3.693461	-1.235500	-1.309586
5	6	2.332059	-0.931604	-1.377867
6	6	1.468492	-1.253022	-0.318451
7	6	0.018306	-0.856512	-0.461851

8	7	-1.001934	-1.823457	0.100094
9	6	-0.955266	-3.228654	-0.332566
10	6	-4.327092	0.718745	-0.119721
11	6	-4.571116	-0.649366	-0.276621
12	6	-3.529742	-1.591623	-0.239101
13	6	-2.244656	-1.104596	-0.055034
14	6	-1.986036	0.269092	0.087042
15	6	-0.500548	0.390992	0.335701
16	8	-0.314453	-0.208214	1.761005
17	6	-3.021870	1.194576	0.076578
18	6	1.620268	4.102324	-0.142611
19	6	0.607917	3.740951	-1.036140
20	6	-0.091163	2.545294	-0.859818
21	6	0.224529	1.694366	0.211698
22	6	1.249114	2.053993	1.099544
23	6	1.937158	3.256919	0.924023
24	1	-0.201857	-0.668846	-1.517905
25	1	3.746238	-2.729037	1.746858
26	1	5.266069	-2.125702	-0.129468
27	1	4.344559	-0.975806	-2.138572
28	1	1.937302	-0.440183	-2.262772
29	1	-0.657940	-1.225255	1.434129
30	1	-0.925220	0.197255	2.404755
31	1	-1.664685	-3.803474	0.264649
32	1	-1.207023	-3.321396	-1.394413
33	1	-5.154064	1.420245	-0.151621
34	1	-5.587993	-0.996738	-0.429768
35	1	-3.734899	-2.649965	-0.351677
36	1	-2.831124	2.254602	0.205390
37	1	2.157989	5.035884	-0.276794
38	1	0.355471	4.389883	-1.868895
39	1	-0.873826	2.275662	-1.561194
40	1	1.508785	1.402295	1.925772
41	1	2.723401	3.528688	1.621473
42	1	1.361615	-2.188522	1.640059
43	1	0.045370	-3.622112	-0.160062

1j (D, NMP)

Number	Atomic Number	X	Y	Z
1	6	1.069015	-1.651637	1.261407
2	6	2.139548	-2.257432	1.919599
3	6	3.269363	-2.663346	1.199120

4	6	3.321074	-2.465229	-0.182105
5	6	2.246883	-1.860896	-0.844442
6	6	1.119426	-1.449277	-0.125655
7	6	-0.052105	-0.792324	-0.850590
8	7	-1.302820	-1.553209	-0.710607
9	6	-1.453481	-2.926077	-1.180661
10	6	-3.970208	1.268256	0.671880
11	6	-4.447472	-0.066339	0.439549
12	6	-3.638409	-1.075888	-0.024862
13	6	-2.273017	-0.761468	-0.251561
14	6	-1.761614	0.575545	-0.002074
15	6	-0.419886	0.590842	-0.351406
16	6	-2.659966	1.595462	0.453142
17	6	2.394754	3.790491	-0.123866
18	6	2.471292	2.862531	-1.168558
19	6	1.560332	1.811959	-1.239881
20	6	0.537338	1.682616	-0.273905
21	6	0.475350	2.624236	0.777750
22	6	1.399452	3.663396	0.851361
23	1	0.182123	-0.735391	-1.923493
24	1	2.093099	-2.410685	2.993400
25	1	4.101981	-3.133390	1.713559
26	1	4.191418	-2.782105	-0.748418
27	1	2.291196	-1.714787	-1.919948
28	1	-1.892651	-2.945086	-2.183145
29	1	-0.470388	-3.395743	-1.207324
30	1	-4.672634	2.022322	1.009064
31	1	-5.496509	-0.277059	0.623433
32	1	-4.027971	-2.068507	-0.215012
33	1	-2.309189	2.609841	0.597761
34	1	3.110407	4.604757	-0.067233
35	1	3.239801	2.958878	-1.928756
36	1	1.620641	1.114410	-2.068183
37	1	-0.263147	2.511083	1.563218
38	1	1.348968	4.368803	1.674582
39	1	0.195212	-1.341335	1.827574
40	1	-2.088637	-3.486071	-0.492289

1j (2j, NMP)

Number	Atomic Number	X	Y	Z
1	6	-2.051986	-2.057377	-0.879787
2	6	-3.413337	-2.366806	-0.832637

3	6	-4.219332	-1.841763	0.182736
4	6	-3.654069	-1.006516	1.151945
5	6	-2.292427	-0.699212	1.107324
6	6	-1.472593	-1.218744	0.089981
7	6	-0.036663	-0.867311	0.040830
8	7	0.958449	-1.843489	0.050014
9	6	0.785788	-3.282504	0.201090
10	6	4.372052	0.484505	-0.116108
11	6	4.560863	-0.914606	-0.067436
12	6	3.474912	-1.785514	-0.007086
13	6	2.190542	-1.222339	0.011479
14	6	1.977615	0.183818	-0.017838
15	6	0.550073	0.393800	0.000828
16	6	3.094845	1.038527	-0.094671
17	6	-1.408794	4.224043	-0.215871
18	6	-0.357924	4.014324	0.682829
19	6	0.269813	2.767883	0.754841
20	6	-0.134519	1.701315	-0.071722
21	6	-1.188044	1.931920	-0.977605
22	6	-1.821090	3.175034	-1.044890
23	1	-3.844267	-3.012511	-1.592255
24	1	-5.277894	-2.081733	0.218547
25	1	-4.271637	-0.597688	1.946423
26	1	-1.856332	-0.056203	1.865494
27	1	1.471294	-3.656627	0.966394
28	1	-0.234113	-3.498159	0.514882
29	1	5.238897	1.136692	-0.172684
30	1	5.568509	-1.319551	-0.084887
31	1	3.623834	-2.860414	0.013822
32	1	2.964814	2.115650	-0.136748
33	1	-1.898322	5.192014	-0.271514
34	1	-0.029443	4.819231	1.334594
35	1	1.070959	2.612613	1.471395
36	1	-1.506116	1.131376	-1.638244
37	1	-2.631465	3.326860	-1.752621
38	1	-1.437942	-2.455847	-1.682255
39	1	0.985726	-3.806150	-0.739845

1ae (S0, NMP)

Number	Atomic Number	X	Y	Z
1	6	2.561731	-0.546958	0.494217
2	6	3.901154	-0.829227	0.206620

3	6	4.596553	-0.067217	-0.738391
4	6	3.945982	0.972119	-1.411191
5	6	2.603109	1.249980	-1.134723
6	6	1.910068	0.498211	-0.179333
7	6	1.721191	-1.334884	1.465352
8	6	0.487351	0.831028	0.210856
9	7	-0.337560	-0.364979	0.478959
10	6	0.351042	-1.615077	0.839451
11	6	-4.252496	-0.561999	-1.117713
12	6	-3.489765	-1.720843	-0.899146
13	6	-2.228325	-1.657400	-0.322032
14	6	-1.649184	-0.418251	0.066031
15	6	-2.488943	0.746955	-0.024472
16	6	-2.298411	2.004437	0.699756
17	8	-1.524749	2.227274	1.632934
18	6	-3.744736	0.646745	-0.671084
19	1	4.400178	-1.647007	0.720745
20	1	5.637404	-0.289990	-0.954856
21	1	4.478380	1.559631	-2.153558
22	1	2.096020	2.054360	-1.661992
23	1	1.586407	-0.777914	2.402979
24	1	2.196329	-2.286603	1.720524
25	1	0.009099	1.404743	-0.588354
26	1	0.491530	1.480901	1.094716
27	1	-0.278450	-2.165309	1.545774
28	1	0.496423	-2.250961	-0.046575
29	1	-5.224781	-0.616375	-1.595638
30	1	-3.873127	-2.688765	-1.210260
31	1	-1.661979	-2.573802	-0.222642
32	1	-4.343117	1.550191	-0.762143
33	1	-3.007342	2.797839	0.389896

1ae (S1, NMP)

Number	Atomic Number	X	Y	Z
1	6	2.425207	0.414404	0.548621
2	6	3.806898	0.599035	0.703554
3	6	4.718653	-0.137147	-0.053815
4	6	4.253952	-1.081926	-0.975818
5	6	2.881919	-1.278108	-1.132333
6	6	1.964565	-0.531082	-0.379259
7	6	1.428394	1.219227	1.348988
8	6	0.488037	-0.765707	-0.609644

9	7	-0.399933	-0.096625	0.332772
10	6	0.132928	0.444133	1.578990
11	6	-4.553868	-0.705948	-0.070963
12	6	-3.772401	-1.664543	0.611917
13	6	-2.393108	-1.447880	0.737437
14	6	-1.812581	-0.306964	0.196268
15	6	-2.577834	0.688205	-0.497938
16	6	-1.939601	1.841364	-1.025377
17	8	-0.675498	2.067183	-0.916055
18	6	-3.978933	0.432517	-0.609433
19	1	4.166091	1.326680	1.426782
20	1	5.785142	0.018572	0.078968
21	1	4.955398	-1.665132	-1.564654
22	1	2.518648	-2.014987	-1.844477
23	1	1.180270	2.145975	0.820701
24	1	1.845906	1.491274	2.322414
25	1	0.256567	-1.838378	-0.557592
26	1	0.184028	-0.433424	-1.607759
27	1	-0.642260	1.066360	2.025642
28	1	0.306756	-0.413058	2.246468
29	1	-5.623904	-0.863750	-0.177144
30	1	-4.223689	-2.556636	1.031550
31	1	-1.769987	-2.171641	1.256312
32	1	-4.595911	1.158434	-1.132990
33	1	-2.572921	2.571130	-1.552351

1ae (T1, NMP)

Number	Atomic Number	X	Y	Z
1	6	2.405056	0.364570	0.596970
2	6	3.785210	0.604235	0.691640
3	6	4.691561	-0.065223	-0.130252
4	6	4.223166	-0.996604	-1.064844
5	6	2.854660	-1.245443	-1.163957
6	6	1.940511	-0.570059	-0.341137
7	6	1.427817	1.115935	1.473071
8	6	0.467986	-0.898350	-0.482499
9	7	-0.410347	-0.059401	0.331857
10	6	0.106638	0.366622	1.635775
11	6	-4.576092	-0.588405	-0.138863
12	6	-3.841998	-1.547208	0.590078
13	6	-2.456903	-1.378436	0.749003
14	6	-1.821769	-0.273942	0.192543

15	6	-2.548121	0.711319	-0.549668
16	6	-1.811885	1.796765	-1.074088
17	8	-0.525156	1.910667	-0.889084
18	6	-3.953275	0.516562	-0.698955
19	1	4.146943	1.324852	1.421094
20	1	5.755601	0.133410	-0.041042
21	1	4.919072	-1.525702	-1.709094
22	1	2.488856	-1.970864	-1.886913
23	1	1.216116	2.096258	1.031871
24	1	1.860158	1.288358	2.464145
25	1	0.296209	-1.950127	-0.199662
26	1	0.145092	-0.796112	-1.522893
27	1	-0.651094	0.994448	2.106902
28	1	0.246143	-0.527601	2.264365
29	1	-5.647910	-0.716514	-0.264438
30	1	-4.337067	-2.409010	1.025181
31	1	-1.879218	-2.109906	1.307740
32	1	-4.531869	1.247179	-1.257812
33	1	-2.308725	2.577782	-1.658684

1ae (TS1, NMP)

Number	Atomic Number	X	Y	Z
1	6	2.472720	-0.680159	0.483882
2	6	3.856960	-0.852770	0.597380
3	6	4.736764	-0.047373	-0.130769
4	6	4.231447	0.934141	-0.990873
5	6	2.851881	1.106468	-1.115219
6	6	1.966489	0.305521	-0.378174
7	6	1.478890	-1.526031	1.240681
8	6	0.490371	0.566500	-0.468520
9	7	-0.373362	-0.506252	-0.033449
10	6	0.230436	-1.777268	0.389855
11	6	-4.570844	-0.332897	-0.409188
12	6	-3.867877	-1.519251	-0.716885
13	6	-2.483046	-1.512915	-0.562534
14	6	-1.770936	-0.373673	-0.140466
15	6	-2.476868	0.872533	0.185610
16	6	-2.004716	2.105535	0.749248
17	8	-0.810419	2.514048	1.003006
18	6	-3.899753	0.794147	0.032166
19	1	4.245963	-1.624914	1.256318
20	1	5.808973	-0.190534	-0.034930

21	1	4.908499	1.558364	-1.566298
22	1	2.458600	1.866009	-1.786105
23	1	1.184904	-1.036332	2.178516
24	1	1.911631	-2.494877	1.507611
25	1	0.194852	0.864883	-1.483732
26	1	0.199901	1.452935	0.173614
27	1	-0.514735	-2.338786	0.951184
28	1	0.505717	-2.353144	-0.505733
29	1	-5.652180	-0.299320	-0.511050
30	1	-4.380939	-2.407879	-1.065620
31	1	-1.927425	-2.411384	-0.808492
32	1	-4.476441	1.677019	0.295461
33	1	-2.821943	2.794293	1.012194

1ae (TS1', NMP)

Number	Atomic Number	X	Y	Z
1	6	2.471377	-0.680472	0.484630
2	6	3.855518	-0.852599	0.599748
3	6	4.735916	-0.047751	-0.128451
4	6	4.231369	0.932720	-0.990260
5	6	2.851873	1.104696	-1.116220
6	6	1.965901	0.304296	-0.379138
7	6	1.476875	-1.525637	1.241468
8	6	0.490081	0.564476	-0.470754
9	7	-0.373428	-0.507183	-0.036652
10	6	0.229060	-1.777754	0.390018
11	6	-4.571898	-0.330491	-0.404634
12	6	-3.870078	-1.515335	-0.718517
13	6	-2.484586	-1.510344	-0.567411
14	6	-1.771686	-0.372977	-0.143103
15	6	-2.475564	0.872049	0.187582
16	6	-2.000411	2.104046	0.750479
17	8	-0.803576	2.513158	0.997173
18	6	-3.899081	0.794940	0.038628
19	1	4.244041	-1.624035	1.259763
20	1	5.808044	-0.190712	-0.031437
21	1	4.908940	1.556217	-1.565855
22	1	2.459114	1.863112	-1.788677
23	1	1.182330	-1.034977	2.178637
24	1	1.909397	-2.494169	1.509718
25	1	0.194495	0.865531	-1.485185
26	1	0.198218	1.451840	0.172455

27	1	-0.517129	-2.337811	0.951441
28	1	0.504712	-2.355267	-0.504367
29	1	-5.653524	-0.296386	-0.503086
30	1	-4.384234	-2.402790	-1.068705
31	1	-1.929846	-2.408514	-0.816484
32	1	-4.474553	1.677305	0.306308
33	1	-2.815398	2.792503	1.020262

