Electronic Supplementary Material (ESI) for Green Chemistry.

Supporting information

Catalyst-Free Photoinduced Selective Oxidative C(sp^3)–C(sp^3) bond Cleavage in Arylamines

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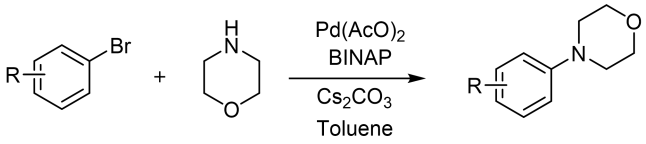
1. General Information

^{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). Chemical shifts of carbon were referenced to the carbon resonances of the solvent ($CDCl_3$: δ 77.0). 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. Substrates of **1a-5a**, **13a**, **16a**, **21a**, **24a-28a**, **30a-33a**, **43a** and **51a** were purchased from *J&K* in analysis pure. Substrates of **39a-42a** were purchased from DOW in analysis pure.

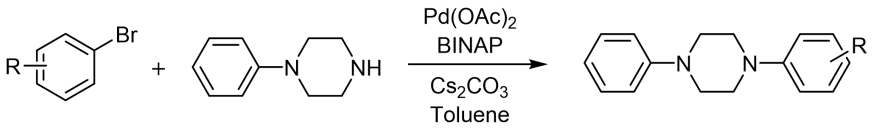
2. General Procedures

2.1 Typical procedure for the preparation of substrates **7a-9a**, **11a**, **14a-15a**, **17a-20a**, **22a-23a**, **29a and 34a-38a**.



The compound was synthesized according to a known procedure.[1] To a solution of potassium carbonate (1.95 g, 6.0 mmol) in toluene (10 mL), 1-bromo-2-methylbenzene (513 mg, 3.0 mmol), $Pd(AcO)_2$ (37 mg, 0.15 mmol), BINAP (186 mg, 0.3 mmol) and morpholine (392 mg, 4.5 mmol) were added in sequence. The reaction mixture was stirred at 100 °C for 15 h. Then, toluene was removed through vacuum distillation. And the crude production was purified by flash chromatography to give a yellow oil **14a** (318 mg, yield: 60%).

2.2 Typical procedure for the preparation of substrates **44a-49a**.

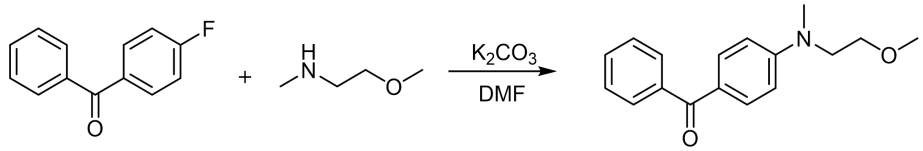


The compound was synthesized according to a known procedure.[1] To a solution of potassium carbonate (1.95 g, 6.0 mmol) in toluene (10 mL), 1-bromo-4-methylbenzene (513 mg, 3.0 mmol), $Pd(AcO)_2$ (37 mg, 0.15 mmol), BINAP (186 mg, 0.3 mmol) and 1-phenylpiperazine (729 mg, 4.5 mmol) were added in sequence. The reaction mixture was stirred at 100 °C for 15 h. Then, toluene was removed through vacuum distillation. And the crude production was purified by flash chromatography to give a white solid **44a** (567 mg, yield: 75%).

2.3 Typical procedure for the preparation of substrates **6a** and **50a**.

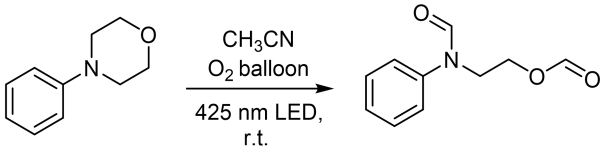
The compound was synthesized according to a known procedure.[2] To a solution of 1-phenylpiperazine (810 mg, 5 mmol) in DCM (15 mL), Acetyl chloride (785 mg, 10 mmol) was added dropwise at 0 °C. Two hours later, the reaction mixture was allowed to continue stirring at room temperature for 8h. Then, the crude production was purified through recrystallization to give a white solid **50a** (714 mg, yield: 70%).

2.4 Typical procedure for the preparation of substrates **10a** and **12a**.



The compound was synthesized according to the similar procedures.[3] To a solution of 4-fluorobenzophenone (600 mg, 3 mmol) in DMF (10 mL) was added (2-methoxyethyl)methylamine (405 mg, 4.5 mmol), K_2CO_3 (621 mg, 4.5 mmol). The reaction mixture was allowed to stir at 100 °C for 15h. Then, DMF was removed through vacuum distillation. And the crude production was purified by flash chromatography, giving a yellow oil **10a** (485 mg, yield: 60%).

2.5 Typical procedure for oxidative C(sp^3)–C(sp^3) bond cleavage.



4-phenylmorpholine **13a** (48.9 mg, 0.3 mmol) was added to 10 mL quartz tube containing 2 mL CH_3CN, the reaction mixture was stirred and irradiated using a 10 W 425 nm LED lamp (WATTCAS: WP-TEC-1020HSL) at room temperature under O_2 atmosphere condition for 48 h. Then, the crude product was purified by flash chromatography to give a colourless oil **13b** (55 mg, yield: 95%).

3. Computational Method

All the calculations were carried out in Gaussian09 package[4] by employing the density-functional theory (DFT) method[5]. For geometry optimization, all the structures including ground states (**a**, **1**, **2**, **3**, **4**, **5**, **6**, **pre_b**, **b**, **c** and **d**), excited states (**a***) and transition states (**1_TS_2**, **3_TS_4**, **4_TS_pre_b**, **3_TS_c**, **1_TS_5** and **5_TS_6**) were performed at B3LYP method[6] with cc-PVTZ basis set[7]. For vibration frequency calculation, same computational method was carried out to make sure that the optimized structures were true energy minima, and obtained the absolute free energies of the optimized molecules. All the calculations considered the solvation effect (CH_3CN) provided by the PCM solvent continuum models.[8]

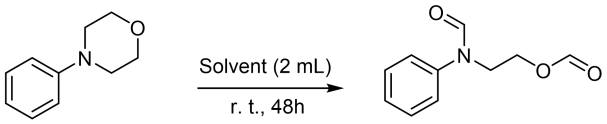
4. Reaction Condition Optimization (Tables S1-S2 and Figure S1)

A morpholine arylamine substrate (**13a**) was chosen to initiate the reaction condition optimization (Table S1). We first screened a series of solvents under operationally simple (425 nm LED and 1 bar oxygen atmosphere) and very mild (room temperature and 48 h reaction time) photochemical reaction conditions (entries 1-12). Except that in CH_3COCH_3 and DMSO only trace amounts of oxidative cleavage product (**13b**) were detected, in all other tested solvents it yielded measurable amounts of oxidative cleavage product (**13b**), such as CH_3OH, CH_3CH_2OH, Toluene, DMF, THF, DMA, DCE, Dioxane, NMP and CH_3CN. In particular, in NMP and CH_3CN solvents, the yields were the highest (65% in NMP and 95% in CH_3CN). We then explored the influence of visible light using the determined NMP and CH_3CN solvents (entries 13-20). Obviously, oxidative cleavage reaction was likely to present the best effect under the specific 425 nm LED. Under the specific light close to 425 nm, such as 405 nm and 365 nm, it also yielded oxidative cleavage product (**13b**) with good yield, especially under 405 nm, its yield was almost equal to that under 425 nm. However, under the specific light far away from 425 nm, it hardly occurred (avoided light, 254 nm and 570 nm). At the same time, we also tested the quantum yield of our oxidative cleavage reaction under different light sources. The results as shown in Table S2 also showed that our oxidative cleavage reaction had the best quantum yield under the light around 425 nm, indicating the specificity of 425 nm to our oxidative cleavage reaction. Surprisingly, a completely acceptable yield was obtained under the widespread sunlight (70%). We finally investigated the influence of oxygen atmosphere (entries 21-22). It revealed that when the oxygen atmosphere was replaced by air atmosphere which could still maintain the oxygen atmosphere to some extent, the yield of oxidative cleavage product (**13b**) would only have a small decrease and still high to 72% which was also an excellent yield. However, once the oxygen atmosphere was completely destroyed and replaced by anoxic environment (nitrogen atmosphere), the oxidative cleavage would hardly occur. To sum up, the following optimized reaction conditions were employed in our catalyst-free photoinduced oxidative cleavage of C(sp^3)–C(sp^3) bond: 0.3 mmol substrate, 425 nm LED, 1 bar O_2, room temperature, 2 mL CH_3CN solvent and 48 h reaction time. Meanwhile, we also investigated the influence of radical scavengers (BHT and TEMPO) on our oxidative cleavage reaction (entries 23-24). It revealed that the oxidative cleavage could be inhibited by the radical scavengers, implicating some radical intermediates formed during our oxidative cleavage reaction.

UV absorption spectra to some extent could explain why NMP and CH_3CN solvents had the better performance than other solvents. As shown in Figure S1a, in NMP and CH_3CN solvents, in addition to the main absorption peak near 340 nm, the morpholine arylamine substrate (**13a**) also had a certain absorption near 425 nm. Moreover, as the concentration of the substrate **(13a)** increased, the absorption intensity at 425nm was also increasing (Figure S1b). While in other solvents

(CH_3COCH_3, DMSO, CH_3OH, CH_3CH_2OH, Toluene, DMF, THF, DMA, DCE and Dioxane), there was only a main absorption peak near 340 nm and at 425 nm, there was almost no absorption. To sum up, that our oxidative cleavage reaction was likely to occur under the light around 425 nm and only in NMP and CH_3CN solvents the substrate (**13a**) had stronger absorption around 425 nm, determined the best performance of NMP and CH_3CN solvents.

Table S1. Reaction conditions optimization for substrate **13a**.



13a (0.3 mmol) **13b**

Entry	Solvent	Additive	Light source	Isolated Yield
1	CH_3COCH_3	O_2	425 nm	trace
2	DMSO	O_2	425 nm	trace
3	CH_3OH	O_2	425 nm	10%
4	CH_3CH_2OH	O_2	425 nm	10%
5	Toluene	O_2	425 nm	25%
6	DMF	O_2	425 nm	27%
7	THF	O_2	425 nm	30%
8	DMA	O_2	425 nm	30%
9	DCE	O_2	425 nm	40%
10	Dioxane	O_2	425 nm	47%
11	NMP	O_2	425 nm	65%
12	***CH_3CN***	***O_2***	***425 nm***	***95%***
13	NMP	O_2	405 nm	60%
14	CH_3CN	O_2	405 nm	93%
15	CH_3CN	O_2	avoided light (72 h)	-
16	CH_3CN	O_2	avoided light (72 h, 60°C)	-
17	CH_3CN	O_2	254 nm	-
18	CH_3CN	O_2	365 nm	45%
19	CH_3CN	O_2	570 nm	-
20	CH_3CN	O_2	sunlight	70%
21	CH_3CN	air	425 nm	72%
22	CH_3CN	N_2	425 nm	-
23	CH_3CN	O_2	425 nm (0.3 mmol BHT)	10%
24	CH_3CN	O_2	425 nm (0.3 mmol TEMPO)	-

Optimized reaction conditions: 0.3 mmol substrate, 425 nm LED, 1 bar O_2, room temperature, 2 mL CH_3CN solvent and 48 h reaction time.

Table S2. Quantum yield of oxidative cleavage reaction under different light sources.

Entry	Substrate	Solvent	Light source	Quantum Yield
1	**13a**	CH_3CN	570 nm	-
2	**13a**	CH_3CN	425 nm	0.160
3	**13a**	CH_3CN	405 nm	0.100
4	**13a**	CH_3CN	365 nm	0.035
5	**13a**	CH_3CN	254 nm	-

The quantum yield was measured under the optimized reaction conditions, and calculated according the following formula[9-10]: Quantum yield = [number of formed products (mol)] / [number of incident photons (mol)] * 100%.

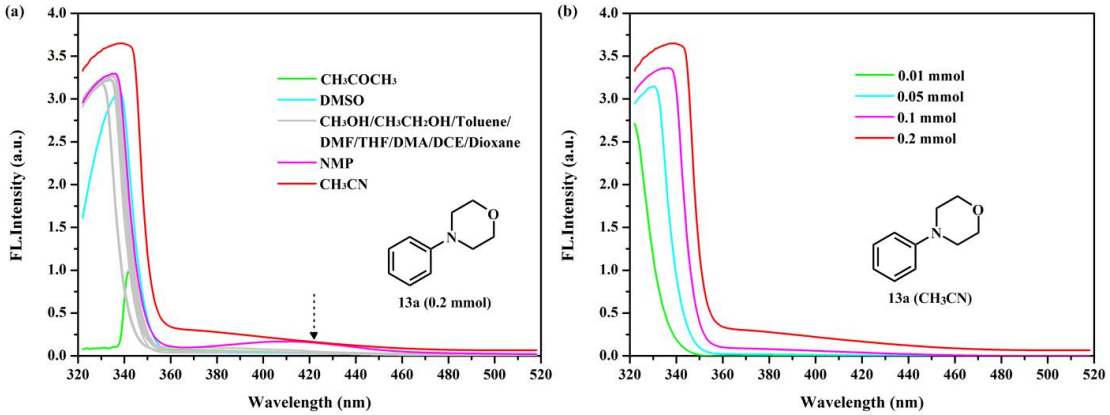
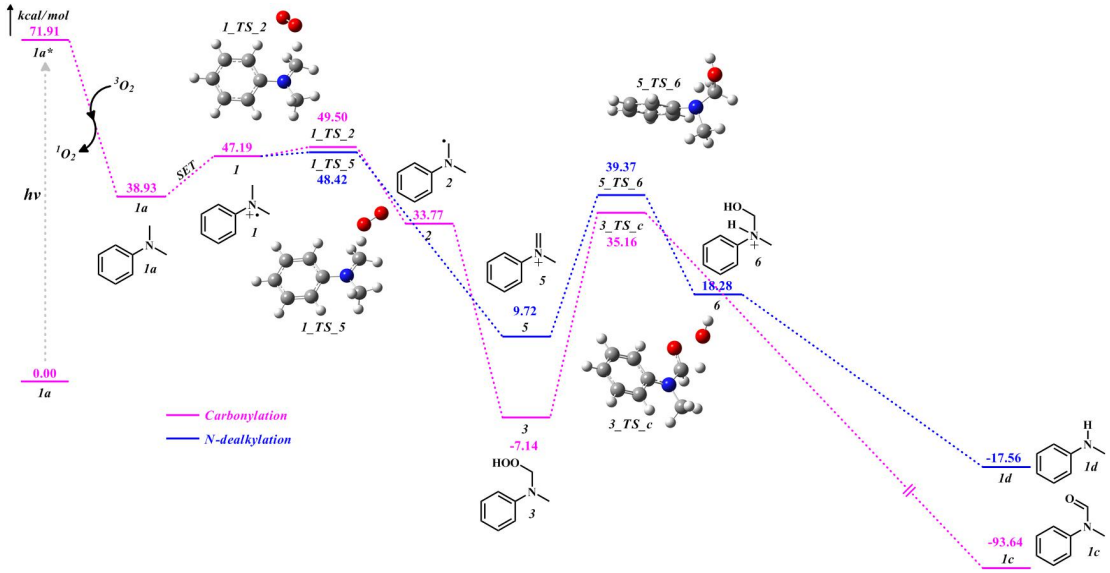
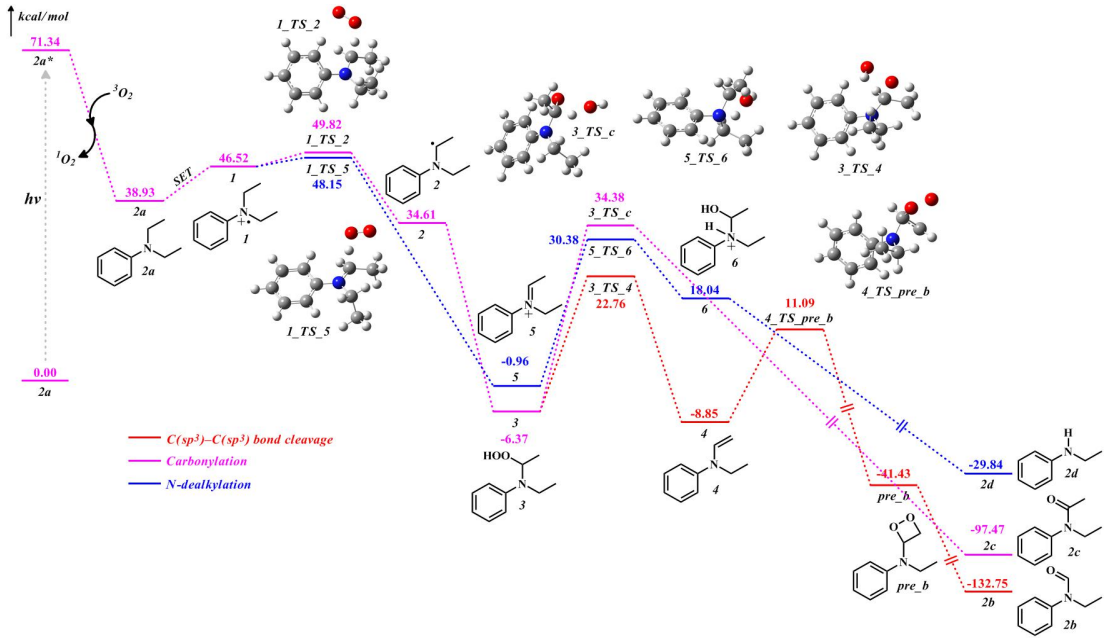


Figure S1. (a) UV absorption spectra of substrate **13a** in different solvents. (b) UV absorption spectra of different concentrations of substrate **13a**.

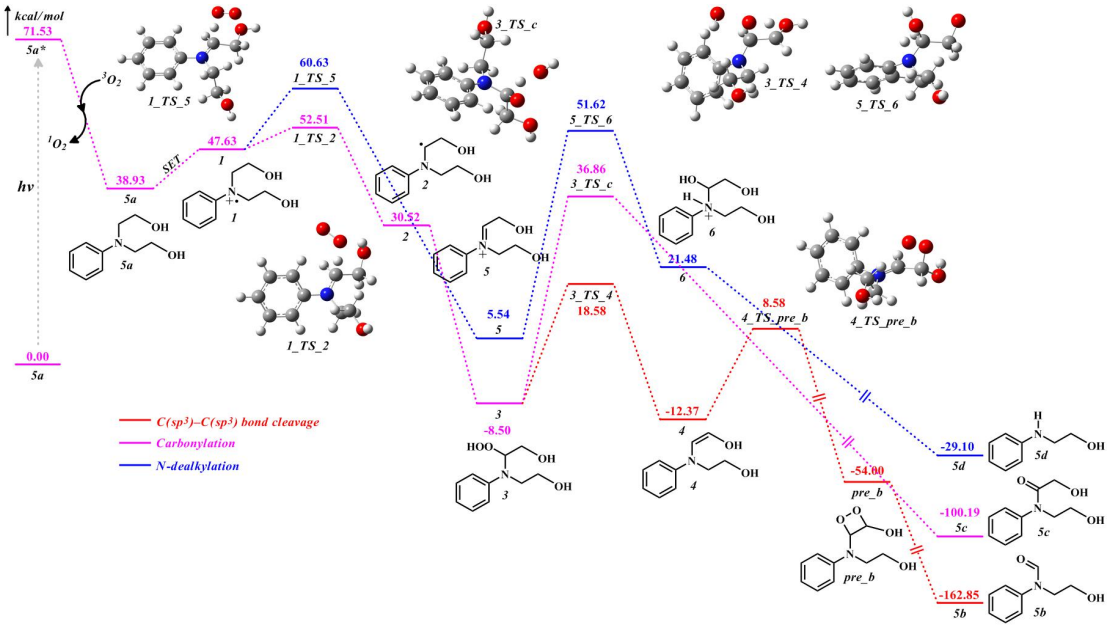
5. Mechanism studies (Figures S2-S8)



Figures S2. Reaction profiles of **1a** based on the mechanisms (carbonylation and N-dealkylation) in Figure 1d. **1_TS_2**, **1_TS_5**, **3_TS_c** and **5_TS_6** were the transition states of proton transfer, HAT, dehydration and hydrolysis reactions, respectively. And dehydration and hydrolysis reactions were the rate-limiting steps of carbonylation and N-dealkylation, respectively.

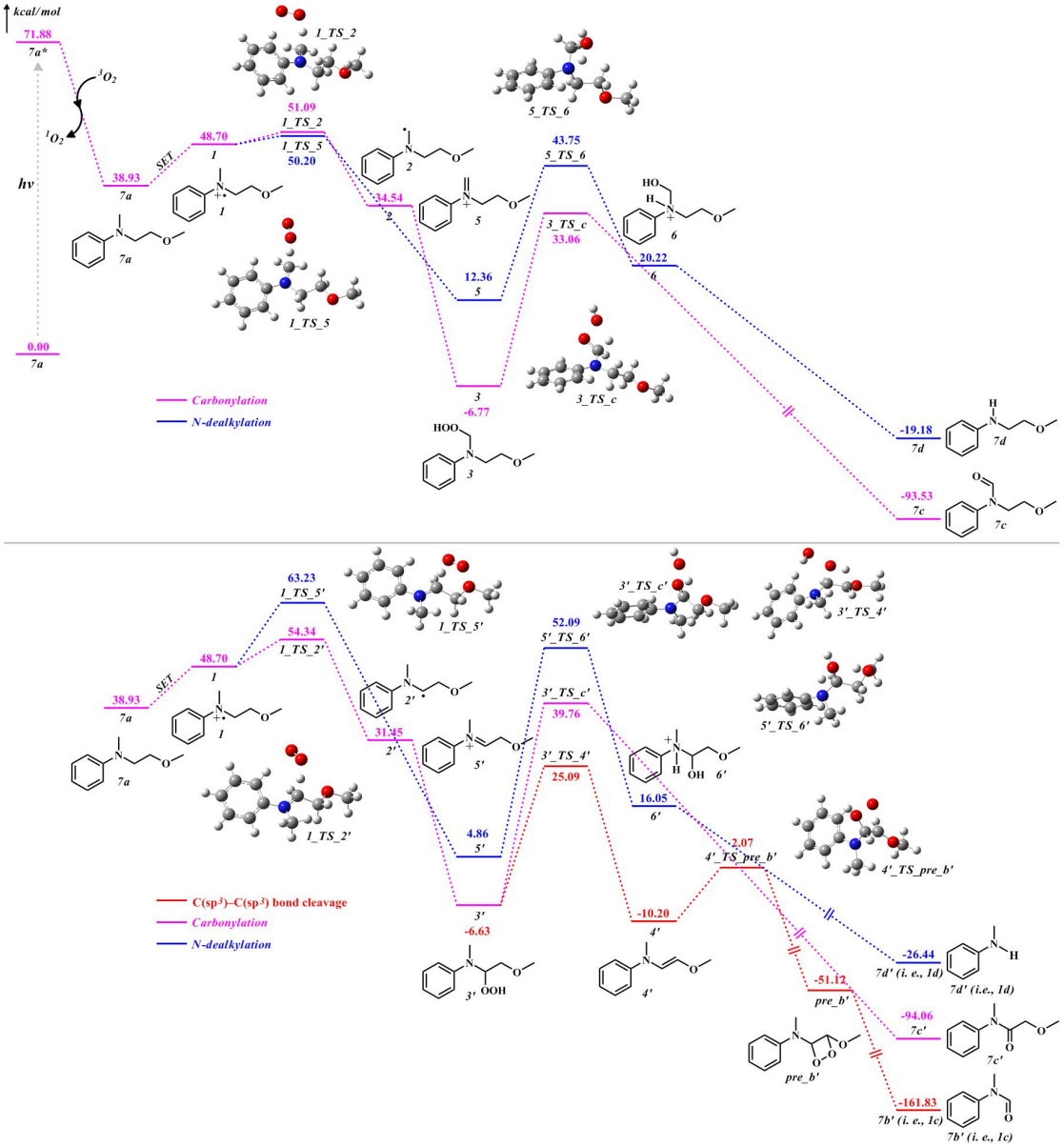


Figures S3. Reaction profiles of **2a** based on the mechanisms (C(sp^3)–C(sp^3) bond cleavage, carbonylation and N-dealkylation) in Figure 1d. **1_TS_2**, **1_TS_5**, **3_TS_4**, **3_TS_c**, **4_TS_pre_b** and **5_TS_6** were the transition states of proton transfer, HAT, dehydroperoxide, dehydration, 1, 2-addition and hydrolysis reactions, respectively. And dehydroperoxide, dehydration and hydrolysis reactions were the rate-limiting steps of C(sp^3)–C(sp^3) bond cleavage, carbonylation and N-dealkylation, respectively.

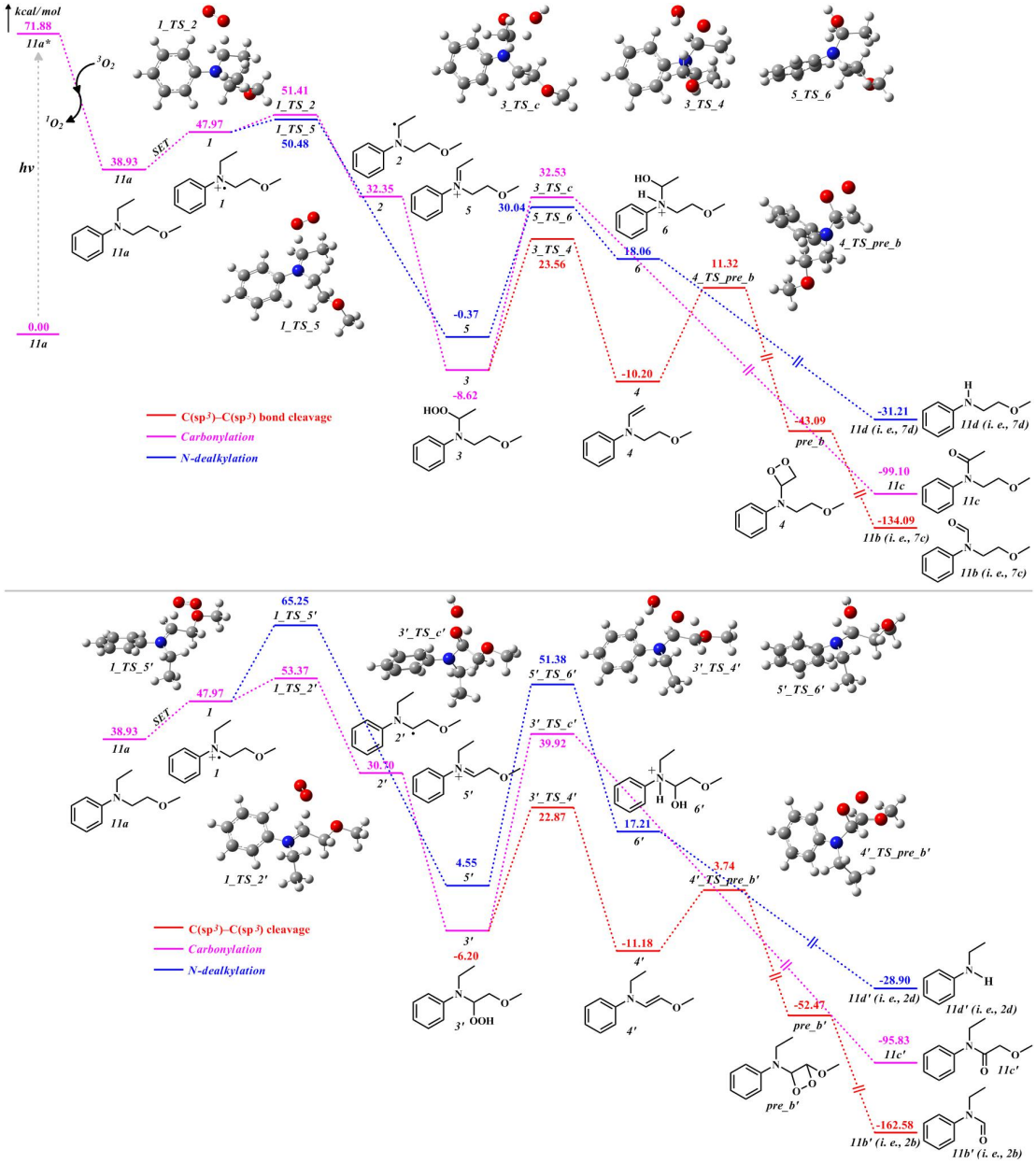


Figures S4. Reaction profiles of **5a** based on the mechanisms (C(sp^3)–C(sp^3) bond cleavage, carbonylation and N-dealkylation) in Figure 1d. **1_TS_2**, **1_TS_5**, **3_TS_4**, **3_TS_c**, **4_TS_pre_b** and **5_TS_6** were the transition states of proton transfer, HAT, dehydroperoxide, dehydration, 1, 2-addition and hydrolysis reactions, respectively. And dehydroperoxide, dehydration and hydrolysis reactions were the rate-limiting

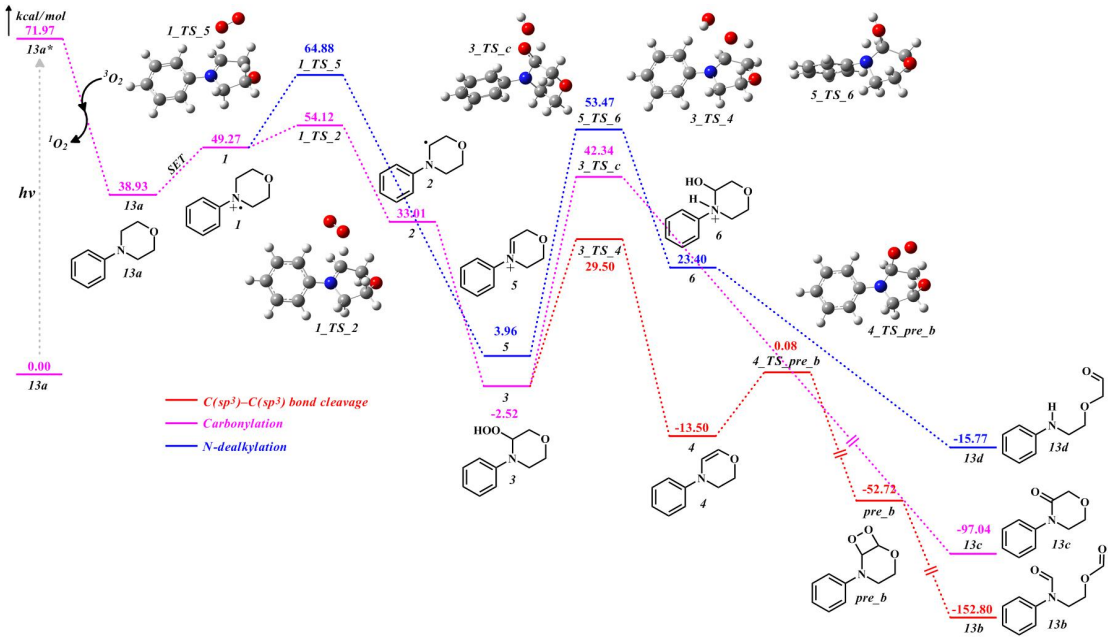
steps of C(sp^3)–C(sp^3) bond cleavage, carbonylation and N-dealkylation, respectively.



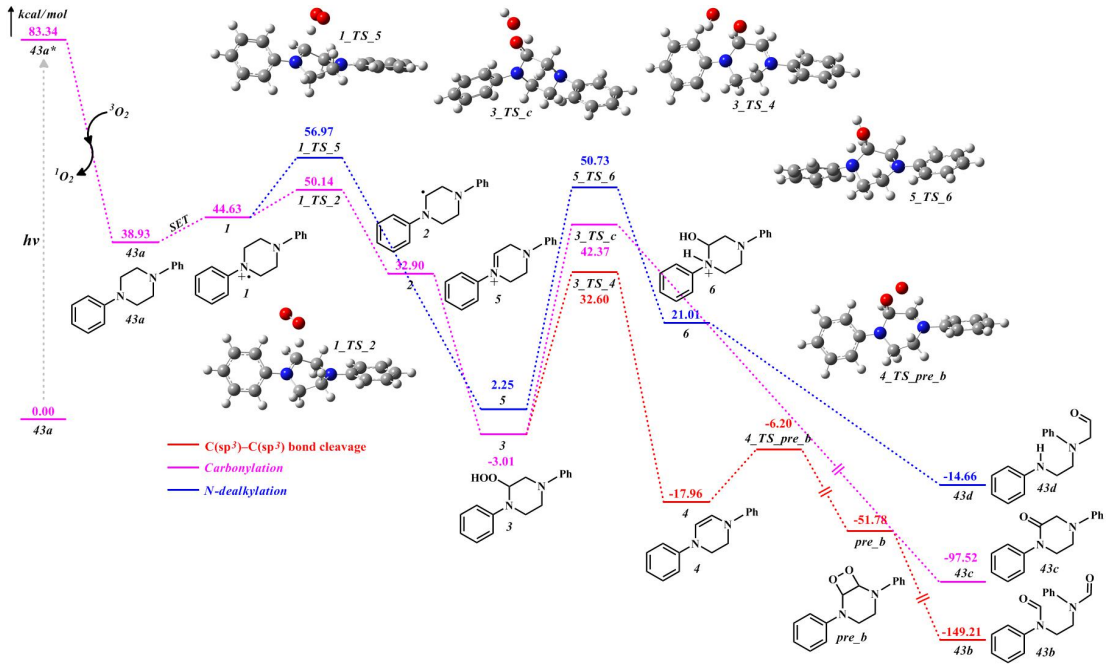
Figures S5. Reaction profiles of **7a** based on the mechanisms (C(sp^3)–C(sp^3) bond cleavage, carbonylation and N-dealkylation) in Figure 1d. The upper figure referred to the reaction profiles that occurred on the N-methyl group and the lower figure referred to the reaction profiles that occurred on the N-methoxyethyl group. **1_TS_2** (**1_TS_2'**), **1_TS_5** (**1_TS_5'**), **3'_TS_4'**, **3_TS_c** (**3'_TS_c'**), **4'_TS_pre_b'** and **5_TS_6** (**5'_TS_6'**) were the transition states of proton transfer, HAT, dehydroperoxide, dehydration, 1, 2-addition and hydrolysis reactions, respectively. And dehydroperoxide, dehydration and hydrolysis reactions were the rate-limiting steps of C(sp^3)–C(sp^3) bond cleavage, carbonylation and N-dealkylation, respectively.



Figures S6. Reaction profiles of **11a** based on the mechanisms (C(sp^3)–C(sp^3) bond cleavage, carbonylation and N-dealkylation) in Figure 1d. The upper figure referred to the reaction profiles that occurred on the N-methyl group and the lower figure referred to the reaction profiles that occurred on the N-methoxyethyl group. **1_TS_2** (**1_TS_2'**), **1_TS_5** (**1_TS_5'**), **3_TS_4** (**3'_TS_4'**), **3_TS_c** (**3'_TS_c'**), **4_TS_pre_b** (**4'_TS_pre_b'**) and **5_TS_6** (**5'_TS_6'**) were the transition states of proton transfer, HAT, dehydroperoxide, dehydration, 1, 2-addition and hydrolysis reactions, respectively. And dehydroperoxide, dehydration and hydrolysis reactions were the rate-limiting steps of C(sp^3)–C(sp^3) bond cleavage, carbonylation and N-dealkylation, respectively.



Figures S7. Reaction profiles of **13a** based on the mechanisms (C(sp^3)–C(sp^3) bond cleavage, carbonylation and N-dealkylation) in Figure 1d. **1_TS_2**, **1_TS_5**, **3_TS_4**, **3_TS_c**, **4_TS_pre_b** and **5_TS_6** were the transition states of proton transfer, HAT, dehydroperoxide, dehydration, 1, 2-addition and hydrolysis reactions, respectively. And dehydroperoxide, dehydration and hydrolysis reactions were the rate-limiting steps of C(sp^3)–C(sp^3) bond cleavage, carbonylation and N-dealkylation, respectively.



Figures S8. Reaction profiles of **43a** based on the mechanisms (C(sp^3)–C(sp^3) bond cleavage, carbonylation and N-dealkylation) in Figure 1d. **1_TS_2**, **1_TS_5**, **3_TS_4**, **3_TS_c**, **4_TS_pre_b** and **5_TS_6** were the transition states of proton transfer, HAT, dehydroperoxide, dehydration, 1, 2-addition and hydrolysis reactions, respectively.

And dehydroperoxide, dehydration and hydrolysis reactions were the rate-limiting steps of C(sp^3)–C(sp^3) bond cleavage, carbonylation and N-dealkylation, respectively.

6. ESR Spectra (Figure S9)

In order to determine whether the substrate itself acted as the photosensitizer to excite the conversion of triplet oxygen ($^3O_2$) to singlet oxygen ($^1O_2$), ESR experiments were employed to look for the traces of $^1O_2$. Our oxidative cleavage reaction only involved solvent (CH_3CN or NMP), UV light irradiation, $^3O_2$ and substrate, and no external photocatalysts or auxiliary agents were involved, therefore, if we captured the $^1O_2$, then we can confirm that to some extent the occurrence of this $^1O_2$ was likely to be related to the substrate. In our ESR experiments TEMP was used to trap $^1O_2$. As shown in Figure S9a, for the case of no substrate and the case of no UV light irradiation, in both there was only a very weak characteristic signal of the $^1O_2$ adduct with TEMP. However, a strong characteristic signal of the $^1O_2$ adduct with TEMP was observed in the presence of both substrate (**13a**) and UV light irradiation, and a series of stronger characteristic signals were collected with prolonged time. Obviously, from the above described ESR spectra, we can see that during our oxidation cleavage reaction, a $^1O_2$ was produced and this $^1O_2$ was very likely to be converted from $^3O_2$ by the photosensitizer effect of substrate.

In order to determine the active species of oxygen involved in our oxidative cleavage reaction, besides the determination of singlet oxygen species ($^1O_2$), we also employed the ESR experiments to determine the superoxide radical ($O_2^{\bullet-}$). DMPO was employed to capture $O_2^{\bullet-}$. As shown in Figure S9b, similar to the determination results of $^1O_2$, only in the presence of both substrate (**13a**) and UV light irradiation, a stronger characteristic signal of the $O_2^{\bullet-}$ adduct with DMPO was observed, and a series of stronger characteristic signals were collected with prolonged tome. Therefore, during our oxidative cleavage reaction $O_2^{\bullet-}$ coexisted with $^1O_2$, which further supported our proposed mechanism in Figure 1d.

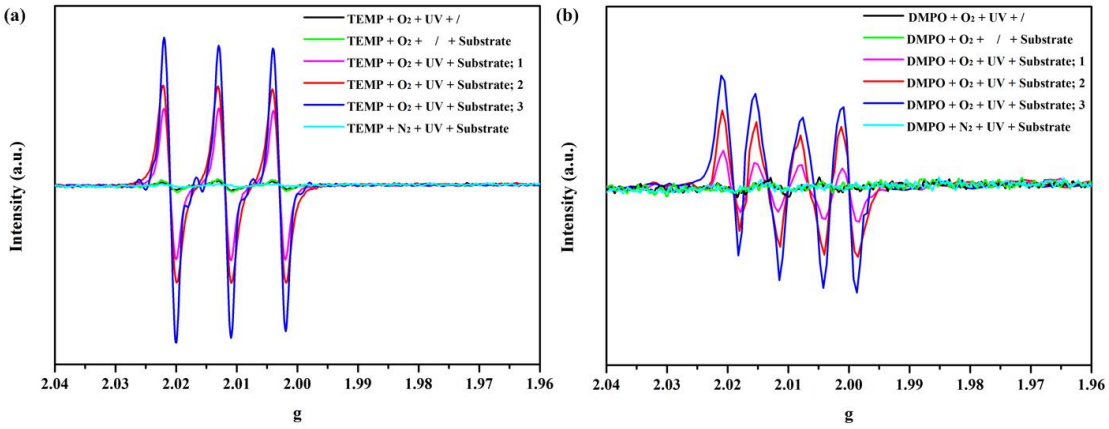


Figure S9. (a) Determination of singlet oxygen species ($^1O_2$) via the ESP experiments. (b) Determination of superoxide radical ($O_2^{\bullet-}$) via the ESR experiments. TEMP =

2,2,6,6-tetramethylpiperidine, DMPO = 5,5-dimethyl-pyrroline-N-oxide. After 5 h reaction time for each reaction, TEMP and DMPO were added to capture $^1O_2$ and $O_2^{\bullet-}$, respectively. ESR spectrum was measured 1-5 min after the TEMP/DMPO was added.

Figure S9a:

TEMP + O_2 + UV + /: a solution of TEMP (0.3 mmol) added in NMP solvent without substrate under O_2 atmosphere and 425 nm light irradiation. ESR spectrum was measured 5 min after the TEMP was added.

TEMP + O_2 + / + Substrate: a solution of TEMP (0.3 mmol) added in NMP solvent containing substrate (**13a**) under O_2 atmosphere and without UV irradiation. ESR spectrum was measured 5 min after the TEMP was added.

TEMP + O_2 + UV + Substrate; 1: a solution of TEMP (0.3 mmol) added in NMP solvent containing substrate (**13a**) under O_2 atmosphere and 425 nm light irradiation. ESR spectrum was measured 1 min after the TEMP was added.

TEMP + O_2 + UV + Substrate; 2: a solution of TEMP (0.3 mmol) added in NMP solvent containing substrate (**13a**) under O_2 atmosphere and 425 nm light irradiation. ESR spectrum was measured 3 min after the TEMP was added.

TEMP + O_2 + UV + Substrate; 3: a solution of TEMP (0.3 mmol) added in NMP solvent containing substrate (**13a**) under O_2 atmosphere and 425 nm light irradiation. ESR spectrum was measured 5 min after the TEMP was added.

TEMP + N_2 + UV + Substrate: a solution of TEMP (0.3 mmol) added in NMP solvent containing substrate (**13a**) under N_2 atmosphere and 425 nm light irradiation. ESR spectrum was measured 5 min after the TEMP was added.

Figure S9b:

DMPO + O_2 + UV + /: a solution of DMPO (0.3 mmol) added in NMP solvent without substrate under O_2 atmosphere and 425 nm light irradiation. ESR spectrum was measured 5 min after the DMPO was added.

DMPO + O_2 + / + Substrate: a solution of DMPO (0.3 mmol) added in NMP solvent containing substrate (**13a**) under O_2 atmosphere and without UV irradiation. ESR spectrum was measured 5 min after the DMPO was added.

DMPO + O_2 + UV + Substrate; 1: a solution of DMPO (0.3 mmol) added in NMP solvent containing substrate (**13a**) under O_2 atmosphere and 425 nm light irradiation. ESR spectrum was measured 1 min after the DMPO was added.

DMPO + O_2 + UV + Substrate; 2: a solution of DMPO (0.3 mmol) added in NMP solvent containing substrate (**13a**) under O_2 atmosphere and 425 nm light irradiation. ESR spectrum was measured 3 min after the DMPO was added.

DMPO + O_2 + UV + Substrate; 3: a solution of DMPO (0.3 mmol) added in NMP solvent containing substrate (**13a**) under O_2 atmosphere and 425 nm light irradiation. ESR spectrum was measured 5 min after the DMPO was added.

DMPO+ N_2 + UV + Substrate: a solution of DMPO (0.3 mmol) added in NMP solvent containing substrate (**13a**) under N_2 atmosphere and 425 nm light irradiation. ESR spectrum was measured 5 min after the DMPO was added.

7. Verification Experiments (Figure S10)

As a well-known photocatalyst, $[Ru(bpy)_3]Cl_2•6H_2O$ is able to rapidly convert the triplet $^3O_2$ to the singlet $^1O_2$ under the UV irradiation. Thus, 1.0 mol% $[Ru(bpy)_3]Cl_2•6H_2O$ was added to the oxidative cleavage reaction of substrate (**43a**) to expect to accelerate the reaction rate (or shorten the reaction time). Unsurprisingly, as shown in Figure S10, it also improve the yield of cleavage product (**43b**) in addition to improvement of reaction rate. Obviously, this result indicated the positive effect of the $^1O_2$-generating photosensitizer. And to some extent it is thought that in the absence of an external photosensitizer, the substrate molecule is likely to act as a photosensitizer to convert the triplet $^3O_2$ to the singlet $^1O_2$ which subsequently could trigger the following oxidative cleavage reaction.

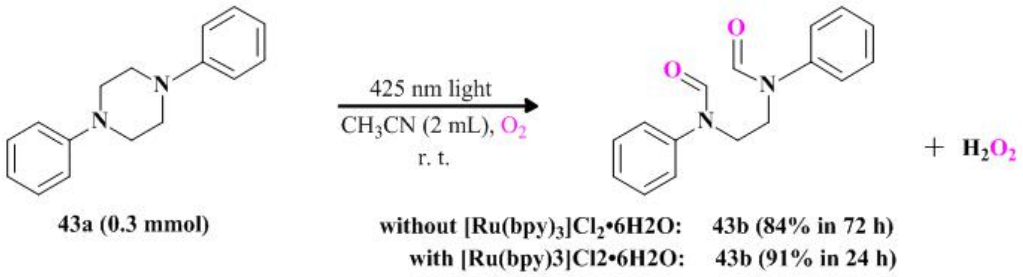


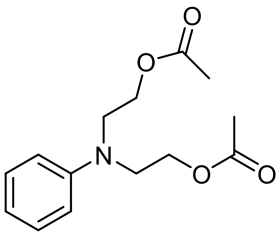
Figure S10. Verification experiments to further verify the photosensitizer effect of substrate.

8. Characterization Data

8.1 Characterizations of substrates **7a**, **15a**, **19a**, **22a-23a**, **29a** and **36a** have been reported in the Supporting Information of our previous reported literature.[11]

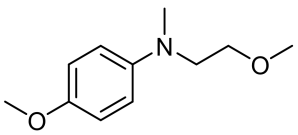
8.2 Characterizations of substrates **6a**, **8a-12a**, **14a**, **17a-18a**, **20a**, **34a-35a**, **37a-38a** and **44a-50a**.

(phenylazanediyl)bis(ethane-2,1-diyl) diacetate (6a)



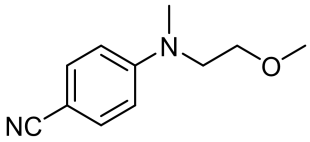
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.27 (t, *J* = 7.8 Hz, 2H), 6.93–6.87 (m, 3H), 3.75 (t, *J* = 5.2 Hz, 2H), 3.59 (t, *J* = 5.2 Hz, 2H), 3.17–3.11 (m, 4H), 2.12 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 169.02, 150.96, 129.26, 120.54, 116.66, 49.68, 49.35, 46.23, 41.35, 21.40. **HRMS** (ESI) calculated for $C_{14}H_{20}NO_4$ $(M+H)^+$: 266.1387, found: 266.1395.

4-methoxy-*N*-(2-methoxyethyl)-*N*-methylaniline (8a)



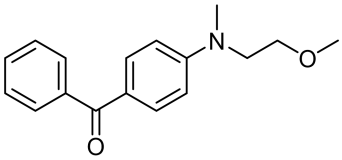
Yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 6.76 (d, *J* = 9.0 Hz, 2H), 6.66 (d, *J* = 9.0 Hz, 2H), 3.68 (s, 3H), 3.47 (t, *J* = 6.0 Hz, 2H), 3.35 (t, *J* = 6.0 Hz, 2H), 3.29 (s, 3H), 2.83 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 150.74, 143.43, 113.71, 113.51, 69.29, 57.99, 54.76, 52.72, 38.54. **HRMS** (ESI) calculated for $C_{11}H_{18}NO_2$ $(M+H)^+$: 196.1332, found: 196.1338.

4-((2-methoxyethyl)(methyl)amino)benzonitrile (9a)



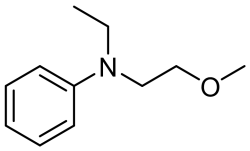
Yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.50–7.38 (m, 2H), 6.74–6.60 (m, 2H), 3.56 (d, *J* = 2.5 Hz, 4H), 3.35 (s, 3H), 3.04 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 151.71, 133.47, 120.69, 111.46, 97.40, 69.95, 59.14, 51.94, 38.92. **HRMS** (ESI) calculated for $C_{11}H_{15}N_2O$ $(M+H)^+$: 191.1179, found: 191.1185.

(4-((2-methoxyethyl)(methyl)amino)phenyl)(phenyl)methanone (10a)



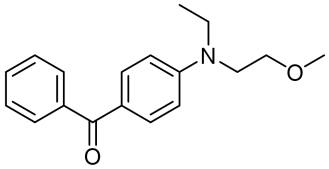
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.79 (t, *J* = 2.4 Hz, 1H), 7.77 (t, *J* = 4.4 Hz, 1H), 7.73 (t, *J* = 2.4 Hz, 1H), 7.71 (t, *J* = 2.4 Hz, 1H), 7.54–7.48 (m, 1H), 7.47–7.40 (m, 2H), 6.69 (d, *J* = 9.2 Hz, 2H), 3.66–3.54 (m, 4H), 3.35 (s, 3H), 3.08 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 195.10, 152.42, 139.27, 132.87, 131.15, 129.46, 128.03, 124.82, 110.54, 70.06, 59.15, 52.01, 39.14. **HRMS** (ESI) calculated for $C_{17}H_{20}NO_2$ $(M+H)^+$: 270.1489, found: 270.1495.

***N*-ethyl-*N*-(2-methoxyethyl)aniline (11a)**



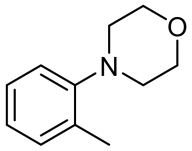
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.24 (d, *J* = 7.2 Hz, 1H), δ 7.21 (d, *J* = 7.2 Hz, 1H), 6.70 (d, *J* = 8.0 Hz, 2H), 6.66 (t, *J* = 7.2 Hz, 1H), 3.58–3.52 (m, 2H), 3.51–3.46 (m, 2H), 3.41 (q, *J* = 7.2 Hz, 2H), 3.37 (s, 3H), 1.15 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 147.81, 129.30, 115.74, 111.80, 70.42, 59.06, 50.00, 45.39, 12.09. **HRMS** (ESI) calculated for $C_{11}H_{18}NO$ $(M+H)^+$: 180.1383, found: 180.1390.

(4-(ethyl(2-methoxyethyl)amino)phenyl)(phenyl)methanone (12a)



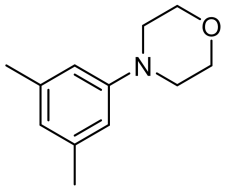
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 9.2 Hz, 2H), 7.72 (dd, *J* = 8.0, 1.2 Hz, 2H), 7.52 (t, *J* = 7.2 Hz, 1H), 7.44 (t, *J* = 7.2 Hz, 2H), 6.68 (d, *J* = 9.2 Hz, 2H), 3.57 (s, 4H), 3.50 (q, *J* = 7.2 Hz, 2H), 3.37 (s, 3H), 1.20 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 194.95, 151.29, 139.33, 133.03, 131.08, 129.42, 128.01, 124.49, 110.33, 70.18, 59.14, 50.01, 45.68, 12.04. **HRMS** (ESI) calculated for $C_{18}H_{22}NO_2$ $(M+H)^+$: 284.1645, found: 284.1652.

4-(*o*-tolyl)morpholine (14a)



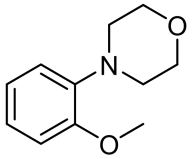
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.17 (t, *J* = 7.0 Hz, 2H), 7.06–6.94 (m, 2H), 3.89–3.77 (m, 4H), 2.96–2.83 (m, 4H), 2.31 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 151.31, 132.65, 131.21, 126.70, 123.44, 118.98, 67.49, 52.28, 17.91. **HRMS** (ESI) calculated for $C_{11}H_{16}NO$ $(M+H)^+$: 178.1227, found: 178.1230.

4-(3,5-dimethylphenyl)morpholine (17a)



Colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 6.53 (s, 3H), 3.88–3.70 (m, 4H), 3.16–3.00 (m, 4H), 2.27 (s, 6H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 151.57, 138.74, 122.09, 113.83, 67.07, 49.66, 21.76. HRMS (ESI) calculated for $C_{12}H_{18}NO$ $(M+H)^+$: 192.1383, found: 192.1386.

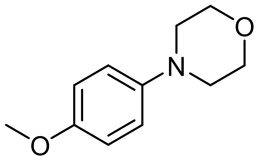
4-(2-methoxyphenyl)morpholine (18a)



Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.06–6.99 (m, 1H), 6.93 (d, *J* = 4.2 Hz, 2H), 6.88 (d, *J* = 7.8 Hz, 1H), 3.93–3.88 (m, 4H), 3.87 (s, 3H), 3.12–3.01 (m, 4H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 152.27, 141.13, 123.18, 121.06, 118.03, 111.32, 67.23,

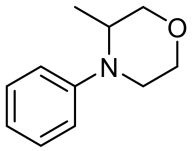
55.38, 51.18. **HRMS** (ESI) calculated for $C_{11}H_{16}NO_2$ $(M+H)^+$: 194.1176, found: 194.1180.

4-(4-methoxyphenyl)morpholine (20a)



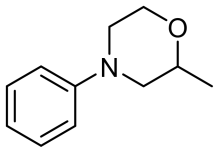
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 6.94–6.87 (m, 2H), 6.87–6.83 (m, 2H), 3.91–3.81 (m, 4H), 3.77 (s, 3H), 3.11–2.99 (m, 4H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 154.00, 145.65, 117.85, 114.52, 67.06, 55.59, 50.85. **HRMS** (ESI) calculated for $C_{11}H_{16}NO_2$ $(M+H)^+$: 194.1176, found: 194.1181.

3-methyl-4-phenylmorpholine (34a)



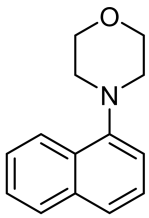
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.30–7.24 (m, 2H), 6.91–6.84 (m, 3H), 3.96 (dt, *J* = 11.2, 3.2 Hz, 1H), 3.86 (dd, *J* = 11.2, 2.8 Hz, 1H), 3.81–3.63 (m, 3H), 3.23–3.00 (m, 2H), 1.07 (d, *J* = 6.4 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 149.99, 129.23, 119.85, 116.73, 72.07, 67.24, 51.02, 44.44, 11.68. **HRMS** (ESI) calculated for $C_{11}H_{16}NO$ $(M+H)^+$: 178.1227, found: 178.1220.

2-methyl-4-phenylmorpholine (35a)



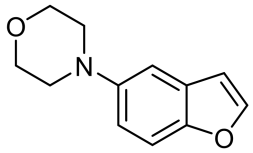
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.28 (t, *J* = 8.4 Hz, 2H), 6.92 (d, *J* = 8.8 Hz, 2H), 6.87 (t, *J* = 7.4 Hz, 1H), 4.01 (ddd, *J* = 11.6, 3.2, 1.2 Hz, 1H), 3.86–3.71 (m, 2H), 3.47 (d, *J* = 11.6 Hz, 1H), 3.41 (dd, *J* = 12.0, 1.6 Hz, 1H), 2.82 (td, *J* = 11.6, 3.6 Hz, 1H), 2.48 (dd, *J* = 11.6, 10.4 Hz, 1H), 1.25 (d, *J* = 6.4 Hz, 3H). **^{13}C NMR** (100 MHz, CDCl3) δ 151.15, 129.21, 119.96, 115.79, 71.81, 66.76, 55.63, 48.61, 19.09. **HRMS** (ESI) calculated for $C_{11}H_{16}NO$ $(M+H)^+$: 178.1227, found: 178.1225.

4-(naphthalen-1-yl)morpholine (37a)



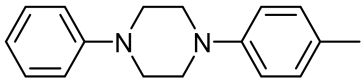
Pale white solid. M. p. 81–82 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.25 (dd, *J* = 6.0, 3.2 Hz, 1H), 7.86 (dd, *J* = 6.0, 3.2 Hz, 1H), 7.60 (d, *J* = 8.2 Hz, 1H), 7.54–7.49 (m, 2H), 7.44 (t, *J* = 7.8 Hz, 1H), 7.13 (d, *J* = 7.4 Hz, 1H), 4.11–3.94 (m, 4H), 3.25–3.06 (m, 4H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 149.42, 134.81, 128.79, 128.50, 125.92, 125.88, 125.49, 123.83, 123.41, 114.70, 67.50, 53.52. **HRMS** (ESI) calculated for $C_{14}H_{16}NO$ $(M+H)^+$: 214.1227, found: 214.1230.

4-(benzofuran-5-yl)morpholine (38a)



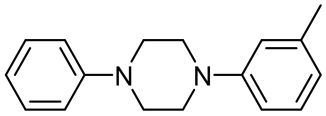
Yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.57 (s, 1H), 7.08 (s, 1H), 6.97 (d, *J* = 9.0 Hz, 1H), 6.69 (s, 1H), 3.88 (d, *J* = 4.5 Hz, 4H), 3.12 (d, *J* = 4.5 Hz, 4H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 150.34, 148.08, 145.54, 128.00, 115.83, 111.64, 107.87, 106.66, 67.13, 51.47. **HRMS** (ESI) calculated for $C_{12}H_{14}NO_2$ $(M+H)^+$: 204.1019, found: 204.1025.

1-phenyl-4-(*p*-tolyl)piperazine (44a)



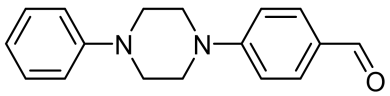
White solid. M. p. 130–131 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.29 (t, *J* = 7.5 Hz, 2H), 7.11 (d, *J* = 8.0 Hz, 2H), 6.99 (d, *J* = 8.0 Hz, 2H), 6.92–6.87 (m, 3H), 3.34 (d, *J* = 3.5 Hz, 4H), 3.30 (d, *J* = 3.5 Hz, 4H), 2.29 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 151.29, 149.13, 129.75, 129.21, 120.08, 116.77, 116.38, 50.07, 49.48, 20.49. **HRMS** (ESI) calculated for $C_{17}H_{21}N_2$ $(M+H)^+$: 253.1699, found: 253.1707.

1-phenyl-4-(*m*-tolyl)piperazine (45a)



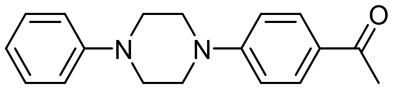
White solid. M. p. 125–127 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.29 (t, *J* = 7.3 Hz, 2H), 7.18 (t, *J* = 7.8 Hz, 1H), 6.98 (d, *J* = 7.8 Hz, 2H), 6.89 (t, *J* = 7.0 Hz, 1H), 6.81 – 6.79 (m, 2H), 6.72 (d, *J* = 7.0 Hz, 1H), 3.33 (s, 8H), 2.33 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 151.28, 138.93, 129.22, 129.07, 121.05, 120.10, 117.26, 116.38, 113.53, 49.56, 49.49, 21.83. **HRMS** (ESI) calculated for $C_{17}H_{21}N_2$ $(M+H)^+$: 253.1699, found: 253.1705.

4-(4-phenylpiperazin-1-yl)benzaldehyde (46a)



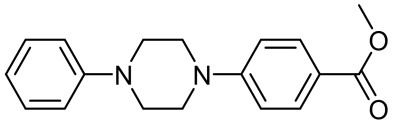
White solid. M. p. 123–125 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.80 (s, 1H), 7.78 (d, *J* = 9.0 Hz, 2H), 7.31 (t, *J* = 7.8 Hz, 2H), 7.01–6.95 (m, 4H), 6.92 (t, *J* = 7.3 Hz, 1H), 3.57 (t, *J* = 5.0 Hz, 4H), 3.35 (t, *J* = 5.3 Hz, 4H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 190.49, 154.90, 150.81, 131.92, 129.31, 127.38, 120.42, 116.36, 113.69, 49.04, 47.19. **HRMS** (ESI) calculated for $C_{17}H_{19}N_2O$ $(M+H)^+$: 267.1492, found: 267.1499.

1-(4-(4-phenylpiperazin-1-yl)phenyl)ethan-1-one (47a)



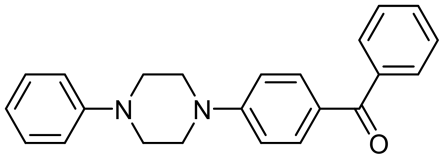
White solid. M. p. 146–148 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 8.4 Hz, 1H), 7.91 (d, *J* = 9.0 Hz, 2H), 7.73 (d, *J* = 8.6 Hz, 1H), 7.31 (dd, *J* = 8.8, 7.6 Hz, 2H), 6.98 (d, *J* = 7.6 Hz, 1H), 6.93 (d, *J* = 8.4 Hz, 2H), 3.52 (dd, *J* = 6.4, 4.0 Hz, 4H), 3.35 (dd, *J* = 6.2, 4.2 Hz, 4H), 2.54 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 196.58, 154.04, 130.44, 129.28, 129.04, 127.48, 120.34, 116.37, 113.59, 49.10, 47.48, 26.18. **HRMS** (ESI) calculated for $C_{18}H_{21}N_2O$ $(M+H)^+$: 281.1649, found: 281.1659.

methyl 4-(4-phenylpiperazin-1-yl)benzoate (48a)



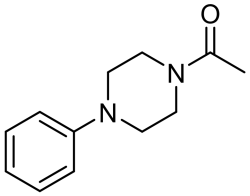
White solid. M. p. 172–175 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.5 Hz, 2H), 7.30 (t, *J* = 7.8 Hz, 2H), 6.98 (d, *J* = 8.0 Hz, 2H), 6.92–6.89 (m, 3H), 3.87 (s, 3H), 3.49 (t, *J* = 5.0 Hz, 4H), 3.34 (t, *J* = 5.0 Hz, 4H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 167.12, 154.03, 150.99, 131.28, 129.27, 120.31, 120.06, 116.38, 113.84, 51.72, 49.15, 47.65. **HRMS** (ESI) calculated for $C_{18}H_{21}N_2O_2$ $(M+H)^+$: 297.1598, found: 297.1603.

phenyl(4-(4-phenylpiperazin-1-yl)phenyl)methanone (49a)



White solid. M. p. 108–109 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.82 (d, *J* = 9.0 Hz, 2H), 7.75 (d, *J* = 7.5 Hz, 2H), 7.54 (t, *J* = 7.3 Hz, 1H), 7.46 (t, *J* = 7.5 Hz, 2H), 7.30 (t, *J* = 7.8 Hz, 2H), 6.98 (d, *J* = 8.0 Hz, 2H), 6.95 (d, *J* = 9.0 Hz, 2H), 6.91 (t, *J* = 7.5 Hz, 1H), 3.53 (t, *J* = 5.0 Hz, 4H), 3.35 (t, *J* = 5.0 Hz, 4H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 195.26, 153.85, 150.98, 138.81, 132.56, 131.54, 129.62, 129.29, 128.13, 127.52, 120.33, 116.37, 113.49, 49.11, 47.50. **HRMS** (ESI) calculated for $C_{23}H_{23}N_2O$ $(M+H)^+$: 343.1805, found: 343.1809.

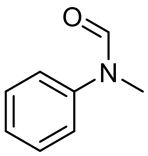
1-(4-phenylpiperazin-1-yl)ethan-1-one (50a)



White solid. M. p. 86–88 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.27 (dd, *J* = 8.4, 7.2 Hz, 2H), 6.93–6.88 (m, 3H), 3.75 (t, *J* = 5.2, 2H), 3.59 (t, *J* = 5.2, 2H), 3.28–3.08 (m, 4H), 2.12 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 169.02, 150.96, 129.26, 120.54, 116.66, 49.68, 49.35, 46.23, 41.35, 21.40. **HRMS** (ESI) calculated for $C_{12}H_{17}N_2O$ $(M+H)^+$: 205.1336, found: 205.1339.

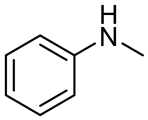
8.3 Characterizations of products.

***N*-methyl-*N*-phenylformamide (1c)**



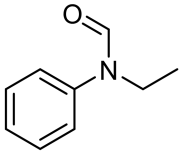
Colorless oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.48 (s, 1H), 7.41 (t, *J* = 7.8 Hz, 2H), 7.28 (t, *J* = 7.3 Hz, 1H), 7.17 (d, *J* = 8.0 Hz, 2H), 3.32 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 162.34, 142.20, 129.63, 126.41, 122.37, 32.04. **HRMS** (ESI) calculated for $C_8H_{10}NO$ $(M+H)^+$: 136.0757, found: 136.0770.

***N*-methylaniline (1d)**



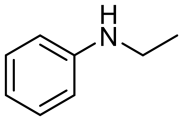
Colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.25–7.12 (m, 2H), 6.70 (t, *J* = 7.2 Hz, 1H), 6.59 (d, *J* = 7.6 Hz, 2H), 3.62 (s, 1H), 2.80 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 149.42, 129.27, 117.29, 112.48, 30.78. **HRMS** (ESI) calculated for $C_7H_{10}N$ $(M+H)^+$: 108.0808, found: 108.0815.

***N*-ethyl-*N*-phenylformamide (2b)**



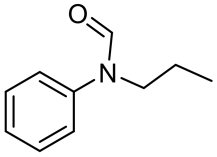
Colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.39 (s, 1H), 7.44 (t, *J* = 7.8 Hz, 2H), 7.34 (d, *J* = 7.4 Hz, 1H), 7.21–7.18 (m, 2H), 3.89 (q, *J* = 7.2 Hz, 2H), 1.19 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 162.06, 140.85, 129.65, 126.88, 124.29, 40.10, 13.07. **HRMS** (ESI) calculated for $C_9H_{12}NO$ $(M+H)^+$: 150.0914, found: 150.0920.

***N*-ethylaniline (2d)**



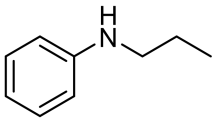
Colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.20–7.13 (m, 2H), 6.69 (t, *J* = 7.4 Hz, 1H), 6.59 (dd, *J* = 8.6, 1.0 Hz, 2H), 3.51 (s, 1H), 3.14 (q, *J* = 7.2 Hz, 2H), 1.24 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 148.51, 129.27, 117.25, 112.78, 38.50, 14.94. **HRMS** (ESI) calculated for $C_8H_{12}N$ $(M+H)^+$: 122.0964, found: 122.0970.

_N_-phenyl-_N_-propylformamide (3b)



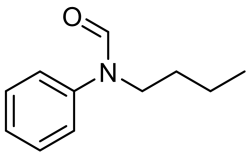
Colorless oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.39 (s, 1H), 7.41 (t, *J* = 7.8 Hz, 2H), 7.31 (d, *J* = 7.0 Hz, 1H), 7.18 (d, *J* = 8.0 Hz, 2H), 3.78 (t, *J* = 7.5 Hz, 2H), 1.60 - 1.53 (m, 2H), 0.90 (t, *J* = 7.5 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 162.46, 141.05, 129.64, 126.85, 124.28, 46.57, 20.89, 11.22. **HRMS** (ESI) calculated for $C_{10}H_{14}NO$ $(M+H)^+$: 164.1070, found: 164.1075.

_N_-propylaniline (3d)



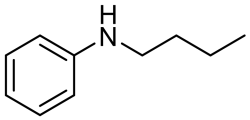
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.17 (dd, *J* = 8.4, 7.2 Hz, 2H), 6.68 (t, *J* = 7.4 Hz, 1H), 6.60 (dd, *J* = 8.6, 1.0 Hz, 2H), 3.61 (s, 1H), 3.08 (t, *J* = 7.2 Hz, 2H), 1.70–1.58 (m, 2H), 0.99 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 148.54, 129.24, 117.09, 112.71, 45.82, 22.76, 11.68. **HRMS** (ESI) calculated for $C_9H_{14}N$ $(M+H)^+$: 136.1121, found: 136.1129.

_N_-butyl-_N_-phenylformamide (4b)



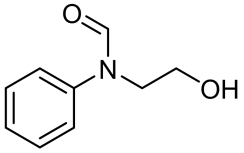
Colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.37 (s, 1H), 7.41 (t, *J* = 7.8 Hz, 2H), 7.30 (t, *J* = 7.4 Hz, 1H), 7.17 (d, *J* = 7.6 Hz, 2H), 3.82 (t, *J* = 7.4 Hz, 2H), 1.56–1.48 (m, 2H), 1.37–1.29 (m, 2H), 0.89 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR** (100 MHz, CDCl3) δ 162.34, 141.09, 129.63, 126.81, 124.25, 44.73, 29.70, 20.01, 13.70. **HRMS** (ESI) calculated for $C_{11}H_{16}NO$ $(M+H)^+$: 178.1227, found: 178.1225.

_N_-butylaniline (4d)



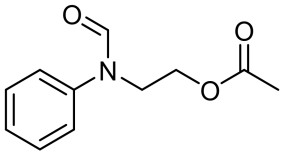
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.16 (t, *J* = 8.0 Hz, 2H), 6.69 (d, *J* = 7.2 Hz, 1H), 6.60 (d, *J* = 7.6 Hz, 2H), 3.57 (s, 1H), 3.11 (t, *J* = 7.2 Hz, 2H), 1.64–1.56 (m, 2H), 1.48–1.40 (m, 2H), 0.96 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 148.58, 129.23, 117.09, 112.70, 43.70, 31.72, 20.32, 13.92. **HRMS** (ESI) calculated for $C_{10}H_{16}N$ $(M+H)^+$: 150.1277, found: 150.1285.

_N_-(2-hydroxyethyl)-_N_-phenylformamide (5b)



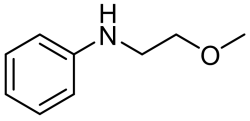
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.10 (s, 1H), 7.23–7.16 (m, 2H), 6.75 (t, *J* = 7.4 Hz, 1H), 6.64 (dd, *J* = 8.6, 1.0 Hz, 2H), 4.43–4.35 (m, 2H), 3.90 (s, 1H), 3.45 (t, *J* = 5.6 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 160.93, 147.40, 129.40, 118.12, 113.01, 62.59, 42.69. **HRMS** (ESI) calculated for $C_9H_{12}NO_2$ $(M+H)^+$: 166.0863, found: 166.0870.

2-(_N_-phenylformamido)ethyl acetate (6b)



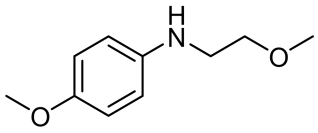
Colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.40 (s, 1H), 7.43 (t, *J* = 7.6 Hz, 2H), 7.32 (t, *J* = 7.4 Hz, 1H), 7.24–7.18 (m, 2H), 4.25 (t, *J* = 5.6 Hz, 2H), 4.08 (t, *J* = 5.6 Hz, 2H), 1.91 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 170.72, 162.57, 140.96, 129.75, 127.15, 124.44, 61.36, 44.27, 20.65. **HRMS** (ESI) calculated for $C_{11}H_{14}NO_3$ $(M+H)^+$: 208.0968, found: 208.0970.

_N_-(2-methoxyethyl)aniline (7d)



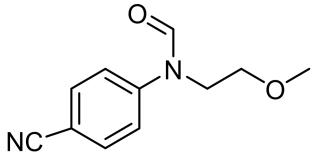
Colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.18 (t, *J* = 7.6 Hz, , 2H), 6.72 (t, *J* = 7.2 Hz, 1H), 6.64 (d, *J* = 7.6 Hz, 2H), 4.09 (s, 1H), 3.61 (t, *J* = 5.2 Hz, 2H), 3.39 (s, 3H), 3.29 (t, *J* = 5.2 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 148.22, 129.25, 117.63, 113.11, 71.05, 58.78, 43.49. **HRMS** (ESI) calculated for $C_9H_{14}NO$ $(M+H)^+$: 152.1070, found: 152.1065.

4-methoxy-_N_-(2-methoxyethyl)aniline (8d)



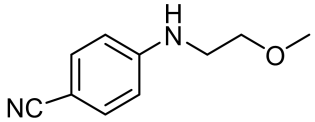
Colorless oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 6.78 (d, *J* = 8.5 Hz, 2H), 6.61 (d, *J* = 9.0 Hz, 2H), 3.75 (s, 3H), 3.60 (t, *J* = 5.0 Hz, 2H), 3.38 (s, 3H), 3.24 (t, *J* = 5.3 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 152.32, 142.46, 114.87, 114.53, 71.15, 58.78, 55.80, 44.58. **HRMS** (ESI) calculated for $C_{10}H_{15}NO_2$ $(M+H)^+$: 182.1176, found: 182.1178.

_N_-(4-cyanophenyl)-_N_-(2-methoxyethyl)formamide (9c)



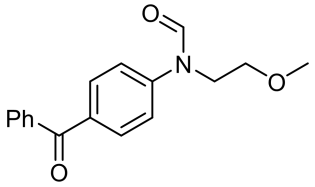
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.56 (s, 1H), 7.71 (d, *J* = 8.4 Hz, 2H), 7.42 (d, *J* = 8.4 Hz, 2H), 3.99 (t, *J* = 5.2 Hz, 2H), 3.62 (t, *J* = 5.2 Hz, 2H), 3.33 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 161.79, 145.70, 133.62, 123.45, 118.25, 109.87, 69.58, 58.92, 46.02. **HRMS** (ESI) calculated for $C_{11}H_{13}N_2O_2$ $(M+H)^+$: 205.0972, found: 205.0977.

4-((2-methoxyethyl)amino)benzonitrile (9d)



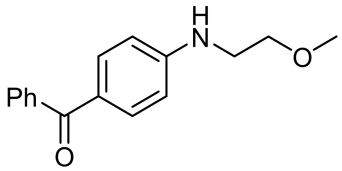
Yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.42 (d, *J* = 8.5 Hz, 2H), 6.58 (d, *J* = 8.5 Hz, 2H), 4.57 (s, 1H), 3.61 (t, *J* = 5.0 Hz, 2H), 3.40 (s, 3H), 3.32 (t, *J* = 5.0 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 151.31, 133.72, 120.47, 112.37, 98.87, 70.43, 58.87, 42.68. **HRMS** (ESI) calculated for $C_{10}H_{13}N_2O$ $(M+H)^+$: 177.1023, found: 177.1027.

_N_-(4-benzoylphenyl)-_N_-(2-methoxyethyl)formamide (10c)



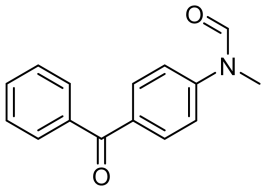
Colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.58 (s, 1H), 7.87 (d, J = 8.4 Hz, 2H), 7.79 (d, J = 7.2 Hz, 2H), 7.61 (t, J = 7.4 Hz, 1H), 7.50 (t, J = 7.6 Hz, 2H), 7.39 (d, J = 8.4 Hz, 2H), 4.03 (t, J = 5.4 Hz, 2H), 3.63 (t, J = 5.4 Hz, 2H), 3.34 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 195.49, 162.20, 145.16, 137.37, 135.41, 132.62, 131.69, 129.95, 128.42, 122.85, 69.50, 58.88, 45.68. **HRMS** (ESI) calculated for $C_{17}H_{18}NO_3$ $(M+H)^+$: 284.1281, found: 284.1285.

(4-((2-methoxyethyl)amino)phenyl)(phenyl)methanone (10d)



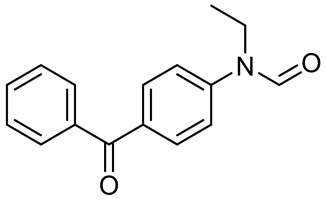
Colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.79–7.68 (m, 4H), 7.53 (t, *J* = 7.4 Hz, 1H), 7.45 (t, *J* = 7.6 Hz, 2H), 6.61 (d, *J* = 8.8 Hz, 2H), 4.60 (s, 1H), 3.63 (t, *J* = 5.2 Hz, 2H), 3.40 (s, 3H), 3.38 (t, *J* = 5.0 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 195.21, 152.01, 139.13, 133.00, 131.24, 129.48, 128.05, 126.34, 111.53, 70.61, 58.86, 42.80. **HRMS** (ESI) calculated for $C_{16}H_{18}NO_2$ $(M+H)^+$: 256.1332, found: 256.1335.

***N*-(4-benzoylphenyl)-*N*-methylformamide (10b')**



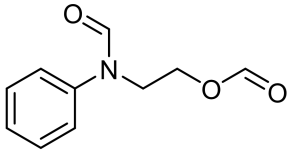
Yellow solid. M. p. 92–94 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.56 (s, 1H), 7.76 (d, *J* = 8.4 Hz, 2H), 7.67 (d, *J* = 7.2 Hz, 2H), 7.49 (t, *J* = 7.4 Hz, 1H), 7.38 (t, *J* = 7.6 Hz, 2H), 7.18 (d, *J* = 8.4 Hz, 2H), 3.26 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 195.19, 161.86, 145.61, 137.38, 134.76, 132.54, 131.74, 129.85, 128.38, 120.46, 31.42. **HRMS** (ESI) calculated for $C_{15}H_{14}NO_2$ $(M+H)^+$: 240.1019, found: 240.1026.

***N*-(4-benzoylphenyl)-*N*-ethylformamide (12b')**



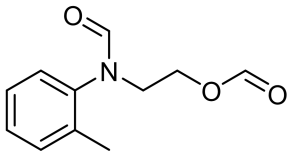
Colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.55 (s, 1H), 8.12 (d, *J* = 8.0 Hz, 1H), 7.89 (d, *J* = 8.4 Hz, 2H), 7.80 (d, *J* = 7.2 Hz, 2H), 7.61 (d, *J* = 7.4 Hz, 1H), 7.52–7.48 (m, 2H), 7.29 (d, *J* = 8.6 Hz, 2H), 3.96 (q, *J* = 7.2 Hz, 2H), 1.22 (d, *J* = 7.2 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 195.39, 161.72, 144.49, 137.34, 133.65, 132.65, 131.80, 129.95, 128.43, 122.26, 39.77, 13.13. **HRMS** (ESI) calculated for $C_{16}H_{16}NO_2$ $(M+H)^+$: 254.1176, found: 254.1177.

2-(*N*-phenylformamido)ethyl formate (13b)



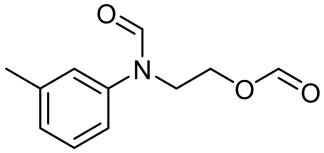
Colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.40 (s, 1H), 7.97 (s, 1H), 7.42 (d, *J* = 8.0 Hz, 2H), 7.33 (t, *J* = 7.4 Hz, 1H), 7.24–7.20 (m, 2H), 4.34 (t, *J* = 5.6 Hz, 2H), 4.11 (t, *J* = 5.6 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 162.71, 160.62, 140.60, 129.84, 127.34, 124.46, 60.62, 44.17. **HRMS** (ESI) calculated for $C_{10}H_{12}NO_3$ $(M+H)^+$: 194.0812, found: 194.0815.

2-(*N*-*o*-tolylformamido)ethyl formate (14b)



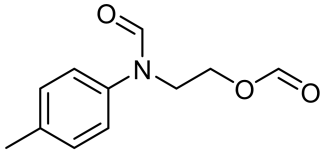
Colorless oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.15 (s, 1H), 7.98 (s, 1H), 7.31 (dd, *J* = 5.0, 1.0 Hz, 2H), 7.16 (t, *J* = 6.5 Hz, 2H), 4.30 (t, *J* = 5.5 Hz, 2H), 3.98 (t, *J* = 5.0 Hz, 2H), 2.27 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 177.39, 163.38, 160.61, 135.81, 131.63, 128.79, 128.75, 127.23, 60.62, 44.11, 28.21. **HRMS** (ESI) calculated for $C_{11}H_{14}NO_3$ $(M+H)^+$: 208.0968, found: 208.0971.

