

**Supporting Information**

**Function-oriented ionic polymers featuring high-density active sites for sustainable carbon dioxide conversion**

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## Section 1 Characterization

Fourier transform infrared spectroscopy (FTIR) spectra of the samples were obtained under ambient conditions at a resolution of  $4\text{ cm}^{-1}$  in the wave number range of  $4000\text{-}400\text{ cm}^{-1}$  by using an EQUINOX 55 spectrometer. Elemental analyses for C, H, N and O were detected on a Vario EL cube instrument. Thermogravimetry and differential thermogravimetric (TG-DTG) was carried out in a NETZSCH TG 209 F3 Tarsus instrument by heating samples from  $40\text{ }^{\circ}\text{C}$  to  $850\text{ }^{\circ}\text{C}$  at a heating rate of  $10\text{ }^{\circ}\text{C}\cdot\text{min}^{-1}$  under air atmosphere. Liquid  $^1\text{H}$  and  $^{13}\text{C}$  NMR data were collected on a Bruker Varian INOVA500NB or Bruker AVANCE 400 spectrometer using TMS as an internal standard. The Solid-state  $^{13}\text{C}$  NMR spectrum was recorded on Bruker AVANCE 400 spectrometer. The bromine content was measured by oxygen flask combustion and mercury nitrate titration technique. X-ray photoelectron spectroscopy (XPS) analysis was carried out on an ESCALAB 250 spectrometer. Field emission scanning electron microscopy (SEM) images were obtained by a FEI Quanta 400 FEG. Transmission electron microscopy (TEM) and EDS-mapping experiments were performed on JEM-2100F field emission electron microscope (JEOL, Japan) with an acceleration voltage of 200 kV, which incorporated a probe corrector and a super-X EDS system. The  $\text{N}_2$  adsorption and desorption measurements were performed on a Micromeritic ASAP2020M analyzer at 77 K. Specific surface areas ( $S_{\text{BET}}$ ) were calculated using Brunauer-Emmett-Teller (BET) methods and the pore size distributions were analyzed by using nonlocal density functional theory (NLDFT). All samples were degassed at  $130\text{ }^{\circ}\text{C}$  for 10 h under vacuum before analysis. X-Ray diffraction patterns of the powder samples were obtained with a Bruker AXS D8 Advanced SWAX diffractometer by depositing powder on glass substrate, from  $2\theta = 4.0^{\circ}$  to  $60^{\circ}$  with  $0.1^{\circ}$  increment at  $25\text{ }^{\circ}\text{C}$ . Isotherms of carbon dioxide were collected from Micromeritic ASAP2020M at 273 K and 298 K. Fluorescence property of sample was recorded by a FLS980 steady-state fluorescence spectrometer with a Xe lamp as the excitation light source. Gas chromatographic (GC) analysis was performed on a GC2010 gas chromatograph (Shimadzu) equipped with a flame ionization detection and a capillary column (Rtx-5,  $30\text{ m} \times 0.32\text{ mm} \times 0.25\text{ }\mu\text{m}$ ).

## **Sction 2 Catalyst testing**

### **Typical procedures for the cycloaddition reaction of epoxides with CO<sub>2</sub>**

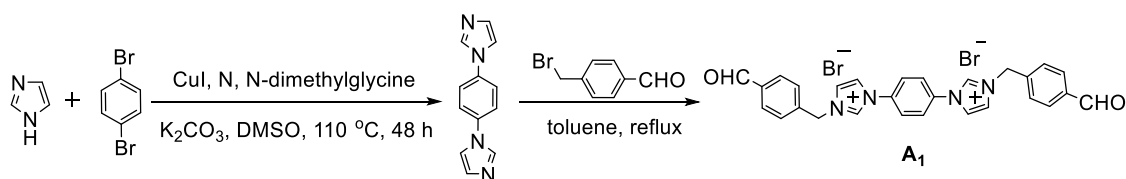
The reaction was performed in a stainless steel autoclave with a Teflon tube. Firstly, the epoxide and catalyst were quickly added into the autoclave. After sealing and purging with CO<sub>2</sub> for 3 times, the autoclave was pressurized with CO<sub>2</sub> to the requested pressure, followed by stirring at the needed temperature. After reaction, the autoclave was cooled to 0 °C and the excess of CO<sub>2</sub> was released slowly. Subsequently, the reaction mixture was extracted with ethyl acetate (3 × 2 mL), and the product yield and selectivity were determined by GC analysis through the internal standard method. The purity and structure of products were also confirmed by <sup>1</sup>H NMR, <sup>13</sup>C NMR spectra, and GC-MS analysis. For catalytic evaluation under low CO<sub>2</sub> concentration, simulated flue gas, a gas mixture of 15% CO<sub>2</sub> and 85% N<sub>2</sub> in volume, was used under defined conditions. The recycled catalyst was obtained through filtering, washing and drying, and then used for the next run without further purification. For each recyclability test, three parallel experiments were done, and the yield was taken as the average.

### **Typical procedures for the *N*-formylation reaction of amine with CO<sub>2</sub> and PhSiH<sub>3</sub>**

The reaction was performed in a stainless steel autoclave with a Teflon tube. Firstly, the amine, PhSiH<sub>3</sub> and catalyst were quickly added into the autoclave. After sealing and purging with CO<sub>2</sub> for 3 times, the autoclave was pressurized with CO<sub>2</sub> to the requested pressure, followed by stirring at the needed temperature. After reaction, the excess of CO<sub>2</sub> was vented at 0 °C. Subsequently, the reaction mixture was extracted with ethyl ether (3 × 2 mL), and the product yield and selectivity were determined by GC analysis through the internal standard method. The purity and structure of products were also confirmed by <sup>1</sup>H NMR, <sup>13</sup>C NMR spectra, and GC-MS analysis. For catalytic evaluation under low CO<sub>2</sub> concentration, simulated flue gas, a gas mixture of 15% CO<sub>2</sub> and 85% N<sub>2</sub> in volume, was used under defined conditions. The recycled catalyst was obtained through filtering, washing and drying, and then used for the next run without further purification. For each recyclability test, three parallel experiments were done, and the yield was taken as the average.

## Section 3 Synthesis

### Synthesis of A<sub>1</sub>

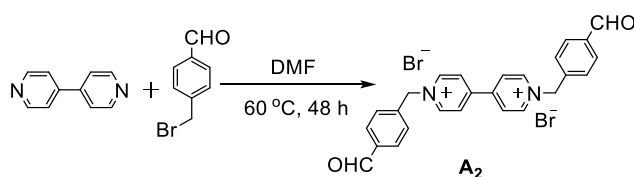


**Scheme S1.** Synthesis of A<sub>1</sub>

Following a modified procedure from reference 1: 1,4-Dibromobenzene (4.72 g, 20 mmol), 1H-imidazole (3.40 g, 50 mmol), copper iodide (0.76 g, 4 mmol), N, N-dimethylglycine (0.83 g, 8 mmol), potassium carbonate (11.06 g, 80 mmol) and Methyl sulfoxide (50 mL) was added to a 100 mL Schlenk flash, then the system was degassed by stirring under vacuum and backfilling with nitrogen three times. After the reaction mixture was heated at 110 °C for 48 h, water and ethyl acetate were added. The organic phase was separated, and the aqueous phase was extracted with ethyl acetate for three times. Then the combined organic phase was washed with brine, dried over anhydrous magnesium sulfate, and concentrated in vacuo. The residue was purified by silica gel column chromatography with CH<sub>2</sub>Cl<sub>2</sub>/MeOH (10/1, v/v) as eluent to afford 1, 4-bis(1-imidazolyl)benzene as pale yellow solid. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.87 (t, *J* = 1.1 Hz, 2H), 7.51 (s, 4H), 7.30 (t, *J* = 1.4 Hz, 2H), 7.23 (t, *J* = 1.1 Hz, 2H).

A solution of 1, 4-bis(1-imidazolyl)benzene (0.53 g, 2.5 mmol) and 4-(bromomethyl)benzaldehyde (1.0 g, 5.0 mmol) in acetonitrile (20 mL) was stirred at 80 °C for 24 h under N<sub>2</sub> atmosphere. The resulting precipitate was filtered, washed with acetonitrile and diethyl ether, and dried in vacuo to afford the target product (A<sub>1</sub>) as a white solid (1.45 g, 95 %). <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>) δ 10.30 (s, 2H), 10.07 (s, 2H), 8.52 (s, 2H), 8.17 (m, 6H), 8.00 (d, *J* = 8.0 Hz, 2H), 7.78 (d, *J* = 7.8 Hz, 4H), 5.72 (s, 4H).

### Synthesis of A<sub>2</sub>

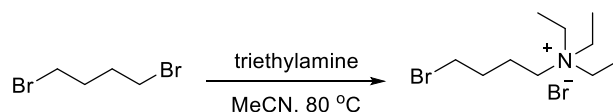


**Scheme S2.** Synthesis of A<sub>2</sub>

A solution of 4,4'-bipyridine (0.39 g, 2.5 mmol) and 4-(bromomethyl)benzaldehyde (1.0 g, 5.0

mmol) in N,N-Dimethylformamide (20 mL) was stirred at 60 °C for 48 h under N<sub>2</sub> atmosphere. The resulting precipitate was filtered, washed with N,N-dimethylformamide and diethyl ether, and dried in vacuo to yield the target product (**A<sub>2</sub>**) as a white solid (1.28 g, 92 %). <sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>): δ 10.03 (s, 2H), 9.56 (d, *J* = 6.5 Hz, 4H), (d, *J* = 6.4 Hz, 4H), 7.99 (d, *J* = 7.9 Hz, 4H), 7.80 (d, *J* = 8.0 Hz, 4H), 6.09 (s, 4H). <sup>13</sup>C NMR (126 MHz, DMSO-*d*<sub>6</sub>): δ 193.2, 149.8, 146.5, 140.6, 137.1, 130.6, 130.0, 127.8, 63.3.