1ae (A, NMP)

Number	Atomic Number	X	Y	Z
1	6	2.506657	0.449202	0.558209
2	6	3.879425	0.510518	0.780657
3	6	4.775855	-0.261410	0.025152
4	6	4.280376	-1.113268	-0.978284
5	6	2.915463	-1.200246	-1.213905
6	6	1.992045	-0.430793	-0.446882
7	6	1.519517	1.313472	1.308505
8	6	0.599623	-0.526397	-0.670768
9	7	-0.331124	0.203461	0.085027
10	6	0.153844	0.634717	1.425528
11	6	-4.336250	-1.244736	0.203556
12	6	-3.272216	-2.079905	0.591979
13	6	-1.962424	-1.588804	0.532341
14	6	-1.696114	-0.296763	0.085104
15	6	-2.762019	0.563017	-0.339317
16	6	-2.578292	1.864336	-0.855443
17	8	-1.372101	2.446182	-1.058811
18	6	-4.090507	0.040717	-0.248783
19	1	4.261187	1.176091	1.551900
20	1	5.843128	-0.198724	0.214269
21	1	4.967842	-1.710643	-1.570875
22	1	2.534686	-1.865223	-1.985044
23	1	1.400390	2.276925	0.791817
24	1	1.888949	1.543576	2.313464
25	1	0.192873	-1.124045	-1.477608
26	1	-0.691437	1.791480	-0.763483
27	1	-0.587829	1.317384	1.846658
28	1	0.219569	-0.243786	2.083448
29	1	-5.358138	-1.609787	0.252251
30	1	-3.460517	-3.090628	0.939249
31	1	-1.130623	-2.216363	0.840935
32	1	-4.917087	0.674337	-0.559155

33	1	-3.418211	2.483774	-1.148412

1ae (A', NMP)

Number	Atomic Number	X	Y	Z
1	6	2.601006	-0.691054	0.439367
2	6	3.979316	-0.725980	0.631680
3	6	4.813731	0.243565	0.054754
4	6	4.249621	1.263539	-0.727590
5	6	2.874758	1.313174	-0.933918
6	6	2.022029	0.337244	-0.355513
7	6	1.645924	-1.673008	1.069219
8	6	0.608265	0.391348	-0.540970
9	7	-0.225662	-0.630588	-0.191230
10	6	0.423581	-1.915160	0.180914
11	6	-4.458518	-0.503776	-0.245686
12	6	-3.753614	-1.708429	-0.476170
13	6	-2.368703	-1.698888	-0.465749
14	6	-1.615157	-0.527650	-0.217052
15	6	-2.322704	0.729619	0.034660
16	6	-1.727420	1.945450	0.381683
17	8	-2.420238	2.994339	0.933140
18	6	-3.766878	0.659759	-0.006778
19	1	0.171594	1.195017	-1.118132
20	1	4.411256	-1.518502	1.238794
21	1	5.887390	0.201430	0.210687
22	1	4.888275	2.017575	-1.179269
23	1	2.443280	2.101664	-1.545475
24	1	1.307857	-1.292890	2.044371
25	1	2.134115	-2.634931	1.256178
26	1	-3.259137	2.694342	1.314846
27	1	-0.301498	-2.525281	0.715235
28	1	0.717079	-2.439174	-0.737188
29	1	-5.543846	-0.488437	-0.283686
30	1	-4.286170	-2.629820	-0.688373
31	1	-1.846091	-2.621928	-0.687775
32	1	-4.333625	1.579620	0.104048
33	1	-0.680382	2.182208	0.292128

1ae (TS2, NMP)

Number	Atomic Number	X	Y	Z
1	6	2.454459	-0.752445	0.456706
2	6	3.808757	-0.787625	0.785203

3	6	4.696326	0.176519	0.287930
4	6	4.216438	1.185594	-0.558941
5	6	2.867088	1.231537	-0.900389
6	6	1.961201	0.270936	-0.392934
7	6	1.451064	-1.754580	0.974528
8	6	0.558464	0.336050	-0.711803
9	7	-0.284281	-0.704499	-0.448795
10	6	0.332016	-1.993688	-0.042077
11	6	-4.416138	-0.299838	0.163170
12	6	-3.872498	-1.533530	-0.278095
13	6	-2.522522	-1.627902	-0.544362
14	6	-1.650758	-0.516523	-0.391368
15	6	-2.204573	0.787832	-0.056403
16	6	-1.464236	1.977612	0.071347
17	8	-1.894120	3.003197	0.884917
18	6	-3.608168	0.805806	0.276580
19	1	0.232363	1.036800	-1.466169
20	1	4.178146	-1.579809	1.432646
21	1	5.748938	0.135418	0.551299
22	1	4.897903	1.933045	-0.955446
23	1	2.499475	2.013704	-1.560068
24	1	1.010504	-1.394716	1.915579
25	1	1.932561	-2.712732	1.195369
26	1	-2.430942	2.656080	1.613122
27	1	-0.439091	-2.624495	0.394644
28	1	0.727483	-2.488956	-0.936716
29	1	-5.479013	-0.215934	0.370338
30	1	-4.512403	-2.400373	-0.409742
31	1	-2.115830	-2.575598	-0.879915
32	1	-4.059116	1.757576	0.542181
33	1	-0.689585	2.331373	-0.579447

1ae (TS2', NMP)

Number	Atomic Number	X	Y	Z
1	6	-2.255913	0.795880	0.251997
2	6	-3.633697	0.836359	0.465696
3	6	-4.470654	-0.188073	-0.002325
4	6	-3.917267	-1.258611	-0.718096
5	6	-2.544250	-1.309460	-0.947252
6	6	-1.689873	-0.296517	-0.454912
7	6	-1.339812	1.906302	0.720165
8	6	-0.247158	-0.397429	-0.659072

9	7	0.515485	0.764700	-0.387065
10	6	-0.142574	2.062625	-0.226687
11	6	4.404159	-0.599729	-0.200002
12	6	4.231744	0.828272	-0.316208
13	6	2.940969	1.368795	-0.349026
14	6	1.857565	0.513493	-0.140827
15	6	2.038842	-0.896478	0.208336
16	6	0.788895	-1.551514	0.511309
17	8	0.156015	-1.363500	1.754132
18	6	3.336608	-1.449760	0.023758
19	1	-4.063456	1.684435	0.994029
20	1	-5.540785	-0.140694	0.175658
21	1	-4.557820	-2.049077	-1.099161
22	1	-2.116872	-2.140330	-1.503409
23	1	-0.969941	1.699441	1.733860
24	1	-1.881019	2.856774	0.768814
25	1	0.047475	-0.911760	-1.578455
26	1	0.520084	-0.571399	2.177420
27	1	0.585687	2.769985	0.171823
28	1	-0.477366	2.418866	-1.209023
29	1	5.406993	-1.012972	-0.269009
30	1	5.096819	1.466562	-0.459157
31	1	2.785655	2.415872	-0.595902
32	1	3.496700	-2.518686	0.140198
33	1	0.665812	-2.596846	0.227587

1ae (B', NMP)

Number	Atomic Number	X	Y	Z
1	6	-2.193293	0.896665	0.224612
2	6	-3.554709	0.945857	0.564375
3	6	-4.397301	-0.140916	0.331344
4	6	-3.885457	-1.298724	-0.265880
5	6	-2.537312	-1.355453	-0.616320
6	6	-1.681389	-0.273589	-0.362830
7	6	-1.298346	2.093104	0.481453
8	6	-0.228589	-0.378869	-0.787285
9	7	0.546928	0.833070	-0.458148
10	6	-0.108125	2.128187	-0.485591
11	6	4.350379	-0.597423	0.217815
12	6	4.206494	0.854184	0.227054
13	6	2.927746	1.428046	-0.018151
14	6	1.854502	0.567877	-0.201425

15	6	1.983498	-0.905776	-0.151802
16	6	0.636415	-1.519916	-0.179412
17	8	0.101864	-1.831506	1.151064
18	6	3.291772	-1.461115	0.035960
19	1	-0.205215	-0.505305	-1.881901
20	1	-3.954084	1.852747	1.011781
21	1	-5.447335	-0.082257	0.602579
22	1	-4.533075	-2.148251	-0.461411
23	1	-2.141386	-2.252099	-1.086061
24	1	-0.914970	2.065034	1.509657
25	1	-1.869968	3.021300	0.380175
26	1	0.814738	-2.259005	1.646958
27	1	0.610299	2.897781	-0.202650
28	1	-0.450018	2.334357	-1.508656
29	1	5.345677	-1.012244	0.362790
30	1	5.079208	1.480760	0.365813
31	1	2.805650	2.504370	-0.085137
32	1	3.443581	-2.536735	0.046201
33	1	0.575783	-2.432712	-0.785117

1ae (B, NMP)

Number	Atomic Number	X	Y	Z
1	6	-2.291893	0.914640	0.115949
2	6	-3.678313	0.929640	0.339710
3	6	-4.454901	-0.215468	0.160889
4	6	-3.848282	-1.405614	-0.256302
5	6	-2.472607	-1.434164	-0.485353
6	6	-1.684933	-0.289014	-0.294234
7	6	-1.482779	2.183454	0.336156
8	6	-0.207773	-0.312718	-0.616156
9	7	0.492288	0.848255	-0.050327
10	6	-0.101222	2.142031	-0.328668
11	6	4.422465	-0.542766	0.006338
12	6	4.232872	0.843263	0.075600
13	6	2.952508	1.414271	0.047392
14	6	1.851846	0.554490	-0.050209
15	6	2.036549	-0.844126	-0.128603
16	6	0.671343	-1.508120	-0.147702
17	8	0.309520	-2.045061	1.134225
18	6	3.310382	-1.395710	-0.092676
19	1	-0.094770	-0.284869	-1.718626
20	1	-4.151502	1.856826	0.654777

21	1	-5.525817	-0.179001	0.339133
22	1	-4.442009	-2.303200	-0.402727
23	1	-2.003214	-2.357672	-0.812060
24	1	-1.346523	2.334554	1.415215
25	1	-2.044228	3.049220	-0.032594
26	1	0.408231	-1.346474	1.798287
27	1	0.534709	2.932328	0.077056
28	1	-0.187407	2.307900	-1.417021
29	1	5.426360	-0.955493	0.022342
30	1	5.097348	1.497953	0.145722
31	1	2.830175	2.491350	0.096650
32	1	3.445286	-2.473064	-0.145281
33	1	0.599624	-2.352195	-0.835165

1ae (C, NMP)

Number	Atomic Number	X	Y	Z
1	6	-2.338172	0.921246	0.004212
2	6	-3.732038	0.934081	0.159159
3	6	-4.479336	-0.238251	0.050238
4	6	-3.837633	-1.453292	-0.211706
5	6	-2.451876	-1.484998	-0.361058
6	6	-1.699867	-0.307322	-0.252114
7	6	-1.565100	2.223523	0.166997
8	6	-0.214704	-0.319831	-0.512996
9	7	0.461671	0.838627	0.222333
10	6	-0.092804	2.155912	-0.248535
11	6	4.421544	-0.513440	-0.200294
12	6	4.248398	0.856969	0.024264
13	6	2.967191	1.409230	0.171863
14	6	1.904008	0.528757	0.077513
15	6	2.044497	-0.841210	-0.138642
16	6	0.680138	-1.512922	-0.136972
17	8	0.305491	-1.954720	1.169079
18	6	3.320651	-1.377420	-0.282939
19	1	-0.018848	-0.109202	-1.570168
20	1	-4.233356	1.876503	0.363334
21	1	-5.558152	-0.204103	0.167662
22	1	-4.411745	-2.370535	-0.296646
23	1	-1.953183	-2.427661	-0.560884
24	1	-1.626399	2.542946	1.214946
25	1	-2.039389	3.016784	-0.418705
26	1	0.226821	0.744435	1.219722

27	1	0.924741	-2.638392	1.462811
28	1	0.485453	2.957976	0.209651
29	1	0.048484	2.185583	-1.330301
30	1	5.423826	-0.912354	-0.318210
31	1	5.114437	1.507771	0.081439
32	1	2.833627	2.470967	0.345209
33	1	3.461945	-2.438445	-0.462831
34	1	0.596750	-2.321092	-0.869935

1ae (TS3, NMP)

Number	Atomic Number	X	Y	Z
1	6	-2.322366	0.845641	0.043638
2	6	-3.722359	0.857430	0.148009
3	6	-4.476321	-0.288411	-0.102025
4	6	-3.837141	-1.477823	-0.470029
5	6	-2.448399	-1.505674	-0.583311
6	6	-1.688159	-0.356447	-0.320727
7	6	-1.535678	2.107482	0.357634
8	6	-0.190441	-0.393556	-0.516349
9	7	0.489976	0.787639	0.123106
10	6	-0.107360	2.094621	-0.191397
11	6	4.403446	-0.643012	-0.271764
12	6	4.241379	0.744917	-0.329753
13	6	2.975060	1.347837	-0.222616
14	6	1.891015	0.500468	-0.066729
15	6	2.042356	-0.898458	-0.005590
16	6	0.660202	-1.448417	0.219962
17	8	0.277096	-1.065486	1.656589
18	6	3.295034	-1.487851	-0.097679
19	1	0.063492	-0.438460	-1.583073
20	1	-4.222364	1.781170	0.427535
21	1	-5.558229	-0.253697	-0.016342
22	1	-4.415856	-2.373947	-0.670924
23	1	-1.952434	-2.425799	-0.880262
24	1	-1.494623	2.239389	1.446745
25	1	-2.060546	2.981478	-0.040133
26	1	0.307193	0.037349	1.408512
27	1	0.963118	-1.321281	2.300425
28	1	0.491784	2.874500	0.282482
29	1	-0.088280	2.254937	-1.277019
30	1	5.395751	-1.071852	-0.363478
31	1	5.112889	1.377718	-0.464838

32	1	2.865550	2.425525	-0.269274
33	1	3.415036	-2.565287	-0.047601
34	1	0.449311	-2.503798	0.085144

1ae (D, NMP)