2-(*N*-*m*-tolylformamido)ethyl formate (15b)



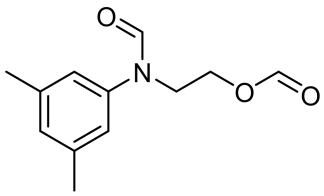
Colorless oil, **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.38 (s, 1H), 7.98 (s, 1H), 7.30 (t, *J* = 8.2 Hz, 1H), 7.13 (d, *J* = 7.6 Hz, 1H), 7.01 (s, 1H), 7.00 (d, *J* = 6.0 Hz, 1H), 4.33 (t, *J* = 5.8 Hz, 2H), 4.09 (t, *J* = 5.8 Hz, 2H), 2.39 (s, 3H). **^{13}C NMR** (100 MHz, CDCl3) δ 162.71, 160.63, 140.50, 139.93, 129.59, 128.11, 125.11, 121.50, 60.59, 44.07, 21.37. **HRMS** (ESI) calculated for $C_{11}H_{14}NO_3$ $(M+H)^+$: 208.0968, found: 208.0972.

2-(*N*-*p*-tolylformamido)ethyl formate (16b)



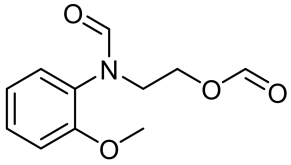
Colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.35 (s, 1H), 7.97 (s, 1H), 7.22 (d, *J* = 8.0 Hz, 2H), 7.09 (d, *J* = 8.4 Hz, 2H), 4.32 (t, *J* = 5.6 Hz, 2H), 4.07 (t, *J* = 5.6 Hz, 2H), 2.37 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 162.75, 160.62, 137.98, 137.40, 130.38, 124.62, 60.60, 44.20, 20.95. **HRMS** (ESI) calculated for $C_{11}H_{14}NO_3$ $(M+H)^+$: 208.0968, found: 208.0975.

2-(*N*-(3,5-dimethylphenyl)formamido)ethyl formate (17b)



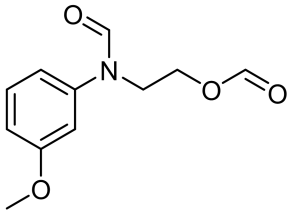
Yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.36 (s, 1H), 7.99 (s, 1H), 6.96 (s, 1H), 6.80 (s, 2H), 4.32 (t, *J* = 5.8 Hz, 2H), 4.07 (t, *J* = 5.8 Hz, 2H), 2.34 (s, 6H). **^{13}C NMR** (125 MHz, CDCl3) δ 162.73, 160.64, 140.40, 139.65, 129.01, 122.22, 60.58, 43.99, 21.27. **HRMS** (ESI) calculated for $C_{12}H_{16}NO_3$ $(M+H)^+$: 222.1125, found: 222.1129.

2-(*N*-(2-methoxyphenyl)formamido)ethyl formate (18b)



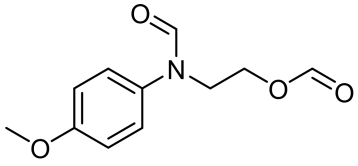
Colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.15 (s, 1H), 7.96 (s, 1H), 7.35 (td, *J* = 8.0, 1.6 Hz, 1H), 7.16 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.01-6.97 (m, 2H), 4.28 (t, *J* = 5.8 Hz, 2H), 4.01 (t, *J* = 5.6 Hz, 2H), 3.84 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 163.74, 160.69, 155.30, 129.67, 129.06, 128.72, 120.97, 111.93, 60.91, 55.60, 43.62. **HRMS** (ESI) calculated for $C_{11}H_{14}NO_4$ $(M+H)^+$: 224.0918, found: 224.0920.

2-(*N*-(3-methoxyphenyl)formamido)ethyl formate (19b)



Colorless oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.42 (s, 1H), 7.99 (s, 1H), 7.33 (t, *J* = 8.0 Hz, 1H), 6.86 (dd, *J* = 8.0, 2.0 Hz, 1H), 6.79 (dd, *J* = 8.0, 2.0 Hz, 1H), 6.75 (t, *J* = 2.2 Hz, 1H), 4.34 (t, *J* = 5.8 Hz, 2H), 4.09 (t, *J* = 5.8 Hz, 2H), 3.83 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 162.64, 160.64, 160.60, 141.79, 130.57, 116.46, 112.43, 110.57, 60.61, 55.47, 44.14. **HRMS** (ESI) calculated for $C_{11}H_{14}NO_4$ $(M+H)^+$: 224.0918, found: 224.0921.

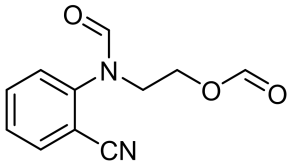
2-(*N*-(4-methoxyphenyl)formamido)ethyl formate (20b)



Colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.30 (s, 1H), 7.99 (s, 1H), 7.13 (d, *J* = 8.8 Hz, 2H), 6.94 (d, *J* = 8.8 Hz, 2H), 4.32 (t, *J* = 5.6 Hz, 2H), 4.04 (t, *J* = 5.6 Hz, 2H), 3.83 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 162.89, 160.63, 158.90, 133.33, 126.70,

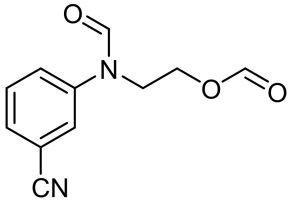
114.92, 60.60, 55.56, 44.51. **HRMS** (ESI) calculated for $C_{11}H_{14}NO_4$ $(M+H)^+$: 224.0918, found: 224.0920.

2-(*N*-(2-cyanophenyl)formamido)ethyl formate (21b)



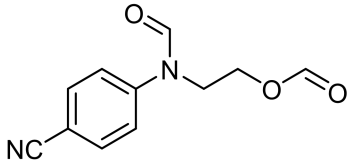
Yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.32 (s, 1H), 7.94 (s, 1H), 7.80 (d, *J* = 7.5 Hz, 1H), 7.74 (t, *J* = 8.0 Hz, 1H), 7.53 (t, *J* = 7.5 Hz, 1H), 7.42 (d, *J* = 8.0 Hz, 1H), 4.35 (t, *J* = 5.4 Hz, 2H), 4.19 (t, *J* = 5.4 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 162.15, 160.48, 143.11, 134.43, 134.24, 128.72, 128.47, 116.02, 111.51, 60.85, 44.92. **HRMS** (ESI) calculated for $C_{11}H_{11}N_2O_3$ $(M+H)^+$: 219.0764, found: 219.0767.

2-(*N*-(3-cyanophenyl)formamido)ethyl formate (22b)



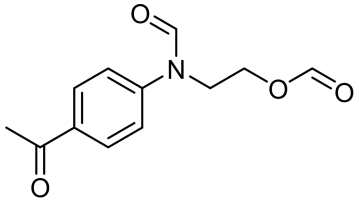
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.37 (s, 1H), 7.91 (s, 1H), 7.55 (t, *J* = 7.2 Hz, 1H), 7.52–7.48 (m, 2H), 7.45–7.41 (m, 1H), 4.30 (t, *J* = 5.6 Hz, 2H), 4.05 (t, *J* = 5.4 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 162.09, 160.52, 141.77, 130.94, 130.59, 128.35, 127.22, 117.70, 114.03, 60.60, 44.37. **HRMS** (ESI) calculated for $C_{11}H_{11}N_2O_3$ $(M+H)^+$: 219.0764, found: 219.0766.

2-(*N*-(4-cyanophenyl)formamido)ethyl formate (23b)



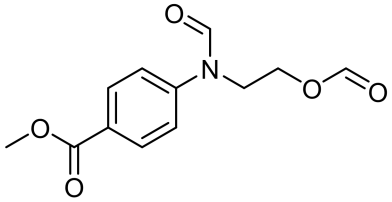
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.55 (s, 1H), 7.98 (s, 1H), 7.83–7.73 (m, 2H), 7.46–7.33 (m, 2H), 4.39 (t, *J* = 5.4 Hz, 2H), 4.16 (t, *J* = 5.6 Hz, 2H). **^{13}C NMR** (100 MHz, CDCl3) δ 161.90, 160.47, 144.78, 133.91, 123.29, 118.00, 110.35, 60.60, 43.98. **HRMS** (ESI) calculated for $C_{11}H_{11}N_2O_3$ $(M+H)^+$: 219.0764, found: 219.0768.

2-(*N*-(4-acetylphenyl)formamido)ethyl formate (24b)



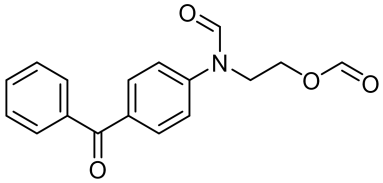
Colorless oil, **^{1}H NMR** (500 MHz, CDCl3) δ 8.55 (s, 1H), 8.04 (d, *J* = 8.5 Hz, 2H), 7.97 (s, 1H), 7.33 (d, *J* = 8.5 Hz, 2H), 4.38 (t, *J* = 5.6 Hz, 2H), 4.18 (t, *J* = 5.6 Hz, 2H), 2.62 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 196.70, 162.15, 160.52, 144.79, 135.23, 130.11, 122.80, 60.60, 43.83, 26.58. **HRMS** (ESI) calculated for $C_{12}H_{14}NO_4$ $(M+H)^+$: 236.0913, found: 236.0915.

methyl 4-(*N*-(2-(formyloxy)ethyl)formamido)benzoate (25b)



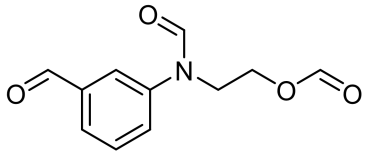
Colorless oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.53 (s, 1H), 8.11 (d, *J* = 8.5 Hz, 2H), 7.96 (s, 1H), 7.29 (d, *J* = 8.5 Hz, 2H), 4.38 (t, *J* = 5.5 Hz, 2H), 4.16 (t, *J* = 5.5 Hz, 2H), 3.94 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 166.05, 162.18, 160.48, 144.73, 131.34, 128.50, 122.79, 60.64, 52.33, 43.91. **HRMS** (ESI) calculated for $C_{12}H_{14}NO_5$ $(M+H)^+$: 252.0867, found: 252.0869.

2-(*N*-(4-benzoylphenyl)formamido)ethyl formate (26b)



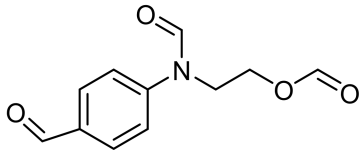
Colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.57 (s, 1H), 7.99 (s, 1H), 7.90 (d, *J* = 8.6 Hz, 2H), 7.80 (d, *J* = 7.0 Hz, 2H), 7.62 (t, *J* = 7.4 Hz, 1H), 7.51 (t, *J* = 7.6 Hz, 2H), 7.39–7.32 (m, 2H), 4.40 (t, *J* = 5.6 Hz, 2H), 4.19 (t, *J* = 5.6 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 195.28, 162.22, 160.54, 144.29, 137.19, 135.82, 132.74, 131.87, 129.94, 128.47, 122.74, 60.65, 43.98. **HRMS** (ESI) calculated for $C_{17}H_{16}NO_4$ $(M+H)^+$: 298.1074, found: 298.1077.

2-(*N*-(3-formylphenyl)formamido)ethyl formate (27b)



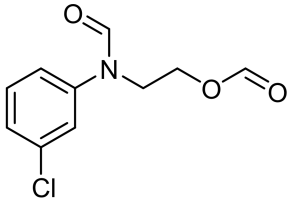
Yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.98 (s, 1H), 8.41 (s, 1H), 7.90 (s, 1H), 7.77 (d, *J* = 7.5 Hz, 1H), 7.69 (s, 1H), 7.57 (t, *J* = 7.8 Hz, 1H), 7.43 (d, *J* = 7.5 Hz, 1H), 4.31 (t, *J* = 5.5 Hz, 2H), 4.09 (t, *J* = 5.5 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 191.05, 162.35, 160.50, 141.76, 137.85, 130.72, 129.67, 128.90, 123.86, 60.64, 44.29. **HRMS** (ESI) calculated for $C_{11}H_{12}NO_4$ $(M+H)^+$: 222.0761, found: 222.0768.

2-(*N*-(4-formylphenyl)formamido)ethyl formate (28b)



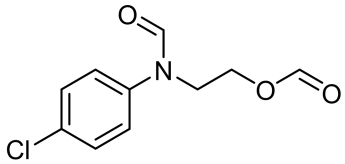
Yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.95 (s, 1H), 8.51 (s, 1H), 7.93–7.86 (m, 3H), 7.32 (d, *J* = 8.5 Hz, 2H), 4.33 (t, *J* = 5.5 Hz, 2H), 4.11 (t, *J* = 5.5 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 190.67, 162.03, 160.46, 146.01, 134.46, 131.42, 123.05, 60.65, 43.94. **HRMS** (ESI) calculated for $C_{11}H_{12}NO_4$ $(M+H)^+$: 222.0761, found: 222.0770.

2-(*N*-(3-chlorophenyl)formamido)ethyl formate (29b)



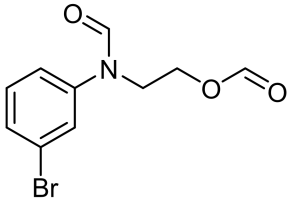
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.41 (s, 1H), 7.98 (s, 1H), 7.37 (t, *J* = 8.0 Hz, 1H), 7.33–7.29 (m, 1H), 7.24 (t, *J* = 2.0 Hz, 1H), 7.11 (ddd, *J* = 7.6, 2.0, 1.2 Hz, 1H), 4.35 (t, *J* = 5.6 Hz, 2H), 4.09 (t, *J* = 5.6 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 162.29, 160.50, 141.95, 135.48, 130.84, 127.46, 124.44, 122.32, 60.60, 44.29. **HRMS** (ESI) calculated for $C_{10}H_{11}NO_3Cl$ $(M+H)^+$: 228.0422, found: 228.0426.

2-(*N*-(4-chlorophenyl)formamido)ethyl formate (30b)



Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.37 (s, 1H), 7.97 (s, 1H), 7.41 (d, *J* = 8.8 Hz, 2H), 7.16 (d, *J* = 8.8 Hz, 2H), 4.34 (t, *J* = 5.6 Hz, 2H), 4.08 (t, *J* = 5.6 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 162.37, 160.53, 139.25, 133.12, 130.01, 125.72, 60.62, 44.35. **HRMS** (ESI) calculated for $C_{10}H_{11}NO_3Cl$ $(M+H)^+$: 228.0422, found: 228.0425.

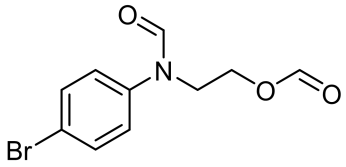
2-(*N*-(3-bromophenyl)formamido)ethyl formate (31b)



Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.40 (s, 1H), 7.99 (s, 1H), 7.47 (ddd, *J* = 8.0, 1.8, 0.8 Hz, 1H), 7.40 (t, *J* = 2.5 Hz, 1H), 7.31 (t, *J* = 8.0 Hz, 1H), 7.16 (ddd, *J* = 8.0, 2.0, 0.8 Hz, 1H), 4.35 (t, *J* = 5.4 Hz, 2H), 4.09 (t, *J* = 5.6 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 162.32, 160.53, 142.05, 131.10, 130.41, 127.35, 123.30, 122.85,

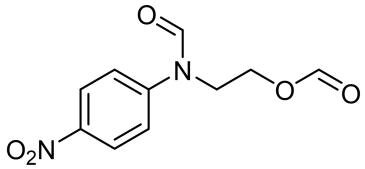
60.60, 44.31. **HRMS** (ESI) calculated for $C_{10}H_{11}NO_3Br$ $(M+H)^+$: 271.9917, found: 271.9920.

2-(*N*-(4-bromophenyl)formamido)ethyl formate (32b)



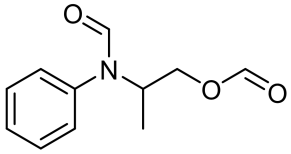
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.37 (s, 1H), 7.97 (s, 1H), 7.56 (d, *J* = 8.8 Hz, 2H), 7.10 (d, *J* = 8.8 Hz, 2H), 4.34 (t, *J* = 5.4 Hz, 2H), 4.08 (t, *J* = 5.8 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 162.32, 160.55, 132.99, 132.02, 125.95, 119.69, 60.62, 44.29. **HRMS** (ESI) calculated for $C_{10}H_{11}NO_3Br$ $(M+H)^+$: 271.9917, found: 271.9921.

2-(*N*-(4-nitrophenyl)formamido)ethyl formate (33b)



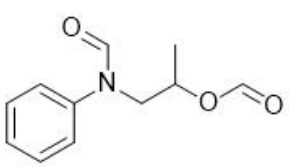
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.62 (s, 1H), 8.34 (d, *J* = 8.8 Hz, 2H), 7.99 (s, 1H), 7.41 (d, *J* = 8.8 Hz, 2H), 4.43 (t, *J* = 5.4 Hz, 2H), 4.21 (t, *J* = 5.4 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 161.73, 160.38, 146.47, 145.78, 125.54, 122.76, 60.63, 44.13. **HRMS** (ESI) calculated for $C_{10}H_{11}N_2O_5$ $(M+H)^+$: 239.0663, found: 239.0666.

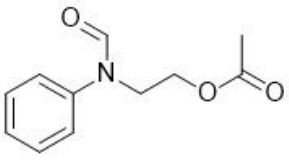
2-(*N*-phenylformamido)propyl formate (34b)



Colorless oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.25 (s, 1H), 8.07 (s, 1H), 7.52–7.36 (m, 3H), 7.21 (d, *J* = 8.0 Hz, 2H), 4.86 (dq, *J* = 13.9, 7.1 Hz, 1H), 4.31 (dd, *J* = 11.5, 5.0 Hz, 1H), 4.21 (dd, *J* = 11.5, 8.0 Hz, 1H), 1.26 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 163.16, 160.55, 138.19, 129.61, 128.58, 128.52, 64.11, 49.43, 15.49. **HRMS** (ESI) calculated for $C_{11}H_{14}NO_3$ $(M+H)^+$: 208.0968, found: 208.0960.

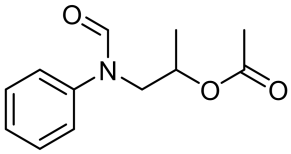
1-(*N*-phenylformamido)propan-2-yl formate (35b)
2-(*N*-phenylformamido)ethyl acetate (35b′)





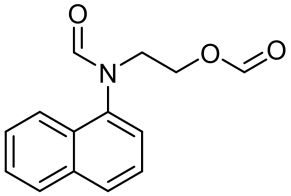
Colorless oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.40 (s, 1H), 8.38 (s, 1.4H), 7.88 (s, 1.4H), 7.44–7.39 (m, 5.4H), 7.33–7.28 (m, 2.48H), 7.23–7.16 (m, 5.19H), 5.33–5.21 (m, 1.47H), 4.25 (t, *J* = 5.6 Hz, 2.06H), 4.07 (t, *J* = 5.6 Hz, 2.07H), 4.03 (dd, *J* = 14.3, 7.9 Hz, 1.48H), 3.96 (dd, *J* = 14.3, 4.3 Hz, 1.46H), 1.90 (s, 3.01H), 1.28 (d, *J* = 6.5 Hz, 4.70H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 170.73, 162.85, 162.59, 160.35, 140.94, 140.90, 129.79, 129.75, 127.20, 127.15, 124.44, 124.29, 68.32, 61.36, 49.04, 44.27, 20.64, 17.81. **HRMS** (ESI) calculated for $C_{11}H_{14}NO_3$ $(M+H)^+$: 208.0968, found: 208.0971.

1-(*N*-phenylformamido)propan-2-yl acetate (36b)



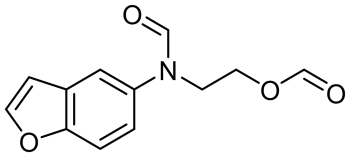
Colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.36 (s, 1H), 7.40 (t, *J* = 7.8 Hz, 2H), 7.28 (t, *J* = 7.4 Hz, 1H), 7.21–7.09 (m, 2H), 5.21–5.01 (m, 1H), 3.97 (qd, *J* = 14.2, 5.8 Hz, 2H), 1.75 (s, 3H), 1.22 (d, *J* = 6.4 Hz, 3H). **^{13}C NMR** (100 MHz, CDCl3) δ 170.36, 162.81, 141.21, 129.69, 126.97, 124.24, 68.76, 48.82, 20.88, 17.78. **HRMS** (ESI) calculated for $C_{12}H_{16}NO_3$ $(M+H)^+$: 222.1125, found: 222.1125.

2-(*N*-(naphthalen-1-yl)formamido)ethyl formate (37b)



Yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.30 (s, 1H), 7.97 (s, 1H), 7.96–7.89 (m, 2H), 7.84–7.79 (m, 1H), 7.63–7.57 (m, 2H), 7.55–7.50 (m, 1H), 7.41 (dd, *J* = 7.5, 1.0 Hz, 1H), 4.51 (t, *J* = 6.0 Hz, 1H), 4.33 (t, *J* = 5.5 Hz, 2H), 3.84 (t, *J* = 6.5 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 163.77, 160.62, 136.24, 134.69, 130.73, 129.45, 128.76, 127.64, 126.92, 126.45, 125.51, 122.12, 60.78, 44.95. **HRMS** (ESI) calculated for $C_{14}H_{14}NO_3$ $(M+H)^+$: 244.0968, found: 244.0970.

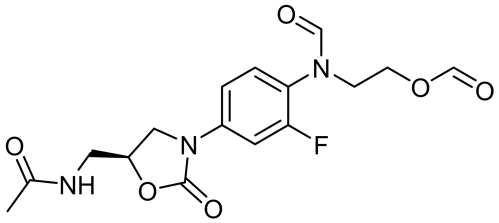
2-(*N*-(benzofuran-5-yl)formamido)ethyl formate (38b)



Colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.31 (s, 1H), 7.92 (s, 1H), 7.64 (d, *J* = 2.4 Hz, 1H), 7.48 (d, *J* = 8.8 Hz, 1H), 7.37 (d, *J* = 2.0 Hz, 1H), 7.07 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.73 (dd, *J* = 2.4, 0.8 Hz, 1H), 4.27 (t, *J* = 5.6 Hz, 2H), 4.05 (t, *J* = 5.6 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 163.11, 160.64, 153.79, 146.82, 135.81, 128.53,

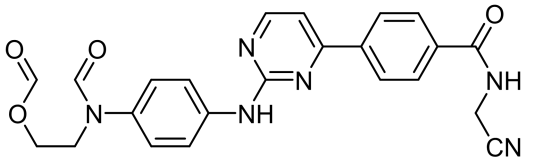
121.98, 118.40, 112.49, 106.72, 60.62, 44.89. **HRMS** (ESI) calculated for $C_{12}H_{12}NO_4$ $(M+H)^+$: 234.0761, found: 234.0769.

(S)-2-(N-(4-(5-(acetamidomethyl)-2-oxooxazolidin-3-yl)-2-fluorophenyl)formamido)ethyl formate (39b)



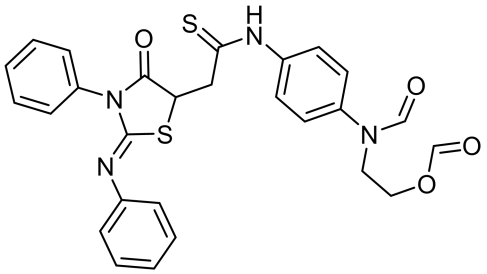
Yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.20 (s, 1H), 7.96 (s, 1H), 7.63 (d, J = 13.0 Hz, 1H), 7.27 (d, J = 12.0 Hz, 1H), 7.25 (s, 1H), 6.67 (t, J = 5.8 Hz, 1H), 4.87–4.78 (m, 1H), 4.30 (t, J = 5.3 Hz, 2H), 4.08 (t, J = 9.0 Hz, 1H), 4.03 (t, J = 5.3 Hz, 2H), 3.87–3.81 (m, 1H), 3.68 (t, J = 5.0 Hz, 2H), 2.03 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 171.51, 163.04, 160.60, 158.00 ($^1J_{C\text{-}F}$ = 257.8 Hz), 154.19, 139.14 ($^3J_{C\text{-}F}$ = 10.4 Hz), 129.26, 123.65 ($^3J_{C\text{-}F}$ = 12.3 Hz), 113.88 ($^4J_{C\text{-}F}$ = 3.5 Hz), 107.01 ($^2J_{C\text{-}F}$ = 25.8 Hz), 72.20, 60.72, 47.43, 44.20, 41.83, 23.02. **HRMS** (ESI) calculated for $C_{16}H_{19}N_3O_6F$ $(M+H)^+$: 368.1253, found: 368.1260.

2-(*N*-(4-((4-(4-((cyanomethyl)carbamoyl)phenyl)pyrimidin-2-yl)amino)phenyl)formamido)ethyl formate (40b)



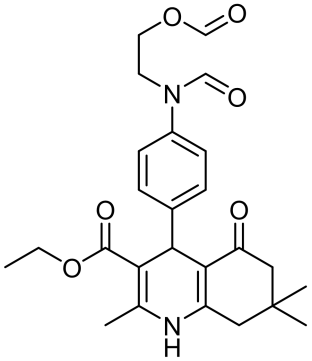
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.85 (t, J = 5.6 Hz, 1H), 8.53 (d, J = 5.2 Hz, 1H), 8.37 (s, 1H), 8.13 (d, J = 8.6 Hz, 2H), 8.08 (d, J = 8.6 Hz, 2H), 8.02 (s, 1H), 7.93 (s, 1H), 7.83 (d, J = 8.8 Hz, 2H), 7.33 (s, 1H), 7.24–7.19 (m, 2H), 4.38 (d, J = 5.6 Hz, 2H), 4.36 (t, J = 5.6 Hz, 2H), 4.09 (t, J = 5.6 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 166.84, 163.82, 162.78, 160.61, 160.07, 158.87, 140.19, 139.23, 134.87, 134.52, 128.17, 127.13, 125.63, 120.08, 116.42, 109.05, 60.57, 44.36, 27.96. **HRMS** (ESI) calculated for $C_{23}H_{21}N_6O_4$ $(M+H)^+$: 445.1619, found: 445.1625.

(Z)-2-(*N*-(4-(2-(4-oxo-3-phenyl-2-(phenylimino)thiazolidin-5-yl)ethanethioamido)phenyl)formamido)ethyl formate (41b)



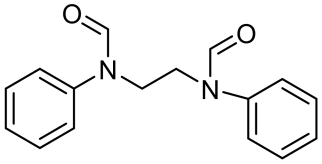
Colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.50 (s, 1H), 8.30 (s, 1H), 7.95 (s, 1H), 7.51–7.40 (m, 7H), 7.30–7.25 (m, 2H), 7.12–7.05 (m, 3H), 6.90 (dd, *J* = 8.4, 1.0 Hz, 2H), 4.56 (dd, *J* = 9.6, 3.6 Hz, 1H), 4.29 (t, *J* = 5.4 Hz, 2H), 4.03 (t, *J* = 5.6 Hz, 2H), 3.40–3.34 (m, 1H), 3.02–2.95 (m, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 174.18, 167.33, 162.71, 160.66, 154.77, 147.91, 137.03, 136.36, 134.78, 129.45, 129.21, 129.16, 128.05, 125.29, 124.78, 120.92, 60.55, 44.33, 43.81, 40.08. **HRMS** (ESI) calculated for $C_{27}H_{24}N_4O_4S_2$ $(M+H)^+$: 533.1312, found: 533.1320.

4-(4-(*N*-(2-(formyloxy)ethyl)formamido)phenyl)-2,7,7-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (42b)



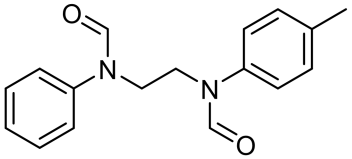
Colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.47 (s, 1H), 8.01 (s, 1H), 7.25 (d, *J* = 8.6 Hz, 2H), 7.20 (d, *J* = 8.6 Hz, 2H), 4.37 (t, *J* = 5.6 Hz, 2H), 4.15 (t, *J* = 5.6 Hz, 2H), 4.02 (q, *J* = 7.0 Hz, 2H), 3.74 (t, *J* = 7.0 Hz, 1H), 3.11 (s, 2H), 2.61 (s, 3H), 2.48 (s, 2H), 1.13 (s, 6H), 0.98 (t, *J* = 7.0 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 197.16, 167.15, 162.38, 160.60, 160.14, 158.43, 140.08, 136.34, 129.88, 129.08, 123.23, 122.64, 61.41, 60.61, 53.48, 49.33, 47.29, 44.01, 32.35, 23.13, 17.54, 13.61. **HRMS** (ESI) calculated for $C_{25}H_{31}N_2O_6$ $(M+H)^+$: 455.2177, found: 455.2182.

***N,N′*-(ethane-1,2-diyl)bis(*N*-phenylformamide) (43b)**



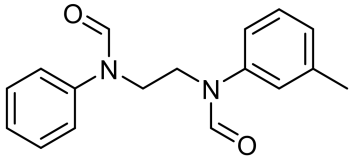
White solid. M. p. 119–120 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.32 (s, 2H), 7.38 (t, *J* = 7.6 Hz, 4H), 7.29 (d, *J* = 7.2 Hz, 2H), 7.06 (d, *J* = 8.0 Hz, 4H), 4.05 (s, 4H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 162.65, 140.69, 129.71, 126.86, 123.50, 43.27. **HRMS** (ESI) calculated for $C_{16}H_{17}N_2O_2$ $(M+H)^+$: 269.1285, found: 269.1290.

***N*-phenyl-*N*-(2-(*N*-*p*-tolylformamido)ethyl)formamide (44b)**



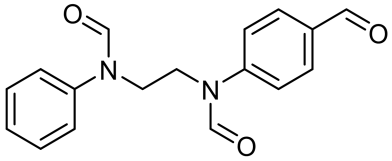
White solid. M. p. 109–111 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.24 (s, 1H), 8.18 (s, 1H), 7.30 (t, *J* = 7.8 Hz, 2H), 7.20 (t, *J* = 7.3 Hz, 1H), 7.08 (d, *J* = 8.0 Hz, 2H), 7.00 (d, *J* = 8.0 Hz, 2H), 6.85 (d, *J* = 8.5 Hz, 2H), 3.94 (s, 4H), 2.27 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 162.67, 162.60, 140.76, 138.08, 136.84, 130.22, 129.68, 126.84, 123.67, 123.58, 43.31, 43.22, 20.92. **HRMS** (ESI) calculated for $C_{17}H_{19}N_2O_2$ $(M+H)^+$: 283.1441, found: 283.1448.

***N*-phenyl-*N*-(2-(*N*-*m*-tolylformamido)ethyl)formamide (45b)**



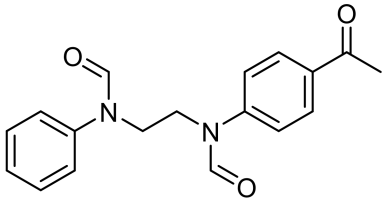
Colorless oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.32 (s, 1H), 8.28 (s, 1H), 7.38 (t, *J* = 7.5 Hz, 2H), 7.31–7.22 (m, 2H), 7.09 (d, *J* = 8.0 Hz, 1H), 7.05 (d, *J* = 8.70 Hz, 2H), 6.85 (d, *J* = 8.0 Hz, 1H), 6.76 (s, 1H), 4.04 (s, 4H), 2.33 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 162.67, 162.62, 140.77, 140.55, 139.72, 129.65, 129.45, 127.62, 126.80, 124.28, 123.53, 120.58, 43.28, 21.38. **HRMS** (ESI) calculated for $C_{17}H_{19}N_2O_2$ $(M+H)^+$: 283.1441, found: 283.1450.

***N*-(4-formylphenyl)-*N*-(2-(*N*-phenylformamido)ethyl)formamide (46b)**



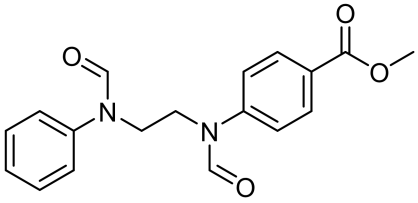
White solid. M. p. 125–127 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 10.00 (s, 1H), 8.51 (s, 1H), 8.35 (s, 1H), 7.92 (d, *J* = 8.5 Hz, 2H), 7.39 (t, *J* = 7.5 Hz, 2H), 7.31 (d, *J* = 7.0 Hz, 1H), 7.27 (d, *J* = 8.0 Hz, 2H), 7.07 (d, *J* = 8.0 Hz, 2H), 4.14 (t, *J* = 6.3 Hz, 2H), 4.08 (t, *J* = 6.3 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 190.75, 162.69, 162.05, 145.87, 140.59, 134.10, 131.35, 129.83, 127.00, 123.28, 122.12, 43.26, 42.85. **HRMS** (ESI) calculated for $C_{17}H_{17}N_2O_3$ $(M+H)^+$: 297.1234, found: 297.1238.

***N*-(4-acetylphenyl)-*N*-(2-(*N*-phenylformamido)ethyl)formamide (47b)**



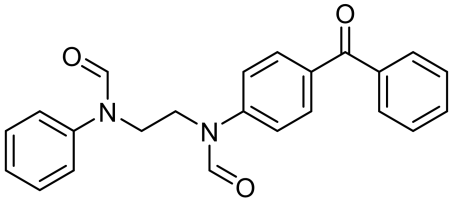
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.47 (s, 1H), 8.34 (s, 1H), 7.99 (d, *J* = 8.4 Hz, 2H), 7.39 (t, *J* = 7.8 Hz, 2H), 7.33–7.27 (m, 1H), 7.19 (d, *J* = 8.4 Hz, 2H), 7.07 (d, *J* = 8.0 Hz, 2H), 4.12 (t, *J* = 5.8 Hz, 2H), 4.06 (t, *J* = 5.8 Hz, 2H), 2.62 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 196.72, 162.67, 162.13, 144.70, 140.63, 134.90, 130.08, 129.81, 126.98, 123.33, 121.88, 43.27, 42.84, 26.61. **HRMS** (ESI) calculated for $C_{18}H_{19}N_2O_3$ $(M+H)^+$: 311.1390, found: 311.1395.

methyl 4-(*N*-(2-(*N*-phenylformamido)ethyl)formamido)benzoate (48b)



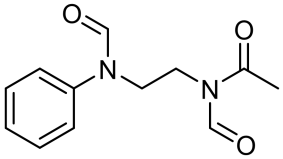
White solid. M. p. 107–109 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.45 (s, 1H), 8.33 (s, 1H), 8.05 (d, *J* = 8.5 Hz, 2H), 7.38 (t, *J* = 7.8 Hz, 2H), 7.31–7.29 (m, 1H), 7.13 (d, *J* = 8.5 Hz, 2H), 7.05 (d, *J* = 8.0 Hz, 2H), 4.11 (t, *J* = 6.0 Hz, 2H), 4.06 (t, *J* = 6.0 Hz, 2H), 3.94 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 166.14, 162.64, 162.18, 144.61, 140.63, 131.25, 129.78, 128.05, 126.92, 123.31, 121.87, 52.30, 43.24, 42.91. **HRMS** (ESI) calculated for $C_{18}H_{19}N_2O_4$ $(M+H)^+$: 327.1340, found: 327.1349.

***N*-(4-benzoylphenyl)-*N*-(2-(*N*-phenylformamido)ethyl)formamide (49b)**



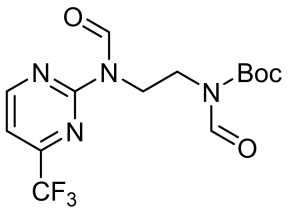
White solid. M. p. 99–101 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.50 (s, 1H), 8.36 (s, 1H), 7.85 (d, *J* = 8.5 Hz, 2H), 7.80 (d, *J* = 8.0 Hz, 2H), 7.62 (t, *J* = 7.3 Hz, 1H), 7.51 (t, *J* = 7.8 Hz, 2H), 7.40 (t, *J* = 7.8 Hz, 2H), 7.31 (d, *J* = 7.5 Hz, 1H), 7.21 (d, *J* = 8.0 Hz, 2H), 7.10 (d, *J* = 8.0 Hz, 2H), 4.14 (t, *J* = 6.0 Hz, 2H), 4.09 (t, *J* = 6.0 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 195.29, 162.71, 162.22, 144.22, 140.66, 137.28, 135.39, 132.67, 131.83, 129.94, 129.82, 128.45, 126.98, 123.34, 121.81, 43.29, 42.97. **HRMS** (ESI) calculated for $C_{23}H_{21}N_2O_3$ $(M+H)^+$: 373.1547, found: 373.1548.

***N*-formyl-*N*-(2-(*N*-phenylformamido)ethyl)acetamide (50b)**



Colorless oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.02 (s, 1H), 8.32 (s, 1H), 7.42 (t, *J* = 7.8 Hz, 2H), 7.31 (t, *J* = 7.6 Hz, 1H), 7.23–7.19 (m, 2H), 4.03 (t, *J* = 5.8 Hz, 2H), 3.96 (t, *J* = 5.8 Hz, 2H), 2.30 (s, 3H).**^{13}C NMR** (100 MHz, $CDCl_3$) δ 171.34, 162.92, 162.85, 140.92, 129.75, 127.05, 123.97, 43.35, 38.12, 22.71. **HRMS** (ESI) calculated for $C_{12}H_{15}N_2O_3$ $(M+H)^+$: 235.1077, found: 235.1085.

***tert*-butyl-formyl(2-(*N*-(4-(trifluoromethyl)pyrimidin-2-yl)formamido)ethyl)carbamate (51b)**



Brown oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.86 (s, 1H), 9.07 (s, 1H), 8.80 (d, J = 5.0 Hz, 1H), 7.37 (d, J = 4.9 Hz, 1H), 4.30 (t, J = 5.0 Hz, 2H), 3.98 (t, J = 5.0 Hz, 2H), 1.47 (s, 9H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 163.26, 162.89, 160.63, 159.37, 156.51 (q, $^2J_{CF3}$ = 36.8 Hz), 152.28, 120.01 (q, $^1J_{CF3}$ = 273.6 Hz), 112.04 (q, $^3J_{CF3}$ = 2.6 Hz), 84.17, 39.19, 38.44, 27.86. **HRMS** (ESI) calculated for $C_{14}H_{18}F_3N_4O_4$ $(M+H)^+$: 363.1275, found: 363.1280.

9. References

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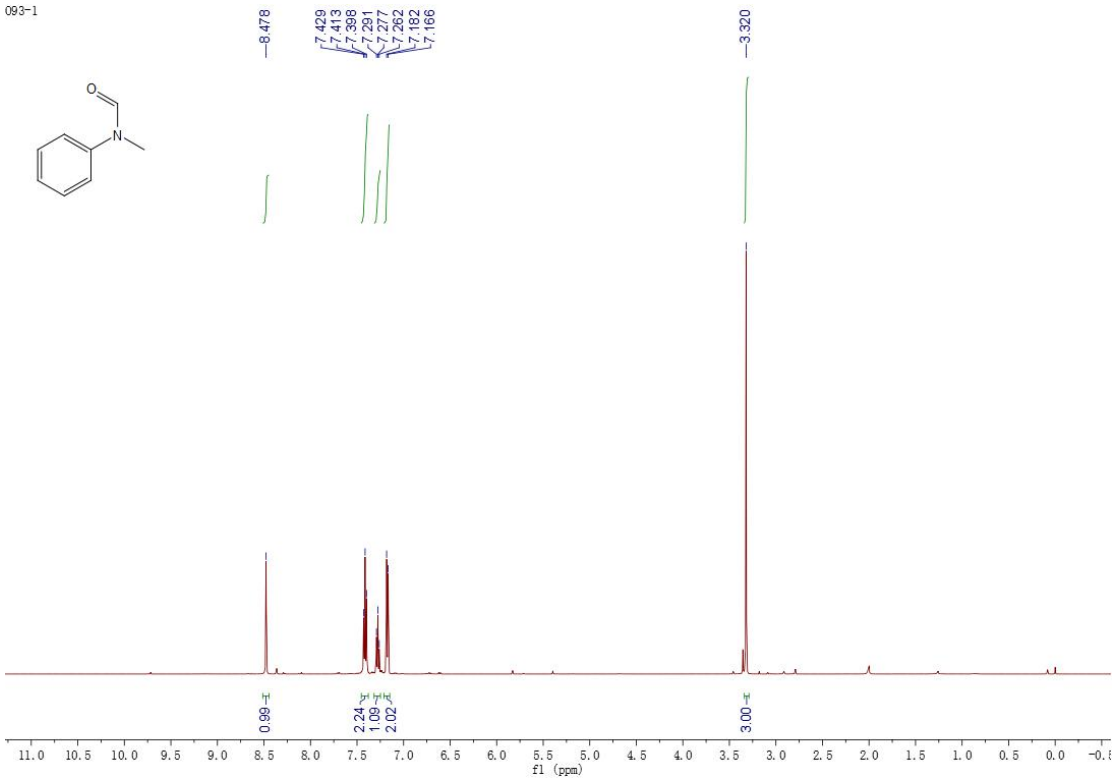
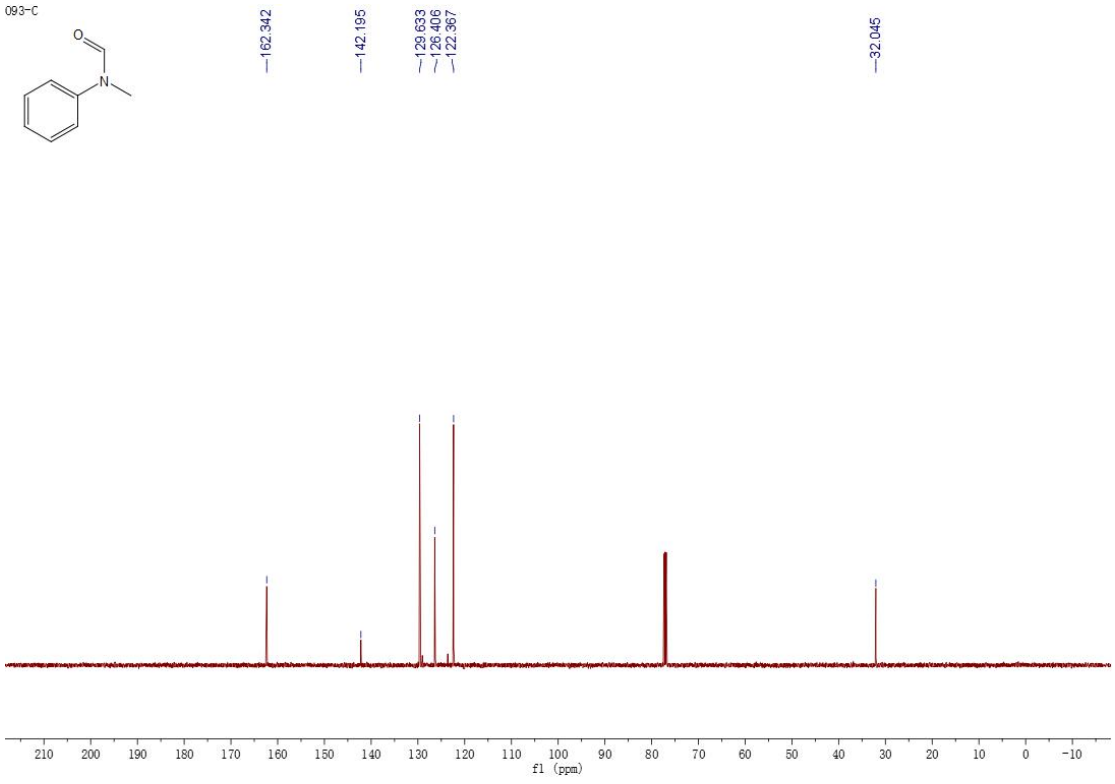
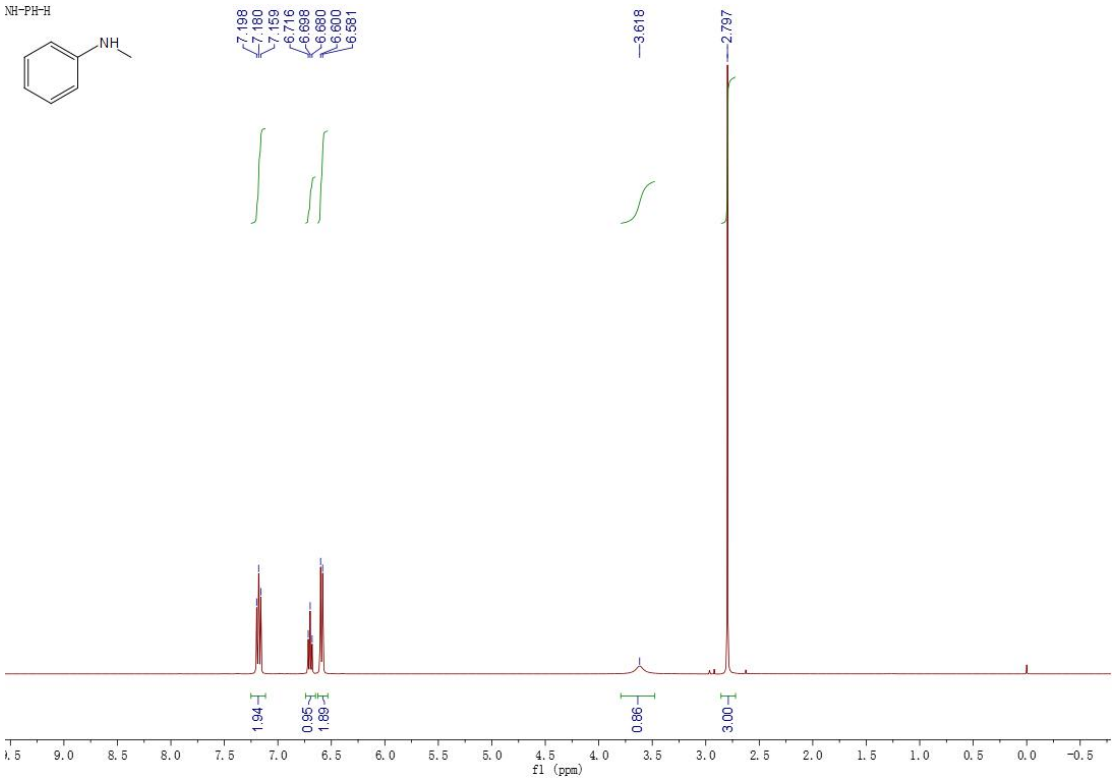
10. ^{1}H and ^{13}C NMR Spectra

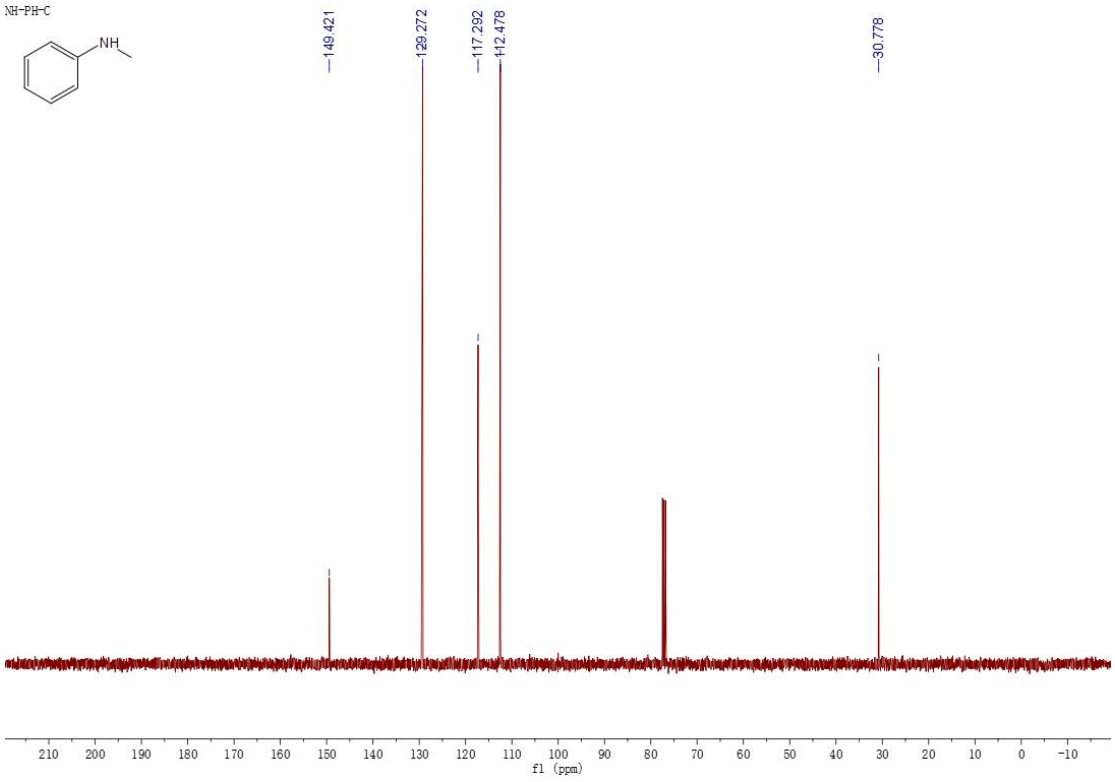
NMR of 1c



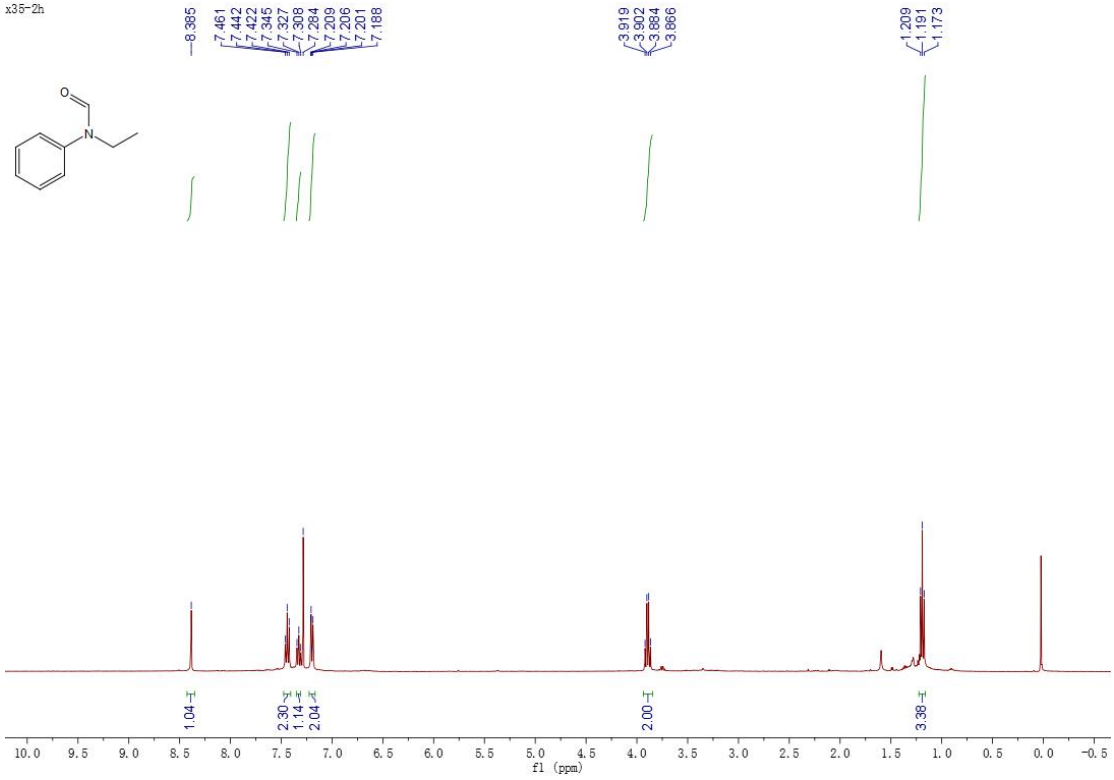


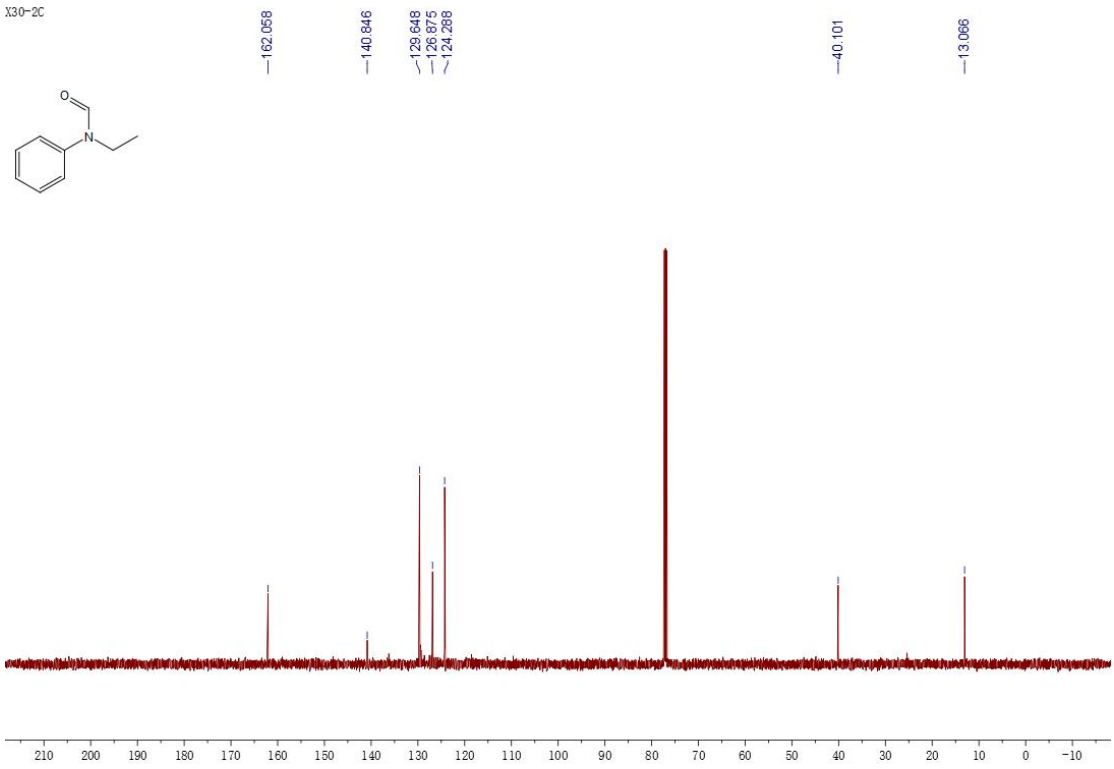
NMR of 1d


NH-PH-H
NH
7.198
7.180
7.159
6.716
6.698
6.680
6.600
6.581
3.618
2.797
1.94
0.95
1.89
0.86
3.00
f1 (ppm)

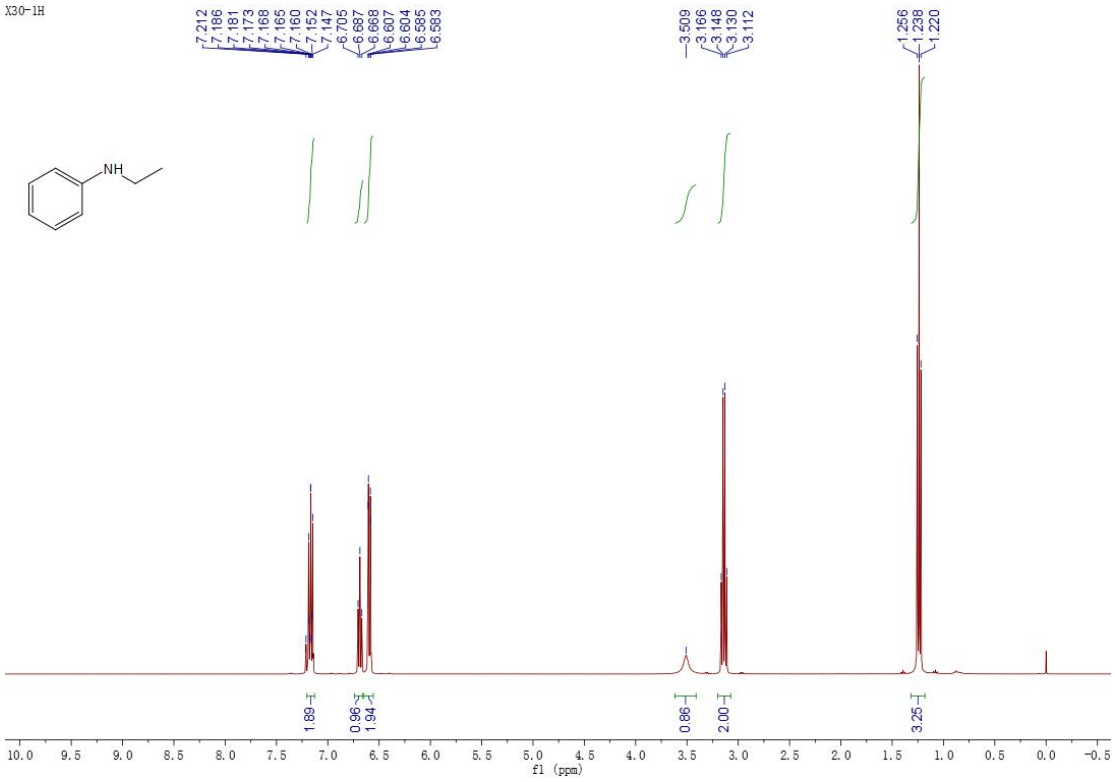

NH-PH-C
NH
149.421
129.272
117.292
112.478
30.778
f1 (ppm)

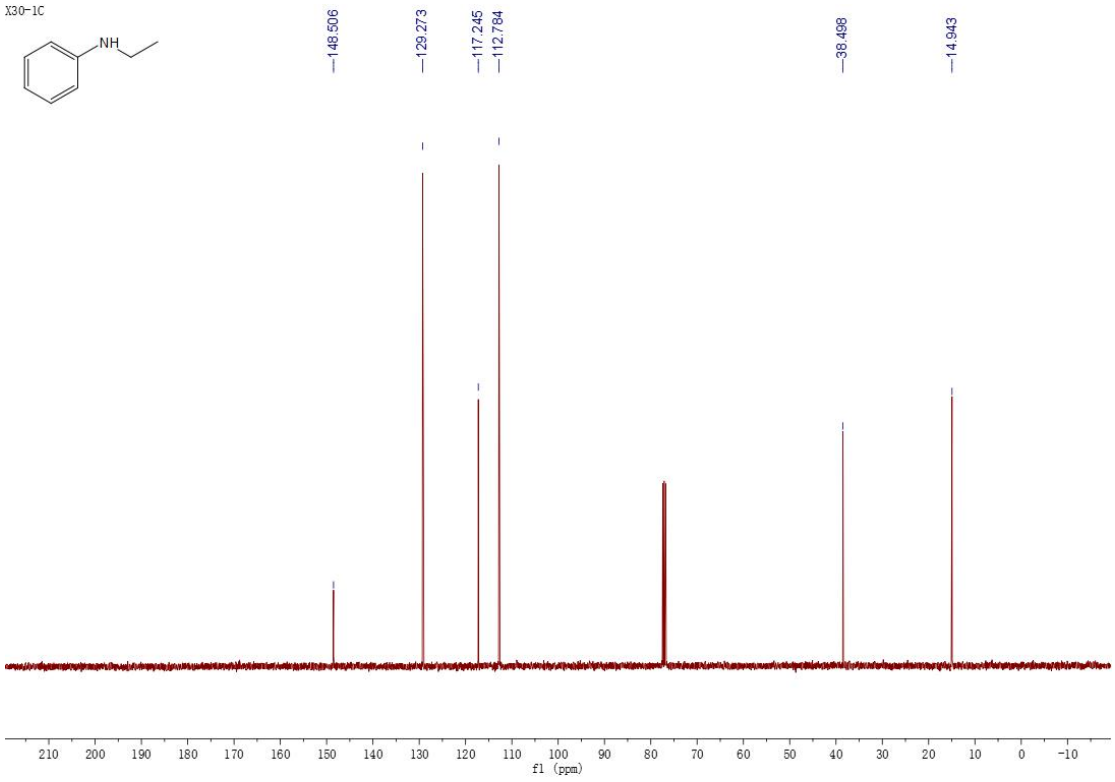
NMR of 2b


x35-2h
8.385
7.461
7.442
7.422
7.345
7.327
7.308
7.284
7.209
7.206
7.201
7.188
3.919
3.902
3.884
3.866
1.209
1.191
1.173
1.04
2.30
1.14
2.04
2.00
3.38
f1 (ppm)

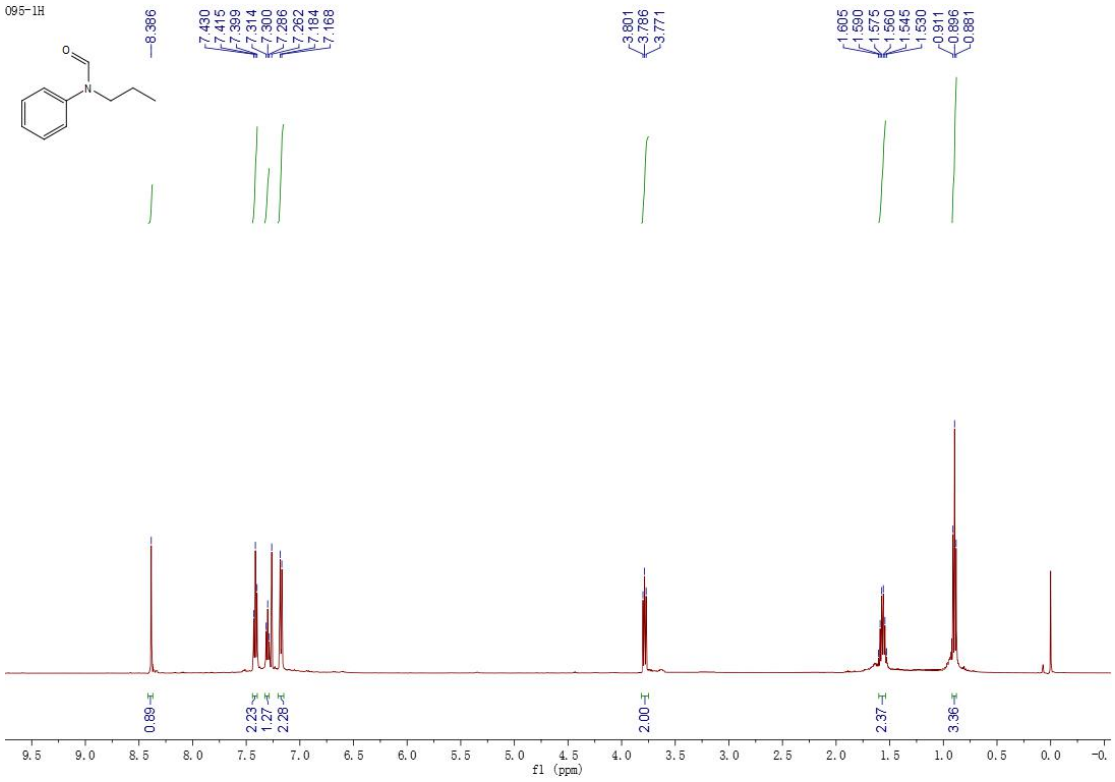

X30-2C
162.058
140.846
129.648
126.875
124.288
40.101
13.066

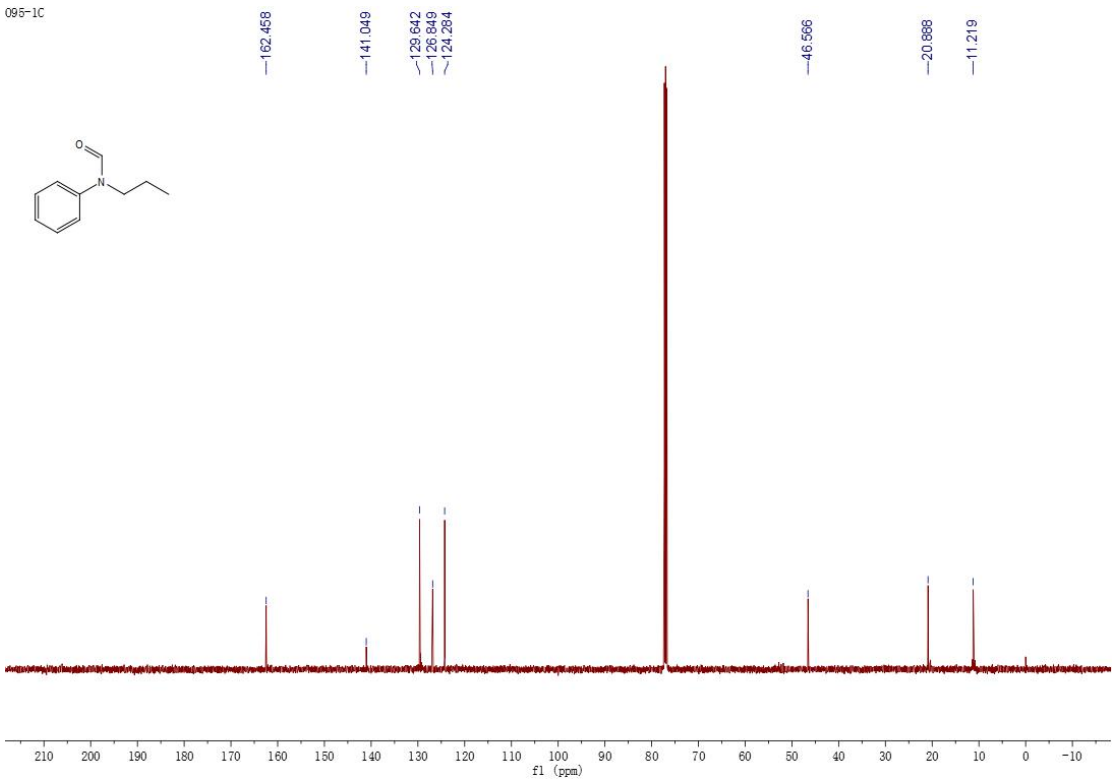
NMR of 2d


X30-1H
7.212
7.186
7.181
7.173
7.168
7.165
7.160
7.152
7.147
6.705
6.687
6.668
6.607
6.604
6.585
6.583
3.509
3.166
3.148
3.130
3.112
1.256
1.238
1.220
NH
1.89
0.96
1.94
0.86
2.00
3.25
f1 (ppm)

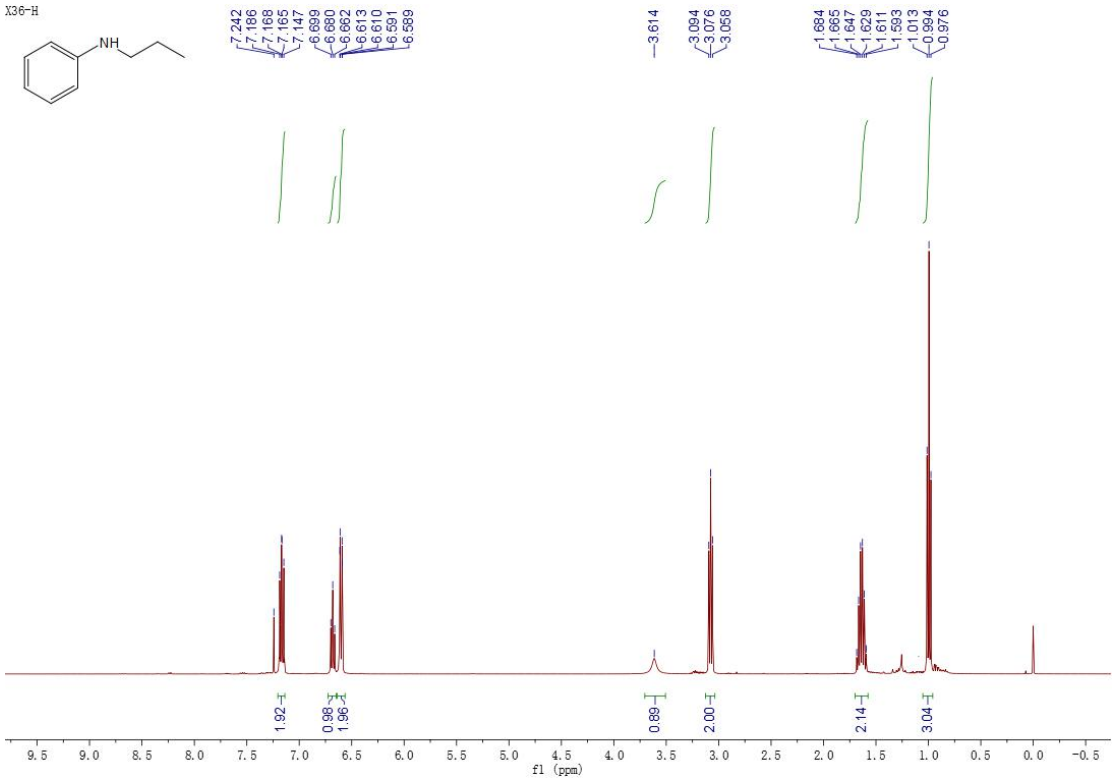

X30-1C
148.506
129.273
117.245
112.784
38.498
14.943
NH
f1 (ppm)

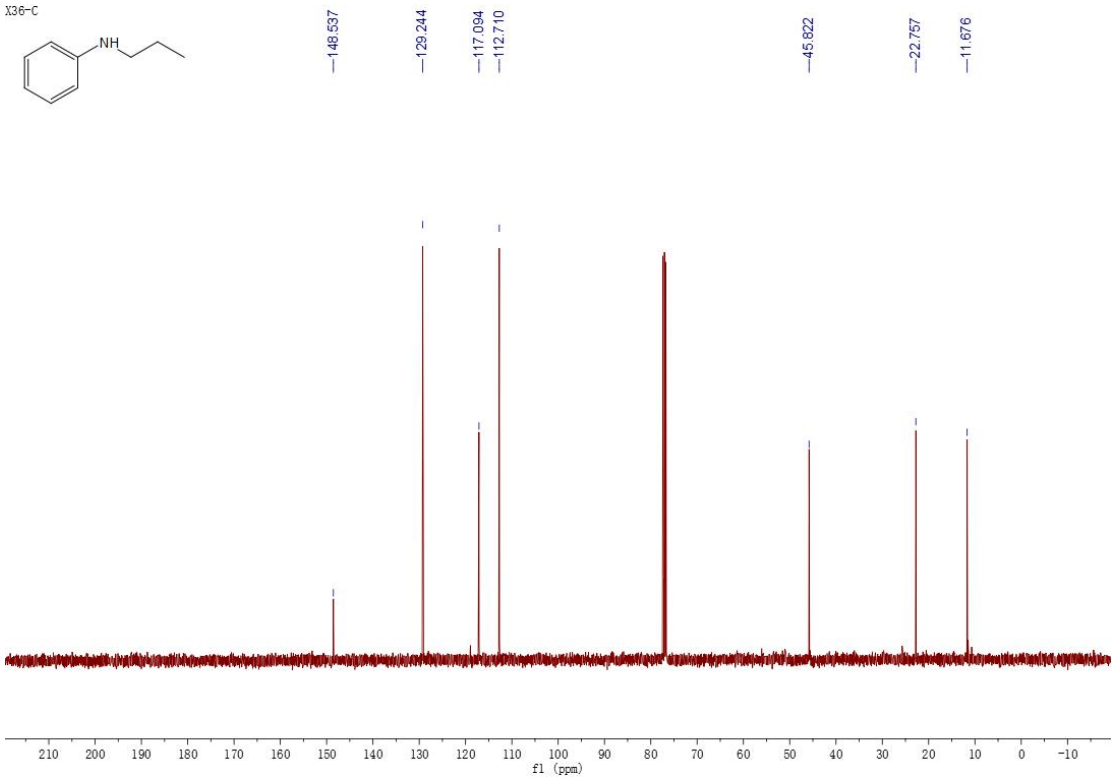
NMR of 3b


095-1H
8.386
7.430
7.415
7.399
7.314
7.300
7.286
7.262
7.184
7.168
3.801
3.786
3.771
1.605
1.590
1.575
1.560
1.545
1.530
0.911
0.896
0.881
0.89
2.23
1.27
2.28
2.00
2.37
3.36
f1 (ppm)

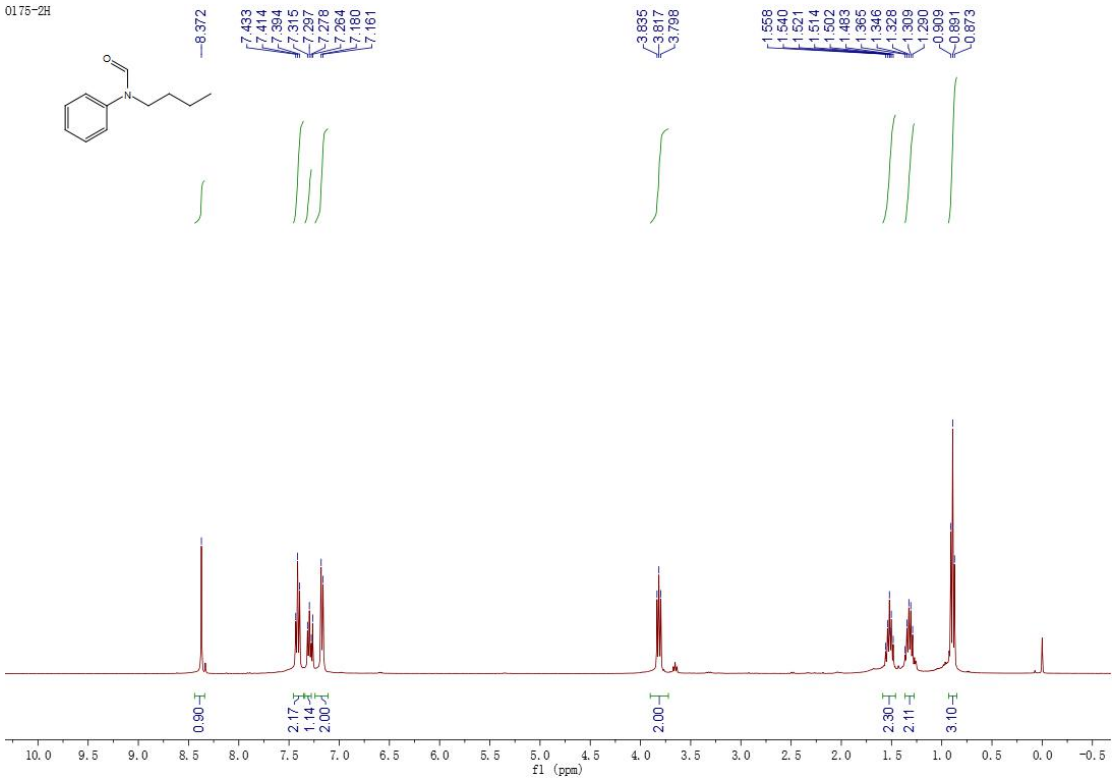

095-1C
162.458
141.049
129.642
126.849
124.284
46.566
20.888
11.219
f1 (ppm)

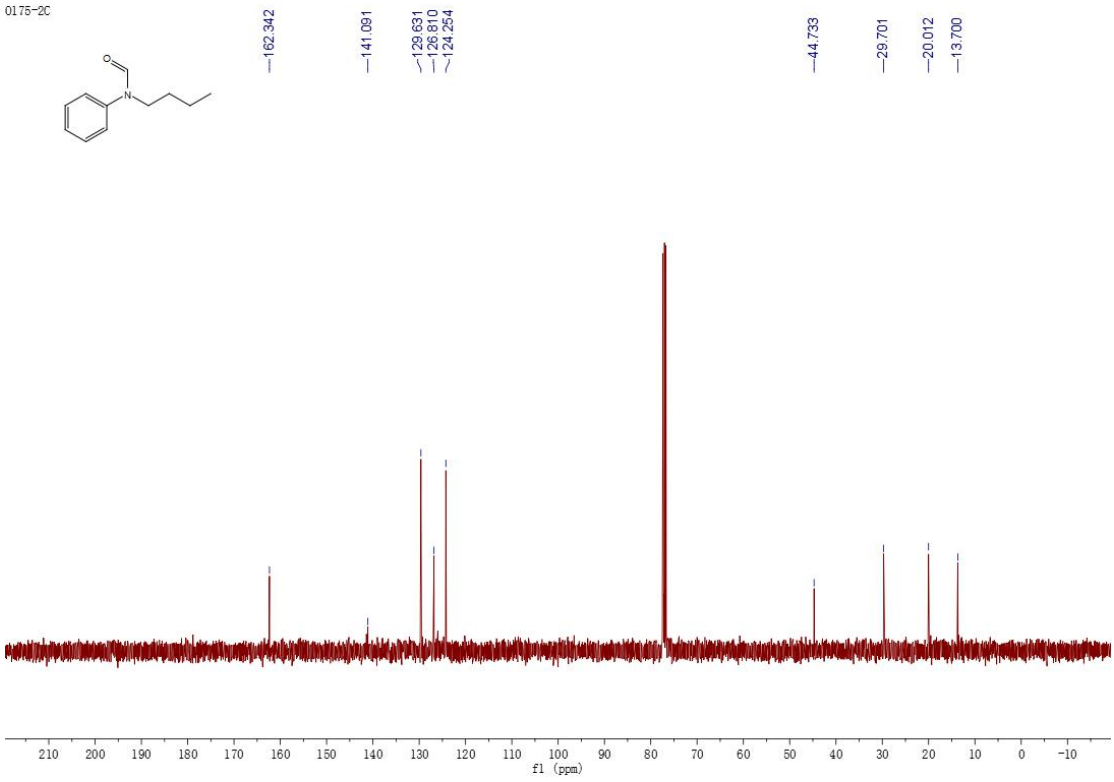
NMR of 3d


X36-H
NH
7.242
7.186
7.168
7.165
7.147
6.699
6.680
6.662
6.613
6.610
6.591
6.589
3.614
3.094
3.076
3.058
1.684
1.665
1.647
1.629
1.611
1.593
1.013
0.994
0.976
1.92
0.98
1.96
0.89
2.00
2.14
3.04
f1 (ppm)

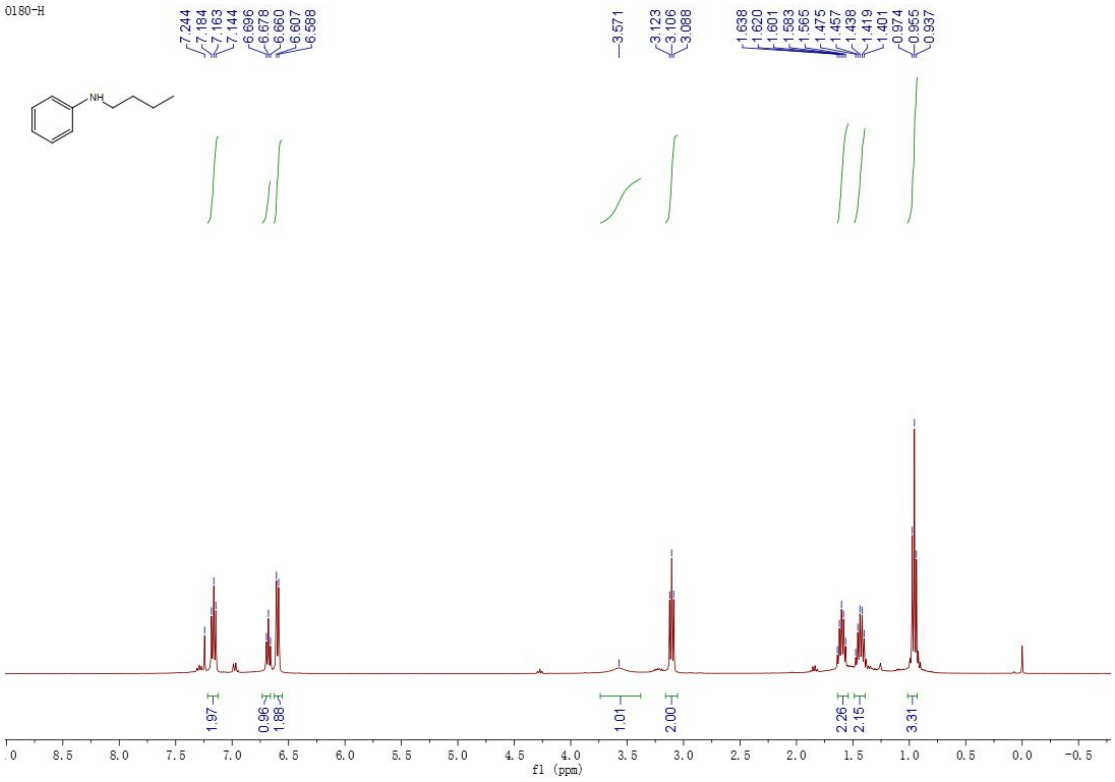

X36-C
NH
148.537
129.244
117.094
112.710
45.822
22.757
11.676
f1 (ppm)