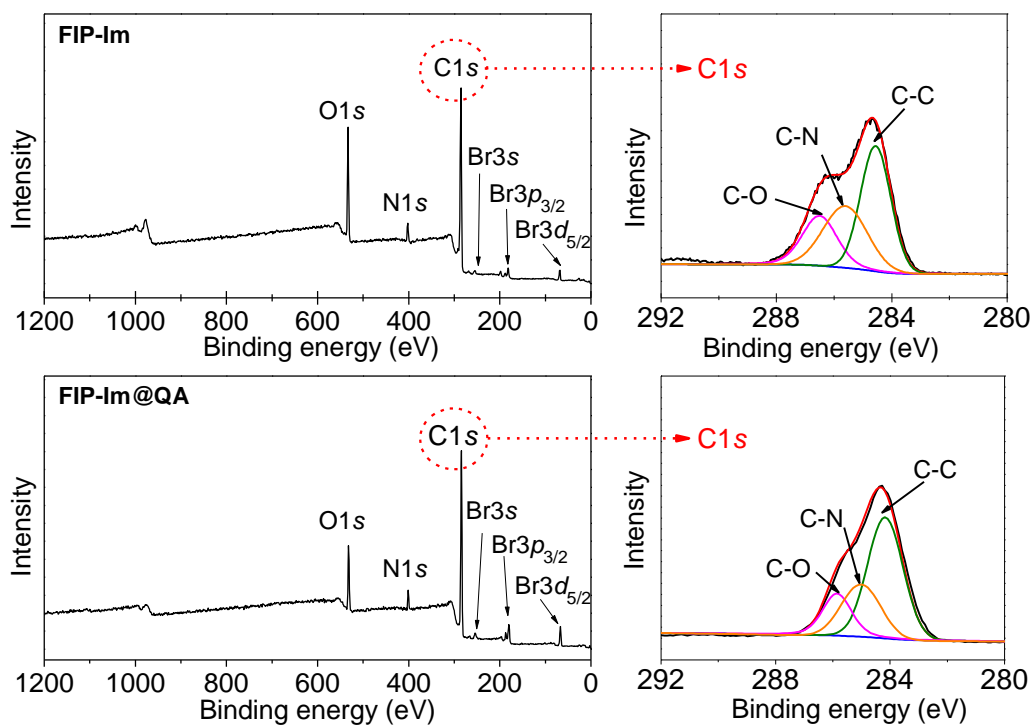
### Synthesis of (2-bromobutyl)triethylammonium bromide ([BrBuNEt<sub>3</sub>]Br)



**Scheme S3.** Synthesis of [BrBuNEt<sub>3</sub>]Br

Following a modified procedure from reference 2: Triethylamine (0.33 g, 3.3 mmol), 1,4-dibromobutane (1.4 g, 6.6 mmol) and CH<sub>3</sub>CN (35 mL) were refluxed at 80 °C under N<sub>2</sub> for 4 h. Upon cooling, the solvent was evaporated under reduced pressure, and then the residue was dissolved into hot CH<sub>3</sub>CN. Cooling of this solution gave precipitate which was mostly the dicationic product. After removing the precipitate by filtration, ethyl acetate was added to the filtrate. Simultaneously, the white solid was appeared, which was obtained by filtration and dried under vacuum to give **BrBuNEt<sub>3</sub>]Br** (0.52 g, 50% yield). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 1.30 (t, *J* = 7.4 Hz, 9 H), 1.80-1.86 (m, 2 H), 1.91-2.97 (m, 2 H), 3.42-3.37 (m, 8 H), 3.47-3.45 (t, *J* = 6.3 Hz, 2H). <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 56.56, 53.57, 32.9, 28.98, 20.49, 8.15.

## Section 4 XPS Spectra



**Figure S1.** Full XPS survey spectrum for **FIP-Im** and **FIP-Im@QA** recorded from 0 to 1200 eV

## Section 5 Elemental Analysis

**Table S1** Elemental analysis for catalysts.

Sample	CHN Elemental Analysis (wt%)				Br content (mmol g <sup>-1</sup> )
	C	H	N	O	
<b>IL-free</b>	77.18	4.12	0	0	0
<b>FIP-Im@M</b>	60.35	3.94	7.52	8.18	2.44
<b>FIP-Im</b>	58.37	3.86	7.56	8.26	2.51
<b>FIP-Im</b> after 6 cycles	58.42	3.82	7.59	8.32	2.48
<b>FIP-Py</b>	59.50	3.82	4.08	9.78	2.64
<b>FIP-Im@QA</b>	55.73	5.76	7.78	5.13	4.40
<b>FIP-Im@QA</b> after 6 cycles	55.62	5.83	6.81	5.16	4.34

## Section 6 Thermogravimetric Analysis

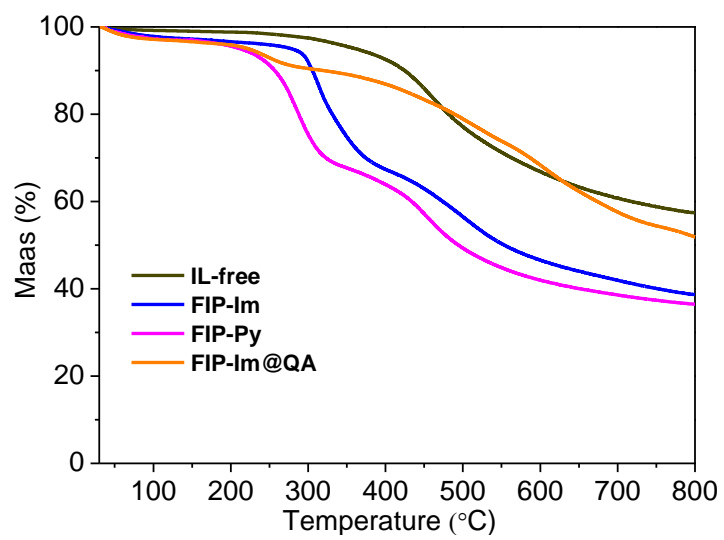
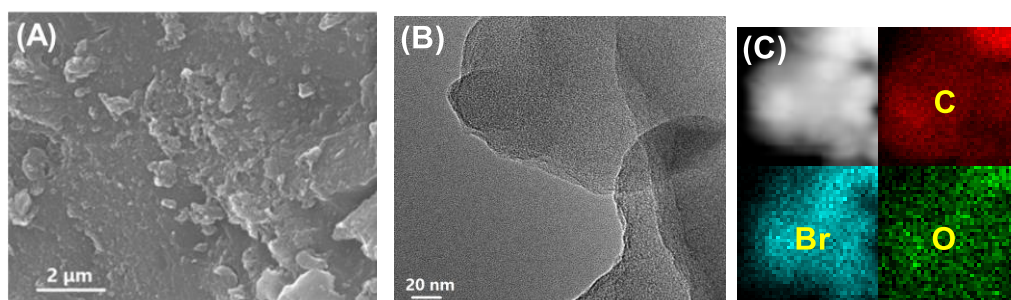


Figure S2. TGA curves of the obtained catalysts

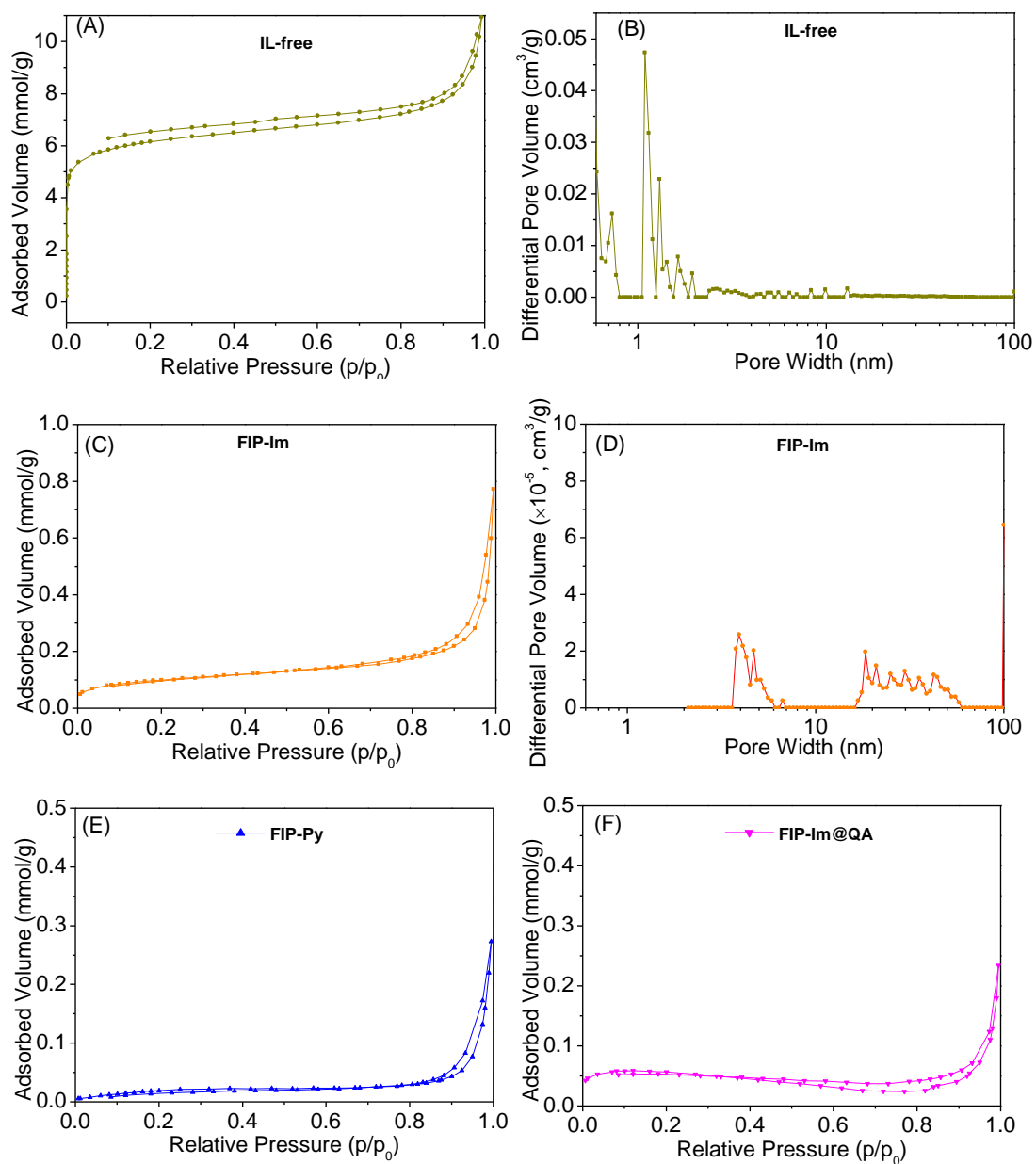


## Section 7 SEM and TEM Analysis



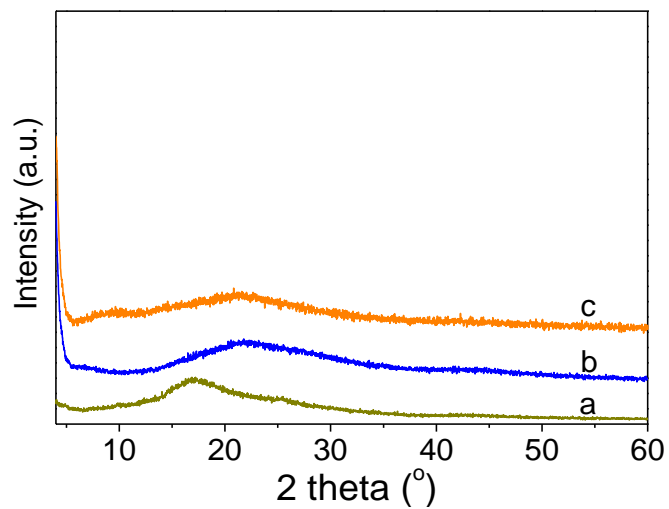
**Figure S3.** (A) SEM, (B) TEM, and (C) EDS elemental mapping images of FIP-Im