Number	Atomic Number	X	Y	Z
1	6	2.054146	0.803435	-0.220176
2	6	3.348331	0.845291	-0.763755
3	6	4.169165	-0.281240	-0.770542
4	6	3.708418	-1.481821	-0.219852
5	6	2.428074	-1.542331	0.327742
6	6	1.599542	-0.412111	0.321096
7	6	1.187992	2.047595	-0.243147
8	6	0.212301	-0.505085	0.964987
9	7	-0.576704	0.705318	0.744079
10	6	0.083899	2.006022	0.821828
11	6	-4.118236	-0.799538	-0.737353
12	6	-3.986537	0.630158	-0.596941
13	6	-2.854262	1.241350	-0.116877
14	6	-1.773732	0.395962	0.249674
15	6	-1.881852	-1.054804	0.104822
16	6	-0.693613	-1.596958	0.499587
17	6	-3.097168	-1.636454	-0.394856
18	1	0.335167	-0.630990	2.055933
19	1	3.711200	1.779815	-1.183011
20	1	5.166299	-0.221923	-1.195956
21	1	4.341530	-2.363423	-0.212306
22	1	2.076809	-2.471686	0.766443
23	1	0.724188	2.157176	-1.231518
24	1	1.803069	2.938058	-0.081253
25	1	-0.653444	2.793569	0.669329
26	1	0.500894	2.115756	1.827182
27	1	-5.051162	-1.197630	-1.120593
28	1	-4.831117	1.249119	-0.883795
29	1	-2.793823	2.318160	-0.019173
30	1	-3.179424	-2.713375	-0.491427
31	1	-0.432079	-2.646685	0.534169

1ae (2ae, NMP)

Number	Atomic Number	X	Y	Z
1	6	-2.284402	0.789213	0.156401
2	6	-3.681845	0.845755	0.120199

3	6	-4.444882	-0.312609	-0.051273
4	6	-3.806158	-1.550184	-0.195065
5	6	-2.414405	-1.621748	-0.171862
6	6	-1.640329	-0.460995	0.007681
7	6	-1.444137	2.025904	0.398181
8	6	-0.178447	-0.509993	0.037272
9	7	0.537255	0.679081	-0.062286
10	6	-0.104035	1.960846	-0.339521
11	6	4.426778	-0.724900	0.057706
12	6	4.262644	0.670398	-0.100094
13	6	2.995579	1.248318	-0.158999
14	6	1.887247	0.395444	-0.055572
15	6	2.030311	-1.018576	0.092449
16	6	0.709096	-1.566524	0.146980
17	6	3.325613	-1.570511	0.154807
18	1	-4.176846	1.807355	0.231114
19	1	-5.528735	-0.249929	-0.077510
20	1	-4.391007	-2.454512	-0.334734
21	1	-1.921417	-2.580300	-0.302887
22	1	-1.248796	2.126757	1.475027
23	1	-1.985603	2.924191	0.087091
24	1	0.555792	2.763960	-0.004861
25	1	-0.253088	2.073515	-1.422158
26	1	5.429678	-1.140025	0.100896
27	1	5.140318	1.305560	-0.177223
28	1	2.880109	2.320641	-0.281514
29	1	3.460579	-2.642392	0.272534
30	1	0.446466	-2.607418	0.274498

1aj (S0, NMP)

Number	Atomic Number	X	Y	Z
1	6	2.719504	-2.698122	-0.281143
2	6	3.305644	-1.614594	-0.946154
3	6	2.734398	-0.347692	-0.890015
4	6	1.534613	-0.100773	-0.170365
5	6	0.885061	-1.231384	0.417816
6	6	-0.495203	-1.249729	1.000894
7	8	-0.700291	-1.781667	2.097037
8	6	1.519487	-2.488036	0.390996
9	6	-3.905549	0.052484	-1.281214
10	6	-2.688560	-0.173793	-1.931450
11	6	-1.567075	-0.572377	-1.200529

12	6	-1.655538	-0.756835	0.189260
13	6	-2.887050	-0.537884	0.832719
14	6	-4.002797	-0.129672	0.104288
15	1	3.172103	-3.683921	-0.309353
16	1	4.228815	-1.749638	-1.503207
17	1	3.236760	0.469038	-1.392079
18	1	1.015696	-3.319524	0.874640
19	1	-4.775585	0.366541	-1.850444
20	1	-2.612811	-0.043184	-3.006746
21	1	-0.628337	-0.753765	-1.712449
22	1	-2.952028	-0.687092	1.905430
23	1	-4.946694	0.045869	0.611671
24	6	1.740674	2.318324	-0.701449
25	6	0.670546	3.135463	1.272993
26	6	1.010692	3.552361	-0.165313
27	1	1.685878	2.223508	-1.791393
28	1	2.803791	2.355338	-0.418032
29	1	-0.127877	3.732385	1.721998
30	1	1.558831	3.221056	1.909361
31	1	0.093927	3.733687	-0.738170
32	1	1.630818	4.450804	-0.222023
33	7	1.059377	1.188934	-0.043322
34	6	0.267125	1.662810	1.113847
35	1	0.494191	1.062821	2.001856
36	1	-0.806608	1.583573	0.914806

1aj (S1, NMP)

Number	Atomic Number	X	Y	Z
1	6	2.348737	-3.024450	-0.264662
2	6	3.120365	-2.051707	-0.880136
3	6	2.734554	-0.698111	-0.843948
4	6	1.577184	-0.252188	-0.154254
5	6	0.713055	-1.277637	0.340474
6	6	-0.654850	-1.054105	0.914006
7	8	-0.687107	-1.433121	2.162263
8	6	1.146215	-2.619003	0.340111
9	6	-4.083603	0.323695	-1.204641
10	6	-2.851061	0.177386	-1.868485
11	6	-1.721919	-0.263340	-1.193210
12	6	-1.783918	-0.583129	0.199481
13	6	-3.045222	-0.430159	0.860994
14	6	-4.161177	0.012907	0.164186

15	1	2.646722	-4.066730	-0.254372
16	1	4.038449	-2.315697	-1.395872
17	1	3.342086	0.018411	-1.381907
18	1	0.497854	-3.358649	0.797869
19	1	-4.960792	0.668987	-1.742351
20	1	-2.777791	0.410199	-2.927694
21	1	-0.783828	-0.373203	-1.727346
22	1	-3.119571	-0.669343	1.917148
23	1	-5.107656	0.118574	0.688458
24	6	2.218066	2.098250	-0.645062
25	6	1.029423	3.107667	1.172768
26	6	1.618232	3.437296	-0.205909
27	1	2.258927	1.988754	-1.734208
28	1	3.240003	1.983309	-0.253458
29	1	0.273492	3.824398	1.504344
30	1	1.825266	3.078728	1.926011
31	1	0.824212	3.741623	-0.897240
32	1	2.369173	4.230996	-0.179776
33	7	1.317527	1.093990	-0.049726
34	6	0.438910	1.705330	0.970415
35	1	0.443435	1.108748	1.887406
36	1	-0.593756	1.765726	0.610200

1aj (T1, NMP)

Number	Atomic Number	X	Y	Z
1	6	0.411306	3.431259	-0.259988
2	6	1.806585	3.288149	-0.183927
3	6	2.352606	2.002454	-0.082398
4	6	1.516735	0.889210	-0.039085
5	6	0.094368	1.007776	-0.082117
6	6	-0.651507	-0.228155	-0.072206
7	8	0.035232	-1.344007	-0.159033
8	6	-0.428105	2.324373	-0.214424
9	6	-4.926488	-0.732889	0.099557
10	6	-4.333769	0.378342	0.712261
11	6	-2.952456	0.567683	0.662352
12	6	-2.114379	-0.351401	-0.014157
13	6	-2.728805	-1.484906	-0.602900
14	6	-4.109299	-1.666162	-0.552432
15	1	-0.024198	4.420698	-0.368693
16	1	2.456988	4.156067	-0.215700
17	1	3.429564	1.866359	-0.036523

18	1	-1.495848	2.471806	-0.317091
19	1	-6.002398	-0.874770	0.139276
20	1	-4.949592	1.096747	1.246815
21	1	-2.520953	1.410726	1.189602
22	1	-2.103493	-2.212220	-1.109928
23	1	-4.551998	-2.538635	-1.025822
24	6	2.521127	-0.998785	1.329838
25	6	3.225570	-2.390095	-0.537967
26	6	3.548566	-2.076954	0.937065
27	1	1.646471	-1.411975	1.841973
28	1	2.941209	-0.203867	1.954989
29	1	2.400326	-3.105065	-0.610084
30	1	4.082010	-2.794668	-1.082475
31	1	3.480829	-2.956915	1.580849
32	1	4.563273	-1.674645	1.022955
33	7	2.073919	-0.423584	0.044217
34	6	2.782500	-1.033978	-1.089835
35	1	3.645872	-0.404130	-1.352703
36	1	2.115303	-1.083888	-1.952510

1aj (TS1, NMP)

Number	Atomic Number	X	Y	Z
1	6	0.333521	3.326435	-0.395584
2	6	1.672443	3.294988	-0.010766
3	6	2.276501	2.060407	0.224855
4	6	1.565776	0.850903	0.106512
5	6	0.171339	0.860755	-0.249028
6	6	-0.694446	-0.325761	-0.490001
7	8	-0.184184	-1.393415	-1.119417
8	6	-0.379105	2.130654	-0.522471
9	6	-4.877301	-0.553082	0.464324
10	6	-4.088305	0.464523	1.024883
11	6	-2.736178	0.572255	0.718474
12	6	-2.101087	-0.348497	-0.168590
13	6	-2.917273	-1.391224	-0.702040
14	6	-4.271581	-1.479881	-0.398262
15	1	-0.160177	4.269560	-0.609526
16	1	2.247167	4.208769	0.098945
17	1	3.316792	2.030489	0.528130
18	1	-1.403215	2.176602	-0.873985
19	1	-5.933777	-0.627905	0.703706
20	1	-4.533397	1.176500	1.715223

21	1	-2.153437	1.353678	1.192945
22	1	-2.457325	-2.119968	-1.359614
23	1	-4.863815	-2.281074	-0.833391
24	6	1.700100	-1.578513	0.598608
25	6	3.922419	-1.954835	-0.209457
26	6	2.824999	-2.603435	0.654029
27	1	0.887207	-1.696272	-0.361659
28	1	0.996552	-1.556065	1.438212
29	1	3.752090	-2.175809	-1.268178
30	1	4.929381	-2.287159	0.052188
31	1	2.511049	-3.582093	0.281644
32	1	3.168252	-2.737151	1.688287
33	7	2.290229	-0.329061	0.330654
34	6	3.735598	-0.452058	0.043122
35	1	4.304078	-0.120493	0.922187
36	1	4.009929	0.177322	-0.806018

1aj (TS1', NMP)

Number	Atomic Number	X	Y	Z
1	6	0.334616	3.327330	-0.394751
2	6	1.673547	3.294837	-0.010218
3	6	2.277187	2.059864	0.224826
4	6	1.565852	0.850845	0.105950
5	6	0.171545	0.861735	-0.249716
6	6	-0.694326	-0.324660	-0.491270
7	8	-0.183529	-1.392192	-1.121458
8	6	-0.378623	2.131878	-0.522145
9	6	-4.876690	-0.553190	0.465159
10	6	-4.087396	0.464278	1.025709
11	6	-2.735421	0.572202	0.718688
12	6	-2.100607	-0.348175	-0.169126
13	6	-2.917162	-1.390745	-0.702609
14	6	-4.271357	-1.479616	-0.398149
15	1	-0.158627	4.270840	-0.607969
16	1	2.248784	4.208242	0.099884
17	1	3.317470	2.029403	0.527976
18	1	-1.402897	2.178571	-0.873130
19	1	-5.933031	-0.628162	0.705058
20	1	-4.532151	1.175985	1.716528
21	1	-2.152558	1.353533	1.193124
22	1	-2.457875	-2.119305	-1.360865
23	1	-4.863772	-2.280653	-0.833311

24	6	1.698673	-1.578360	0.598549
25	6	3.921185	-1.956698	-0.208047
26	6	2.822647	-2.604124	0.654937
27	1	0.884576	-1.695112	-0.363833
28	1	0.994231	-1.554925	1.437352
29	1	3.751883	-2.178424	-1.266788
30	1	4.927673	-2.289289	0.054957
31	1	2.508271	-3.582733	0.282733
32	1	3.165060	-2.737646	1.689484
33	7	2.289413	-0.329798	0.329675
34	6	3.735032	-0.453648	0.043249
35	1	4.302765	-0.121750	0.922603
36	1	4.010338	0.175028	-0.806073

1aj (A, NMP)

Number	Atomic Number	X	Y	Z
1	6	-0.821790	3.440423	0.065291
2	6	-2.156707	3.104684	-0.193824
3	6	-2.553448	1.771691	-0.236845
4	6	-1.630121	0.721779	-0.021633
5	6	-0.276693	1.058576	0.311771
6	6	0.704796	0.065776	0.784691
7	8	0.366530	-0.688669	1.885412
8	6	0.089995	2.418431	0.324193
9	6	4.650984	-0.547907	-0.722107
10	6	3.749118	0.281134	-1.408939
11	6	2.463609	0.491056	-0.924364
12	6	2.024394	-0.124731	0.285213
13	6	2.952246	-0.970702	0.964077
14	6	4.234645	-1.170875	0.464608
15	1	-0.503980	4.477819	0.092607
16	1	-2.891821	3.882596	-0.379624
17	1	-3.583178	1.536479	-0.479306
18	1	1.114033	2.668808	0.585244
19	1	5.653828	-0.707954	-1.106110
20	1	4.053085	0.762455	-2.334622
21	1	1.779250	1.123765	-1.479388
22	1	2.647745	-1.458164	1.883190
23	1	4.920803	-1.817874	1.004910
24	6	-1.270921	-1.673259	-0.576600
25	6	-3.422137	-2.511400	-0.015584
26	6	-2.136536	-2.878776	-0.788784

27	1	-0.531282	-0.464018	2.168288
28	1	-0.320633	-1.483898	-1.057421
29	1	-3.326136	-2.806687	1.034564
30	1	-4.320160	-2.982384	-0.422311
31	1	-1.680349	-3.807974	-0.427950
32	1	-2.359407	-3.033198	-1.858229
33	7	-2.052011	-0.596629	-0.159980
34	6	-3.477892	-0.981400	-0.121430
35	1	-3.979241	-0.667672	-1.048325
36	1	-3.981973	-0.503365	0.722643

1aj (A', NMP)

Number	Atomic Number	X	Y	Z
1	6	3.368954	-2.053190	-0.362863
2	6	3.805310	-0.763139	-0.746591
3	6	2.937962	0.300657	-0.611932
4	6	1.612450	0.148354	-0.119230
5	6	1.091782	-1.190762	0.134063
6	6	-0.247091	-1.576683	0.434154
7	8	-0.414825	-2.830492	1.055267
8	6	2.077775	-2.244524	0.068764
9	6	-3.979727	0.053678	-0.916001
10	6	-3.938745	-1.008787	0.011207
11	6	-2.730664	-1.533511	0.441800
12	6	-1.480925	-1.020083	-0.029259
13	6	-1.546298	0.057455	-0.962694
14	6	-2.778857	0.563589	-1.401791
15	6	-0.188072	1.462025	0.925675
16	6	0.360022	3.648718	0.219617
17	6	-0.485817	2.886429	1.256747
18	7	0.940768	1.327289	0.233021
19	6	1.499561	2.677365	-0.109453
20	1	-0.649379	0.601773	1.380467
21	1	0.194856	-2.898822	1.802666
22	1	4.040914	-2.903704	-0.438853
23	1	4.812308	-0.600033	-1.116677
24	1	3.306615	1.289148	-0.851636
25	1	1.751207	-3.252563	0.294577
26	1	-4.930485	0.458719	-1.249733
27	1	-4.866482	-1.424827	0.396406
28	1	-2.720791	-2.353506	1.150000
29	1	-0.643184	0.405325	-1.448622