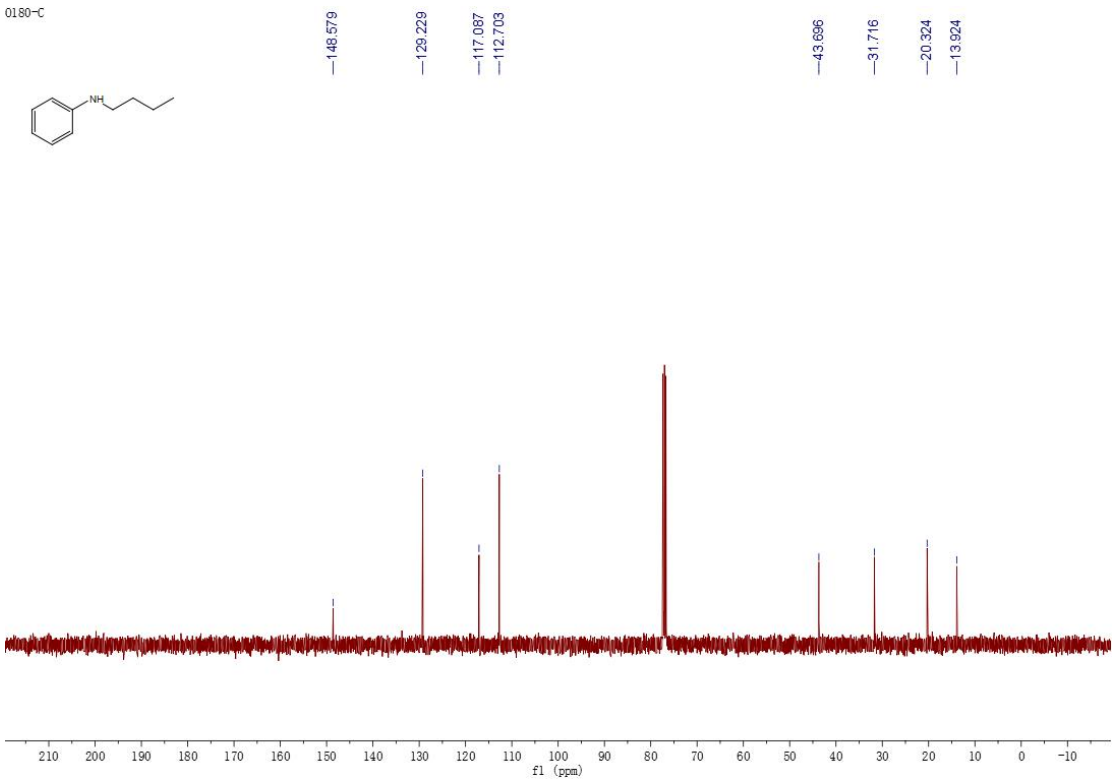
NMR of 4b


0175-2H
8.372
7.433
7.414
7.394
7.315
7.297
7.278
7.284
7.180
7.161
3.835
3.817
3.798
1.558
1.540
1.521
1.514
1.502
1.483
1.365
1.346
1.328
1.309
1.290
0.909
0.891
0.873
0.90
2.17
1.14
2.00
2.00
2.30
2.11
3.10
f1 (ppm)

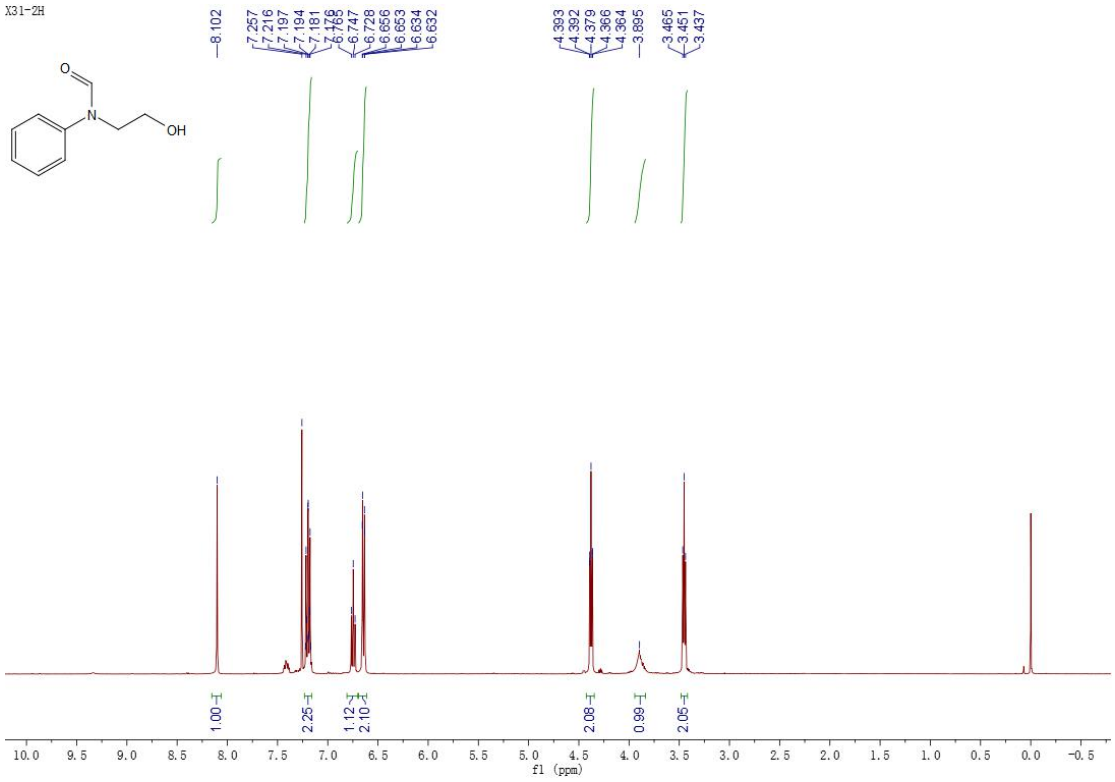

0175-2C
162.342
141.091
129.631
126.810
124.254
44.733
29.701
20.012
13.700
f1 (ppm)

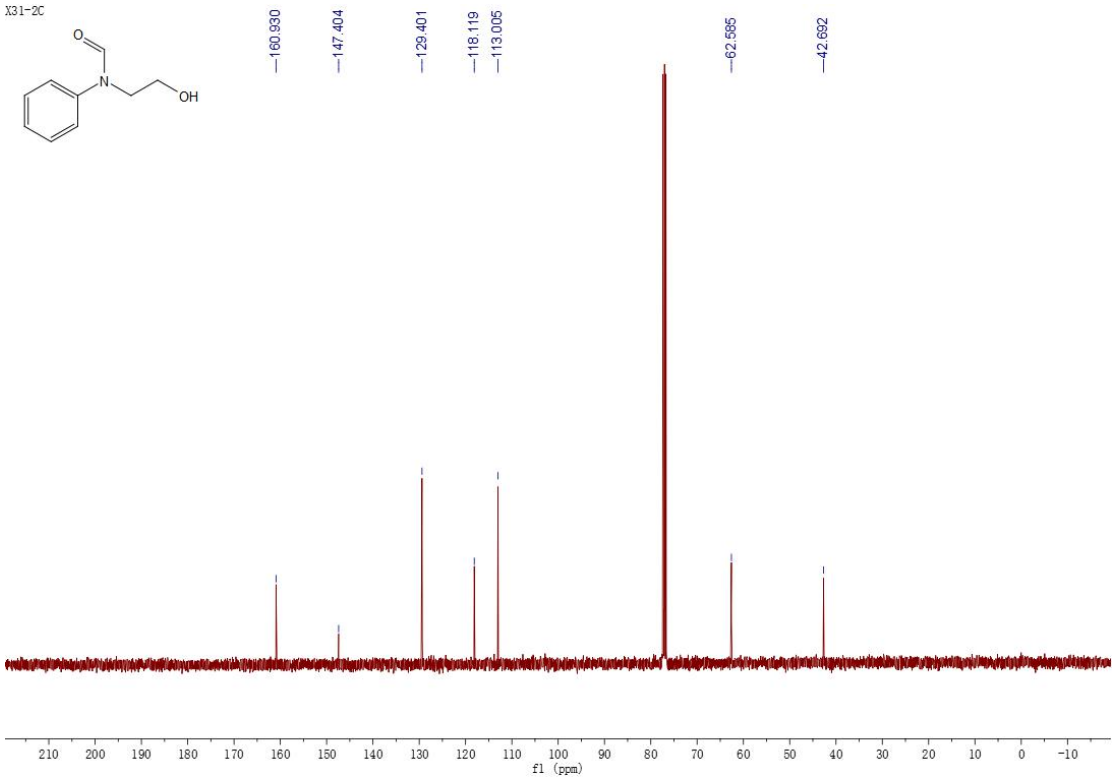
NMR of 4d


0180-H
7.244
7.184
7.163
7.144
6.696
6.678
6.660
6.607
6.588
3.571
3.123
3.106
3.088
1.638
1.620
1.601
1.583
1.565
1.475
1.457
1.438
1.419
1.401
0.974
0.955
0.937
NH
1.97
0.96
1.88
1.01
2.00
2.26
2.15
3.31
f1 (ppm)

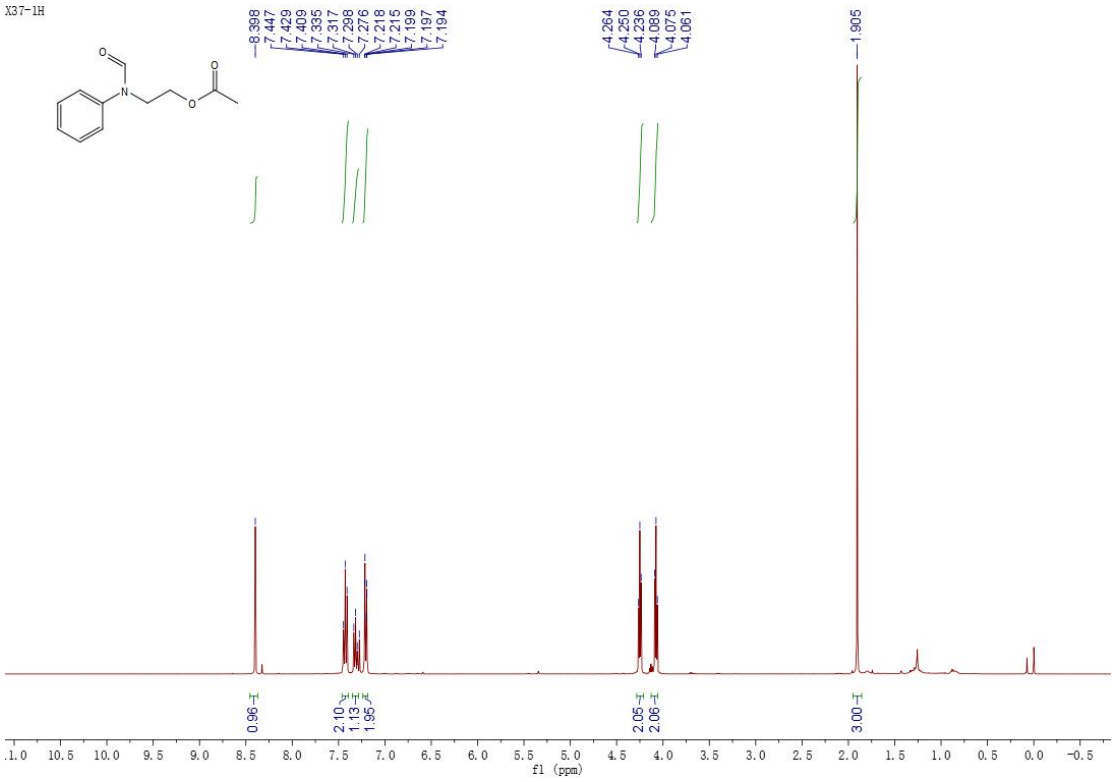

0180-C
148.579
129.229
117.087
112.703
43.696
31.716
20.324
13.924
NH
f1 (ppm)

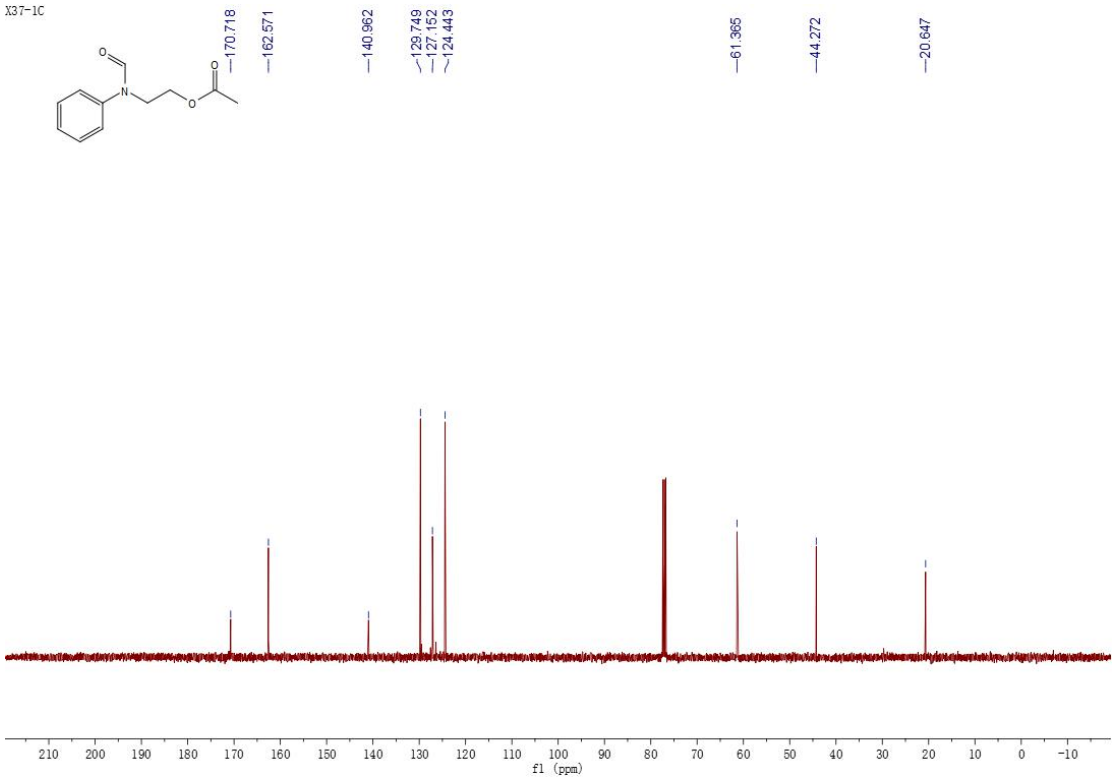
NMR of 5b


X31-2H
8.102
7.257
7.216
7.197
7.194
7.181
6.747
6.728
6.656
6.653
6.634
6.632
4.393
4.392
4.379
4.366
4.364
3.895
3.465
3.451
3.437
1.00
2.25
1.12
2.10
2.08
0.99
2.05
f1 (ppm)

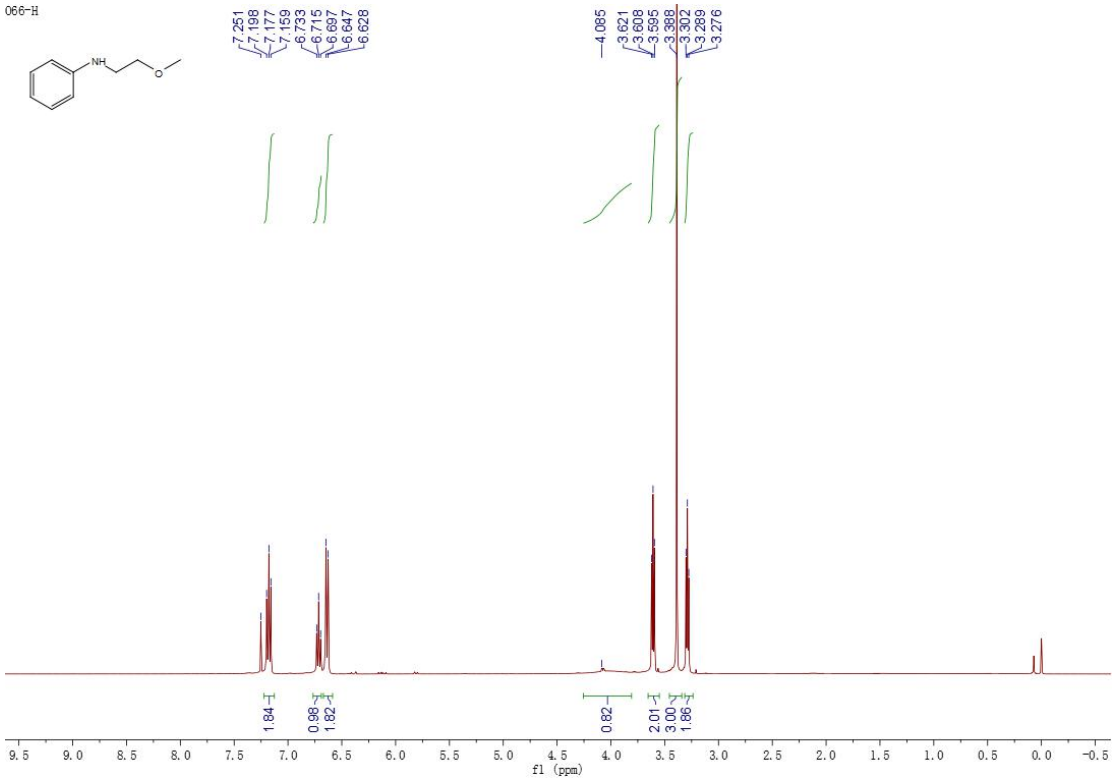

X31-2C
160.930
147.404
129.401
118.119
113.005
62.585
42.692
f1 (ppm)

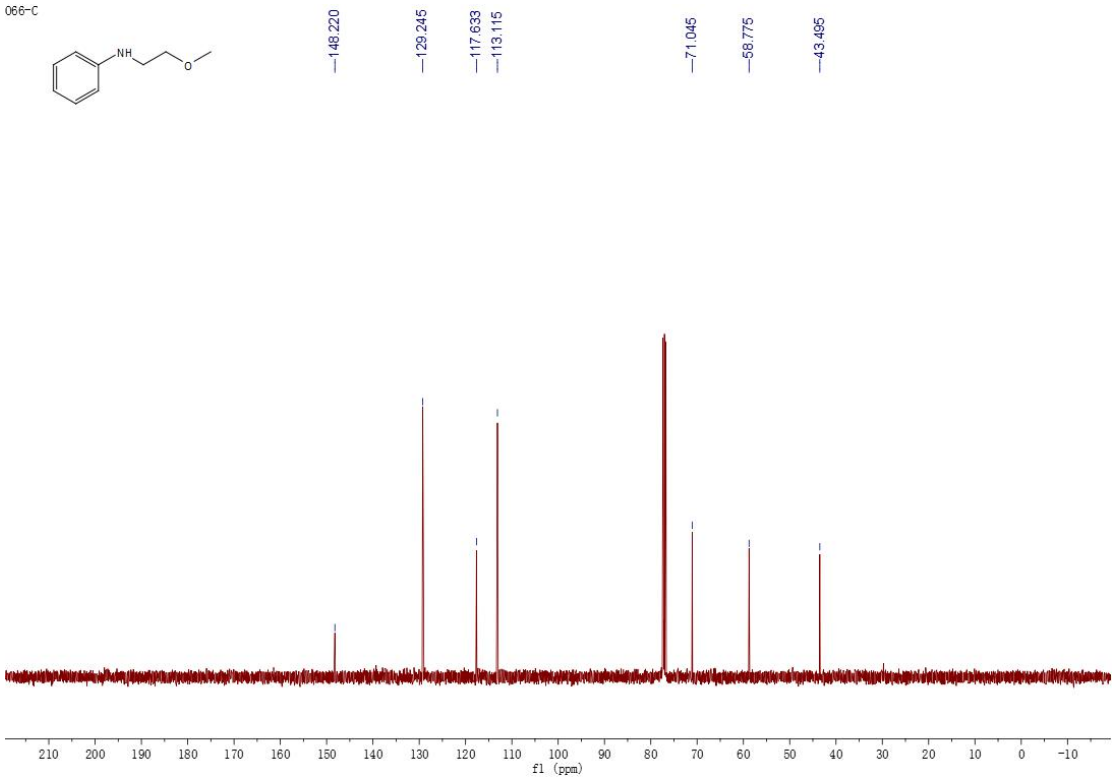
NMR of 6b


X37-1H
8.398
7.447
7.429
7.409
7.335
7.317
7.298
7.276
7.218
7.215
7.199
7.197
7.194
4.264
4.250
4.236
4.089
4.075
4.061
1.905
0.96
2.10
1.13
1.95
2.05
2.06
3.00
f1 (ppm)

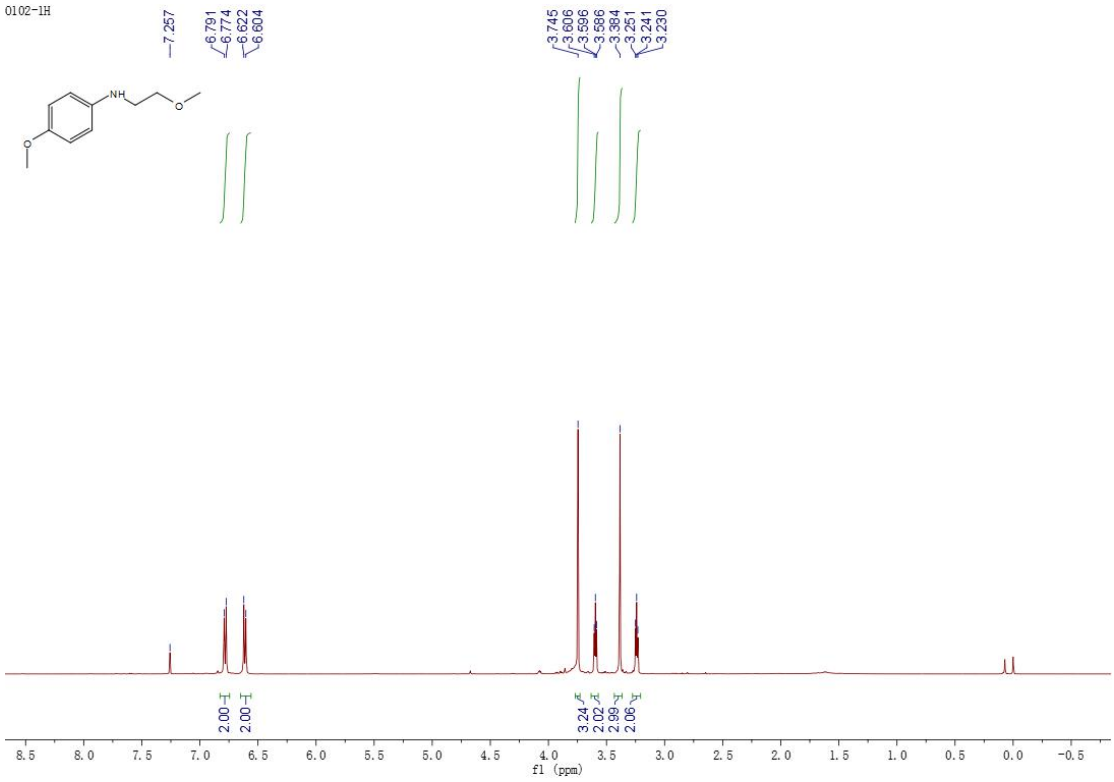

X37-1C
170.718
162.571
140.962
129.749
127.152
124.443
61.365
44.272
20.647
f1 (ppm)

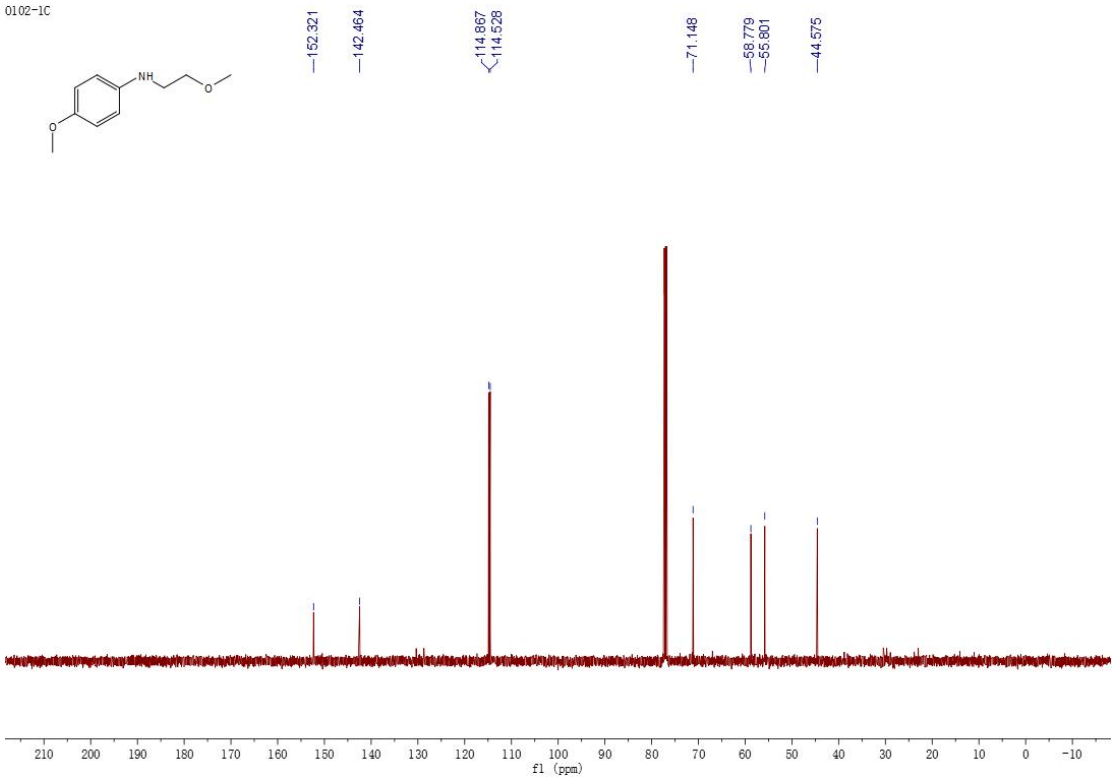
NMR of 7d


066-H
7.251
7.198
7.177
7.159
6.733
6.715
6.697
6.647
6.628
4.085
3.621
3.608
3.595
3.388
3.302
3.289
3.276
1.84
0.98
1.82
0.82
2.01
3.00
1.86
f1 (ppm)

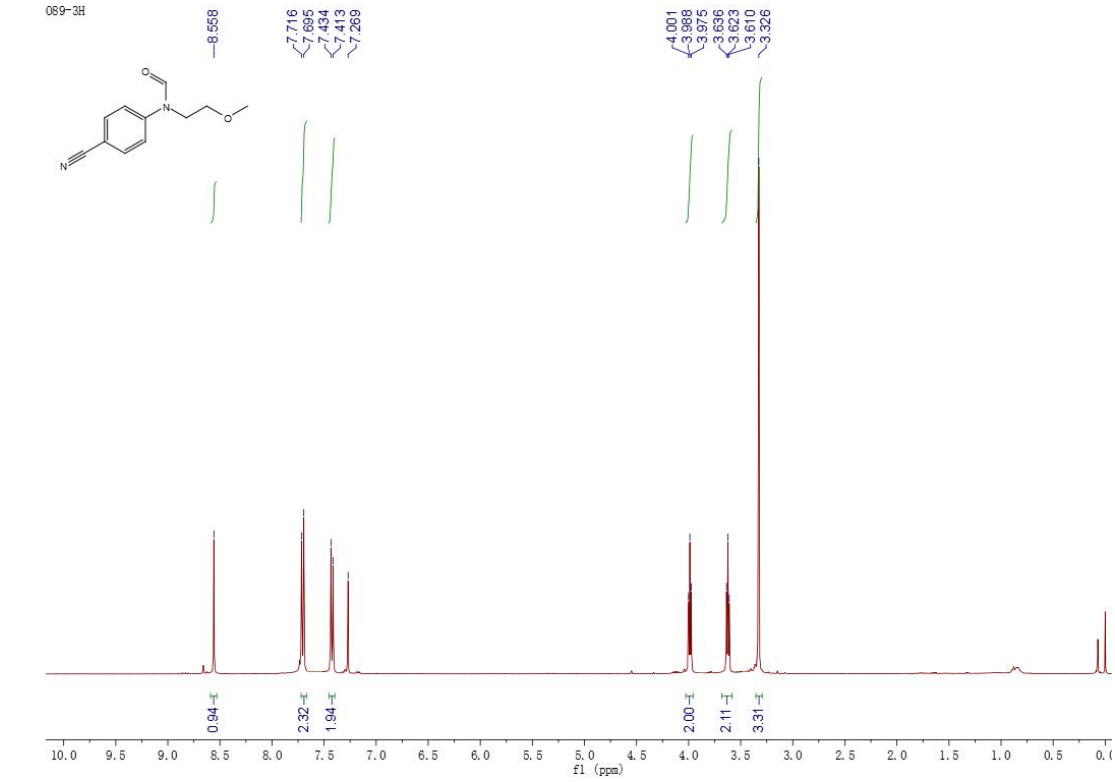

066-C
148.220
129.245
117.633
113.115
71.045
58.775
43.495
f1 (ppm)

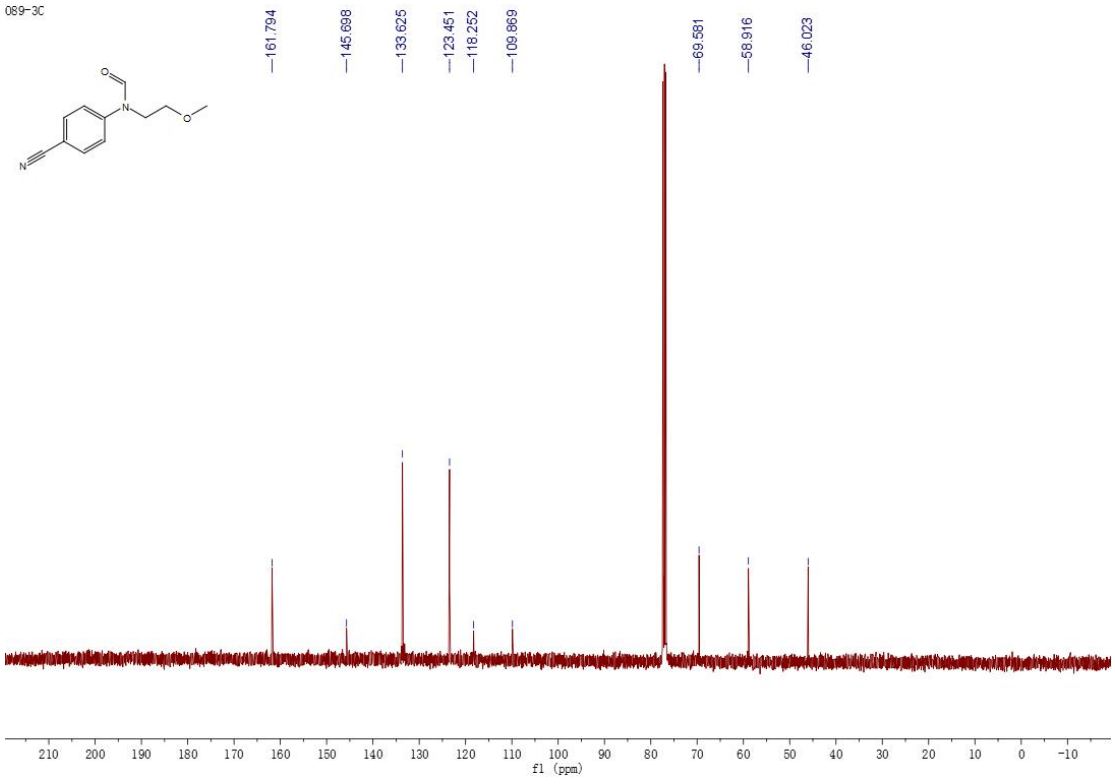
NMR of 8d


0102-1H
7.257
6.791
6.774
6.622
6.604
3.745
3.606
3.596
3.586
3.384
3.251
3.241
3.230
2.00
2.00
3.24
2.02
2.99
2.06
f1 (ppm)

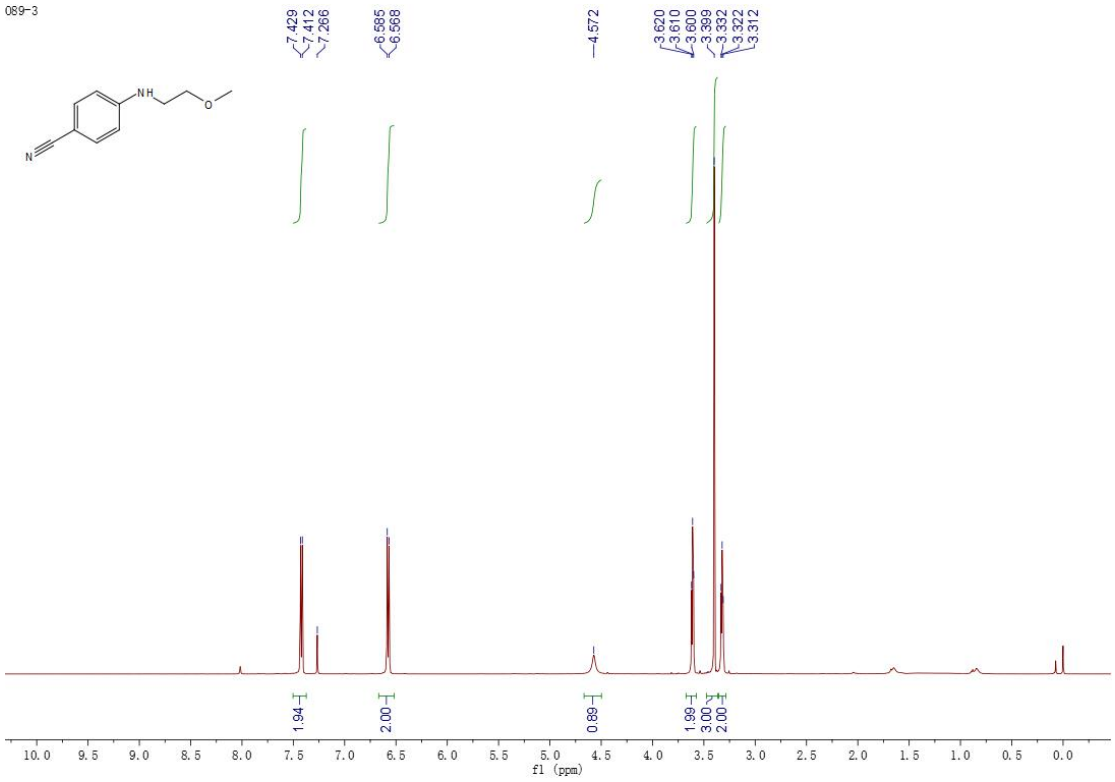

0102-1C
152.321
142.464
114.867
114.528
71.148
58.779
55.801
44.575
f1 (ppm)

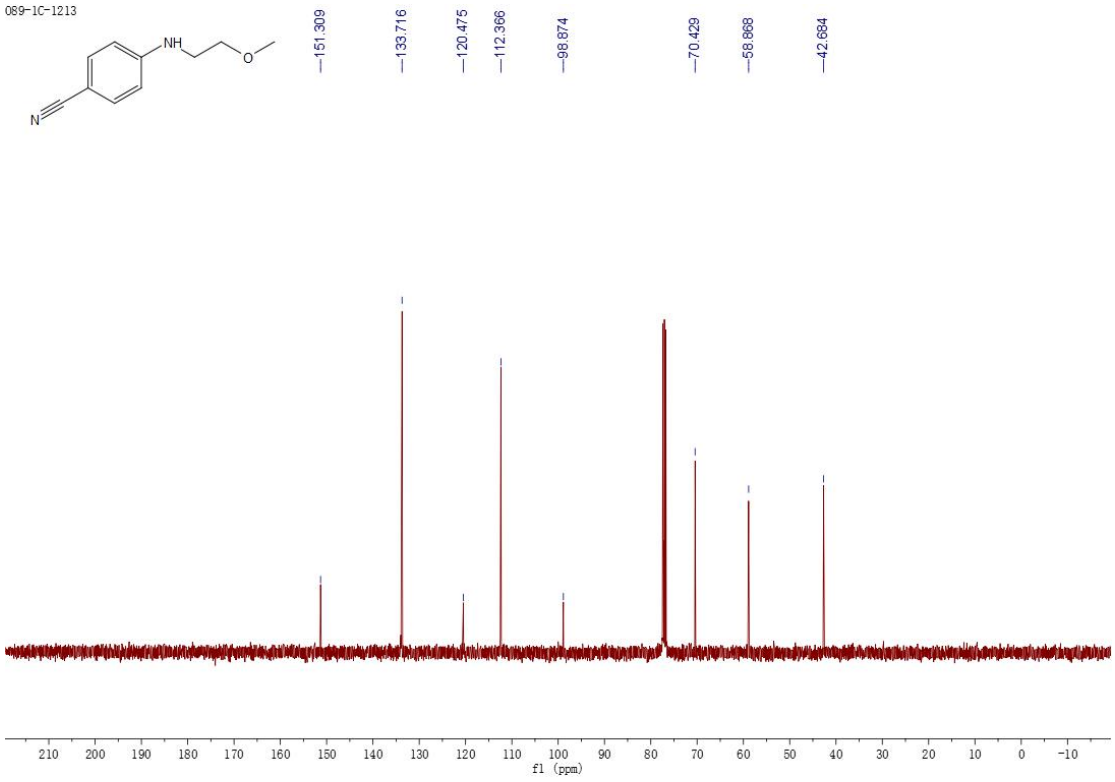
NMR of 9c


089-3H
8.558
7.716
7.695
7.434
7.413
7.269
4.001
3.988
3.975
3.636
3.623
3.610
3.326
0.94
2.32
1.94
2.00
2.11
3.31
f1 (ppm)

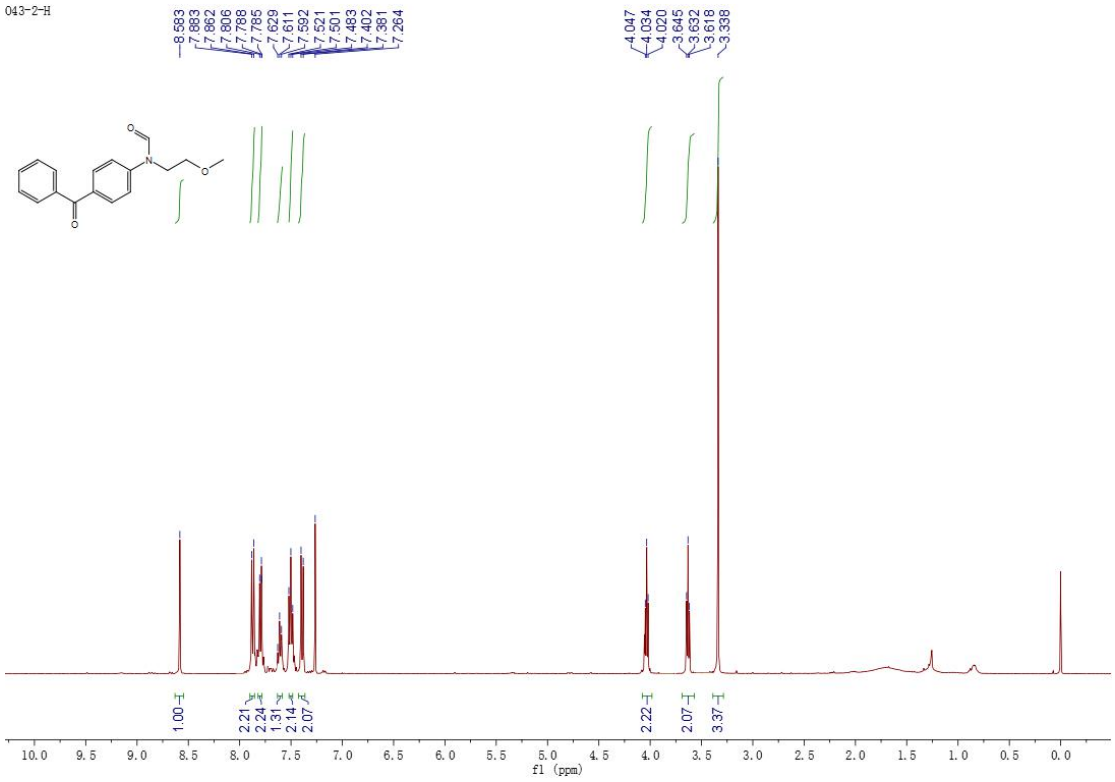

089-3C
161.794
145.698
133.625
123.451
118.252
109.869
69.581
58.916
46.023
f1 (ppm)

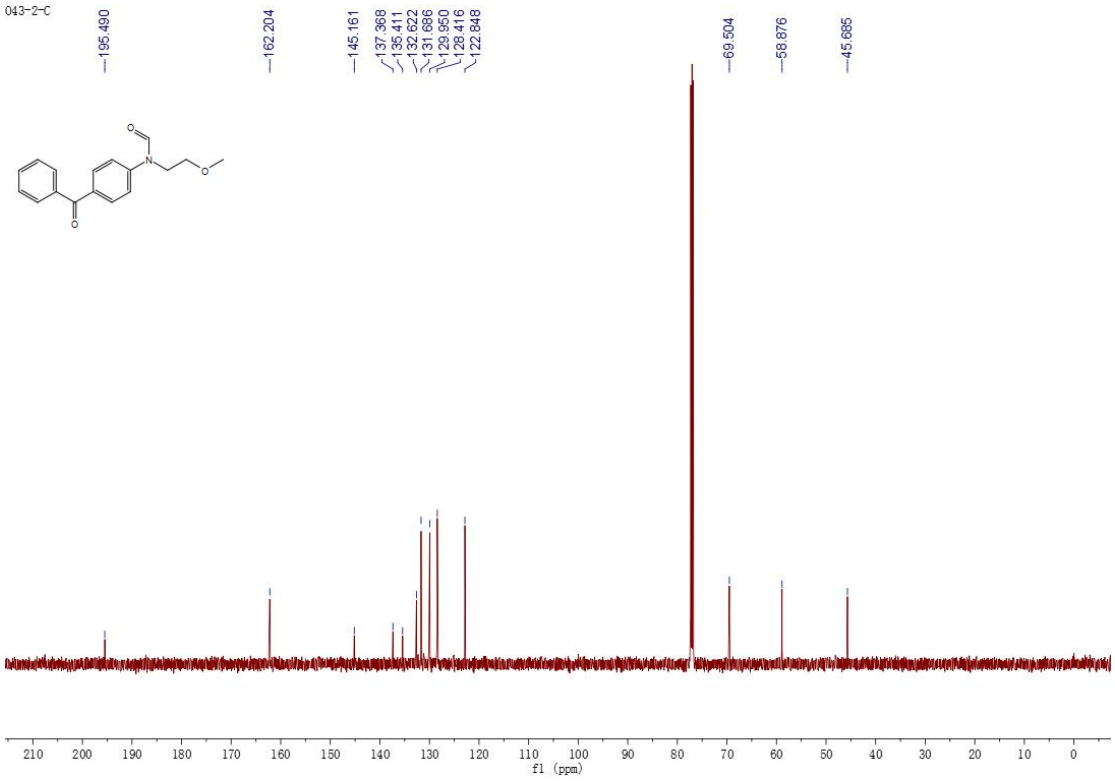
NMR of 9d


089-3
7.429
7.412
7.266
6.585
6.568
4.572
3.620
3.610
3.600
3.399
3.332
3.322
3.312
NH
O
N
1.94
2.00
0.89
1.99
3.00
2.00
f1 (ppm)

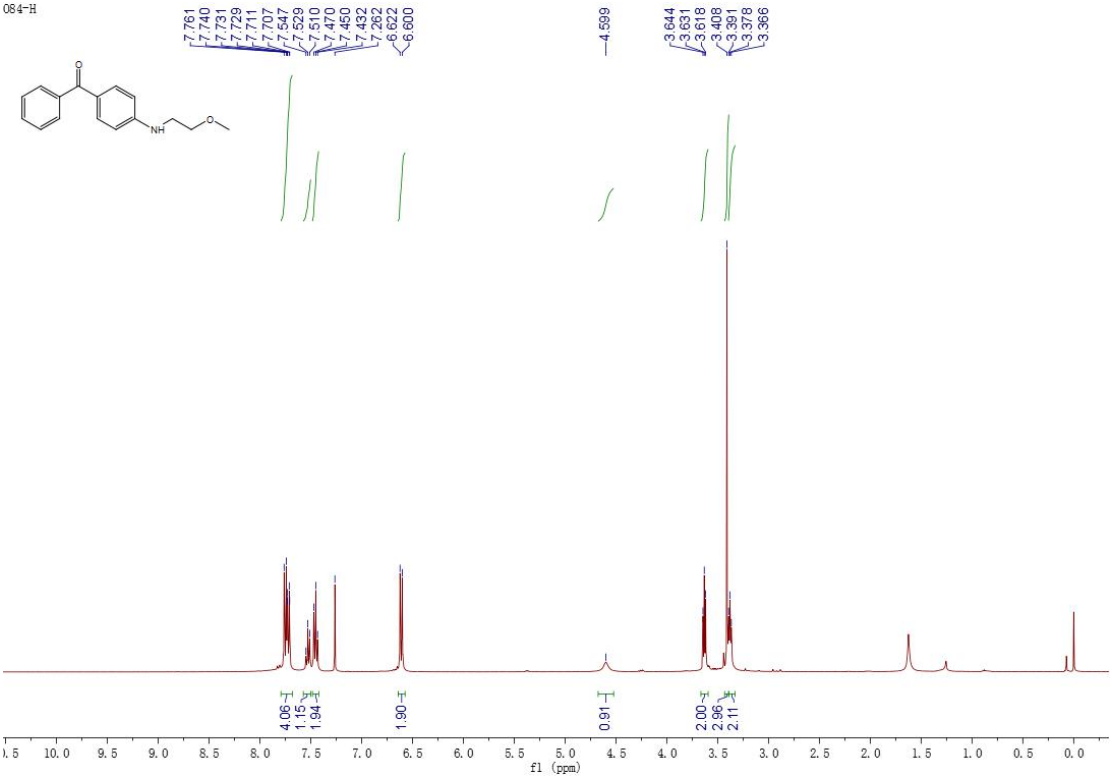

089-1C-1213
151.309
133.716
120.475
112.366
98.874
70.429
58.868
42.684
NH
O
N
f1 (ppm)

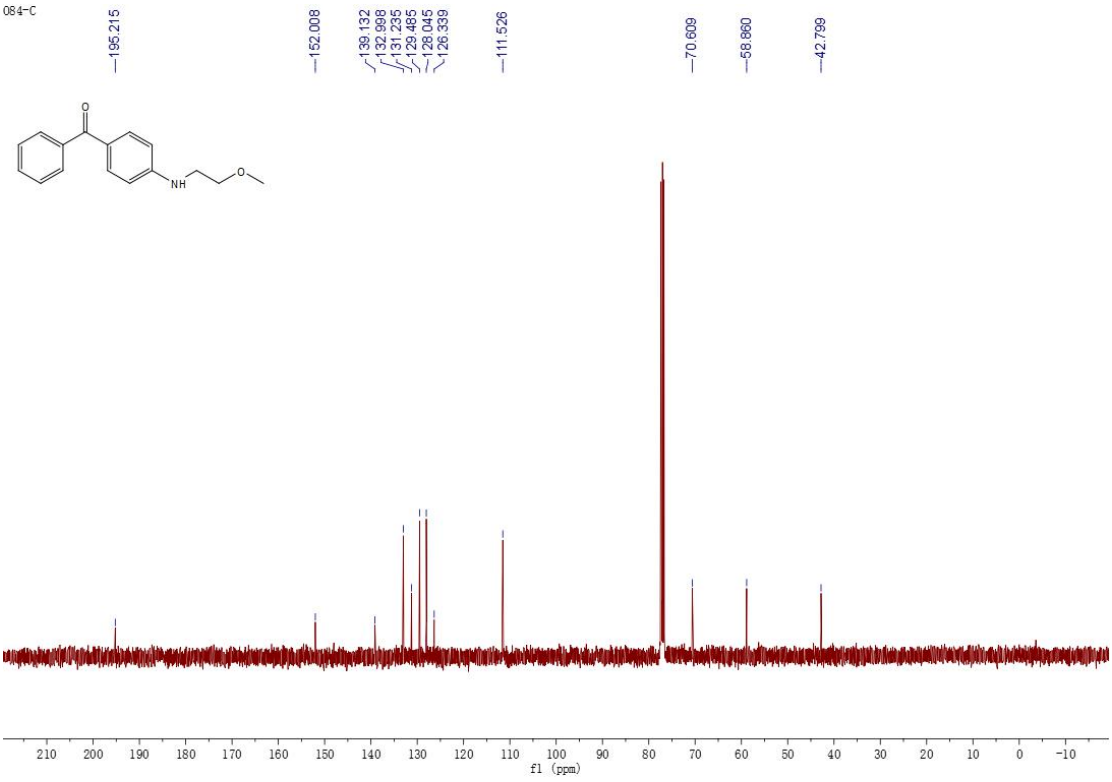
NMR of 10c


043-2-H
8.583
7.883
7.862
7.806
7.788
7.785
7.629
7.611
7.592
7.521
7.501
7.483
7.402
7.381
7.264
4.047
4.034
4.020
3.645
3.632
3.618
3.338
1.00
2.21
2.24
1.31
2.14
2.07
2.22
2.07
3.37
f1 (ppm)

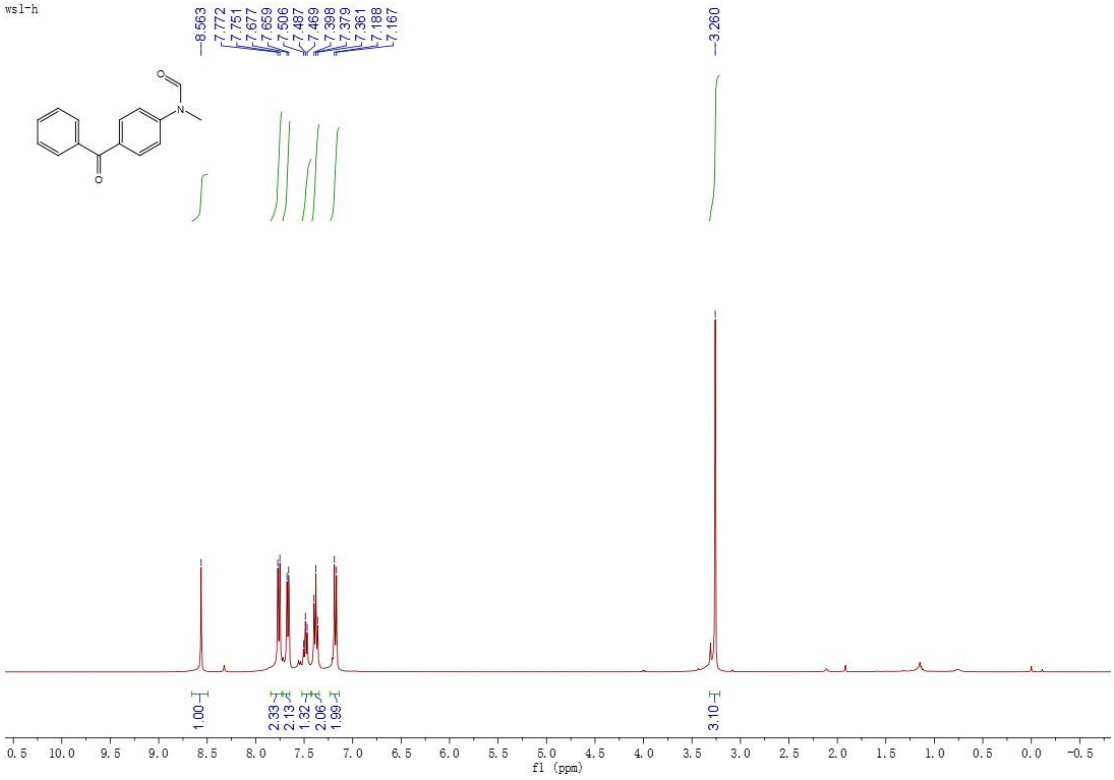

043-2-C
195.490
162.204
145.161
137.368
135.411
132.622
131.686
129.950
128.416
122.848
69.504
58.876
45.685
f1 (ppm)

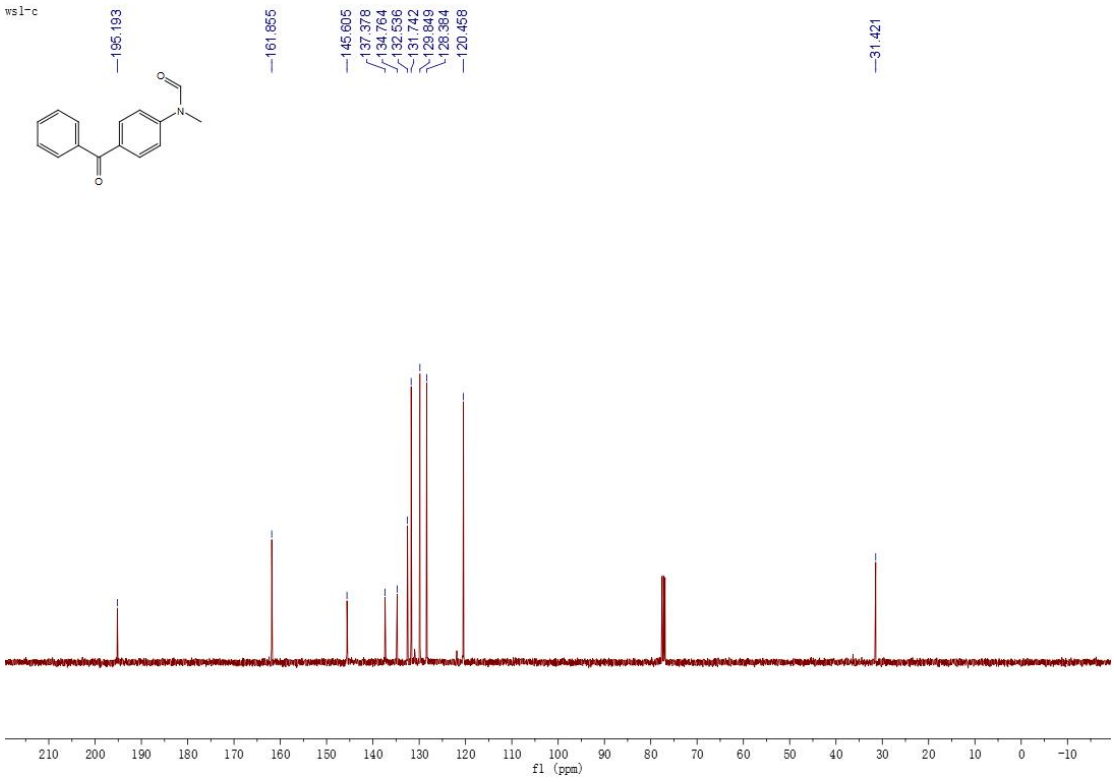
NMR of 10d


084-H
7.761
7.740
7.731
7.729
7.711
7.707
7.547
7.529
7.510
7.470
7.450
7.432
7.262
6.622
6.600
4.599
3.644
3.631
3.618
3.408
3.391
3.378
3.366
4.06
1.15
1.94
1.90
0.91
2.00
2.96
2.11
f1 (ppm)

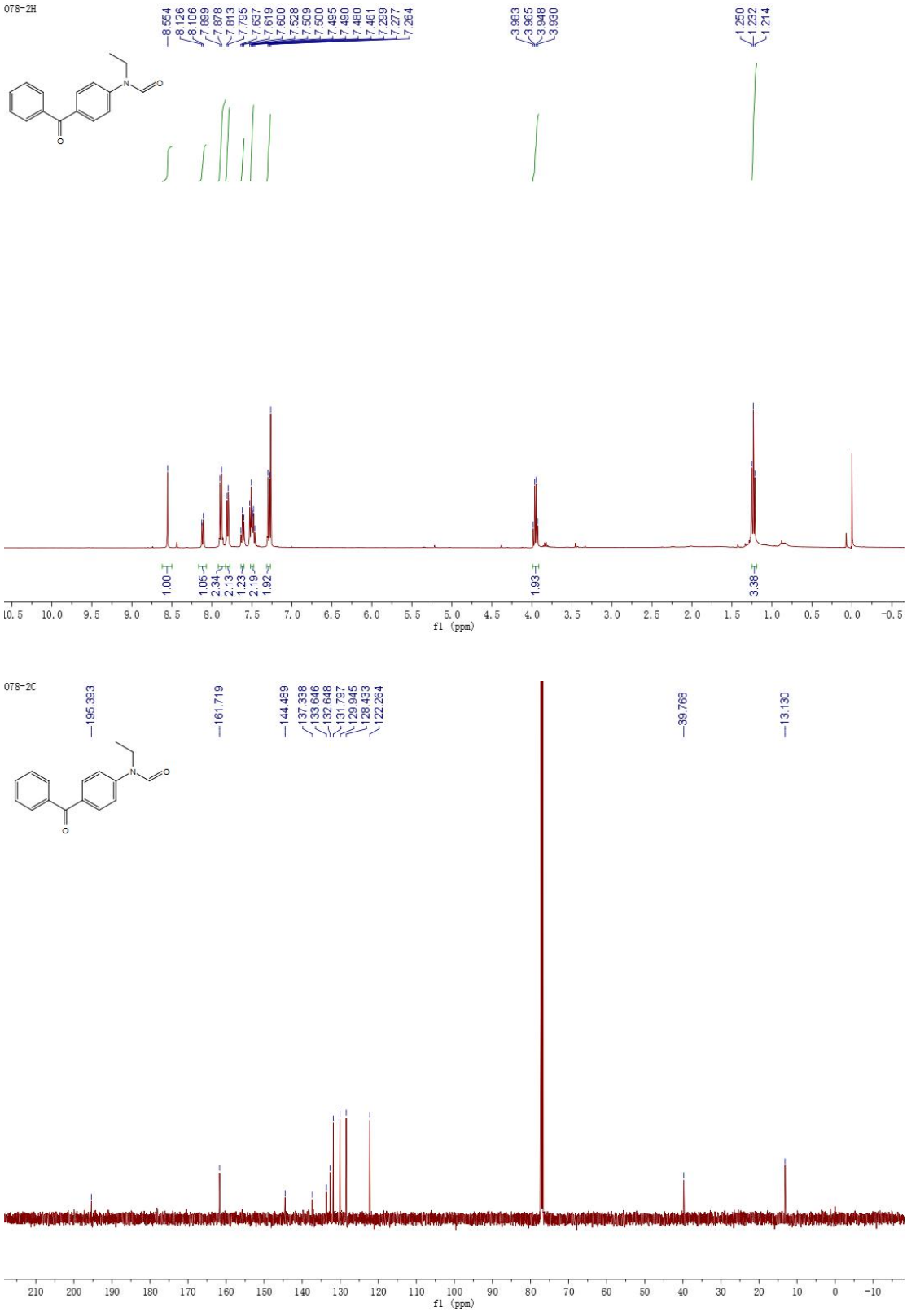

084-C
195.215
152.008
139.132
132.998
131.235
129.485
128.045
126.339
111.526
70.609
58.860
42.799
f1 (ppm)

NMR of 10b’

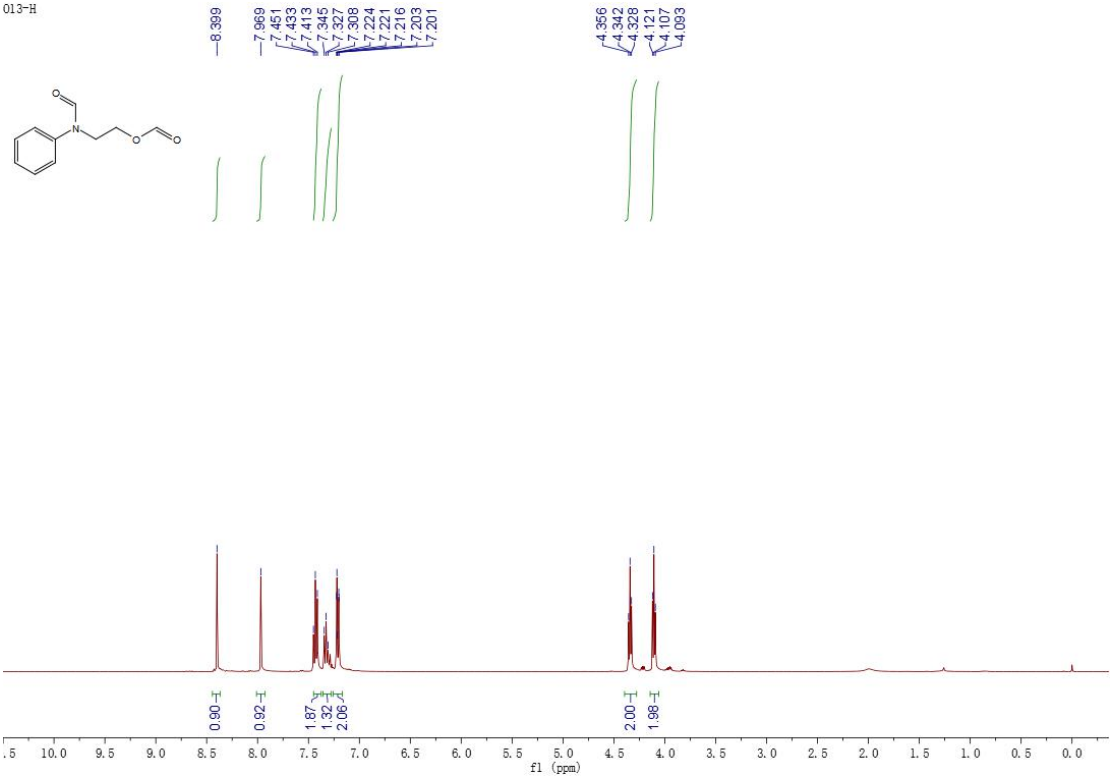

ws1-h
8.563
7.772
7.751
7.677
7.659
7.506
7.487
7.469
7.398
7.379
7.361
7.188
7.167
3.260
1.00
2.33
2.13
1.32
2.06
1.99
3.10
f1 (ppm)

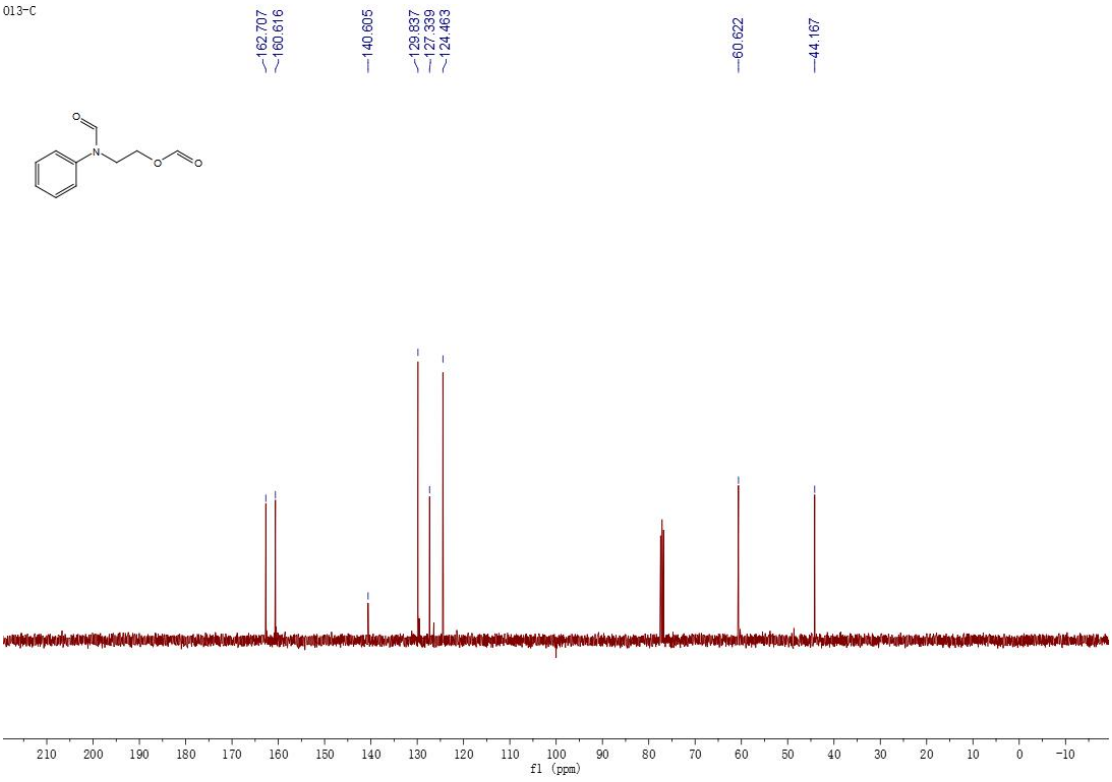

ws1-c
195.193
161.865
145.605
137.378
134.764
132.536
131.742
129.849
128.384
120.458
31.421
f1 (ppm)

NMR of 12b’

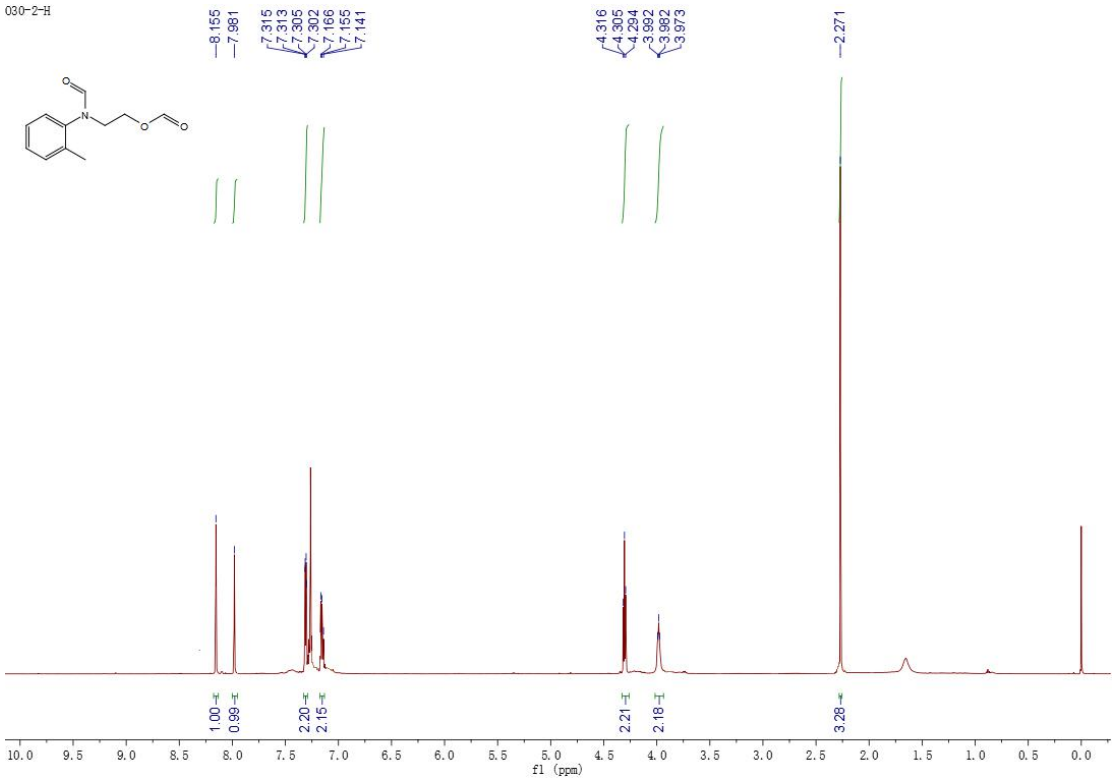

078-2H
8.554
8.126
8.106
7.899
7.878
7.813
7.795
7.637
7.619
7.600
7.528
7.509
7.500
7.495
7.490
7.480
7.461
7.299
7.277
7.264
3.983
3.965
3.948
3.930
1.250
1.232
1.214
1.00
1.05
2.34
2.13
1.23
2.19
1.92
1.93
3.38
f1 (ppm)
078-2C
196.393
161.719
144.489
137.338
133.646
132.648
131.797
129.945
128.433
122.264
39.768
13.130
f1 (ppm)

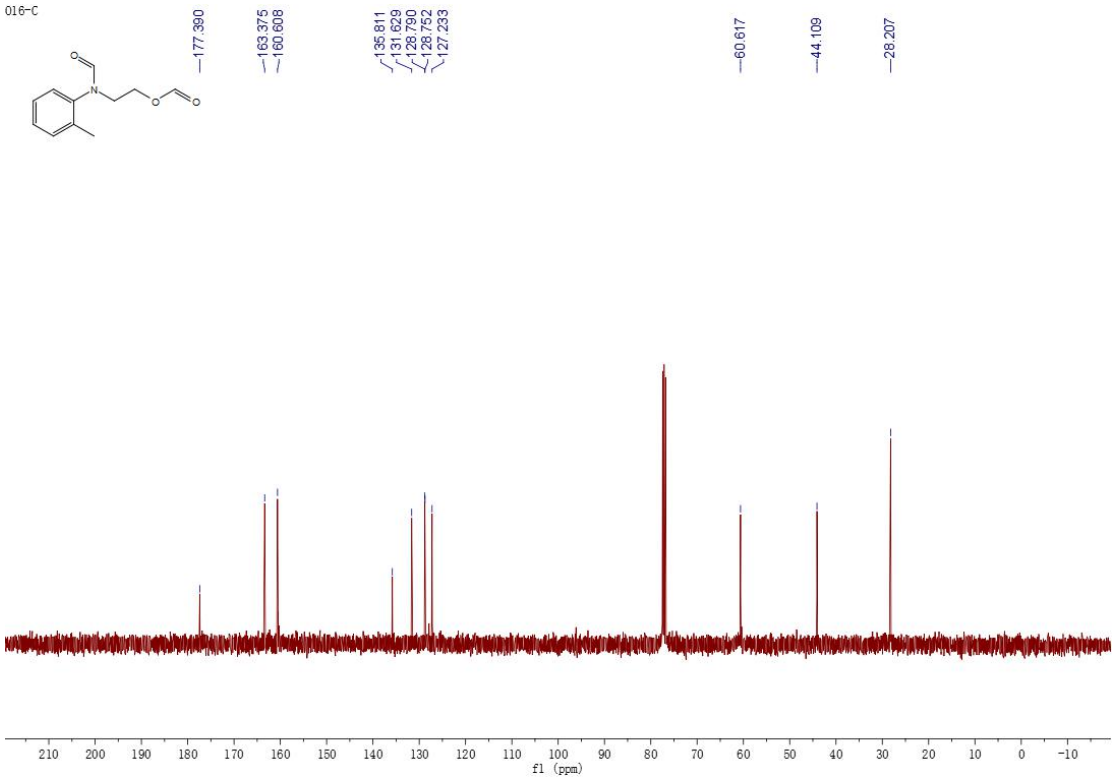
NMR of 13b


013-H
8.399
7.969
7.451
7.433
7.413
7.345
7.327
7.308
7.224
7.221
7.216
7.203
7.201
4.356
4.342
4.328
4.121
4.107
4.093
0.90
0.92
1.87
1.32
2.06
2.00
1.98
f1 (ppm)

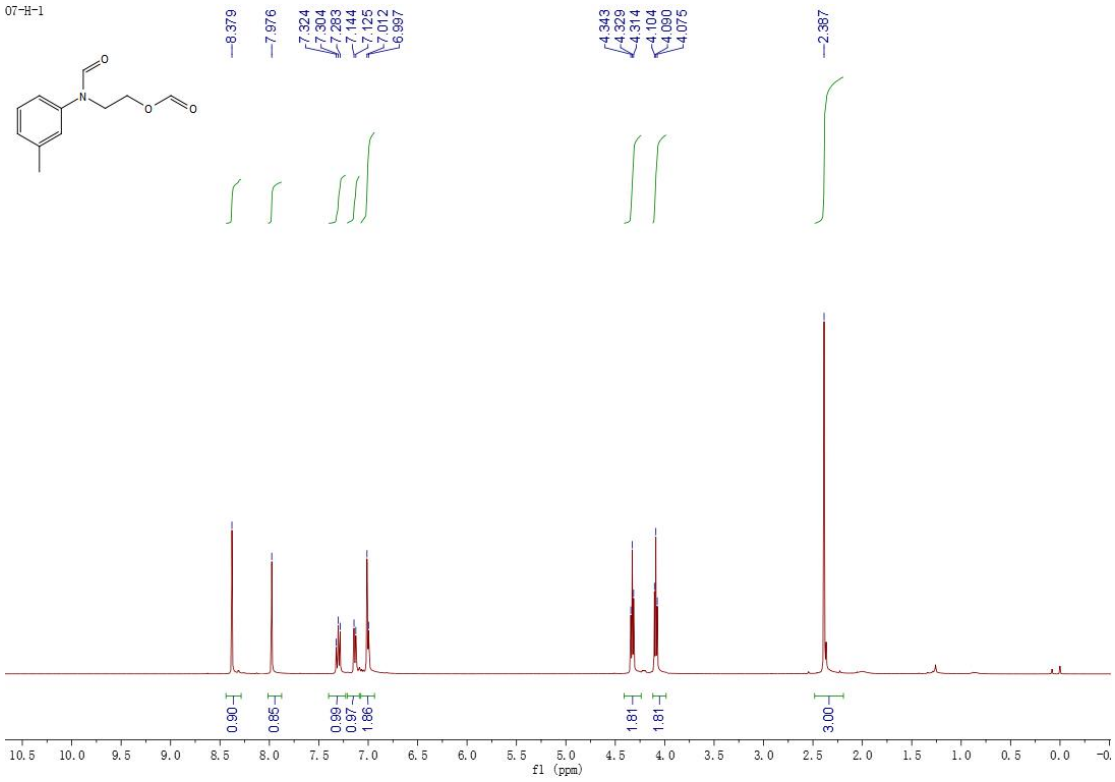

013-C
162.707
160.616
140.605
129.837
127.339
124.463
60.622
44.167
f1 (ppm)

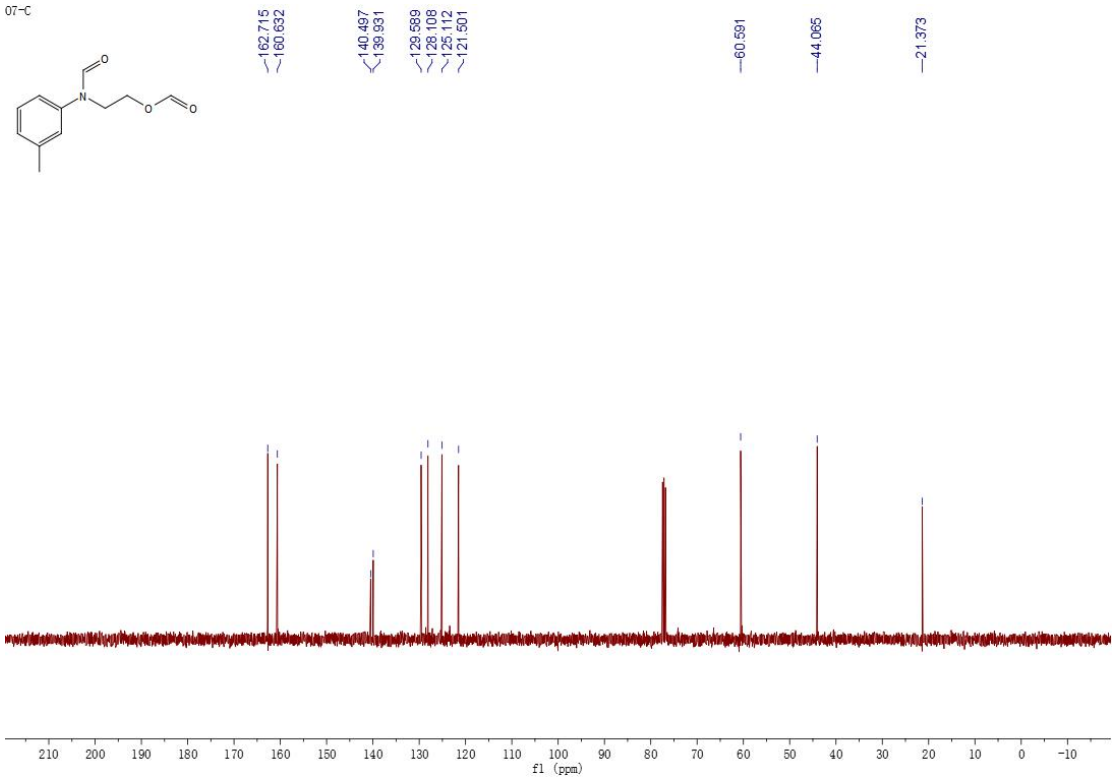
NMR of 14b


030-2-H
8.155
7.981
7.315
7.313
7.305
7.302
7.166
7.155
7.141
4.316
4.305
4.294
3.992
3.982
3.973
2.271
1.00
0.99
2.20
2.15
2.21
2.18
3.28
f1 (ppm)