## Section 8 N<sub>2</sub> Sorption Isotherms



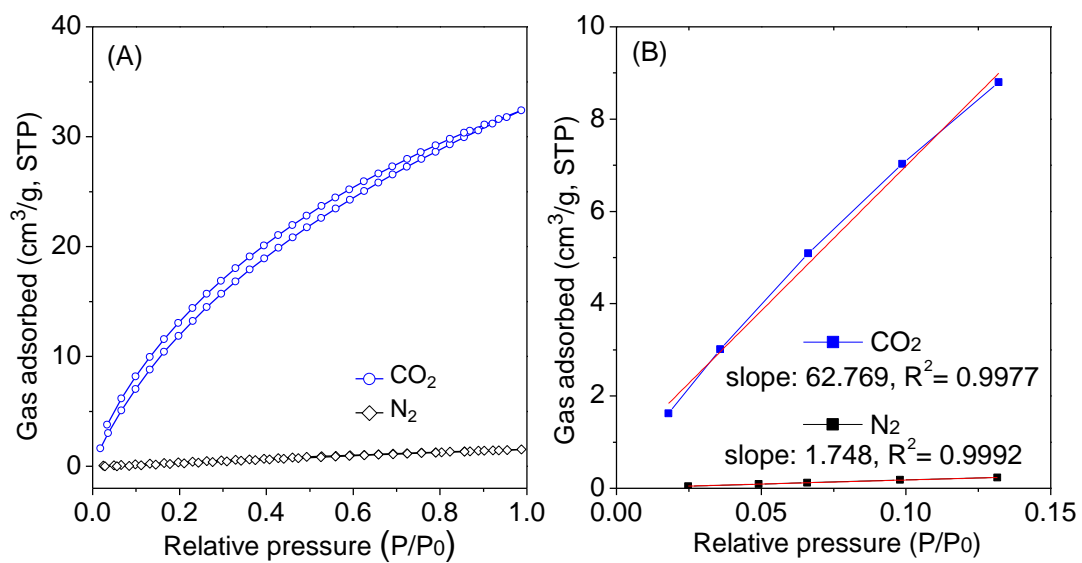
**Figure S4.** (A) N<sub>2</sub> sorption isotherms of samples at 77 K and (B) corresponding pore size distribution curve based on the DFT calculation model.

## Section 9 PXRD Patterns



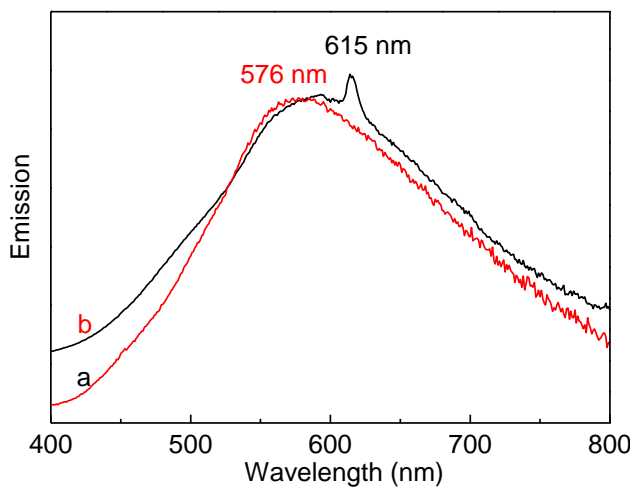
**Figure S5.** PXRD curves of **IL-free(a)**, **FIP-Im(b)** and **FIP-Im@QA(c)**. (The PXRD pattern shows a very broad peak at  $2\theta = 10 \sim 30^\circ$  for each sample)

## Section 10 CO<sub>2</sub> Sorption Isotherms and Selectivity of CO<sub>2</sub> over N<sub>2</sub>



**Figure S6.** (A) Gas sorption isotherms and (B) adsorption selectivity of CO<sub>2</sub> over N<sub>2</sub> for FIP-Im from initial slope calculations of CO<sub>2</sub> and N<sub>2</sub> isotherms at 273 K

## Section 11 Fluorescence Property



**Figure S7.** Fluorescence emission spectra of **FIP-Im** (a) and **FIP-Im@QA** (b) with excitation at 303 nm.

## Section 12 Activity Comparison

**Table S2. Activity comparison in the propylene oxide to propylene carbonate conversion reaction**

Catalyst (mol%)	Additive (mol%)	Solvent	T (°C)	CO <sub>2</sub> (MPa)	t (h)	Yield (%)	Ref.
FIP-Im (5)	- <sup>a</sup>	-	80	1.0	10	99	This work
PDBA-Cl-SCD (2.4)	-	-	90	0.1	6	99.6	<sup>3</sup>
NP-NHC (5 wt%)	-	-	120	0.1	24	98	<sup>4</sup>
NPILs-BPA (0.5)	-	-	150	2.0	4	98	<sup>5</sup>
SBA-[V0.15OH0.60]R <sub>2</sub> 37 (0.65)	-	-	140	2.0	6	99	<sup>6</sup>
TBB-Bpy-a (80 mg)	-	-	120	1.0	4	99	<sup>7</sup>
PDmBr (1.3)	-	-	110	1.0	4	98.7	<sup>8</sup>
TBB-Bpy-a (4 wt%)	-	-	90	1.0	12	99	<sup>9</sup>
mesoPILC (50 mg)	-	-	150	1.0	6	92	<sup>10</sup>
DVB-HTA (0.22)	-	-	120	1.2	6	93	<sup>11</sup>
SYSU-Zn@IL2 (0.16)	-	-	80	1.0	12	99	<sup>12</sup>
DVB@ISA (0.25)	-	-	60	1.0	24	17	<sup>13</sup>
Al-CPOP (1)	-	-	120	0.1	24	67	<sup>14</sup>
TBB-Bpy@Salen-Co (0.2)	-	-	60	1.0	6	99.2	<sup>15</sup>
Mg-por/pho@POP (0.5)	-	-	140	3.0	1	78	<sup>16</sup>
PPh <sub>3</sub> -ILBr-ZnBr <sub>2</sub> @POPs (0.0125)	-	-	120	3.0	1	44	<sup>17</sup>
1P <sup>+</sup> Br-&ZnBr <sub>2</sub> -1PPh <sub>3</sub> @POPs (0.0125)	-	-	120	3.0	1	49.8	<sup>18</sup>
Py-Zn@MA (0.28)	-	-	150	2.0	6	96	<sup>19</sup>
POM3-IM (5)	-	EtOH	120	1.0	8	96	<sup>20</sup>
HIP-Br-2 (4)	ZnBr <sub>2</sub> (4)	DMF	25	0.1	96	99	<sup>21</sup>
Zn@SBMMP (1.2)	TBAB (1.8)	DCE	80	2.0	4	95	<sup>22</sup>
g-C <sub>3</sub> N <sub>4</sub> -475-NaOH (0.4 g)	ZnI <sub>2</sub> (38 mg)	-	140	2.0	6	89.5	<sup>23</sup>
Bp-Zn@MA (0.086)	TBAB (0.55)	-	100	1.0	1.5	99	<sup>24</sup>
PPS-COF-TpBpy-Cu (0.1)	-	-	25	0.1	72	94	<sup>25</sup>
IL-ZIF-90 (0.5)	-	-	120	1.0	3	697	<sup>26</sup>
HF-MOP (5)	TBAI (5)	-	80	2.0	18	89	<sup>27</sup>
Co-CMP	TBAB (7.2)	-	100	3.0	1	98.1	<sup>28</sup>
Al-MON (0.05)	TBAC (0.15)	-	60	1.0	12	71	<sup>29</sup>
In-MOF (0.23)	TBAB (2.5)	-	80	2.0	4	93.9	<sup>30</sup>
Cu-MOF (0.2)	TBAB (10)	-	25	0.1	48	96	<sup>31</sup>
Co/POP-TPP (0.22)	TBAB (0.7)	-	29	0.1	24	94.8	<sup>32</sup>
Cu/POP-Bpy (0.5)	TBAB (7)	-	29	0.1	48	99	<sup>33</sup>

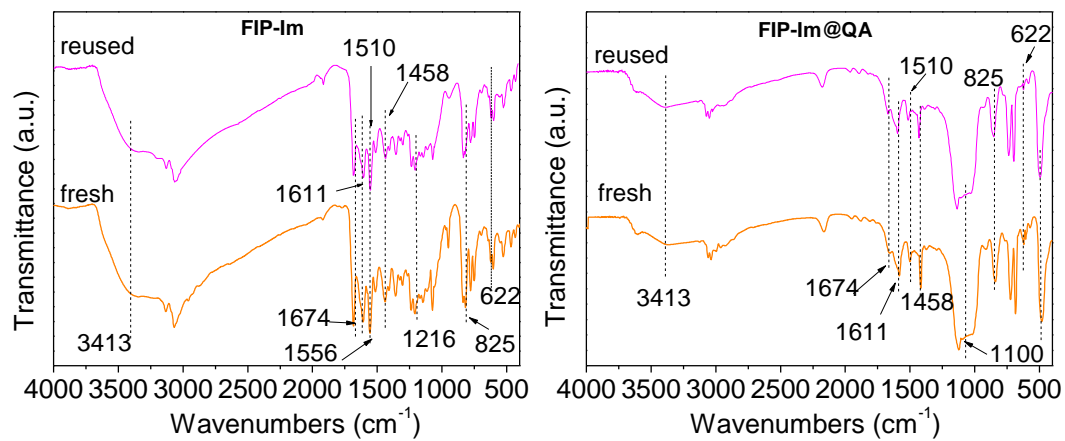
<sup>a</sup> Not added additive or solvent.

**Table S3. Activity Comparison in the *N*-formylation reaction of *N*-methylaniline with CO<sub>2</sub> and hydrosilanes**

Catalyst (mol%)	Hydrosilane (mmol)	Solvent	T (°C)	CO <sub>2</sub> (MPa)	t (h)	Yield (h <sup>-1</sup> )	Ref.
FIP-Im@QA (6)	PhSiH <sub>3</sub> (1.0 eq.)	- <sup>a</sup>	35	1.0	14	99	This work
F-PNHC-Zn (5.0)	PhSiH <sub>3</sub> (3 eq.)	THF	80	1.0	24	71	34
ILSZ1 (1)	PhSiH <sub>3</sub> (1.0 eq.)	-	40	1.5	3	100	35
DVB@ISZ (0.25)	PhSiH <sub>3</sub> (1.0 eq.)	-	40	1.0	20	96	13
[Et <sub>4</sub> NBr]50%-Py-COF (5)	PhSiH <sub>3</sub> (2.0 eq.)	DMF	30	0.1	24	94	36
Cs <sub>2</sub> CO <sub>3</sub> (5)	PhSiH <sub>3</sub> (1.0 eq.)	CH <sub>3</sub> CN	25	0.1	12	94	37
[BMIm]Cl (100)	PhSiH <sub>3</sub> (2.0 eq.)	-	30	1.0	5	95	38
Glycine Betaine (3)	PhSiH <sub>3</sub> (2.0 eq.)	CH <sub>3</sub> CN	25	0.5	4	95	39
Glycine Betaine (10)	Ph <sub>2</sub> SiH <sub>2</sub> (4.0 eq.)	CH <sub>3</sub> CN	50	1.0	12	96	40
Fe(acac) <sub>2</sub> (5)+PP <sub>3</sub> (5)	PhSiH <sub>3</sub> (1.0 eq.)	THF	25	0.1	18	95	41
Cu(OAc) <sub>2</sub> (0.07)+dppb (0.21)	PMHS (2.3 eq.)	Dioxane	80	0.1	30	87	42
TBAF (5)	(EtO) <sub>3</sub> SiH	CH <sub>3</sub> CN	30	0.1	4	90	43
TBAF·3H <sub>2</sub> O (10)	PhSiH <sub>3</sub> (1.2 eq.)	-	25	0.1	6	99	44
IPr (5)	PhSiH <sub>3</sub> (1 eq.)	THF	25	0.1	24	99	45
ZnPc (0.5) + DMF (200)	PhSiH <sub>3</sub> (1 eq.)	-	25	0.1	6	99	46
Ph <sub>3</sub> P <sup>+</sup> CHRCOO <sup>-</sup> (5.0)	PhSiH <sub>3</sub> (2 eq.)	CH <sub>3</sub> CN	100	2.0	24	91	47
NHP-H (5.0)	PhSi <sub>2</sub> H <sub>2</sub> (3.0 eq.)	CD <sub>3</sub> CN	25	0.1	4	97	48
CsF (10.0)	PhSi(Me) <sub>2</sub> H	DMSO	80	0.1	39	60	49
TBD (5.0)	PhSiH <sub>3</sub> (1 eq.)	-	100	0.1	24	100	50
Poly-NHC	PhSiH <sub>3</sub> (2.5 eq.)	DMF	25	0.1	20	66	51

<sup>a</sup> Not added solvent.