30	1	-2.785514	1.365010	-2.136483
31	1	0.740202	4.601944	0.591812
32	1	-0.235465	3.844711	-0.676568
33	1	-0.167644	3.109319	2.287249
34	1	-1.554864	3.112715	1.199361
35	1	1.790053	2.703019	-1.160096
36	1	2.385159	2.849132	0.509576

1aj (TS2, NMP)

Number	Atomic Number	X	Y	Z
1	6	2.316131	-2.978840	-0.285875
2	6	3.083083	-2.036840	-1.009018
3	6	2.703836	-0.709205	-1.010729
4	6	1.542755	-0.267094	-0.321966
5	6	0.664576	-1.235932	0.291354
6	6	-0.616601	-0.957635	0.874993
7	8	-0.958623	-1.731117	2.000019
8	6	1.159883	-2.578056	0.350637
9	6	-4.109974	0.481274	-1.177439
10	6	-4.186987	0.012593	0.144072
11	6	-3.054453	-0.443640	0.810733
12	6	-1.777674	-0.456944	0.178902
13	6	-1.722856	0.018341	-1.162195
14	6	-2.866755	0.476826	-1.817947
15	6	0.346708	1.737843	0.446336
16	6	2.060208	3.374912	0.290892
17	6	0.726369	3.071660	1.005079
18	7	1.400391	1.102385	-0.085330
19	6	2.608241	1.992271	-0.086787
20	1	-0.656797	1.388679	0.322560
21	1	-0.200307	-1.755098	2.598393
22	1	2.610895	-4.024190	-0.265221
23	1	3.973820	-2.345115	-1.547462
24	1	3.322646	0.009404	-1.534067
25	1	0.545790	-3.316830	0.855513
26	1	-4.997401	0.837576	-1.691767
27	1	-5.144012	0.005368	0.660108
28	1	-3.136873	-0.799062	1.831193
29	1	-0.782939	-0.011076	-1.705030
30	1	-2.782734	0.824297	-2.844603
31	1	2.765066	3.927639	0.915118
32	1	1.873076	3.962480	-0.612386

33	1	0.861873	3.004970	2.095030
34	1	-0.042320	3.829124	0.826831
35	1	3.072269	1.987843	-1.073021
36	1	3.325233	1.597024	0.639703

1aj (TS2', NMP)

Number	Atomic Number	X	Y	Z
1	6	-1.483205	3.263222	0.240799
2	6	-2.834222	2.767708	0.045829
3	6	-3.046449	1.408848	-0.174405
4	6	-1.946383	0.543917	-0.143954
5	6	-0.594728	1.011620	0.190367
6	6	0.313072	-0.093649	0.490990
7	8	0.001825	-0.724663	1.728277
8	6	-0.396752	2.410945	0.299992
9	6	4.499355	0.214672	-0.477646
10	6	4.103297	-0.393881	0.719759
11	6	2.751376	-0.485195	1.054766
12	6	1.755787	0.033894	0.199032
13	6	2.171098	0.627448	-1.015871
14	6	3.522287	0.725909	-1.342374
15	6	-0.606119	-1.299125	-0.746985
16	6	-2.055608	-3.032193	0.135773
17	6	-0.688321	-2.806222	-0.556478
18	7	-1.895849	-0.780829	-0.514380
19	6	-2.906961	-1.822317	-0.298677
20	1	0.391133	-1.613980	1.751467
21	1	-1.329879	4.331424	0.367915
22	1	-3.666873	3.462874	0.040524
23	1	-4.037628	1.031261	-0.413891
24	1	0.597756	2.806120	0.490249
25	1	5.551815	0.285701	-0.735545
26	1	4.850900	-0.790316	1.401214
27	1	2.471182	-0.933326	2.002303
28	1	1.423052	1.013750	-1.701935
29	1	3.815393	1.194575	-2.277756
30	1	-0.125199	-0.943362	-1.659258
31	1	-1.941307	-3.025938	1.223337
32	1	-2.519395	-3.978586	-0.151600
33	1	0.146280	-3.207037	0.030389
34	1	-0.647998	-3.310810	-1.531060
35	1	-3.437297	-2.017909	-1.239003

36	1	-3.630727	-1.494941	0.451587

1aj (B', NMP)

Number	Atomic Number	X	Y	Z
1	6	1.642660	-3.185697	0.323288
2	6	2.929331	-2.679715	-0.134495
3	6	3.066112	-1.293323	-0.422402
4	6	1.944241	-0.489399	-0.284769
5	6	0.618066	-0.999654	0.143520
6	6	-0.274111	0.148894	0.514885
7	8	-0.244903	0.415137	1.953382
8	6	0.522198	-2.397624	0.469939
9	6	-4.431240	-0.278770	-0.681517
10	6	-4.119443	0.181852	0.600014
11	6	-2.784369	0.314296	1.000095
12	6	-1.741613	-0.013551	0.123207
13	6	-2.064843	-0.473821	-1.163569
14	6	-3.396021	-0.607199	-1.563984
15	6	0.421448	1.327459	-0.262200
16	6	1.927584	3.194749	-0.345997
17	6	0.638335	2.709477	0.358604
18	7	1.801225	0.844375	-0.459776
19	6	2.787445	1.920022	-0.521883
20	1	-0.060192	1.433190	-1.244359
21	1	0.607153	0.106219	2.291585
22	1	1.571162	-4.243710	0.567790
23	1	3.770268	-3.355700	-0.232755
24	1	4.007648	-0.877264	-0.768028
25	1	-0.411675	-2.820067	0.828250
26	1	-5.467442	-0.383361	-0.990007
27	1	-4.914412	0.438002	1.294905
28	1	-2.550384	0.666855	1.997432
29	1	-1.267315	-0.741063	-1.851970
30	1	-3.623863	-0.970392	-2.562133
31	1	2.456834	3.960686	0.225543
32	1	1.685741	3.617030	-1.326673
33	1	0.793471	2.610610	1.436727
34	1	-0.207623	3.380104	0.190606
35	1	3.333490	1.897158	-1.471257
36	1	3.513087	1.781998	0.289303

1aj (B, NMP)

Number	Atomic Number	X	Y	Z
1	6	-1.522773	3.196599	0.476934
2	6	-2.694824	2.768160	-0.164276
3	6	-2.850884	1.445692	-0.592831
4	6	-1.798534	0.544153	-0.367269
5	6	-0.633547	0.962920	0.302647
6	6	0.271811	-0.232155	0.579513
7	8	0.305183	-0.499738	1.994164
8	6	-0.487170	2.283206	0.719205
9	6	4.378122	0.220535	-0.777537
10	6	4.115346	-0.252636	0.509942
11	6	2.796325	-0.389923	0.959314
12	6	1.720343	-0.054841	0.126794
13	6	1.994458	0.421107	-1.166005
14	6	3.309155	0.558488	-1.615391
15	6	-0.452318	-1.376743	-0.246982
16	6	-2.152450	-3.072723	-0.299438
17	6	-0.877248	-2.667037	0.465245
18	7	-1.729714	-0.790601	-0.739968
19	6	-2.853424	-1.729111	-0.571087
20	1	0.176405	-1.622071	-1.110089
21	1	-0.571498	-0.311773	2.356750
22	1	-1.422082	4.230667	0.791787
23	1	-3.498681	3.478192	-0.339125
24	1	-3.758263	1.128812	-1.097705
25	1	0.414958	2.598098	1.237508
26	1	5.401570	0.328092	-1.124984
27	1	4.935820	-0.517399	1.171162
28	1	2.601601	-0.755393	1.960458
29	1	1.175590	0.695310	-1.825585
30	1	3.498091	0.932813	-2.617537
31	1	-2.788175	-3.760341	0.265036
32	1	-1.890965	-3.557745	-1.246803
33	1	-1.114489	-2.465208	1.514491
34	1	-0.099082	-3.434597	0.439813
35	1	-3.487158	-1.759830	-1.463283
36	1	-3.481433	-1.429683	0.281905

1aj (C, NMP)

Number	Atomic Number	X	Y	Z
1	6	1.580540	-3.233676	0.083502
2	6	2.845325	-2.714201	-0.212845

3	6	3.064900	-1.328759	-0.247707
4	6	1.968880	-0.526128	0.008345
5	6	0.691292	-1.013411	0.304865
6	6	-0.272118	0.155472	0.595710
7	8	-0.155441	0.535694	1.973002
8	6	0.491185	-2.389488	0.345455
9	6	-4.383374	-0.330562	-0.695011
10	6	-4.099352	0.231174	0.551925
11	6	-2.774022	0.379831	0.973486
12	6	-1.717989	-0.039335	0.154165
13	6	-2.009793	-0.602243	-1.098680
14	6	-3.333108	-0.745041	-1.520772
15	6	0.460104	1.262035	-0.194536
16	6	1.792778	3.221953	-0.589414
17	6	0.423606	2.764994	0.024443
18	7	1.919232	0.943076	0.097411
19	6	2.678992	1.946438	-0.730533
20	1	2.071833	1.183377	1.086567
21	1	0.335467	1.039913	-1.258762
22	1	-0.352587	-0.227292	2.536471
23	1	1.437458	-4.309222	0.104115
24	1	3.670684	-3.387603	-0.418418
25	1	4.042713	-0.915260	-0.467754
26	1	-0.488071	-2.804032	0.562024
27	1	-5.412509	-0.445456	-1.021801
28	1	-4.907087	0.558044	1.200008
29	1	-2.560319	0.825886	1.938248
30	1	-1.207245	-0.937108	-1.749594
31	1	-3.541965	-1.184076	-2.491720
32	1	2.276101	3.960684	0.052216
33	1	1.652816	3.674669	-1.572510
34	1	0.365081	3.003539	1.089797
35	1	-0.427123	3.224373	-0.479897
36	1	2.717375	1.564604	-1.751055
37	1	3.689200	2.053560	-0.338201

1aj (TS3, NMP)

Number	Atomic Number	X	Y	Z
1	6	1.711412	-3.223636	0.057494
2	6	2.975091	-2.637052	-0.065682
3	6	3.140915	-1.241509	-0.080307
4	6	1.993475	-0.470404	0.010886

5	6	0.709714	-1.049966	0.124157
6	6	-0.275660	0.100961	0.289100
7	8	0.036772	0.651174	1.714854
8	6	0.558364	-2.429480	0.166876
9	6	-4.502369	-0.352494	-0.376689
10	6	-4.049772	0.422644	0.694294
11	6	-2.680797	0.566410	0.932577
12	6	-1.751342	-0.078097	0.103028
13	6	-2.208621	-0.857223	-0.971873
14	6	-3.578178	-0.988059	-1.210803
15	6	0.477681	1.194290	-0.507186
16	6	1.771231	3.213421	-0.610894
17	6	0.318663	2.701461	-0.347705
18	7	1.821396	0.945659	0.101900
19	6	2.736067	2.017037	-0.335358
20	1	1.070546	0.949961	1.418827
21	1	0.472026	0.899651	-1.563671
22	1	0.044767	-0.060786	2.381618
23	1	1.619467	-4.304596	0.068716
24	1	3.851979	-3.271530	-0.148466
25	1	4.125224	-0.793304	-0.159915
26	1	-0.420626	-2.885704	0.270203
27	1	-5.566906	-0.461178	-0.559999
28	1	-4.760234	0.920460	1.346929
29	1	-2.341584	1.175578	1.762611
30	1	-1.501683	-1.355779	-1.626942
31	1	-3.919447	-1.591733	-2.045953
32	1	2.003865	4.068113	0.027174
33	1	1.877740	3.537961	-1.648477
34	1	-0.010174	2.964212	0.661361
35	1	-0.399845	3.113662	-1.057586
36	1	3.271455	1.712535	-1.240901
37	1	3.464231	2.223636	0.450850

1aj (D, NMP)

Number	Atomic Number	X	Y	Z
1	6	-1.624310	-3.134303	-0.452810
2	6	-2.927176	-2.568082	-0.254155
3	6	-3.119576	-1.242542	0.061366
4	6	-1.962875	-0.437315	0.203899
5	6	-0.632409	-0.985167	0.007958
6	6	0.287621	0.059176	0.103252

7	6	-0.494004	-2.370149	-0.329098
8	6	4.551003	-0.149935	-0.011856
9	6	3.890980	0.975810	-0.517203
10	6	2.501385	1.052617	-0.469794
11	6	1.741171	-0.011246	0.064964
12	6	2.422768	-1.138348	0.577975
13	6	3.813178	-1.201915	0.542306
14	6	-0.487813	1.310828	0.420761
15	6	-1.935829	3.165248	-0.039566
16	6	-0.588313	2.558923	-0.490081
17	7	-1.881279	0.866511	0.483586
18	6	-2.849407	1.946563	0.220412
19	1	-0.167519	1.629866	1.425827
20	1	-1.546280	-4.182356	-0.720048
21	1	-3.792724	-3.213592	-0.367335
22	1	-4.110992	-0.828916	0.203987
23	1	0.484263	-2.796756	-0.513035
24	1	5.634859	-0.203214	-0.041807
25	1	4.459537	1.794072	-0.947293
26	1	2.004934	1.924625	-0.878123
27	1	1.864975	-1.939973	1.048186
28	1	4.321879	-2.067079	0.955330
29	1	-2.359430	3.835186	-0.790215
30	1	-1.797955	3.737235	0.882887
31	1	-0.625578	2.247949	-1.538620
32	1	0.245724	3.246931	-0.349992
33	1	-3.518336	2.086471	1.072864
34	1	-3.446767	1.683001	-0.657697

1aj (2ae, NMP)

Number	Atomic Number	X	Y	Z
1	6	-1.911932	-3.111340	-0.178238
2	6	-3.162310	-2.457488	-0.141373
3	6	-3.241668	-1.067231	-0.076069
4	6	-2.039600	-0.349986	-0.038878
5	6	-0.757549	-0.987054	-0.058784
6	6	0.252243	0.059677	-0.028789
7	6	-0.717633	-2.392861	-0.138993
8	6	4.538704	-0.364174	0.021150
9	6	3.939006	0.698876	-0.662767
10	6	2.548758	0.828519	-0.687666
11	6	1.716173	-0.092743	-0.018656