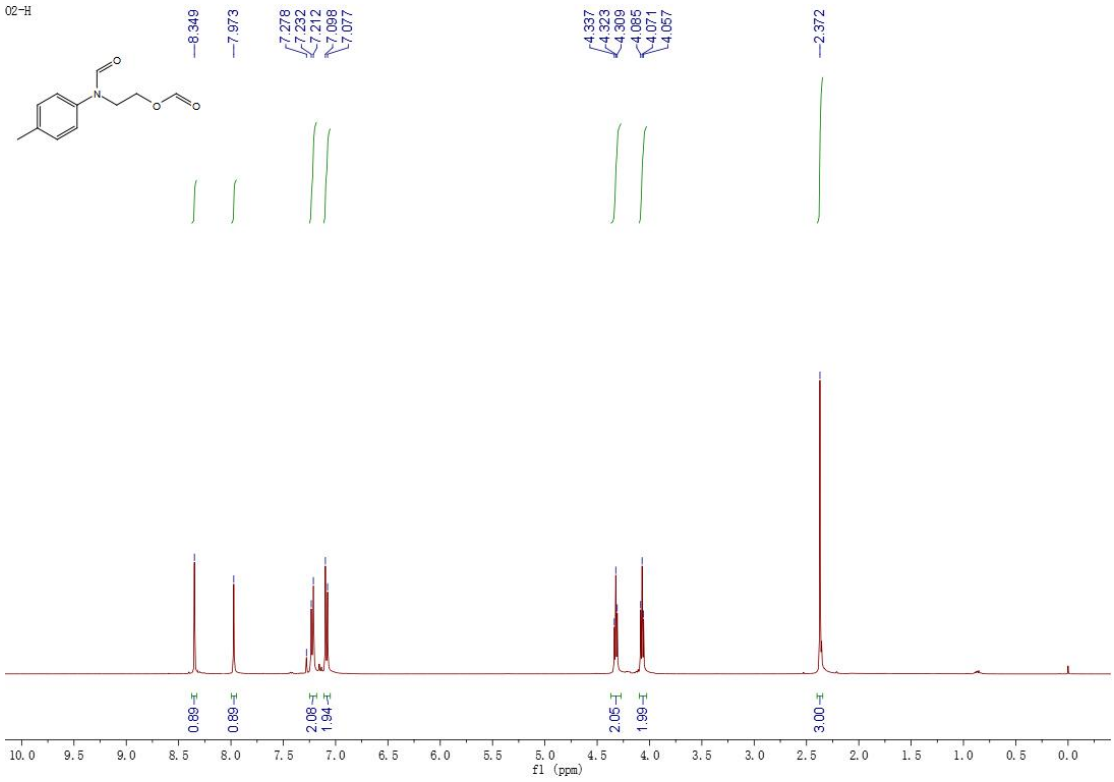

016-C
177.390
163.375
160.608
135.811
131.629
128.790
128.752
127.233
60.617
44.109
28.207
f1 (ppm)

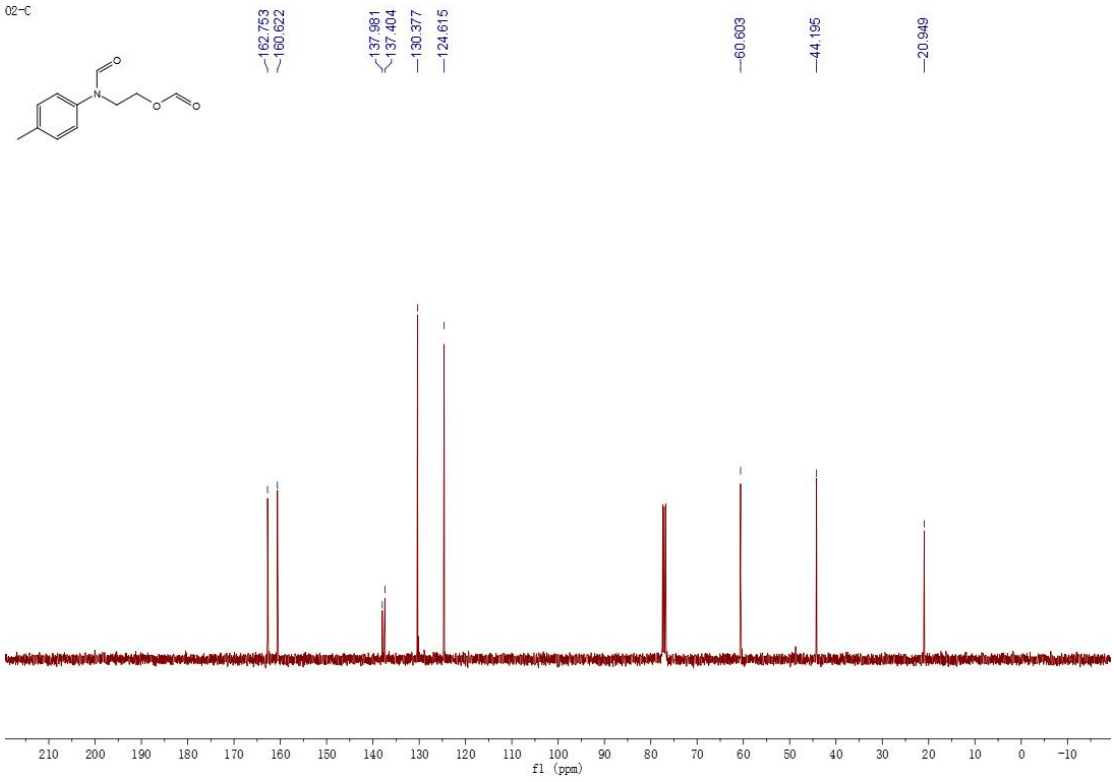
NMR of 15b


07-H-1
8.379
7.976
7.324
7.304
7.283
7.144
7.125
7.012
6.997
4.343
4.329
4.314
4.104
4.090
4.075
2.387
0.90
0.85
0.99
0.97
1.86
1.81
1.81
3.00
f1 (ppm)

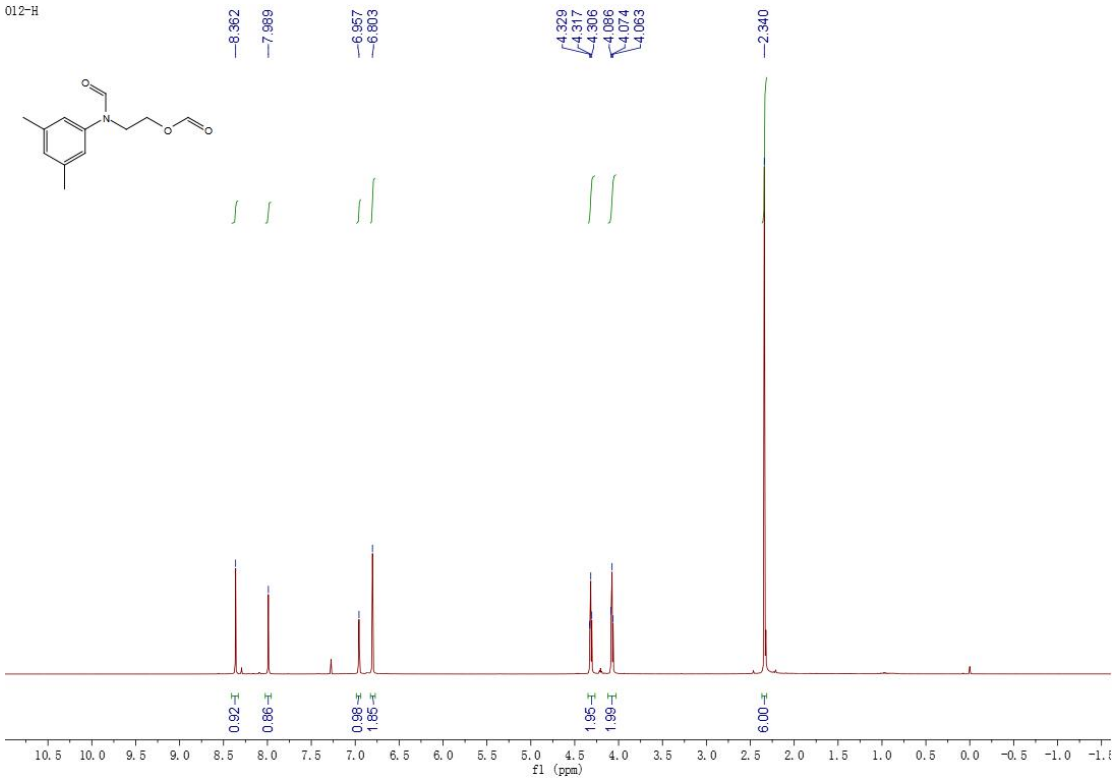

07-C
162.715
160.632
140.497
139.931
129.589
128.108
125.112
121.501
60.591
44.065
21.373
f1 (ppm)

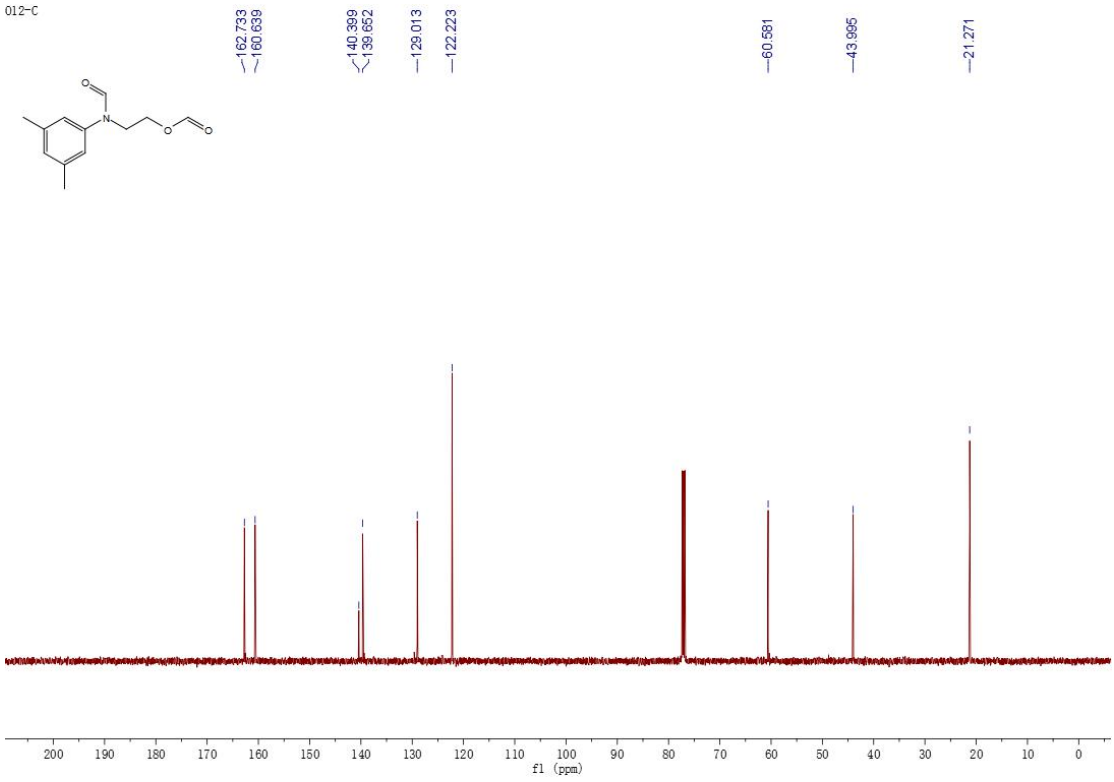
NMR of 16b


02-H
8.349
7.973
7.278
7.232
7.212
7.098
7.077
4.337
4.323
4.309
4.085
4.071
4.057
2.372
0.89
0.89
2.08
1.94
2.05
1.99
3.00
f1 (ppm)

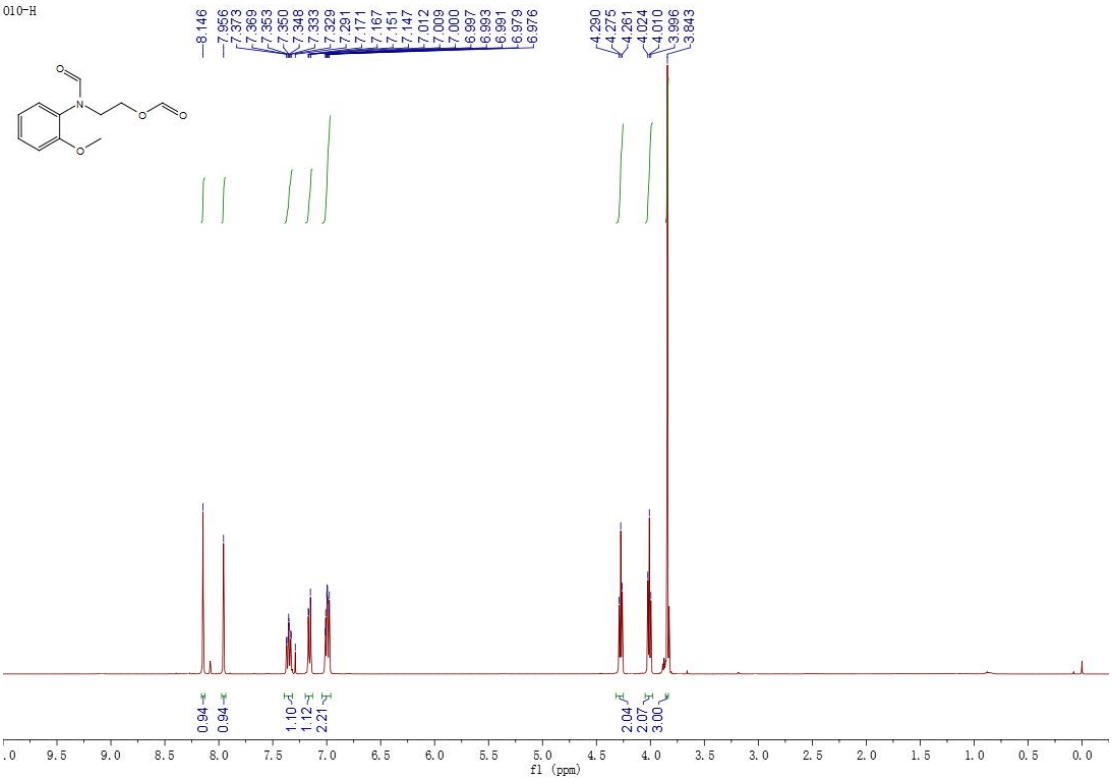

02-C
162.753
160.622
137.981
137.404
130.377
124.615
60.603
44.195
20.949
f1 (ppm)

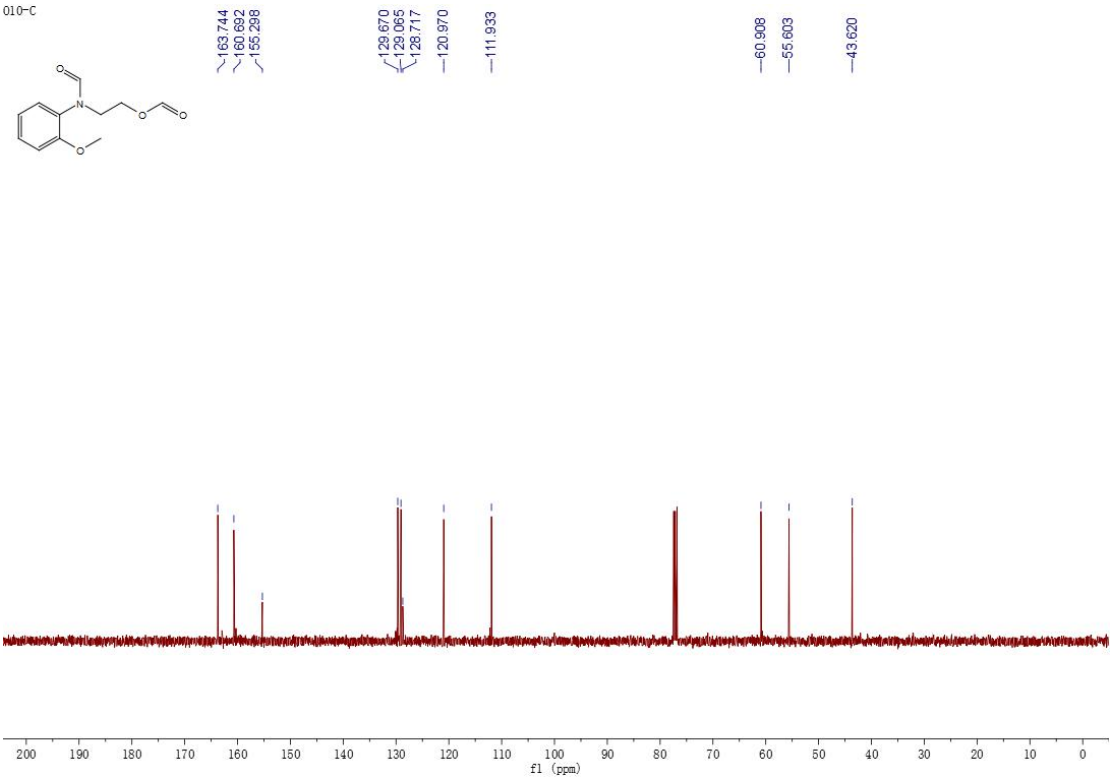
NMR of 17b


012-H
8.362
7.989
6.957
6.803
4.329
4.317
4.306
4.086
4.074
4.063
2.340
0.92
0.86
0.98
1.85
1.95
1.99
6.00
f1 (ppm)

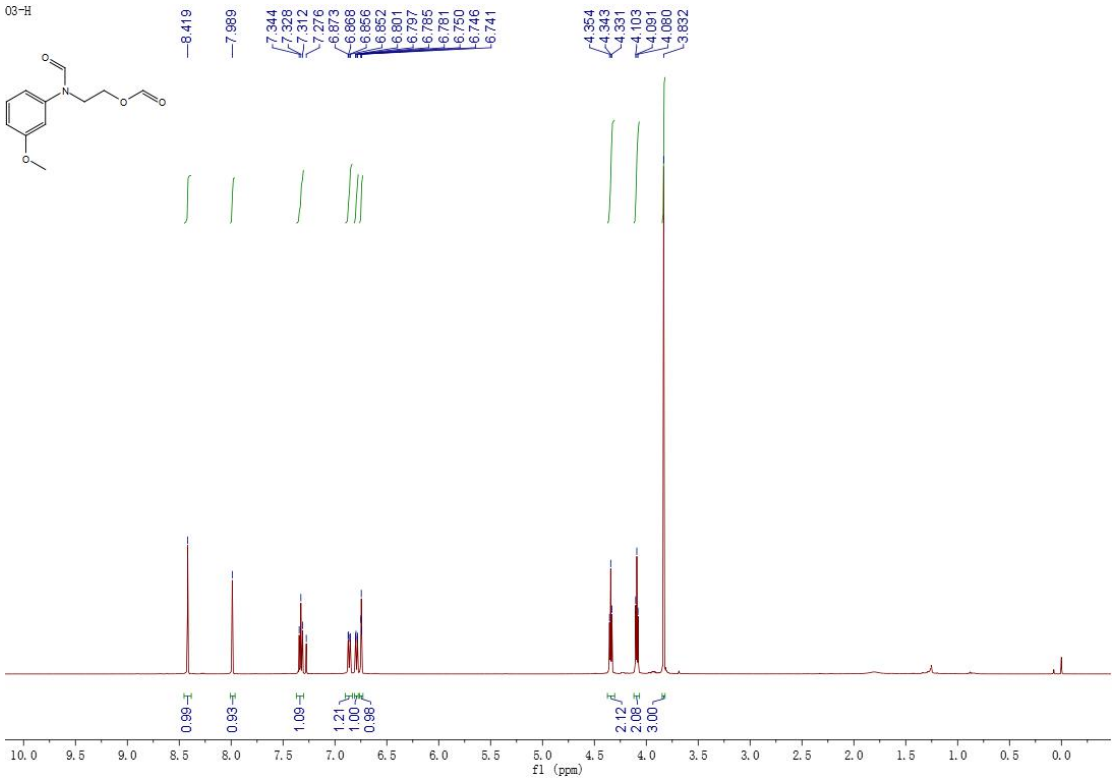

012-C
162.733
160.639
140.399
139.652
129.013
122.223
60.581
43.995
21.271
f1 (ppm)

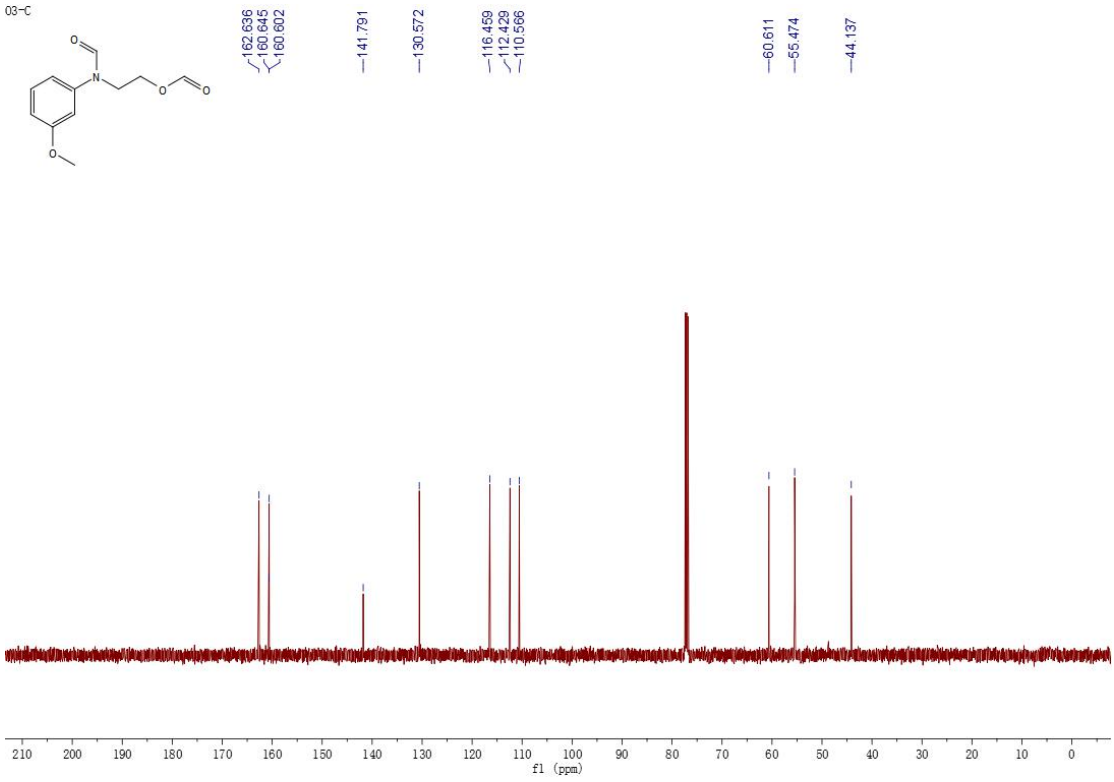
NMR of 18b


010-H
8.146
7.956
7.373
7.369
7.353
7.350
7.348
7.333
7.329
7.291
7.171
7.167
7.151
7.147
7.012
7.009
7.000
6.997
6.993
6.991
6.979
6.976
4.290
4.275
4.261
4.024
4.010
3.996
3.843
0.94
0.94
1.10
1.12
2.21
2.04
2.07
3.00
f1 (ppm)

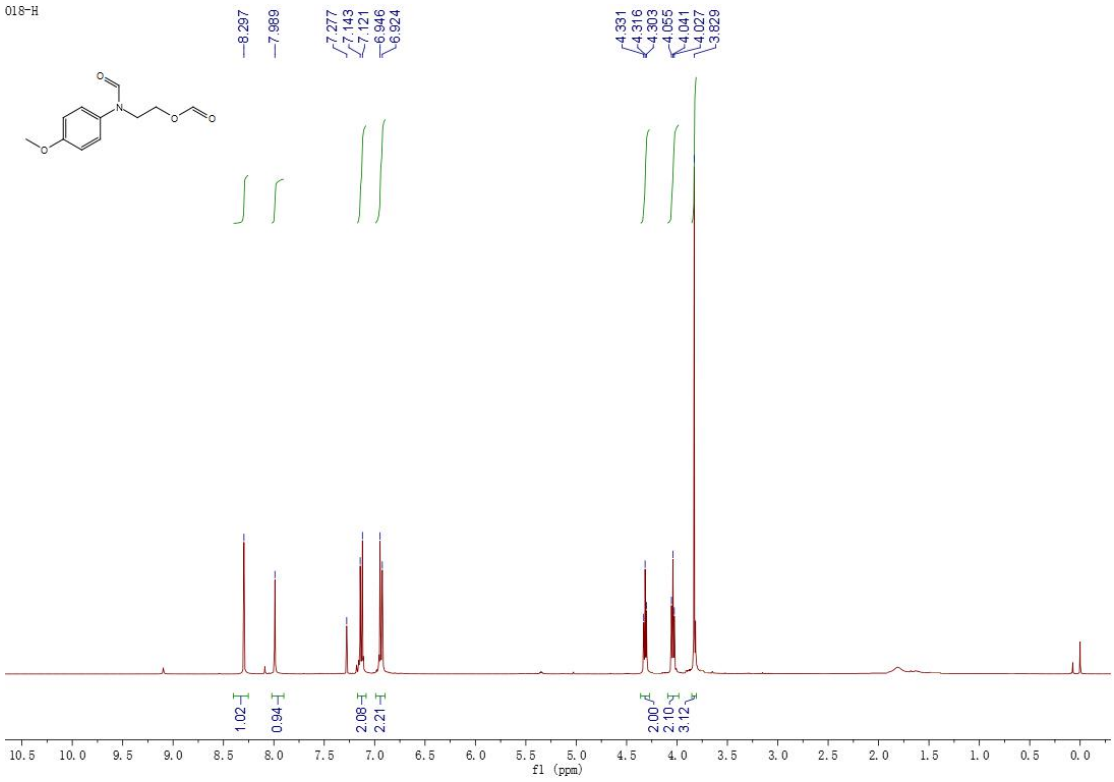

010-C
163.744
160.692
155.298
129.670
129.065
128.717
120.970
111.933
60.908
55.603
43.620
f1 (ppm)

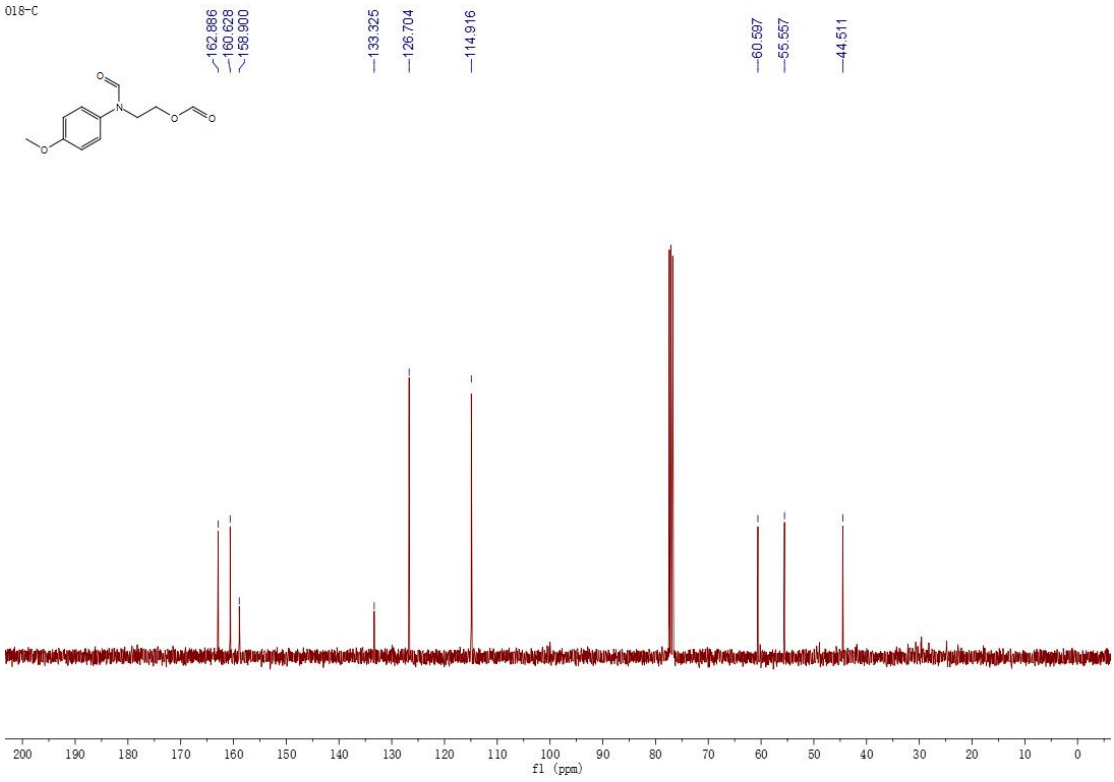
NMR of 19b


03-H
8.419
7.989
7.344
7.328
7.312
7.276
6.873
6.868
6.856
6.852
6.801
6.797
6.785
6.781
6.750
6.746
6.741
4.354
4.343
4.331
4.103
4.091
4.080
3.832
0.99
0.93
1.09
1.21
1.00
0.98
2.12
2.08
3.00
f1 (ppm)

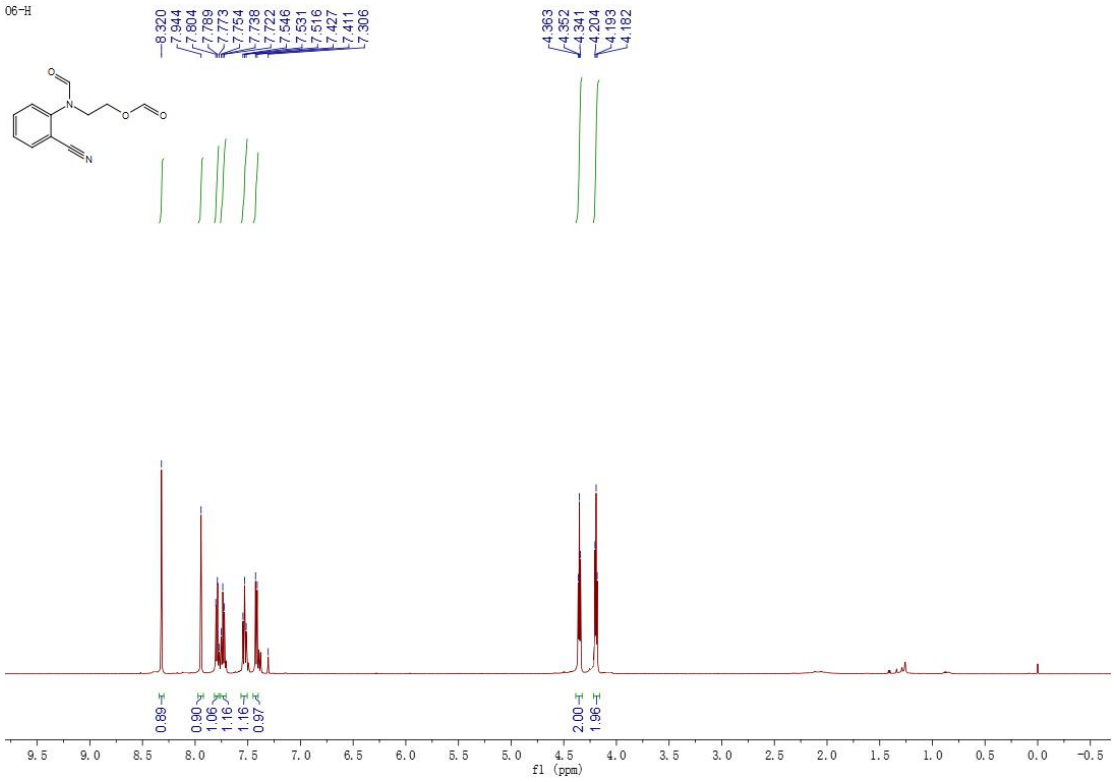

03-C
162.636
160.645
160.602
141.791
130.572
116.459
112.429
110.566
60.611
55.474
44.137
f1 (ppm)

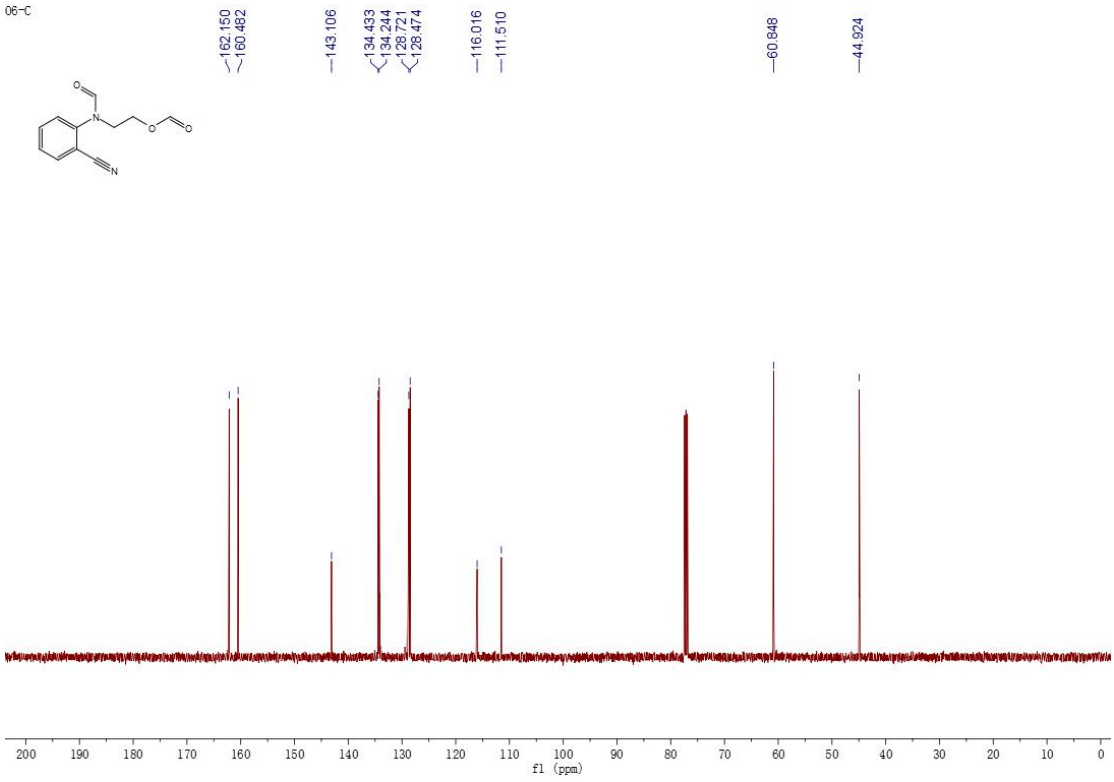
NMR of 20b


018-H
8.297
7.989
7.277
7.143
7.121
6.946
6.924
4.331
4.316
4.303
4.055
4.041
4.027
3.829
1.02
0.94
2.08
2.21
2.00
2.10
3.12
f1 (ppm)

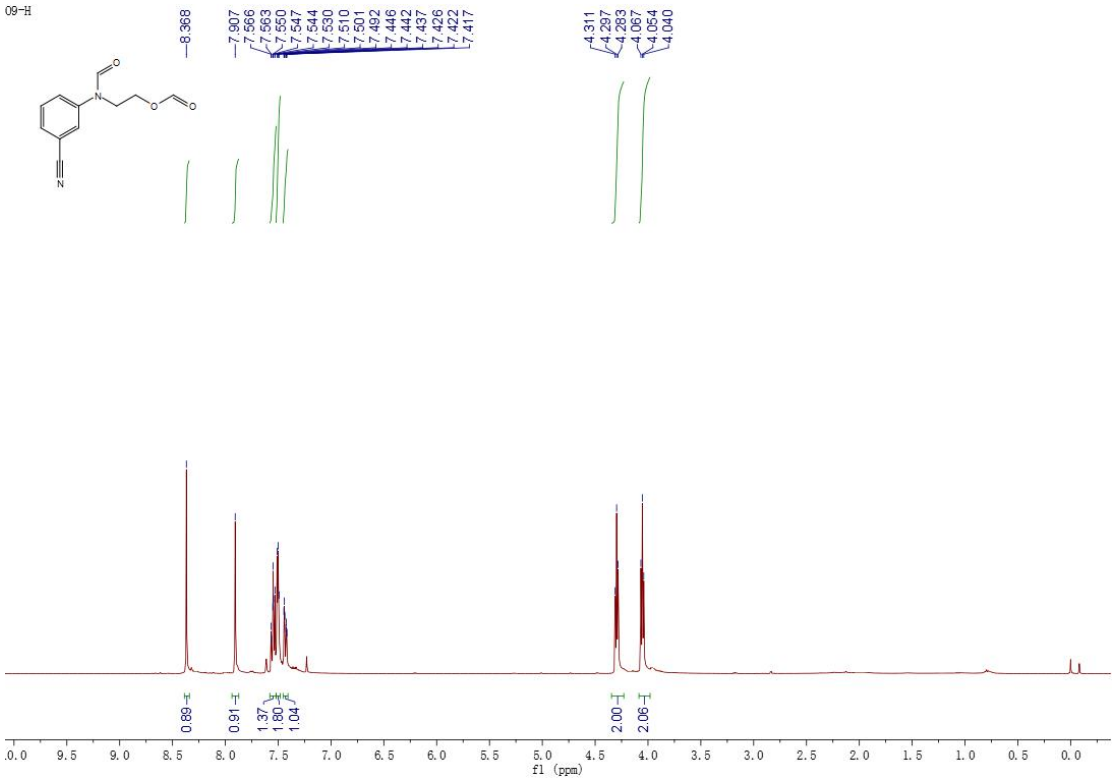

018-C
162.886
160.628
158.900
133.325
126.704
114.916
60.597
55.557
44.511
f1 (ppm)

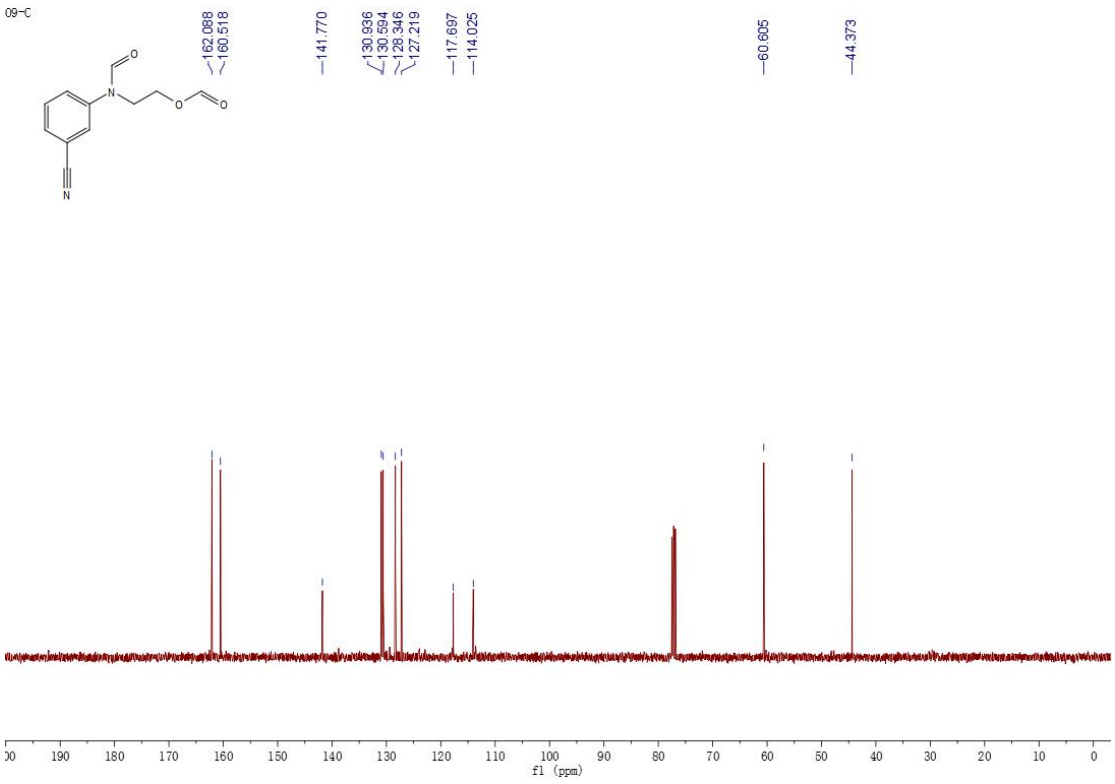
NMR of 21b


06-H
8.320
7.944
7.804
7.789
7.773
7.754
7.738
7.722
7.546
7.531
7.516
7.427
7.411
7.306
4.363
4.352
4.341
4.204
4.193
4.182
0.89
0.90
1.06
1.16
1.16
0.97
2.00
1.96
f1 (ppm)

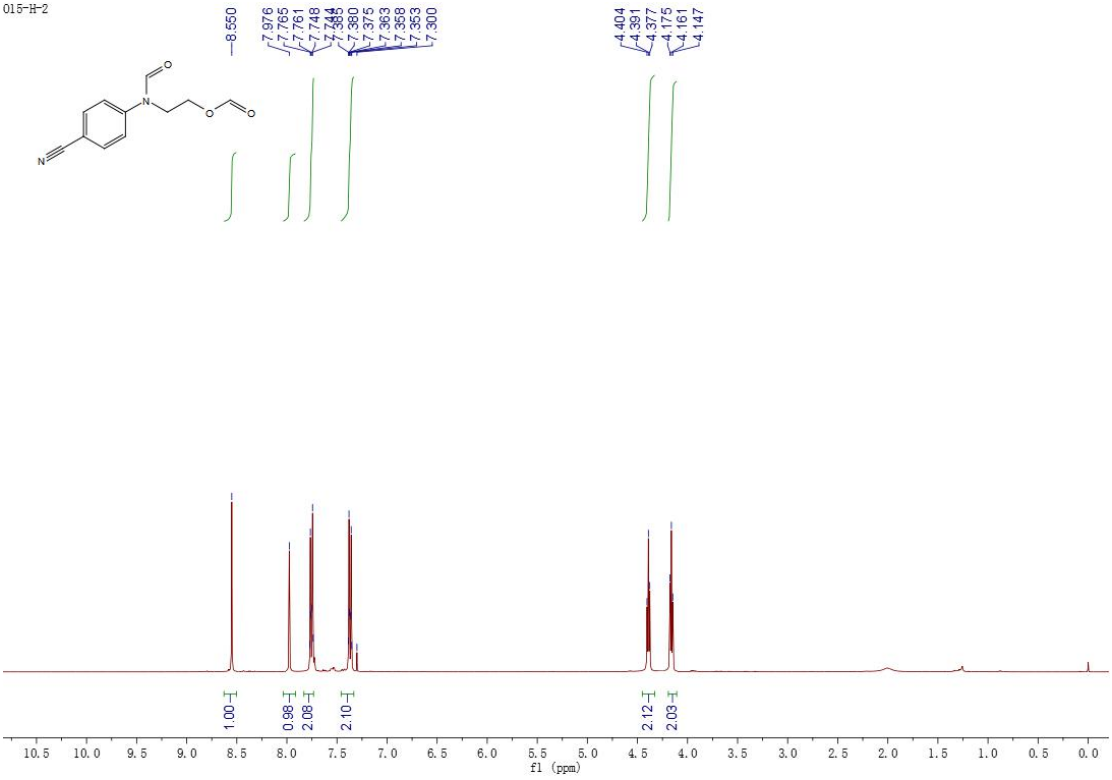

06-C
162.150
160.482
143.106
134.433
134.244
128.721
128.474
116.016
111.510
60.848
44.924
f1 (ppm)

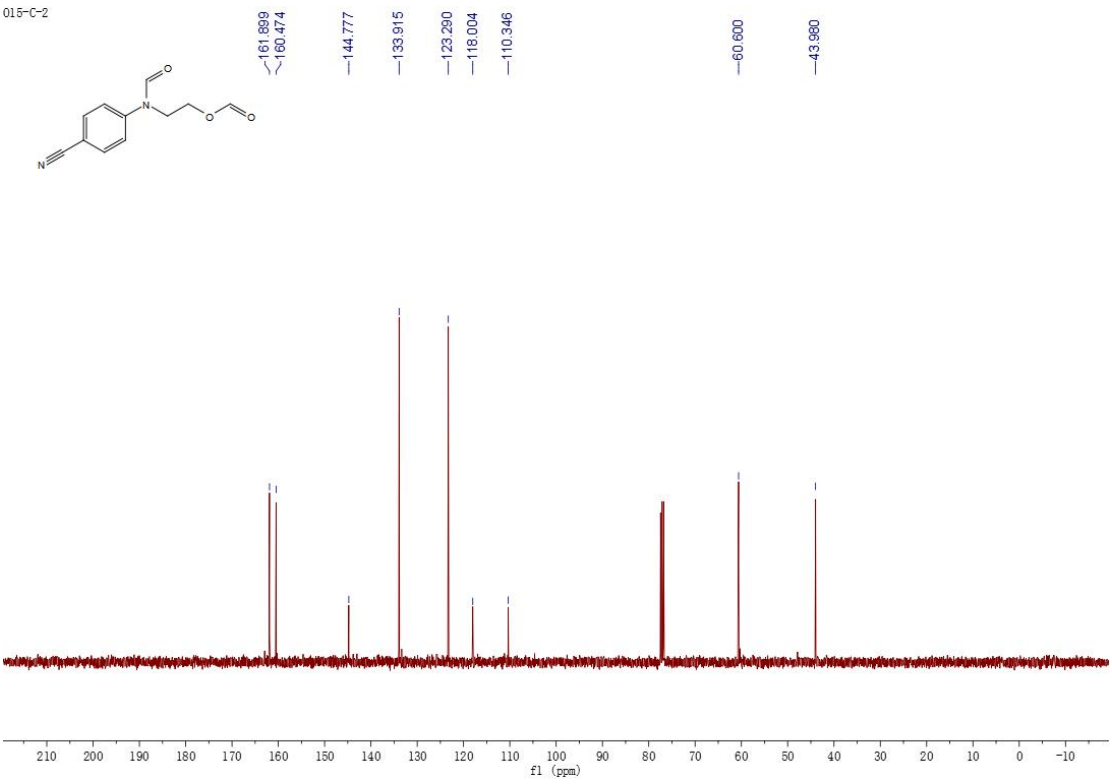
NMR of 22b


09-H
8.368
7.907
7.566
7.563
7.550
7.547
7.544
7.530
7.510
7.501
7.492
7.446
7.442
7.437
7.426
7.422
7.417
4.311
4.297
4.283
4.067
4.054
4.040
0.89
0.91
1.37
1.80
1.04
2.00
2.06
f1 (ppm)

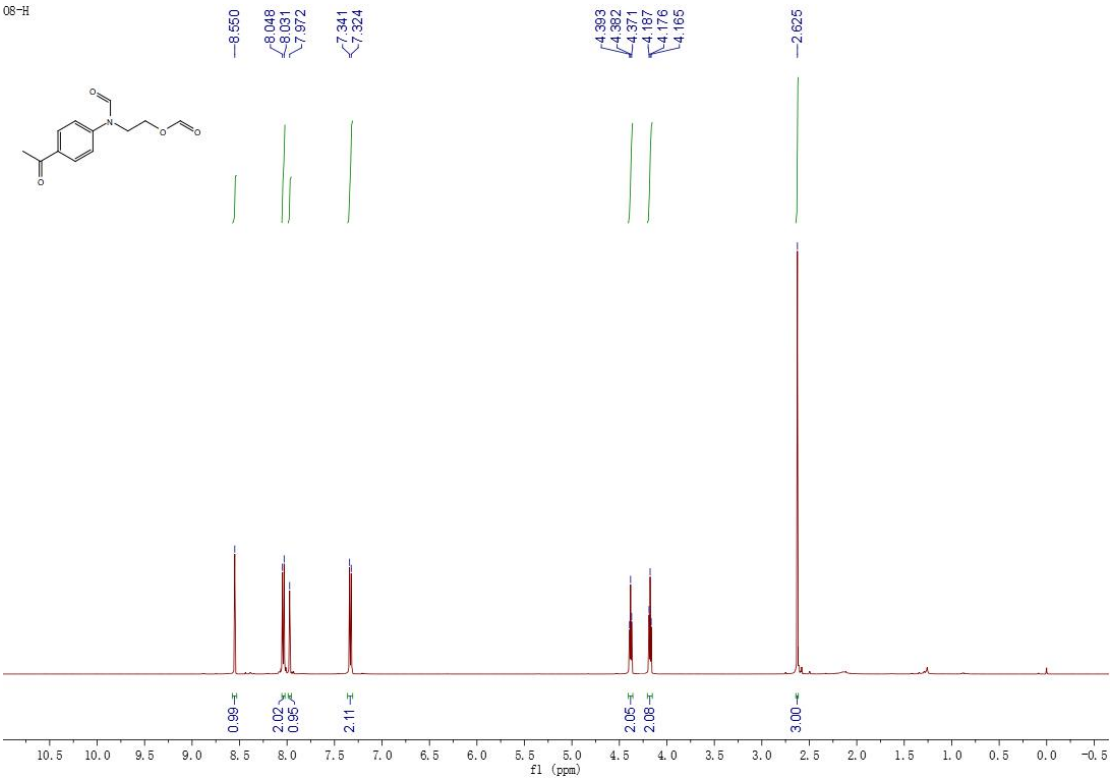

09-C
162.088
160.518
141.770
130.936
130.594
128.346
127.219
117.697
114.025
60.605
44.373
f1 (ppm)

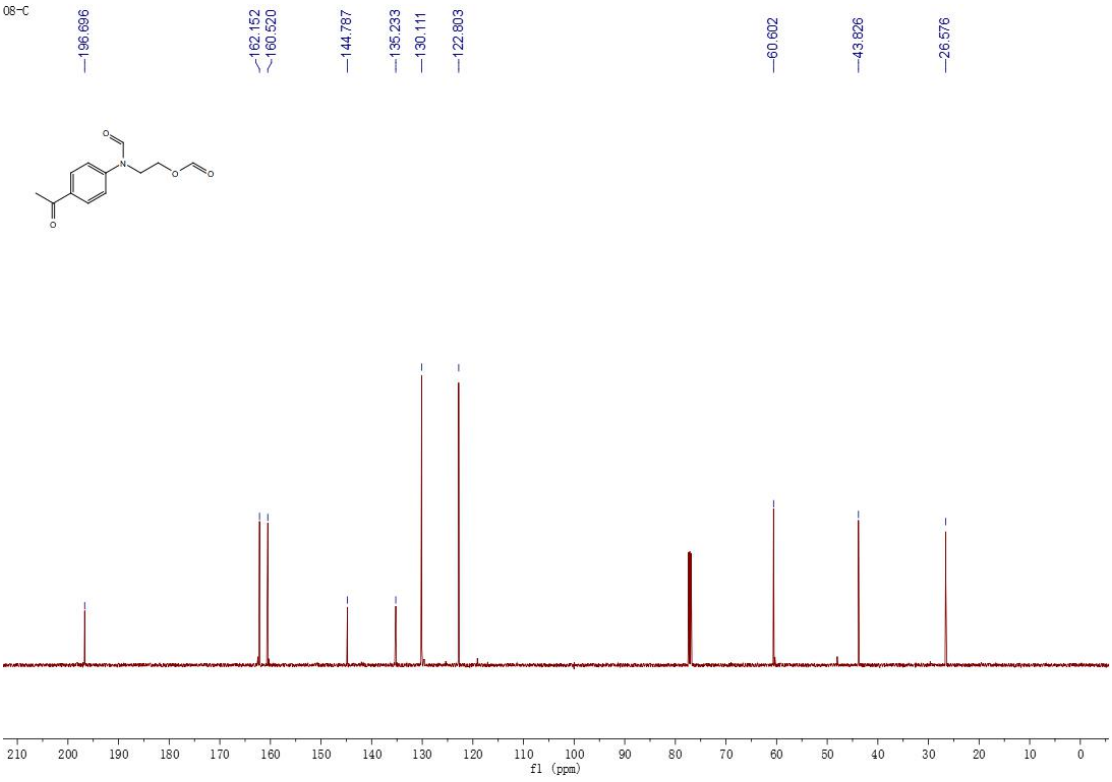
NMR of 23b


015-H-2
8.550
7.976
7.765
7.761
7.748
7.744
7.385
7.380
7.375
7.363
7.358
7.353
7.300
4.404
4.391
4.377
4.175
4.161
4.147
1.00
0.98
2.08
2.10
2.12
2.03
f1 (ppm)

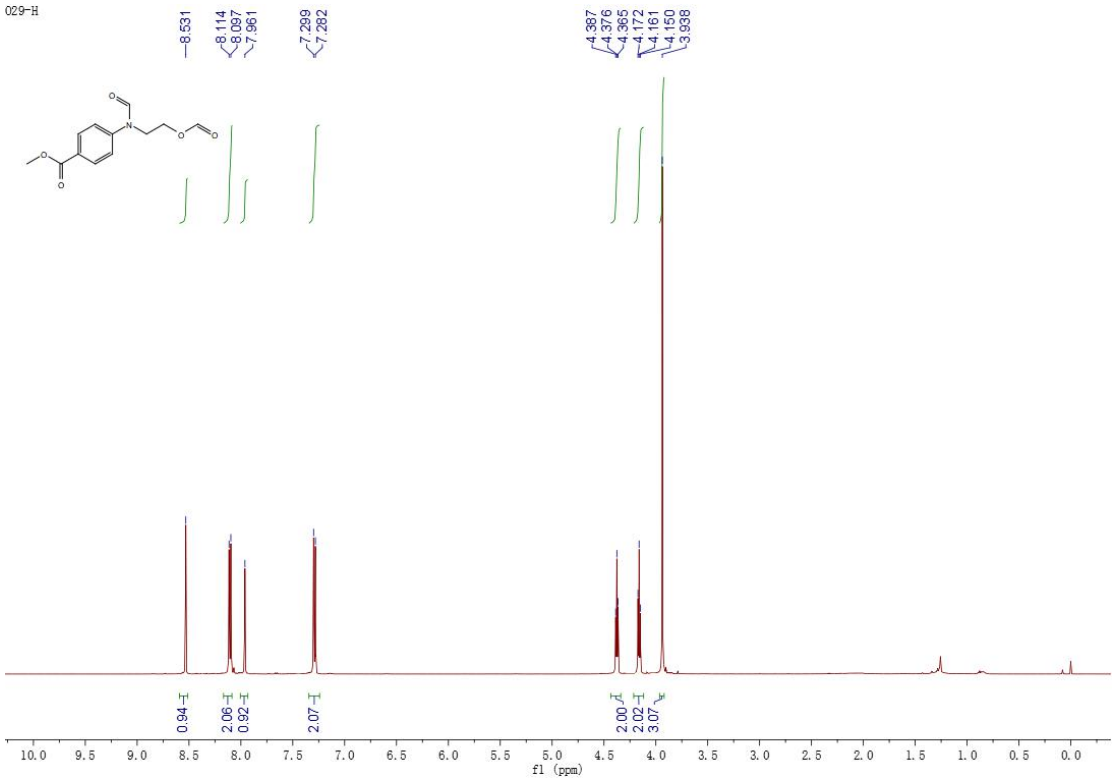

015-C-2
161.899
160.474
144.777
133.915
123.290
118.004
110.346
60.600
43.980
f1 (ppm)

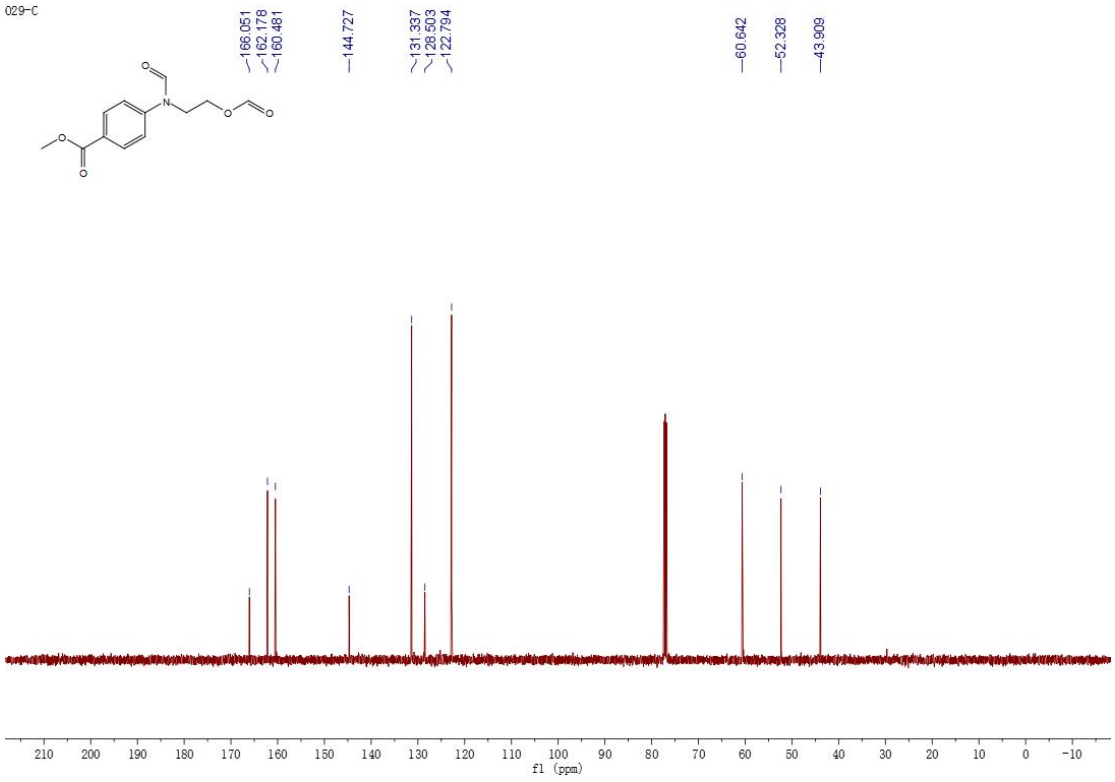
NMR of 24b


08-H
8.550
8.048
8.031
7.972
7.341
7.324
4.393
4.382
4.371
4.187
4.176
4.165
2.625
0.99
2.02
0.95
2.11
2.05
2.08
3.00
f1 (ppm)

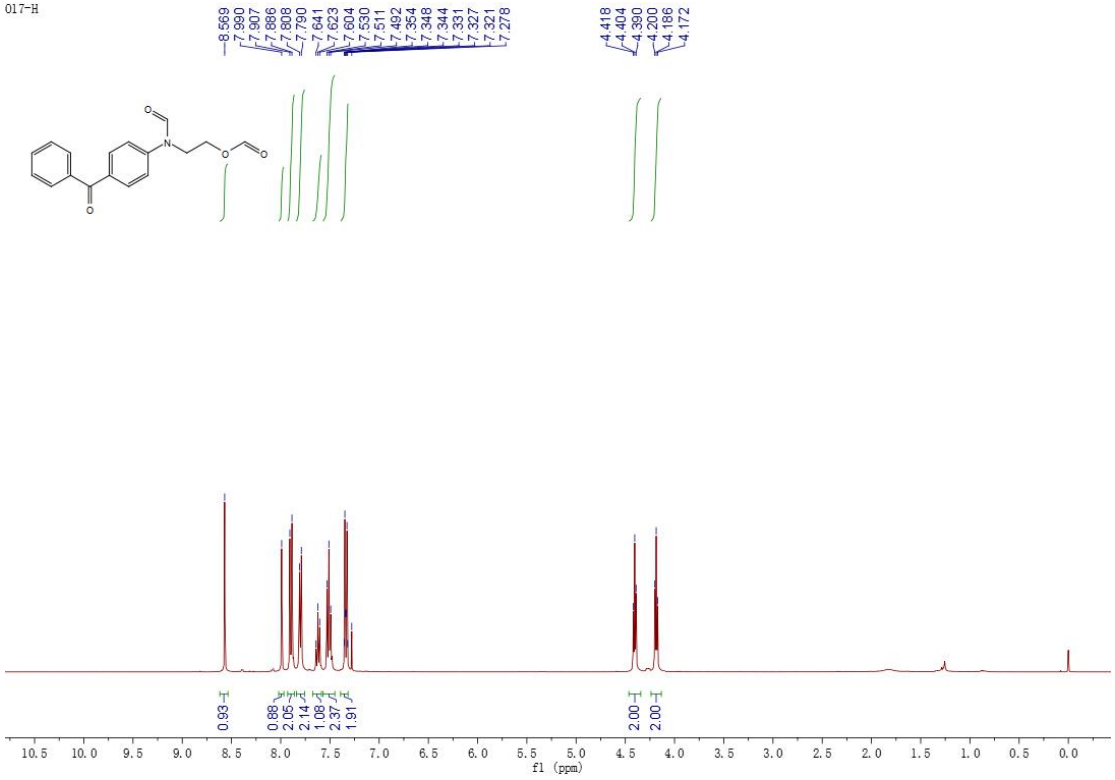

08-C
196.696
162.152
160.520
144.787
135.233
130.111
122.803
60.602
43.826
26.576
f1 (ppm)

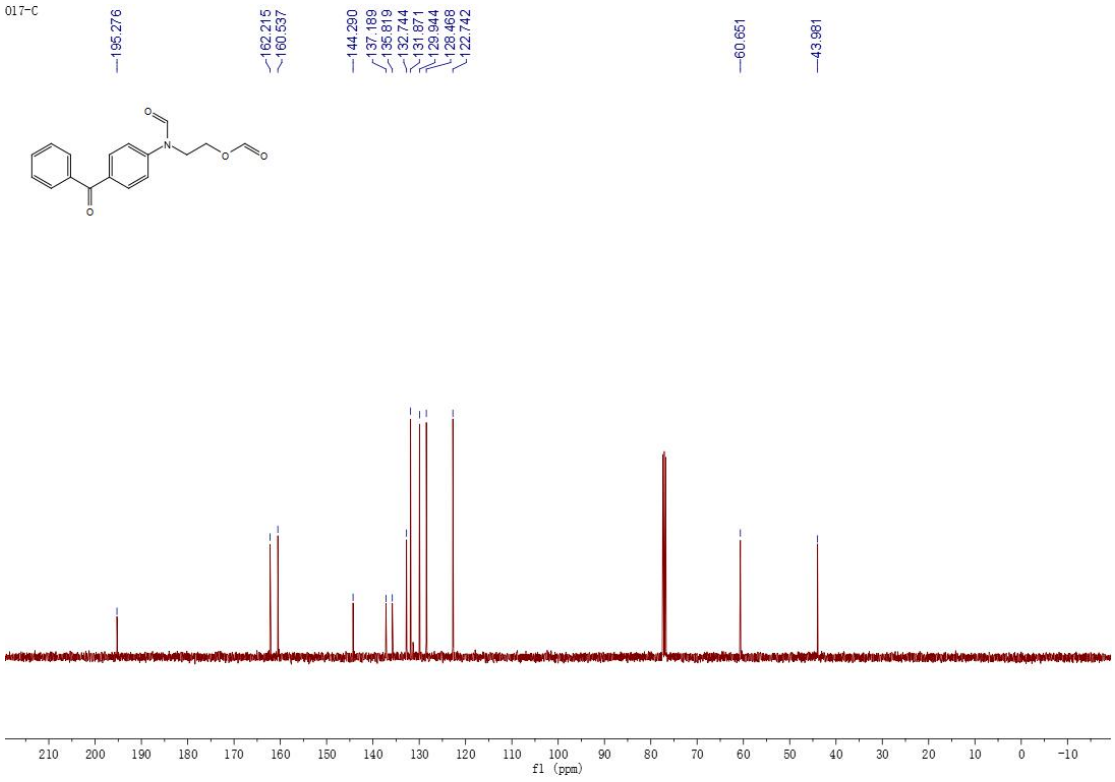
NMR of 25b


029-H
8.531
8.114
8.097
7.961
7.299
7.282
4.387
4.376
4.365
4.172
4.161
4.150
3.938
0.94
2.06
0.92
2.07
2.00
2.02
3.07
f1 (ppm)

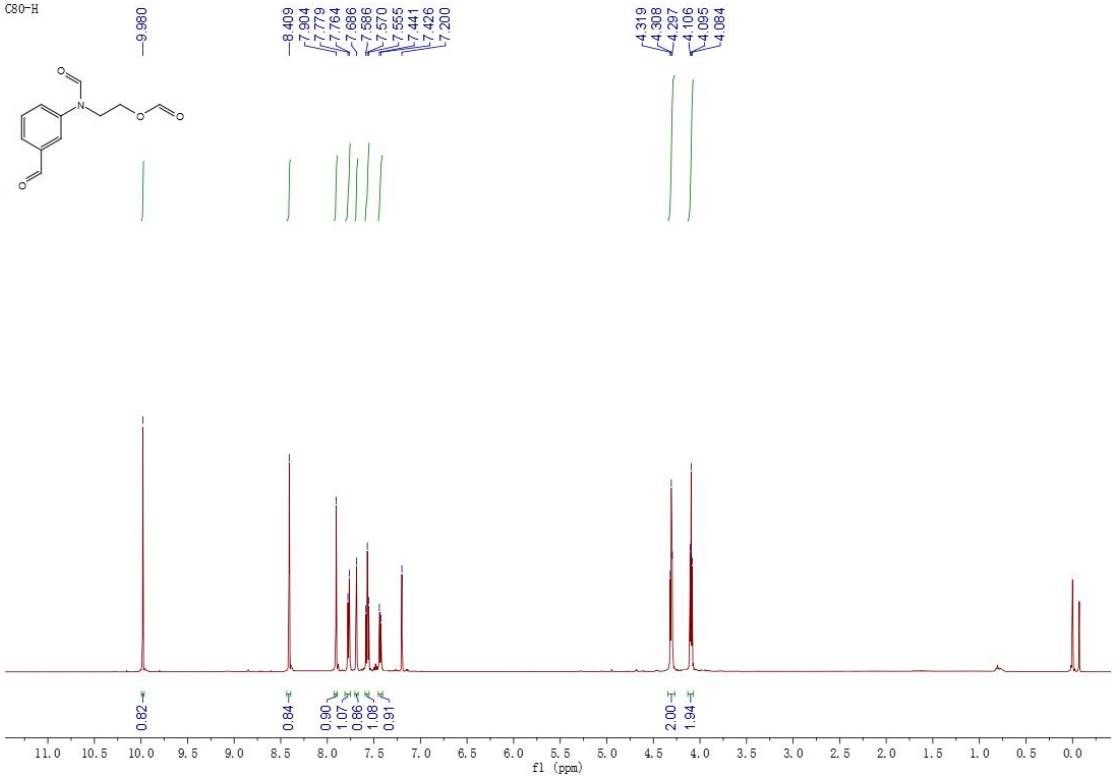

029-C
166.051
162.178
160.481
144.727
131.337
128.503
122.794
60.642
52.328
43.909
f1 (ppm)

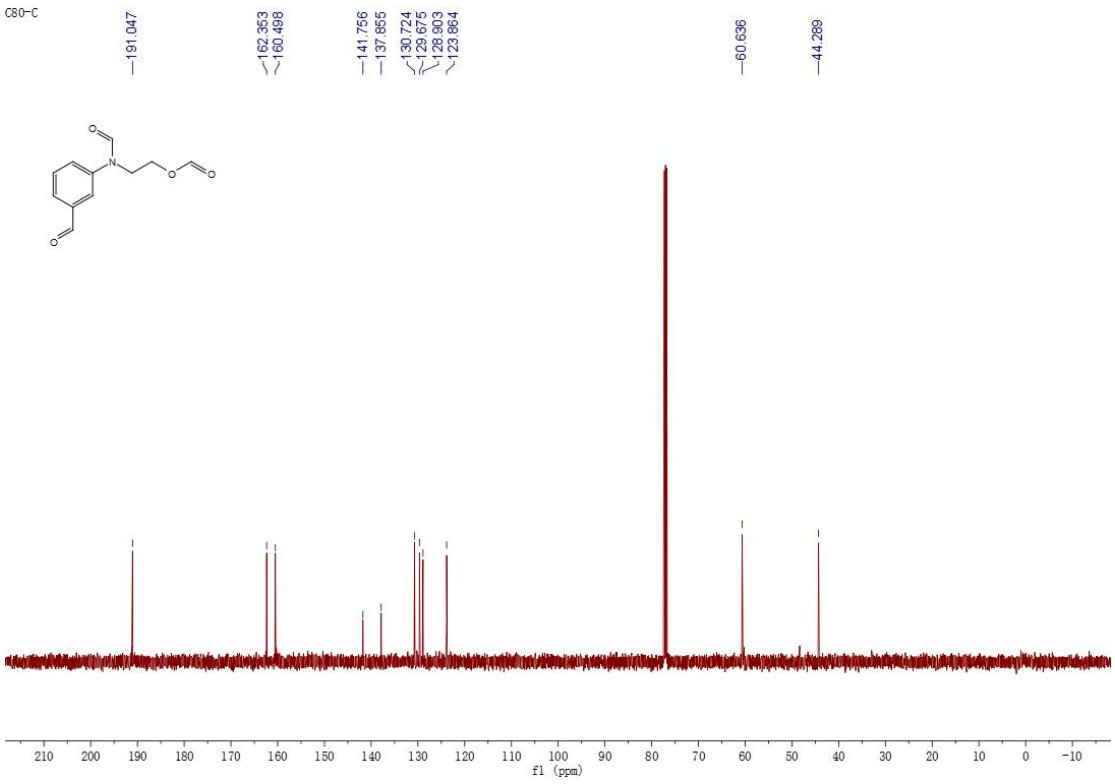
NMR of 26b


017-H
8.569
7.990
7.907
7.886
7.808
7.790
7.641
7.623
7.604
7.530
7.511
7.492
7.354
7.348
7.344
7.331
7.327
7.321
7.278
4.418
4.404
4.390
4.200
4.186
4.172
0.93
0.88
2.05
2.14
1.08
2.37
1.91
2.00
2.00
f1 (ppm)

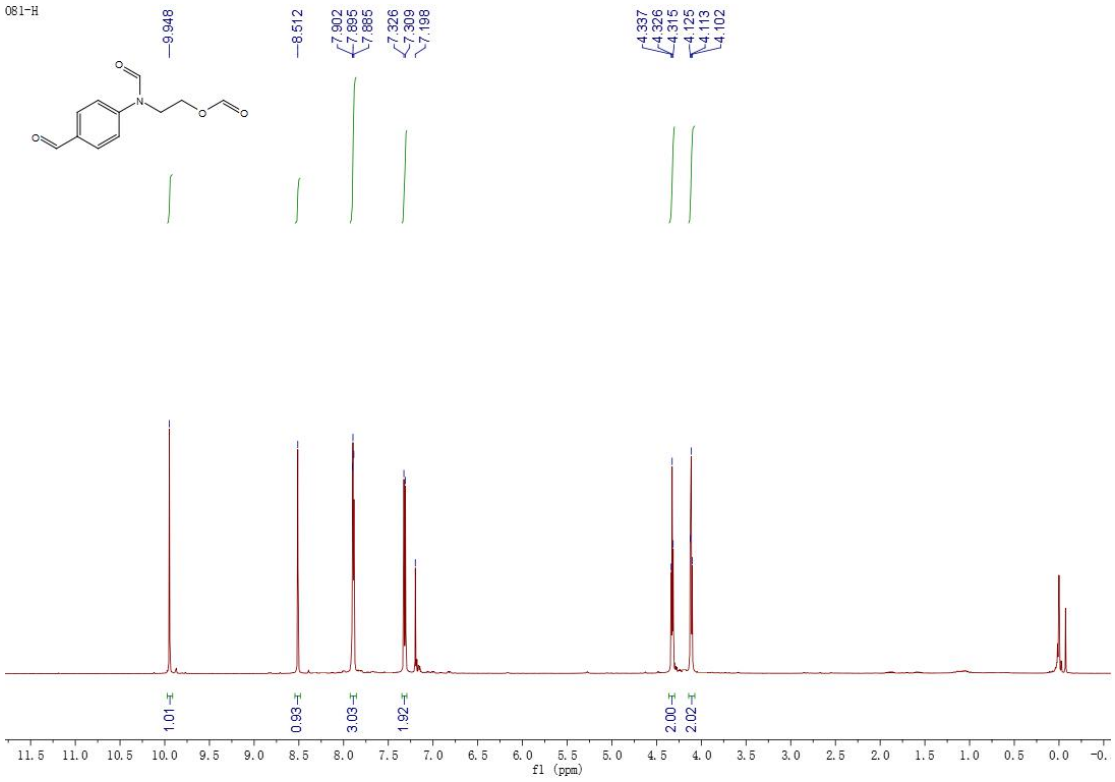

017-C
195.276
162.215
160.537
144.290
137.189
135.819
132.744
131.871
129.944
128.468
122.742
60.651
43.961
f1 (ppm)

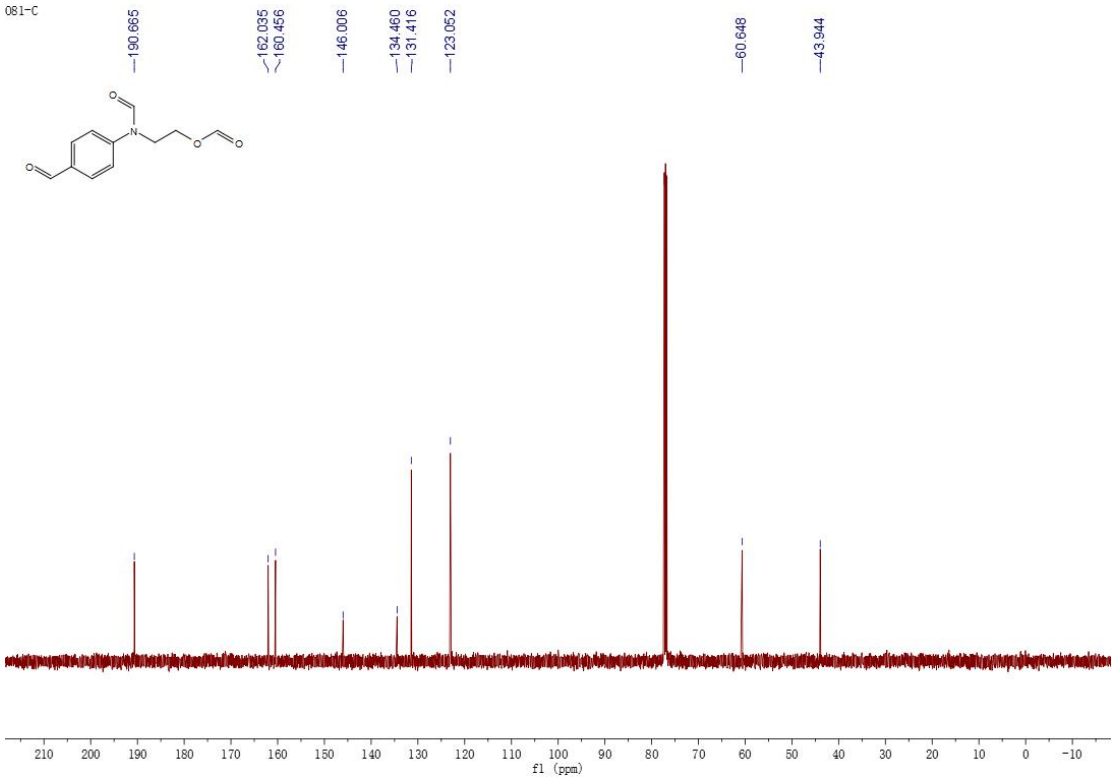
NMR of 27b


C80-H
9.980
8.409
7.904
7.779
7.764
7.686
7.586
7.570
7.555
7.441
7.426
7.200
4.319
4.308
4.297
4.106
4.095
4.084
0.82
0.84
0.90
1.07
0.86
1.08
0.91
2.00
1.94
f1 (ppm)

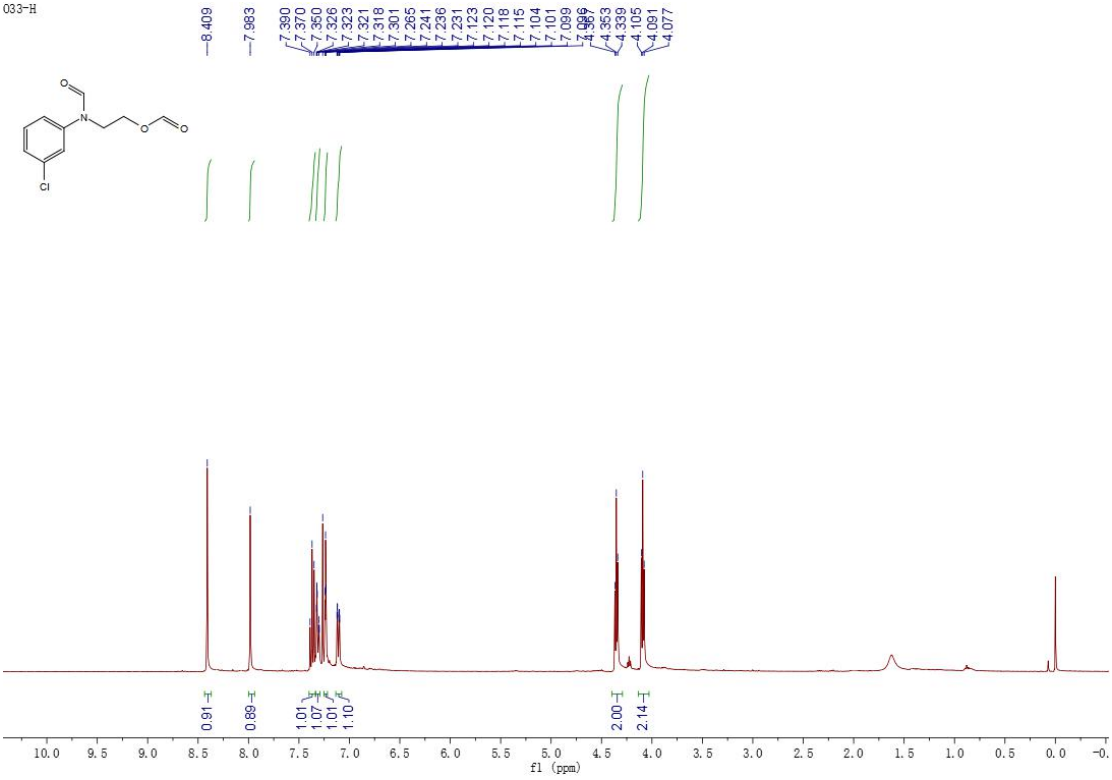

C80-C
191.047
162.353
160.498
141.756
137.855
130.724
129.675
128.903
123.864
60.636
44.289
f1 (ppm)

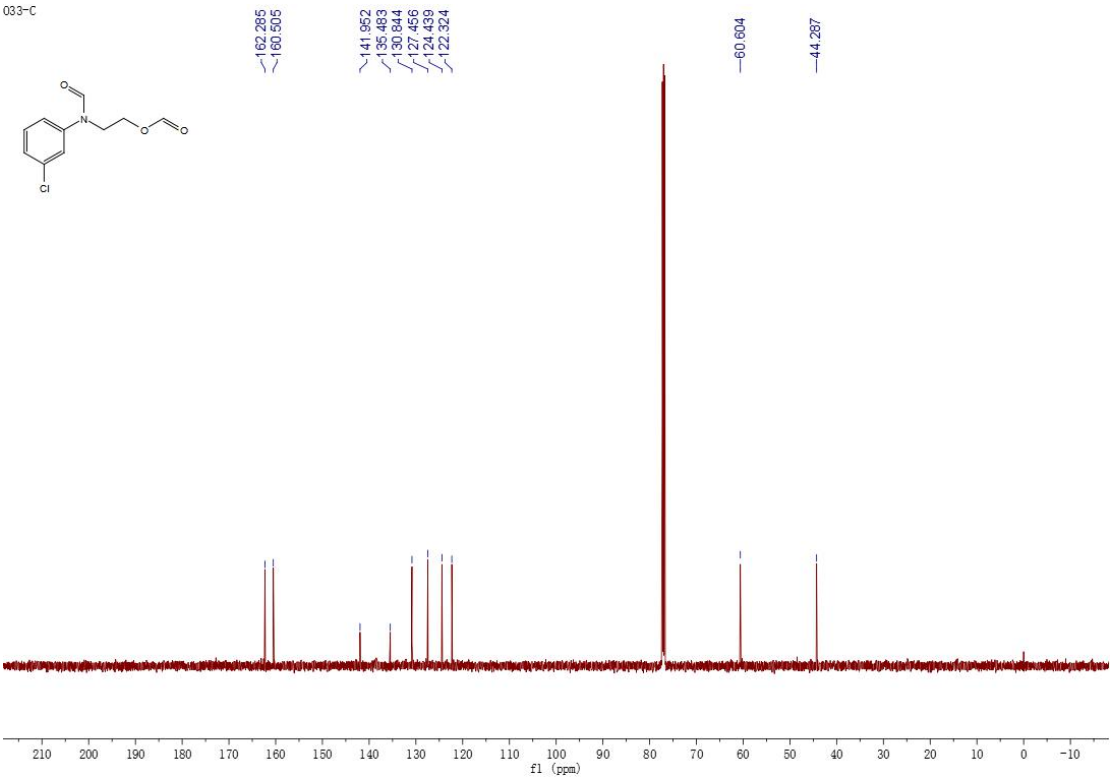
NMR of 28b


081-H
9.948
8.512
7.902
7.895
7.885
7.326
7.309
7.198
4.337
4.326
4.315
4.125
4.113
4.102
1.01
0.93
3.03
1.92
2.00
2.02
f1 (ppm)