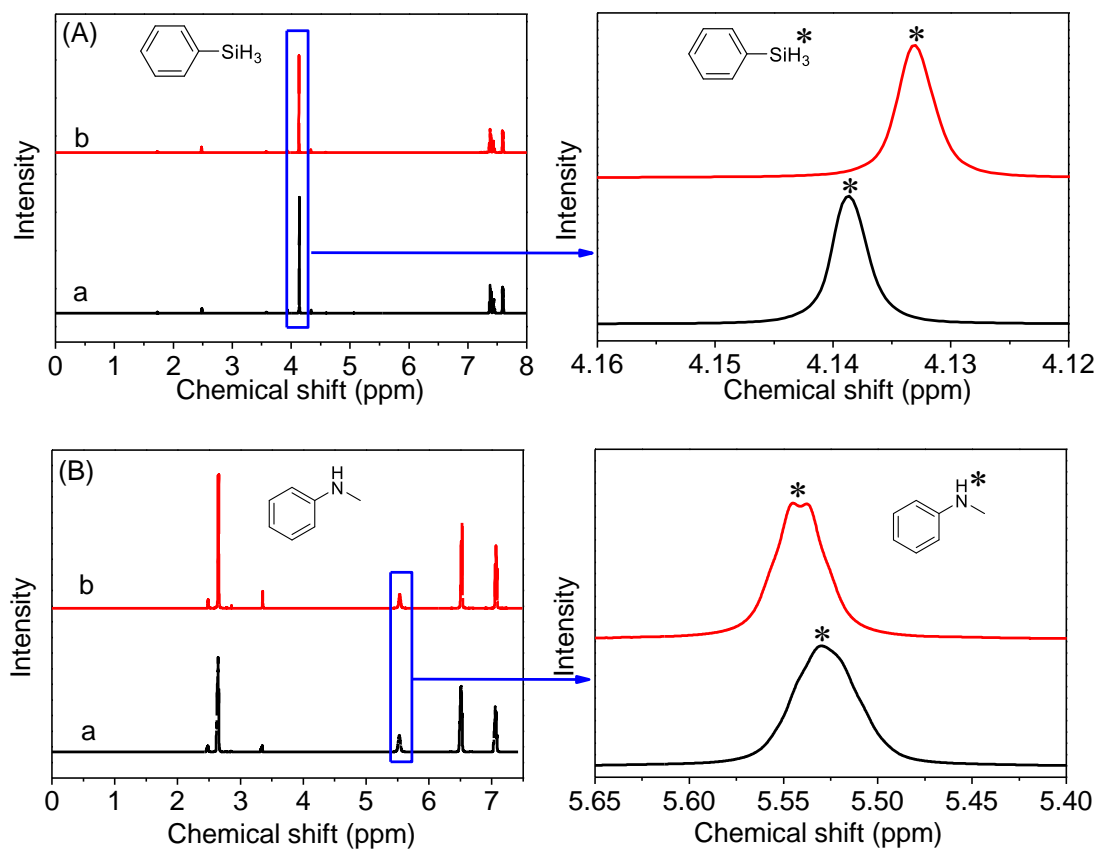
### Section 13 Characterization for the Reused Catalyst



**Figure S8.** FTIR spectra of the fresh and reused **FIP-Im** and **FIP-Im@QA**

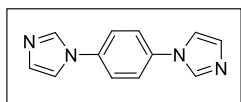


Section 14  $^1\text{H}$  NMR spectra of  $\text{PhSiH}_3$  or *N*-methylaniline and its mixture with catalyst

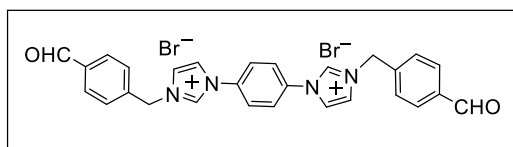


**Figure S9.**  $^1\text{H}$  NMR spectra of (A)  $\text{PhSiH}_3$  (a) and its mixture with **FIP-Im@QA** (b) and (B) *N*-methylaniline and its mixture with **FIP-Im@QA** (b) ( $\text{DMSO-}d_6$ , 298 K)

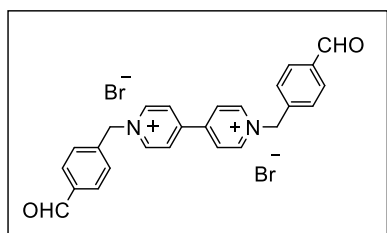
## Section 14 NMR Spectra



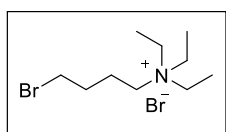
$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ , 25 °C, TMS):  $\delta$  (ppm) = 7.87 (t,  $J$  = 1.1 Hz, 2H), 7.51 (s, 4H), 7.30 (t,  $J$  = 1.4 Hz, 2H), 7.23 (t,  $J$  = 1.1 Hz, 2H).



$^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ , 25 °C, TMS):  $\delta$  (ppm) = 10.30 (s, 2H), 10.07 (s, 2H), 8.52 (s, 2H), 8.17 (m, 6H), 8.00 (d,  $J$  = 8.0 Hz, 2H), 7.78 (d,  $J$  = 7.8 Hz, 4H), 5.72 (s, 4H).

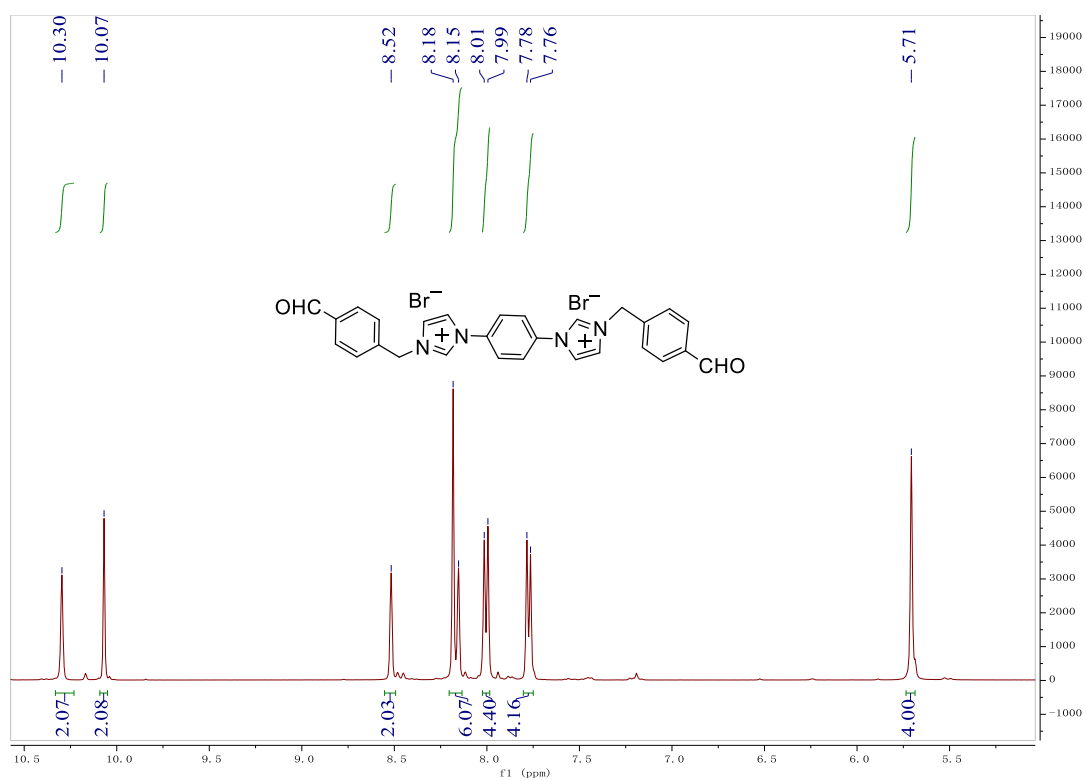
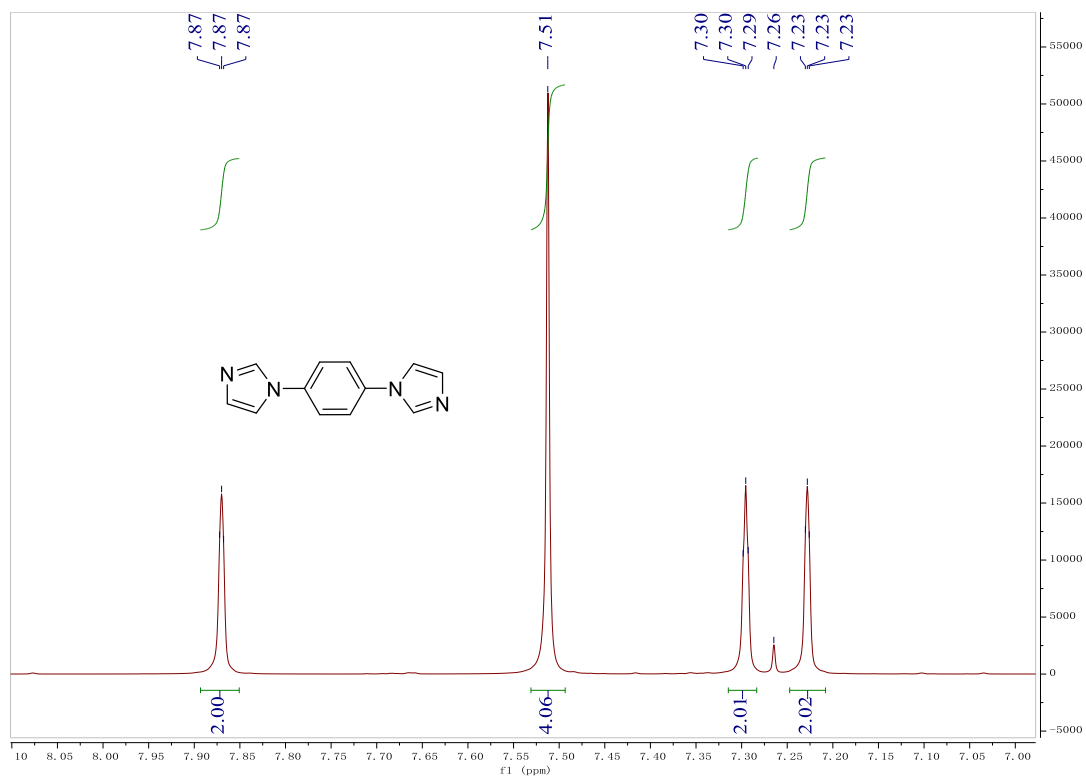