12	6	2.338262	-1.154270	0.670737
13	6	3.728329	-1.290220	0.686234
14	6	-0.454929	1.251864	0.002991
15	6	-1.615702	3.283213	0.475213
16	6	-0.226472	2.736633	0.036993
17	7	-1.807594	1.004143	0.012200
18	6	-2.637530	2.206409	0.034413
19	1	-1.880422	-4.195431	-0.241113
20	1	-4.075656	-3.044489	-0.171738
21	1	-4.200978	-0.558678	-0.060853
22	1	0.230360	-2.919863	-0.180731
23	1	5.619587	-0.469104	0.035276
24	1	4.553974	1.424126	-1.188719
25	1	2.101005	1.644806	-1.246332
26	1	1.729492	-1.865323	1.219648
27	1	4.178914	-2.117111	1.228505
28	1	-1.838984	4.259731	0.040325
29	1	-1.642864	3.383626	1.564543
30	1	0.043112	3.109974	-0.959528
31	1	0.575780	3.030162	0.719888
32	1	-3.470033	2.096429	0.734295
33	1	-3.047033	2.405200	-0.963982

1e (S0, NMP)

Number	Atomic Number	X	Y	Z
1	6	2.593722	-1.159565	0.907710
2	6	3.970733	-0.938620	0.791430
3	6	4.462992	0.253859	0.265726
4	6	3.565581	1.256875	-0.165852
5	6	2.187866	1.027885	-0.068210
6	6	1.705993	-0.173035	0.469787
7	6	1.977163	-2.425755	1.441817
8	6	0.223502	-0.402732	0.666454
9	7	-0.187145	-1.790493	0.397279
10	6	0.818774	-2.855100	0.535342
11	6	-3.768243	-2.683550	-1.686192
12	6	-2.695324	-3.582796	-1.653299
13	6	-1.540025	-3.291987	-0.938354
14	6	-1.395272	-2.081362	-0.206998
15	6	-2.528743	-1.200785	-0.172619
16	6	-2.703739	-0.113691	0.832610
17	8	-2.338378	-0.265504	2.004899

18	6	-3.665917	-1.509573	-0.950081
19	6	-4.601677	3.616445	-0.188796
20	6	-3.916625	2.901086	-1.175787
21	6	-3.322467	1.675091	-0.866805
22	6	-3.393575	1.160660	0.438949
23	6	-4.072019	1.894578	1.427475
24	6	-4.680749	3.109125	1.114184
25	8	5.827351	0.462573	0.229477
26	6	6.426778	0.371238	-1.075542
27	8	4.127549	2.401693	-0.656253
28	6	3.260963	3.448589	-1.100397
29	1	4.684209	-1.692392	1.113466
30	1	7.493188	0.555695	-0.935161
31	1	6.008537	1.121653	-1.752666
32	1	6.279975	-0.631909	-1.492942
33	1	3.917021	4.250452	-1.439006
34	1	2.629447	3.812892	-0.282434
35	1	2.631039	3.114648	-1.932503
36	1	1.483627	1.782874	-0.399114
37	1	1.603276	-2.274379	2.464323
38	1	2.709122	-3.237701	1.484613
39	1	-0.338963	0.259167	0.001130
40	1	-0.055673	-0.120251	1.691636
41	1	0.332697	-3.742207	0.954560
42	1	1.229417	-3.132999	-0.447256
43	1	-4.667201	-2.904164	-2.252163
44	1	-2.747614	-4.515847	-2.207714
45	1	-0.722235	-3.998809	-0.978478
46	1	-4.512194	-0.831157	-0.916581
47	1	-5.070544	4.565390	-0.432114
48	1	-3.845070	3.296013	-2.184724
49	1	-2.789109	1.126271	-1.636125
50	1	-4.118602	1.497482	2.436200
51	1	-5.214653	3.661359	1.881809

1e (S1, NMP)

Number	Atomic Number	X	Y	Z
1	6	2.176190	-1.477401	0.806601
2	6	3.574677	-1.431242	0.790078
3	6	4.247317	-0.313159	0.304333
4	6	3.514261	0.792063	-0.189091
5	6	2.116245	0.735031	-0.197068

6	6	1.455329	-0.393547	0.305527
7	6	1.373677	-2.654285	1.292837
8	6	-0.053893	-0.407415	0.389603
9	7	-0.642053	-1.741892	0.142223
10	6	0.220170	-2.929934	0.323913
11	6	-4.536170	-2.313821	-1.282354
12	6	-3.537612	-3.270235	-1.526120
13	6	-2.264632	-3.070527	-1.030241
14	6	-1.937167	-1.890780	-0.295770
15	6	-2.964907	-0.914249	-0.025680
16	6	-2.815982	0.228500	0.952503
17	8	-2.795951	-0.141321	2.189644
18	6	-4.239936	-1.173630	-0.529162
19	6	-2.653969	4.316263	-0.340544
20	6	-2.696524	3.275836	-1.285484
21	6	-2.756172	1.944642	-0.887594
22	6	-2.778797	1.583211	0.498600
23	6	-2.724874	2.658786	1.443831
24	6	-2.668071	3.981510	1.028004
25	8	5.623008	-0.276755	0.372605
26	6	6.310139	-0.408311	-0.886392
27	8	4.246502	1.856252	-0.625312
28	6	3.552616	3.005532	-1.121001
29	1	4.163162	-2.266011	1.160113
30	1	7.375653	-0.365313	-0.655691
31	1	6.045293	0.407289	-1.564916
32	1	6.073209	-1.373426	-1.348926
33	1	4.327837	3.719274	-1.398923
34	1	2.911828	3.442685	-0.347513
35	1	2.952072	2.754807	-2.002278
36	1	1.536080	1.567590	-0.577511
37	1	0.970160	-2.473116	2.297897
38	1	1.984728	-3.558962	1.351053
39	1	-0.481603	0.292518	-0.326834
40	1	-0.379237	-0.091737	1.389215
41	1	-0.404537	-3.744488	0.690339
42	1	0.630064	-3.214167	-0.653262
43	1	-5.537886	-2.460153	-1.672858
44	1	-3.754152	-4.155003	-2.114465
45	1	-1.492818	-3.792386	-1.261906
46	1	-5.027604	-0.458901	-0.313195
47	1	-2.611009	5.353146	-0.658300
48	1	-2.684609	3.510516	-2.347461

49	1	-2.795350	1.169294	-1.647209
50	1	-2.733434	2.415220	2.501124
51	1	-2.633460	4.772141	1.774479

1e (T1, NMP)

Number	Atomic Number	X	Y	Z
1	6	2.391056	-1.068180	-0.944027
2	6	3.761732	-1.220332	-1.180191
3	6	4.700482	-0.829335	-0.227740
4	6	4.273068	-0.262710	0.995445
5	6	2.903004	-0.086419	1.224142
6	6	1.972025	-0.494696	0.261362
7	6	1.313058	-1.448397	-1.929654
8	6	0.482139	-0.385324	0.496757
9	7	-0.234805	0.074320	-0.716981
10	6	0.286106	-0.316026	-2.037212
11	6	-2.621582	3.541678	-0.512032
12	6	-1.248348	3.666922	-0.777722
13	6	-0.462180	2.510322	-0.851039
14	6	-1.037804	1.259561	-0.641184
15	6	-2.424826	1.105274	-0.339515
16	6	-2.901240	-0.250079	-0.192852
17	8	-2.060866	-1.213010	-0.496536
18	6	-3.201471	2.295954	-0.301637
19	6	-6.805955	-1.567361	1.059281
20	6	-6.306378	-0.342512	1.519527
21	6	-5.048301	0.109193	1.120707
22	6	-4.247216	-0.651561	0.234730
23	6	-4.757133	-1.901648	-0.197658
24	6	-6.015701	-2.345355	0.202519
25	8	6.038370	-1.061335	-0.469071
26	6	6.820385	0.107401	-0.778366
27	8	5.254764	0.073645	1.881632
28	6	4.874361	0.651991	3.133530
29	1	4.121957	-1.651876	-2.109912
30	1	7.840763	-0.243767	-0.939991
31	1	6.802186	0.821754	0.049528
32	1	6.446837	0.583600	-1.692356
33	1	5.805959	0.830129	3.670378
34	1	4.244658	-0.034253	3.710375
35	1	4.348498	1.601805	2.986353
36	1	2.552995	0.353328	2.151013

37	1	0.804527	-2.368529	-1.611293
38	1	1.729394	-1.639572	-2.922460
39	1	0.245493	0.303916	1.308209
40	1	0.065369	-1.365952	0.759308
41	1	-0.567407	-0.598758	-2.659402
42	1	0.756096	0.566119	-2.492514
43	1	-3.248949	4.428240	-0.485036
44	1	-0.799568	4.641651	-0.938163
45	1	0.599812	2.582956	-1.066942
46	1	-4.271381	2.235649	-0.146753
47	1	-7.786663	-1.914036	1.371211
48	1	-6.893801	0.260019	2.207228
49	1	-4.670516	1.036261	1.536039
50	1	-4.151956	-2.510854	-0.860727
51	1	-6.384490	-3.302637	-0.156457

1i (S0, NMP)

Number	Atomic Number	X	Y	Z
1	6	3.952224	-1.054533	-0.532002
2	6	5.075978	-1.828940	-0.225673
3	6	4.992220	-2.846914	0.730518
4	6	3.784263	-3.082573	1.395004
5	6	2.661429	-2.301851	1.100065
6	6	2.740546	-1.291625	0.135336
7	6	3.948889	0.079951	-1.522955
8	6	1.530609	-0.479037	-0.269298
9	7	1.844013	0.937203	-0.520986
10	6	3.215230	1.284664	-0.923304
11	6	-0.703126	4.053209	0.807408
12	6	0.661174	4.269498	0.577980
13	6	1.478890	3.247384	0.111487
14	6	0.972501	1.947011	-0.158630
15	6	-0.440440	1.751016	-0.000694
16	6	-1.186455	0.604525	-0.594376
17	8	-0.895418	0.171337	-1.715994
18	6	-1.229373	2.800022	0.517893
19	6	-4.477062	-1.255329	1.455175
20	6	-3.478299	-0.627024	2.192247
21	6	-2.412824	0.013189	1.547936
22	6	-2.346689	0.005739	0.148382
23	6	-3.346266	-0.641819	-0.602022
24	6	-4.414039	-1.262652	0.049708

25	8	-5.440056	-1.901754	-0.585956
26	6	-5.430278	-1.956167	-2.015944
27	1	6.017163	-1.635454	-0.734429
28	1	5.867763	-3.446796	0.961771
29	1	3.717367	-3.865615	2.144734
30	1	1.723893	-2.480638	1.620797
31	1	3.450004	-0.223772	-2.453921
32	1	4.967051	0.380939	-1.786559
33	1	0.777715	-0.532011	0.522558
34	1	1.072285	-0.927985	-1.162368
35	1	3.169498	2.093044	-1.660613
36	1	3.794308	1.651973	-0.062425
37	1	-1.341286	4.847505	1.180242
38	1	1.101918	5.241409	0.782523
39	1	2.534210	3.450968	-0.010716
40	1	-2.295384	2.633546	0.633722
41	1	-5.311671	-1.746938	1.945174
42	1	-3.528633	-0.634265	3.276794
43	1	-1.635709	0.494916	2.130517
44	1	-3.260140	-0.640951	-1.681027
45	1	-6.326252	-2.509735	-2.296078
46	1	-4.543226	-2.482959	-2.384352
47	1	-5.469788	-0.950726	-2.449299

1i (S1, NMP)

Number	Atomic Number	X	Y	Z
1	6	3.355076	-1.529366	-0.484752
2	6	4.247142	-2.588029	-0.288668
3	6	3.915569	-3.634805	0.577049
4	6	2.696906	-3.616310	1.263158
5	6	1.807998	-2.552664	1.080933
6	6	2.134201	-1.513981	0.202495
7	6	3.632808	-0.342951	-1.369148
8	6	1.148456	-0.401882	-0.076866
9	7	1.792934	0.916894	-0.258131
10	6	3.217753	0.945216	-0.652811
11	6	-0.123852	4.554550	0.520275
12	6	1.273114	4.447992	0.613118
13	6	1.886276	3.243152	0.332964
14	6	1.119699	2.092718	-0.023387
15	6	-0.314014	2.202862	-0.142207
16	6	-1.195232	1.147306	-0.769190

17	8	-1.062821	1.047932	-2.049606
18	6	-0.883370	3.446776	0.131047
19	6	-3.959188	-1.178573	1.525417
20	6	-3.102698	-0.270692	2.162141
21	6	-2.200621	0.508300	1.443308
22	6	-2.123162	0.400812	0.020337
23	6	-2.997272	-0.536515	-0.624041
24	6	-3.889565	-1.296934	0.119505
25	8	-4.762432	-2.210951	-0.429581
26	6	-4.759933	-2.386455	-1.844930
27	1	5.199924	-2.592337	-0.811486
28	1	4.609989	-4.456859	0.723021
29	1	2.441233	-4.422970	1.943498
30	1	0.863687	-2.534079	1.618251
31	1	3.087300	-0.423299	-2.318568
32	1	4.695387	-0.265509	-1.613845
33	1	0.425174	-0.322488	0.733383
34	1	0.587925	-0.617026	-0.995832
35	1	3.370667	1.810502	-1.297696
36	1	3.828105	1.069802	0.250308
37	1	-0.614591	5.496012	0.744217
38	1	1.871291	5.299023	0.919298
39	1	2.958562	3.159780	0.450111
40	1	-1.958324	3.549860	0.022930
41	1	-4.666068	-1.784936	2.081045
42	1	-3.146484	-0.171551	3.244104
43	1	-1.560943	1.207510	1.972322
44	1	-2.935050	-0.622182	-1.700771
45	1	-5.517887	-3.142335	-2.054180
46	1	-3.784911	-2.738710	-2.201867
47	1	-5.020059	-1.455470	-2.362320

1i (T1, NMP)

Number	Atomic Number	X	Y	Z
1	6	3.784011	-1.422092	-0.356781
2	6	5.103981	-1.862660	-0.494633
3	6	6.052817	-1.567505	0.490355
4	6	5.688427	-0.814889	1.611291
5	6	4.373054	-0.358991	1.748625
6	6	3.421495	-0.668269	0.772223
7	6	2.700629	-1.671551	-1.377860
8	6	1.971097	-0.260074	0.900894