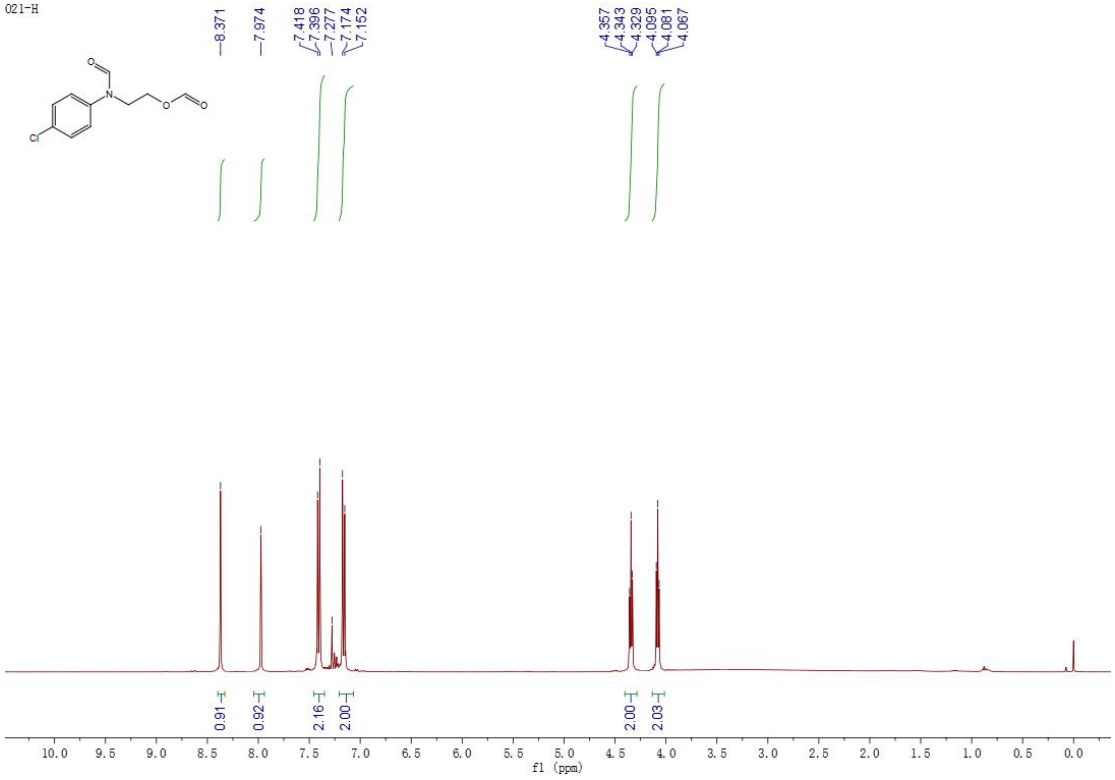

081-C
190.665
162.035
160.456
146.006
134.460
131.416
123.052
60.648
43.944
f1 (ppm)

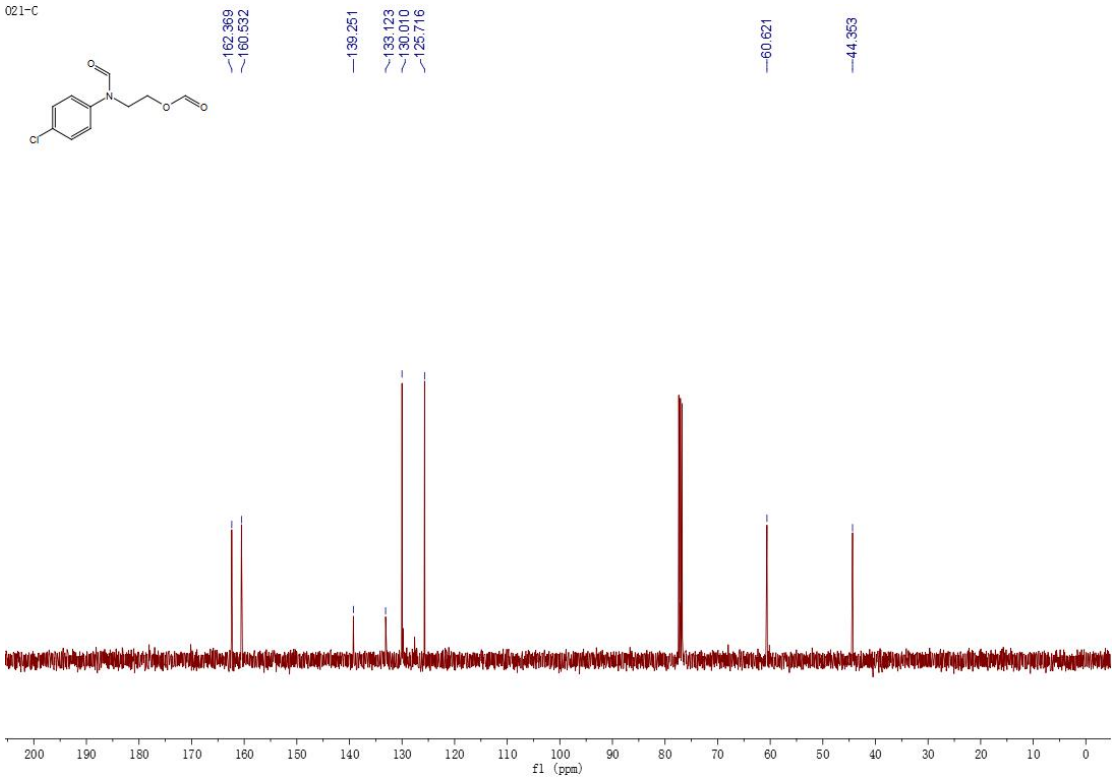
NMR of 29b


033-H
8.409
7.983
7.390
7.370
7.350
7.326
7.323
7.321
7.318
7.301
7.265
7.241
7.236
7.231
7.123
7.120
7.118
7.115
7.104
7.101
7.099
4.353
4.339
4.105
4.091
4.077
0.91
0.89
1.01
1.07
1.01
1.10
2.00
2.14
f1 (ppm)

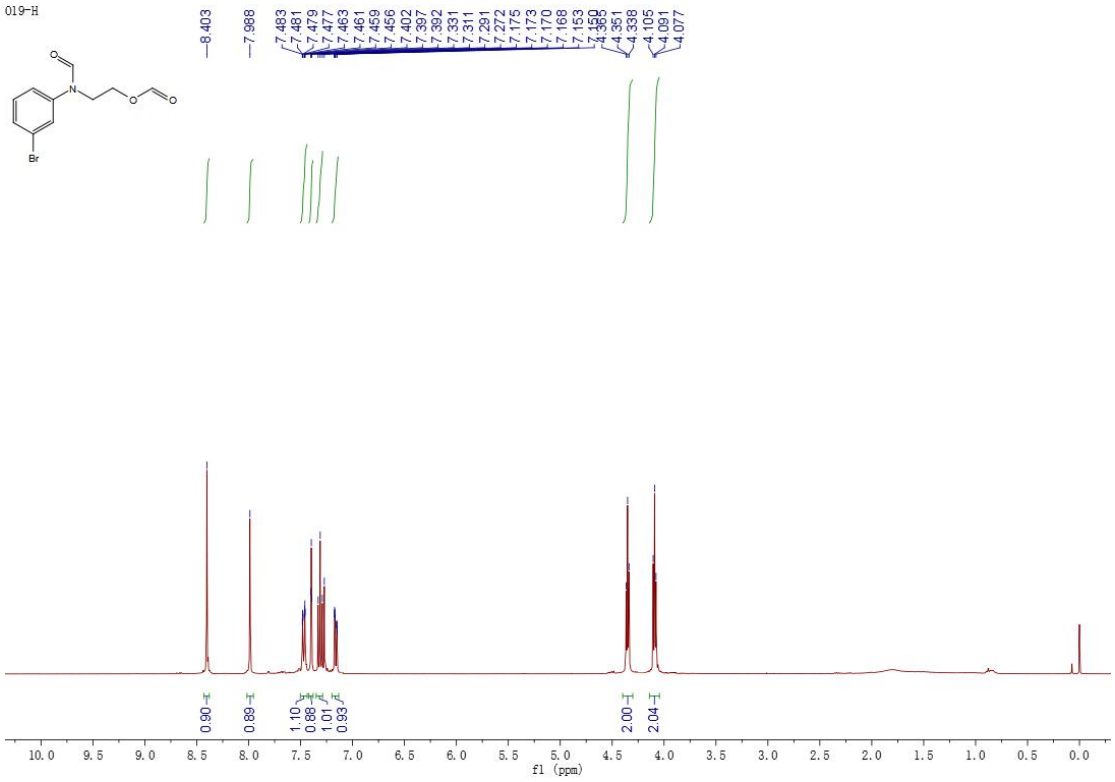

033-C
162.285
160.505
141.952
135.483
130.844
127.456
124.439
122.324
60.604
44.287
f1 (ppm)

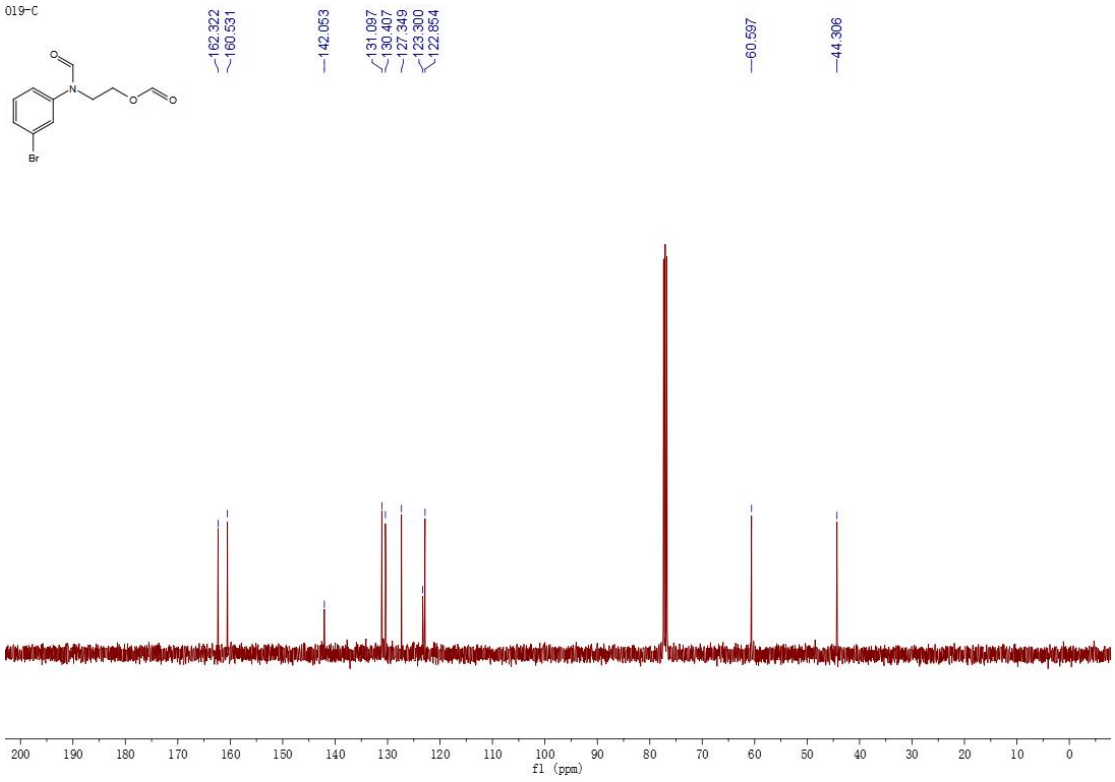
NMR of 30b


021-H
8.371
7.974
7.418
7.396
7.277
7.174
7.152
4.357
4.343
4.329
4.095
4.081
4.067
0.91
0.92
2.16
2.00
2.00
2.03
f1 (ppm)

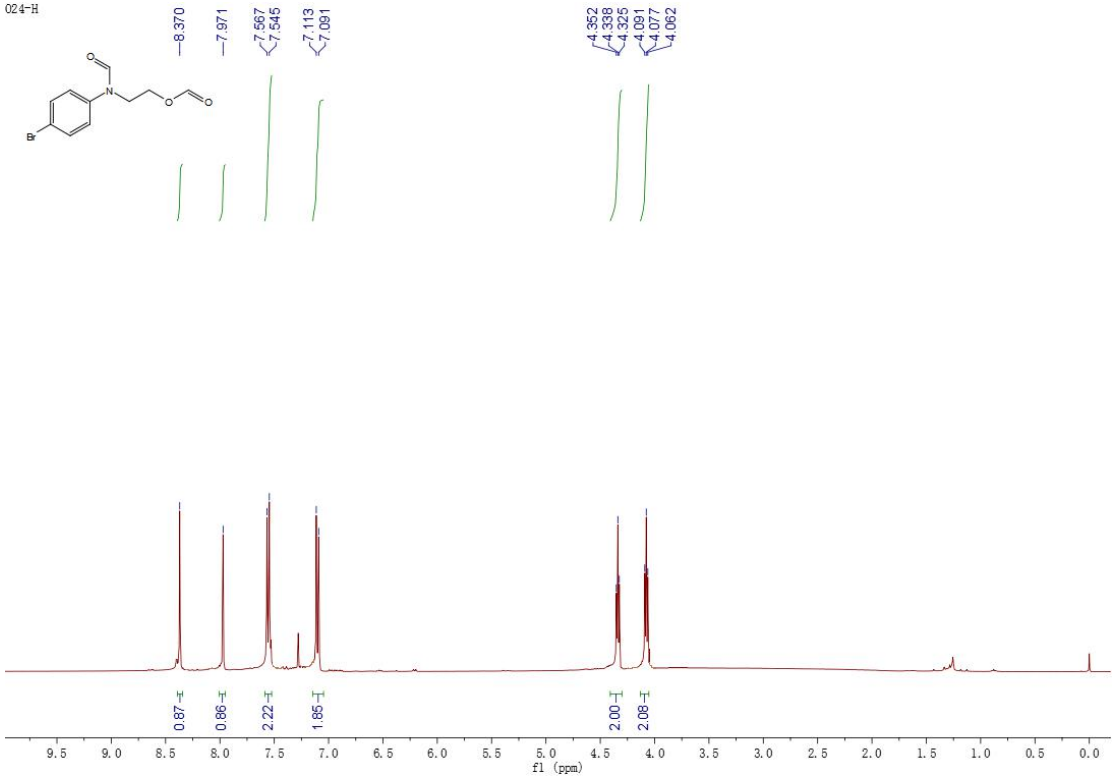

021-C
162.369
160.532
139.251
133.123
130.010
125.716
60.621
44.353
f1 (ppm)

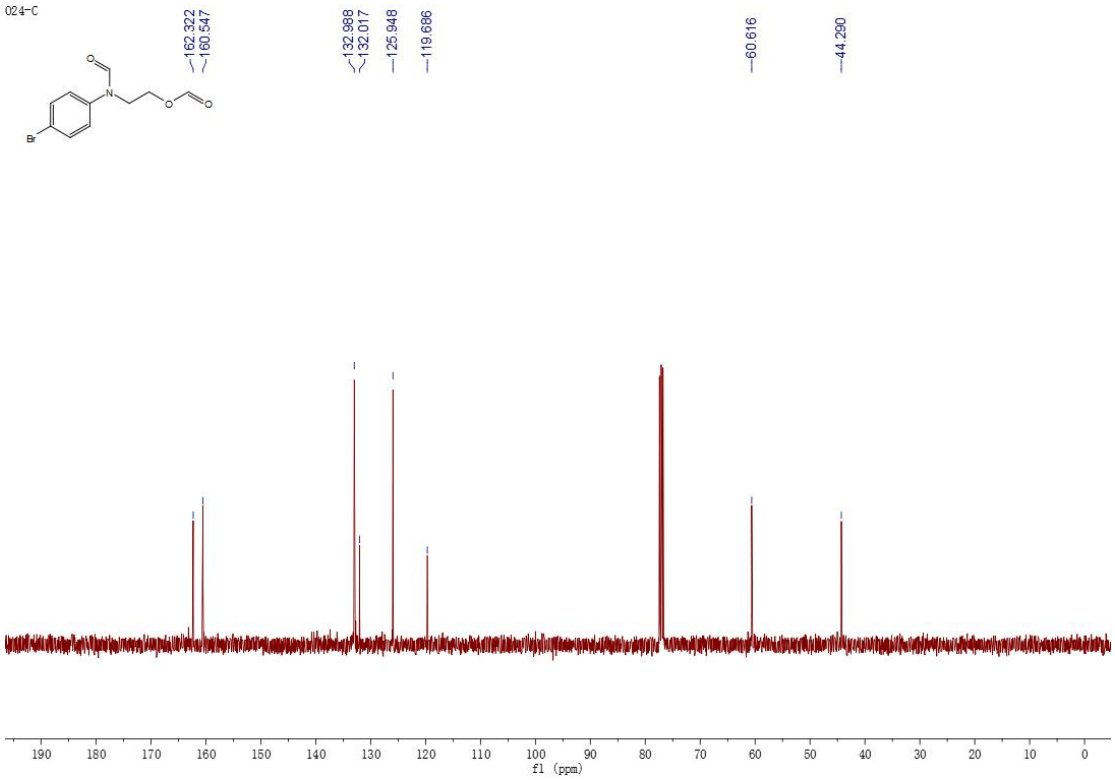
NMR of 31b


019-H
8.403
7.988
7.483
7.481
7.479
7.477
7.463
7.461
7.459
7.456
7.402
7.397
7.392
7.331
7.311
7.291
7.272
7.175
7.173
7.170
7.168
7.153
4.351
4.338
4.105
4.091
4.077
0.90
0.89
1.10
0.88
1.01
0.93
2.00
2.04
f1 (ppm)

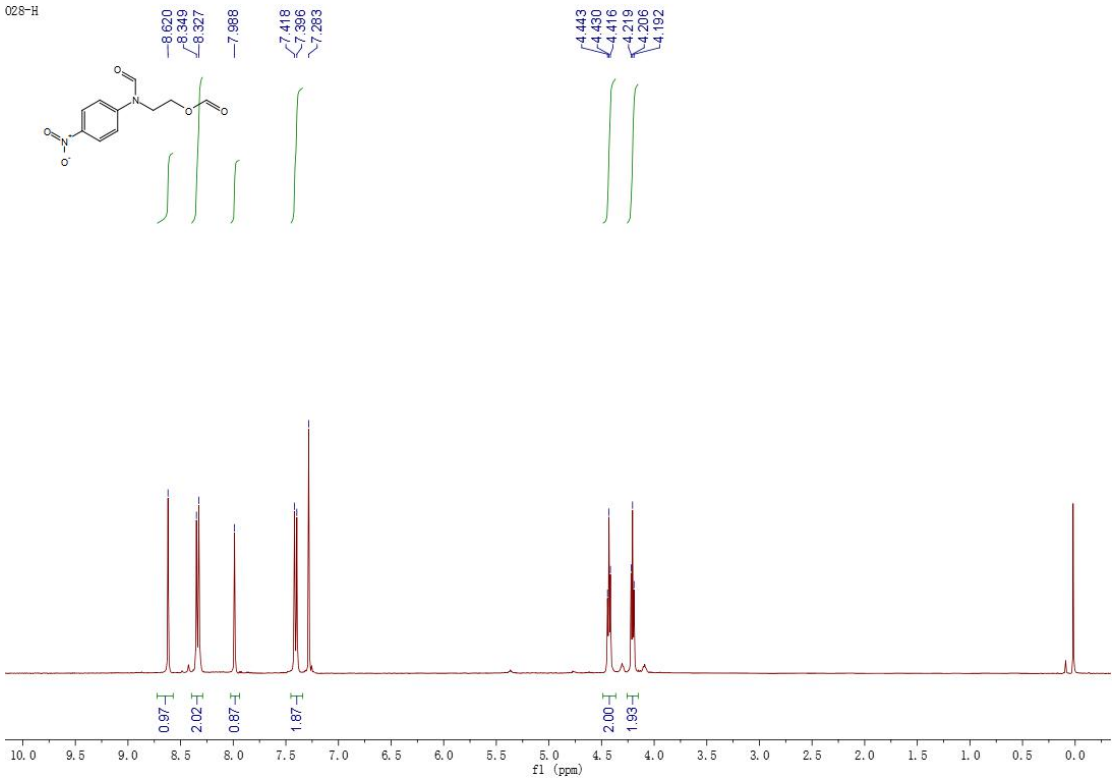

019-C
162.322
160.531
142.053
131.097
130.407
127.349
123.300
122.854
60.597
44.306
f1 (ppm)

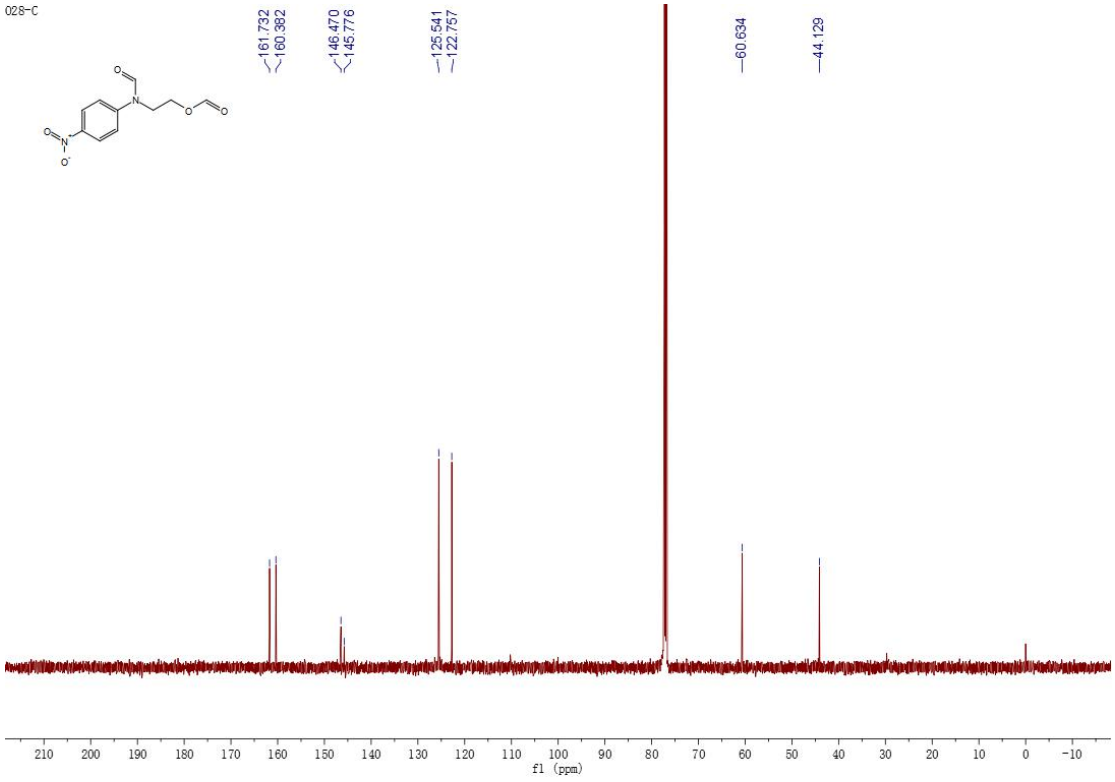
NMR of 32b


024-H
8.370
7.971
7.567
7.545
7.113
7.091
4.352
4.338
4.325
4.091
4.077
4.062
0.87
0.86
2.22
1.85
2.00
2.08
f1 (ppm)

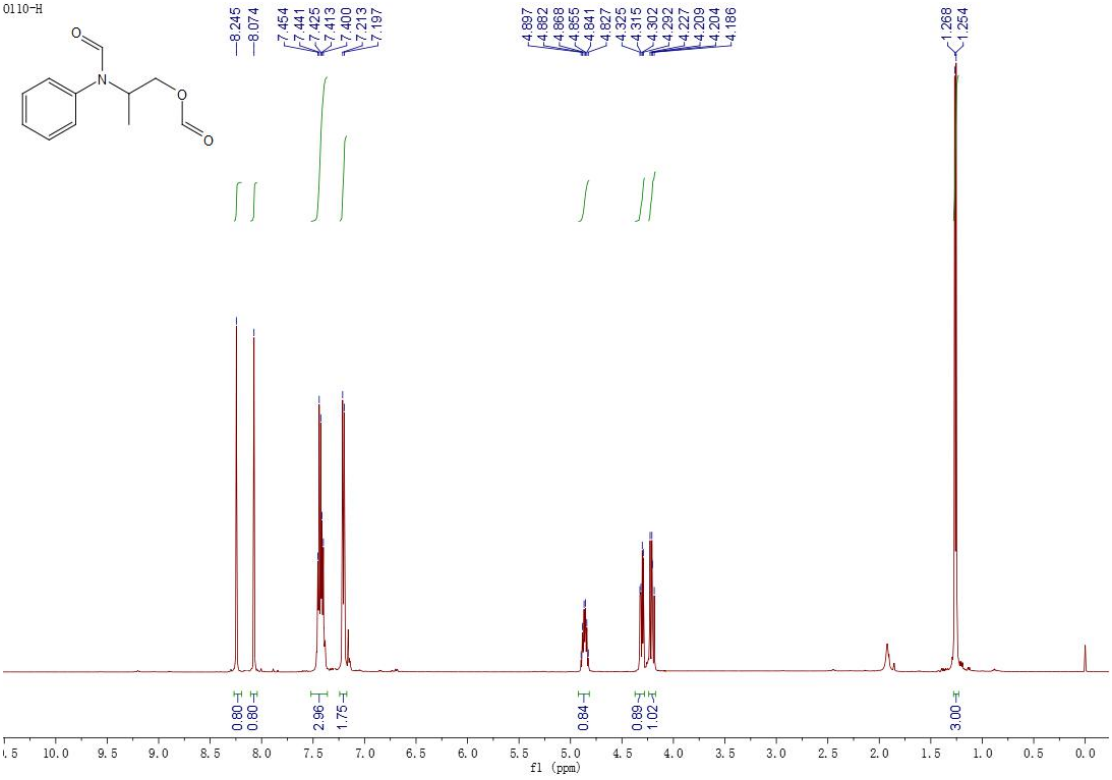

024-C
162.322
160.547
132.988
132.017
125.948
119.686
60.616
44.290
f1 (ppm)

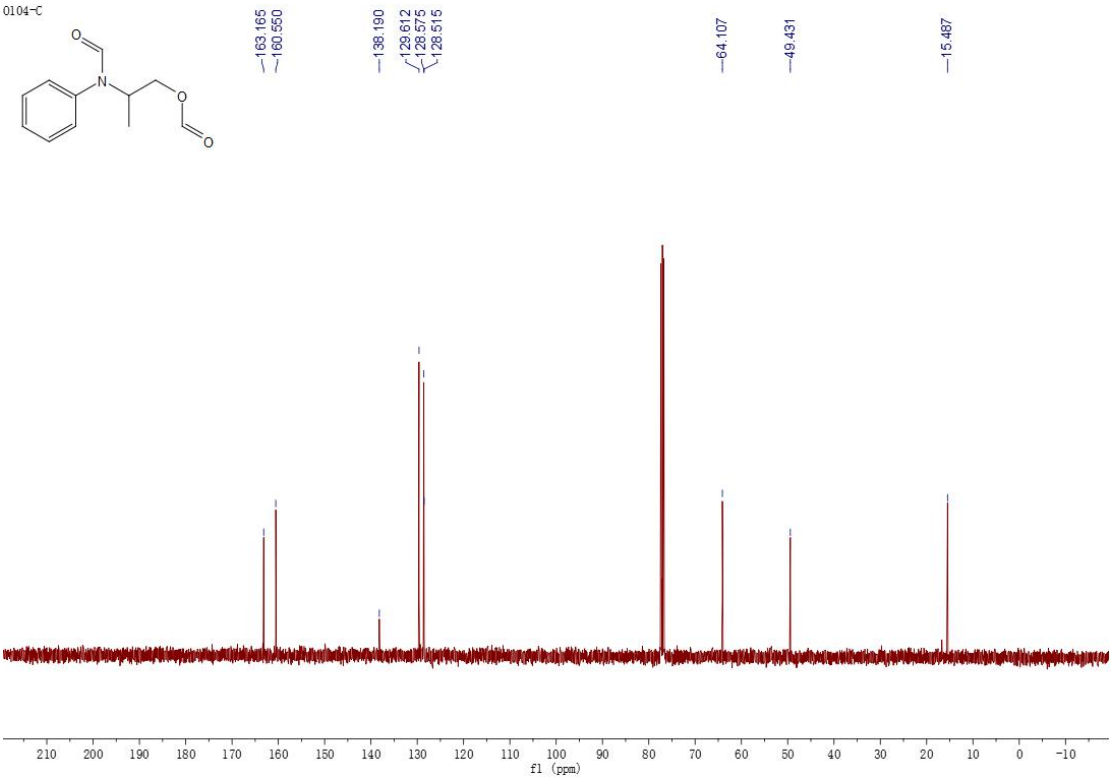
NMR of 33b


028-H
8.620
8.349
8.327
7.988
7.418
7.396
7.283
4.443
4.430
4.416
4.219
4.206
4.192
0.97
2.02
0.87
1.87
2.00
1.93
f1 (ppm)

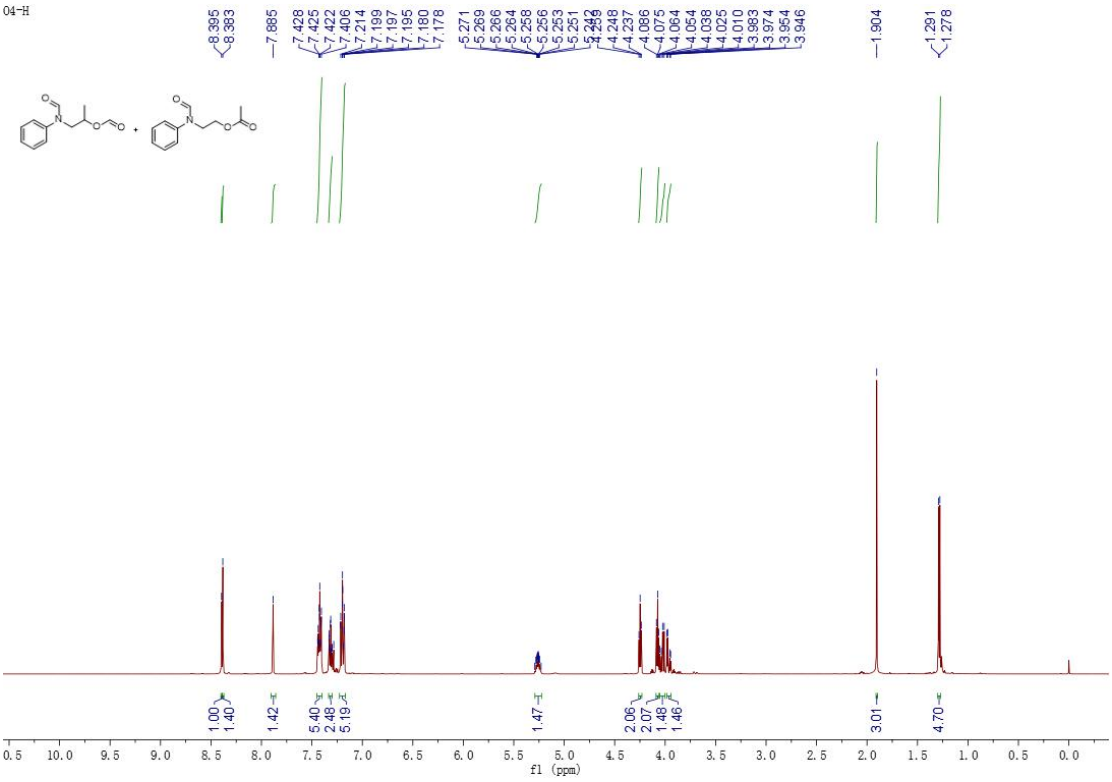

028-C
161.732
160.382
146.470
145.776
125.541
122.757
60.634
44.129
f1 (ppm)

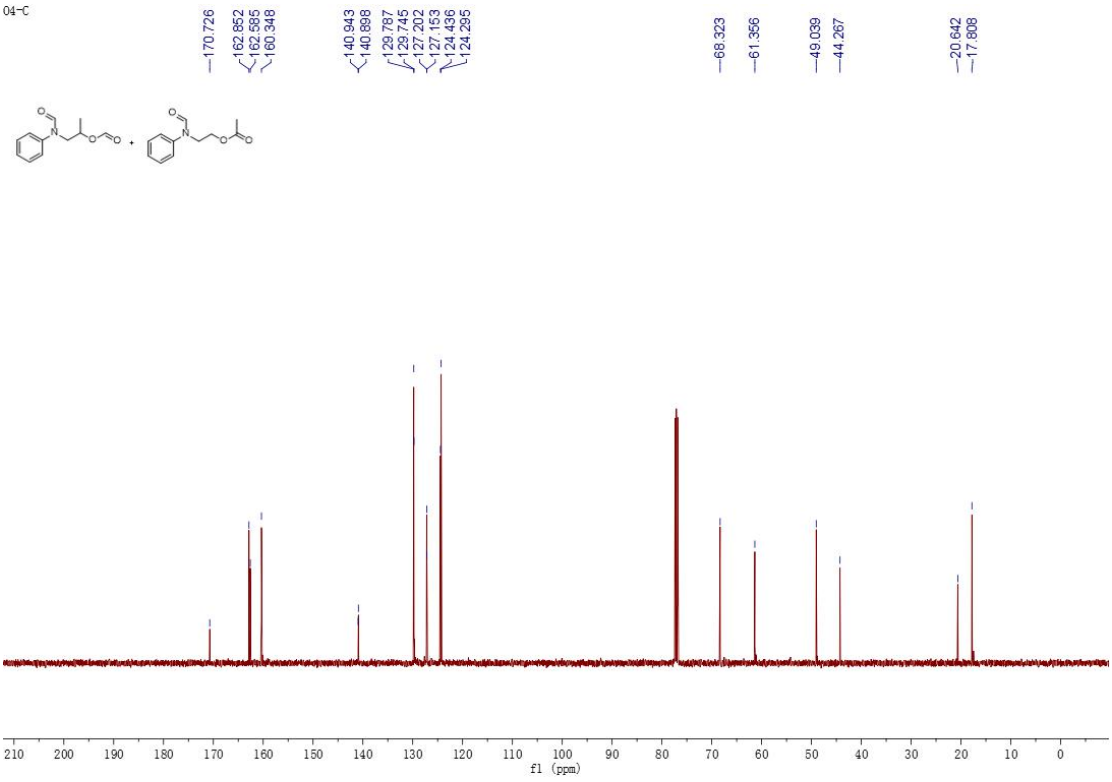
NMR of 34b


0110-H
8.245
8.074
7.454
7.441
7.425
7.413
7.400
7.213
7.197
4.897
4.882
4.868
4.855
4.841
4.827
4.325
4.315
4.302
4.292
4.227
4.209
4.204
4.186
1.268
1.254
0.80
0.80
2.96
1.75
0.84
0.89
1.02
3.00
f1 (ppm)

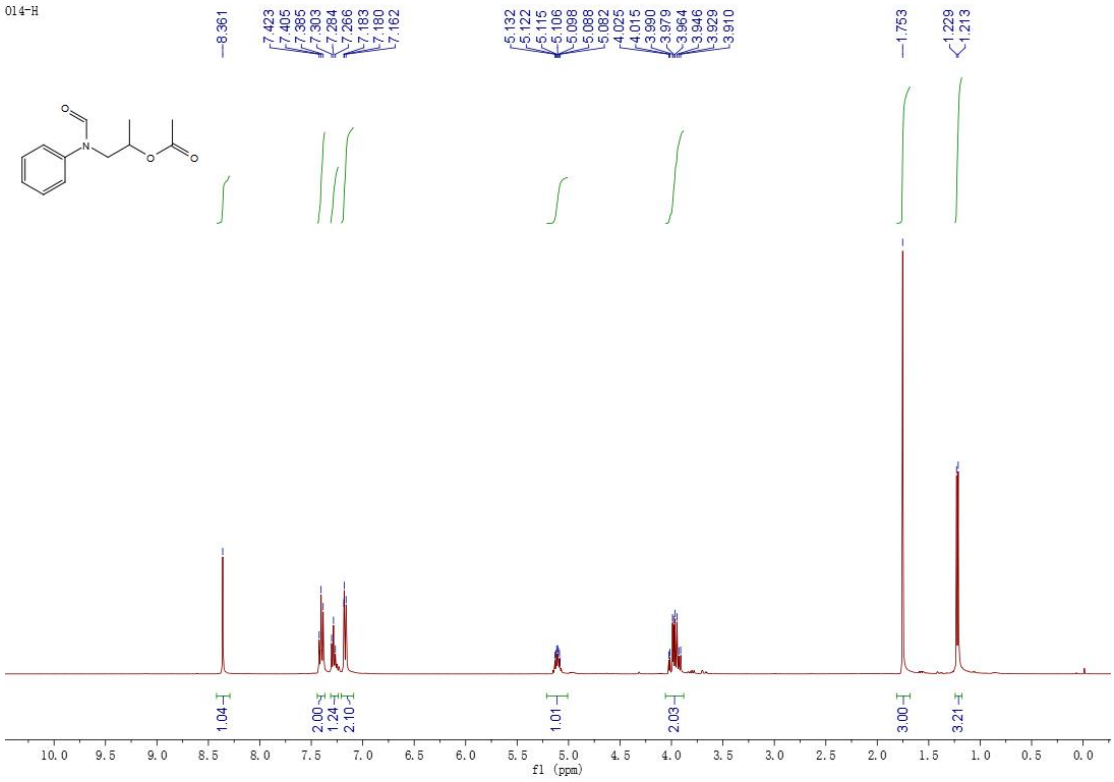

0104-C
163.165
160.550
138.190
129.612
128.575
128.515
64.107
49.431
15.487
f1 (ppm)

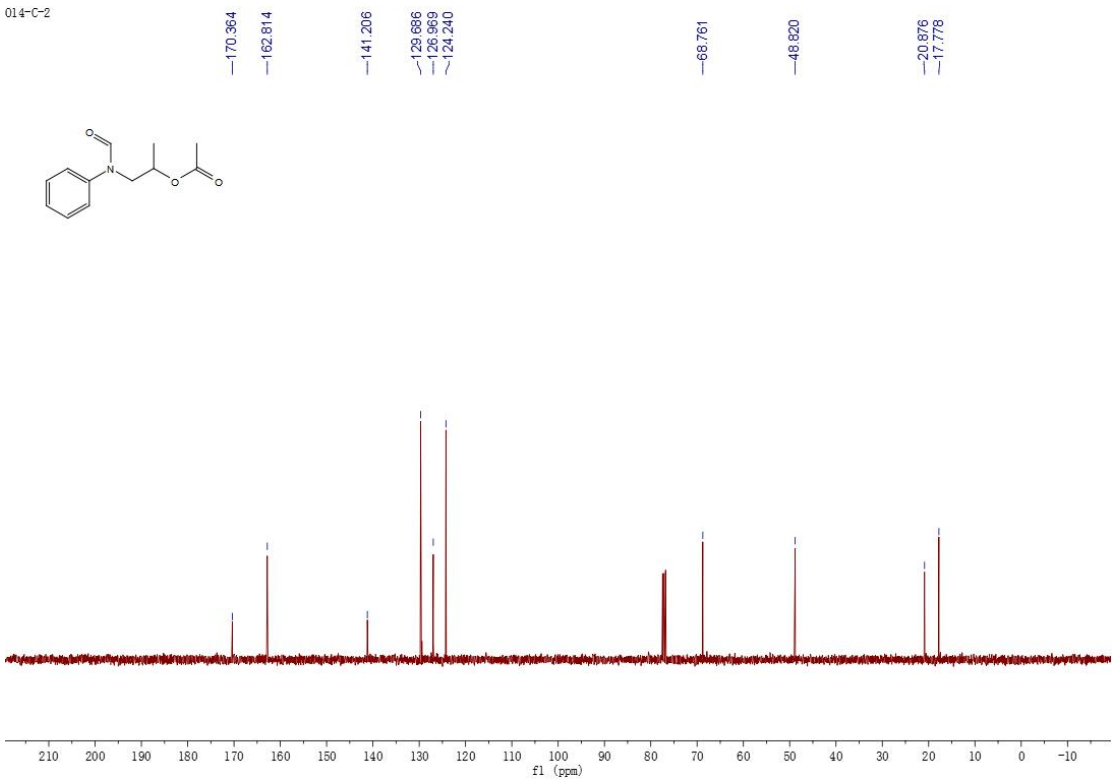
NMR of 35b and 35b’



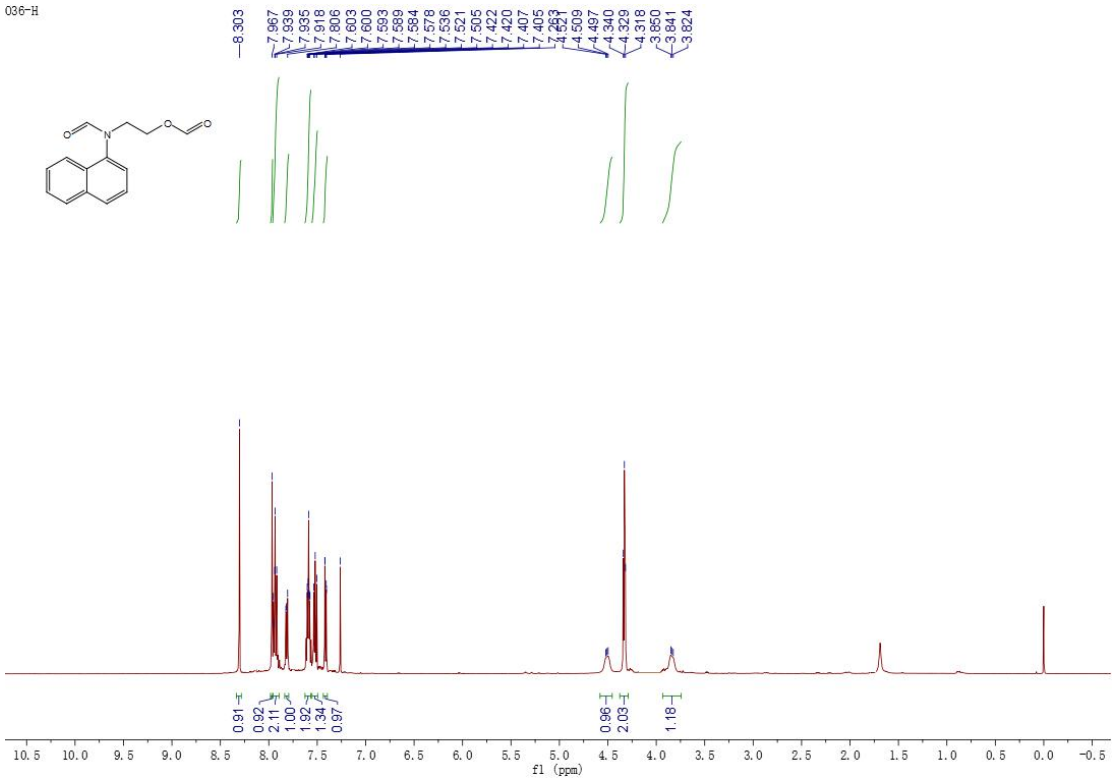


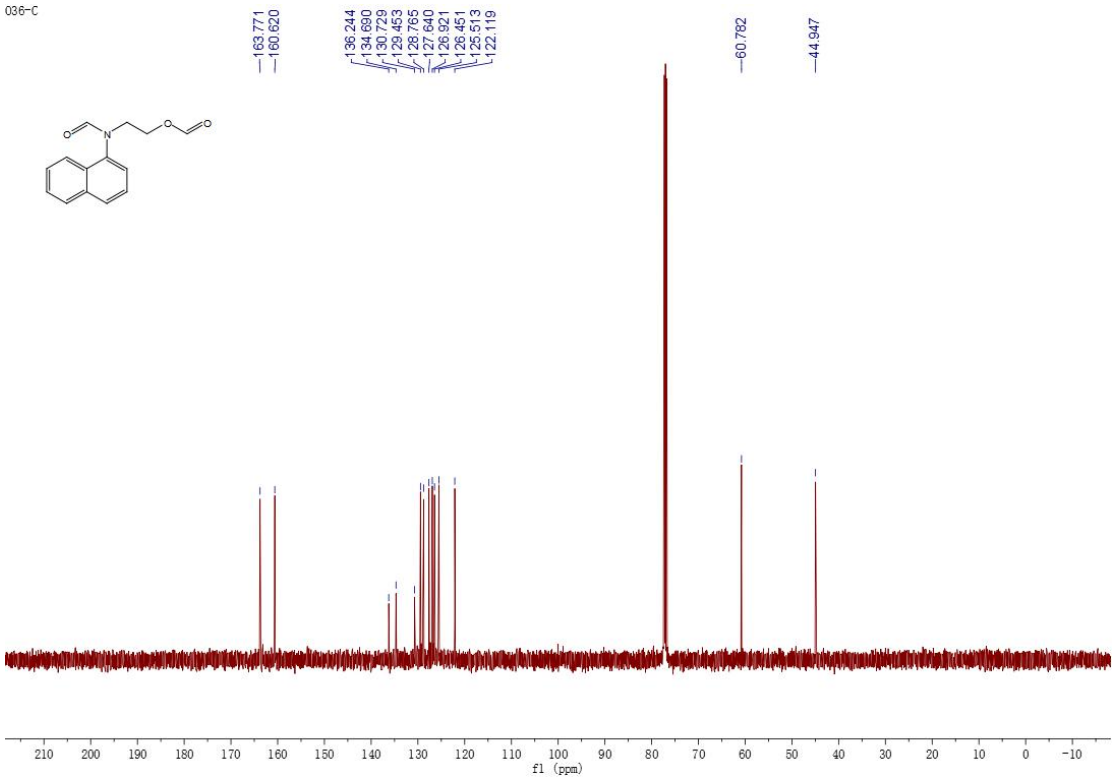
NMR of 36b


014-H
8.361
7.423
7.405
7.385
7.303
7.284
7.266
7.183
7.180
7.162
5.132
5.122
5.115
5.106
5.098
5.088
5.082
4.025
4.015
3.990
3.979
3.964
3.946
3.929
3.910
1.753
1.229
1.213
1.04
2.00
1.24
2.10
1.01
2.03
3.00
3.21
f1 (ppm)

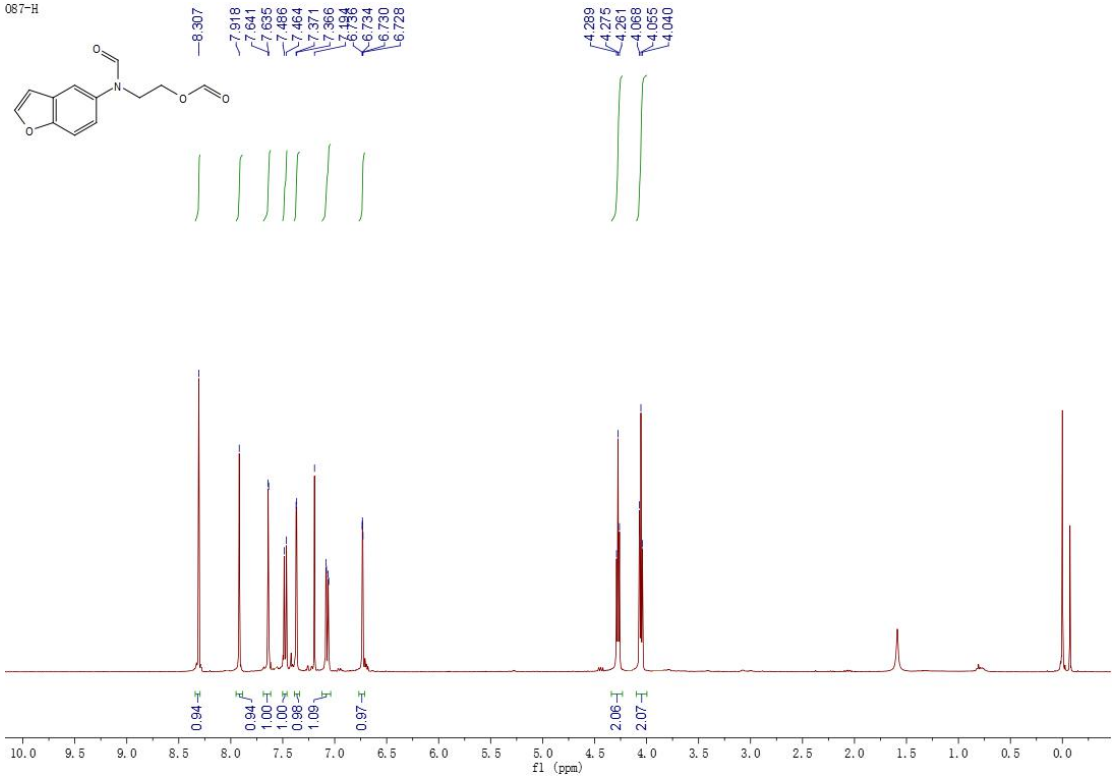

014-C-2
170.364
162.814
141.206
129.686
126.969
124.240
68.761
48.820
20.876
17.778
f1 (ppm)

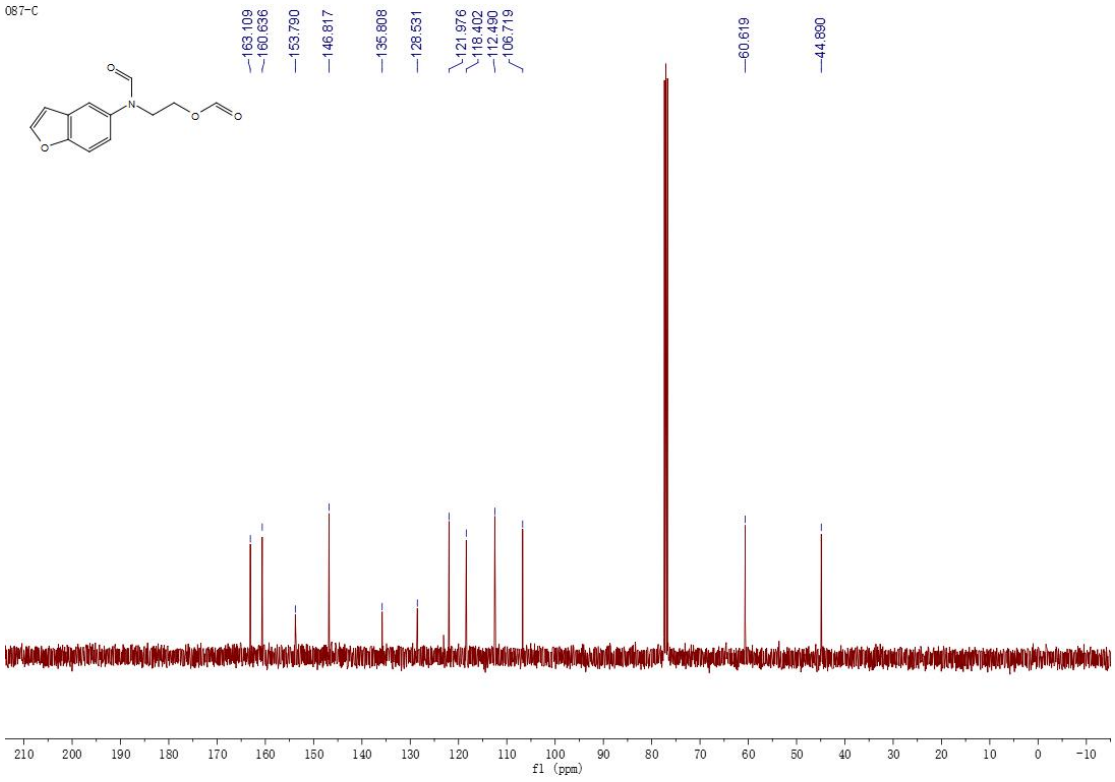
NMR of 37b


036-H
8.303
7.967
7.939
7.935
7.918
7.806
7.603
7.600
7.593
7.589
7.584
7.578
7.536
7.521
7.505
7.422
7.420
7.407
7.405
4.509
4.497
4.340
4.329
4.318
3.850
3.841
3.824
0.91
0.92
2.11
1.00
1.92
1.34
0.97
0.96
2.03
1.18
f1 (ppm)

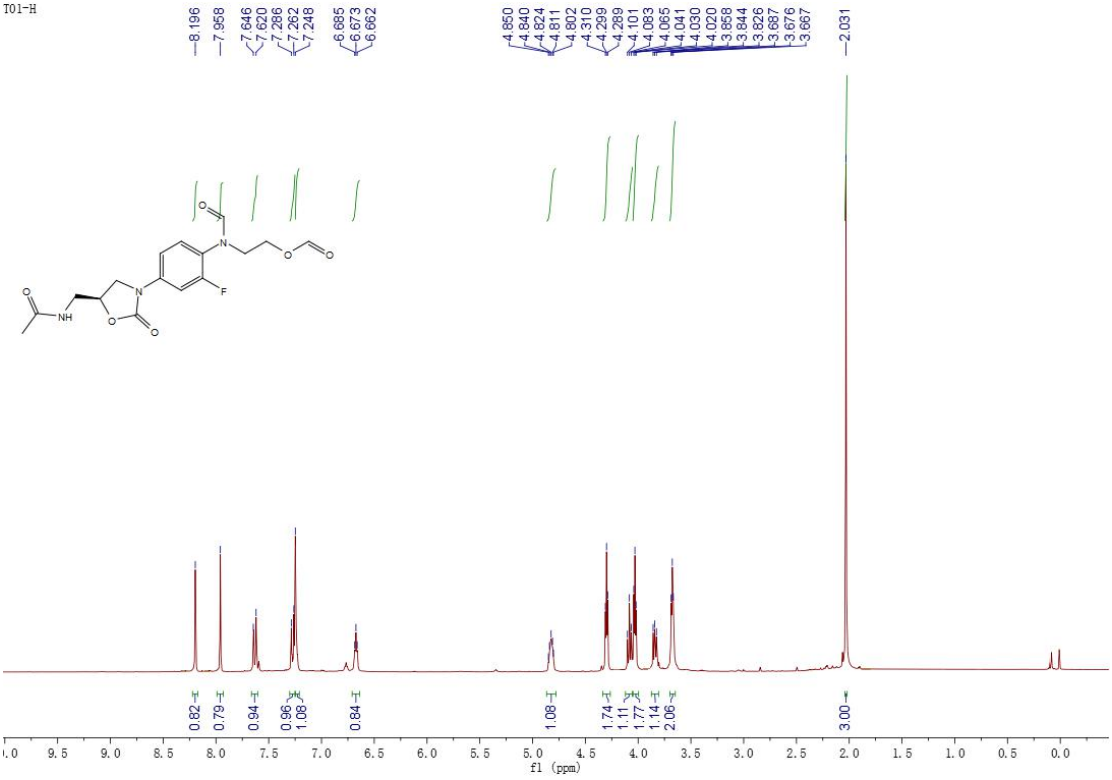

036-C
163.771
160.620
136.244
134.690
130.729
129.453
128.765
127.640
126.921
126.451
125.513
122.119
60.782
44.947
f1 (ppm)

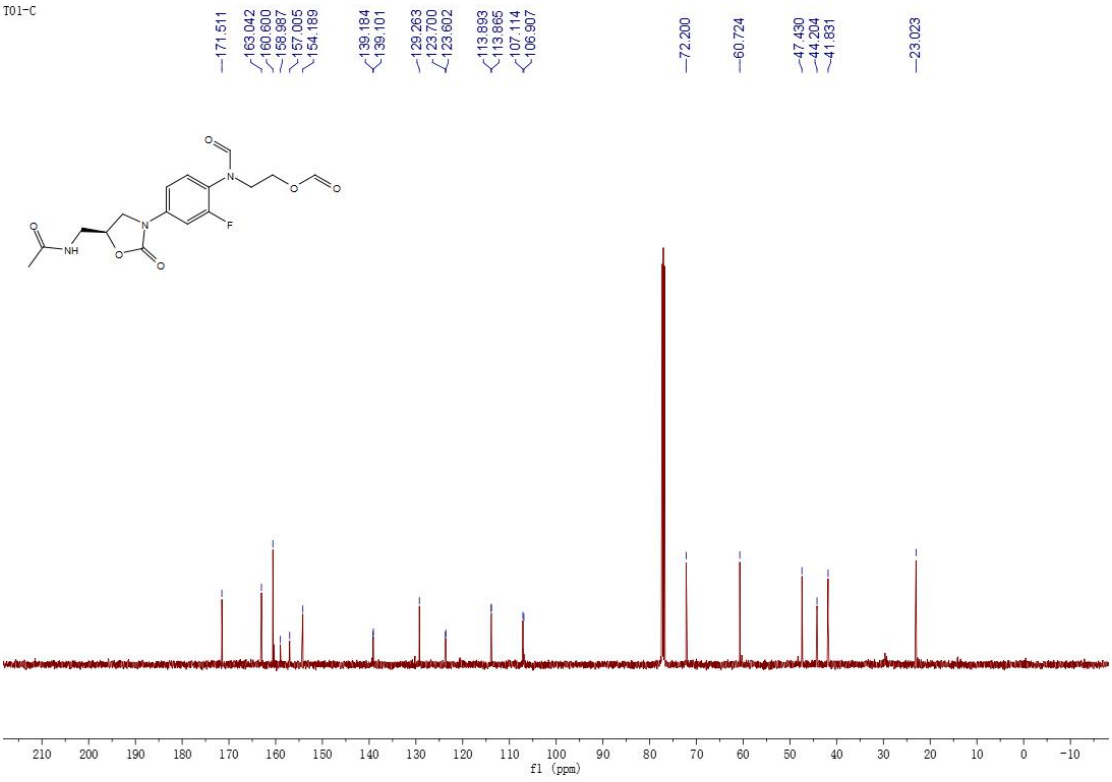
NMR of 38b


087-H
8.307
7.918
7.641
7.635
7.486
7.464
7.371
7.366
6.734
6.730
6.728
4.289
4.275
4.261
4.068
4.055
4.040
0.94
0.94
1.00
1.00
0.98
1.09
0.97
2.06
2.07
f1 (ppm)

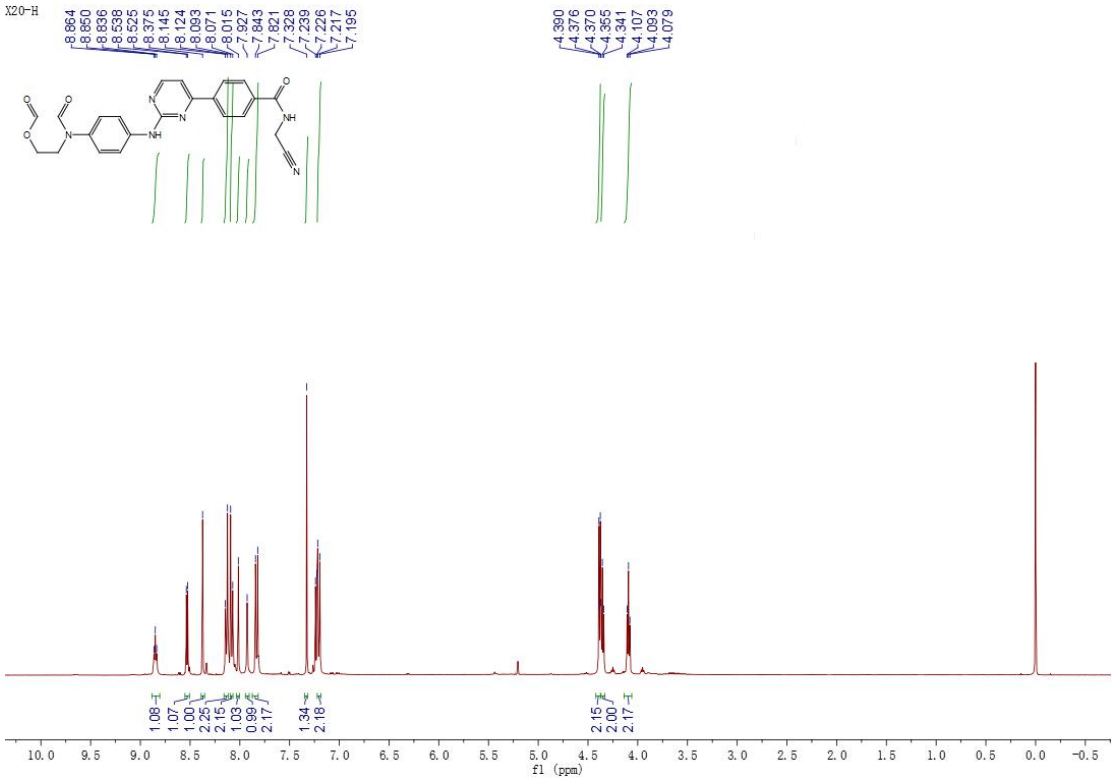

087-C
163.109
160.636
153.790
146.817
135.808
128.531
121.976
118.402
112.490
106.719
60.619
44.890
f1 (ppm)

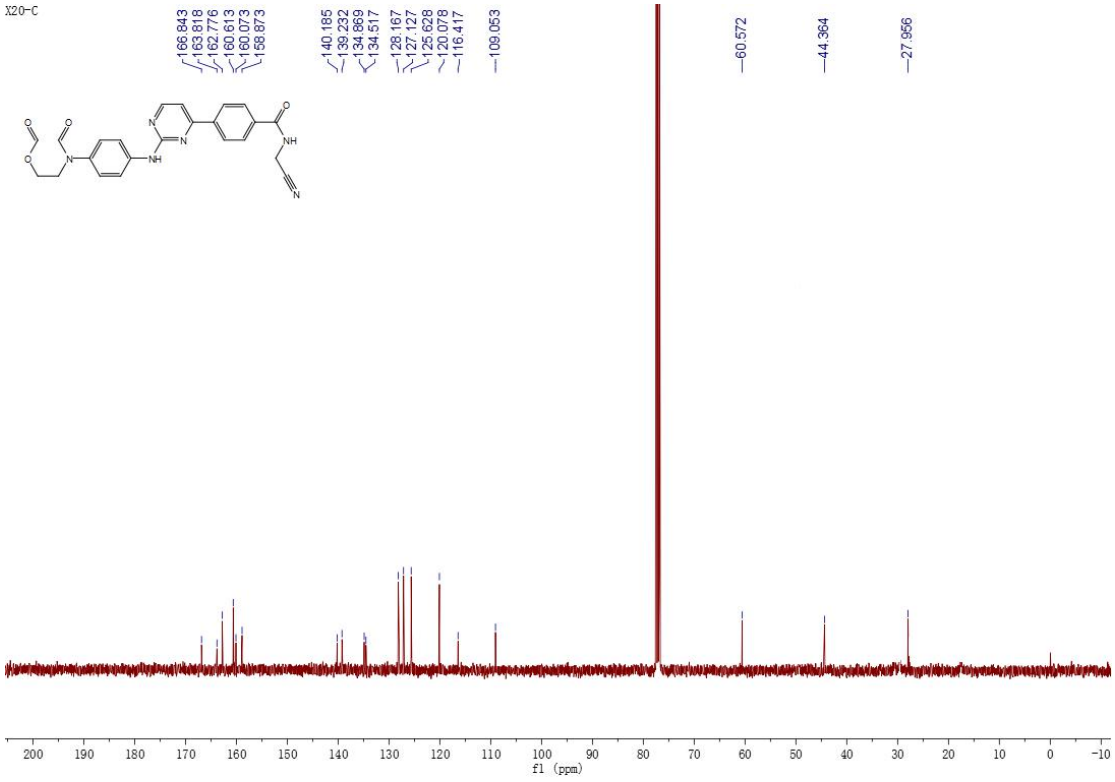
NMR of 39b


T01-H
8.196
7.958
7.646
7.620
7.286
7.262
7.248
6.685
6.673
6.662
4.850
4.840
4.824
4.811
4.802
4.310
4.299
4.289
4.101
4.083
4.065
4.041
4.030
4.020
3.858
3.844
3.826
3.687
3.676
3.667
2.031
0.82
0.79
0.94
0.96
1.08
0.84
1.08
1.74
1.11
1.77
1.14
2.06
3.00
f1 (ppm)

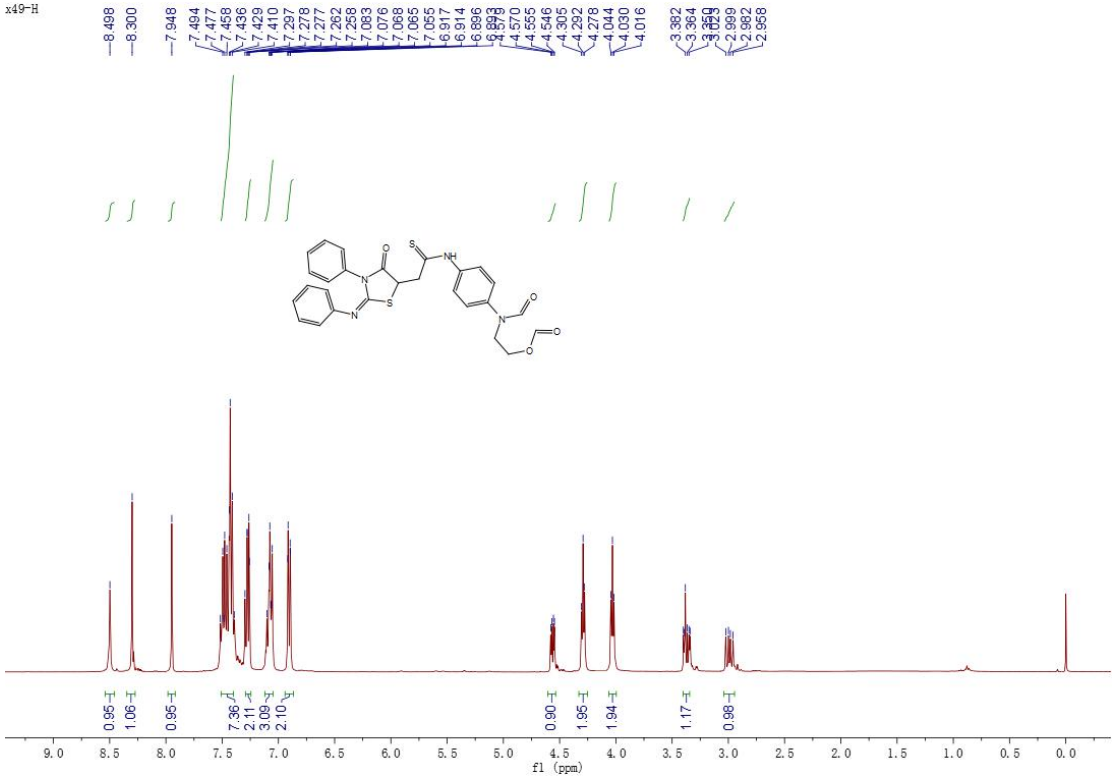

T01-C
171.511
163.042
160.600
158.967
157.005
154.189
139.184
139.101
129.263
123.700
123.602
113.893
113.865
107.114
106.907
72.200
60.724
47.430
44.204
41.831
23.023
f1 (ppm)

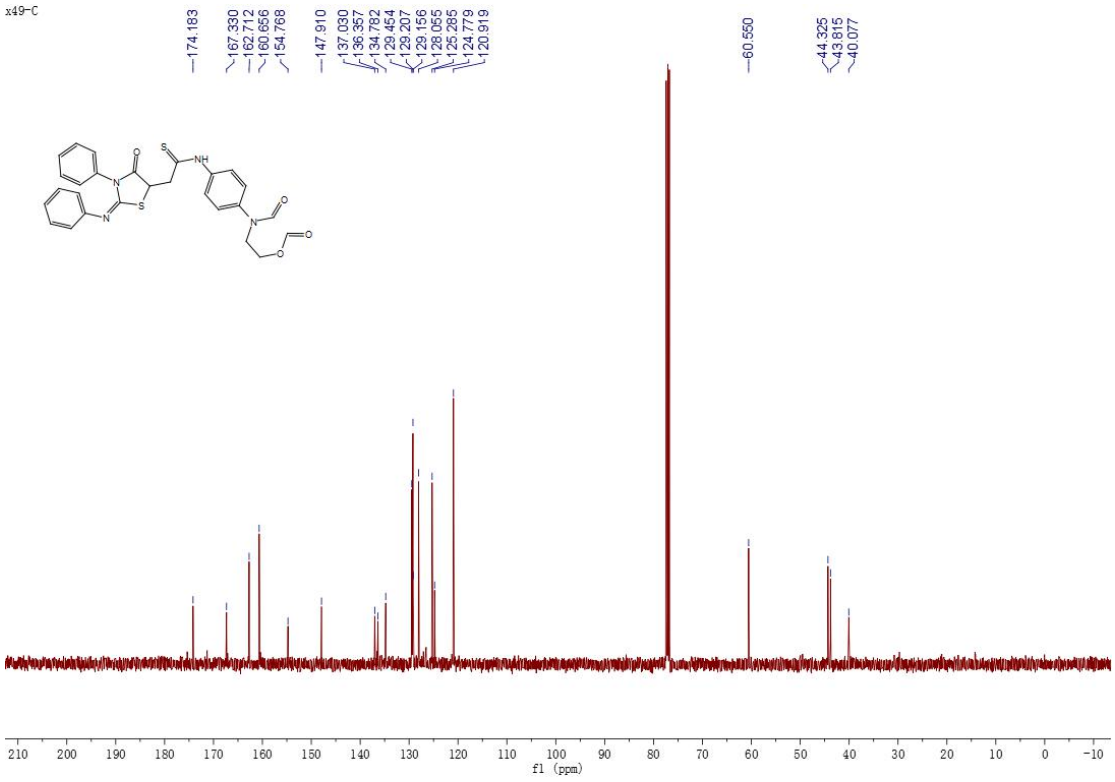
NMR of 40b


X20-H
8.864
8.850
8.836
8.538
8.525
8.375
8.145
8.124
8.093
8.071
8.015
7.927
7.843
7.821
7.328
7.239
7.226
7.217
7.195
4.390
4.376
4.370
4.355
4.341
4.107
4.093
4.079
1.08
1.07
1.00
2.25
2.15
1.03
0.99
2.17
1.34
2.18
2.15
2.00
2.17
f1 (ppm)

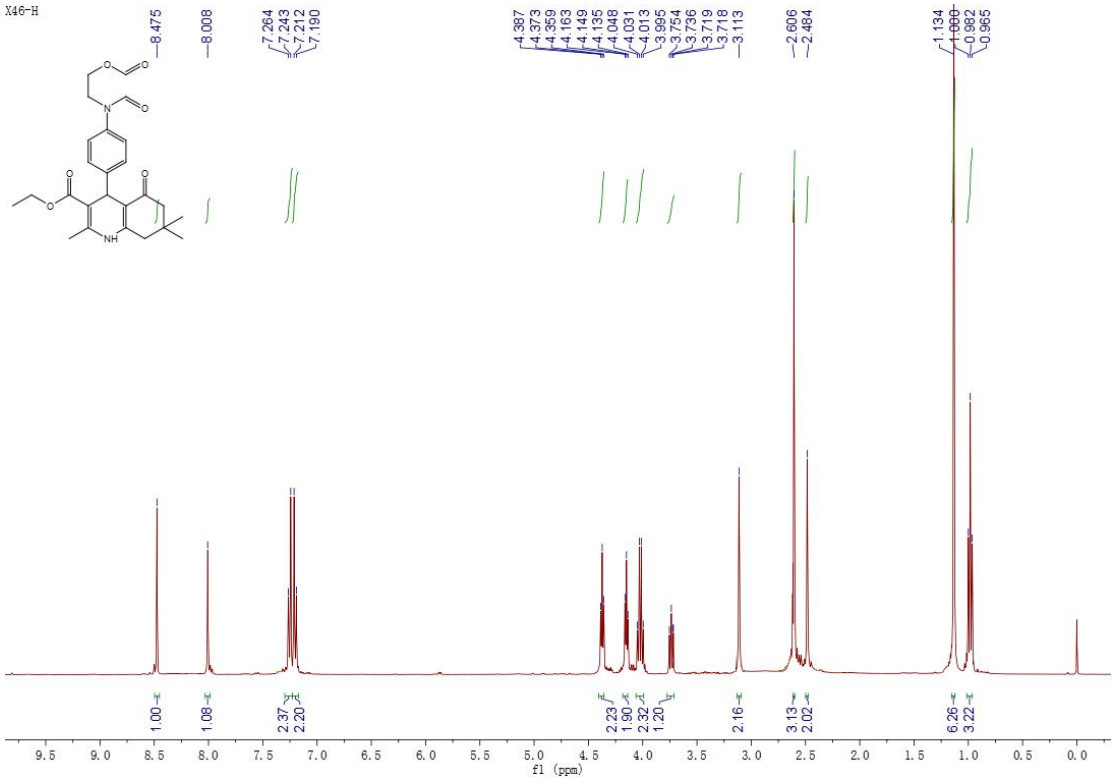

X20-C
166.843
163.818
162.776
160.613
160.073
158.873
140.185
139.232
134.869
134.517
128.167
127.127
125.628
120.078
116.417
109.053
60.572
44.364
27.956
f1 (ppm)

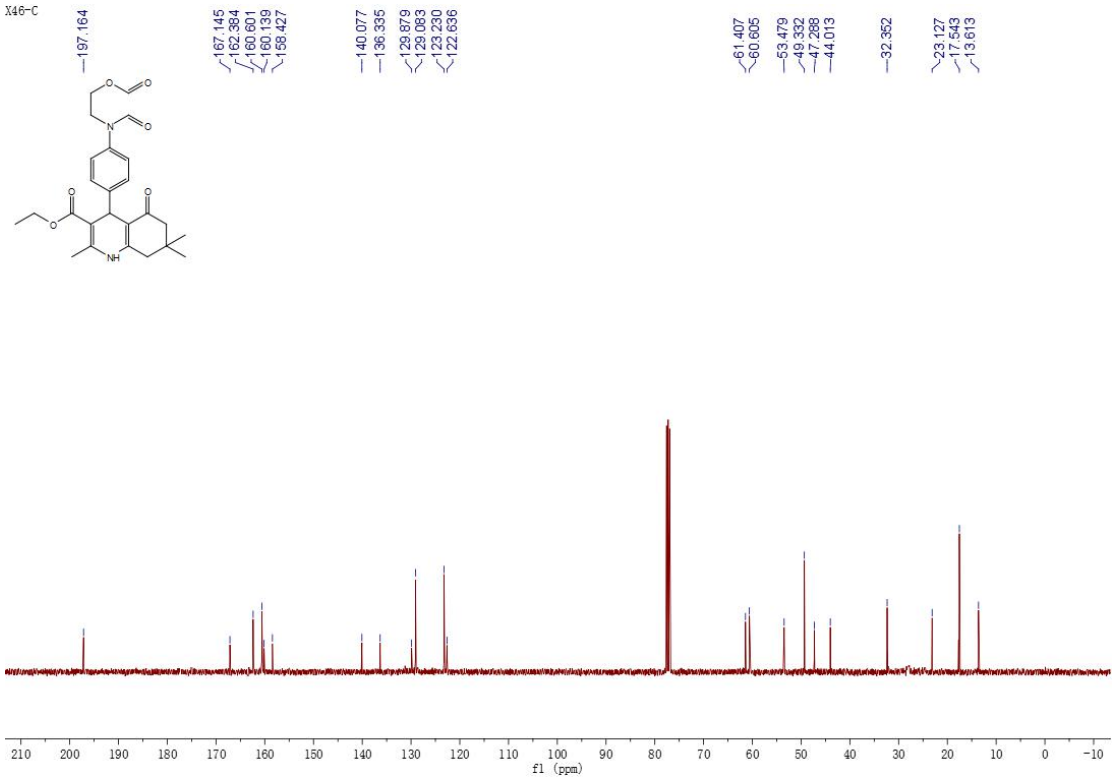
NMR of 41b


x49-H
8.498
8.300
7.948
7.494
7.477
7.458
7.436
7.429
7.410
7.297
7.278
7.277
7.262
7.258
7.083
7.076
7.068
7.065
7.055
6.917
6.914
6.896
4.570
4.555
4.546
4.305
4.292
4.278
4.044
4.030
4.016
3.382
3.364
2.999
2.982
2.958
0.95
1.06
0.95
7.36
2.11
3.09
2.10
0.90
1.95
1.94
1.17
0.98
f1 (ppm)

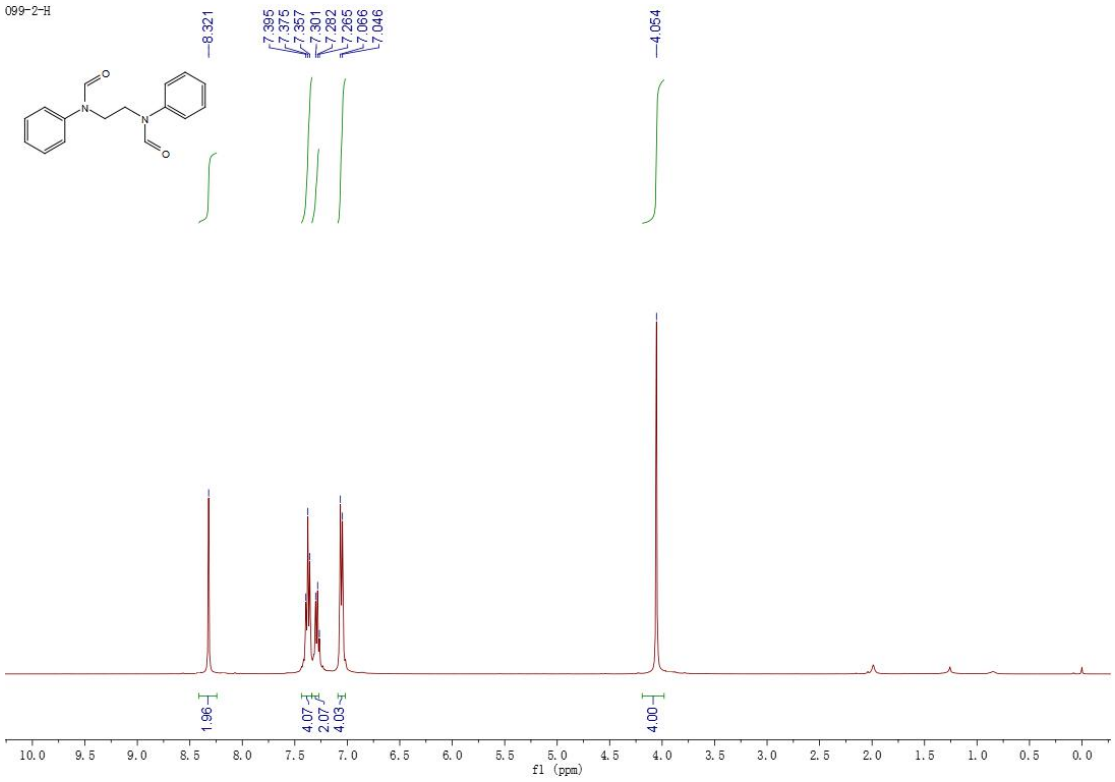

x49-C
174.183
167.330
162.712
160.656
154.768
147.910
137.030
136.357
134.782
129.454
129.207
129.156
128.055
125.285
124.779
120.919
60.550
44.325
43.815
40.077
f1 (ppm)