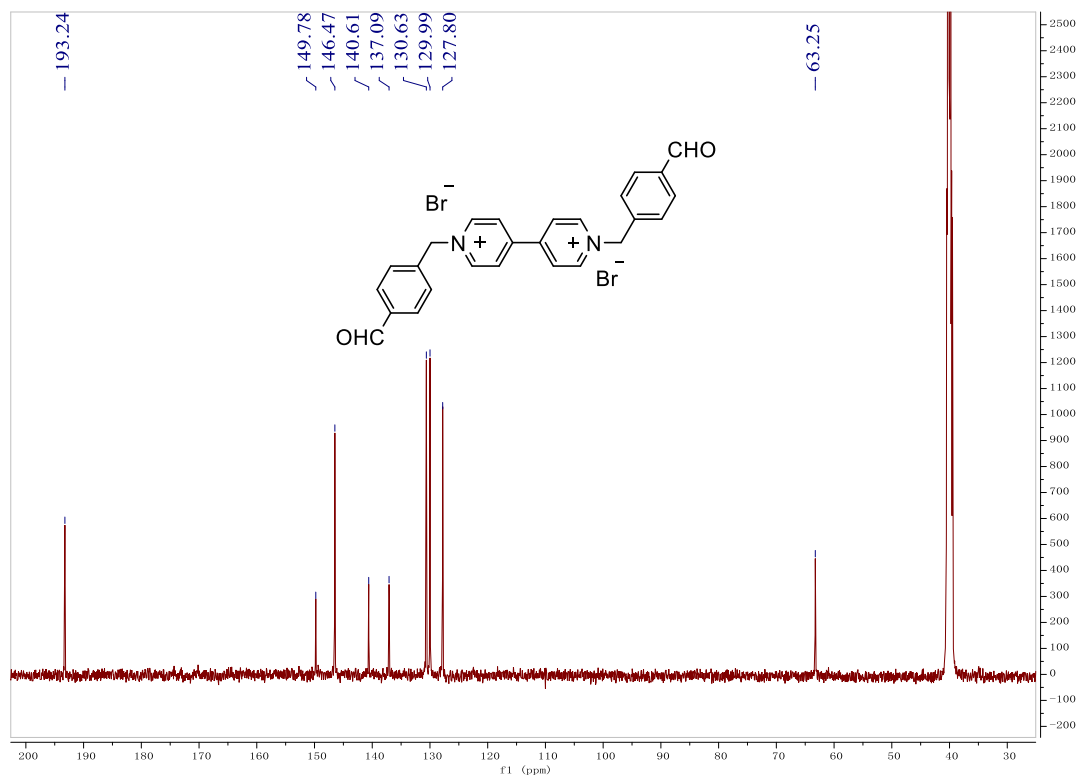
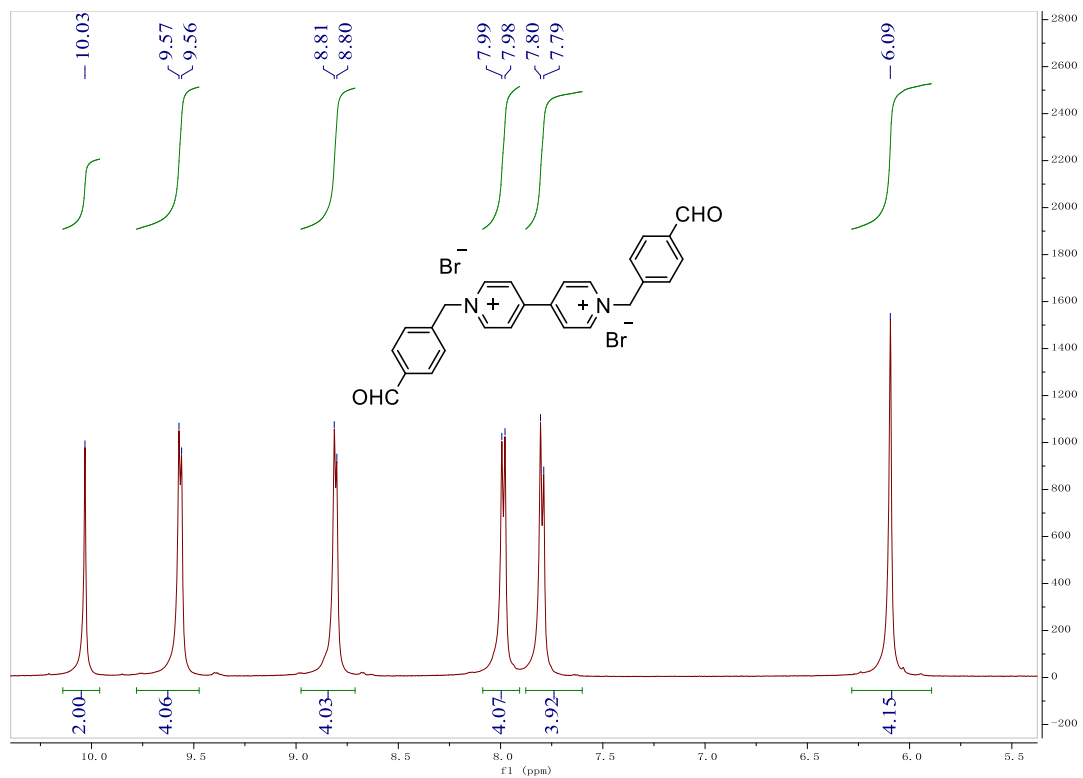
$^1\text{H}$  NMR (500 MHz,  $\text{DMSO-}d_6$ , 25 °C, TMS):  $\delta$  (ppm) = 10.03 (s, 2H), 9.56 (d,  $J$  = 6.5 Hz, 4H), (d,  $J$  = 6.4 Hz, 4H), 7.99 (d,  $J$  = 7.9 Hz, 4H), 7.80 (d,  $J$  = 8.0 Hz, 4H), 6.09 (s, 4H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{DMSO-}d_6$ ), 25 °C, TMS):  $\delta$  (ppm) = 193.2, 149.8, 146.5, 140.6, 137.1, 130.6, 130.0, 127.8, 63.3.

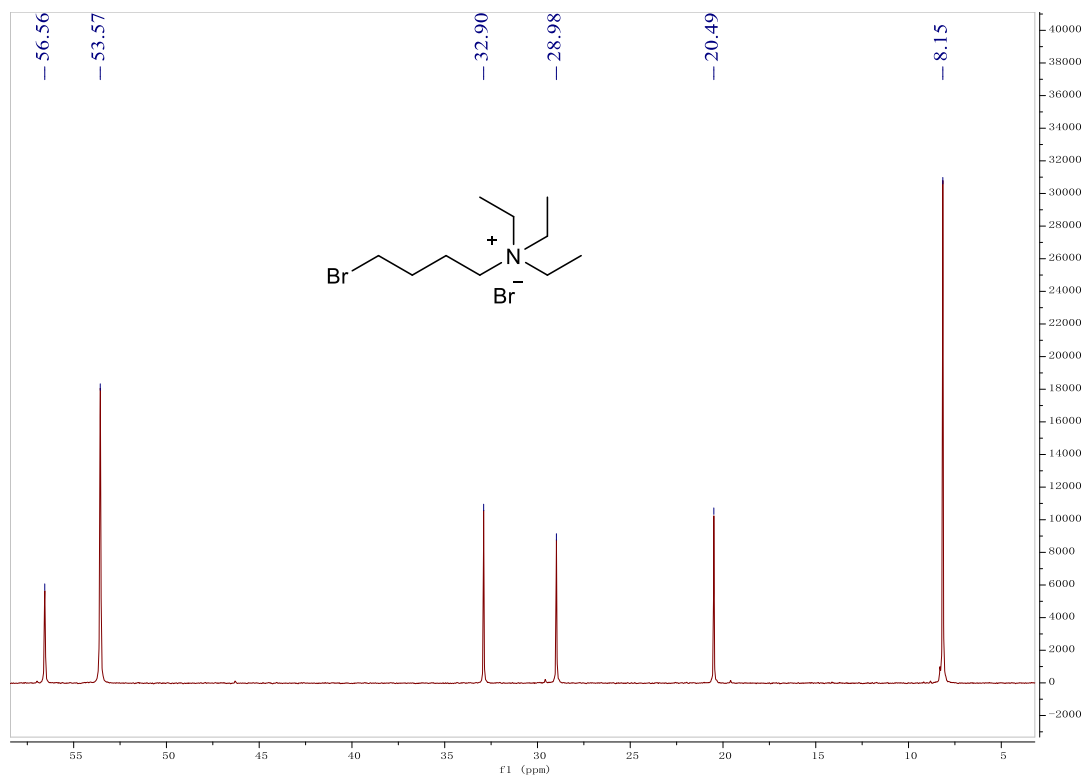
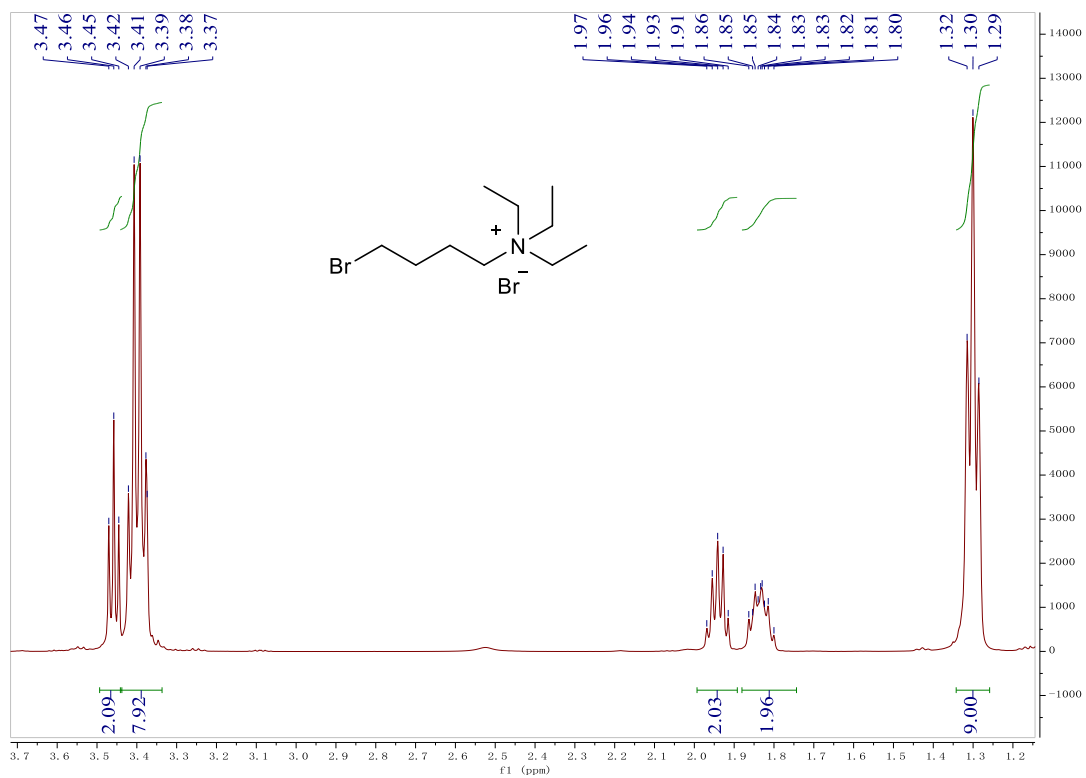


$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ), 25 °C, TMS)  $\delta$  (ppm) = 1.30 (t,  $J$  = 7.4 Hz, 9 H), 1.80-1.86 (m, 2 H), 1.91-2.97 (m, 2 H), 3.42-3.37 (m, 8 H), 3.47-3.45 (t,  $J$  = 6.3 Hz, 2H).  $^{13}\text{C}$  NMR

(126 MHz, CDCl<sub>3</sub>, 25 °C, TMS):  $\delta$  (ppm) = 56.56, 53.57, 32.9, 28.98, 20.49, 8.15.