9	7	1.405494	0.203380	-0.388376
10	6	1.922633	-0.377302	-1.637126
11	6	-0.379743	4.015283	-0.594558
12	6	1.008261	3.895850	-0.769786
13	6	1.594250	2.625540	-0.707370
14	6	0.806938	1.504811	-0.454288
15	6	-0.601720	1.600320	-0.243694
16	6	-1.305157	0.354628	-0.042277
17	8	-0.617999	-0.751360	-0.217191
18	6	-1.170226	2.899962	-0.342331
19	6	-5.444037	-0.229300	0.962061
20	6	-4.788052	0.928887	1.378333
21	6	-3.446783	1.157002	1.061435
22	6	-2.725603	0.209868	0.300744
23	6	-3.388764	-0.980337	-0.098072
24	6	-4.730042	-1.189163	0.222588
25	8	-5.442175	-2.302604	-0.142858
26	6	-4.782598	-3.318900	-0.900409
27	1	5.390625	-2.436915	-1.371931
28	1	7.074996	-1.917110	0.378345
29	1	6.425574	-0.576967	2.372407
30	1	4.088613	0.232233	2.615210
31	1	2.006504	-2.444733	-1.021882
32	1	3.119204	-2.026601	-2.323480
33	1	1.836542	0.536137	1.634211
34	1	1.365001	-1.116215	1.223791
35	1	1.071199	-0.541826	-2.302585
36	1	2.581879	0.362465	-2.111713
37	1	-0.851424	4.990901	-0.671960
38	1	1.621521	4.769635	-0.963797
39	1	2.664540	2.508837	-0.850838
40	1	-2.242399	3.025057	-0.260373
41	1	-6.486115	-0.410409	1.204968
42	1	-5.327307	1.661988	1.972034
43	1	-2.957170	2.042606	1.446917
44	1	-2.828588	-1.711174	-0.665880
45	1	-5.530658	-4.093182	-1.072122
46	1	-3.938095	-3.742967	-0.345534
47	1	-4.430703	-2.930432	-1.862956

1n (S0, NMP)

Number	Atomic Number	X	Y	Z

1	6	-2.284841	2.658360	-0.825637
2	6	-3.175660	3.663722	-0.430816
3	6	-3.341610	3.958217	0.924692
4	6	-2.609087	3.246014	1.883175
5	6	-1.721449	2.245222	1.484065
6	6	-1.553031	1.936613	0.124803
7	6	-0.560156	0.871894	-0.308516
8	7	-0.908902	-0.487052	0.137477
9	6	1.864311	-3.078271	2.032724
10	6	0.482708	-3.195962	2.238815
11	6	-0.401591	-2.349654	1.581923
12	6	0.049597	-1.364767	0.673411
13	6	1.446059	-1.288241	0.414582
14	6	2.025093	-0.546265	-0.750328
15	8	1.483101	-0.607367	-1.857887
16	6	2.327362	-2.123553	1.135055
17	6	5.653530	1.736223	-0.369920
18	6	4.860846	1.512544	0.759840
19	6	3.694281	0.751429	0.656371
20	6	3.302042	0.219397	-0.583937
21	6	4.098993	0.461449	-1.717036
22	6	5.271500	1.207011	-1.609347
23	6	-4.471221	-2.185462	-1.433221
24	6	-3.222939	-2.554065	-1.947242
25	6	-2.055899	-1.989684	-1.427899
26	6	-2.122898	-1.058659	-0.378782
27	6	-3.374450	-0.697212	0.138962
28	6	-4.541897	-1.255455	-0.391780
29	1	-3.738189	4.212154	-1.181068
30	1	-4.031946	4.737586	1.234231
31	1	-2.727694	3.474325	2.938659
32	1	-1.155666	1.694911	2.231722
33	1	0.408290	1.113207	0.136391
34	1	-0.431798	0.905499	-1.397705
35	1	2.561846	-3.725638	2.554184
36	1	0.094746	-3.932914	2.936310
37	1	-1.464569	-2.418022	1.787720
38	1	3.391890	-2.052431	0.935009
39	1	6.564530	2.321581	-0.286866
40	1	5.149742	1.929159	1.719942
41	1	3.081233	0.584625	1.535925
42	1	3.789498	0.052892	-2.673373
43	1	5.887653	1.377634	-2.487030

44	1	-2.161333	2.430843	-1.881521
45	1	-5.379390	-2.621806	-1.838510
46	1	-3.157355	-3.274891	-2.757283
47	1	-1.084870	-2.263418	-1.829074
48	1	-3.430758	0.008556	0.959558
49	1	-5.505917	-0.970608	0.019808

1n (S1, NMP)

Number	Atomic Number	X	Y	Z
1	6	3.343471	-1.452279	-0.676527
2	6	4.186680	-2.549927	-0.486665
3	6	3.685410	-3.850837	-0.600339
4	6	2.335163	-4.047535	-0.902342
5	6	1.491159	-2.948124	-1.085900
6	6	1.986882	-1.641664	-0.980552
7	6	1.049440	-0.471787	-1.243459
8	7	1.014077	0.510474	-0.141691
9	6	-1.002243	-0.861445	3.304944
10	6	0.401949	-0.819298	3.281434
11	6	1.033594	-0.340692	2.130617
12	6	0.285804	0.084414	1.033687
13	6	-1.145679	0.032215	1.009865
14	6	-1.895678	0.554728	-0.128606
15	8	-1.316838	1.374718	-0.940184
16	6	-1.746453	-0.447578	2.207361
17	6	-6.007114	-0.437866	-1.031776
18	6	-5.216108	-1.349392	-0.319903
19	6	-3.892635	-1.045005	0.001042
20	6	-3.309334	0.188143	-0.377220
21	6	-4.117634	1.083977	-1.118343
22	6	-5.441861	0.780431	-1.431484
23	6	2.997071	4.194005	-0.226261
24	6	2.130502	3.878042	0.831041
25	6	1.479786	2.657446	0.865118
26	6	1.678362	1.706831	-0.179569
27	6	2.558994	2.042308	-1.249007
28	6	3.204386	3.266997	-1.259445
29	1	5.234042	-2.387849	-0.249900
30	1	4.341892	-4.703038	-0.452130
31	1	1.935501	-5.053436	-0.990109
32	1	0.441008	-3.107346	-1.314823
33	1	0.027025	-0.837684	-1.345751

34	1	1.294264	0.043382	-2.171377
35	1	-1.519469	-1.200722	4.198316
36	1	0.988974	-1.138143	4.135855
37	1	2.117208	-0.295978	2.078668
38	1	-2.827490	-0.445438	2.282326
39	1	-7.037488	-0.676461	-1.278348
40	1	-5.628515	-2.310467	-0.023416
41	1	-3.297463	-1.787284	0.522446
42	1	-3.681657	2.024440	-1.438673
43	1	-6.038103	1.497300	-1.990619
44	1	3.751194	-0.450618	-0.580068
45	1	3.505098	5.151800	-0.246331
46	1	1.960430	4.595050	1.626751
47	1	0.800384	2.424160	1.673232
48	1	2.748395	1.345259	-2.053384
49	1	3.877450	3.505370	-2.075630

1n (T1, NMP)

Number	Atomic Number	X	Y	Z
1	6	3.182548	-1.601132	-1.853071
2	6	4.252841	-2.491410	-1.721812
3	6	4.329367	-3.334628	-0.610273
4	6	3.321142	-3.292833	0.358439
5	6	2.248550	-2.408519	0.220600
6	6	2.174473	-1.539223	-0.879803
7	6	0.983422	-0.609425	-1.073818
8	7	0.826870	0.454472	-0.042533
9	6	-1.313555	-0.714346	3.401631
10	6	0.075631	-0.508723	3.480220
11	6	0.761081	-0.092548	2.336581
12	6	0.079122	0.106493	1.134701
13	6	-1.337568	-0.078582	1.029498
14	6	-1.986197	0.306395	-0.205424
15	8	-1.295497	0.994893	-1.069742
16	6	-2.001550	-0.505096	2.213785
17	6	-6.061699	-0.540573	-1.329907
18	6	-5.375226	-1.429163	-0.492559
19	6	-4.059885	-1.170333	-0.106044
20	6	-3.388309	-0.003752	-0.541998
21	6	-4.088338	0.869166	-1.409896
22	6	-5.403782	0.608067	-1.789226
23	6	3.019728	4.047785	-0.167748

24	6	1.998930	3.867756	0.775731
25	6	1.282550	2.679053	0.824188
26	6	1.576581	1.628216	-0.080872
27	6	2.600677	1.822085	-1.037087
28	6	3.309680	3.018655	-1.071044
29	1	5.021256	-2.525381	-2.488508
30	1	5.160744	-4.025217	-0.504171
31	1	3.362895	-3.956306	1.217337
32	1	1.462891	-2.403576	0.968824
33	1	0.057552	-1.183685	-1.038506
34	1	1.024503	-0.124823	-2.049188
35	1	-1.866503	-1.013637	4.287618
36	1	0.611653	-0.667178	4.409922
37	1	1.835827	0.057729	2.365934
38	1	-3.079773	-0.607032	2.209665
39	1	-7.086035	-0.744963	-1.627134
40	1	-5.861784	-2.338291	-0.149288
41	1	-3.539817	-1.898655	0.506465
42	1	-3.583290	1.758926	-1.771224
43	1	-5.920051	1.303736	-2.445594
44	1	3.128291	-0.962816	-2.731472
45	1	3.576901	4.978437	-0.201157
46	1	1.753232	4.663941	1.471279
47	1	0.479069	2.561253	1.540086
48	1	2.859112	1.041866	-1.737600
49	1	4.097938	3.144911	-1.806370

1ah (S0, NMP)

Number	Atomic Number	X	Y	Z
1	6	2.898896	-0.710593	0.572947
2	6	4.113029	-1.352039	0.306952
3	6	4.891645	-0.963511	-0.788571
4	6	4.447300	0.059959	-1.631917
5	6	3.227438	0.695245	-1.376249
6	6	2.453998	0.317733	-0.272759
7	6	1.975212	-1.082951	1.703792
8	6	1.177492	1.044390	0.086390
9	7	0.122278	0.145257	0.601950
10	6	0.535317	-1.142051	1.183414
11	6	-3.827189	0.575047	-0.840584
12	6	-3.330993	-0.677508	-0.417749
13	6	-2.044459	-0.801912	0.105265

14	6	-1.190496	0.325178	0.231317
15	6	-1.743276	1.620955	-0.065661
16	6	-1.240681	2.905053	0.401299
17	8	-0.361220	3.122323	1.241609
18	6	-3.033653	1.684818	-0.653109
19	8	-4.176597	-1.725652	-0.595479
20	6	-3.770175	-3.036307	-0.182965
21	1	4.449165	-2.157011	0.955873
22	1	5.835151	-1.463530	-0.987731
23	1	5.043294	0.357900	-2.489689
24	1	2.879385	1.486645	-2.035557
25	1	2.039971	-0.346467	2.516803
26	1	2.239022	-2.056035	2.128204
27	1	0.786264	1.561765	-0.793721
28	1	1.391870	1.821583	0.829647
29	1	-0.150345	-1.388128	2.000488
30	1	0.470287	-1.947831	0.436727
31	1	-4.821805	0.642975	-1.266632
32	1	-4.617607	-3.686428	-0.398426
33	1	-3.551183	-3.059836	0.889490
34	1	-2.896131	-3.373166	-0.750232
35	1	-1.667640	-1.783265	0.347287
36	1	-3.426026	2.665411	-0.911052
37	1	-1.793506	3.766211	-0.025052

1ah (S1, NMP)

Number	Atomic Number	X	Y	Z
1	6	2.929723	0.012611	0.663336
2	6	4.305823	-0.141199	0.888158
3	6	5.120506	-0.775508	-0.050334
4	6	4.560732	-1.275422	-1.231626
5	6	3.192486	-1.133339	-1.461692
6	6	2.374116	-0.487911	-0.523225
7	6	2.043328	0.716776	1.663731
8	6	0.900926	-0.344187	-0.836926
9	7	0.088274	0.199392	0.244810
10	6	0.608225	0.197471	1.609502
11	6	-4.046346	0.654055	-0.421025
12	6	-3.531005	-0.613771	-0.052164
13	6	-2.158629	-0.758683	0.166276
14	6	-1.319231	0.351096	0.018495
15	6	-1.801471	1.646327	-0.345748

16	6	-0.900352	2.733989	-0.471362
17	8	0.371281	2.623802	-0.260398
18	6	-3.211090	1.741621	-0.562254
19	8	-4.453729	-1.628590	0.059431
20	6	-3.987652	-2.922861	0.434649
21	1	4.737420	0.240582	1.809908
22	1	6.183833	-0.885967	0.140603
23	1	5.184706	-1.776290	-1.965600
24	1	2.754459	-1.524575	-2.376717
25	1	2.022407	1.792216	1.456880
26	1	2.424020	0.578446	2.679680
27	1	0.469994	-1.319583	-1.102561
28	1	0.742137	0.308624	-1.701139
29	1	-0.066621	0.797771	2.219289
30	1	0.559266	-0.841341	1.968534
31	1	-5.114678	0.750723	-0.590316
32	1	-4.869782	-3.562978	0.463765
33	1	-3.518031	-2.904545	1.425753
34	1	-3.275295	-3.317962	-0.299857
35	1	-1.730160	-1.713685	0.447931
36	1	-3.628448	2.704338	-0.845752
37	1	-1.314092	3.710404	-0.763073

1ah (T1, NMP)

Number	Atomic Number	X	Y	Z
1	6	2.903045	2.903045	0.703614
2	6	4.291116	4.291116	0.893330
3	6	5.129218	5.129218	-0.122957
4	6	4.582142	4.582142	-1.354861
5	6	3.204303	3.204303	-1.552280
6	6	2.359437	2.359437	-0.532701
7	6	2.006866	2.006866	1.802011
8	6	0.869001	0.869001	-0.800840
9	7	0.096858	0.096858	0.265852
10	6	0.559182	0.559182	1.636381
11	6	-4.022421	-4.022421	-0.447792
12	6	-3.554329	-3.554329	-0.099738
13	6	-2.188308	-2.188308	0.139705
14	6	-1.309621	-1.309621	0.035304
15	6	-1.755059	-1.755059	-0.306060
16	6	-0.783284	-0.783284	-0.368743
17	8	0.479807	0.479807	-0.107643

18	6	-3.151883	-3.151883	-0.549477
19	8	-4.511166	-4.511166	-0.025509
20	6	-4.096273	-4.096273	0.318811
21	1	4.713498	4.713498	1.851881
22	1	6.200462	6.200462	0.043943
23	1	5.224045	5.224045	-2.153785
24	1	2.776441	2.776441	-2.507678
25	1	2.024438	2.024438	1.795742
26	1	2.372306	2.372306	2.780902
27	1	0.484138	0.484138	-0.941911
28	1	0.660916	0.660916	-1.726563
29	1	-0.106845	-0.106845	2.313219
30	1	0.470304	0.470304	1.854951
31	1	-5.084286	-5.084286	-0.631962
32	1	-5.001684	-5.001684	0.319268
33	1	-3.639302	-3.639302	1.315307
34	1	-3.389829	-3.389829	-0.418655
35	1	-1.800353	-1.800353	0.403471
36	1	-3.532683	-3.532683	-0.814990
37	1	-1.057487	-1.057487	-0.641137