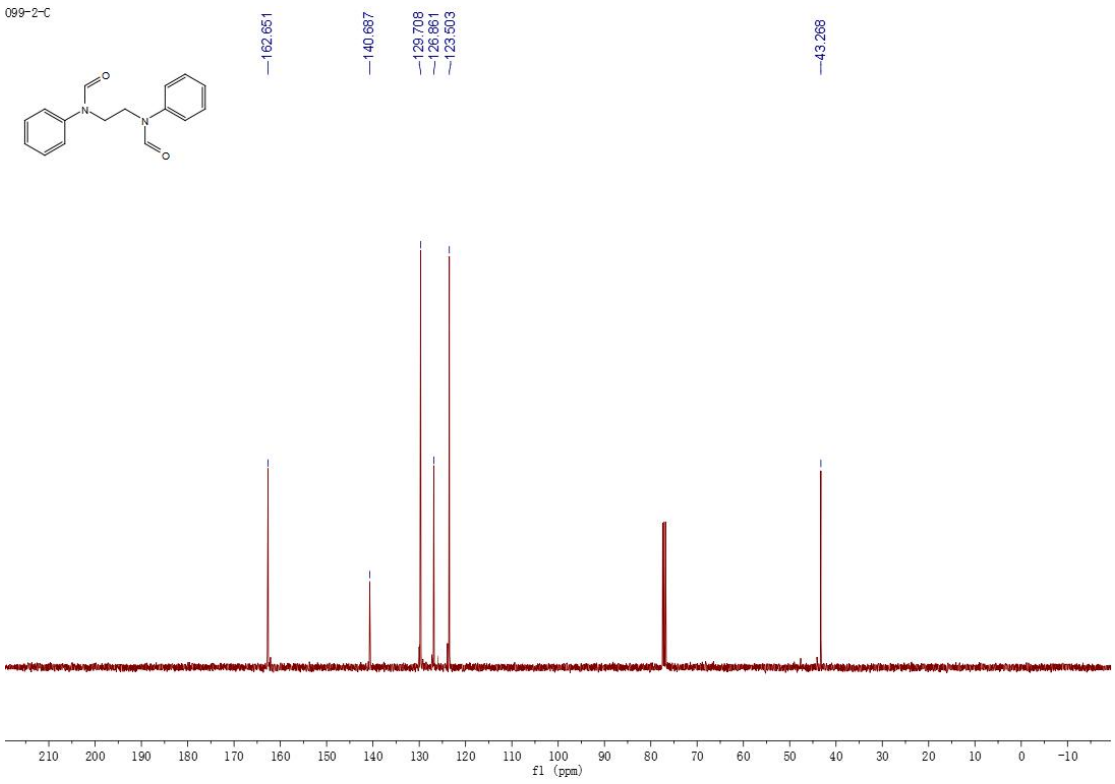
NMR of 42b


X46-H
8.475
8.008
7.264
7.243
7.212
7.190
4.387
4.373
4.359
4.163
4.149
4.135
4.048
4.031
4.013
3.995
3.754
3.736
3.719
3.718
3.113
2.606
2.484
1.134
1.000
0.982
0.965
1.00
1.08
2.37
2.20
2.23
1.90
2.32
1.20
2.16
3.13
2.02
6.26
3.22
f1 (ppm)

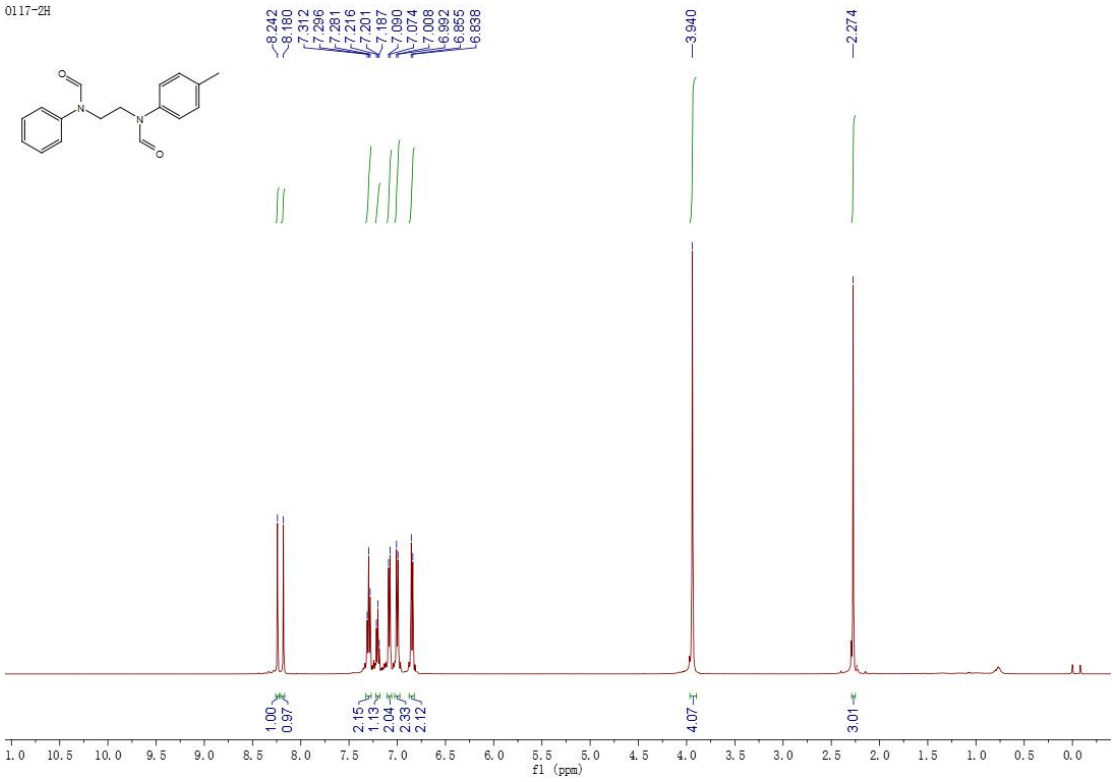

X46-C
197.164
167.145
162.384
160.601
160.139
158.427
140.077
136.335
129.879
129.083
123.230
122.636
61.407
60.605
53.479
49.332
47.288
44.013
32.352
23.127
17.543
13.613
f1 (ppm)

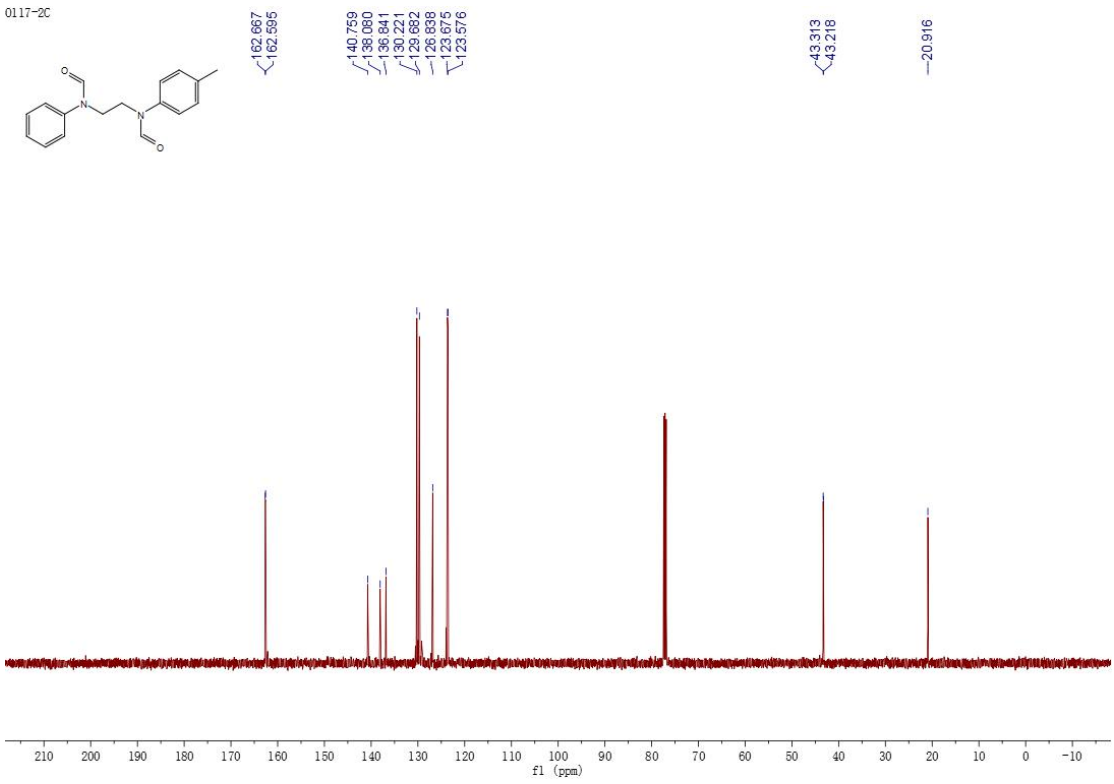
NMR of 43b


099-2-H
8.321
7.395
7.375
7.357
7.301
7.282
7.265
7.066
7.046
4.054
1.96
4.07
2.07
4.03
4.00
f1 (ppm)

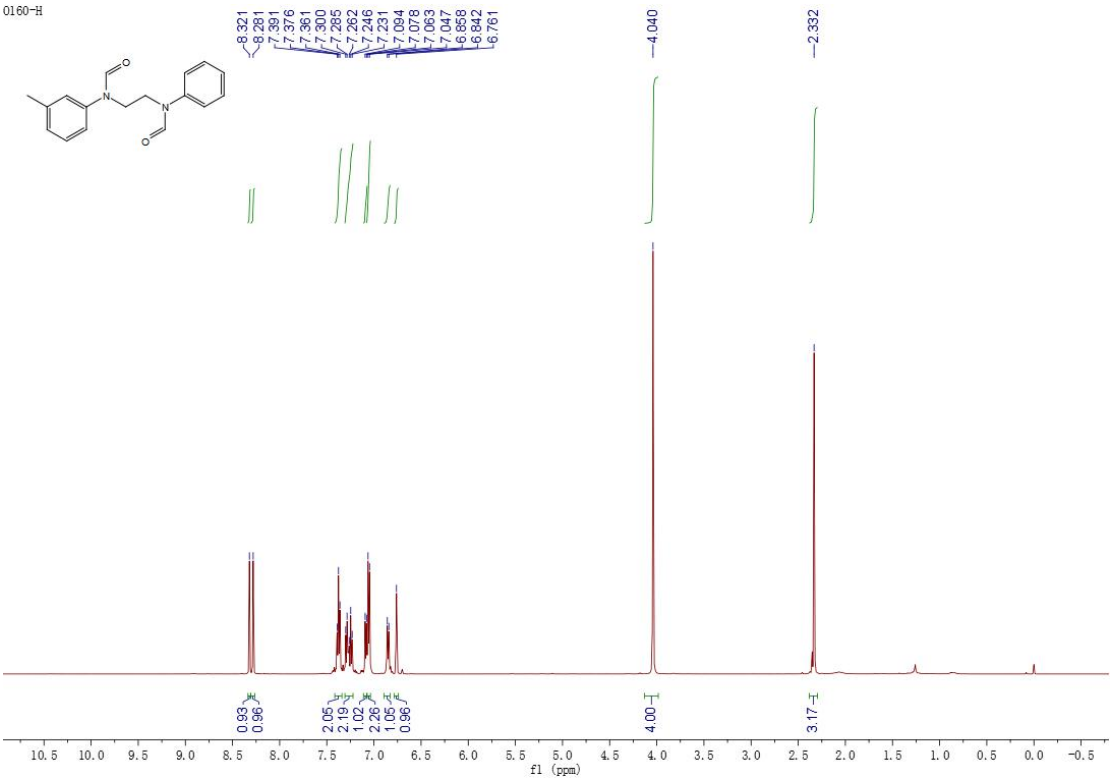

099-2-C
162.651
140.687
129.708
126.861
123.503
43.268
f1 (ppm)

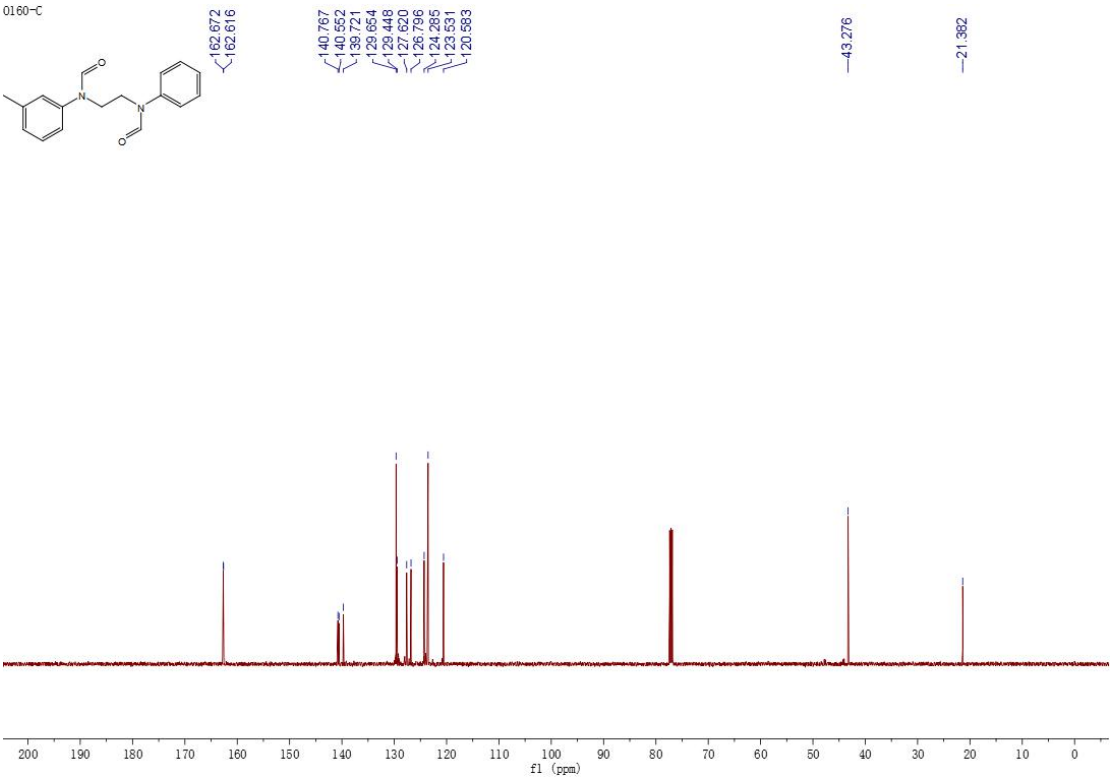
NMR of 44b


0117-2H
8.242
8.180
7.312
7.296
7.281
7.216
7.201
7.187
7.090
7.074
7.008
6.992
6.855
6.838
3.940
2.274
1.00
0.97
2.15
1.13
2.04
2.33
2.12
4.07
3.01
f1 (ppm)

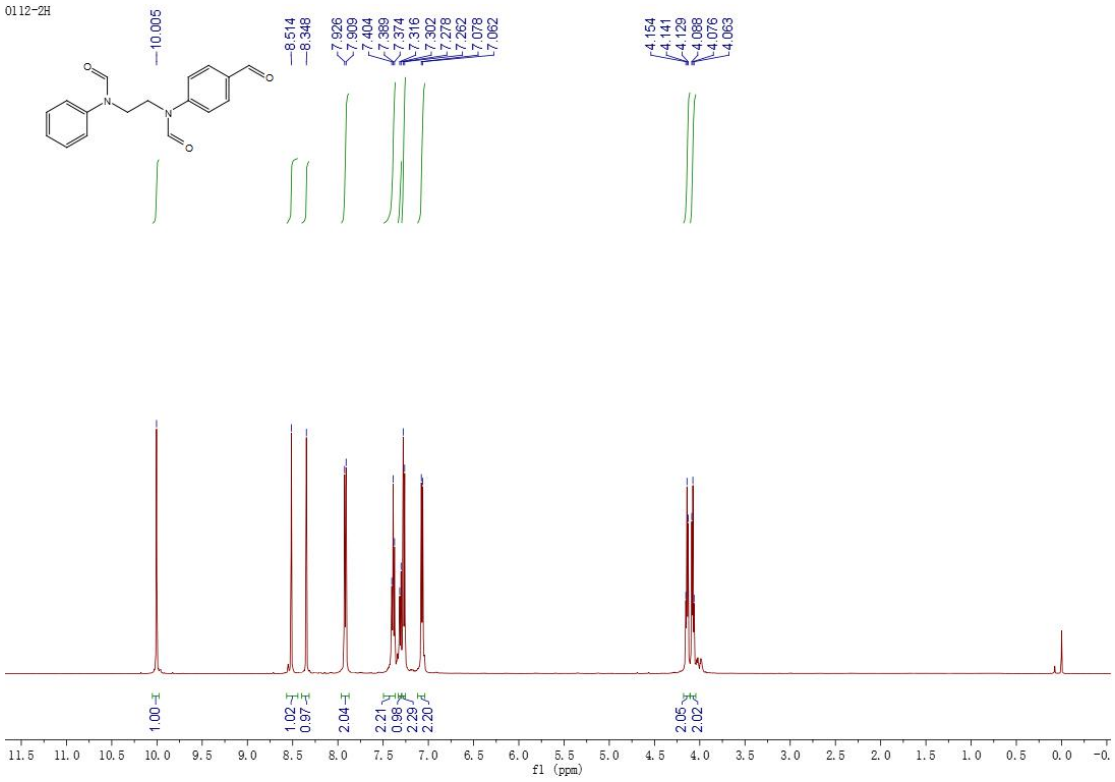

0117-2C
162.667
162.595
140.759
138.080
136.841
130.221
129.682
126.838
123.675
123.576
43.313
43.218
20.916
f1 (ppm)

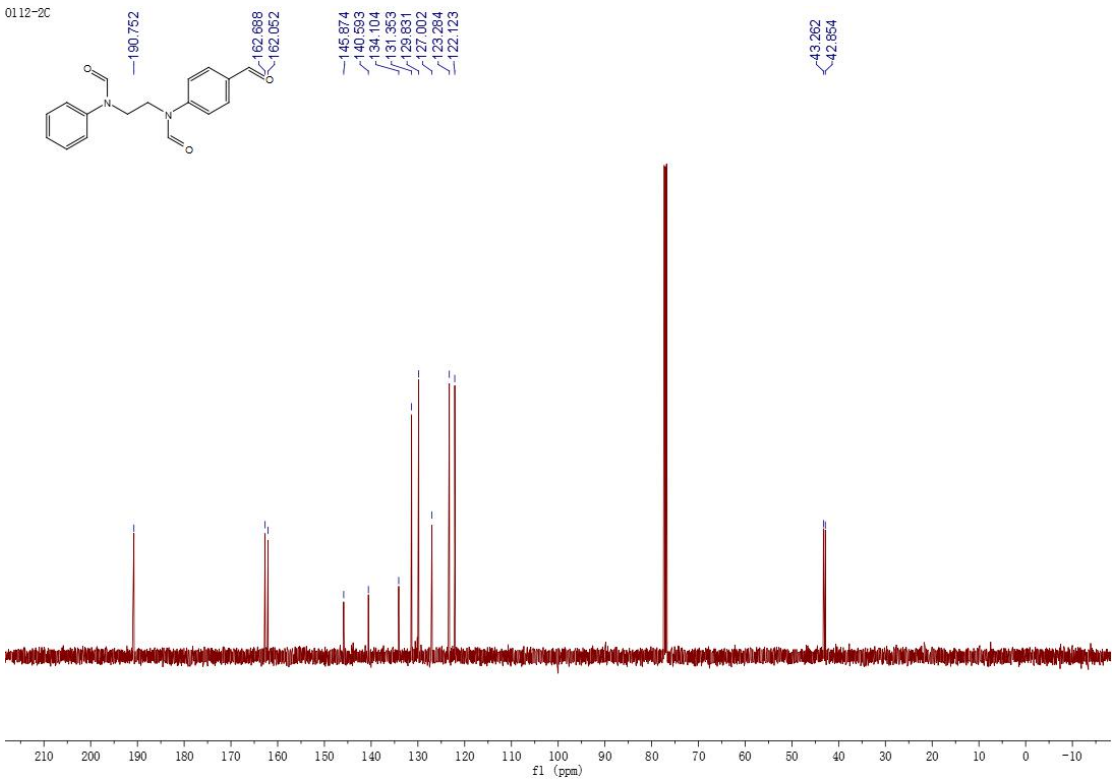
NMR of 45b


0160-H
8.321
8.281
7.391
7.376
7.361
7.300
7.285
7.262
7.246
7.231
7.094
7.078
7.063
7.047
6.858
6.842
6.761
4.040
2.332
0.93
0.96
2.05
2.19
1.02
2.26
1.05
0.96
4.00
3.17
f1 (ppm)

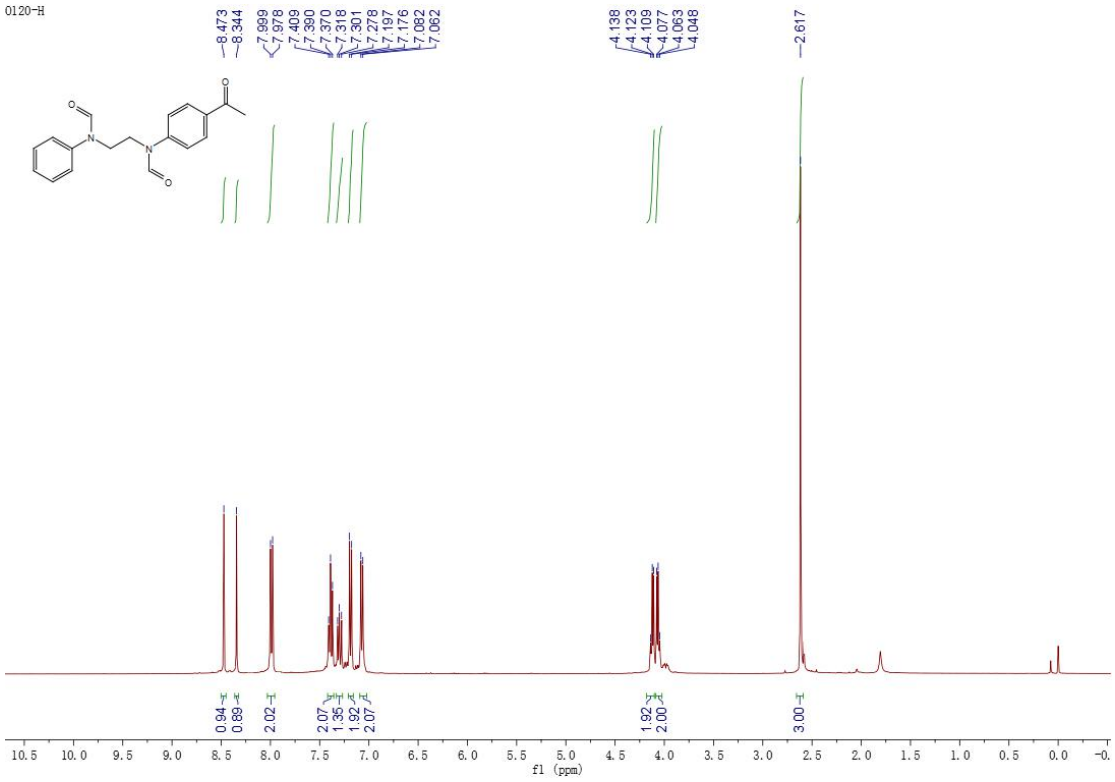

0160-C
162.672
162.616
140.767
140.552
139.721
129.654
129.448
127.620
126.796
124.285
123.531
120.583
43.276
21.382
f1 (ppm)

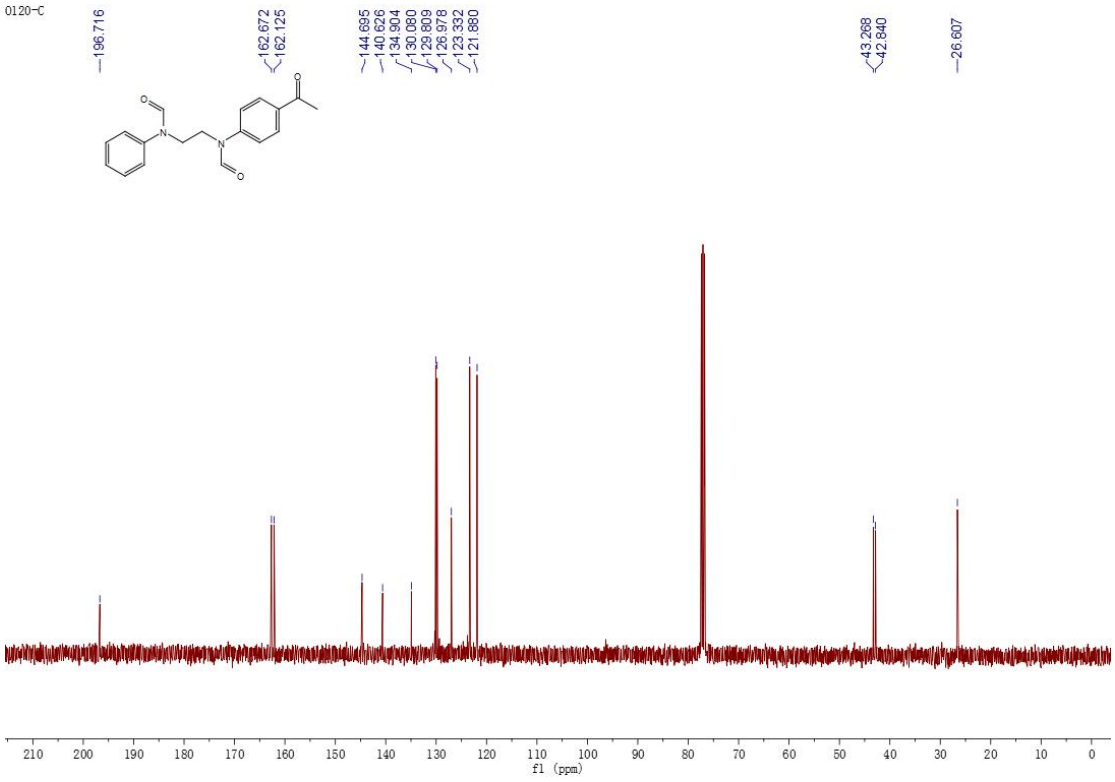
NMR of 46b


0112-2H
10.005
8.514
8.348
7.926
7.909
7.404
7.389
7.374
7.316
7.302
7.278
7.262
7.078
7.062
4.154
4.141
4.129
4.088
4.076
4.063
1.00
1.02
0.97
2.04
2.21
0.98
2.29
2.20
2.05
2.02
f1 (ppm)

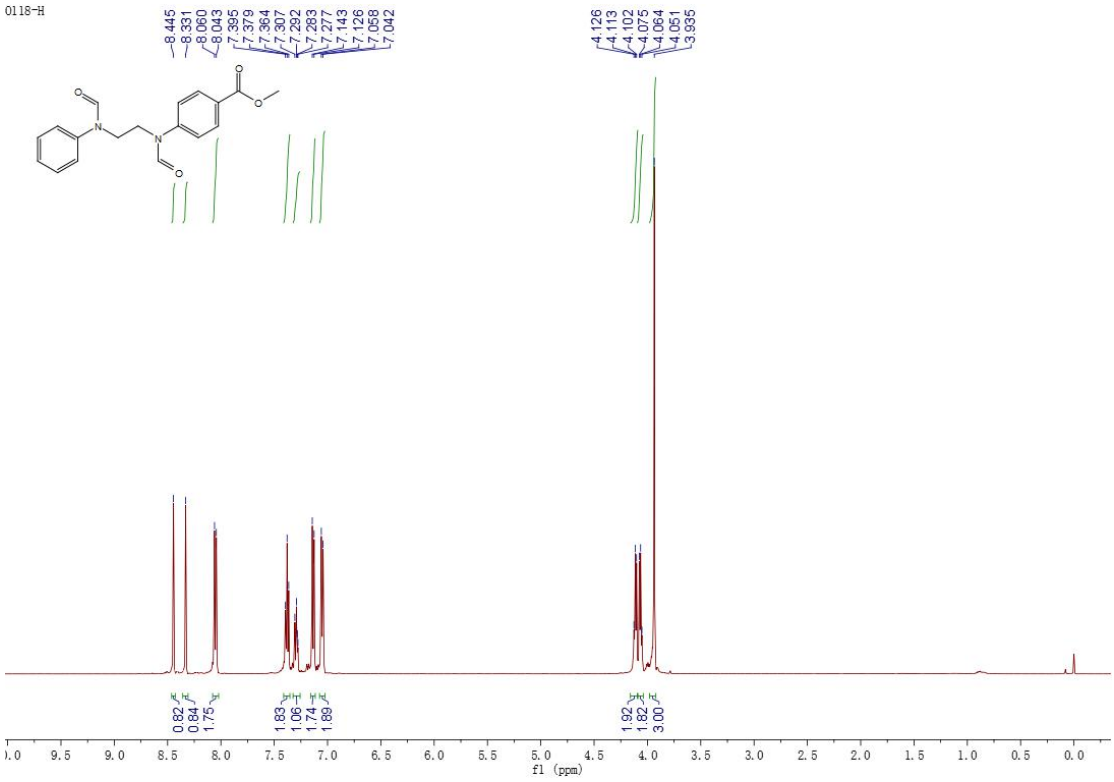

0112-2C
190.752
162.688
162.052
145.874
140.593
134.104
131.353
129.831
127.002
123.284
122.123
43.262
42.854
f1 (ppm)

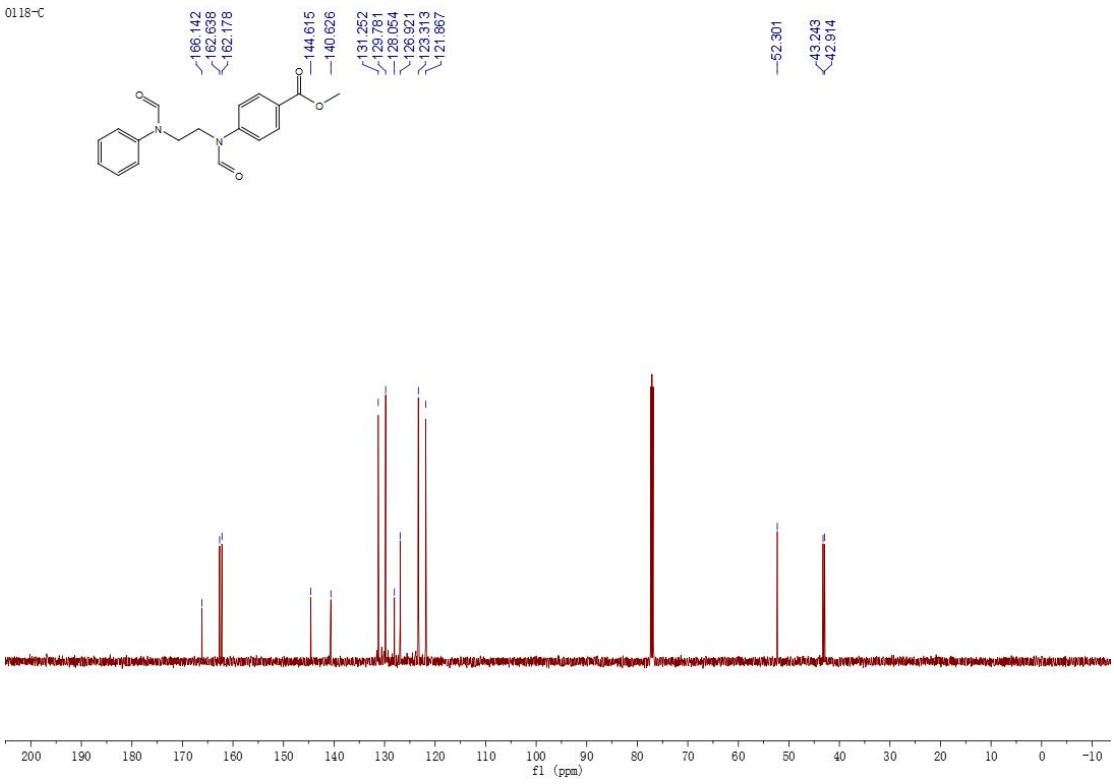
NMR of 47b


0120-H
8.473
8.344
7.999
7.978
7.409
7.390
7.370
7.318
7.301
7.278
7.197
7.176
7.082
7.062
4.138
4.123
4.109
4.077
4.063
4.048
2.617
0.94
0.89
2.02
2.07
1.35
1.92
2.07
1.92
2.00
3.00
f1 (ppm)

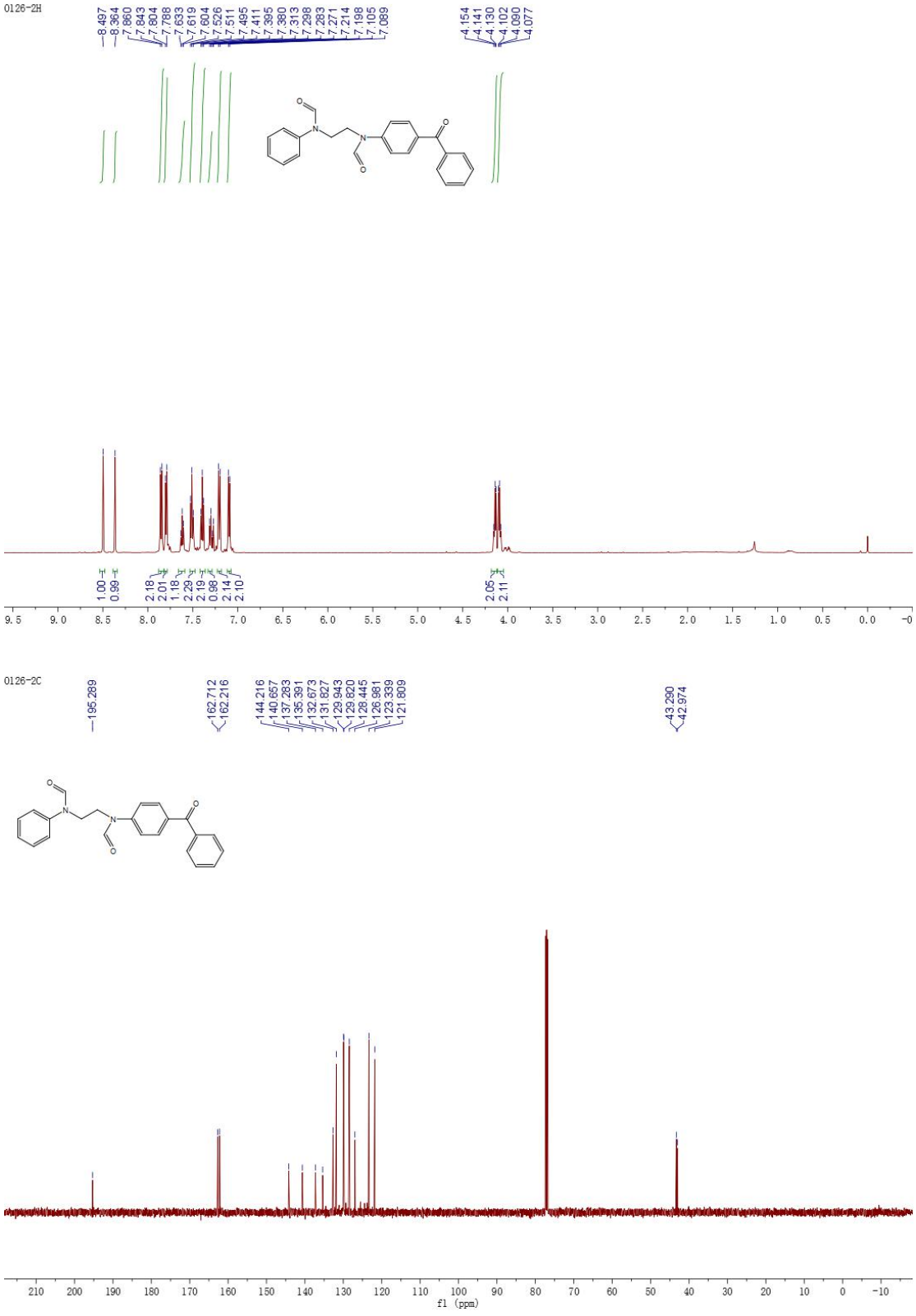

0120-C
196.716
162.672
162.125
144.695
140.626
134.904
130.080
129.809
126.978
123.332
121.880
43.268
42.840
26.607
f1 (ppm)

NMR of 48b

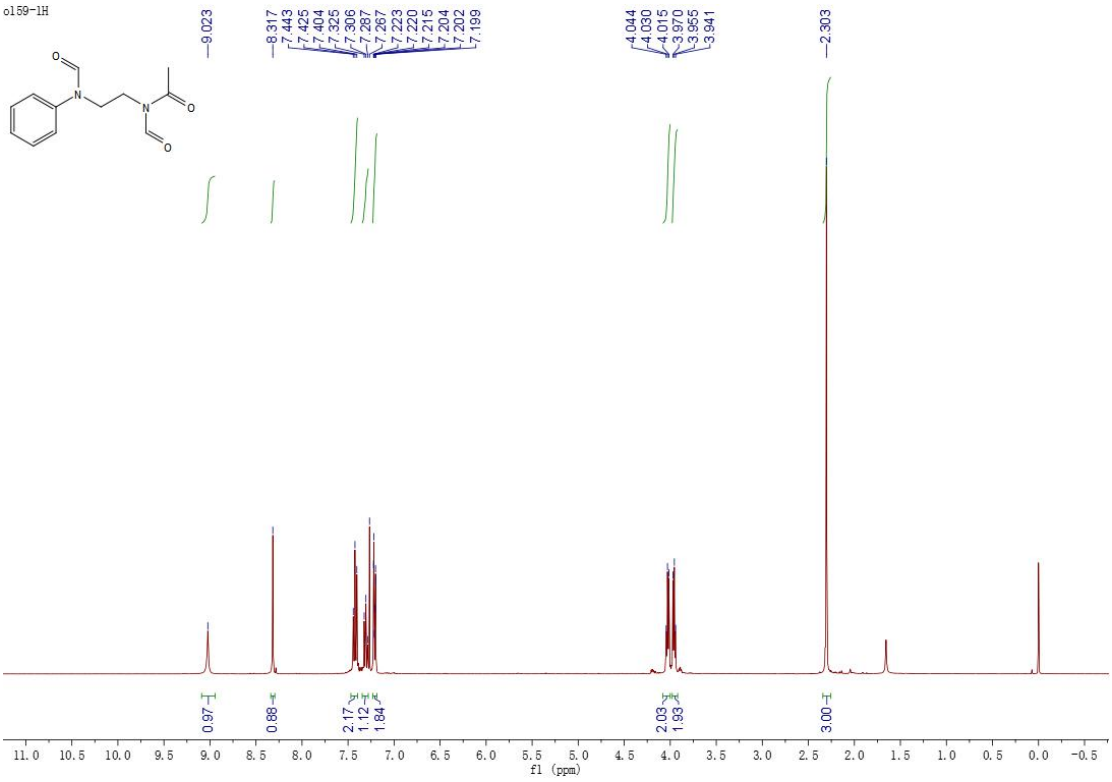

0118-H
8.445
8.331
8.060
8.043
7.395
7.379
7.364
7.307
7.292
7.283
7.277
7.143
7.126
7.058
7.042
4.126
4.113
4.102
4.075
4.064
4.051
3.935
0.82
0.84
1.75
1.83
1.06
1.74
1.89
1.92
1.82
3.00
f1 (ppm)

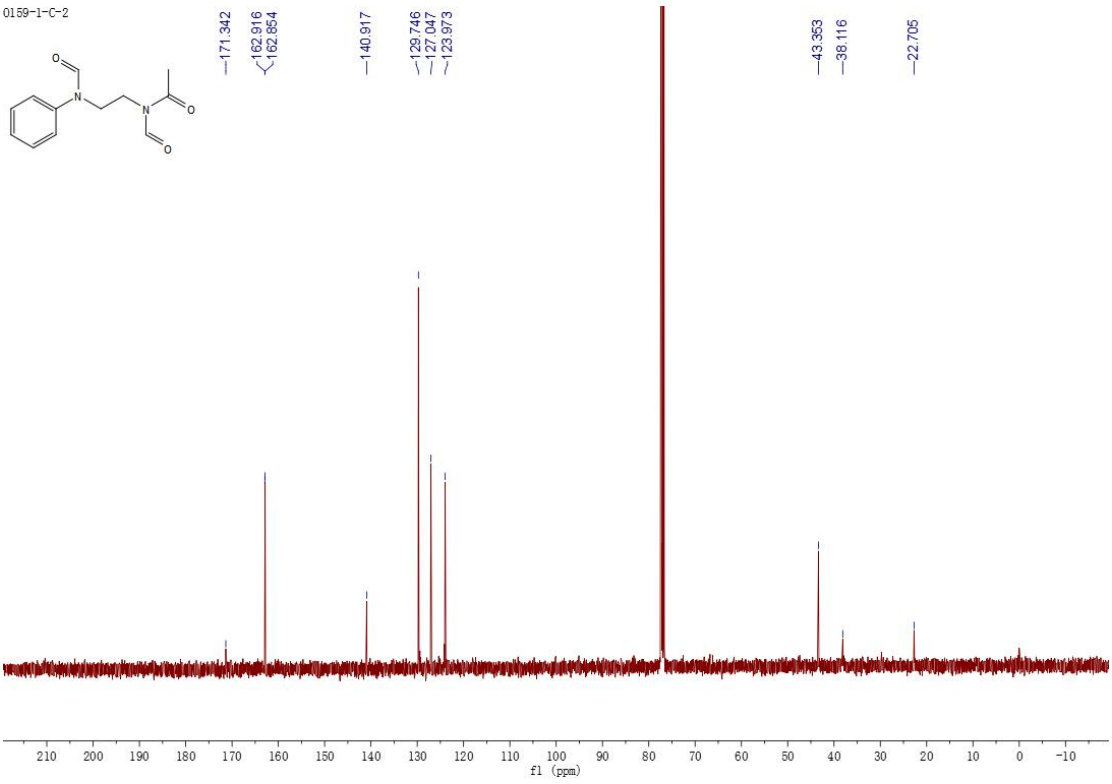

0118-C
166.142
162.638
162.178
144.615
140.626
131.252
129.781
128.054
126.921
123.313
121.867
52.301
43.243
42.914
f1 (ppm)

NMR of 49b

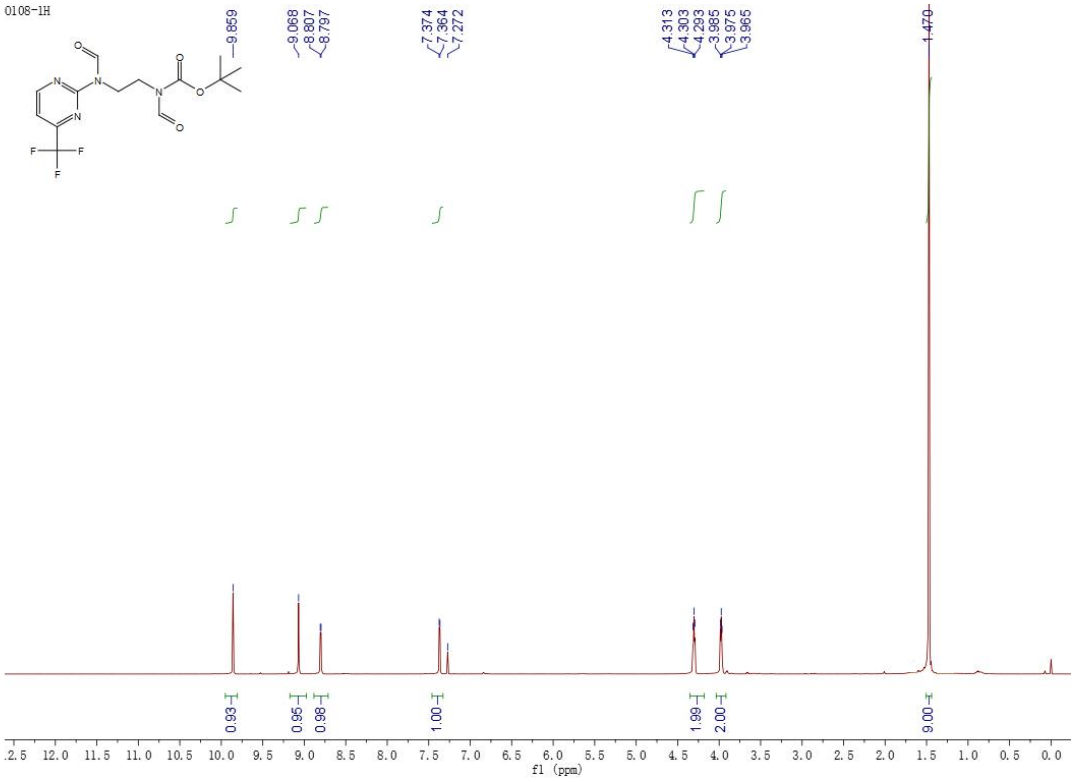

0126-2H
8.497
8.364
7.860
7.843
7.804
7.788
7.633
7.619
7.604
7.526
7.511
7.495
7.411
7.395
7.380
7.313
7.298
7.283
7.271
7.214
7.198
7.105
7.089
4.154
4.141
4.130
4.102
4.090
4.077
1.00
0.99
2.18
2.01
1.18
2.29
2.19
0.98
2.14
2.10
2.05
2.11
0126-2C
195.289
162.712
162.216
144.216
140.657
137.283
136.391
132.673
131.627
129.943
129.820
128.445
126.981
123.339
121.809
43.290
42.974
f1 (ppm)

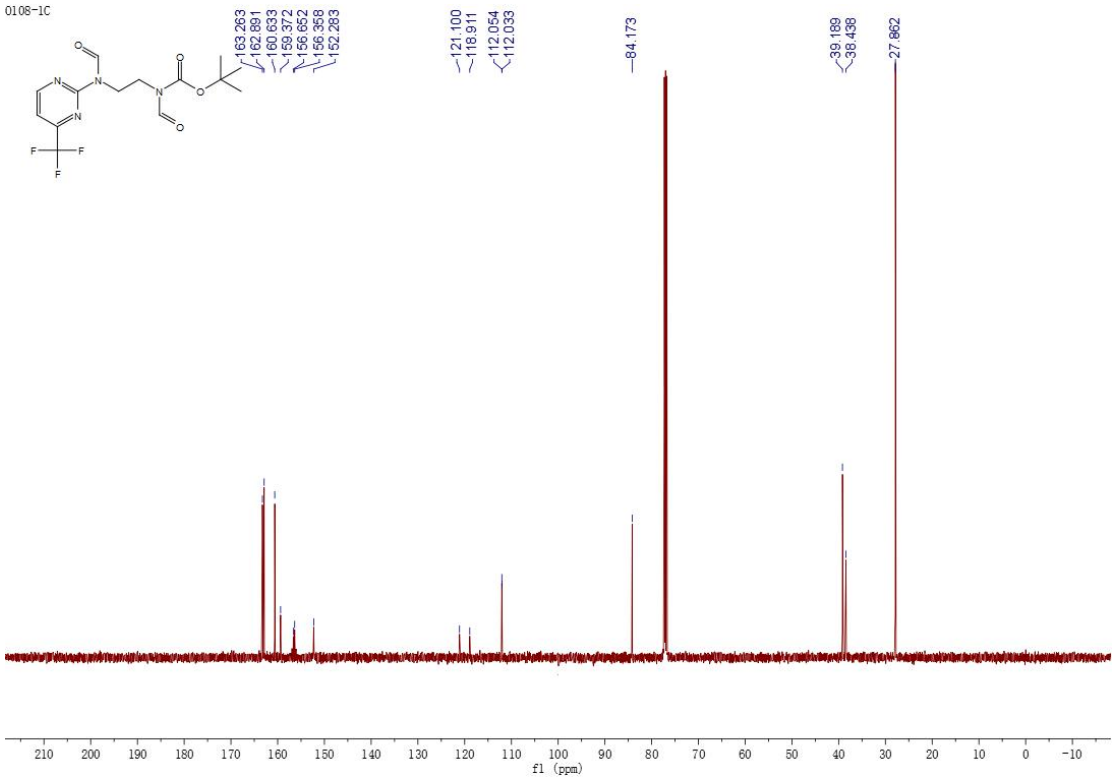
NMR of 50b


o159-1H
9.023
8.317
7.443
7.425
7.404
7.325
7.306
7.287
7.267
7.223
7.220
7.215
7.204
7.202
7.199
4.044
4.030
4.015
3.970
3.955
3.941
2.303
0.97
0.88
2.17
1.12
1.84
2.03
1.93
3.00
f1 (ppm)


0159-1-C-2
171.342
162.916
162.854
140.917
129.746
127.047
123.973
43.353
38.116
22.705
f1 (ppm)

NMR of 51b


0108-1H
9.859
9.068
8.807
8.797
7.374
7.364
7.272
4.313
4.303
4.293
3.985
3.975
3.965
1.470
0.93
0.95
0.98
1.00
1.99
2.00
9.00
f1 (ppm)


0108-1C
163.263
162.891
160.633
159.372
156.652
156.358
152.283
121.100
118.911
112.054
112.033
84.173
39.189
38.438
27.862
f1 (ppm)

11. Molecular Coordinates and Free Energies

1a

ΔG = -366.212666 hartree

C	-1.938574	1.194352	0.013735
C	-0.551358	1.204607	-0.024232
C	0.184263	-0.000001	-0.058967
C	-0.551360	-1.204609	-0.024238
C	-1.938576	-1.194351	0.013729
C	-2.651727	0.000001	0.030112
H	-2.466095	2.139650	0.036118
H	-0.039982	2.154408	-0.027278
H	-0.039986	-2.154411	-0.027292
H	-2.466098	-2.139648	0.036107
H	-3.732381	0.000002	0.061777
N	1.563360	-0.000001	-0.134004
C	2.291883	-1.242993	0.050591
H	3.353450	-1.053317	-0.080209
H	2.141393	-1.678914	1.046042
H	1.996384	-1.987206	-0.690439
C	2.291880	1.242995	0.050579
H	3.353444	1.053327	-0.080255
H	1.996353	1.987209	-0.690437
H	2.141416	1.678909	1.046038

1a (*1a)**

ΔG = -366.098067 hartree

C	2.001833	-1.188403	-0.118547
C	0.581507	-1.258784	-0.154373
C	-0.177586	0.024740	-0.025160
C	0.515275	1.223931	0.113009
C	1.914568	1.262991	0.148436
C	2.651814	0.001310	0.033241
H	2.571336	-2.100825	-0.244895
H	0.097788	-2.122170	-0.585843
H	-0.038122	2.141890	0.253069
H	2.441508	2.189181	0.316243
H	3.734388	0.021461	0.056584
N	-1.542672	-0.038384	-0.105168
C	-2.333392	1.171139	-0.252177
H	-3.327250	0.899538	-0.600220
H	-2.435837	1.700892	0.700665
H	-1.869405	1.836464	-0.975771
C	-2.299444	-1.204582	0.331555
H	-3.116879	-1.395052	-0.362989
H	-1.659265	-2.075674	0.400378
H	-2.727009	-1.021075	1.323049

1a (*1*)

ΔG = -366.023978 hartree

C	1.932788	1.210193	-0.075122
C	0.559648	1.224375	-0.069554
C	-0.168085	-0.000044	0.000008
C	0.559701	-1.224429	0.069582
C	1.932842	-1.210183	0.075115
C	2.631919	0.000018	-0.000020
H	2.474186	2.142321	-0.144529
H	0.039273	2.164109	-0.151618
H	0.039382	-2.164187	0.151697
H	2.474281	-2.142288	0.144521
H	3.712388	0.000040	-0.000041
N	-1.520648	-0.000030	0.000002
C	-2.306972	1.225504	0.139569
H	-3.253597	0.967910	0.604968
H	-1.792449	1.950506	0.758373
H	-2.505290	1.650390	-0.846288
C	-2.307118	-1.225450	-0.139577
H	-3.253113	-0.967931	-0.606326
H	-1.792088	-1.951104	-0.757169
H	-2.506770	-1.649464	0.846390

1a (*1_TS_2*)

ΔG = -516.531092 hartree

C	0.585033	0.409500	-0.078743
C	0.346737	-0.974448	-0.099872
C	1.415253	-1.858053	-0.046234
C	2.722867	-1.394332	0.049555
C	2.957199	-0.023910	0.090387
C	1.903461	0.875284	0.029375
C	-1.725944	0.918313	-0.557401
N	-0.481645	1.320970	-0.166551
C	-0.277667	2.711190	0.242875
H	-0.659915	-1.367778	-0.136752
H	1.217588	-2.921342	-0.061688
H	3.547688	-2.091257	0.101530
H	3.967971	0.353032	0.165821
H	2.113119	1.933203	0.045070
H	-1.756542	0.105012	-1.290200
H	-2.337760	0.214046	0.303096
H	0.342382	3.239174	-0.482315
H	0.202953	2.754149	1.218500
O	-2.909617	-1.752294	-0.199867
O	-2.987849	-0.796296	0.697307
H	-2.405704	1.738569	-0.755252
H	-1.242165	3.203863	0.298867

1a (*2*)

ΔG = -365.574002 hartree

C	-1.948194	1.160741	0.088895
C	-0.563103	1.222449	0.099880
C	0.208250	0.046395	0.007526
C	-0.472591	-1.182803	-0.084210
C	-1.859268	-1.224826	-0.091675
C	-2.613704	-0.058110	-0.009099

H	-2.513198	2.080620	0.167724
H	-0.081122	2.181120	0.210319
H	0.076537	-2.107903	-0.163833
H	-2.352825	-2.184975	-0.168244
H	-3.694012	-0.097692	-0.016517
N	1.600494	0.095503	0.004872
C	2.357646	-1.143978	0.147861
H	2.306241	-1.750358	-0.759360
H	3.397313	-0.897200	0.338099
H	1.981555	-1.732969	0.983456
C	2.305455	1.264856	-0.148604
H	1.810417	2.134493	-0.541402
H	3.378686	1.197990	-0.147784

1a (*3*)

ΔG = -516.621361 hartree

C	-0.578395	0.285729	0.108130
C	-0.749914	-1.109083	0.172330
C	-2.014043	-1.672820	0.081336
C	-3.144253	-0.879573	-0.093097
C	-2.981818	0.497485	-0.179310
C	-1.723084	1.078302	-0.082224
C	1.811344	0.118459	0.612417
N	0.680673	0.874801	0.232176
C	0.863740	2.282523	-0.095302
O	2.371655	-0.486713	-0.586695
O	3.480132	-1.322946	-0.163437
H	4.237767	-0.750335	-0.352438
H	0.106416	-1.759506	0.263991
H	-2.110800	-2.749576	0.133342
H	-4.125748	-1.326282	-0.169932
H	-3.843005	1.137557	-0.321252
H	-1.638488	2.152119	-0.145339
H	1.555240	-0.678515	1.309168
H	2.568096	0.762266	1.060451
H	0.357727	2.935968	0.620036
H	1.924892	2.512240	-0.073799
H	0.487433	2.511604	-1.094082

1a (*3_TS_c*)

ΔG = -516.553949 hartree

C	0.467472	0.301233	-0.118325
C	0.737455	-1.061938	-0.389390
C	2.025408	-1.556427	-0.267648
C	3.074048	-0.742967	0.148140
C	2.815463	0.594252	0.443336
C	1.541163	1.114173	0.317440
N	-0.780804	0.858366	-0.300237
C	-0.987634	2.284696	-0.068813
O	-2.071812	-1.149313	-0.670199
O	-2.960046	-1.065264	1.231308
H	-3.204257	-1.708539	1.919044
H	-0.066194	-1.715232	-0.673406
H	2.205979	-2.599992	-0.487893
H	4.072537	-1.143643	0.252911
H	3.616442	1.240636	0.775600
H	1.379841	2.153822	0.550475
H	-2.724222	0.440009	0.208433
H	-0.310477	2.877592	-0.681599
H	-2.007915	2.538266	-0.342377
H	-0.838688	2.544039	0.980679
C	-1.999632	0.142222	-0.626673
H	-2.445009	0.629621	-1.517488

1a (*1c*)

ΔG = -440.295838 hartree

C	0.027331	0.157541	0.053875
C	0.584116	-1.075995	0.407579
C	1.959847	-1.256970	0.359767
C	2.802091	-0.221598	-0.032371
C	2.251092	1.006944	-0.373852
C	0.875156	1.199163	-0.332017
C	-2.299202	-0.586448	-0.172635
N	-1.378533	0.377803	0.116638
C	-1.864653	1.727270	0.411716
O	-2.074547	-1.732617	-0.522727
H	-3.325213	-0.208538	-0.058309
H	-0.055633	-1.884770	0.717695
H	2.374640	-2.216099	0.639966
H	3.872712	-0.369787	-0.065618
H	2.889956	1.825286	-0.677543
H	0.469480	2.161309	-0.605665
H	-1.728882	2.402088	-0.433412
H	-1.339926	2.130328	1.275695
H	-2.925700	1.677062	0.640171

1a (*1_TS_5*)

ΔG = -516.357301 hartree

C	-0.736405	0.278393	0.174971
C	-0.864952	-1.101503	0.420326
C	-2.081264	-1.722820	0.224357
C	-3.186459	-0.993165	-0.213930
C	-3.061866	0.369476	-0.465232
C	-1.848676	1.007560	-0.281203
C	1.551083	0.349991	0.969691
N	0.485745	0.933864	0.380519
C	0.659394	2.309241	-0.118797
H	-0.021914	-1.695853	0.733560
H	-2.168749	-2.784093	0.406235
H	-4.135794	-1.487431	-0.363157
H	-3.913442	0.940647	-0.805069
H	-1.779382	2.065387	-0.472667
H	1.357045	-0.501410	1.607774
H	2.300262	-0.265362	0.028990
H	0.035981	2.984537	0.464483
H	0.378536	2.359280	-1.166713
O	4.200254	-0.978653	-0.318348
O	3.042347	-0.866795	-0.763740

H	2.323253	1.035818	1.299435
H	1.698054	2.591975	-0.000894

1a (*5*)

ΔG = -365.436792 hartree

C	-0.175983	-0.035826	-0.033251
C	0.533176	-1.184758	0.299156
C	1.920358	-1.134586	0.323802
C	2.582354	0.050134	0.022662
C	1.857507	1.192782	-0.300126
C	0.470135	1.160315	-0.324292
C	-2.232270	-1.033317	-0.685564
N	-1.623862	-0.094450	-0.070839
C	-2.367998	0.949360	0.664364
H	0.012138	-2.094064	0.562848
H	2.479377	-2.020467	0.588967
H	3.662412	0.085274	0.044843
H	2.370122	2.113678	-0.538365
H	-0.087532	2.045126	-0.591224
H	-1.664864	-1.766927	-1.238305
H	-2.161092	1.915186	0.213450
H	-2.028305	0.947877	1.696082
H	-3.310091	-1.083728	-0.648852
H	-3.428809	0.734581	0.605929

1a (*5_TS_6*)

ΔG = -441.852923 hartree

C	-0.201221	-0.008066	0.132481
C	-0.891329	1.174987	0.364476
C	-2.268774	1.211470	0.180786
C	-2.948319	0.071871	-0.234767
C	-2.250035	-1.109107	-0.462323
C	-0.873767	-1.155924	-0.273169
C	2.071529	-0.503624	-0.749398
O	2.741365	0.815598	-0.986602
N	1.239783	-0.022595	0.355476
C	1.631353	-0.513703	1.702848
H	1.517546	-0.804576	-1.628256
H	2.556684	1.193932	-1.863467
H	1.979466	1.100953	-0.145886
H	-0.354329	2.057928	0.683257
H	-2.806674	2.132541	0.356706
H	-4.018976	0.103460	-0.381638
H	-2.774216	-1.998267	-0.783737
H	-0.336950	-2.079862	-0.440727
H	1.358627	-1.561113	1.826479
H	1.113577	0.086178	2.444670
H	2.834851	-1.212461	-0.457637
H	2.704371	-0.392746	1.829111

1a (*6*)

ΔG = -441.886525 hartree

C	0.293835	-0.102231	0.172062
C	1.077379	-1.236210	0.320984
C	2.446935	-1.140683	0.104612
C	3.011782	0.075784	-0.259580
C	2.209023	1.201594	-0.408183
C	0.838746	1.120402	-0.192516
C	-1.943513	-0.086798	-0.939733
O	-3.259325	-0.444942	-0.757556
N	-1.164047	-0.223588	0.389794
C	-1.694185	0.680591	1.466591
H	-1.463893	-0.786384	-1.617824
H	-3.810395	0.332059	-0.609978
H	-1.341683	-1.179922	0.699331
H	0.633639	-2.181926	0.603172
H	3.066621	-2.018029	0.222045
H	4.077197	0.147463	-0.427000
H	2.645612	2.148565	-0.691414
H	0.223563	2.001071	-0.305799
H	-1.571489	1.712519	1.156568
H	-1.132982	0.488263	2.374697
H	-1.800105	0.936858	-1.274899
H	-2.743175	0.449411	1.617565

1a (*1d*)

ΔG = -326.923055 hartree

C	1.405893	0.342404	0.533731
N	2.126053	0.965658	1.533597
C	3.244404	0.325330	2.197377
C	1.486793	-1.040753	0.303293
C	0.708903	-1.637220	-0.683943
C	-0.157460	-0.886252	-1.468891
C	-0.235996	0.489280	-1.250185
C	0.528907	1.096772	-0.269047
H	2.203884	1.964169	1.437295
H	4.013358	-0.026120	1.499202
H	2.911723	-0.529154	2.789247
H	3.699449	1.041534	2.877499
H	2.153643	-1.651466	0.894093
H	0.789510	-2.705661	-0.839277
H	-0.756831	-1.357168	-2.235600
H	-0.900239	1.095964	-1.852445
H	0.455007	2.165681	-0.108946

2a

ΔG = -444.817128 hartree

C	0.341681	-0.000014	-0.000051
N	-1.037300	0.000002	-0.000088
C	-1.807135	-1.143412	0.477150
C	-2.097077	-2.195815	-0.595549
C	-1.807083	1.143525	-0.477151
C	-2.096825	2.195880	0.595651
C	1.083883	1.149463	-0.354751
C	2.471224	1.138946	-0.354765
C	3.186924	-0.000062	0.000027
C	2.471169	-1.139045	0.354779

C	1.083827	-1.149514	0.354690
H	-1.294500	-1.600319	1.324010
H	-1.176425	-2.621303	-0.994688
H	-2.655695	-1.760914	-1.425434
H	-2.693533	-3.008087	-0.176366
H	-2.749733	-0.761074	0.871164
H	-1.294499	1.600441	-1.324036
H	-1.176105	2.621308	0.994696
H	-2.655356	1.760954	1.425580
H	-2.693304	3.008201	0.176593
H	-2.749757	0.761300	-0.871090
H	0.577088	2.064114	-0.619555
H	2.997269	2.044230	-0.631093
H	4.267969	-0.000075	0.000063
H	2.997167	-2.044349	0.631132
H	0.576985	-2.064151	0.619457

2a (*2a)**

ΔG = -444.703440 hartree

C	0.365795	0.044867	0.008053
N	-1.000739	-0.005343	-0.015053
C	-1.781904	-1.136393	0.501756
C	-2.211812	-2.119372	-0.586951
C	-1.799654	1.121472	-0.500744
C	-2.139481	2.139085	0.590166
C	1.087367	1.194308	-0.306100
C	2.494290	1.204123	-0.313992
C	3.198610	-0.042589	-0.017950
C	2.520128	-1.185384	0.297913
C	1.100878	-1.206238	0.361421
H	-1.213355	-1.640762	1.275392
H	-1.345085	-2.588100	-1.051928
H	-2.793166	-1.624917	-1.365317
H	-2.833428	-2.900285	-0.147510
H	-2.663383	-0.716703	0.987462
H	-1.267133	1.598286	-1.320629
H	-1.239418	2.583925	1.011383
H	-2.704803	1.676322	1.399220
H	-2.750807	2.935433	0.165075
H	-2.718842	0.708517	-0.914639
H	0.562450	2.112299	-0.523186
H	3.043644	2.105182	-0.536328
H	4.281038	-0.057772	-0.057275
H	3.064781	-2.099493	0.497493
H	0.577376	-2.137805	0.484731

2a (*1*)

ΔG = -444.629509 hartree

C	-0.350465	-0.000011	-0.000014
N	1.002479	-0.000003	-0.000004
C	1.796147	1.146262	0.477460
C	2.099511	2.146111	-0.639165
C	1.796196	-1.146245	-0.477452
C	2.099531	-2.146105	0.639169
C	-1.082859	-1.163571	-0.383730
C	-2.455743	-1.152130	-0.375377
C	-3.155970	0.000001	0.000008
C	-2.455727	1.152127	0.375380
C	-1.082843	1.163553	0.383714
H	1.277156	1.619828	1.304379
H	1.187610	2.591533	-1.032976
H	2.637770	1.673310	-1.459145
H	2.725237	2.939475	-0.232987
H	2.721291	0.732700	0.872411
H	1.277261	-1.619806	-1.304408
H	1.187624	-2.591567	1.032919
H	2.637726	-1.673300	1.459189
H	2.725308	-2.939439	0.233012
H	2.721349	-0.732652	-0.872351
H	-0.566790	-2.065104	-0.666781
H	-2.996218	-2.043243	-0.659368
H	-4.236403	0.000006	0.000022
H	-2.996187	2.043246	0.659379
H	-0.566756	2.065078	0.666765

2a (*1_TS_2*)

ΔG = -595.135057 hartree

C	-0.827968	-0.299052	-0.234283
C	-1.004836	1.070134	0.021634
C	-2.284495	1.600605	0.131088
C	-3.406174	0.790615	0.010348
C	-3.235107	-0.569251	-0.230904
C	-1.965749	-1.112129	-0.352898
C	1.512247	-0.009720	-0.770287
N	0.464645	-0.845576	-0.398549
C	0.747349	-2.189537	0.126676
H	-0.157297	1.725346	0.160457
H	-2.397561	2.657451	0.332434
H	-4.398326	1.208952	0.107617
H	-4.096179	-1.215104	-0.336988
H	-1.868776	-2.163629	-0.573862
H	1.156454	0.792297	-1.422841
H	1.848252	0.720967	0.152069
H	1.593454	-2.595726	-0.417995
H	-0.097809	-2.833196	-0.094481
O	1.786322	2.897692	0.259135
O	2.247254	1.819750	0.811709
C	2.805584	-0.629055	-1.254960
H	3.479444	0.172413	-1.550332
H	3.305348	-1.219738	-0.489600
H	2.630239	-1.265197	-2.124937
C	1.025166	-2.188640	1.630178
H	1.217701	-3.207727	1.965942
H	1.896630	-1.579839	1.870534
H	0.171208	-1.801591	2.185527

2a (*2*)

ΔG = -444.177120 hartree

C	-0.243957	-0.037635	-0.136507
N	1.155774	-0.000701	-0.296241
C	1.885805	-1.275526	-0.359507
C	2.126436	-1.910319	1.009653
C	1.899288	1.141097	-0.034755
C	1.459293	2.494744	-0.489211
C	-0.884899	0.764968	0.820074
C	-2.266324	0.735771	0.960074
C	-3.044254	-0.098975	0.164545
C	-2.415179	-0.908361	-0.778995
C	-1.037294	-0.878780	-0.933751
H	1.333424	-1.965724	-0.992819
H	1.183375	-2.130112	1.511273
H	2.710047	-1.249262	1.650707
H	2.674908	-2.846574	0.896012
H	2.834409	-1.082930	-0.859185
H	0.531872	2.840620	-0.029504
H	1.296464	2.527125	-1.576744
H	2.233912	3.223628	-0.252870
H	2.960550	0.955363	0.043641
H	-0.288084	1.388914	1.469091
H	-2.734673	1.360765	1.709530
H	-4.119435	-0.120766	0.277206
H	-3.003274	-1.561375	-1.410625
H	-0.577387	-1.496665	-1.691745

2a (*3*)

ΔG = -595.224601 hartree

C	-0.813964	0.132772	0.200062
N	0.475402	0.614229	0.538274
C	0.733587	2.054422	0.400383
C	0.863805	2.549918	-1.040242
C	1.602387	-0.245753	0.656620
C	1.361869	-1.527399	1.437892
O	2.093945	-0.537066	-0.704428
O	3.447664	-1.058022	-0.601126
C	-1.009214	-0.907235	-0.717060
C	-2.288660	-1.369854	-1.005303
C	-3.403191	-0.788460	-0.412765
C	-3.220632	0.259301	0.485038
C	-1.944476	0.708642	0.795511
H	-0.064823	2.601860	0.900286
H	-0.047780	2.351938	-1.605820
H	1.694468	2.061954	-1.548213
H	1.036038	3.627854	-1.049034
H	1.647798	2.272977	0.952225
H	0.586230	-2.143922	0.990710
H	1.068860	-1.280157	2.458094
H	2.283881	-2.104027	1.483032
H	2.401782	0.320144	1.135976
H	3.304983	-2.003579	-0.748123
H	-0.154833	-1.344915	-1.211456
H	-2.410985	-2.179162	-1.713371
H	-4.397643	-1.142664	-0.647468
H	-4.075734	0.721139	0.961089
H	-1.822007	1.503552	1.517772

2a (*3_TS_4*)

ΔG = -595.178173 hartree

C	-1.120340	-0.221665	-0.227333
C	-1.011298	1.150318	-0.022483
C	-2.164892	1.909089	0.138632
C	-3.414004	1.300368	0.101467
C	-3.511051	-0.073822	-0.098358
C	-2.365830	-0.841753	-0.262473
C	2.347126	-1.047188	-1.383456
C	0.988735	-0.589084	-1.254551
N	0.083139	-0.997426	-0.401377
C	0.318701	-2.116078	0.539710
O	2.757639	1.158168	-0.049238
O	3.616821	2.212185	0.512616
H	-0.029162	1.602538	0.024926
H	-2.083275	2.974735	0.302404
H	-4.309681	1.892412	0.229111
H	-4.480836	-0.550337	-0.134983
H	-2.444929	-1.905764	-0.434245
H	2.917009	-0.201085	-0.811707
H	0.676761	0.232367	-1.884873
H	3.629153	1.973128	1.445919
H	0.978151	-2.828148	0.053022
H	-0.636478	-2.609361	0.695348
H	2.578498	-2.006530	-0.933082
C	0.900810	-1.635686	1.864248
H	1.839104	-1.105996	1.708490
H	0.209281	-0.967942	2.377248
H	1.083441	-2.495815	2.507720
H	2.687565	-0.992035	-2.415109

2a (*4*)

ΔG = -443.614008 hartree

C	-0.437268	-0.099423	0.066375
N	0.965117	-0.174110	0.140168
C	1.736112	0.949115	0.678003
C	2.407454	1.817163	-0.385183
C	1.634658	-1.319279	-0.251749
C	2.938522	-1.599044	-0.114787
C	-1.234429	-1.253626	0.132755
C	-2.617489	-1.167921	0.046626
C	-3.250248	0.063322	-0.085795
C	-2.469920	1.213229	-0.132152
C	-1.085047	1.139098	-0.062743
H	1.069017	1.549101	1.292576
H	1.671377	2.293174	-1.032941
H	3.076774	1.227395	-1.010161
H	2.995286	2.601076	0.094249
H	2.489549	0.541415	1.354067
H	1.003172	-2.038517	-0.753303
H	3.310446	-2.535729	-0.500908
H	3.653095	-0.937221	0.350199

H	-0.778668	-2.220878	0.282670
H	-3.203613	-2.075767	0.105136
H	-4.327943	0.125706	-0.144903
H	-2.938474	2.183111	-0.236413
H	-0.509916	2.050099	-0.129533

2a (*4_TS_pre_b*)

ΔG = -593.917502 hartree

C	-0.861027	-0.046546	0.134342
N	0.534098	0.220238	0.330630
C	0.944065	1.633919	0.505960
C	0.736028	2.466345	-0.753976
C	1.534251	-0.751920	-0.159706
C	1.796032	-0.985606	1.239947
C	-1.335921	-0.507434	-1.092647
C	-2.695185	-0.743490	-1.262148
C	-3.583425	-0.517339	-0.216843
C	-3.106516	-0.054062	1.005669
C	-1.749424	0.176931	1.185274
O	2.675813	-0.279765	-0.767533
O	3.640656	-1.204614	-0.120783
H	0.375498	2.042280	1.338883
H	-0.312760	2.499068	-1.046618
H	1.319406	2.069741	-1.584026
H	1.064478	3.488311	-0.562352
H	1.993982	1.637155	0.782810
H	1.042594	-1.565202	-0.692185
H	2.408339	-0.274426	1.762911
H	1.281754	-1.756358	1.796266
H	-0.653647	-0.668715	-1.915270
H	-3.057997	-1.097616	-2.217291
H	-4.639984	-0.702525	-0.352520
H	-3.789939	0.118261	1.825750
H	-1.375429	0.518601	2.140516

2a (*pre_b*)

ΔG = -594.001198 hartree

C	0.885212	0.006915	-0.202414
N	-0.481968	0.341181	-0.366713
C	-0.894412	1.743435	-0.198322
C	-0.662689	2.290361	1.208616
C	-1.438744	-0.677473	-0.362722
C	-2.777241	-0.558433	-1.089133
C	1.279649	-1.144924	0.490511
C	2.623901	-1.477720	0.606482
C	3.606833	-0.659595	0.062373
C	3.223798	0.499260	-0.604955
C	1.882172	0.829791	-0.741332
O	-2.224014	-0.827100	0.907999
O	-3.472749	-0.965127	0.112931
H	-0.379705	2.362336	-0.933124
H	0.391966	2.253822	1.481128
H	-1.228412	1.716762	1.942204
H	-0.986472	3.330940	1.258471
H	-1.951301	1.807604	-0.439077
H	-0.947240	-1.622542	-0.574649
H	-3.066331	0.444276	-1.400002
H	-2.932074	-1.263905	-1.903393
H	0.538417	-1.774694	0.962263
H	2.900173	-2.374217	1.145676
H	4.652519	-0.915326	0.163126
H	3.973397	1.150292	-1.035207
H	1.612070	1.724500	-1.282506

2a (*2b*)

ΔG = -479.597498 hartree

C	0.294669	0.032614	0.110968
N	-1.110546	0.228969	0.243375
C	-1.968091	-0.868736	0.737291
C	-2.674297	-1.659164	-0.360443
C	-1.735414	1.392636	-0.093756
C	1.190093	1.086068	0.324493
C	2.558006	0.871605	0.219605
C	3.060234	-0.387674	-0.090550
C	2.173549	-1.437844	-0.292392
C	0.802376	-1.232977	-0.196044
O	-1.229759	2.384184	-0.592838
H	-1.346967	-1.518186	1.349017
H	-1.970363	-2.129013	-1.045884
H	-3.330837	-1.012791	-0.943328
H	-3.285225	-2.442912	0.089002
H	-2.709187	-0.427443	1.403392
H	-2.810453	1.349512	0.136006
H	0.816942	2.065543	0.572009
H	3.234951	1.697774	0.391940
H	4.126654	-0.548321	-0.169326
H	2.543948	-2.425466	-0.532189
H	0.135694	-2.064126	-0.366590

2a (*3_TS_c*)

ΔG = -595.159820 hartree

C	-1.159494	-0.281381	0.130610
C	-1.248112	-1.680193	0.333612
C	-2.427588	-2.358836	0.091620
C	-3.559008	-1.688599	-0.368960
C	-3.480268	-0.319608	-0.599812
C	-2.301654	0.375693	-0.386598
N	-0.016602	0.405795	0.492783
O	-0.489593	2.492261	-0.558576
O	1.341865	2.565069	-1.621728
H	-0.403317	-2.235990	0.704731
H	-2.463547	-3.425487	0.267269
H	-4.474084	-2.228719	-0.567282
H	-4.338545	0.214442	-0.984873
H	-2.242545	1.418631	-0.644091
H	1.240359	1.982203	0.056709
H	1.667264	2.864809	-2.488232
C	0.148824	1.848683	0.375344

C	0.036601	2.529429	1.779178
H	-0.996468	2.457719	2.114377
H	0.688374	2.048473	2.503509
H	0.317146	3.573262	1.669988
C	1.181956	-0.306252	0.953783
H	0.897684	-1.064409	1.680733
H	1.791952	0.421624	1.486001
C	2.002154	-0.908421	-0.187492
H	1.444407	-1.677431	-0.720270
H	2.285410	-0.134854	-0.900558
H	2.909087	-1.360613	0.214359

2a (*2c*)

ΔG = -518.906400 hartree

C	-0.530078	-0.000744	0.113408
N	0.900330	0.073547	0.232265
C	1.471126	1.388482	0.568525
C	1.594845	2.323896	-0.630868
C	1.643169	-1.051554	0.005923
C	3.150527	-0.933509	0.109687
O	1.117069	-2.130285	-0.258256
C	-1.320072	0.048508	1.258780
C	-2.706029	0.009399	1.152345
C	-3.307873	-0.085759	-0.097789
C	-2.518010	-0.138753	-1.241972
C	-1.132683	-0.092708	-1.138504
H	0.827511	1.838746	1.323772
H	0.623780	2.500274	-1.093480
H	2.263256	1.911160	-1.387025
H	1.995880	3.286153	-0.309955
H	2.439610	1.240429	1.036898
H	3.579642	-1.874308	-0.220953
H	3.457553	-0.753607	1.140981
H	3.547178	-0.123969	-0.501336
H	-0.848475	0.113457	2.230258
H	-3.313386	0.047679	2.046599
H	-4.385816	-0.118140	-0.180335
H	-2.979860	-0.211870	-2.217424
H	-0.515255	-0.132105	-2.025008

2a (*1_TS_5*)

ΔG = -594.962193 hartree

C	-0.957848	0.024365	0.069425
C	-1.298259	-1.237232	0.594191
C	-2.603880	-1.682321	0.538139
C	-3.600051	-0.892124	-0.033439
C	-3.271119	0.351366	-0.560440
C	-1.965872	0.809031	-0.520064
C	1.335830	-0.140436	0.842251
N	0.364549	0.504712	0.126774
C	0.739455	1.693751	-0.677416
H	-0.554098	-1.890863	1.018460
H	-2.845215	-2.657895	0.934774
H	-4.619755	-1.247674	-0.071962
H	-4.033347	0.973767	-1.006320
H	-1.750138	1.781822	-0.926995
H	0.937785	-0.771994	1.627526
H	1.781219	-1.108000	0.050997
H	0.171911	1.661202	-1.600784
H	1.785102	1.580295	-0.940964
O	3.485654	-1.589372	-1.041665
O	2.375118	-1.993077	-0.656939
C	2.648547	0.518336	1.181663
H	3.233002	-0.180948	1.773783
H	3.237958	0.795666	0.308357
H	2.484343	1.414649	1.781373
C	0.523501	3.010425	0.069741
H	-0.520858	3.162002	0.332772
H	1.115883	3.060315	0.980316
H	0.836351	3.823295	-0.584228