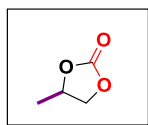






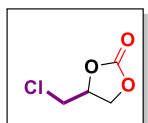
**The  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectral copies of various synthesized cyclic carbonates:**

**4-methyl-1,3-dioxolan-2-one:**



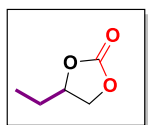
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, 25 °C, TMS):  $\delta$  (ppm) = 4.77-4.86 (m, 1H, ring CH- $\text{CH}_3$ ), 4.49-4.53 (t, 1H,  $J$  = 8 Hz, ring  $\text{CH}_2$ ), 1.41-1.43 (d, 3H,  $J$  = 8 Hz,  $\text{CH}_3$ );  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 101 MHz, 25 °C, TMS):  $\delta$  (ppm) = 155.15, 73.70, 70.72, 19.31.

**4-(chloromethyl)-1,3-dioxolan-2-one:**



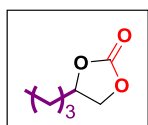
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, 25 °C, TMS):  $\delta$  (ppm) = 4.98-5.04 (m, 1H, CH- $\text{CH}_2$ ), 4.59-4.63 (t,  $J$  = 8 Hz, 1H, ring  $\text{CH}_2$ ), 4.40-4.44 (dd,  $J$  = 8 Hz, 4 Hz, 1H, ring  $\text{CH}_2$ ), 3.72-3.84 (m, 2 H,  $\text{CH}_2$ -Cl);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 101 MHz, 25 °C, TMS):  $\delta$  (ppm) = 154.35, 74.38, 67.00, 43.86.

**4-ethyl-1,3-dioxolan-2-one:**



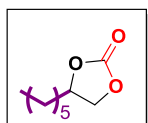
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz, 25 °C, TMS):  $\delta$  (ppm) = 4.58-4.63 (m, 1H), 4.45-4.48 (t,  $J$  = 10 Hz, 1H), 4.00-4.03 (t,  $J$  = 10 Hz, 1H), 1.64-1.75 (m, 2H), 0.92-0.95 (t,  $J$  = 10 Hz, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 101 MHz, 25 °C, TMS):  $\delta$  (ppm) = 155.21, 78.11, 69.06, 26.79, 8.38.

**4-butyl-1,3-dioxolan-2-one:**



$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz, 25 °C, TMS):  $\delta$  (ppm) = 4.59-4.64 (m, 1H), 4.42-4.45 (t,  $J$  = 10 Hz, 1H), 3.95-3.98 (t,  $J$  = 10 Hz, 1H), 1.63-1.71 (m, 1H), 1.55-1.62 (m, 1H), 1.19-1.36 (m, 4H), 0.79-0.82 (t,  $J$  = 10 Hz, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 126 MHz, 25 °C, TMS):  $\delta$  (ppm) = 155.16, 77.15, 69.41, 33.35, 26.33, 22.13, 13.66.

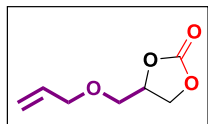
**4-hexyl-1,3-dioxolan-2-one:**



$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz, 25 °C, TMS):  $\delta$  (ppm) = 4.62-4.68 (m, 1H), 4.46-4.49 (t,  $J$  = 10 Hz, 1H), 3.99-4.02 (t,  $J$  = 10 Hz, 1H), 1.69-1.76 (m, 1H), 1.59-1.65 (m, 1H), 1.34-1.44 (m, 1H),

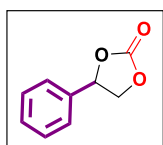
1.20-1.33 (m, 7H), 0.80-0.83 (t,  $J = 10$  Hz, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 126 MHz, 25 °C, TMS):  $\delta$  (ppm) = 155.16, 77.14, 69.42, 33.77, 31.46, 28.73, 24.26, 22.39, 13.92.

**4-((allyloxy)methyl)-1,3-dioxolan-2-one:**

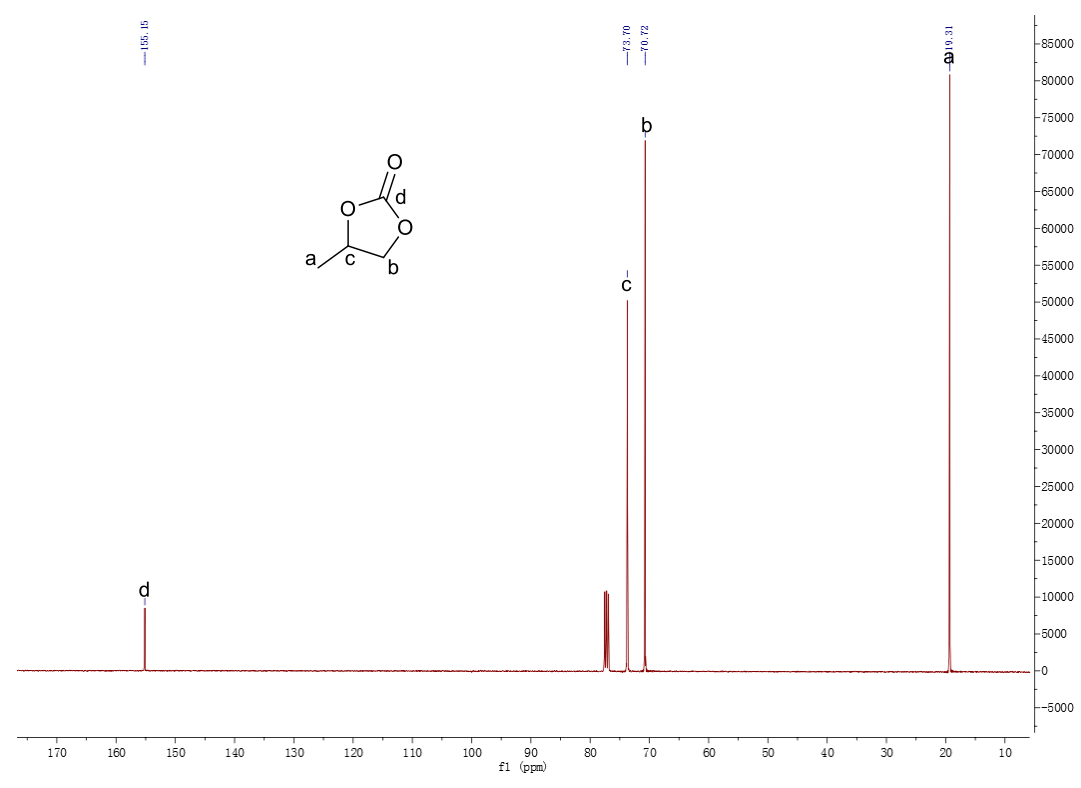
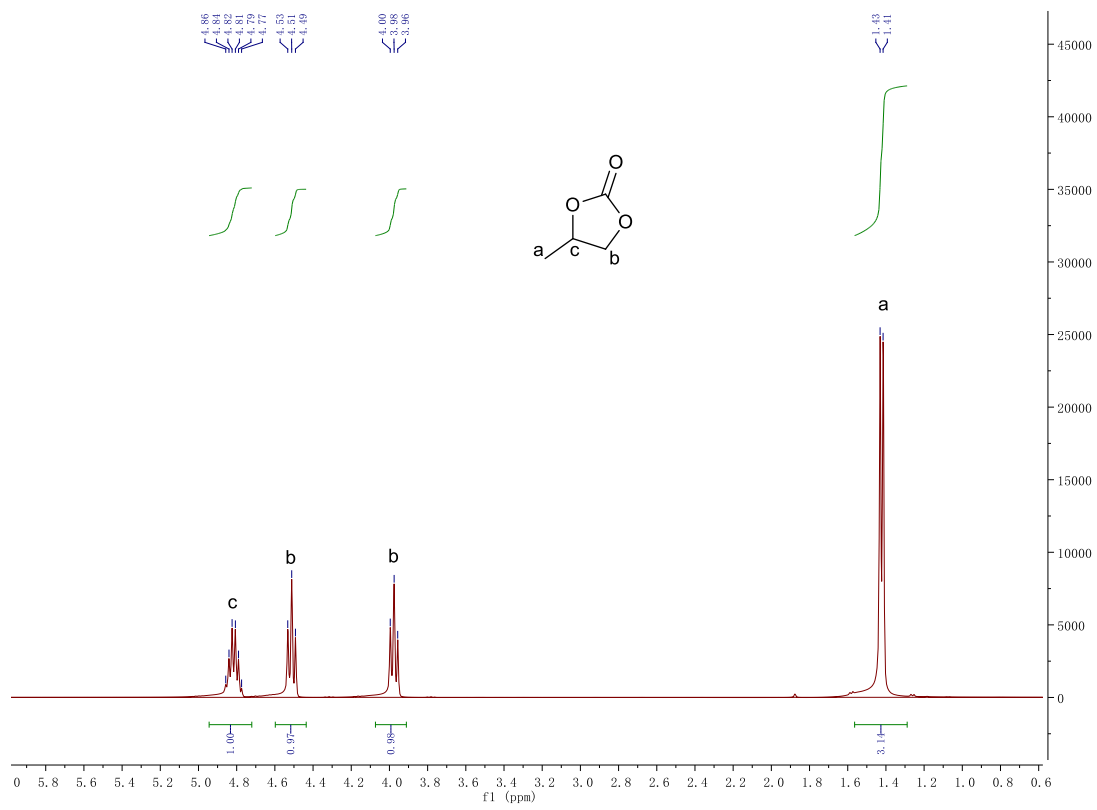


$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, 25 °C, TMS):  $\delta$  (ppm) = 5.83-5.92 (m, 1H), 5.19-5.31 (dd,  $J = 10$  Hz, 2H), 4.84-4.87 (m, 1H), 4.50-4.54 (t,  $J = 8$  Hz, 1H), 4.38-4.42 (d,  $J = 8$  Hz, 1H), 4.01-4.10 (m, 2H), 3.60-3.73 (m, 2H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 101 MHz, 25 °C, TMS):  $\delta$  (ppm) = 155.06, 133.17, 117.79, 75.17, 72.51, 68.86, 66.27.