1al (S0, NMP)

Number	Atomic Number	X	Y	Z
1	6	0.247386	3.745341	-0.519020
2	6	-0.792032	3.072849	-1.170911
3	6	-0.963611	1.702170	-1.014831
4	6	-0.092906	0.920251	-0.208593
5	6	1.029054	1.595897	0.366714
6	6	2.219936	0.965427	1.033529
7	8	2.551728	1.310936	2.170428
8	6	1.140312	2.993761	0.238480
9	6	4.820115	-1.663279	-1.170191
10	6	3.831067	-0.945743	-1.849450
11	6	2.969807	-0.101798	-1.144437
12	6	3.095050	0.036037	0.248255
13	6	4.100208	-0.682240	0.921557
14	6	4.953149	-1.530025	0.218294
15	6	-1.467301	-1.122542	-0.688310
16	6	-0.653619	-2.504905	1.109854
17	6	-1.181445	-2.599268	-0.327213
18	7	-0.378084	-0.414547	0.009879
19	6	0.232124	-1.253154	1.061763

20	6	-5.540513	-0.092873	0.437546
21	6	-5.260047	-0.647439	-0.816066
22	6	-3.942223	-0.950179	-1.168514
23	6	-2.884162	-0.710671	-0.278066
24	6	-3.174853	-0.147774	0.971430
25	6	-4.492608	0.158147	1.328106
26	1	0.372821	4.818491	-0.618828
27	1	-1.493028	3.620655	-1.794769
28	1	-1.807854	1.230958	-1.499593
29	1	1.987065	3.480330	0.713874
30	1	5.486770	-2.322206	-1.718725
31	1	3.731301	-1.040567	-2.926458
32	1	2.208497	0.457465	-1.677371
33	1	4.194644	-0.569462	1.996463
34	1	5.720811	-2.086906	0.747160
35	1	-1.367314	-0.970884	-1.769776
36	1	-0.089940	-3.389051	1.418074
37	1	-1.481389	-2.369522	1.813084
38	1	-0.405188	-2.992215	-0.993520
39	1	-2.070165	-3.226237	-0.427834
40	1	0.260799	-0.713843	2.015951
41	1	1.254615	-1.537737	0.798433
42	1	-6.563197	0.146957	0.713692
43	1	-6.064716	-0.839442	-1.520272
44	1	-3.732920	-1.375286	-2.147843
45	1	-2.368322	0.068258	1.665441
46	1	-4.697871	0.596659	2.300678

1al (S1, NMP)

Number	Atomic Number	X	Y	Z
1	6	0.435188	3.661882	-0.280468
2	6	-0.739188	3.211671	-0.911537
3	6	-1.041972	1.869194	-0.920413
4	6	-0.178601	0.904961	-0.298793
5	6	1.037642	1.368533	0.338598
6	6	2.019506	0.505926	1.093661
7	8	1.736918	0.355238	2.346358
8	6	1.286061	2.741570	0.334417
9	6	5.495765	-1.139089	-0.805168
10	6	4.574826	-0.379155	-1.548851
11	6	3.445605	0.168501	-0.950940
12	6	3.176629	-0.020594	0.443523

13	6	4.123371	-0.804739	1.180009
14	6	5.247436	-1.340316	0.566658
15	6	-1.761829	-0.887921	-1.061123
16	6	-0.739703	-2.748308	0.087628
17	6	-1.502515	-2.404829	-1.194277
18	7	-0.548272	-0.406463	-0.334821
19	6	0.187484	-1.545679	0.269072
20	6	-5.536750	-0.087913	0.922490
21	6	-5.477327	-0.296883	-0.459547
22	6	-4.248799	-0.532048	-1.080288
23	6	-3.063863	-0.566100	-0.329388
24	6	-3.129515	-0.351134	1.053048
25	6	-4.360067	-0.114029	1.674906
26	1	0.683308	4.717970	-0.278429
27	1	-1.410717	3.916810	-1.388746
28	1	-1.959013	1.547786	-1.392008
29	1	2.194072	3.092934	0.813764
30	1	6.376782	-1.561158	-1.277992
31	1	4.746100	-0.211195	-2.609695
32	1	2.762857	0.758455	-1.555756
33	1	3.942025	-0.970918	2.236792
34	1	5.946326	-1.927581	1.158492
35	1	-1.779981	-0.419223	-2.047269
36	1	-0.170550	-3.676675	0.008570
37	1	-1.423451	-2.842516	0.937004
38	1	-0.876911	-2.589379	-2.073844
39	1	-2.435679	-2.957517	-1.313057
40	1	0.435216	-1.315587	1.305173
41	1	1.121440	-1.679011	-0.286031
42	1	-6.490705	0.099257	1.406179
43	1	-6.384528	-0.270284	-1.055842
44	1	-4.210498	-0.687558	-2.155555
45	1	-2.225879	-0.354945	1.654409
46	1	-4.393960	0.052648	2.747413

1al (T1, NMP)

Number	Atomic Number	X	Y	Z
1	6	0.518161	3.643103	-0.203412
2	6	-0.699984	3.241911	-0.792391
3	6	-1.051531	1.912948	-0.819044
4	6	-0.197324	0.900744	-0.259939
5	6	1.060300	1.313939	0.339769

6	6	2.034686	0.409665	1.037108
7	8	1.684463	0.192044	2.270444
8	6	1.354394	2.686040	0.361887
9	6	5.623613	-1.073607	-0.761526
10	6	4.725381	-0.288886	-1.510782
11	6	3.558914	0.205043	-0.940937
12	6	3.229366	-0.066022	0.425836
13	6	4.151426	-0.872801	1.168003
14	6	5.314831	-1.356295	0.582108
15	6	-1.815145	-0.828493	-1.083744
16	6	-0.820528	-2.749920	-0.011604
17	6	-1.568039	-2.340222	-1.283721
18	7	-0.597937	-0.395782	-0.336744
19	6	0.111383	-1.563079	0.242753
20	6	-5.591225	-0.084238	0.920982
21	6	-5.528720	-0.229620	-0.469078
22	6	-4.300097	-0.448161	-1.095890
23	6	-3.117933	-0.528969	-0.344048
24	6	-3.187041	-0.377289	1.046729
25	6	-4.417396	-0.156948	1.675078
26	1	0.804060	4.690066	-0.198058
27	1	-1.369176	3.980925	-1.220506
28	1	-2.004984	1.635280	-1.245311
29	1	2.291802	2.992774	0.814983
30	1	6.534769	-1.454610	-1.212800
31	1	4.945551	-0.062086	-2.551425
32	1	2.886692	0.811098	-1.542714
33	1	3.922783	-1.101169	2.204359
34	1	5.995588	-1.964350	1.173988
35	1	-1.826389	-0.314851	-2.048027
36	1	-0.257213	-3.677914	-0.130267
37	1	-1.515674	-2.882384	0.823439
38	1	-0.935582	-2.489329	-2.165222
39	1	-2.504288	-2.879789	-1.436692
40	1	0.328416	-1.371566	1.295648
41	1	1.065181	-1.683575	-0.282017
42	1	-6.545068	0.089991	1.409796
43	1	-6.433515	-0.166358	-1.066400
44	1	-4.259366	-0.553704	-2.177228
45	1	-2.284894	-0.417599	1.649188
46	1	-4.453783	-0.039790	2.754109

1ao (S0, NMP)

Number	Atomic Number	X	Y	Z
1	6	-0.268738	-1.659341	-0.785913
2	6	-0.762620	-0.341705	-0.978670
3	6	-0.658117	0.728234	-0.551006
4	6	-0.030700	0.517683	0.062759
5	6	0.458970	-0.822781	0.196300
6	6	1.104186	-1.205159	0.696242
7	8	2.397115	-2.072232	1.568274
8	6	0.326106	-1.885613	-0.190584
9	6	-1.246941	0.346215	-1.097508
10	6	-1.875001	0.415277	-1.801035
11	6	-1.132247	-0.054469	-1.217435
12	6	0.300094	-0.614796	0.070615
13	6	0.918984	-0.691800	0.765356
14	6	0.160546	-0.204960	0.189099
15	6	-0.816391	2.925887	0.031521
16	7	0.055250	1.589507	0.525528
17	6	1.066472	1.608240	1.945126
18	1	-0.357238	-2.493977	-1.103798
19	1	-1.212530	-0.139642	-1.443779
20	1	-1.001349	1.736744	-0.671251
21	1	0.679310	-2.900032	-0.057271
22	1	-1.833323	0.719141	-1.550134
23	1	-2.960604	0.835345	-2.802054
24	1	-1.653651	0.001449	-1.765812
25	1	2.002556	-1.129376	1.758171
26	1	0.665229	-0.256576	0.738196
27	1	-1.797839	2.912318	-1.054384
28	1	-0.363405	3.353709	0.483311
29	1	-0.925626	3.587458	0.275683
30	1	1.913954	0.602511	2.323707
31	1	1.388422	2.066156	2.557178
32	1	0.624800	2.190610	2.078150

1ao (S1, NMP)

Number	Atomic Number	X	Y	Z
1	6	2.571875	-2.346319	-0.268738
2	6	3.404078	-1.325990	-0.762620
3	6	3.009984	-0.008913	-0.658117
4	6	1.773651	0.341485	-0.030700
5	6	0.907709	-0.704481	0.458970
6	6	-0.438987	-0.483119	1.104186

7	8	-0.418653	-0.463828	2.397115
8	6	1.351441	-2.021222	0.326106
9	6	-3.997750	-0.025458	-1.246941
10	6	-2.754362	-0.221965	-1.875001
11	6	-1.589314	-0.373118	-1.132247
12	6	-1.610282	-0.337345	0.300094
13	6	-2.887478	-0.135504	0.918984
14	6	-4.039924	0.014460	0.160546
15	6	2.082467	2.665777	-0.816391
16	7	1.450604	1.670689	0.055250
17	6	0.558353	2.238925	1.066472
18	1	2.872928	-3.384894	-0.357238
19	1	4.360747	-1.567545	-1.212530
20	1	3.678346	0.769766	-1.001349
21	1	0.700743	-2.814682	0.679310
22	1	-4.903466	0.091565	-1.833323
23	1	-2.698189	-0.257541	-2.960604
24	1	-0.649212	-0.527649	-1.653651
25	1	-2.933405	-0.102806	2.002556
26	1	-4.991736	0.166096	0.665229
27	1	2.290162	2.244552	-1.797839
28	1	3.008000	3.037691	-0.363405
29	1	1.390839	3.501580	-0.925626
30	1	0.449616	1.568254	1.913954
31	1	0.994257	3.188086	1.388422
32	1	-0.423394	2.440039	0.624800

1ao (T1, NMP)

Number	Atomic Number	X	Y	Z
1	6	3.355878	-1.437290	-0.731159
2	6	3.691360	-0.069011	-0.895264
3	6	2.795133	0.895074	-0.475159
4	6	1.546077	0.534483	0.106647
5	6	1.120703	-0.869103	0.106077
6	6	-0.231525	-1.370409	0.394934
7	8	-0.317333	-2.497250	1.013507
8	6	2.116385	-1.813825	-0.231883
9	6	-3.873498	0.530635	-0.917591
10	6	-2.646528	0.925853	-1.467987
11	6	-1.453830	0.338660	-1.046121
12	6	-1.443725	-0.670915	-0.049023
13	6	-2.698180	-1.073601	0.477562

14	6	-3.885447	-0.480804	0.055194
15	6	0.963258	2.928963	0.356832
16	7	0.789752	1.518384	0.700890
17	6	0.028741	1.292705	1.932996
18	1	4.065389	-2.203488	-1.030057
19	1	4.657037	0.219512	-1.294761
20	1	3.092327	1.936688	-0.492974
21	1	1.848463	-2.862452	-0.173184
22	1	-4.799935	0.992087	-1.246413
23	1	-2.619421	1.689713	-2.240925
24	1	-0.528557	0.641877	-1.524299
25	1	-2.713849	-1.858279	1.226424
26	1	-4.829043	-0.805554	0.486762
27	1	1.148501	3.040686	-0.710779
28	1	1.791478	3.370480	0.925101
29	1	0.045736	3.456715	0.622112
30	1	0.037233	0.243001	2.209347
31	1	0.504759	1.878677	2.728392
32	1	-0.998518	1.641165	1.804628

1ap (S0, NMP)

Number	Atomic Number	X	Y	Z
1	6	-1.629516	3.500151	-0.256597
2	6	-2.474605	2.631079	-0.957936
3	6	-2.253404	1.256553	-0.944805
4	6	-1.158481	0.690835	-0.249246
5	6	-0.253937	1.587646	0.390791
6	6	1.052355	1.180342	0.998723
7	8	1.388321	1.623615	2.102418
8	6	-0.535104	2.965800	0.417370
9	6	3.932919	-1.170463	-1.169479
10	6	2.937708	-0.481132	-1.871042
11	6	1.975968	0.256455	-1.178600
12	6	2.010149	0.325957	0.224021
13	6	3.020820	-0.358981	0.919864
14	6	3.970937	-1.110725	0.228581
15	6	-1.537364	-1.580410	-1.203111
16	7	-0.968877	-0.688334	-0.187248
17	6	-0.699624	-1.372666	1.086372
18	6	-2.813129	-2.299420	-0.737177
19	6	-2.553536	-3.036987	0.585171
20	6	-1.953839	-2.082137	1.627161

21	1	-0.770928	-2.337028	-1.431031
22	1	-1.703473	-1.016760	-2.123301
23	1	-0.341685	-0.651813	1.821529
24	1	0.103707	-2.106411	0.929227
25	1	-1.813009	4.569726	-0.249598
26	1	-3.333697	3.022208	-1.496099
27	1	-2.963621	0.608298	-1.444732
28	1	0.158335	3.619780	0.937509
29	1	4.676269	-1.749647	-1.709527
30	1	2.910969	-0.518336	-2.955983
31	1	1.207762	0.790640	-1.727471
32	1	3.047673	-0.298050	2.002928
33	1	4.740661	-1.646384	0.776199
34	1	-3.136926	-3.000115	-1.516337
35	1	-3.621482	-1.569345	-0.601031
36	1	-1.851708	-3.864388	0.405861
37	1	-3.479290	-3.484856	0.964268
38	1	-1.685887	-2.625224	2.541904
39	1	-2.697984	-1.324266	1.906707