2a (*5*)

ΔG = -444.058283 hartree

C	-0.218453	0.024009	-0.121535
N	1.228881	0.084446	-0.248990
C	1.928500	-1.211018	-0.498275
C	1.869906	-2.140238	0.703074
C	1.890129	1.181774	-0.146844
C	1.334015	2.527211	0.065180
C	-0.801687	0.178405	1.129036
C	-2.184503	0.091958	1.239679
C	-2.962607	-0.146621	0.112643
C	-2.361446	-0.300693	-1.132367
C	-0.980389	-0.220531	-1.256892
H	1.446591	-1.658215	-1.365250
H	0.846170	-2.403096	0.962477
H	2.352617	-1.692276	1.570593
H	2.399950	-3.057706	0.450834
H	2.954027	-0.969864	-0.763858
H	0.251560	2.566224	0.021163
H	1.771134	3.196743	-0.678218
H	1.675771	2.891437	1.038316
H	2.966164	1.089552	-0.235055
H	-0.187617	0.356981	2.000162
H	-2.649051	0.209383	2.208362
H	-4.037730	-0.212638	0.203711
H	-2.965222	-0.480900	-2.010396
H	-0.507326	-0.332284	-2.222111

2a (*5_TS_6*)

ΔG = -520.471714 hartree

C	0.739997	0.066440	0.012510
C	1.497359	0.982347	0.732949
C	2.884742	0.901217	0.702992
C	3.510660	-0.093801	-0.039543
C	2.746548	-1.007394	-0.757302
C	1.358734	-0.927876	-0.738640
C	-1.438058	-1.033148	0.449274

O	-2.021983	-0.376182	1.694387
N	-0.712296	0.195029	0.041572
C	-1.261638	0.998909	-1.104606
H	-0.730753	-1.782366	0.783224
H	-1.765844	-0.814906	2.523419
H	-1.305032	0.458843	1.311642
H	1.004155	1.751568	1.311150
H	3.473130	1.612521	1.265731
H	4.589745	-0.158021	-0.058194
H	3.227761	-1.782271	-1.337652
H	0.771950	-1.635665	-1.308200
H	-1.512568	0.325291	-1.923763
H	-0.438695	1.621712	-1.442849
C	-2.440058	1.879130	-0.716952
H	-3.298090	1.310754	-0.361837
H	-2.153337	2.589049	0.058959
C	-2.526248	-1.600639	-0.409099
H	-2.996684	-2.425320	0.123087
H	-3.285311	-0.866737	-0.661528
H	-2.091966	-1.996434	-1.326862
H	-2.758753	2.445119	-1.591928

2a (*6*)

ΔG = -520.491375 hartree

C	-0.751746	0.103872	-0.216588
C	0.715049	0.123479	-0.412532
C	1.347107	1.475602	-0.111318
C	2.733501	1.642780	-0.704787
C	1.409957	-1.141804	0.256383
C	1.702244	-0.921310	1.717881
C	2.578338	-1.406695	-0.434592
O	-1.329128	0.659003	0.916215
N	-2.709753	0.593442	1.066651
C	-3.496324	-0.017034	0.097133
H	-2.902997	-0.565387	-1.033933
H	-1.524495	-0.507369	-1.194703
H	0.867803	-0.034776	-1.408881
H	0.659998	2.205182	-0.531614
H	2.727535	1.484180	-1.783303
H	3.464918	0.975076	-0.259930
H	3.047719	2.669763	-0.521708
H	1.352738	1.599227	0.966144
H	0.661351	-1.917588	0.111041
H	0.813988	-0.622062	2.268599
C	2.492090	-0.187407	1.862790
H	2.044877	-1.870890	2.124496
H	2.405472	-1.985723	-1.186457
C	-0.733581	1.145934	1.672829
H	-3.166233	1.025727	1.945594
H	-4.569224	-0.061111	0.220515
H	-3.507988	-1.035660	-1.795877
H	-1.063711	-0.931437	-2.077389

2a (*2d*)

ΔG = -366.227438 hartree

C	2.417854	-0.379844	0.068307
N	3.732577	-0.021846	0.301762
C	4.637560	0.374277	-0.766832
C	5.982333	0.799554	-0.196792
C	1.945146	-0.712199	-1.211950
C	0.625777	-1.114695	-1.393659
C	-0.257293	-1.190360	-0.323599
C	0.203613	-0.852968	0.948924
C	1.514824	-0.454317	1.145933
H	3.883596	0.461351	1.173462
H	4.781012	-0.471162	-1.443518
H	6.438825	-0.011496	0.371770
H	5.874122	1.661864	0.464036
H	6.662146	1.078966	-1.000968
H	4.212140	1.189639	-1.366710
H	2.604649	-0.658625	-2.065577
H	0.288474	-1.366849	-2.391060
H	-1.281667	-1.501769	-0.473831
H	-0.467036	-0.899564	1.797480
H	1.859348	-0.198959	2.140822

5a

ΔG = -595.295845 hartree

C	0.938511	-0.209848	-0.166981
N	-0.442102	-0.121573	-0.344888
C	-1.281680	-1.193928	0.181621
C	-2.692252	-1.229663	-0.393379
O	-3.250813	-2.474413	0.026704
C	-1.058070	1.182887	-0.559128
C	-1.161551	2.036567	0.703019
O	-1.784138	3.263666	0.324255
C	1.807106	0.805374	-0.622067
C	3.182756	0.687526	-0.494452
C	3.760474	-0.431848	0.096757
C	2.918842	-1.430862	0.568286
C	1.538075	-1.326748	0.450747
H	-3.302354	-0.402131	-0.024164
H	-2.652197	-1.167666	-1.485959
H	-4.184291	-2.479499	-0.205387
H	-1.347644	-1.169760	1.277523
H	-0.827724	-2.146586	-0.086679
H	-0.508495	1.734822	-1.318758
H	-0.166170	2.215000	1.119729
H	-1.756112	1.515314	1.460220
H	-1.863069	3.820234	1.104928
H	-2.055674	1.042327	-0.967358
H	1.414604	1.695592	-1.087202
H	3.809421	1.489022	-0.864504
H	4.833791	-0.516710	0.194184
H	3.333955	-2.308256	1.047829
H	0.933007	-2.121460	0.855617

5a (*5a)**

ΔG = -595.181858 hartree

C	-0.942055	-0.229399	0.111489
N	0.420237	-0.109727	0.273002
C	1.298105	-1.167658	-0.221701
C	2.626503	-1.272053	0.520873
O	3.211451	-2.494757	0.080207
C	1.016374	1.202614	0.516405
C	1.286640	1.981313	-0.772626
O	1.854859	3.225350	-0.376256
C	-1.810679	0.701881	0.907974
C	-3.219044	0.590294	0.746375
C	-3.768930	-0.342238	-0.081449
C	-2.925322	-1.281229	-0.832885
C	-1.537447	-1.183055	-0.708474
H	3.285423	-0.432447	0.289805
H	2.449727	-1.285651	1.601179
H	4.105388	-2.546425	0.432013
H	1.493503	-1.048462	-1.292940
H	0.779597	-2.114017	-0.089474
H	0.339069	1.793518	1.125373
H	0.345407	2.127257	-1.311429
H	1.971742	1.429497	-1.422740
H	2.074981	3.726855	-1.167392
H	1.945939	1.083383	1.067831
H	-1.413975	1.155742	1.804717
H	-3.861370	1.239972	1.328047
H	-4.845127	-0.406595	-0.181373
H	-3.371902	-1.980191	-1.522645
H	-0.915423	-1.821919	-1.319476

5a (*1*)

ΔG = -595.106453 hartree

C	0.819454	-0.000378	-0.000085
N	-0.534367	0.000046	-0.000029
C	-1.320700	1.134241	-0.497940
C	-1.582025	2.174290	0.596987
O	-2.404960	3.158567	-0.003784
C	-1.321933	-1.133229	0.497843
C	-1.583800	-2.173505	-0.596943
O	-2.407652	-3.157032	0.003880
C	1.551370	-1.146271	0.436686
C	2.923412	-1.135115	0.428482
C	3.623887	-0.001045	-0.000081
C	2.923892	1.133403	-0.428466
C	1.551850	1.145257	-0.436638
H	-2.076025	1.701319	1.449686
H	-0.634947	2.597471	0.943720
H	-2.677792	3.786315	0.673042
H	-2.272581	0.742217	-0.847615
H	-0.822002	1.593478	-1.345480
H	-0.824052	-1.592923	1.345544
H	-0.636956	-2.597620	-0.943181
H	-2.077281	-1.700402	-1.449816
H	-2.681446	-3.784224	-0.673078
H	-2.273624	-0.740280	0.847068
H	1.036046	-2.031905	0.767303
H	3.463803	-2.011160	0.755734
H	4.704267	-0.001309	-0.000204
H	3.464729	2.009260	-0.755490
H	1.036894	2.031270	-0.766865

5a (*1_TS_2*)

ΔG = -745.609489 hartree

C	1.184849	0.032044	-0.345802
C	1.404671	-1.203065	0.281628
C	2.699723	-1.678552	0.445050
C	3.790155	-0.935742	0.010454
C	3.574042	0.294866	-0.602341
C	2.287608	0.778249	-0.782699
C	-1.161198	-0.413517	-0.669402
N	-0.133393	0.503724	-0.563039
C	-0.424928	1.929579	-0.394850
H	0.579814	-1.786698	0.666907
H	2.851696	-2.630423	0.935470
H	4.795843	-1.306543	0.151140
H	4.411530	0.880667	-0.955735
H	2.148027	1.717758	-1.294844
H	-0.833973	-1.342610	-1.142904
H	-1.440665	-0.917997	0.430024
H	-1.301278	2.190852	-0.980984
H	0.402171	2.513942	-0.785260
O	-1.373599	-2.965002	1.114729
O	-1.944638	-1.805026	1.261918
C	-2.528000	0.026731	-1.175467
H	-2.946961	0.818339	-0.549115
H	-2.439369	0.412466	-2.193007
C	-0.645563	2.307641	1.069827
H	-1.502335	1.761244	1.475810
H	0.238046	2.039949	1.656163
O	-3.396802	-1.090153	-1.232281
H	-3.399771	-1.499186	-0.354430
O	-0.874854	3.710685	1.088413
H	-0.998027	3.988741	2.001426

5a (*2*)

ΔG = -594.662358 hartree

C	-1.054328	-0.180087	0.099415
N	0.331820	-0.356853	0.216618
C	0.923266	-1.554337	-0.140104
C	2.269403	-1.966463	0.300264
O	3.315684	-1.328776	-0.486262
C	1.169917	0.755487	0.665692
C	1.713693	1.598482	-0.485174
O	2.491238	2.639249	0.106810
C	-1.634900	1.101228	0.073081
C	-3.008998	1.255138	-0.041824
C	-3.849485	0.150642	-0.140468
C	-3.285092	-1.120587	-0.108945
C	-1.913958	-1.291399	0.013316

H	2.431564	-1.734633	1.358363
H	2.343947	-3.050310	0.182924
H	4.163418	-1.613666	-0.124877
H	0.368214	-2.179286	-0.819316
H	0.600330	1.379865	1.350916
H	0.895214	2.013547	-1.079898
H	2.326038	0.965121	-1.129260
H	2.892742	3.156554	-0.597866
H	2.014046	0.356351	1.222468
H	-1.020032	1.985693	0.128419
H	-3.422683	2.254895	-0.061949
H	-4.918999	0.277807	-0.233537
H	-3.918557	-1.996347	-0.165180
H	-1.510465	-2.290029	0.076566

5a (*3*)

ΔG = -745.706713 hartree

C	1.164926	-0.146427	-0.279205
N	-0.157560	0.298005	-0.478303
C	-1.219581	-0.637573	-0.325505
C	-2.505653	-0.273881	-1.060837
O	-3.379787	-1.400547	-0.919360
O	-1.511959	-0.791299	1.098552
O	-2.028975	-2.129950	1.338564
C	-0.442567	1.729953	-0.545300
C	-0.418484	2.423071	0.814065
O	-0.648985	3.810129	0.573383
C	2.261495	0.674631	-0.592237
C	3.563565	0.213541	-0.451927
C	3.823937	-1.071838	0.008022
C	2.747705	-1.885529	0.339951
C	1.440139	-1.434772	0.212400
H	-2.969189	0.608477	-0.620686
H	-2.290366	-0.082698	-2.115410
H	-4.275377	-1.126476	-1.140301
H	-0.899051	-1.616805	-0.680025
H	-2.842758	-2.111617	0.800594
H	0.267349	2.218437	-1.209409
H	0.548789	2.264712	1.299825
H	-1.194367	1.998866	1.458006
H	-0.652451	4.269730	1.418425
H	-1.416641	1.881641	-1.000097
H	2.112463	1.677924	-0.958017
H	4.380989	0.873888	-0.710765
H	4.839694	-1.425964	0.115725
H	2.919312	-2.884207	0.720136
H	0.639277	-2.085677	0.524447

5a (*3_TS_4*)

ΔG = -745.663558 hartree

C	1.056962	-0.193457	-0.246389
C	1.500229	-1.177963	0.646830
C	2.845248	-1.517612	0.707733
C	3.781744	-0.871578	-0.093292
C	3.350135	0.126408	-0.959458
C	2.004045	0.461676	-1.043147
C	-2.490898	-0.893351	-1.062794
C	-1.285539	-0.880602	-0.200779
N	-0.316284	0.131759	-0.347965
C	-0.724115	1.510819	-0.606980
O	-2.206694	-0.732826	0.979852
O	-1.178086	-0.903043	2.577101
H	0.790037	-1.625872	1.327748
H	3.164738	-2.279512	1.406949
H	4.829393	-1.132809	-0.034701
H	4.062041	0.645480	-1.587803
H	1.695384	1.227207	-1.740038
H	-3.106369	-0.611214	0.247106
H	-0.808765	-1.850981	-0.140977
H	-0.953910	0.034275	2.613040
H	-1.807076	1.538990	-0.705048
H	-0.317722	1.881171	-1.550204
H	-2.781751	-0.018855	-1.634355
C	-0.331356	2.467455	0.522829
H	-0.800705	2.144843	1.456512
H	0.747374	2.457722	0.670014
O	-0.675327	3.812455	0.207547
H	-1.633664	3.900918	0.240074
O	-2.865219	-2.100393	-1.528472
H	-3.701137	-2.033994	-2.008100

5a (*4*)

ΔG = -594.098328 hartree

C	0.897578	-0.173833	-0.158550
N	-0.485117	-0.136360	-0.344957
C	-1.228653	-1.328504	-0.297134
C	-2.498622	-1.439032	0.099292
O	-3.248802	-2.584543	0.026753
C	-1.172480	1.122173	-0.605659
C	-1.381235	1.975684	0.642211
O	-2.034538	3.170453	0.218932
C	1.717920	0.926288	-0.475370
C	3.094989	0.856881	-0.317517
C	3.708987	-0.294446	0.164366
C	2.906972	-1.378783	0.502213
C	1.527835	-1.324015	0.355364
H	-0.709370	-2.207120	-0.662573
H	-3.076237	-0.620628	0.503126
H	-2.719662	-3.299698	-0.347194
H	-0.626382	1.706998	-1.347115
H	-0.418252	2.200342	1.109491
H	-1.989293	1.432017	1.371786
H	-2.154211	3.740930	0.984145
H	-2.139322	0.887053	-1.045370
H	1.290405	1.843486	-0.848463
H	3.692539	1.721450	-0.576586
H	4.782198	-0.339806	0.286052
H	3.353731	-2.280660	0.900634
H	0.936642	-2.171601	0.665987

5a (*4_TS_pre_b*)

ΔG = -744.400210 hartree

C	1.294167	-0.228784	-0.224243
N	-0.109319	0.004970	-0.515966
C	-0.939034	-0.973580	-0.435775
C	-2.449029	-0.929635	-0.433274
O	-2.959142	-1.861344	-1.346719
C	-0.505455	1.402067	-0.817038
C	-0.610623	2.251072	0.456589
O	-0.858241	3.605687	0.102747
C	1.637850	-0.749892	1.017337
C	2.977102	-0.989863	1.299826
C	3.952447	-0.706990	0.350658
C	3.591991	-0.181833	-0.886713
C	2.257680	0.064977	-1.181565
O	-2.371053	-0.136148	1.716625
O	-2.781765	-1.279686	0.863330
H	-0.514323	-1.950378	-0.236323
H	-2.855314	0.045202	-0.700577
H	-2.738329	-2.750595	-1.039227
H	0.253843	1.814317	-1.476099
H	0.337510	2.233244	0.993068
H	-1.387630	1.828562	1.094708
H	-1.802209	3.715330	-0.050925
H	-1.448761	1.388026	-1.352345
H	0.868856	-0.939006	1.753034
H	3.254315	-1.389240	2.265104
H	4.993642	-0.892802	0.574446
H	4.348621	0.031383	-1.628457
H	1.974037	0.457873	-2.147327

5a (*pre_b*)

ΔG = -744.499943 hartree

C	1.223651	-0.114701	0.000657
N	-0.157199	0.159124	-0.041991
C	-1.099759	-0.797552	0.386069
C	-2.169802	-1.396504	-0.544893
O	-2.167874	-2.750042	-0.786786
C	-0.652983	1.393829	-0.649734
C	-0.865709	2.542640	0.335059
O	-1.242978	3.675714	-0.446395
C	2.161983	0.927696	-0.040191
C	3.524297	0.660927	-0.005131
C	3.995690	-0.643826	0.081467
C	3.074439	-1.683861	0.108820
C	1.709927	-1.430864	0.052795
O	-2.187204	-0.210122	1.181374
O	-3.192285	-0.975845	0.397819
H	-0.599107	-1.572383	0.963808
H	-2.296711	-0.907448	-1.509167
H	-2.024803	-3.229544	0.040414
H	0.043452	1.710451	-1.425587
H	0.050844	2.743112	0.896879
H	-1.648220	2.273700	1.046564
H	-1.468150	4.395676	0.150400
H	-1.603634	1.190424	-1.142178
H	1.835613	1.954821	-0.087238
H	4.220288	1.488907	-0.035077
H	5.057122	-0.845972	0.114626
H	3.414412	-2.710308	0.149398
H	1.031611	-2.269642	0.013489

5a (*5b*)

ΔG = -554.837977 hartree

C	0.669560	0.084556	0.094901
N	-0.625738	0.673411	0.208149
C	-0.879941	1.974316	-0.118277
C	-1.758844	-0.128066	0.693871
C	-2.660253	-0.651061	-0.420014
O	-3.701616	-1.384316	0.215477
C	0.803010	-1.256698	-0.270799
C	2.060652	-1.843305	-0.346821
C	3.202145	-1.102384	-0.067826
C	3.070960	0.232579	0.299676
C	1.818416	0.825685	0.386429
O	-0.099000	2.774478	-0.602676
H	-1.921675	2.247755	0.106139
H	-1.368622	-0.957404	1.278473
H	-2.096656	-1.284045	-1.110792
H	-3.062272	0.190771	-0.992601
H	-4.298282	-1.718143	-0.461375
H	-2.356390	0.487123	1.366739
H	-0.068231	-1.850750	-0.501726
H	2.141949	-2.883429	-0.632184
H	4.180180	-1.559094	-0.131781
H	3.949263	0.819995	0.531764
H	1.731609	1.858312	0.681053

5a (*3_TS_c*)

ΔG = -745.634426 hartree

C	-1.032521	0.245535	0.101486
C	-1.558112	1.409042	-0.471990
C	-2.899574	1.480089	-0.824814
C	-3.739319	0.390596	-0.626278
C	-3.220931	-0.765693	-0.054454
C	-1.884338	-0.845213	0.318394
N	0.340324	0.202671	0.486169
O	0.698630	-2.100962	0.215736
O	0.142010	-2.813489	2.036042
H	-0.924599	2.264233	-0.652605
H	-3.282558	2.390991	-1.265117
H	-4.782626	0.444981	-0.905595
H	-3.865416	-1.616776	0.122674
H	-1.504040	-1.735167	0.796017
H	2.142088	-0.748771	0.742510
H	-0.073435	-1.949677	2.407647
C	1.139207	-0.916368	0.338492

C	1.711682	-1.212704	-1.644867
H	0.807555	-1.615077	-2.072054
H	1.883766	-0.147711	-1.743795
O	2.756305	-2.020638	-1.747465
C	0.985683	1.413375	1.012846
H	0.209230	2.062498	1.410780
H	1.623556	1.128222	1.850301
C	1.825929	2.198361	0.007940
H	1.231641	2.469828	-0.869229
H	2.672027	1.593233	-0.333094
H	3.582156	-1.560748	-1.544539
O	2.285628	3.356473	0.695733
H	2.871563	3.848051	0.112005

5a (*5c*)

ΔG = -669.389449 hartree

C	-0.983940	-0.130039	0.119866
N	0.444742	-0.005687	0.259153
C	1.225705	-1.093482	0.050355
C	2.742392	-0.957977	0.209249
O	3.354555	-2.184133	-0.114974
O	0.774327	-2.197651	-0.251581
C	0.976136	1.309751	0.630736
C	1.084782	2.257900	-0.558182
O	1.575929	3.493067	-0.047249
C	-1.785973	-0.115868	1.256753
C	-3.167346	-0.211832	1.131014
C	-3.747214	-0.329631	-0.127518
C	-2.941940	-0.348257	-1.261840
C	-1.561151	-0.245003	-1.140938
H	3.119408	-0.164603	-0.441264
H	2.974317	-0.677466	1.241956
H	2.610454	-2.784292	-0.300318
H	0.315685	1.747643	1.378012
H	0.103669	2.386471	-1.023886
H	1.764294	1.841121	-1.308243
H	1.618546	4.127256	-0.769412
H	1.950669	1.196827	1.097751
H	-1.329717	-0.034132	2.234084
H	-3.787627	-0.200429	2.016860
H	-4.821622	-0.406429	-0.224260
H	-3.387818	-0.439185	-2.242969
H	-0.930643	-0.256615	-2.018921

5a (*1_TS_5*)

ΔG = -745.421018 hartree

C	1.267816	-0.221170	-0.063764
C	1.602441	-1.522464	-0.485111
C	2.920384	-1.931593	-0.488106
C	3.934126	-1.066377	-0.077562
C	3.610850	0.216554	0.348303
C	2.293911	0.640505	0.364688
C	-1.079197	-0.536616	-0.577888
N	-0.069623	0.221796	-0.064210
H	0.847816	-2.230587	-0.784921
H	3.159120	-2.936366	-0.805304
H	4.963564	-1.394726	-0.084295
H	4.386273	0.895825	0.671184
H	2.082813	1.642398	0.696463
H	-0.763118	-1.276058	-1.304675
H	-1.456090	-1.385495	0.376559
O	-3.023234	-1.626433	1.704206
O	-1.986825	-2.137707	1.248469
C	-2.440385	0.042891	-0.901779
H	-2.971676	0.363631	-0.000120
H	-2.318723	0.919152	-1.547883
O	-3.134825	-0.996549	-1.560204
C	-0.409607	1.505979	0.580859
H	-1.438390	1.452171	0.921627
H	0.215055	1.636386	1.457943
C	-0.254897	2.705712	-0.362667
H	0.773345	2.777034	-0.724351
H	-0.909526	2.596825	-1.229848
H	-4.073015	-0.781199	-1.575630
O	-0.612321	3.830612	0.420907
H	-0.625100	4.608526	-0.146132

5a (*5*)

ΔG = -594.526646 hartree

C	-1.036503	-0.106609	0.051276
N	0.411577	-0.164360	0.144123
C	1.029266	-1.240134	-0.195438
C	2.479453	-1.505509	-0.019271
O	2.715625	-2.806573	-0.507298
C	1.129082	1.003706	0.718849
C	1.728596	1.933486	-0.338995
O	2.525009	2.847460	0.394983
C	-1.652829	0.981672	-0.554802
C	-3.038452	1.010310	-0.633858
C	-3.795134	-0.031228	-0.107100
C	-3.165594	-1.107443	0.506623
C	-1.780178	-1.149278	0.593268
H	3.066711	-0.750391	-0.552251
H	2.723985	-1.409514	1.047953
H	3.655201	-3.000409	-0.425181
H	0.436935	-2.036420	-0.628154
H	0.423006	1.539195	1.344530
H	0.943120	2.449607	-0.892893
H	2.327546	1.364070	-1.054937
H	2.809848	3.551533	-0.196368
H	1.928363	0.626907	1.353290
H	-1.072185	1.785737	-0.979187
H	-3.523989	1.847952	-1.113740
H	-4.873757	0.000241	-0.168963
H	-3.748619	-1.911786	0.931854
H	-1.288516	-1.967136	1.100385

5a (*5_TS_6*)

ΔG = -670.916573 hartree

C	1.188179	0.037764	0.040902
C	1.987965	0.513563	1.071804
C	3.372053	0.449728	0.950789
C	3.948320	-0.087880	-0.193562
C	3.139572	-0.560072	-1.222464
C	1.755984	-0.496277	-1.111583
C	-0.962622	-1.176804	0.236796
O	-1.388602	-1.006887	1.677522
N	-0.263857	0.128337	0.187897
C	-0.882203	1.248278	-0.592069
H	-0.256239	-1.997789	0.188370
H	-1.046523	-1.692759	2.275127
H	-0.720320	-0.056350	1.517968
H	1.535238	0.935136	1.958640
H	3.995022	0.818178	1.753750
H	5.024348	-0.138919	-0.285057
H	3.583606	-0.977254	-2.115438
H	1.133186	-0.857524	-1.918539
H	-1.327788	0.874771	-1.512255
H	-0.075608	1.919541	-0.871151
C	-2.182913	-1.425590	-0.626111
H	-2.927070	-0.646875	-0.473943
H	-1.877559	-1.411173	-1.674309
C	-1.905402	2.024332	0.226423
H	-2.722491	1.376516	0.558769
H	-1.418759	2.435611	1.116421
O	-2.783037	-2.651197	-0.260010
H	-2.326879	-3.374981	-0.703268
O	-2.385449	3.051723	-0.627022
H	-3.022066	3.584156	-0.139833

5a (*6*)

ΔG = -670.964605 hartree

C	-1.180276	-0.232725	0.192833
N	0.280736	-0.261935	0.476147
C	0.878367	1.152716	0.544052
C	1.206145	1.754580	-0.817961
O	1.874522	2.966833	-0.491664
O	2.005587	1.030693	1.350177
C	1.019398	-1.291236	-0.360562
C	2.409380	-1.640689	0.158266
O	2.755106	-2.822135	-0.552693
C	-2.043827	-0.284749	1.276259
C	-3.413781	-0.244313	1.048699
C	-3.901947	-0.152398	-0.249277
C	-3.020598	-0.103342	-1.322967
C	-1.647570	-0.143616	-1.109297
H	0.369498	-0.581958	1.443578
H	0.102478	1.741239	1.037032
H	0.293873	1.940381	-1.386408
H	1.861241	1.094426	-1.388047
H	2.320858	3.299540	-1.276978
H	2.612671	1.743946	1.101126
H	0.402139	-2.185186	-0.325522
H	2.378918	-1.820496	1.237338
H	3.122361	-0.840181	-0.030624
H	3.694737	-2.988589	-0.428340
H	1.057758	-0.941312	-1.385531
H	-1.662332	-0.357843	2.286179
H	-4.093412	-0.287616	1.887530
H	-4.968027	-0.122647	-0.424476
H	-3.396000	-0.035805	-2.333865
H	-0.975385	-0.112860	-1.952843

5a (*5d*)

ΔG = -441.467937 hartree

C	3.167332	0.228521	0.048060
N	4.469563	-0.206857	-0.138459
C	5.298205	0.280675	-1.225460
C	6.667793	-0.373806	-1.167795
O	7.429071	0.137052	-2.258256
C	2.317031	-0.486879	0.911187
C	1.024924	-0.053531	1.156144
C	0.533307	1.103513	0.552346
C	1.364597	1.812122	-0.306072
C	2.663604	1.386084	-0.565317
H	4.608020	-1.181001	0.082624
H	4.850199	0.090226	-2.209558
H	6.563754	-1.462505	-1.242534
H	7.145244	-0.145241	-0.210026
H	8.305115	-0.259003	-2.228057
H	5.427406	1.360399	-1.132477
H	2.686331	-1.385113	1.391144
H	0.394196	-0.625340	1.824752
H	-0.475763	1.439734	0.746206
H	1.002028	2.709437	-0.791186
H	3.281044	1.955515	-1.244265

7a

ΔG = -520.044295 hartree

C	-1.066285	0.282797	-0.107772
N	0.154694	0.917285	-0.214501
C	1.362024	0.204545	-0.599279
C	2.114843	-0.383336	0.603240
O	3.262492	-1.125026	0.216538
C	4.414169	-0.333142	-0.032700
C	0.249538	2.352068	-0.008888
C	-2.245090	1.016687	0.148094
C	-3.476426	0.383085	0.247859
C	-3.593891	-0.994299	0.099601
C	-2.439000	-1.730463	-0.148636
C	-1.199529	-1.116278	-0.248076
H	1.123111	-0.597796	-1.297727
H	1.465045	-1.076825	1.137664
H	2.392095	0.417494	1.298356
H	5.231599	-1.017614	-0.250717
H	4.676472	0.267177	0.845006
H	4.282970	0.336348	-0.887772

H	2.008016	0.898122	-1.136609
H	-0.300645	2.915946	-0.769832
H	1.293401	2.648056	-0.060473
H	-0.132632	2.647324	0.971161
H	-2.203299	2.088437	0.263384
H	-4.356158	0.983612	0.442270
H	-4.555665	-1.481471	0.179132
H	-2.496785	-2.805752	-0.261377
H	-0.332433	-1.733829	-0.423924

7a (*7a)**

ΔG = -519.929753 hartree

C	-1.108942	0.301232	-0.106599
N	0.156929	0.819195	-0.143468
C	1.326597	0.059534	-0.580593
C	2.181501	-0.422455	0.603483
O	3.351761	-1.085570	0.163095
C	4.444339	-0.222089	-0.120382
C	0.376666	2.236581	0.105936
C	-2.240525	1.100044	0.028724
C	-3.526900	0.544119	0.111194
C	-3.657898	-0.916944	0.086765
C	-2.564484	-1.725106	-0.041913
C	-1.258966	-1.185043	-0.172155
H	1.016138	-0.790210	-1.178285
H	1.608485	-1.143574	1.187291
H	2.434131	0.416405	1.261030
H	5.281428	-0.853337	-0.410472
H	4.723451	0.360160	0.763553
H	4.225594	0.467363	-0.940863
H	1.919092	0.707779	-1.226810
H	0.010439	2.841413	-0.728491
H	1.440317	2.419546	0.223283
H	-0.138995	2.547576	1.012820
H	-2.134734	2.175043	0.041263
H	-4.401657	1.170472	0.186289
H	-4.642276	-1.358577	0.180080
H	-2.685352	-2.801020	-0.036568
H	-0.396989	-1.828082	-0.121372

7a (*1*)

ΔG = -519.853204 hartree

C	1.074667	0.267780	0.139009
N	-0.140111	0.857801	0.269489
C	-1.342958	0.119904	0.636632
C	-2.108169	-0.388662	-0.614986
O	-3.260857	-1.093021	-0.234102
C	-4.408254	-0.282818	0.004770
C	-0.321983	2.288918	0.005825
C	2.228692	1.055538	-0.141274
C	3.458412	0.457543	-0.271700
C	3.592827	-0.929082	-0.139612
C	2.469692	-1.717438	0.132226
C	1.230174	-1.142529	0.275322
H	-1.092583	-0.718701	1.276119
H	-1.470757	-1.083239	-1.161591
H	-2.350395	0.449451	-1.275075
H	-5.234014	-0.961061	0.203930
H	-4.642860	0.327611	-0.871473
H	-4.274637	0.371529	0.870345
H	-1.973054	0.799147	1.205393
H	0.144917	2.874841	0.797807
H	-1.383426	2.505898	-0.009825
H	0.113028	2.559553	-0.952466
H	2.148642	2.125660	-0.235561
H	4.326925	1.066716	-0.475216
H	4.563952	-1.390405	-0.246555
H	2.572414	-2.788329	0.228830
H	0.380886	-1.774037	0.474459

7a (*1_TS_2*)

ΔG = -670.360192 hartree

C	0.793671	-0.573434	0.434855
C	1.949930	-0.133641	-0.227605
C	2.864644	-1.060202	-0.710519
C	2.641577	-2.424324	-0.567853
C	1.485945	-2.860398	0.072575
C	0.566900	-1.949999	0.570468
C	0.271537	1.650483	1.212154
N	-0.118015	0.363337	0.972997
C	-1.539119	0.026401	1.103570
H	2.134155	0.919848	-0.391012
H	3.749886	-0.705632	-1.220854
H	3.352650	-3.139137	-0.957874
H	1.297560	-3.918290	0.193975
H	-0.307664	-2.318798	1.082830
H	1.317275	1.777802	1.499622
H	0.408246	2.355994	0.153445
H	-1.998314	0.765167	1.754859
H	-1.648705	-0.941307	1.586731
O	2.239817	3.160086	-0.499538
O	0.937250	3.115793	-0.676444
H	-0.441499	2.223710	1.793031
C	-2.260967	0.012003	-0.242529
H	-2.199860	1.001126	-0.712646
H	-1.796519	-0.712345	-0.921458
O	-3.603888	-0.337893	0.019026
C	-4.401355	-0.381368	-1.153967
H	-5.407918	-0.658797	-0.849371
H	-4.432167	0.594492	-1.649569
H	-4.023032	-1.124202	-1.863934

7a (*2*)

ΔG = -519.404407 hartree

C	1.086773	0.315999	0.096777
N	-0.156914	0.948393	0.174086
C	-1.346352	0.209752	0.599204
C	-2.132738	-0.368153	-0.585609

O	-3.281684	-1.082356	-0.160942
C	-4.417896	-0.268466	0.094198
C	-0.325782	2.281820	-0.119262
C	2.269781	1.071614	-0.017065
C	3.504393	0.445330	-0.105028
C	3.609982	-0.941661	-0.077791
C	2.446380	-1.695939	0.043913
C	1.203353	-1.086251	0.127804
H	-1.061671	-0.589924	1.279135
H	-1.512560	-1.077293	-1.134087
H	-2.409133	0.437976	-1.273691
H	-5.237720	-0.937276	0.347890
H	-4.691833	0.312533	-0.792465
H	-4.258178	0.419752	0.929107
H	-1.975471	0.898986	1.161046
H	-1.312371	2.691120	0.010346
H	0.399546	2.786776	-0.732276
H	2.226153	2.149437	-0.004098
H	4.395347	1.054715	-0.184763
H	4.575183	-1.423576	-0.146870
H	2.500478	-2.776550	0.066267
H	0.326743	-1.710854	0.200561

7a (*3*)

ΔG = -670.452403 hartree

C	1.146925	-0.178915	0.303914
N	-0.112132	0.319384	0.672850
C	-1.276050	-0.557627	0.774218
C	-1.835438	-0.976972	-0.592650
O	-2.878799	-1.932117	-0.478072
C	-4.147422	-1.378471	-0.160456
C	-0.319954	1.710942	0.818431
O	-0.626083	2.271507	-0.489616
O	-0.910709	3.680683	-0.289420
C	2.169772	0.681175	-0.132497
C	3.430663	0.189939	-0.441189
C	3.713477	-1.168322	-0.348914
C	2.701011	-2.030047	0.055762
C	1.437167	-1.551393	0.376406
H	-1.032828	-1.450861	1.349531
H	-1.049183	-1.452554	-1.179037
H	-2.177383	-0.092347	-1.140095
H	-4.867520	-2.193772	-0.188626
H	-4.439636	-0.618697	-0.892966
H	-4.168150	-0.929721	0.836897
H	-2.035153	-0.021964	1.340271
H	-1.168565	1.903444	1.472959
H	-0.077578	4.088024	-0.567807
H	0.565765	2.210363	1.211481
H	1.976812	1.735084	-0.259914
H	4.193898	0.881859	-0.772893
H	4.694864	-1.546907	-0.598421
H	2.889749	-3.093281	0.127557
H	0.683636	-2.256797	0.689825

7a (*3_TS_c*)

ΔG = -670.388935 hartree

C	-1.148649	-0.301513	-0.083053
C	-2.185163	0.177981	-0.910800
C	-3.432138	-0.420916	-0.889423
C	-3.701472	-1.484690	-0.030830
C	-2.694585	-1.947836	0.808967
C	-1.435177	-1.369237	0.789266
N	0.135567	0.231790	-0.166159
C	1.264363	-0.505084	0.407929
O	-0.571527	2.483961	-0.608813
O	-0.167504	3.087607	1.330311
H	-0.588382	3.650952	2.004235
H	-2.008267	1.013475	-1.566450
H	-4.206199	-0.046412	-1.545582
H	-4.683537	-1.936115	-0.009609
H	-2.888783	-2.763598	1.492005
H	-0.680790	-1.741789	1.463788
H	0.953642	2.012475	0.455789
H	1.047839	-1.566578	0.333788
H	1.389351	-0.262097	1.468021
C	0.390054	1.626363	-0.471729
H	1.146569	1.709127	-1.273894
C	2.586816	-0.277254	-0.322956
H	2.972252	0.736678	-0.175908
H	2.453813	-0.438356	-1.400230
O	3.494590	-1.218192	0.215191
C	4.799445	-1.096609	-0.328375
H	5.418118	-1.854989	0.145945
H	4.795955	-1.261672	-1.410943
H	5.224020	-0.107871	-0.125335

7a (*7c*)

ΔG = -594.127285 hartree

C	-1.095895	0.072068	0.113715
N	0.063099	0.890477	0.264712
C	0.103098	2.205190	-0.103714
C	1.295566	0.323123	0.831158
C	2.316903	-0.089123	-0.225022
O	3.428531	-0.628497	0.460333
C	4.474142	-1.029456	-0.410059
C	-0.961830	-1.295292	-0.140289
C	-2.085978	-2.104201	-0.254801
C	-3.359480	-1.564994	-0.124119
C	-3.495246	-0.205227	0.133841
C	-2.378536	0.611025	0.256722
O	-0.777165	2.839775	-0.657519
H	1.067510	2.664564	0.158773
H	1.895003	-0.826044	-0.918460
H	4.138183	-1.808284	-1.102858
H	5.276659	-1.425017	0.208496
H	4.853530	-0.182742	-0.991828
H	2.615779	0.784089	-0.818933
H	1.031292	-0.531012	1.449255

H	1.749043	1.066186	1.486485
H	0.015406	-1.738754	-0.254787
H	-1.958346	-3.159890	-0.452689
H	-4.233271	-2.194999	-0.217675
H	-4.479287	0.228843	0.250721
H	-2.500581	1.660818	0.463418

7a (*1_TS_5*)

ΔG = -670.186094 hartree

C	-0.650557	0.275004	0.196717
C	-0.798986	-1.121306	0.273693
C	-2.023677	-1.698825	0.004049
C	-3.118185	-0.907075	-0.339924
C	-2.974487	0.474417	-0.420832
C	-1.752604	1.069267	-0.163558
C	1.588323	0.210258	1.095283
N	0.589210	0.878480	0.480425
C	0.800484	2.275825	0.039287
H	0.036913	-1.761640	0.503891
H	-2.123206	-2.773499	0.050529
H	-4.073771	-1.366303	-0.549054
H	-3.818912	1.095168	-0.682698
H	-1.673800	2.142107	-0.216471
H	1.299264	-0.635346	1.707398
H	2.311361	-0.486964	0.191429
H	0.187216	2.915388	0.675292
H	0.432895	2.358507	-0.980313
O	3.616963	-2.083169	0.094473
O	3.021980	-1.195872	-0.544345
H	2.391629	0.820734	1.483668
C	2.239797	2.774533	0.073735
H	2.620818	2.849439	1.098212
H	2.902517	2.111321	-0.494181
O	2.183607	4.051414	-0.520150
C	3.446356	4.705759	-0.543438
H	3.294830	5.669571	-1.022543
H	3.829046	4.861570	0.469701
H	4.179023	4.128719	-1.115686

7a (*5*)

ΔG = -519.264223 hartree

C	-1.137649	0.291581	0.007685
N	0.163172	0.922670	0.070584
C	1.336077	0.219479	-0.521430
C	2.257914	-0.370946	0.563961
O	3.335282	-1.048647	-0.031088
C	4.432269	-0.217284	-0.403710
C	0.314226	2.072562	0.611126
C	-2.243609	1.070279	-0.318863
C	-3.497590	0.477191	-0.361842
C	-3.639685	-0.878154	-0.087681
C	-2.523035	-1.647515	0.222324
C	-1.262087	-1.069793	0.265478
H	0.959521	-0.562724	-1.170150
H	1.713458	-1.099415	1.163138
H	2.604782	0.424403	1.232308
H	5.203837	-0.876098	-0.793682
H	4.821749	0.323320	0.463201
H	4.159109	0.501899	-1.180108
H	1.868007	0.947931	-1.126750
H	1.279932	2.555282	0.575955
H	-0.520614	2.554993	1.095987
H	-2.125310	2.114404	-0.569920
H	-4.358491	1.074874	-0.624761
H	-4.617435	-1.337109	-0.125919
H	-2.629553	-2.701565	0.434551
H	-0.404434	-1.674115	0.518484

7a (*5_TS_6*)

ΔG = -595.677569 hartree

C	-1.279720	0.055157	-0.002408
C	-1.812489	-0.357401	1.212006
C	-3.107873	-0.859475	1.254928
C	-3.862748	-0.944449	0.090405
C	-3.320604	-0.529290	-1.121092
C	-2.023599	-0.032138	-1.173963
C	0.291520	1.873553	-0.621690
O	0.727196	2.524141	0.652858
N	0.093798	0.549972	-0.022147
C	1.092689	-0.497246	-0.394184
H	-0.617111	2.334543	-0.985451
H	0.138826	3.240519	0.947242
H	0.454224	1.446058	1.034635
H	-1.218129	-0.286762	2.112378
H	-3.525883	-1.177907	2.199641
H	-4.871363	-1.332036	0.126454
H	-3.903305	-0.595030	-2.029227
H	-1.602519	0.279235	-2.120369
H	1.106578	-0.627053	-1.476893
H	0.749001	-1.425548	0.053287
H	1.111527	1.932580	-1.324717
C	2.488098	-0.180252	0.124548
H	2.864675	0.769088	-0.277636
H	2.469922	-0.095697	1.218563
O	3.316100	-1.245912	-0.283497
C	4.664837	-1.088478	0.133573
H	4.738691	-1.039592	1.224605
H	5.213979	-1.956134	-0.223821
H	5.107283	-0.181792	-0.291279

7a (*6*)

ΔG = -595.715069 hartree

C	-1.330127	0.043626	0.116410
N	0.059024	0.552140	0.210309
C	1.080296	-0.440275	-0.307034
C	2.504570	-0.158367	0.159316
O	3.207251	-1.361950	-0.067948
C	4.594776	-1.249980	0.217891

C	0.154121	1.958309	-0.438624
O	1.354768	2.562063	-0.150632
C	-1.835192	-0.368576	-1.108205
C	-3.147180	-0.822771	-1.168200
C	-3.932177	-0.859261	-0.021127
C	-3.408787	-0.438422	1.195631
C	-2.098822	0.019143	1.269906
H	0.255701	0.685541	1.203662
H	0.776672	-1.410869	0.076021
H	2.515598	0.102148	1.226015
H	2.955663	0.667598	-0.392772
H	5.042236	-2.219288	0.012576
H	4.762233	-0.991177	1.268222
H	5.068884	-0.492002	-0.413221
H	1.009554	-0.451499	-1.390365
H	0.078109	1.788298	-1.508068
H	1.287237	3.083645	0.658110
H	-0.712385	2.501379	-0.070258
H	-1.231796	-0.348078	-2.003689
H	-3.551498	-1.149300	-2.115578
H	-4.950952	-1.216086	-0.075904
H	-4.014242	-0.465103	2.090189
H	-1.689200	0.348342	2.215757

7a (*7d*)

ΔG = -480.757264 hartree

C	1.162992	-0.281320	0.047127
N	-0.169523	-0.653989	0.129813
C	-1.249117	0.287845	-0.102347
C	-2.589145	-0.402300	0.090274
O	-3.608034	0.551869	-0.137581
C	-4.909214	0.014037	0.020304
C	1.573567	1.060533	0.063167
C	2.926796	1.383014	0.030649
C	3.900572	0.393995	-0.028990
C	3.497890	-0.940959	-0.055620
C	2.154994	-1.276894	-0.018908
H	-0.352119	-1.586744	-0.207824
H	-1.178339	1.108433	0.613252
H	-2.660375	-0.809091	1.106600
H	-2.691730	-1.241325	-0.611848
H	-5.618208	0.815999	-0.173849
H	-5.064413	-0.362833	1.037229
H	-5.091298	-0.803518	-0.685943
H	-1.211436	0.728054	-1.107227
H	0.842051	1.854018	0.100730
H	3.216371	2.426093	0.045972
H	4.949710	0.653498	-0.057160
H	4.238160	-1.729155	-0.106722
H	1.856556	-2.318159	-0.035192

7a (*1_TS_2'*)

ΔG = -670.355010 hartree

C	-1.409096	-0.444581	0.047824
C	-1.642406	0.925606	-0.147050
C	-2.922612	1.372162	-0.446756
C	-3.987449	0.483347	-0.539290
C	-3.759208	-0.873062	-0.331085
C	-2.486088	-1.338821	-0.039509
C	0.994146	-0.187385	-0.029351
N	-0.115266	-0.928199	0.319845
H	-0.846184	1.649330	-0.039018
H	-3.087602	2.431785	-0.588610
H	-4.982462	0.842459	-0.762367
H	-4.574901	-1.579435	-0.404371
H	-2.329155	-2.398756	0.088793
H	0.820568	0.448571	-0.902902
H	1.169159	0.774130	0.749316
O	1.013607	2.857331	0.279402
O	1.312284	1.978971	1.196010
C	2.333621	-0.892731	-0.106388
H	2.690612	-1.196152	0.884257
H	2.237061	-1.802444	-0.715785
O	3.239368	0.009519	-0.699146
C	0.031742	-2.194535	1.038027
H	0.024475	-3.043703	0.351971
H	0.968120	-2.199420	1.585985
H	-0.779555	-2.308289	1.751133
C	4.556986	-0.512595	-0.782507
H	5.173166	0.249108	-1.253876
H	4.958068	-0.736612	0.211166
H	4.585602	-1.424177	-1.388232

7a (*2'*)

ΔG = -519.409321 hartree

C	-1.147143	0.079454	0.081020
N	0.233675	0.257292	0.212785
C	0.741762	1.608453	0.435958
C	1.108704	-0.792391	0.022549
C	2.535944	-0.739553	0.386489
O	3.319500	-0.012443	-0.590084
C	4.697188	0.004117	-0.259841
C	-1.725184	-1.202840	0.151566
C	-3.094233	-1.370045	0.009155
C	-3.932959	-0.278794	-0.199922
C	-3.371638	0.992716	-0.257756
C	-2.002890	1.177798	-0.120916
H	1.794444	1.563738	0.683657
H	0.203148	2.088468	1.251694
H	0.637101	2.221578	-0.462979
H	0.727413	-1.643354	-0.515944
H	2.918090	-1.764147	0.446466
H	2.693838	-0.274478	1.368777
H	5.213777	0.563242	-1.037743
H	5.111773	-1.009852	-0.214983
H	4.874630	0.491817	0.706008
H	-1.106058	-2.063760	0.351046
H	-3.509624	-2.367247	0.075812
H	-4.999821	-0.416210	-0.308075

H	-4.003011	1.857134	-0.417052
H	-1.604731	2.178090	-0.185318

7a (*3'*)

ΔG = -670.452185 hartree

C	1.488537	0.178564	-0.226385
N	0.200046	0.725192	-0.379439
C	0.079978	2.177970	-0.486361
C	-0.936124	0.014124	0.124950
O	-1.309187	0.610086	1.396883
O	-2.026568	-0.376494	2.187334
C	-2.120407	0.034090	-0.839501
O	-3.201354	-0.659000	-0.228252
C	-4.395379	-0.629827	-0.999817
C	1.708117	-1.206794	-0.324336
C	2.983842	-1.737018	-0.209973
C	4.087554	-0.911461	-0.013236
C	3.885219	0.459359	0.064398
C	2.608346	1.002407	-0.036938
H	-0.949085	2.442966	-0.704820
H	0.703152	2.542276	-1.302043
H	0.371527	2.695310	0.431884
H	-0.669026	-1.016764	0.333601
H	-2.817623	-0.513125	1.632033
H	-1.828070	-0.460492	-1.772048
H	-2.424105	1.058547	-1.071337
H	-5.149442	-1.184753	-0.447369
H	-4.239857	-1.102392	-1.973790
H	-4.739335	0.397177	-1.153059
H	0.884891	-1.879166	-0.516089
H	3.115091	-2.808131	-0.291325
H	5.081185	-1.329417	0.069276
H	4.725613	1.124628	0.214371
H	2.493541	2.071763	0.042264

7a (*3'_TS_4'*)

ΔG = -670.401627 hartree

C	-1.331672	-0.212610	0.196441
C	-1.750351	0.713614	-0.771908
C	-3.026348	0.638825	-1.311228
C	-3.925764	-0.338102	-0.891622
C	-3.525090	-1.241140	0.084864
C	-2.243575	-1.188291	0.621986
C	2.347400	-0.469533	0.033990
C	1.054928	0.256348	-0.049730
N	-0.037248	-0.158794	0.742132
O	1.761850	1.475132	0.456492
O	0.524305	2.922600	0.420284
H	-1.092272	1.524383	-1.048627
H	-3.326758	1.368406	-2.052141
H	-4.921499	-0.385672	-1.310371
H	-4.207943	-2.006839	0.429435
H	-1.953111	-1.918557	1.362524
H	2.733749	0.839733	0.603293
H	0.743531	0.436353	-1.070650
H	0.053627	2.602149	1.199212
H	2.564728	-1.122574	0.875173
O	2.968626	-0.716352	-1.122311
C	0.226833	-0.757088	2.043317
H	-0.612164	-0.567315	2.709247
H	0.394202	-1.837638	1.997414
H	1.103837	-0.286843	2.484512
C	4.311265	-1.224867	-1.019931
H	4.331889	-2.112778	-0.387693
H	4.617541	-1.477962	-2.029259
H	4.967364	-0.457280	-0.609782

7a (*4'*)

ΔG = -518.843315 hartree

C	-1.123335	0.207416	-0.062562
N	0.154128	0.754313	-0.184222
C	0.359260	2.177138	0.044396
C	1.263236	-0.072902	-0.385474
C	2.516798	0.181337	0.000828
O	3.543250	-0.616492	-0.437060
C	4.634046	-0.719074	0.475052
C	-1.328895	-1.186534	-0.029415
C	-2.608043	-1.718237	0.050699
C	-3.727101	-0.895565	0.122421
C	-3.534306	0.481237	0.124735
C	-2.261979	1.030276	0.040227
H	1.354032	2.445597	-0.296609
H	0.265322	2.447687	1.100093
H	-0.355501	2.767491	-0.526952
H	1.080113	-0.970403	-0.960057
H	2.807523	1.029105	0.610627
H	5.407681	-1.298201	-0.022376
H	4.332495	-1.227580	1.394367
H	5.028217	0.269670	0.725950
H	-0.489102	-1.863030	-0.042242
H	-2.724090	-2.794260	0.071692
H	-4.720641	-1.316084	0.190808
H	-4.384344	1.147429	0.197675
H	-2.164685	2.103773	0.057624

7a (*4'_TS_pre_b'*)

ΔG = -669.159039 hartree

C	1.042552	-0.210104	-0.207363
N	-0.305628	-0.434921	-0.659060
C	-1.317945	0.691263	-0.794337
C	-1.702596	0.004888	0.440269
O	-2.697735	-0.835774	0.452174
C	-2.825775	-1.707659	1.608736
C	-0.574451	-1.588689	-1.525100
C	2.072268	-1.012120	-0.704622
C	3.377040	-0.836111	-0.256792
C	3.675773	0.135086	0.687610
C	2.651478	0.937563	1.178074

C	1.345204	0.774500	0.739529
O	-2.060802	2.684735	-0.295815
O	-0.832163	1.944422	-0.715636
H	-1.975198	0.495788	-1.643973
H	-1.227670	0.283486	1.371923
H	-2.098873	-2.512543	1.532542
H	-3.834874	-2.101041	1.571117
H	-2.672941	-1.133692	2.520289
H	-0.162578	-1.423723	-2.520549
H	-1.648106	-1.723991	-1.606067
H	-0.147253	-2.486674	-1.088521
H	1.877518	-1.770938	-1.444613
H	4.158111	-1.467655	-0.657491
H	4.690685	0.268704	1.035251
H	2.864953	1.704464	1.910067
H	0.579938	1.433503	1.111640

7a (*pre_b'*)

ΔG = -669.243805 hartree

C	1.253407	0.382315	0.028623
N	0.184544	1.291054	0.144740
C	-1.129426	0.899788	0.443031
C	-1.789431	-0.362895	-0.112545
O	-2.897914	-0.070290	-0.868788
C	-3.505075	-1.197004	-1.512767
C	0.413448	2.693472	-0.200845
C	2.392522	0.724920	-0.715982
C	3.457812	-0.159716	-0.834338
C	3.421086	-1.406079	-0.222545
C	2.298677	-1.750102	0.523559
C	1.232019	-0.872614	0.659919
O	-2.089705	-0.795633	1.246149
O	-1.349033	0.361407	1.811151
H	-1.787433	1.751702	0.293993
H	-1.153673	-1.101298	-0.604104
H	-4.269399	-0.801855	-2.175738
H	-3.968172	-1.862321	-0.782501
H	-2.766570	-1.751364	-2.096174
H	1.321695	3.058347	0.277984
H	-0.421157	3.287958	0.158862
H	0.504008	2.848270	-1.278979
H	2.451239	1.678444	-1.217049
H	4.320165	0.134115	-1.418311
H	4.251375	-2.091992	-0.317679
H	2.252908	-2.709239	1.022641
H	0.396200	-1.154523	1.279113

7a (*7b'*)

ΔG = -440.295838 hartree

7b' and ***1c*** are the same structure

7a (*3'_TS_c'*)

ΔG = -670.378254 hartree

C	1.241260	-0.225914	0.337995
C	2.050038	-1.366360	0.258497
C	3.275295	-1.318208	-0.395331
C	3.715012	-0.139671	-0.985368
C	2.916749	0.996772	-0.901965
C	1.694630	0.967320	-0.242874
N	0.004573	-0.280598	1.033696
O	-1.160300	1.322636	-0.226546
O	-0.734531	3.046568	0.790857
H	1.726683	-2.297900	0.697859
H	3.882801	-2.212074	-0.445220
H	4.668488	-0.104397	-1.494443
H	3.252842	1.926475	-1.342202
H	1.097794	1.862473	-0.158435
H	-1.979703	0.204674	1.275730
H	-0.177095	2.608198	1.444829
C	-1.153971	0.340438	0.570558
C	-1.906162	-0.800296	-0.963818
H	-1.129723	-0.626672	-1.692915
H	-1.836637	-1.692585	-0.346750
O	-3.101539	-0.437563	-1.367313
C	-0.168275	-1.286062	2.080172
H	-0.307215	-2.295459	1.684493
H	0.702646	-1.288265	2.732362
H	-1.041085	-1.029466	2.675559
C	-4.229541	-0.811391	-0.549983
H	-4.327218	-0.105385	0.273166
H	-5.101871	-0.753989	-1.191865
H	-4.101982	-1.824333	-0.171342

7a (*7c'*)

ΔG = -594.128139 hartree

C	-1.163417	-0.107972	0.157371
N	0.250522	-0.121979	0.424894
C	0.711179	-1.158451	1.349555
C	1.033975	0.820126	-0.162743
O	0.570738	1.707086	-0.875496
C	2.539307	0.767529	0.090374
O	3.072198	-0.447132	-0.405899
C	4.481626	-0.523657	-0.246460
C	-2.025043	0.580596	1.005039
C	-3.394317	0.562470	0.763929
C	-3.903039	-0.143305	-0.321599
C	-3.038999	-0.832590	-1.166247
C	-1.669383	-0.817529	-0.926824
H	1.780654	-1.089136	1.500033
H	0.486264	-2.146773	0.946940
H	0.204189	-1.051391	2.309089
H	2.754928	0.881607	1.161006
H	2.969108	1.623409	-0.434493
H	4.800571	-1.476032	-0.663438
H	4.763711	-0.479792	0.810812
H	4.984354	0.290052	-0.778931
H	-1.622074	1.129040	1.845803
H	-4.062044	1.100824	1.422886

H	-4.968322	-0.156525	-0.508105
H	-3.429651	-1.382996	-2.011444
H	-0.990150	-1.351367	-1.577645

7a (*1_TS_5'*)

ΔG = -670.165317 hartree

C	-1.576355	-0.237290	0.028542
C	-1.817536	0.967557	-0.654948
C	-3.114079	1.345240	-0.943542
C	-4.187795	0.539129	-0.566916
C	-3.952780	-0.651026	0.113172
C	-2.660861	-1.040047	0.420144
C	0.819706	-0.112362	-0.296009
N	-0.265280	-0.658910	0.315418
H	-1.009979	1.626477	-0.931871
H	-3.290379	2.279732	-1.456257
H	-5.199091	0.841866	-0.798127
H	-4.778123	-1.284470	0.404267
H	-2.502910	-1.976604	0.929140
H	0.598415	0.394037	-1.228738
H	1.184889	0.949829	0.416459
O	2.711164	1.504719	1.704542
O	1.704089	1.894719	1.091470
C	2.151964	-0.834789	-0.326132
H	2.611237	-0.903733	0.668722
H	2.001266	-1.860439	-0.691371
O	2.963187	-0.087609	-1.195181
C	-0.061450	-1.696468	1.337845
H	-0.231042	-2.679244	0.897606
H	0.955073	-1.645224	1.706340
H	-0.747236	-1.536625	2.161888
C	4.288897	-0.600603	-1.295393
H	4.823586	0.046664	-1.984989
H	4.789382	-0.588234	-0.323298
H	4.286088	-1.622355	-1.684908

7a (*5'*)

ΔG = -519.276173 hartree

C	-1.192682	0.166347	0.076333
N	0.168394	0.644938	0.220112
C	0.355587	2.029990	0.704100
C	1.160049	-0.115860	-0.071637
C	2.592950	0.246045	0.068178
O	3.340365	-0.856728	-0.368132
C	4.746204	-0.636121	-0.293312
C	-1.537957	-1.068857	0.611061
C	-2.840860	-1.526470	0.460898
C	-3.780777	-0.752591	-0.209551
C	-3.421313	0.486743	-0.729609
C	-2.123664	0.958457	-0.585792
H	1.292384	2.103799	1.245005
H	-0.468441	2.275955	1.363449
H	0.368970	2.709069	-0.145627
H	0.936017	-1.100632	-0.461369
H	2.809907	0.498970	1.117547
H	2.804540	1.147487	-0.525110
H	5.223936	-1.545038	-0.647756
H	5.058436	-0.438896	0.736004
H	5.046453	0.203301	-0.926655
H	-0.812026	-1.652379	1.159283
H	-3.119483	-2.482623	0.880235
H	-4.794429	-1.110874	-0.321178
H	-4.149540	1.089418	-1.253300
H	-1.843623	1.915595	-1.000275

7a (*5'_TS_6'*)

ΔG = -595.664274 hartree

C	1.238393	-0.238465	0.109821
C	2.295650	-0.924994	-0.474490
C	3.517311	-0.284397	-0.646730
C	3.677218	1.035063	-0.239220
C	2.614142	1.714943	0.345053
C	1.391497	1.079238	0.527512
C	-1.214782	-0.308168	-0.292908
O	-1.412995	-1.402963	-1.321743
N	-0.023418	-0.948870	0.301843
H	-0.952525	0.601531	-0.819215
H	-1.321653	-1.097549	-2.240170
H	-0.429335	-1.756307	-0.798195
H	2.164141	-1.951145	-0.789774
H	4.339486	-0.817078	-1.103748
H	4.626998	1.532903	-0.376830
H	2.733740	2.740693	0.664720
H	0.573354	1.613158	0.990818
C	-2.482236	-0.170269	0.526972
H	-2.823800	-1.152503	0.849525
H	-2.269951	0.431699	1.416034
O	-3.507101	0.393000	-0.256239
C	-0.152988	-1.539787	1.659929
H	-0.220421	-0.766128	2.423286
H	-1.025302	-2.184737	1.704960
H	0.733831	-2.139677	1.838165
C	-3.537395	1.819988	-0.257347
H	-2.622718	2.250736	-0.673365
H	-4.377459	2.112083	-0.881710
H	-3.684549	2.205208	0.754901

7a (*6'*)

ΔG = -595.721721 hartree

C	-1.128505	0.076010	-0.267270
N	0.312775	0.345921	-0.442484
C	0.580352	1.465175	-1.410800
C	1.062127	0.517683	0.918171
O	0.727166	-0.541875	1.736165
C	-1.965249	1.074662	0.211358
C	-3.318176	0.796509	0.363194
C	-3.817922	-0.459619	0.036288
C	-2.964383	-1.446981	-0.441186

C	-1.608280	-1.182682	-0.593157
O	2.800717	-0.607105	-0.220558
C	4.179072	-0.796264	-0.526907
C	2.556353	0.485887	0.637970
H	0.747178	-0.493711	-0.835443
H	0.294239	2.408284	-0.958565
H	-0.009662	1.282504	-2.302431
H	1.635317	1.466296	-1.658629
H	0.750542	1.483544	1.311105
H	-0.098789	-0.366272	2.201886
H	-1.584893	2.054169	0.463800
H	-3.979295	1.565888	0.735505
H	-4.871971	-0.667866	0.154282
H	-3.347877	-2.424798	-0.695214
H	-0.939239	-1.949213	-0.960286
H	2.888563	1.427038	0.190173
H	3.064378	0.369303	1.599119
H	4.238966	-1.643597	-1.204323
H	4.750736	-1.012620	0.379047
H	4.596984	0.089171	-1.013459

7a (*7d'*)

ΔG = -326.923055 hartree

7d' and ***1d*** are the same structure

11a

ΔG = -559.344771 hartree

C	-1.204359	0.133631	0.050086
N	0.006192	0.820876	0.120888
C	0.012678	2.284451	0.138724
C	1.285599	2.907662	-0.426139
C	1.151634	0.159814	0.741696
C	2.149124	-0.416577	-0.260534
O	3.170636	-1.065566	0.476676
C	4.167723	-1.639329	-0.349484
C	-1.227508	-1.276099	-0.010709
C	-2.421172	-1.975573	-0.104551
C	-3.643106	-1.311175	-0.145522
C	-3.638301	0.076629	-0.080290
C	-2.450832	0.791015	0.023375
H	-0.816850	2.630127	-0.471359
H	1.451754	2.591499	-1.456336
H	2.171776	2.661428	0.157496
H	1.181274	3.993229	-0.416631
H	-0.159370	2.661226	1.156824
H	1.652523	-1.126686	-0.932637
H	3.744929	-2.399132	-1.016176
H	4.902121	-2.108264	0.302294
H	4.666201	-0.878777	-0.960675
H	2.573904	0.379527	-0.881889
H	0.809145	-0.643092	1.395470
H	1.671753	0.874562	1.381068
H	-0.304067	-1.834431	-0.006114
H	-2.389637	-3.056568	-0.154402
H	-4.571084	-1.860345	-0.223310
H	-4.573014	0.622792	-0.095556
H	-2.508675	1.864603	0.102394

11a (*11a)**

ΔG = -559.232571 hartree

C	1.085204	0.003425	-0.276495
N	-0.017772	0.755638	-0.598614
C	-0.052951	2.214408	-0.417643
C	-0.109395	2.664913	1.042784
C	-1.269154	0.118573	-0.990784
C	-2.231583	-0.151046	0.168567
O	-3.324266	-0.870981	-0.367610
C	-4.324492	-1.155463	0.596934
C	1.040023	-1.374880	-0.081243
C	2.187935	-2.116985	0.223103
C	3.471080	-1.410096	0.327887
C	3.550265	-0.060459	0.135073
C	2.401322	0.713502	-0.164400
H	0.813198	2.657708	-0.903725
H	0.779969	2.338419	1.580250
H	-0.987530	2.270222	1.552675
H	-0.155149	3.754084	1.082494
H	-0.929855	2.572912	-0.952257
H	-1.733278	-0.729455	0.954877
H	-3.926671	-1.766389	1.414222
H	-5.113974	-1.707243	0.091414
H	-4.743210	-0.235603	1.018888
H	-2.577204	0.789744	0.611624
H	-1.044945	-0.820701	-1.490747
H	-1.763437	0.766050	-1.714809
H	0.090242	-1.888528	-0.114783
H	2.128681	-3.174758	0.425214
H	4.368086	-1.974936	0.548615
H	4.512263	0.434519	0.182959
H	2.511831	1.716982	-0.538416

11a (*1*)

ΔG = -559.154837 hartree

C	-1.087641	0.080023	0.278825
N	-0.015184	0.852209	0.580613
C	-0.075633	2.327170	0.556670
C	0.397628	2.931670	-0.765537
C	1.280967	0.264506	0.943577
C	2.028896	-0.336056	-0.253502
O	3.210968	-0.889581	0.273579
C	4.070179	-1.416893	-0.729291
C	-1.046402	-1.334738	0.467463
C	-2.139358	-2.107386	0.162624
C	-3.305192	-1.522406	-0.344629
C	-3.362780	-0.138202	-0.544022
C	-2.286304	0.657250	-0.239129
H	-1.089602	2.634599	0.785508
H	-0.204009	2.579485	-1.601896

H	1.442408	2.700566	-0.963418
H	0.298550	4.014335	-0.699810
H	0.554938	2.668395	1.374228
H	1.420955	-1.102570	-0.746838
H	3.579483	-2.220170	-1.287438
H	4.945195	-1.815251	-0.221905
H	4.382669	-0.637261	-1.430738
H	2.254408	0.439267	-0.993244
H	1.136450	-0.500254	1.703687
H	1.884945	1.051680	1.382086
H	-0.167194	-1.806677	0.872090
H	-2.096996	-3.174623	0.323449
H	-4.160595	-2.138678	-0.580977
H	-4.258763	0.312153	-0.945415
H	-2.350473	1.716553	-0.420582

11a (*1_TS_2*)

ΔG = -709.660168 hartree

C	1.023291	-0.546497	0.411722
C	1.991477	0.097199	-0.374134
C	3.133177	-0.587398	-0.772592
C	3.327858	-1.916701	-0.420479
C	2.364242	-2.560776	0.349513
C	1.225065	-1.888990	0.764257
C	-0.073104	1.537522	0.973547
N	-0.119471	0.152610	0.869181
C	-1.402057	-0.547041	0.954803
H	1.857293	1.119026	-0.698688
H	3.865618	-0.074274	-1.381128
H	4.213492	-2.445814	-0.743676
H	2.502478	-3.592683	0.642353
H	0.514589	-2.406292	1.389948
H	0.934527	1.876658	1.228102
H	-0.097241	2.071647	-0.138158
H	-2.030693	-0.055850	1.690679
H	-1.241406	-1.562156	1.301972
O	1.397995	3.299817	-1.106618
O	0.164518	2.895107	-1.135932
C	-1.153286	2.250527	1.755957
H	-0.925038	3.314063	1.765392
H	-2.143505	2.125479	1.321986
H	-1.180261	1.898360	2.789298
C	-2.122957	-0.594967	-0.392616
H	-2.340619	0.419913	-0.747571
H	-1.489158	-1.082945	-1.142738
O	-3.318475	-1.321147	-0.196799
C	-4.089369	-1.444805	-1.381558
H	-4.982237	-2.012015	-1.128302
H	-4.384618	-0.463427	-1.767363
H	-3.535248	-1.976605	-2.162091

11a (*2*)

ΔG = -558.708364 hartree

C	1.097860	0.005499	-0.183896
N	-0.078859	0.739608	-0.388721
C	-0.134572	2.123503	-0.279538
C	0.468608	2.868033	0.866211
C	-1.275625	0.066537	-0.891760
C	-2.335523	-0.145932	0.184891
O	-3.465858	-0.729285	-0.435888
C	-4.525711	-0.979952	0.470831
C	1.056747	-1.342196	0.211461
C	2.229051	-2.061350	0.397509
C	3.471725	-1.464213	0.206021
C	3.521029	-0.131365	-0.192252
C	2.356346	0.595545	-0.391810
H	-0.997681	2.557540	-0.764577
H	1.518857	2.633909	1.040110
H	-0.059185	2.655498	1.808073
H	0.392536	3.940488	0.687788
H	-1.956096	-0.797916	0.981218
H	-4.219660	-1.676839	1.258739
H	-5.342325	-1.421473	-0.096553
H	-4.875666	-0.054242	0.940686
H	-2.601008	0.815297	0.641987
H	-0.997718	-0.888513	-1.332509
H	-1.706630	0.678656	-1.687510
H	0.108473	-1.827557	0.390608
H	2.167197	-3.096888	0.705832
H	4.382030	-2.027174	0.358957
H	4.476350	0.346415	-0.367469
H	2.409789	1.615179	-0.743226

11a (*3*)

ΔG = -709.755824 hartree

C	1.039190	-0.564443	0.047575
N	-0.016961	0.362867	0.053329
C	0.232655	1.722857	0.418816
O	0.711573	2.365519	-0.805307
O	1.173206	3.705951	-0.479999
C	-0.953032	2.474096	0.997806
C	-1.265071	0.032927	-0.636389
C	-2.338818	-0.562198	0.272692
O	-3.424339	-0.942720	-0.553467
C	-4.507211	-1.493706	0.175554
C	0.789442	-1.932540	-0.159299
C	1.821388	-2.861372	-0.140962
C	3.134856	-2.468929	0.087218
C	3.395879	-1.118054	0.283997
C	2.374772	-0.177459	0.256573
H	1.047001	1.750015	1.141122
H	2.132658	3.589491	-0.531800
H	-1.268766	2.008771	1.930671
H	-1.796867	2.508942	0.311822
H	-0.647016	3.495419	1.211495
H	-1.948802	-1.429970	0.817393
H	-4.203284	-2.393972	0.720875
H	-5.282004	-1.757216	-0.541402
H	-4.913939	-0.772354	0.892801

H	-2.666005	0.171585	1.017429
H	-1.055728	-0.671839	-1.440318
H	-1.656929	0.928666	-1.113432
H	-0.216477	-2.286354	-0.321068
H	1.585994	-3.905695	-0.299995
H	3.935015	-3.195657	0.104312
H	4.411105	-0.779522	0.445669
H	2.634957	0.862542	0.369829

11a (*3_TS_4*)

ΔG = -709.704542 hartree

C	1.472865	-0.181593	0.362143
C	1.841043	0.920558	-0.403466
C	3.125388	0.984566	-0.931456
C	4.029313	-0.045801	-0.700939
C	3.648362	-1.146087	0.061867
C	2.369005	-1.220371	0.596376
C	-1.679594	1.057988	1.967039
C	-0.322483	0.809588	1.565821
N	0.142015	-0.233102	0.918665
C	-0.700001	-1.393359	0.575157
O	-1.578466	2.507614	-0.178471
O	-2.110411	3.496856	-1.126675
H	1.117962	1.703302	-0.591446
H	3.412993	1.837529	-1.530425
H	5.027146	0.005891	-1.114076
H	4.350719	-1.946143	0.250034
H	2.081157	-2.067150	1.203162
H	-2.029998	1.777659	1.106761
H	0.409575	1.581526	1.758238
H	-2.410411	2.931604	-1.847261
H	-1.408342	-1.558015	1.381607
H	-0.057706	-2.266440	0.509925
H	-2.339269	0.197468	2.001739
C	-1.416641	-1.189448	-0.768912
H	-2.054122	-0.301437	-0.728565
H	-0.674345	-1.034111	-1.552216
O	-2.154231	-2.341330	-1.128388
H	-1.724331	1.642426	2.883000
C	-3.456935	-2.406725	-0.560781
H	-3.932784	-3.298094	-0.963459
H	-3.430931	-2.486992	0.529618
H	-4.048490	-1.528325	-0.836096

11a (*4*)

ΔG = -558.144391 hartree

C	-1.219621	0.150655	0.057774
N	0.022398	0.810024	0.138354
C	0.157544	2.121800	-0.285566
C	1.210757	2.934094	-0.125458
C	1.166065	0.144628	0.751954
C	2.171487	-0.388597	-0.265388
O	3.271643	-0.908065	0.458689
C	4.284550	-1.435450	-0.380110
C	-1.284458	-1.248477	-0.022130
C	-2.508457	-1.899532	-0.099088
C	-3.699082	-1.181502	-0.109974
C	-3.644087	0.205394	-0.026847
C	-2.426705	0.866657	0.067124
H	-0.698151	2.485620	-0.835483
H	1.165986	3.927963	-0.543577
H	2.117974	2.654708	0.388335
H	1.715586	-1.171503	-0.883463
H	3.906128	-2.262430	-0.990843
H	5.080594	-1.804445	0.263248
H	4.690528	-0.666723	-1.046673
H	2.496878	0.414799	-0.935398
H	0.807833	-0.669504	1.377152
H	1.671935	0.849720	1.413367
H	-0.378749	-1.835710	-0.042817
H	-2.525087	-2.979577	-0.163147
H	-4.649694	-1.692206	-0.175516
H	-4.557828	0.784971	-0.013936
H	-2.421821	1.940657	0.177010

11a (*4_TS_pre_b*)

ΔG = -708.444781 hartree

C	-0.839176	-0.503526	0.215851
N	0.042007	0.592453	0.513429
C	-0.186898	1.961805	-0.025183
C	-0.881061	2.167841	1.220040
C	1.415666	0.267109	0.933325
C	2.274878	-0.240102	-0.221368
O	3.567023	-0.469989	0.303111
C	4.474546	-0.969889	-0.666491
C	-1.276398	-1.319258	1.258335
C	-2.085606	-2.414416	0.988524
C	-2.470577	-2.693974	-0.319147
C	-2.037682	-1.875678	-1.356107
C	-1.218821	-0.782585	-1.095741
O	-1.709829	3.391460	-0.536095
O	-1.062559	2.161930	-1.065145
H	0.772610	2.466723	-0.142929
H	-1.886478	1.792380	1.283464
H	-0.390956	2.543746	2.106840
H	1.856110	-1.164185	-0.635558
H	4.131912	-1.926347	-1.074950
H	5.430433	-1.116103	-0.168601
H	4.603990	-0.261788	-1.491691
H	2.310479	0.502916	-1.027997
H	1.369416	-0.483442	1.719293
H	1.868653	1.161150	1.358134
H	-0.989399	-1.089216	2.275174
H	-2.423052	-3.042526	1.801447
H	-3.106330	-3.543512	-0.527450
H	-2.332204	-2.087699	-2.374790
H	-0.879526	-0.150431	-1.901594

11a (*pre_b*)

ΔG = -708.531484 hartree

C	0.899732	-0.497180	-0.288358
N	-0.107745	0.405214	-0.741008
C	0.009425	1.790663	-0.596483
C	1.355739	2.487861	-0.740226
C	-1.437229	-0.131506	-1.041531
C	-2.303433	-0.316582	0.201346
O	-3.534641	-0.878387	-0.212805
C	-4.434219	-1.091427	0.861406
C	1.223351	-1.608535	-1.074437
C	2.200885	-2.504286	-0.664021
C	2.889456	-2.299228	0.528134
C	2.579957	-1.192053	1.307945
C	1.585193	-0.302418	0.914435
O	1.192082	3.122419	0.550493
O	-0.053375	2.352638	0.804377
H	-0.790398	2.260522	-1.164316
H	2.220639	1.826878	-0.757028
H	1.418136	3.219913	-1.543537
H	-1.800850	-0.977779	0.918434
H	-4.015840	-1.783735	1.600163
H	-5.342652	-1.521799	0.445145
H	-4.681958	-0.151094	1.365809
H	-2.469531	0.648049	0.698279
H	-1.335750	-1.089764	-1.546045
H	-1.937812	0.544565	-1.734709
H	0.717396	-1.763603	-2.017271
H	2.435347	-3.357020	-1.287261
H	3.655823	-2.994244	0.842898
H	3.102611	-1.021968	2.239959
H	1.333375	0.539355	1.540746

11a (*11b*)

ΔG = -594.127285 hartree

11b and ***7c*** are the same structure

11a (*3_TS_c*)

ΔG = -709.690247 hartree

C	-1.157746	-0.289094	0.124270
C	-1.247424	-1.686828	0.325654
C	-2.432039	-2.361633	0.095594
C	-3.566151	-1.686956	-0.350341
C	-3.485411	-0.317755	-0.579860
C	-2.301962	0.372888	-0.378615
N	-0.007929	0.397778	0.476058
O	-0.472685	2.477698	-0.584503
O	1.371980	2.566457	-1.601287
H	-0.400279	-2.246696	0.685805
H	-2.469004	-3.428490	0.269485
H	-4.485307	-2.223516	-0.539078
H	-4.346033	0.220043	-0.954191
H	-2.243237	1.416401	-0.635216
H	1.249190	1.985472	0.055377
H	1.721040	2.867881	-2.458282
C	0.152609	1.842234	0.362924
C	0.021488	2.524564	1.763037
H	-1.013965	2.444058	2.088951
H	0.671032	2.049895	2.493534
H	0.294342	3.570548	1.655420
C	1.179939	-0.308233	0.949117
H	0.906319	-1.084650	1.660409
H	1.800347	0.409551	1.483432
C	2.010637	-0.896160	-0.191586
H	1.438430	-1.653363	-0.739805
H	2.280647	-0.103938	-0.899236
O	3.164048	-1.470619	0.390744
C	4.042712	-2.033319	-0.570016
H	4.892560	-2.444830	-0.029946
H	3.554302	-2.834675	-1.134620
H	4.398461	-1.274670	-1.275135

11a (*11c*)

ΔG = -633.436649 hartree

C	-1.094099	0.015292	0.114983
N	0.094556	0.814456	0.249807
C	0.053398	2.130500	-0.129437
O	-0.976278	2.641355	-0.559494
C	1.321217	2.946631	0.017052
C	1.279169	0.157197	0.807734
C	2.046868	-0.653687	-0.231290
O	3.128875	-1.275850	0.434606
C	3.919015	-2.078941	-0.425757
C	-1.807033	-0.356446	1.251228
C	-2.942409	-1.150505	1.132106
C	-3.373368	-1.568917	-0.122143
C	-2.662464	-1.192931	-1.257607
C	-1.523201	-0.405551	-1.140578
H	2.177971	2.474096	-0.461264
H	1.567707	3.096805	1.069147
H	1.145734	3.915332	-0.440400
H	1.391999	-1.405923	-0.687036
H	3.327721	-2.886839	-0.870119
H	4.717041	-2.510474	0.174594
H	4.359644	-1.483660	-1.232816
H	2.411451	-0.000267	-1.033973
H	0.959896	-0.507470	1.609751
H	1.938040	0.897138	1.251711
H	-1.474688	-0.020777	2.224481
H	-3.491872	-1.435781	2.019037
H	-4.257727	-2.184626	-0.214692
H	-2.991695	-1.516122	-2.235975
H	-0.966443	-0.112514	-2.019736

11a (*1_TS_5*)