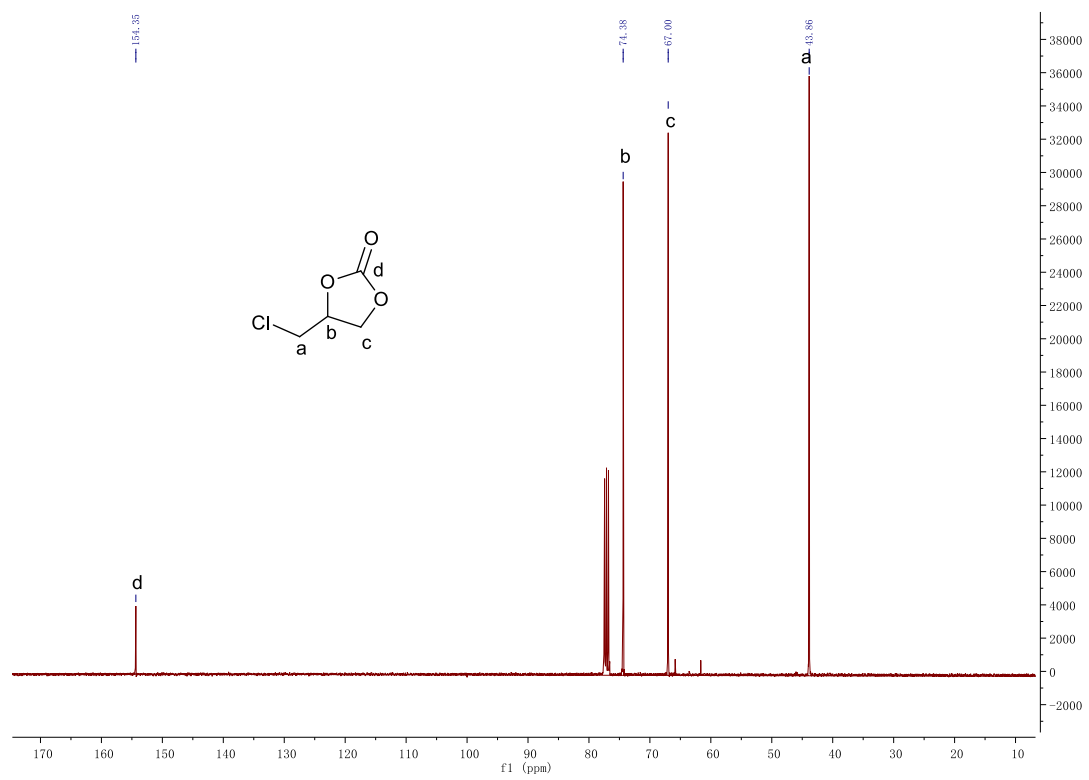
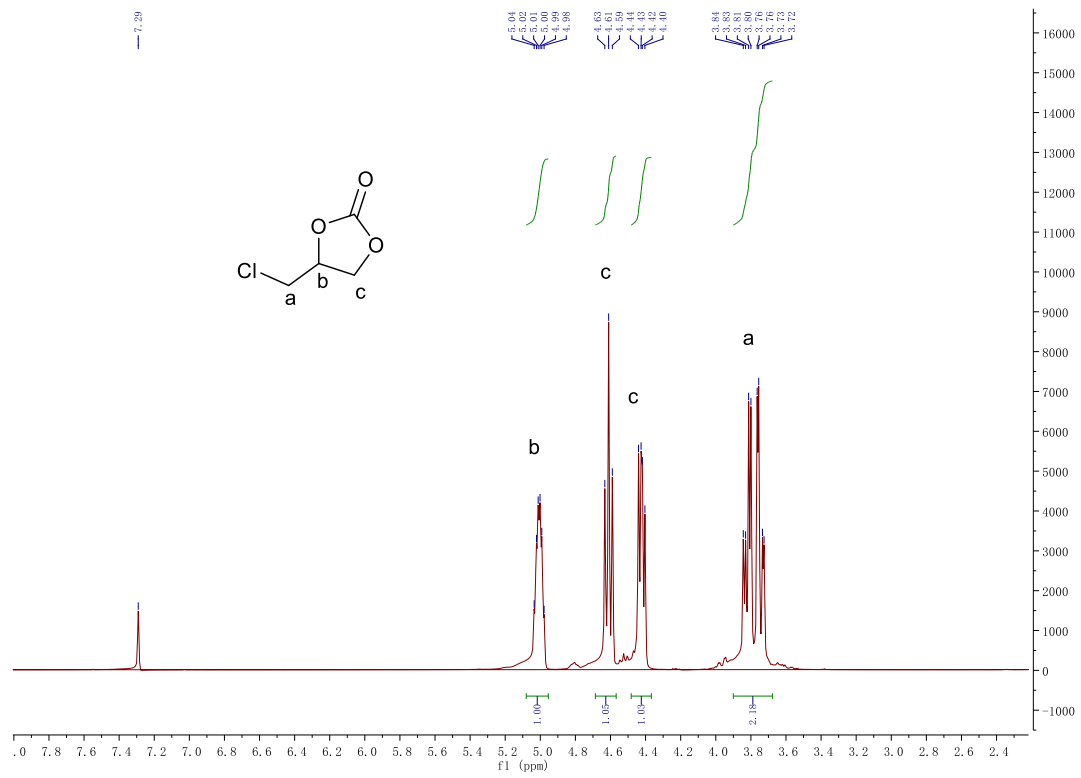
**4-phenyl-1,3-dioxolan-2-one:**

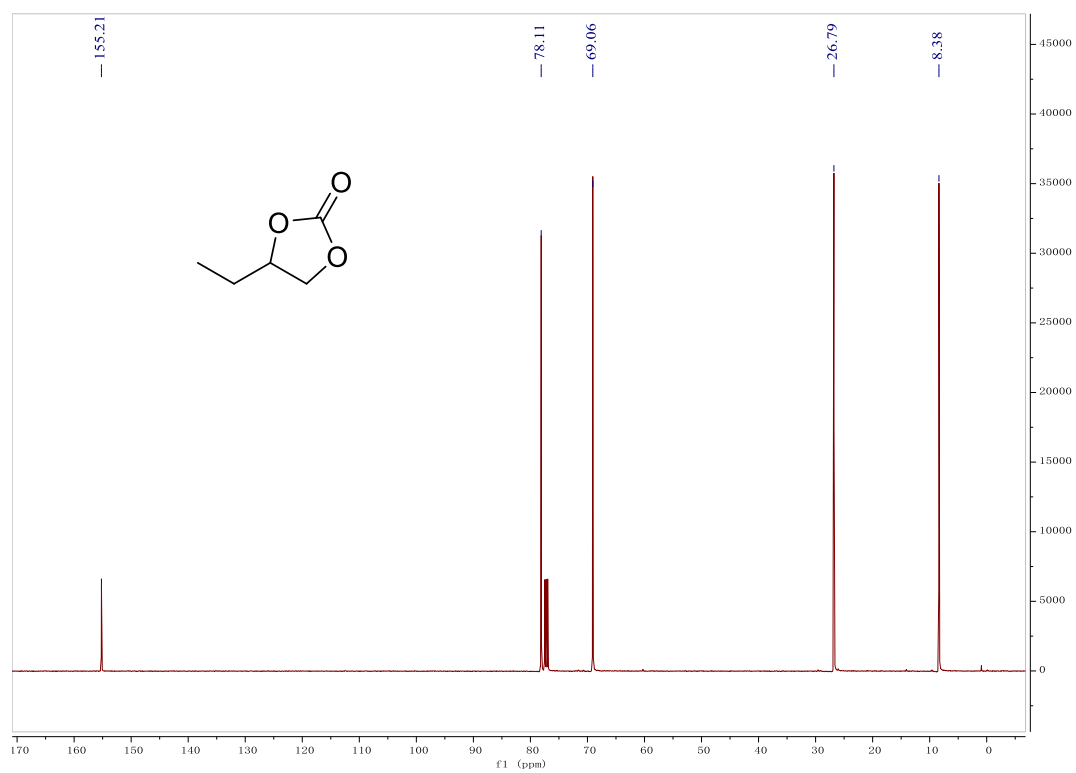
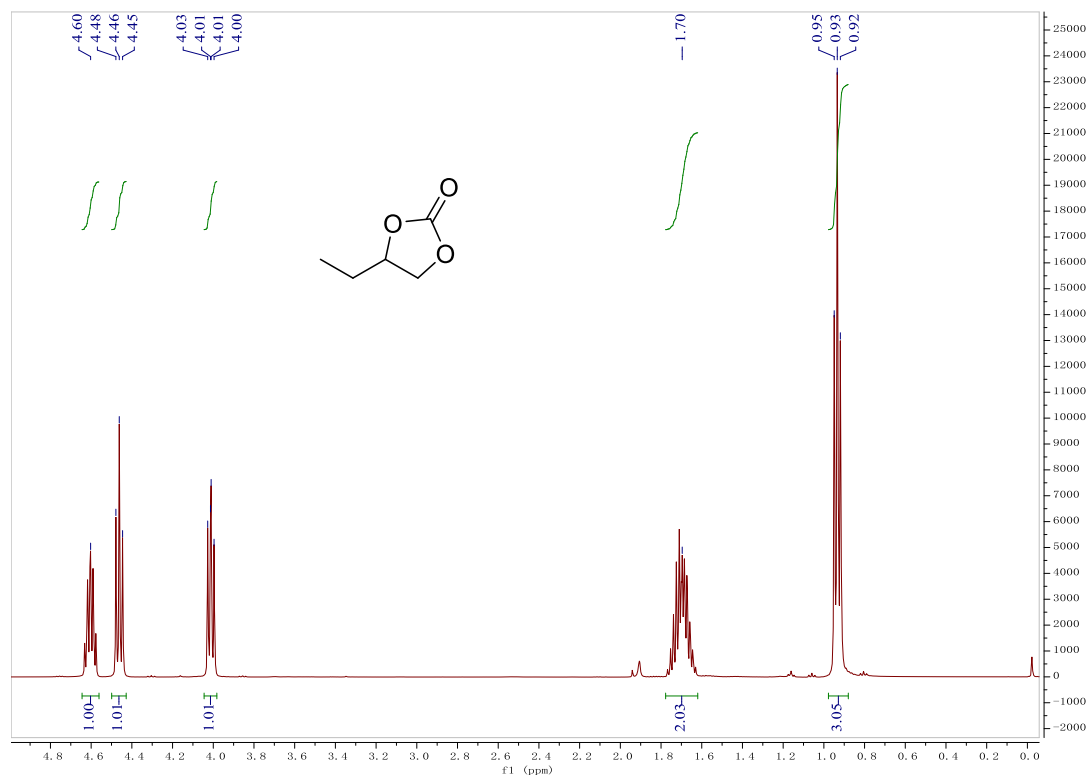