1ap (S1, NMP)

Number	Atomic Number	X	Y	Z
1	6	-0.646252	3.663784	0.090521
2	6	-1.804599	3.211453	-0.561714
3	6	-2.039869	1.856058	-0.677158
4	6	-1.139615	0.901384	-0.114962
5	6	0.054215	1.361406	0.549242
6	6	1.113638	0.466994	1.148648
7	8	0.999270	0.264971	2.421189
8	6	0.256083	2.741193	0.624006
9	6	4.249815	-1.188336	-1.267673
10	6	3.265761	-0.368069	-1.848737
11	6	2.241114	0.177937	-1.084534
12	6	2.150155	-0.069212	0.324534
13	6	3.165253	-0.905816	0.895935
14	6	4.178627	-1.444296	0.116123
15	6	-2.218344	-0.943618	-1.402698
16	7	-1.430663	-0.436015	-0.268287
17	6	-1.121057	-1.467724	0.733142
18	6	-3.554561	-1.549036	-0.939084
19	6	-3.313247	-2.630539	0.119808
20	6	-2.438584	-2.087150	1.253982

21	1	-1.603220	-1.727301	-1.862202
22	1	-2.348842	-0.157406	-2.142290
23	1	-0.559287	-1.029694	1.551733
24	1	-0.510204	-2.235590	0.244905
25	1	-0.447883	4.727284	0.174109
26	1	-2.521795	3.918556	-0.963871
27	1	-2.957229	1.519256	-1.142386
28	1	1.164308	3.096661	1.100231
29	1	5.046010	-1.612736	-1.870858
30	1	3.302036	-0.154842	-2.914699
31	1	1.502236	0.808435	-1.570188
32	1	3.123164	-1.110435	1.960697
33	1	4.931043	-2.075132	0.584764
34	1	-4.062433	-1.958710	-1.817673
35	1	-4.191437	-0.753589	-0.533713
36	1	-2.819748	-3.493852	-0.345738
37	1	-4.268687	-2.985760	0.520557
38	1	-2.165628	-2.879390	1.958439
39	1	-2.983124	-1.321907	1.820395

1ap (T1, NMP)

Number	Atomic Number	X	Y	Z
1	6	-2.026631	3.308721	-0.297971
2	6	-2.793628	2.357605	-1.013405
3	6	-2.388685	1.035458	-1.014826
4	6	-1.216917	0.621655	-0.320306
5	6	-0.333276	1.625758	0.276004
6	6	1.028283	1.400594	0.789216
7	8	1.387223	2.085138	1.820554
8	6	-0.845628	2.941453	0.334188
9	6	3.959340	-1.147646	-1.087748
10	6	2.797375	-0.793597	-1.787469
11	6	1.825890	0.013004	-1.195290
12	6	1.979790	0.498604	0.129685
13	6	3.175106	0.149204	0.811096
14	6	4.139092	-0.660667	0.216323
15	6	-1.495402	-1.741154	-1.101692
16	7	-0.971837	-0.728896	-0.174916
17	6	-0.470071	-1.306803	1.084445
18	6	-2.648457	-2.545657	-0.469565
19	6	-2.216307	-3.145463	0.874961
20	6	-1.615973	-2.066950	1.785421

21	1	-0.657049	-2.416020	-1.314420
22	1	-1.780728	-1.265605	-2.038475
23	1	-0.086455	-0.511956	1.718782
24	1	0.347606	-1.992375	0.839903
25	1	-2.348146	4.345819	-0.267343
26	1	-3.711204	2.647828	-1.512700
27	1	-3.032946	0.290745	-1.465917
28	1	-0.235806	3.690220	0.826669
29	1	4.712491	-1.777878	-1.551367
30	1	2.652418	-1.138710	-2.808116
31	1	0.960409	0.299090	-1.783377
32	1	3.321830	0.527137	1.817340
33	1	5.038524	-0.917525	0.770665
34	1	-2.942865	-3.328910	-1.175739
35	1	-3.515386	-1.888840	-0.329927
36	1	-1.472230	-3.934478	0.702233
37	1	-3.072984	-3.618240	1.367526
38	1	-1.208160	-2.506636	2.701966
39	1	-2.387642	-1.347210	2.083876

1aq (S0, NMP)

Number	Atomic Number	X	Y	Z
1	6	-1.732112	3.459975	-0.263297
2	6	-2.566361	2.568706	-0.948340
3	6	-2.314445	1.199033	-0.928669
4	6	-1.197220	0.665507	-0.246545
5	6	-0.308328	1.583286	0.382192
6	6	1.006410	1.204925	0.994272
7	8	1.320412	1.647552	2.104070
8	6	-0.619538	2.954527	0.403627
9	6	3.950531	-1.064066	-1.172555
10	6	2.930758	-0.411611	-1.873968
11	6	1.949672	0.300297	-1.181839
12	6	1.988467	0.379977	0.220256
13	6	3.023562	-0.268140	0.915990
14	6	3.993666	-0.993637	0.224967
15	6	-1.510684	-1.633444	-1.181776
16	7	-0.968322	-0.710544	-0.183644
17	6	-0.664309	-1.393668	1.079114
18	6	-2.697243	-2.432666	-0.639740
19	8	-2.329627	-3.115885	0.564492
20	6	-1.875609	-2.197497	1.563407

21	1	-0.711952	-2.339762	-1.450505
22	1	-1.784650	-1.092270	-2.089082
23	1	-0.394976	-0.669342	1.848841
24	1	0.189670	-2.068138	0.932387
25	1	-1.938991	4.525252	-0.260704
26	1	-3.440508	2.936988	-1.478004
27	1	-3.017563	0.532336	-1.414418
28	1	0.062687	3.626894	0.914945
29	1	4.709187	-1.623229	-1.712370
30	1	2.900121	-0.457232	-2.958432
31	1	1.163041	0.806936	-1.730740
32	1	3.053148	-0.199131	1.998476
33	1	4.782657	-1.500936	0.772081
34	1	-3.003565	-3.202920	-1.352536
35	1	-3.554628	-1.772354	-0.439114
36	1	-1.609670	-2.797069	2.438357
37	1	-2.695347	-1.514582	1.835255

1aq (S1, NMP)

Number	Atomic Number	X	Y	Z
1	6	-0.717494	3.652937	0.100716
2	6	-1.860817	3.184808	-0.567691
3	6	-2.072813	1.826605	-0.694805
4	6	-1.160871	0.886279	-0.129969
5	6	0.019447	1.360923	0.547114
6	6	1.083929	0.473845	1.146997
7	8	0.956436	0.254945	2.416114
8	6	0.195720	2.743099	0.637414
9	6	4.261362	-1.120577	-1.255220
10	6	3.275807	-0.302717	-1.836702
11	6	2.237756	0.223542	-1.076671
12	6	2.134255	-0.042887	0.327592
13	6	3.150437	-0.877033	0.899475
14	6	4.177758	-1.395378	0.123985
15	6	-2.217058	-0.997451	-1.391831
16	7	-1.417719	-0.458810	-0.288720
17	6	-1.094481	-1.483613	0.708768
18	6	-3.491274	-1.674053	-0.853451
19	8	-3.153373	-2.674775	0.096967
20	6	-2.414214	-2.132448	1.182717
21	1	-1.598088	-1.754379	-1.885632
22	1	-2.450638	-0.224082	-2.119060

23	1	-0.579736	-1.044442	1.559393
24	1	-0.460281	-2.241637	0.239103
25	1	-0.539142	4.719217	0.193055
26	1	-2.585173	3.882469	-0.973363
27	1	-2.979459	1.480107	-1.173433
28	1	1.092425	3.110554	1.126116
29	1	5.068313	-1.529189	-1.854991
30	1	3.321578	-0.075361	-2.899328
31	1	1.498055	0.853431	-1.561934
32	1	3.098421	-1.096170	1.960878
33	1	4.931147	-2.024948	0.592649
34	1	-4.013407	-2.168579	-1.673945
35	1	-4.156071	-0.925227	-0.400964
36	1	-2.176285	-2.958255	1.855288
37	1	-3.016824	-1.388481	1.721928

1aq (T1, NMP)

Number	Atomic Number	X	Y	Z
1	6	-2.195955	3.210848	-0.293316
2	6	-2.922146	2.223182	-1.005041
3	6	-2.454613	0.922259	-1.009943
4	6	-1.259103	0.566928	-0.325593
5	6	-0.418515	1.612511	0.265822
6	6	0.952785	1.451476	0.772320
7	8	1.288096	2.160110	1.794344
8	6	-0.995451	2.901888	0.331170
9	6	3.978023	-0.999208	-1.084489
10	6	2.811341	-0.681264	-1.792934
11	6	1.810951	0.094174	-1.206756
12	6	1.940699	0.581282	0.119020
13	6	3.140184	0.270383	0.809272
14	6	4.133703	-0.508431	0.220875
15	6	-1.426817	-1.822845	-1.069784
16	7	-0.936057	-0.768415	-0.181502
17	6	-0.398246	-1.315143	1.072128
18	6	-2.467963	-2.698224	-0.344921
19	8	-1.923469	-3.214664	0.863459
20	6	-1.493271	-2.175044	1.734377
21	1	-0.563316	-2.446240	-1.327368
22	1	-1.826880	-1.398799	-1.988770
23	1	-0.105147	-0.507932	1.739972
24	1	0.471762	-1.936346	0.842844

25	1	-2.567066	4.231146	-0.260647
26	1	-3.855918	2.469566	-1.497602
27	1	-3.066133	0.148949	-1.458652
28	1	-0.420187	3.678622	0.821663
29	1	4.753575	-1.605682	-1.542816
30	1	2.684804	-1.029953	-2.814718
31	1	0.940476	0.354227	-1.799631
32	1	3.266744	0.651228	1.817222
33	1	5.036576	-0.737999	0.781385
34	1	-2.727298	-3.552908	-0.972482
35	1	-3.376264	-2.116514	-0.134768
36	1	-1.081398	-2.654014	2.624954
37	1	-2.342591	-1.540655	2.024259

PTSA (NMP)

Number	Atomic Number	X	Y	Z
1	6	-2.662997	0.159300	-0.181633
2	6	-4.163347	0.314496	-0.204810
3	6	-1.821787	1.199980	-0.604201
4	6	-0.432934	1.070327	-0.564021
5	6	0.117067	-0.125062	-0.096234
6	6	-0.692334	-1.185182	0.326995
7	6	-2.075652	-1.032688	0.278916
8	16	1.887770	-0.298300	-0.015593
9	8	2.260584	0.076249	1.539174
10	8	2.253243	-1.710939	-0.121441
11	8	2.516843	0.702437	-0.884434
12	1	-4.466799	1.176237	-0.804440
13	1	-4.550825	0.459339	0.810861
14	1	-4.647629	-0.578934	-0.611149
15	1	-2.255318	2.124618	-0.973541
16	1	0.207492	1.878285	-0.899495
17	1	-0.250369	-2.111356	0.677121
18	1	-2.709661	-1.854067	0.600339
19	1	2.264653	1.044261	1.657588

PTSA-noH (NMP)

Number	Atomic Number	X	Y	Z
1	6	-2.660605	0.001522	0.013264
2	6	-4.171305	-0.005064	0.003675
3	6	-1.935547	-1.202064	0.003595
4	6	-0.540415	-1.205736	-0.018471

5	6	0.157157	0.006943	-0.033281
6	6	-0.543154	1.214746	-0.018724
7	6	-1.941102	1.205374	0.004129
8	16	1.966434	0.000405	0.001138
9	8	2.390571	1.346831	-0.496362
10	8	2.346573	-0.235897	1.432968
11	8	2.387090	-1.121298	-0.897630
12	1	-4.570482	-0.822284	0.612527
13	1	-4.554909	-0.141898	-1.015139
14	1	-4.576644	0.937021	0.383691
15	1	-2.469627	-2.149005	0.012661
16	1	0.002400	-2.145376	-0.030978
17	1	0.000554	2.153215	-0.031904
18	1	-2.478298	2.150437	0.014009

PhCOOH (NMP)

Number	Atomic Number	X	Y	Z
1	6	1.538583	0.038147	0.032578
2	8	2.277432	0.775801	-0.603415
3	8	2.023870	-0.887549	0.890598
4	6	-2.733348	0.146982	-0.246706
5	6	-1.948389	1.024841	-1.003512
6	6	-0.558543	0.979337	-0.903505
7	6	0.054935	0.053531	-0.044250
8	6	-0.734979	-0.826220	0.714285
9	6	-2.125828	-0.776754	0.610515
10	1	2.994694	-0.827264	0.876541
11	1	-3.815867	0.183157	-0.325078
12	1	-2.419513	1.741631	-1.668847
13	1	0.061565	1.653875	-1.483893
14	1	-0.262995	-1.541045	1.378282
15	1	-2.734617	-1.457471	1.197407

$PhCOO^-$ (NMP)

Number	Atomic Number	X	Y	Z
1	6	1.579539	-0.014854	0.084133
2	8	2.245116	0.822647	-0.593164
3	8	2.056699	-0.899055	0.854491
4	6	-2.753797	0.169093	-0.271665
5	6	-1.948026	1.033852	-1.021152
6	6	-0.556229	0.972557	-0.903855
7	6	0.052916	0.048615	-0.040869

8	6	-0.765005	-0.814226	0.704768
9	6	-2.157482	-0.755875	0.592916
10	1	-3.835765	0.215697	-0.360486
11	1	-2.404103	1.754258	-1.695156
12	1	0.077491	1.639121	-1.479309
13	1	-0.294294	-1.528684	1.371978
14	1	-2.777062	-1.430148	1.178368

CH_3COOH (NMP)

Number	Atomic Number	X	Y	Z
1	6	-0.082166	0.007949	-0.003914
2	6	1.420504	0.009710	-0.011328
3	8	2.129676	0.248255	-0.973675
4	8	1.935871	-0.292670	1.202081
5	1	-0.450964	0.720037	0.740211
6	1	-0.448614	-0.983349	0.279549
7	1	-0.458237	0.273097	-0.991124
8	1	2.906930	-0.277029	1.134199

CH_3COO^- (NMP)

Number	Atomic Number	X	Y	Z
1	6	-0.063146	0.050571	-0.060670
2	6	1.470584	-0.014713	0.061104
3	8	2.157875	0.315809	-0.951043
4	8	1.933086	-0.392832	1.180070
5	1	-0.456480	0.788022	0.648628
6	1	-0.501702	-0.916922	0.207420
7	1	-0.382216	0.324065	-1.069509

H_2O (NMP)

Number	Atomic Number	X	Y	Z
1	8	-0.594866	0.909060	0.019761
2	1	0.371126	0.947084	0.019761
3	1	-0.881479	1.832337	0.019761