ΔG = -709.486111 hartree

C	1.157166	-0.477445	0.097319

C	2.393470	-0.026666	0.599114
C	3.513879	-0.827111	0.503827
C	3.438694	-2.088596	-0.085366
C	2.223855	-2.538719	-0.588506
C	1.092763	-1.745826	-0.508284
C	-0.009996	1.511202	0.863022
N	-0.002081	0.318555	0.190932
C	-1.221820	-0.095305	-0.527923
H	2.502236	0.949286	1.041643
H	4.456004	-0.461366	0.885787
H	4.320703	-2.708970	-0.154808
H	2.151288	-3.513495	-1.048495
H	0.169767	-2.131224	-0.905411
H	0.780343	1.590718	1.598963
H	0.471038	2.406378	0.006888
H	-0.939085	-0.553011	-1.469727
H	-1.795431	0.795082	-0.757796
O	-0.188867	4.031688	-1.102183
O	0.805207	3.372713	-0.754501
C	-1.292255	2.201913	1.250120
H	-1.036885	3.083351	1.832158
H	-1.889612	2.525464	0.397856
H	-1.909204	1.551651	1.871959
C	-2.092388	-1.056156	0.291364
H	-1.532499	-1.958887	0.557411
H	-2.419967	-0.584414	1.223553
O	-3.191105	-1.363426	-0.533036
C	-4.131166	-2.224707	0.097465
H	-4.547646	-1.762660	0.997749
H	-4.930251	-2.401230	-0.618035
H	-3.671317	-3.179852	0.368627

11a (*5*)

ΔG = -558.584978 hartree

C	-0.963489	0.068958	0.138027
N	0.055158	1.096661	0.297715
C	-0.156987	2.335791	0.022749
C	-1.420901	2.931092	-0.433267
C	1.377803	0.650297	0.799968
C	2.155089	-0.132194	-0.253671
O	3.350304	-0.536605	0.374335
C	4.196822	-1.289084	-0.484097
C	-1.346682	-0.320941	-1.138468
C	-2.305999	-1.317195	-1.275381
C	-2.866423	-1.907902	-0.148674
C	-2.468910	-1.506401	1.122507
C	-1.508109	-0.514908	1.274444
H	0.692124	2.995047	0.158119
H	-2.259306	2.244091	-0.422894
H	-1.273933	3.317446	-1.446081
H	-1.629803	3.800822	0.193087
H	1.581217	-0.999837	-0.596768
H	3.701493	-2.203656	-0.824685
H	5.081093	-1.552917	0.090714
H	4.496392	-0.702042	-1.357868
H	2.361154	0.505144	-1.121906
H	1.201959	0.025418	1.672491
H	1.935950	1.530027	1.106880
H	-0.900409	0.138591	-2.008797
H	-2.610505	-1.629812	-2.264035
H	-3.612456	-2.682109	-0.260524
H	-2.906764	-1.961331	1.999534
H	-1.200027	-0.193737	2.259221

11a (*5_TS_6*)

ΔG = -634.999901 hartree

C	-1.334200	-0.075413	0.044379
C	-1.834552	-0.868454	1.069077
C	-3.125178	-1.377406	0.974725
C	-3.909071	-1.090763	-0.136666
C	-3.400251	-0.296219	-1.158683
C	-2.109085	0.211198	-1.075026
C	0.157266	1.907672	0.104982
O	0.649968	2.001487	1.540510
N	0.033251	0.426045	0.158344
C	1.032693	-0.399771	-0.586726
H	-0.827043	2.358065	0.068586
H	0.071089	2.527082	2.118027
H	0.402640	0.861441	1.457261
H	-1.219510	-1.086502	1.931184
H	-3.515835	-1.992284	1.773459
H	-4.913714	-1.483997	-0.206752
H	-4.005420	-0.071819	-2.025943
H	-1.716847	0.819662	-1.878551
H	1.246966	0.048466	-1.555712
H	0.570255	-1.365457	-0.767276
C	2.319227	-0.612209	0.201048
H	2.805534	0.339264	0.448977
H	2.095567	-1.125118	1.144933
O	3.160513	-1.398437	-0.612508
C	4.403459	-1.700805	0.004557
H	4.971954	-2.305137	-0.698175
H	4.964844	-0.788801	0.231611
H	4.258697	-2.266042	0.930752
C	1.133333	2.555553	-0.826934
H	1.165879	3.621010	-0.607297
H	2.136010	2.148608	-0.731997
H	0.790483	2.434535	-1.853919

11a (*6*)

ΔG = -635.018983 hartree

C	-1.131116	-0.033289	0.237191
N	0.036240	0.826618	0.554461
C	0.269365	1.948172	-0.523777
C	1.401305	2.858663	-0.111946
O	-0.902032	2.680440	-0.589867
C	1.264735	0.046687	0.990376
C	1.966669	-0.733971	-0.110948
O	3.121984	-1.258977	0.505157

C	3.886949	-2.082487	-0.366000
C	-2.114667	-0.166396	1.206400
C	-3.216340	-0.972183	0.947837
C	-3.327732	-1.629963	-0.271422
C	-2.336938	-1.481805	-1.234785
C	-1.227885	-0.680896	-0.986824
H	-0.241444	1.361111	1.379286
H	0.485860	1.418561	-1.447290
H	-1.543554	2.250147	-1.167697
H	2.358004	2.345150	-0.079348
H	1.201169	3.320821	0.854462
H	1.333819	-1.540296	-0.492520
H	1.468671	3.646576	-0.859111
H	3.306223	-2.945993	-0.704072
H	4.748837	-2.428023	0.199070
H	4.229772	-1.520435	-1.240061
H	2.241101	-0.088206	-0.953016
H	0.929293	-0.627864	1.773739
H	1.951784	0.764043	1.428740
H	-2.027454	0.349438	2.153726
H	-3.985317	-1.079266	1.699354
H	-4.186683	-2.254461	-0.472302
H	-2.420370	-1.988522	-2.185452
H	-0.469072	-0.576002	-1.747663

11a (*11d*)

ΔG = -480.757264 hartree

11d and ***7d*** are the same structure

11a (*1_TS_2'*)

ΔG = -709.657043 hartree

C	1.424517	0.221053	-0.005514
C	1.644721	-1.152930	-0.191100
C	2.926504	-1.622598	-0.446035
C	4.009870	-0.754072	-0.501186
C	3.797504	0.605008	-0.295782
C	2.522996	1.092727	-0.050203
C	-0.973066	-0.039511	-0.108547
N	0.125302	0.725964	0.222600
H	0.838245	-1.867146	-0.102924
H	3.076406	-2.685449	-0.580345
H	5.005481	-1.130354	-0.690642
H	4.627124	1.297709	-0.334876
H	2.388766	2.154772	0.079186
H	-0.785405	-0.706077	-0.954258
H	-1.134950	-0.979686	0.716567
O	-0.986475	-3.082061	0.384260
O	-1.236404	-2.135012	1.249587
C	-2.332508	0.620677	-0.213821
H	-2.644358	1.076111	0.732213
H	-2.292364	1.416692	-0.968912
O	-3.246585	-0.377413	-0.607290
C	-0.032696	1.971754	0.999085
H	-0.893318	1.845805	1.653148
H	0.835144	2.060897	1.647256
C	-4.568650	0.119222	-0.751484
H	-5.191739	-0.716167	-1.061229
H	-4.947291	0.519773	0.194428
H	-4.616714	0.905646	-1.511796
C	-0.197190	3.236298	0.155979
H	-1.098422	3.206831	-0.452803
H	-0.271810	4.095598	0.822961
H	0.651792	3.393417	-0.506980

11a (*2'*)

ΔG = -558.71099 hartree

C	-1.250967	-0.079869	0.110146
N	0.137280	0.048245	0.242022
C	0.976625	-0.987948	-0.116785
C	2.382819	-1.094072	0.315046
O	3.269739	-0.271388	-0.479031
C	4.621016	-0.406872	-0.076302
C	0.711962	1.327955	0.681847
C	1.058483	2.274760	-0.467098
C	-2.096721	1.045136	0.084043
C	-3.470165	0.898544	-0.046373
C	-4.050771	-0.360879	-0.160728
C	-3.224195	-1.479681	-0.129126
C	-1.849977	-1.350603	0.007739
H	0.574375	-1.719758	-0.797075
H	2.697157	-2.138677	0.213431
H	2.511125	-0.816509	1.369735
H	4.970947	-1.440311	-0.184567
H	4.763167	-0.102535	0.967456
H	5.219910	0.238014	-0.716634
H	0.015037	1.792749	1.376193
H	0.180862	2.538932	-1.056085
H	1.792739	1.811175	-1.123134
H	1.487663	3.194685	-0.066876
H	1.613725	1.108900	1.248197
H	-1.688997	2.041047	0.150707
H	-4.090301	1.785280	-0.066437
H	-5.121410	-0.467805	-0.265726
H	-3.652239	-2.471505	-0.197082
H	-1.241286	-2.239111	0.071539

11a (*3'*)

ΔG = -709.751971 hartree

C	1.461303	-0.083990	-0.100659
N	0.219389	0.540611	-0.248801
C	-0.981103	-0.041998	0.276099
C	-1.939698	-0.504524	-0.822376
O	-3.115577	-1.020055	-0.211631
C	-4.120746	-1.391476	-1.146785
O	-1.621113	0.947048	1.120043
O	-2.474731	0.257464	2.071870
C	0.113328	1.849835	-0.904935
C	0.425767	3.054670	-0.013609

C	2.649645	0.585961	-0.451366
C	3.886951	-0.033937	-0.336840
C	3.999413	-1.336614	0.132512
C	2.834276	-2.013550	0.473855
C	1.589708	-1.411094	0.355124
H	-0.740978	-0.881406	0.919548
H	-1.447181	-1.281106	-1.418206
H	-2.199265	0.325980	-1.485102
H	-3.757810	-2.177566	-1.814892
H	-4.437003	-0.532461	-1.745610
H	-4.967485	-1.766425	-0.577393
H	-3.126978	-0.151097	1.470554
H	0.759767	1.849666	-1.783560
H	1.425228	2.998631	0.415141
H	-0.289802	3.122716	0.803288
H	0.363904	3.970170	-0.604686
H	-0.903997	1.948869	-1.277075
H	2.620358	1.601797	-0.809270
H	4.773391	0.521404	-0.615146
H	4.965403	-1.812969	0.224299
H	2.883839	-3.035010	0.828362
H	0.721188	-2.000821	0.602970

11a (*3'_TS_4'*)

ΔG = -709.705637 hartree

C	1.358705	0.149815	-0.064027
C	1.742112	-1.124244	-0.513840
C	3.045362	-1.371358	-0.921461
C	4.014657	-0.374551	-0.877106
C	3.651872	0.880481	-0.405587
C	2.346677	1.145717	-0.008830
C	-2.398161	0.085234	-0.182551
C	-1.017375	-0.428351	-0.037074
N	0.034517	0.435471	0.320257
O	-1.539819	-1.316053	1.079960
O	-0.176906	-2.452610	1.757365
H	1.040965	-1.941729	-0.476218
H	3.306815	-2.366785	-1.256688
H	5.029675	-0.575731	-1.190418
H	4.385558	1.674249	-0.351520
H	2.105267	2.139407	0.332976
H	-2.586246	-0.823651	0.963580
H	-0.734817	-1.066516	-0.863989
H	0.219566	-1.750333	2.286587
H	-2.698856	1.022775	0.275091
O	-3.069058	-0.320232	-1.267385
C	-0.249629	1.563425	1.215540
H	0.600013	1.682042	1.886993
H	-1.086865	1.277255	1.852850
C	-4.472258	-0.004677	-1.289905
H	-4.622067	1.063745	-1.132709
H	-4.832353	-0.290994	-2.272310
H	-4.993339	-0.572747	-0.519145
C	-0.553400	2.892300	0.520358
H	-1.417382	2.816599	-0.139468
H	-0.769490	3.655085	1.269871
H	0.286823	3.237439	-0.079905

11a (*4'*)

ΔG = -558.145358 hartree

C	1.166750	-0.031279	-0.143846
N	-0.148064	0.422327	-0.279653
C	-1.213647	-0.477550	-0.210738
C	-2.478374	-0.196131	0.121202
O	-3.420846	-1.194711	0.136343
C	-4.730852	-0.771112	-0.231726
C	-0.438099	1.851154	-0.408815
C	-0.369241	2.624483	0.907675
C	2.264421	0.782776	-0.483560
C	3.564448	0.307955	-0.381109
C	3.827615	-0.982117	0.066829
C	2.753354	-1.786948	0.429223
C	1.447871	-1.324207	0.339599
H	-0.976960	-1.496735	-0.481706
H	-2.829952	0.783201	0.423924
H	-4.762848	-0.452395	-1.277039
H	-5.069526	0.052543	0.403226
H	-5.389673	-1.624602	-0.092836
H	0.243213	2.291045	-1.135929
H	0.629873	2.576656	1.341069
H	-1.074653	2.226581	1.637217
H	-0.612172	3.674072	0.736153
H	-1.431887	1.933816	-0.843808
H	2.114084	1.790940	-0.835355
H	4.380878	0.962564	-0.657825
H	4.842965	-1.344926	0.144910
H	2.927362	-2.787267	0.804460
H	0.647036	-1.966233	0.671944

11a (*4'_TS_pre_b'*)

ΔG = -708.456855 hartree

C	-1.253083	0.118998	-0.198706
N	-0.085021	0.826658	-0.541675
C	1.198078	0.202409	-0.738816
C	1.606980	-0.504720	0.513763
O	2.708337	-0.256741	1.062126
C	3.138090	-0.981731	2.264199
C	-0.125218	2.282116	-0.747718
C	0.282775	3.115147	0.466052
C	-2.347406	0.787654	0.374285
C	-3.508028	0.101106	0.705756
C	-3.613525	-1.268606	0.495181
C	-2.534525	-1.939518	-0.068913
C	-1.374723	-1.263292	-0.423083
O	2.670180	-1.088000	-1.904402
O	1.230869	-0.772676	-1.731960
H	1.935651	0.976761	-0.958381
H	0.966933	-1.275405	0.937868
H	4.070019	-1.467560	1.998038

H	2.375573	-1.698984	2.551690
H	3.294465	-0.228104	3.027699
H	0.535547	2.508790	-1.584799
H	0.219102	4.176713	0.222866
H	1.310821	2.901709	0.760907
H	-0.362616	2.922503	1.322630
H	-1.130642	2.546158	-1.069369
H	-2.296232	1.845360	0.579981
H	-4.331644	0.648247	1.145364
H	-4.517138	-1.799757	0.759960
H	-2.595581	-3.003482	-0.257092
H	-0.570686	-1.797604	-0.903753

11a (*pre_b'*)

ΔG = -708.546438 hartree

C	-1.256722	0.114177	-0.168690
N	-0.178794	0.955179	-0.510452
C	1.127293	0.488572	-0.713372
C	1.790139	-0.582279	0.151199
O	2.901563	-0.101770	0.799498
C	3.510615	-1.018618	1.716930
C	-0.380743	2.408218	-0.640385
C	-0.034116	3.209871	0.612646
C	-2.393387	0.634701	0.469838
C	-3.464581	-0.185231	0.800310
C	-3.435893	-1.545615	0.518285
C	-2.315153	-2.069964	-0.115132
C	-1.243730	-1.258589	-0.465407
O	2.085244	-1.359063	-1.045847
O	1.337908	-0.395820	-1.894094
H	1.790370	1.345499	-0.806142
H	1.155441	-1.163446	0.822415
H	4.282393	-0.464723	2.243590
H	3.964457	-1.857716	1.187526
H	2.775680	-1.392073	2.433420
H	0.232597	2.751171	-1.474011
H	-0.209379	4.271834	0.433976
H	1.015897	3.083598	0.879373
H	-0.636480	2.903971	1.467448
H	-1.414540	2.580976	-0.932216
H	-2.445544	1.680987	0.727067
H	-4.323835	0.249801	1.293693
H	-4.269943	-2.181470	0.780807
H	-2.273805	-3.123325	-0.359948
H	-0.411800	-1.689577	-0.997630

11a (*11b'*)

ΔG = -479.597498 hartree

11b' and ***2b*** are the same structure

11a (*3'_TS_c'*)

ΔG = -709.678479 hartree

C	-1.267314	0.138850	0.034809
C	-2.457601	0.798570	0.375777
C	-3.688341	0.323105	-0.058276
C	-3.773464	-0.819056	-0.843718
C	-2.599338	-1.479061	-1.187805
C	-1.362899	-1.014026	-0.760979
N	-0.023188	0.650062	0.477668
O	1.146802	-1.384343	0.571208
O	0.422193	-2.037864	2.365747
H	-2.437570	1.687675	0.985062
H	-4.585451	0.857091	0.225824
H	-4.732524	-1.186379	-1.181710
H	-2.637728	-2.369712	-1.801207
H	-0.477819	-1.559051	-1.035140
H	1.897615	0.420050	1.158555
H	-0.438117	-2.173726	1.952875
C	1.121945	-0.123813	0.614109
C	2.237887	-0.189729	-1.199834
H	1.578432	-0.797953	-1.797939
H	2.148437	0.890025	-1.266139
O	3.435293	-0.698181	-1.048089
C	0.074409	2.052915	0.914380
H	-0.638039	2.234625	1.719754
H	1.060209	2.176255	1.357430
C	4.447337	0.122274	-0.428215
H	4.367739	0.030318	0.653617
H	5.402386	-0.267908	-0.763124
H	4.331460	1.160814	-0.734040
C	-0.108960	3.072218	-0.206076
H	-1.088443	2.990855	-0.674435
H	-0.013479	4.079434	0.200682
H	0.648937	2.946777	-0.979700

11a (*11c'*)

ΔG = -633.43143 hartree

C	-1.284918	0.016442	0.118504
N	0.083874	0.436624	0.247359
C	1.073033	-0.486523	0.061915
C	2.509711	0.020491	0.199823
O	3.398598	-1.017459	-0.123051
C	4.753767	-0.617210	0.001239
O	0.838459	-1.661333	-0.184650
C	0.316758	1.862346	0.537056
C	0.206989	2.759023	-0.692948
C	-2.081274	-0.088340	1.255426
C	-3.414526	-0.465728	1.138885
C	-3.954143	-0.746101	-0.111846
C	-3.156250	-0.644608	-1.247148
C	-1.825062	-0.260949	-1.134179
H	2.674380	0.363313	1.230272
H	2.668652	0.884347	-0.456839
H	4.988836	-0.314696	1.027539
H	4.988875	0.215629	-0.670351
H	5.366755	-1.474732	-0.266786
H	-0.417725	2.165007	1.282871
H	-0.779372	2.679274	-1.149522

H	0.952842	2.496083	-1.443385
H	0.363464	3.799569	-0.406165
H	1.289926	1.975468	1.006056
H	-1.654956	0.120928	2.227355
H	-4.028016	-0.546255	2.026069
H	-4.990432	-1.042483	-0.201516
H	-3.570318	-0.860583	-2.222803
H	-1.200998	-0.179971	-2.013073

11a (*1_TS_5'*)

ΔG = -709.462576 hartree

C	1.224919	-0.217979	0.114765
C	1.783827	0.533705	1.161316
C	3.120269	0.885962	1.117527
C	3.913778	0.498909	0.041017
C	3.363556	-0.255860	-0.992206
C	2.030494	-0.623091	-0.960254
C	-1.061737	0.295841	0.660811
N	-0.140464	-0.571679	0.159310
H	1.192954	0.791505	2.027002
H	3.547950	1.447898	1.935217
H	4.958007	0.775795	0.011543
H	3.974329	-0.553076	-1.832424
H	1.617353	-1.183646	-1.783440
H	-0.628197	1.155126	1.164434
H	-1.541172	0.955479	-0.370557
O	-3.318504	1.111241	-1.466084
O	-2.179607	1.574935	-1.305610
C	-2.358793	-0.177632	1.287728
H	-3.018935	-0.666648	0.561014
H	-2.133300	-0.909543	2.075401
O	-2.965166	0.976824	1.810506
C	-0.566523	-1.881548	-0.384406
H	-1.647139	-1.868719	-0.463411
H	-0.172348	-1.971424	-1.392941
C	-4.243044	0.719083	2.385220
H	-4.617818	1.669251	2.755658
H	-4.935595	0.321306	1.638311
H	-4.164652	0.011223	3.215113
C	-0.092549	-3.040814	0.489112
H	-0.455199	-3.968619	0.049284
H	0.993630	-3.084518	0.536675
H	-0.486372	-2.962863	1.500918

11a (*5'*)

ΔG = -558.577137 hartree

C	-1.249222	-0.047874	0.075134
N	0.119122	0.410454	0.216498
C	1.088961	-0.350814	-0.145281
C	2.534515	-0.073874	0.049542
O	3.228007	-1.229646	-0.338187
C	4.641319	-1.089583	-0.220560
C	0.353890	1.746676	0.849075
C	0.682055	2.848016	-0.152065
C	-2.216378	0.807009	-0.442073
C	-3.519424	0.347186	-0.573814
C	-3.852544	-0.946129	-0.184804
C	-2.879092	-1.785128	0.344288
C	-1.571381	-1.338659	0.481372
H	0.835395	-1.286956	-0.625958
H	2.727834	0.187901	1.100429
H	2.829721	0.797142	-0.551567
H	4.932210	-0.895465	0.815615
H	5.008963	-0.277816	-0.854483
H	5.076562	-2.029527	-0.547702
H	-0.546199	1.976912	1.408854
H	-0.130628	3.017342	-0.854434
H	1.586507	2.634847	-0.717593
H	0.845446	3.769093	0.405612
H	1.164153	1.615903	1.563420
H	-1.964241	1.807399	-0.757732
H	-4.272889	1.002972	-0.986102
H	-4.870425	-1.295358	-0.285973
H	-3.134959	-2.784441	0.666282
H	-0.821548	-1.976906	0.926455

11a (*5'_TS_6'*)

ΔG = -634.965893 hartree

C	1.251261	0.065518	0.181521
C	2.329436	0.379690	1.001911
C	3.550926	-0.252289	0.805515
C	3.693374	-1.200915	-0.201290
C	2.611581	-1.511782	-1.016646
C	1.388908	-0.874755	-0.834007
C	-1.216675	-0.080923	0.496462
O	-1.466743	0.252319	1.955222
N	-0.007633	0.763527	0.413785
H	-0.953388	-1.129702	0.436913
H	-1.457178	-0.521537	2.543239
H	-0.439767	0.782874	1.761626
H	2.211986	1.108697	1.792024
H	4.386166	-0.009077	1.447314
H	4.642812	-1.696487	-0.348739
H	2.715854	-2.245529	-1.803659
H	0.560342	-1.111751	-1.486622
C	-2.467943	0.249781	-0.294363
H	-2.763703	1.282454	-0.119354
H	-2.262085	0.119554	-1.359825
O	-3.531801	-0.567916	0.132398
C	-0.092984	2.119452	-0.230627
H	-1.015215	2.583172	0.112017
H	0.725509	2.687328	0.205894
C	-3.626651	-1.824747	-0.538193
H	-2.756256	-2.458968	-0.350783
H	-4.510537	-2.319251	-0.144315
H	-3.739764	-1.681903	-1.615811
C	0.009289	2.143613	-1.747868
H	-0.028173	3.182102	-2.076482
H	0.950345	1.718549	-2.092226

H	-0.808290	1.613699	-2.233157

11a (*6'*)

ΔG = -635.020337 hartree

C	-1.346973	0.279774	0.045209
N	0.007312	0.874635	-0.024264
C	0.878227	0.165070	-1.144220
O	1.804028	1.068294	-1.608542
C	0.656049	1.072972	1.343212
C	1.514799	-1.134776	-0.678007
C	1.697375	2.176225	1.361439
C	-1.620729	-0.770574	0.909343
C	-2.898936	-1.318065	0.916766
C	-3.883832	-0.818427	0.073361
C	-3.594521	0.237258	-0.783521
C	-2.320721	0.790790	-0.802331
O	2.704431	-0.799541	0.004997
C	3.555721	-1.916811	0.256149
H	-0.108598	1.813045	-0.411144
H	2.655518	0.855088	-1.193739
H	0.138132	-0.026062	-1.916135
H	-0.166165	1.321547	2.008012
H	0.835243	-1.721718	-0.055147
H	1.734476	-1.721809	-1.575482
H	1.301530	3.107823	0.956536
H	2.603326	1.911479	0.825404
H	1.967031	2.356742	2.401509
H	1.077544	0.121486	1.646458
H	-0.870232	-1.159942	1.579891
H	-3.119620	-2.135117	1.588690
H	-4.875846	-1.247370	0.087211
H	-4.357187	0.636081	-1.436948
H	-2.097367	1.613450	-1.468808
H	3.841024	-2.403393	-0.679876
H	3.061574	-2.643181	0.905431
H	4.442019	-1.531231	0.751948

11a (*11d'*)

ΔG = -366.227438 hartree

11d' and ***2d*** are the same structure

13a

ΔG = -518.857166 hartree

C	0.838233	0.006719	-0.058867
C	1.578459	1.186014	-0.265146
C	2.963896	1.177660	-0.231353
C	3.667921	-0.000898	0.004303
C	2.950579	-1.171362	0.209197
C	1.559312	-1.173346	0.187179
O	-3.393524	-0.036834	0.213411
C	-2.713090	1.197312	0.014593
C	-1.277661	1.126789	0.507176
N	-0.563286	0.022713	-0.143619
C	-1.280620	-1.240432	-0.001086
C	-2.719789	-1.086223	-0.471009
H	1.069829	2.114078	-0.479909
H	3.498454	2.103369	-0.401482
H	4.748894	-0.003197	0.025846
H	3.471734	-2.100440	0.401513
H	1.042852	-2.101898	0.373004
H	-3.263061	1.954846	0.570815
H	-2.727981	1.460495	-1.050434
H	-1.275103	0.991238	1.598730
H	-0.790960	2.072954	0.290230
H	-1.271981	-1.594887	1.040525
H	-0.803901	-2.001245	-0.617225
H	-3.275769	-2.001239	-0.272837
H	-2.735243	-0.891787	-1.550656

13a (*13a)**

ΔG = -518.742477 hartree

C	-0.824093	0.065138	0.085410
C	-1.510773	-1.242037	-0.188583
C	-2.920934	-1.232317	-0.302458
C	-3.644458	-0.085017	-0.137293
C	-2.977966	1.198012	0.143860
C	-1.586595	1.220907	0.234671
O	3.388545	-0.014384	0.016191
C	2.641753	-1.223952	-0.042094
C	1.301121	-1.076701	0.660630
N	0.548170	0.053613	0.109848
C	1.323365	1.289444	0.072838
C	2.671288	1.046472	-0.599544
H	-0.941945	-2.071779	-0.579085
H	-3.429071	-2.156219	-0.550115
H	-4.722942	-0.110079	-0.226183
H	-3.562429	2.087017	0.321867
H	-1.095002	2.152259	0.479254
H	3.236466	-1.989812	0.452103
H	2.486717	-1.517105	-1.087234
H	1.469485	-0.894545	1.729414
H	0.717751	-1.987678	0.573266
H	1.478457	1.663199	1.091609
H	0.775493	2.040111	-0.490275
H	3.287113	1.939950	-0.515281
H	2.518109	0.824767	-1.662426

13a (*1*)

ΔG = -518.665160 hartree

C	-0.788272	0.021608	0.208203
C	-1.450216	-1.217997	-0.026380
C	-2.800453	-1.246441	-0.279963
C	-3.547662	-0.064541	-0.297883
C	-2.917393	1.159982	-0.057287
C	-1.566441	1.215444	0.188454
O	3.271236	-0.022675	-0.329151
C	2.503035	-1.210052	-0.303764

C	1.380898	-1.103254	0.738899
N	0.547860	0.067996	0.458281
C	1.351184	1.291470	0.401974
C	2.475304	1.103998	-0.634226
H	-0.899594	-2.142727	-0.044106
H	-3.283003	-2.193519	-0.472592
H	-4.609872	-0.098350	-0.492440
H	-3.494814	2.072896	-0.051360
H	-1.115819	2.168258	0.408008
H	3.167711	-2.023585	-0.023938
H	2.075889	-1.418280	-1.289839
H	1.825230	-0.945170	1.722865
H	0.794196	-2.010275	0.771520
H	1.786285	1.459643	1.387260
H	0.749739	2.145163	0.122072
H	3.121072	1.978339	-0.606910
H	2.038164	1.011733	-1.633460

13a (*1_TS_2*)

ΔG = -669.168235 hartree

C	1.048959	-0.402205	0.096741
C	1.557850	0.904448	0.034401
C	2.930164	1.107405	-0.018643
C	3.811941	0.032475	-0.028702
C	3.306216	-1.262719	0.022604
C	1.939309	-1.485632	0.085630
O	-3.190771	-1.014941	0.047789
C	-2.585303	-0.116566	0.970801
C	-1.208433	0.363259	0.570639
N	-0.333592	-0.628722	0.186303
C	-0.925987	-1.902200	-0.240660
C	-2.289598	-1.641390	-0.859296
H	0.896335	1.759291	0.005155
H	3.308886	2.119190	-0.071115
H	4.878559	0.200531	-0.080914
H	3.979010	-2.109420	0.023496
H	1.571678	-2.497890	0.157056
H	-2.498498	-0.607325	1.948427
H	-3.244211	0.742498	1.088287
H	-0.783854	1.085313	1.277698
H	-1.365570	1.226159	-0.318544
H	-1.015746	-2.579827	0.612558
H	-0.282134	-2.367150	-0.982404
H	-2.743000	-2.585866	-1.154530
H	-2.166493	-1.022661	-1.754300
O	-0.854080	3.269844	0.020884
O	-1.418966	2.427219	-0.800684

13a (*2*)

ΔG = -518.219709 hartree

C	-0.829320	0.010631	-0.010609
C	-1.559029	-1.174128	-0.212903
C	-2.946910	-1.163094	-0.181177
C	-3.649795	0.016545	0.040954
C	-2.933766	1.194236	0.238772
C	-1.547565	1.199230	0.216500
O	3.404203	-0.034747	-0.234034
C	2.732722	1.219146	-0.067622
C	1.289257	1.136118	-0.410990
N	0.568358	0.018394	-0.037570
C	1.306542	-1.249116	0.005951
C	2.726070	-1.033974	0.511911
H	-1.049736	-2.104002	-0.413383
H	-3.481449	-2.090033	-0.343453
H	-4.730665	0.018707	0.061557
H	-3.458644	2.122245	0.425077
H	-1.018346	2.120831	0.407268
H	3.231754	1.941228	-0.711802
H	2.885966	1.544586	0.977976
H	0.746836	2.012436	-0.719707
H	1.335890	-1.699147	-0.991929
H	0.798487	-1.937858	0.678165
H	3.292204	-1.957910	0.407322
H	2.706330	-0.755437	1.573444

13a (*3*)

ΔG = -669.258499 hartree

C	1.035819	-0.278974	-0.059314
C	1.595679	0.757791	0.692133
C	2.977392	0.896489	0.785459
C	3.825939	0.003624	0.144164
C	3.274825	-1.032001	-0.605625
C	1.898423	-1.167672	-0.711953
O	-3.105278	-0.911884	0.518358
C	-2.704767	0.275931	-0.138415
C	-1.238478	0.630913	0.126821
N	-0.371356	-0.479168	-0.200176
C	-0.846002	-1.756127	0.375251
C	-2.307046	-2.000572	0.062790
O	-0.858815	1.684837	-0.775049
O	-1.427720	2.916341	-0.269989
H	0.966490	1.465990	1.209182
H	3.387232	1.709206	1.370748
H	4.898849	0.115201	0.219818
H	3.918824	-1.731233	-1.122479
H	1.482781	-1.959556	-1.320018
H	-3.339669	1.081402	0.222473
H	-2.832053	0.177923	-1.223204
H	-1.116527	0.996538	1.154891
H	-0.639474	3.360671	0.075840
H	-0.707394	-1.754831	1.465033
H	-0.249238	-2.567754	-0.033315
H	-2.654970	-2.891125	0.582954
H	-2.451558	-2.139018	-1.015118

13a (*3_TS_4*)

ΔG = -669.207477 hartree

C	-1.046785	-0.283592	-0.005464

C	-1.671024	0.953034	-0.226423
C	-3.053008	1.033228	-0.320821
C	-3.849245	-0.100135	-0.181438
C	-3.235919	-1.321765	0.062085
C	-1.851002	-1.421530	0.146253
O	3.077286	-1.035205	-0.495069
C	2.529607	0.072954	-1.022522
C	1.161161	0.513637	-0.669794
N	0.358681	-0.374699	0.069226
C	0.958591	-1.630571	0.521165
C	2.447072	-1.474649	0.726207
O	1.830753	1.658757	0.120149
O	0.610091	2.874741	0.885610
H	-1.070353	1.851576	-0.246647
H	-3.511946	1.999486	-0.486086
H	-4.926068	-0.028609	-0.248823
H	-3.833463	-2.216181	0.180329
H	-1.411365	-2.391530	0.318423
H	2.936707	0.337700	-1.989316
H	2.866984	1.256936	-0.226944
H	0.609604	0.995798	-1.467366
H	0.479333	2.330271	1.671411
H	0.782754	-2.435885	-0.199678
H	0.506762	-1.927271	1.468044
H	2.904448	-2.428171	0.969683
H	2.674106	-0.751233	1.511383

13a (*4*)

ΔG = -517.661453 hartree

N	-0.601185	-0.000517	-0.152244
C	-1.354341	1.153888	-0.370904
C	-2.691386	1.162163	-0.309911
C	-1.382816	-1.227426	-0.100912
C	-2.683241	-0.965767	0.654260
O	-3.450495	0.078274	0.049114
C	3.606464	0.025415	0.104200
C	2.920480	-1.145280	-0.200953
C	1.535166	-1.160626	-0.292825
C	0.787544	0.007989	-0.064372
C	1.488488	1.185910	0.252426
C	2.873976	1.187657	0.326136
H	-0.829411	2.044864	-0.672138
H	-3.279356	2.029544	-0.562884
H	-2.457801	-0.688998	1.687619
H	-3.311548	-1.853326	0.652722
H	-0.829645	-1.999666	0.428365
H	-1.606614	-1.594869	-1.107475
H	4.685557	0.032258	0.168768
H	3.466849	-2.061384	-0.384598
H	1.039370	-2.080108	-0.565363
H	0.949481	2.096202	0.468748
H	3.383372	2.109372	0.576167

13a (*4_TS_pre_b*)

ΔG = -667.975090 hartree

C	-1.149742	-0.187413	0.001999
C	-1.638512	1.126022	0.085840
C	-3.003298	1.370802	0.048329
C	-3.914654	0.323723	-0.052428
C	-3.435275	-0.978400	-0.118740
C	-2.069891	-1.239489	-0.097793
O	2.991384	-0.931121	-0.361939
C	2.457796	0.111171	-0.822185
C	1.123964	0.607441	-0.365030
N	0.230056	-0.428026	0.031413
C	0.751402	-1.781451	0.154724
C	2.191696	-1.745297	0.591075
O	1.621259	1.358742	0.730894
O	2.391622	2.476702	0.088224
H	-0.951788	1.950704	0.211002
H	-3.355415	2.391654	0.115870
H	-4.977530	0.520076	-0.072358
H	-4.125745	-1.807633	-0.198749
H	-1.731817	-2.261776	-0.175070
H	3.077549	0.700357	-1.481377
H	0.684111	1.281653	-1.099906
H	0.661597	-2.347973	-0.779073
H	0.199888	-2.323603	0.923035
H	2.660721	-2.721180	0.569210
H	2.332987	-1.263325	1.555340

13a (*pre_b*)

ΔG = -668.059220 hartree

C	-1.208780	0.111024	0.023011
C	-1.777851	-1.170604	-0.039141
C	-3.155718	-1.333485	-0.013790
C	-4.003601	-0.232396	0.049187
C	-3.446498	1.040022	0.084280
C	-2.068235	1.217492	0.073536
O	2.886813	0.876453	0.588672
C	2.476548	-0.425330	0.780200
C	1.037328	-0.764611	0.368947
N	0.184337	0.285165	0.020009
C	0.756846	1.596189	-0.301095
C	2.250269	1.494942	-0.542203
O	1.607860	-1.543394	-0.771780
O	2.972880	-1.347765	-0.217192
H	-1.148759	-2.043518	-0.137706
H	-3.566671	-2.333157	-0.063409
H	-5.076537	-0.364261	0.059234
H	-4.086542	1.911410	0.127983
H	-1.669291	2.219202	0.117578
H	2.797103	-0.720847	1.775830
H	0.546189	-1.461186	1.041969
H	0.578118	2.298986	0.517281
H	0.278075	1.996157	-1.196715
H	2.679872	2.488764	-0.629667
H	2.475799	0.930480	-1.447638

13a (*13b*)

ΔG = -668.218724 hartree

C	-1.202774	0.333210	0.070035
C	-1.987301	0.004297	1.176176
C	-3.108015	-0.800287	1.017773
C	-3.465193	-1.271346	-0.241949
C	-2.684899	-0.942519	-1.343875
C	-1.549578	-0.154884	-1.189592
O	2.449325	-0.281584	-0.241683
C	3.161249	-1.334108	-0.644921
N	-0.053214	1.168189	0.220979
C	0.114544	2.253703	-0.584466
C	0.951010	0.860135	1.241682
C	1.692165	-0.435548	0.983073
O	1.071553	3.010741	-0.562475
O	3.233163	-2.394992	-0.079649
H	-1.732512	0.384128	2.155409
H	-3.710113	-1.048995	1.881092
H	-4.341451	-1.893481	-0.361343
H	-2.946581	-1.312264	-2.325945
H	-0.924450	0.069157	-2.042536
H	3.679402	-1.088124	-1.578061
H	-0.731070	2.398583	-1.269692
H	0.479912	0.794139	2.222055
H	1.647141	1.693874	1.258754
H	1.015791	-1.281990	0.875613
H	2.376859	-0.641610	1.804644

13a (*3_TS_c*)

ΔG = -669.187013 hartree

C	0.957217	-0.183242	0.102100
C	1.837001	-0.943240	0.900216
C	3.200020	-0.922007	0.665220
C	3.730735	-0.149158	-0.364666
C	2.873449	0.614406	-1.150101
C	1.506830	0.616357	-0.921961
O	-2.980400	-1.072084	-0.510919
C	-2.438407	0.055216	-1.093672
N	-0.416467	-0.239366	0.324576
C	-1.053270	-1.421000	0.900682
C	-2.009033	-2.036957	-0.130792
O	-0.992910	1.894028	-0.571668
O	-1.148181	2.623968	1.548877
H	1.460687	-1.527341	1.725351
H	3.853594	-1.505938	1.298694
H	4.796878	-0.133873	-0.542754
H	3.271718	1.223550	-1.950220
H	0.861944	1.228028	-1.526095
H	-3.222953	0.781758	-1.268541
H	-1.863550	-0.160997	-1.995219
H	-2.006150	0.943583	0.837982
H	-0.801983	3.350102	2.092032
H	-1.607900	-1.152285	1.799851
H	-0.309059	-2.163046	1.163994
H	-2.549871	-2.870530	0.309614
H	-1.450405	-2.381835	-1.005140
C	-1.362168	0.782472	-0.064009

13a (*13c*)

ΔG = -592.945752 hartree

C	0.901571	-0.097631	0.020998
C	1.610744	-0.642564	-1.044540
C	3.001055	-0.639591	-1.023876
C	3.681898	-0.091872	0.058370
C	2.969599	0.451605	1.122655
C	1.579553	0.447418	1.107033
O	-3.280201	-0.203154	0.466927
C	-2.752703	0.916280	-0.220222
C	-1.232877	0.991511	-0.301528
N	-0.535418	-0.130007	0.011106
C	-1.183911	-1.375996	0.453080
C	-2.639923	-1.398479	0.039527
O	-0.707168	2.036874	-0.671604
H	1.073959	-1.061909	-1.884785
H	3.550526	-1.061325	-1.854518
H	4.763335	-0.088595	0.072513
H	3.494914	0.877775	1.966593
H	1.018622	0.866807	1.930978
H	-3.095176	1.810155	0.296992
H	-3.129008	0.956746	-1.250675
H	-1.097751	-1.466492	1.538768
H	-0.657677	-2.218091	0.002966
H	-3.152204	-2.229890	0.519017
H	-2.732716	-1.508982	-1.047156

13a (*1_TS_5*)

ΔG = -668.975566 hartree

C	1.273744	-0.153808	0.086147
C	1.717471	1.132305	0.442479
C	3.063412	1.435607	0.384558
C	3.990696	0.474540	-0.015909
C	3.555915	-0.798669	-0.368591
C	2.210082	-1.116373	-0.329121
O	-2.653061	-1.556668	0.612763
C	-2.359663	-0.296287	1.164848
C	-1.025288	0.293330	0.741747
N	-0.088095	-0.496777	0.145846
C	-0.551100	-1.725602	-0.538921
C	-2.060768	-1.744624	-0.661879
H	1.026253	1.906713	0.733916
H	3.391723	2.431239	0.645678
H	5.042370	0.719859	-0.055325
H	4.267076	-1.552247	-0.674428
H	1.902129	-2.114193	-0.593542
H	-2.334661	-0.406006	2.251566
H	-3.157426	0.424821	0.938159
H	-0.624909	1.000103	1.459716

H	-1.400666	1.186577	-0.155855
H	-0.218850	-2.578876	0.052892
H	-0.084559	-1.771077	-1.520303
H	-2.372790	-2.721496	-1.020910
H	-2.411139	-0.991426	-1.374587
O	-3.105036	2.299574	-0.622640
O	-1.903764	2.124711	-0.882630

13a (*5*)

ΔG = -518.090482 hartree

C	-0.856656	0.015420	-0.045989
C	-1.517837	1.104385	0.508801
C	-2.906501	1.100145	0.543862
C	-3.615665	0.018182	0.035405
C	-2.937499	-1.067813	-0.508914
C	-1.549928	-1.079254	-0.549446
O	3.369817	-0.136169	-0.223254
C	2.733895	1.063527	-0.575479
C	1.253386	1.012375	-0.545568
N	0.590306	0.012366	-0.090423
C	1.304189	-1.181878	0.444771
C	2.710948	-0.791531	0.855795
H	-0.960587	1.929526	0.929169
H	-3.429400	1.939321	0.979876
H	-4.696076	0.017833	0.067835
H	-3.486895	-1.908403	-0.908081
H	-1.023651	-1.916546	-0.983583
H	3.042695	1.332137	-1.588346
H	3.032187	1.902145	0.073589
H	0.700504	1.865392	-0.916283
H	1.315468	-1.942417	-0.333053
H	0.730418	-1.546966	1.292014
H	3.285428	-1.683842	1.087259
H	2.689248	-0.146733	1.739179

13a (*5_TS_6*)

ΔG = -594.474956 hartree

C	1.007514	0.094467	0.038701
C	1.821169	1.011322	0.692709
C	3.202192	0.903468	0.579134
C	3.763204	-0.116768	-0.180969
C	2.941322	-1.029812	-0.832356
C	1.559063	-0.924597	-0.730201
O	-3.238058	0.057317	-0.380380
C	-2.474163	-1.124825	-0.300848
C	-1.220880	-0.941616	0.518539
O	-1.571291	-0.412729	1.886764
N	-0.437902	0.256779	0.149072
C	-1.041741	1.022685	-0.979676
C	-2.522607	1.252262	-0.737764
H	-0.626427	-1.841654	0.621297
H	-1.186001	-0.931033	2.613609
H	-0.908418	0.463770	1.475393
H	1.377699	1.800708	1.283963
H	3.836625	1.614157	1.089986
H	4.837739	-0.200881	-0.265123
H	3.372320	-1.823870	-1.425846
H	0.926413	-1.632419	-1.248096
H	-2.174164	-1.499639	-1.286146
H	-3.101366	-1.881347	0.165840
H	-0.864509	0.483630	-1.911310
H	-0.529489	1.978918	-1.041628
H	-2.965831	1.667227	-1.643519
H	-2.664924	1.968762	0.073381

13a (*6*)

ΔG = -594.522869 hartree

C	1.035150	0.028577	-0.186257
C	1.893755	0.736172	-1.013029
C	3.264204	0.639693	-0.800667
C	3.756552	-0.155305	0.226945
C	2.879695	-0.857195	1.047396
C	1.508157	-0.770293	0.845214
O	-3.186854	-0.337828	0.034100
C	-2.351533	-0.151546	1.164322
C	-1.223751	0.792026	0.788616
O	-1.667499	2.024303	0.361317
N	-0.417681	0.143858	-0.422001
C	-1.045878	-1.149501	-0.894799
C	-2.546169	-0.987327	-1.077499
H	-0.493937	0.929125	1.579334
H	-2.548934	1.924927	-0.029218
H	-0.540184	0.836934	-1.162082
H	1.508145	1.353907	-1.813004
H	3.941048	1.187994	-1.440064
H	4.822545	-0.227866	0.390043
H	3.259123	-1.475025	1.848541
H	0.834908	-1.318092	1.488951
H	-1.974646	-1.090914	1.572916
H	-2.954656	0.328711	1.931564
H	-0.799541	-1.908709	-0.160660
H	-0.575027	-1.419864	-1.835553
H	-2.977424	-1.979753	-1.217221
H	-2.763919	-0.391998	-1.964336

13a (*13d*)

ΔG = -594.113926 hartree

C	1.838417	-0.165227	0.097365
C	2.716668	-1.265825	0.076627
C	4.074561	-1.087240	-0.125168
C	4.608201	0.187964	-0.312471
C	3.749004	1.279669	-0.289019
C	2.382559	1.117302	-0.083936
O	-2.339642	-0.413945	-0.401589
C	-3.594081	-1.026139	-0.278153
C	-4.775856	-0.087165	-0.270549
O	-4.709124	1.115886	-0.333918
N	0.485120	-0.375979	0.261099

C	-0.446761	0.692710	0.565377
C	-1.842965	0.161211	0.806213
H	-5.752655	-0.606383	-0.208625
H	0.231689	-1.282533	0.619092
H	2.316312	-2.262516	0.218145
H	4.724703	-1.952779	-0.135069
H	5.669143	0.323600	-0.470016
H	4.141626	2.278962	-0.428287
H	1.742324	1.987061	-0.068120
H	-3.665720	-1.657261	0.620337
H	-3.727752	-1.697449	-1.132765
H	-0.481691	1.402342	-0.264928
H	-0.145098	1.256694	1.457866
H	-2.484032	0.982239	1.133510
H	-1.833040	-0.599219	1.597508

43a

ΔG = -730.024786 hartree

C	2.832132	0.006411	0.058815
C	3.566876	-1.095617	0.534692
C	4.951930	-1.104383	0.494097
C	5.660026	-0.018002	-0.015156
C	4.947965	1.076169	-0.486309
C	3.556576	1.091517	-0.460265
N	-1.429826	0.014676	-0.150649
C	-0.712292	-1.192331	0.264552
C	0.712292	-1.192332	-0.264552
N	1.429826	0.014676	0.150649
C	0.716962	1.215840	-0.259876
C	-0.716961	1.215840	0.259877
C	-5.660026	-0.018002	0.015156
C	-4.947965	1.076169	0.486309
C	-3.556577	1.091518	0.460265
C	-2.832132	0.006411	-0.058815
C	-3.566876	-1.095616	-0.534692
C	-4.951930	-1.104384	-0.494097
H	3.052050	-1.942786	0.963873
H	5.483298	-1.966917	0.875218
H	6.740889	-0.027379	-0.041065
H	5.473065	1.930653	-0.893571
H	3.042909	1.952921	-0.857646
H	-1.217428	-2.075510	-0.112952
H	-0.691058	-1.262388	1.362241
H	0.691058	-1.262388	-1.362241
H	1.217427	-2.075511	0.112952
H	0.704045	1.321054	-1.355149
H	1.216159	2.089996	0.152948
H	-1.216158	2.089996	-0.152948
H	-0.704045	1.321054	1.355150
H	-6.740889	-0.027380	0.041065
H	-5.473066	1.930652	0.893570
H	-3.042910	1.952921	0.857646
H	-3.052049	-1.942785	-0.963872
H	-5.483297	-1.966918	-0.875218

43a (*43a)**

ΔG = -729.891979 hartree

C	-2.568212	0.020284	-0.352260
C	-3.163078	1.107524	0.296523
C	-4.530097	1.072188	0.639039
C	-5.293807	-0.066469	0.330578
C	-4.715732	-1.147385	-0.310312
C	-3.348993	-1.125446	-0.664608
N	1.221290	0.041894	0.734438
C	0.420297	1.236996	0.661881
C	-0.420297	1.236996	-0.661880
N	-1.221289	0.041893	-0.734437
C	-0.412431	-1.148152	-0.672438
C	0.412431	-1.148151	0.672439
C	5.293806	-0.066469	-0.330579
C	4.715732	-1.147385	0.310311
C	3.348994	-1.125445	0.664608
C	2.568213	0.020284	0.352260
C	3.163078	1.107524	-0.296523
C	4.530097	1.072187	-0.639040
H	-2.581712	1.975383	0.565800
H	-4.977172	1.914339	1.147175
H	-6.344598	-0.094890	0.590816
H	-5.313272	-2.012955	-0.563314
H	-2.931977	-1.932785	-1.245263
H	1.038793	2.125156	0.719826
H	-0.277265	1.242840	1.500495
H	0.277265	1.242840	-1.500494
H	-1.038794	2.125156	-0.719825
H	0.294663	-1.165383	-1.502176
H	-1.023734	-2.042199	-0.691836
H	1.023734	-2.042199	0.691837
H	-0.294662	-1.165383	1.502177
H	6.344597	-0.094890	-0.590817
H	5.313272	-2.012955	0.563314
H	2.931978	-1.932785	1.245263
H	2.581712	1.975383	-0.565800
H	4.977171	1.914338	-1.147176

43a (*1*)

ΔG = -729.840182 hartree

C	2.614114	0.021852	0.343630
C	3.213954	1.136685	-0.274358
C	4.544405	1.095354	-0.655198
C	5.315970	-0.040836	-0.430458
C	4.736158	-1.143012	0.192477
C	3.408830	-1.118353	0.579913
N	-1.237241	0.005902	-0.583062
C	-0.436304	1.203928	-0.575683
C	0.469330	1.231723	0.701343
N	1.278964	0.039932	0.744738
C	0.471101	-1.153414	0.766918
C	-0.440731	-1.193107	-0.517862
C	-5.364312	-0.035031	0.205871

C	-4.740565	-1.141657	-0.364325
C	-3.382061	-1.129564	-0.624374
C	-2.604156	0.002783	-0.310803
C	-3.245976	1.122275	0.252987
C	-4.606217	1.092943	0.507889
H	2.647948	2.030839	-0.480137
H	4.978931	1.959497	-1.138193
H	6.354735	-0.064005	-0.727531
H	5.326576	-2.026145	0.393239
H	3.002761	-1.971295	1.100374
H	-1.051915	2.093088	-0.619964
H	0.218415	1.194836	-1.448322
H	-0.176341	1.248135	1.579005
H	1.075736	2.128207	0.709060
H	-0.171586	-1.151562	1.646569
H	1.076104	-2.050716	0.767937
H	-1.061016	-2.078392	-0.457188
H	0.209833	-1.265217	-1.389256
H	-6.426530	-0.048250	0.404281
H	-5.319163	-2.016987	-0.624697
H	-2.933311	-1.982423	-1.109486
H	-2.688579	2.005980	0.520074
H	-5.075899	1.958149	0.954699

43a (*1_TS_2*)

ΔG = -880.342205 hartree

C	2.696610	-0.489901	0.139919
C	3.421951	0.693431	-0.070942
C	4.808110	0.650560	-0.134090
C	5.492758	-0.552847	-0.007930
C	4.773095	-1.726658	0.191546
C	3.388867	-1.703187	0.266600
C	-0.818044	0.546955	0.972049
C	0.616774	0.702326	0.515040
N	1.296130	-0.463068	0.241549
C	0.496381	-1.662411	-0.026686
C	-0.829749	-1.296714	-0.680431
H	2.917598	1.640145	-0.206502
H	5.353715	1.569334	-0.301720
H	6.571828	-0.577234	-0.068474
H	5.290754	-2.669929	0.300333
H	2.855598	-2.622513	0.454618
H	-0.795335	0.218731	2.021466
H	-1.272660	1.537361	0.961064
H	1.181583	1.405618	1.137208
H	0.597547	1.472380	-0.463787
H	0.320339	-2.205451	0.905566
H	1.047949	-2.311380	-0.700527
H	-1.395546	-2.219775	-0.798466
H	-0.638598	-0.897391	-1.684158
O	1.455623	3.426526	-0.344746
O	0.742929	2.612275	-1.073966
N	-1.579157	-0.365542	0.141563
C	-2.958641	-0.279898	0.071967
C	-3.683702	-0.944476	-0.936789
C	-3.689480	0.474083	1.011570
C	-5.068150	-0.859775	-0.989888
H	-3.168505	-1.513068	-1.695829
C	-5.073115	0.554046	0.937299
H	-3.181784	0.984878	1.815696
C	-5.780156	-0.111165	-0.058763
H	-5.592386	-1.380627	-1.780857
H	-5.602255	1.139600	1.678122
H	-6.858119	-0.047014	-0.108660

43a (*2*)

ΔG = -729.387508 hartree

C	-2.841077	0.015832	-0.018305
C	-3.546392	1.116702	0.502312
C	-4.931938	1.112538	0.545427
C	-5.660371	0.021281	0.078584
C	-4.970637	-1.071484	-0.436177
C	-3.583422	-1.080173	-0.492624
N	1.424795	-0.009247	-0.188094
C	0.719107	1.227623	0.177605
C	-0.719798	1.190732	-0.200325
N	-1.443740	0.023777	-0.063255
C	-0.711421	-1.217994	-0.310994
C	0.692365	-1.175246	0.279834
C	5.651538	0.007807	0.056533
C	4.925863	-1.069096	0.546415
C	3.535176	-1.078971	0.496694
C	2.824974	-0.006889	-0.067532
C	3.573380	1.079087	-0.558552
C	4.957715	1.082687	-0.494386
H	-3.006452	1.961659	0.902883
H	-5.446551	1.969207	0.960981
H	-6.740771	0.022990	0.116868
H	-5.515200	-1.928075	-0.811652
H	-3.084232	-1.934042	-0.924256
H	1.176508	2.082026	-0.312140
H	0.836648	1.392545	1.268744
H	-1.268248	2.114388	-0.260747
H	-0.647353	-1.408538	-1.387544
H	-1.247435	-2.043664	0.150755
H	1.201218	-2.080377	-0.042734
H	0.630379	-1.199059	1.378601
H	6.731810	0.013046	0.101087
H	5.439396	-1.913787	0.987406
H	3.012209	-1.926671	0.910958
H	3.070762	1.917376	-1.018070
H	5.499551	1.932644	-0.888759

43a (*3*)

ΔG = -880.426894 hartree

C	2.700957	-0.373416	-0.020008
C	3.472823	-1.396334	-0.581994
C	4.831891	-1.489206	-0.318900
C	5.456421	-0.553196	0.501091

C	4.699514	0.471503	1.054170
C	3.333351	0.561341	0.803854
N	-1.545846	-0.290213	0.084452
C	-0.848065	0.806918	-0.572617
C	0.607613	0.906965	-0.120879
O	1.283487	1.848743	-0.971863
O	0.870100	3.175694	-0.570517
N	1.303284	-0.343540	-0.320313
C	0.564073	-1.487737	0.250288
C	-0.880663	-1.549696	-0.213540
C	-5.769359	-0.143050	0.290552
C	-5.128079	-1.307512	-0.108339
C	-3.740596	-1.364497	-0.203576
C	-2.952091	-0.249807	0.117285
C	-3.612758	0.922616	0.524460
C	-4.995308	0.972140	0.604046
H	3.001787	-2.111650	-1.242484
H	5.407044	-2.288178	-0.767898
H	6.517540	-0.619230	0.698767
H	5.168900	1.208999	1.691999
H	2.773226	1.366060	1.255397
H	-1.327369	1.754587	-0.355520
H	-0.842875	0.669533	-1.663684
H	0.655454	1.278149	0.911660
H	1.661661	3.489091	-0.108231
H	0.580448	-1.435406	1.347630
H	1.070072	-2.403469	-0.043492
H	-1.364899	-2.358480	0.329306
H	-0.922907	-1.785371	-1.287023
H	-6.847612	-0.101996	0.358965
H	-5.707057	-2.185852	-0.363011
H	-3.281913	-2.281638	-0.539616
H	-3.039318	1.794290	0.805549
H	-5.471279	1.889149	0.926403

43a (*3_TS_4*)

ΔG = -880.370158 hartree

C	2.647076	-0.400640	-0.000181
C	3.525179	0.587878	0.473161
C	4.841383	0.273315	0.778116
C	5.330645	-1.019011	0.608315
C	4.474621	-1.994487	0.115915
C	3.148646	-1.698287	-0.183654
C	-0.829991	0.835380	0.601266
C	0.646388	0.942290	0.413572
N	1.302320	-0.095157	-0.291391
C	0.487713	-1.131840	-0.924832
C	-0.904808	-0.641981	-1.272338
O	0.401094	2.231047	-0.342860
O	2.041552	3.027804	-0.828042
H	3.186595	1.612211	0.522345
H	5.497070	1.057007	1.135585
H	6.359702	-1.254706	0.842283
H	4.830833	-3.005436	-0.033604
H	2.515884	-2.490470	-0.550662
H	-1.219397	1.173820	1.550122
H	-0.792659	2.035494	-0.114826
H	1.192847	1.207287	1.310912
H	2.150850	2.464396	-1.603527
H	0.392808	-2.004687	-0.270370
H	0.975908	-1.458948	-1.843175
H	-1.477981	-1.484916	-1.645572
H	-0.868147	0.123832	-2.053747
N	-1.555408	-0.119388	-0.073236
C	-2.959166	-0.208963	0.086855
C	-3.797570	-0.413435	-1.012910
C	-3.525315	-0.112268	1.363703
C	-5.171888	-0.521016	-0.833298
H	-3.390216	-0.472875	-2.010832
C	-4.898766	-0.208981	1.529152
H	-2.892900	0.010277	2.231218
C	-5.732001	-0.415951	0.433463
H	-5.805026	-0.677262	-1.696233
H	-5.317067	-0.137970	2.524050
H	-6.801524	-0.498067	0.567801

43a (*4*)

ΔG = -728.836181 hartree

C	-2.816285	0.023856	-0.052426
C	-3.519751	1.081150	0.554037
C	-4.905999	1.074088	0.603521
C	-5.638450	0.018330	0.068720
C	-4.951045	-1.034541	-0.525147
C	-3.564190	-1.036079	-0.595206
N	1.425063	0.028365	0.113274
C	0.671689	1.197972	0.027294
C	-0.671680	1.197977	-0.027302
N	-1.425063	0.028375	-0.113279
C	-0.659053	-1.176593	-0.391792
C	0.659044	-1.176599	0.391784
C	5.638450	0.018337	-0.068714
C	4.951051	-1.034538	0.525152
C	3.564196	-1.036085	0.595207
C	2.816285	0.023844	0.052422
C	3.519746	1.081145	-0.554033
C	4.905994	1.074093	-0.603514
H	-2.981932	1.897259	1.012923
H	-5.416705	1.900186	1.081367
H	-6.718515	0.016486	0.115009
H	-5.497057	-1.864478	-0.954775
H	-3.067507	-1.854501	-1.094141
H	1.204739	2.132223	0.060636
H	-1.204722	2.132233	-0.060649
H	-0.444685	-1.264642	-1.461747
H	-1.230180	-2.050196	-0.088617
H	1.230164	-2.050205	0.088606
H	0.444675	-1.264649	1.461738
H	6.718515	0.016502	-0.114999
H	5.497068	-1.864471	0.954781
H	3.067518	-1.854509	1.094145

H	2.981921	1.897253	-1.012914
H	5.416695	1.900196	-1.081355

43a (*4_TS_pre_b*)

ΔG = -879.152715 hartree

C	2.754312	-0.333540	0.001662
C	3.531572	0.834609	0.101967
C	4.898019	0.754676	0.324998
C	5.535838	-0.477444	0.439200
C	4.775471	-1.634653	0.329996
C	3.402512	-1.572838	0.119289
C	-0.759705	0.792905	0.426197
C	0.705389	0.974055	0.129240
N	1.377177	-0.246786	-0.220657
C	0.591566	-1.453829	-0.417588
C	-0.776606	-1.126886	-0.979104
O	0.707013	1.883892	-0.942307
O	0.177615	3.151610	-0.362805
H	3.066293	1.800603	-0.026832
H	5.471317	1.669891	0.395344
H	6.602768	-0.532377	0.604965
H	5.247503	-2.604518	0.418266
H	2.845149	-2.495085	0.061695
H	-1.253176	1.559476	0.999519
H	1.174292	1.448604	0.997178
H	0.476164	-2.025434	0.511585
H	1.087388	-2.100542	-1.140426
H	-1.389427	-2.020552	-1.021811
H	-0.702727	-0.689278	-1.973802
N	-1.462007	-0.140354	-0.103978
C	-2.892838	-0.225564	0.072880
C	-3.698875	-0.496143	-1.027536
C	-3.437494	-0.032810	1.337411
C	-5.075404	-0.553875	-0.854928
H	-3.268724	-0.638362	-2.007935
C	-4.815773	-0.093630	1.495290
H	-2.795793	0.138445	2.189775
C	-5.635192	-0.351619	0.402072
H	-5.708886	-0.752490	-1.707698
H	-5.244777	0.048748	2.476943
H	-6.707331	-0.401660	0.530309

43a (*pre_b*)

ΔG = -879.225356 hartree

C	-2.803703	-0.230332	-0.052497
C	-3.626928	0.881483	-0.294234
C	-4.978699	0.716299	-0.560695
C	-5.555118	-0.549792	-0.570459
C	-4.751902	-1.652000	-0.304823
C	-3.393935	-1.502742	-0.049690
N	1.394424	-0.067661	0.133504
C	0.754288	1.089683	-0.334861
C	-0.772648	1.099240	-0.189024
N	-1.431396	-0.074137	0.194408
C	-0.677266	-1.166009	0.818053
C	0.705553	-0.712255	1.253160
C	5.524611	-0.608727	-0.561160
C	4.714914	-1.686444	-0.213150
C	3.359747	-1.507881	0.023569
C	2.781451	-0.234661	-0.068144
C	3.604360	0.848469	-0.400222
C	4.957590	0.655543	-0.656601
O	-0.636359	2.135590	0.868112
O	0.810831	2.268607	0.562879
H	-3.221568	1.881862	-0.245586
H	-5.588003	1.591650	-0.743225
H	-6.610637	-0.672414	-0.769410
H	-5.179174	-2.646170	-0.300858
H	-2.797772	-2.382451	0.137753
H	1.134997	1.369341	-1.312878
H	-1.270031	1.551132	-1.042860
H	-0.571263	-1.997385	0.115622
H	-1.224648	-1.531362	1.688579
H	1.268134	-1.579495	1.580536
H	0.637445	-0.023542	2.100539
H	6.579085	-0.753693	-0.750806
H	5.136602	-2.680162	-0.139893
H	2.745186	-2.365707	0.256716
H	3.199182	1.849524	-0.439613
H	5.571594	1.508637	-0.913257

43a (*43b*)

ΔG = -879.380620 hartree

C	1.755207	0.200064	0.942253
C	2.237879	1.277964	1.680323
C	1.708976	1.549052	2.936528
C	0.706598	0.742761	3.465762
C	0.228261	-0.334939	2.728599
C	0.745793	-0.604256	1.467007
N	5.332458	-0.853852	-0.475039
C	6.037235	-1.347992	-1.530389
C	2.212093	0.826691	-1.362707
N	2.293236	-0.086836	-0.356988
C	2.874286	-1.406579	-0.610119
C	4.225183	-1.651369	0.069783
C	6.453997	2.781589	1.355684
C	6.152114	2.747254	-0.002003
C	5.777226	1.554735	-0.608232
C	5.708795	0.383719	0.143633
C	6.022317	0.414012	1.500855
C	6.386542	1.612039	2.104413
O	1.717688	1.938186	-1.282528
O	6.994175	-0.818674	-2.068781
H	3.022799	1.896774	1.271680
H	2.087352	2.388122	3.504498
H	0.300767	0.953190	4.445853
H	-0.555093	-0.963664	3.129463
H	0.357619	-1.432076	0.889928
H	5.650176	-2.323578	-1.861005

H	2.648001	0.447250	-2.298340
H	2.977558	-1.524802	-1.687552
H	2.182670	-2.177543	-0.270167
H	4.468220	-2.707362	-0.043703
H	4.149066	-1.458004	1.136699
H	6.740604	3.712469	1.825522
H	6.200754	3.652348	-0.592164
H	5.538810	1.529633	-1.661077
H	5.989247	-0.495765	2.084205
H	6.625389	1.626438	3.159105

43a (*3_TS_c*)

ΔG = -880.354576 hartree

C	2.400678	-0.305992	0.145085
C	3.191168	-1.321044	0.706788
C	4.501418	-1.512989	0.296068
C	5.066151	-0.693475	-0.676546
C	4.295911	0.322720	-1.227454
C	2.978402	0.520990	-0.829351
C	-0.692732	0.763482	-1.109331
N	1.068967	-0.151527	0.595351
C	0.215237	-1.328066	0.733096
C	-0.632464	-1.544243	-0.540870
O	0.864907	2.177453	0.219677
O	2.018952	2.681344	1.851250
H	2.787414	-1.948474	1.488212
H	5.086940	-2.300847	0.751014
H	6.089547	-0.841293	-0.992505
H	4.716833	0.972087	-1.983802
H	2.407816	1.321575	-1.266614
H	-1.242037	1.682371	-1.230153
H	0.127739	0.615449	-1.797630
H	-0.511518	1.030116	1.187384
H	2.784330	2.372168	1.354011
H	-0.433401	-1.202825	1.599918
H	0.820040	-2.212458	0.898435
H	-1.279953	-2.408694	-0.439580
H	0.032620	-1.717211	-1.387083
C	0.326931	1.062442	0.478990
N	-1.431199	-0.354158	-0.833099
C	-2.782964	-0.258023	-0.413542
C	-3.314222	-1.120481	0.551370
C	-3.620861	0.695980	-1.005927
C	-4.650024	-1.018624	0.918821
H	-2.697873	-1.863870	1.032065
C	-4.949453	0.794149	-0.623808
H	-3.245449	1.339559	-1.787864
C	-5.473703	-0.060879	0.341094
H	-5.041321	-1.690939	1.669921
H	-5.581703	1.532524	-1.097505
H	-6.512101	0.014489	0.631718

43a (*43c*)

ΔG = -804.114145 hartree

C	2.765015	-0.107452	0.020220
C	3.570981	-0.471663	-1.053609
C	4.949108	-0.554472	-0.888257
C	5.522012	-0.270739	0.346995
C	4.713103	0.093297	1.418844
C	3.334606	0.172467	1.258520
N	-1.468707	-0.082873	-0.069463
C	-0.802958	1.177713	-0.334595
C	0.717314	1.147711	-0.236682
O	1.322753	2.215035	-0.265896
N	1.338617	-0.054643	-0.147815
C	0.611802	-1.331569	-0.111688
C	-0.773432	-1.193983	-0.706790
C	-5.680847	-0.114110	0.313885
C	-4.939197	-1.283545	0.464346
C	-3.560374	-1.276643	0.326543
C	-2.868002	-0.089853	0.022436
C	-3.625783	1.082585	-0.131587
C	-5.008821	1.064005	0.019893
H	3.118597	-0.684419	-2.012861
H	5.573501	-0.835902	-1.725333
H	6.594215	-0.333172	0.474226
H	5.154122	0.313568	2.381570
H	2.699390	0.453233	2.087295
H	-1.123681	1.928144	0.385612
H	-1.032554	1.575136	-1.335159
H	0.545769	-1.684865	0.920520
H	1.183332	-2.063248	-0.681785
H	-1.309190	-2.123152	-0.549836
H	-0.701987	-1.032819	-1.792055
H	-6.756077	-0.124522	0.425957
H	-5.437357	-2.214443	0.702312
H	-3.018412	-2.197894	0.481293
H	-3.147798	2.017550	-0.378191
H	-5.560432	1.986659	-0.106285

43a (*1_TS_5*)

ΔG = -880.155785 hartree

C	-2.803649	-0.340524	-0.180798
C	-3.492165	0.830927	-0.527568
C	-4.876696	0.871157	-0.460483
C	-5.602048	-0.241571	-0.046940
C	-4.921419	-1.403054	0.300666
C	-3.536442	-1.460357	0.236519
C	0.732939	0.055483	-1.366587
C	-0.651746	0.515878	-0.988201
N	-1.402680	-0.397913	-0.264349
C	-0.643794	-1.408314	0.469677
C	0.691574	-0.851643	0.942707
H	-2.953353	1.718985	-0.820043
H	-5.389238	1.786610	-0.722895
H	-6.680927	-0.202613	0.006048
H	-5.469314	-2.279911	0.617588
H	-3.038176	-2.384604	0.486338
H	0.696503	-0.793662	-2.061000

H	1.247824	0.870269	-1.863339
H	-1.176504	0.972841	-1.819397
H	-0.457853	1.790062	-0.131958
H	-0.491119	-2.296028	-0.149888
H	-1.195296	-1.708376	1.355621
H	1.227575	-1.638284	1.462844
H	0.521647	-0.014577	1.625641
O	-0.183005	2.276736	1.736488
O	-0.332364	2.694977	0.506826
N	1.504314	-0.368579	-0.183703
C	2.853662	-0.304324	-0.132332
C	3.545786	-0.540888	1.092556
C	3.613854	-0.000067	-1.300501
C	4.915711	-0.466714	1.133964
H	2.999225	-0.747914	1.997498
C	4.983722	0.056275	-1.234402
H	3.123496	0.155675	-2.246874
C	5.647440	-0.171658	-0.022847
H	5.429703	-0.632841	2.069304
H	5.551121	0.272960	-2.127584
H	6.725826	-0.120484	0.019365

43a (*5*)

ΔG = -729.260826 hartree

C	-2.864510	0.028690	-0.036911
C	-3.535913	0.882261	0.830663
C	-4.924608	0.874029	0.843422
C	-5.627428	0.017411	0.004039
C	-4.940849	-0.839129	-0.850193
C	-3.552836	-0.842723	-0.873755
N	1.413515	-0.045549	-0.080889
C	0.721173	1.219135	-0.116046
C	-0.749380	1.132676	-0.094840
N	-1.418599	0.037761	-0.066538
C	-0.702634	-1.263924	-0.056531
C	0.673772	-1.116046	0.565567
C	5.643452	0.025749	-0.039805
C	4.950756	-1.077345	0.443195
C	3.562039	-1.104246	0.455385
C	2.818415	-0.018918	-0.034846
C	3.527686	1.098469	-0.507743
C	4.915820	1.111976	-0.510662
H	-2.987618	1.523309	1.505951
H	-5.452911	1.529798	1.520636
H	-6.708151	0.011680	0.020224
H	-5.483717	-1.505560	-1.505116
H	-3.023028	-1.499975	-1.547052
H	0.951791	1.778975	-1.029973
H	1.001591	1.895123	0.708937
H	-1.298988	2.063405	-0.124413
H	-0.633018	-1.613476	-1.084711
H	-1.307523	-1.960535	0.515740
H	1.182680	-2.061484	0.410346
H	0.579568	-0.959739	1.647225
H	6.724234	0.041470	-0.043205
H	5.491154	-1.932260	0.827680
H	3.073375	-1.976580	0.858768
H	3.008332	1.964542	-0.887461
H	5.428087	1.987444	-0.887235

43a (*5_TS_6*)

ΔG = -805.646931 hartree

C	-2.821852	-0.099276	-0.019564
C	-3.744483	-0.998971	0.498944
C	-5.100554	-0.801986	0.264467
C	-5.527615	0.288987	-0.483530
C	-4.597091	1.182911	-1.002826
C	-3.239258	0.990036	-0.777803
C	0.673227	1.105169	0.269923
C	-0.645725	0.727904	0.895075
O	-0.424565	-0.079065	2.155403
N	-1.406123	-0.346913	0.227930
C	-0.682682	-0.953366	-0.923676
C	0.760155	-1.248787	-0.556520
H	-1.255047	1.591072	1.133280
H	-0.838076	0.310651	2.944674
H	-1.088074	-0.817315	1.535475
H	-3.404108	-1.845440	1.079096
H	-5.819533	-1.499522	0.670729
H	-6.582694	0.443040	-0.662287
H	-4.924740	2.031213	-1.587285
H	-2.522654	1.684441	-1.194016
H	0.448492	1.782038	-0.565340
H	1.211945	1.694068	1.010497
H	-0.743160	-0.282891	-1.782389
H	-1.194449	-1.877553	-1.176658
H	1.245281	-1.654372	-1.445501
H	0.789319	-2.030950	0.211244
N	1.456881	-0.046283	-0.116894
C	2.844257	0.014409	-0.144266
C	3.532150	1.236814	-0.030442
C	3.610411	-1.156676	-0.294931
C	4.919818	1.274380	-0.051287
H	2.991971	2.167700	0.051551
C	4.997044	-1.099208	-0.322016
H	3.128042	-2.118897	-0.373600
C	5.668513	0.111967	-0.197311
H	5.416831	2.231790	0.036142
H	5.555333	-2.019495	-0.434714
H	6.748637	0.149474	-0.216807

43a (*6*)

ΔG = -805.694297 hartree

C	-2.840072	-0.166665	-0.031150
C	-3.857621	-0.994013	0.418209
C	-5.177713	-0.630308	0.178729
C	-5.464053	0.547587	-0.500224
C	-4.430411	1.367426	-0.940535
C	-3.106808	1.014799	-0.708796

N	1.422292	-0.140250	0.019367
C	0.566827	0.966316	0.401077
C	-0.633657	0.424403	1.161017
O	-0.287904	-0.275628	2.296796
N	-1.445140	-0.572060	0.232228
C	-0.678798	-0.915802	-1.025640
C	0.773446	-1.231938	-0.715134
C	5.613037	0.276884	-0.272684
C	4.999020	-0.952853	-0.482787
C	3.620258	-1.086415	-0.395740
C	2.809730	0.020798	-0.094138
C	3.435069	1.262277	0.099842
C	4.817152	1.378216	0.018117
H	-3.631957	-1.911089	0.946018
H	-5.976630	-1.270316	0.524710
H	-6.491221	0.828287	-0.685607
H	-4.649369	2.285460	-1.466736
H	-2.313156	1.661357	-1.054618
H	0.248518	1.597153	-0.435372
H	1.088080	1.610915	1.103691
H	0.596164	-0.655168	2.173786
H	-1.341741	1.202525	1.424194
H	-1.488972	-1.416521	0.805772
H	-0.775735	-0.071132	-1.699677
H	-1.167332	-1.774222	-1.477334
H	1.268949	-1.395993	-1.674242
H	0.836997	-2.171579	-0.159226
H	6.687499	0.375175	-0.338561
H	5.596185	-1.825949	-0.710673
H	3.180315	-2.061322	-0.543029
H	2.854776	2.150269	0.298013
H	5.269362	2.349076	0.172391

43a (*43d*)

ΔG = -805.279776 hartree

C	-2.690394	-0.397005	0.208553
C	-3.068664	0.139825	1.453369
C	-4.403792	0.281320	1.791769
C	-5.409584	-0.104046	0.905637
C	-5.045540	-0.628518	-0.328094
C	-3.707542	-0.771858	-0.683003
N	1.431530	0.048096	-0.900006
C	1.303944	1.317715	-1.581780
C	0.494203	2.387034	-0.883639
O	-0.035925	2.272949	0.194902
N	-1.342274	-0.568232	-0.071733
C	-0.867304	-0.793725	-1.424268
C	0.636945	-1.057173	-1.430990
C	4.937294	-0.627195	1.370542
C	4.289861	-1.685832	0.745309
C	3.144682	-1.481115	-0.014598
C	2.594786	-0.195203	-0.160336
C	3.260542	0.868243	0.477461
C	4.410368	0.651509	1.222952
H	-2.298211	0.439412	2.153091
H	-4.662856	0.697803	2.756828
H	-6.451368	0.006284	1.172943
H	-5.809215	-0.927685	-1.034762
H	-3.461095	-1.174505	-1.654387
H	0.849860	1.178551	-2.568991
H	2.285612	1.758647	-1.790271
H	0.422342	3.331860	-1.454729
H	-0.741731	0.061879	0.442972
H	-1.127792	0.034619	-2.097317
H	-1.340809	-1.685329	-1.837331
H	0.941553	-1.312129	-2.453574
H	0.810413	-1.928296	-0.807465
H	5.830110	-0.793168	1.957084
H	4.684220	-2.690056	0.832405
H	2.698775	-2.330186	-0.507863
H	2.864397	1.870859	0.418047
H	4.889580	1.494941	1.702972

$^3O_2$

ΔG = -150.397318 hartree

O	0.000000	0.000000	0.602725
O	0.000000	0.000000	-0.602725

$^1O_2$

ΔG = -150.335276 hartree

O	0.000000	0.000000	0.602873
O	0.000000	0.000000	-0.602873

$O_2^{-\bullet}$

ΔG = -150.510801 hartree

O	0.000000	0.000000	0.674277
O	0.000000	0.000000	-0.674277

$^{\bullet}$OOH

ΔG = -150.982169 hartree

O	0.055295	0.717598	0.000000
O	0.055295	-0.608411	0.000000
H	-0.884727	-0.873496	0.000000

HOOH

ΔG = -151.614548 hartree

O	-3.239383	1.342142	0.299663
H	-3.392075	2.086136	-0.299656
O	-1.791969	1.270527	0.299673
H	-1.639275	0.526420	-0.299505

H_2O

ΔG = -76.463372 hartree

O	-3.190329	1.285401	0.000046
H	-3.467827	2.206852	-0.000044

H	-2.229104	1.331419	0.000042

HCHO

ΔG = -114.549224 hartree

C	0.340270	-0.351609	0.000000
H	0.859045	-1.325375	0.000000
H	-0.762391	-0.389628	0.000000
O	0.942262	0.691496	0.000000

CH_3CHO

ΔG = -153.868878 hartree

C	-2.471863	-0.065011	-0.014357
H	-1.846579	-0.961003	0.015308
H	-2.231659	0.533241	-0.890067
H	-3.506860	-0.412768	-0.065455
C	-2.276723	0.713280	1.246678
H	-2.504517	0.161895	2.178955
O	-1.900516	1.861938	1.299542

$HOCH_2CHO$

ΔG = -229.105909 hartree

C	-2.467559	-0.054439	-0.036502
H	-1.841272	-0.954279	0.044556
H	-3.509188	-0.405798	-0.036873
C	-2.274190	0.719478	1.233730
H	-2.513777	0.133624	2.141587
O	-1.898116	1.863499	1.305405
O	-2.155581	0.727019	-1.165396
H	-2.293512	0.188361	-1.950656

CH_3OCH_2CHO

ΔG = -268.395011 hartree

C	-2.475555	-0.067126	-0.004661
H	-1.853137	-0.972106	0.084439
H	-3.519716	-0.419429	0.004662
C	-2.268270	0.736422	1.246156
H	-2.500995	0.171095	2.168722
O	-1.889302	1.880588	1.289483
O	-2.176089	0.670130	-1.154363
C	-2.359953	-0.077443	-2.348114
H	-3.398126	-0.409029	-2.453074
H	-2.108168	0.578235	-3.178281
H	-1.706049	-0.955368	-2.371480

HCOOH

ΔG = -189.835433 hartree

C	-0.788417	-0.069570	0.245479
O	0.260007	0.492530	0.398287
O	-1.022782	-0.854713	-0.816304
H	-1.916603	-1.221547	-0.771734
H	-1.632357	0.003703	0.944272

$HCOOCH_3$

ΔG = -229.124407 hartree

C	-0.765897	0.030756	0.206908
O	0.346740	0.418080	0.444462
O	-0.997145	-1.118743	-0.428246
H	-1.678664	0.577040	0.485720
C	-2.364017	-1.504744	-0.673620
H	-3.056044	-0.760793	-0.281325
H	-2.498425	-1.602711	-1.747577
H	-2.536106	-2.461067	-0.186910