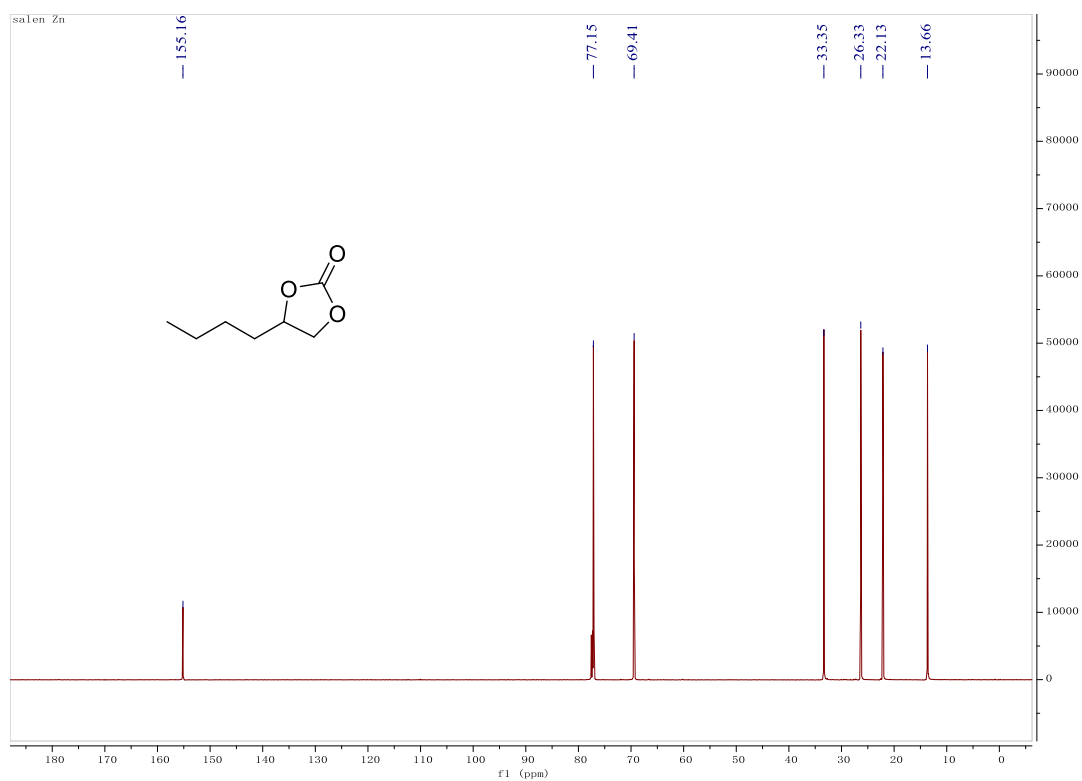
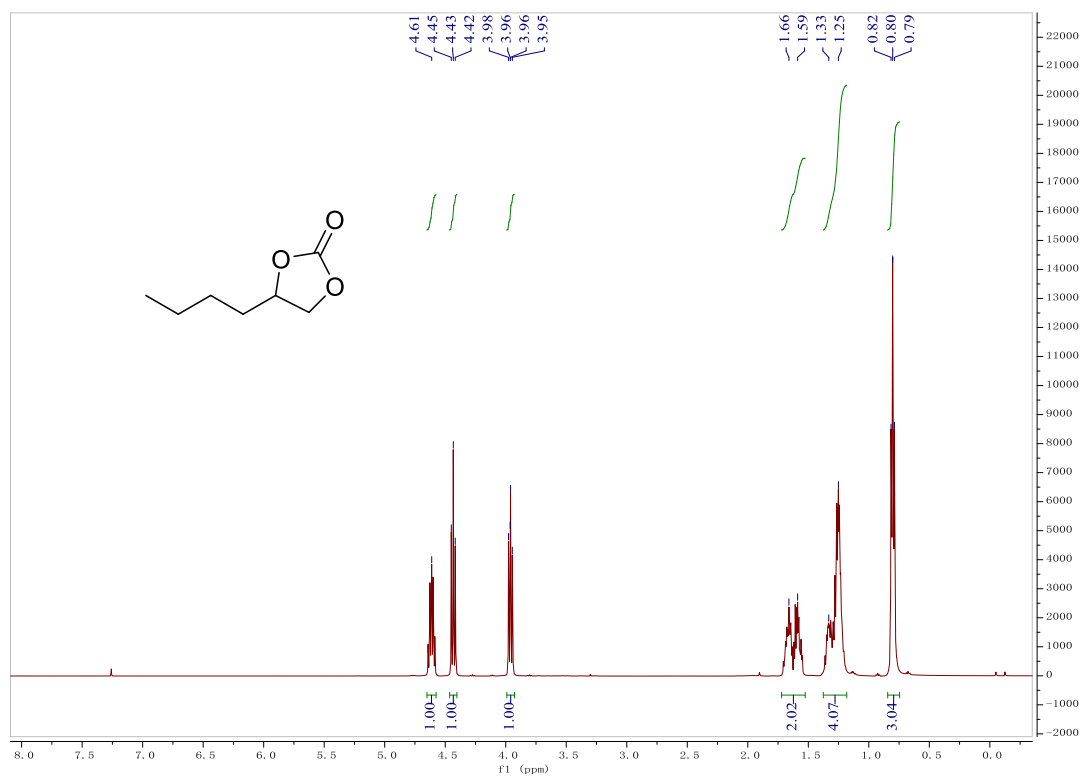
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, 25 °C, TMS):  $\delta$  (ppm) = 7.28-7.38 (m, 4H, ring ArH), 5.58-5.62 (t, 1H,  $J = 8$  Hz, PhCHO), 4.71-4.75 (t, 1H,  $J = 8$  Hz,  $\text{OCH}_2$ ), 4.26-4.30 (t, 1H,  $J = 8$  Hz,  $\text{OCH}_2$ );  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 101 MHz, 25 °C, TMS):  $\delta$  (ppm) = 153.75, 134.78, 128.72, 128.23, 124.83, 76.95, 70.13.

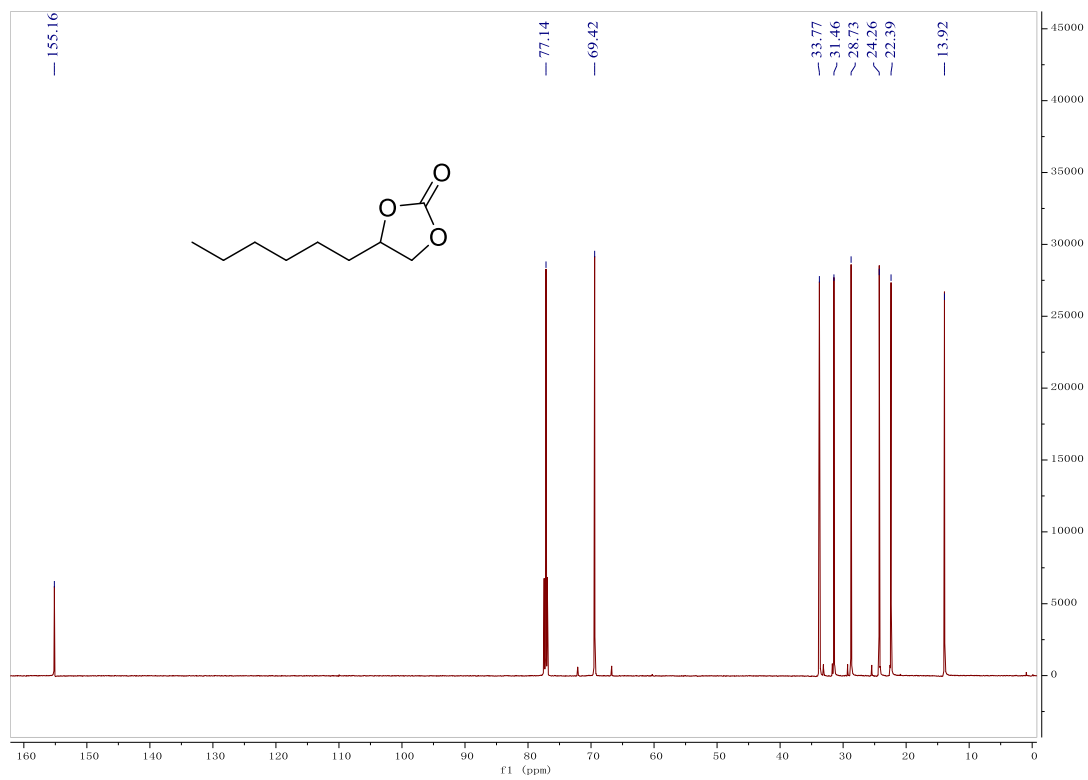
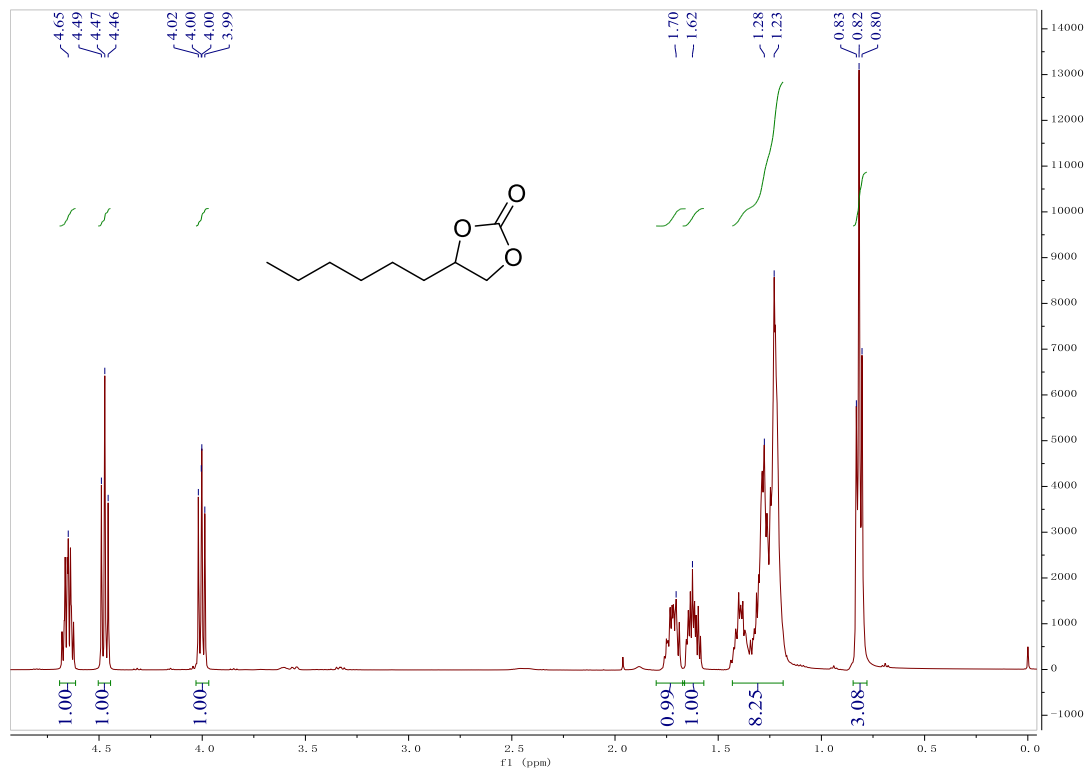


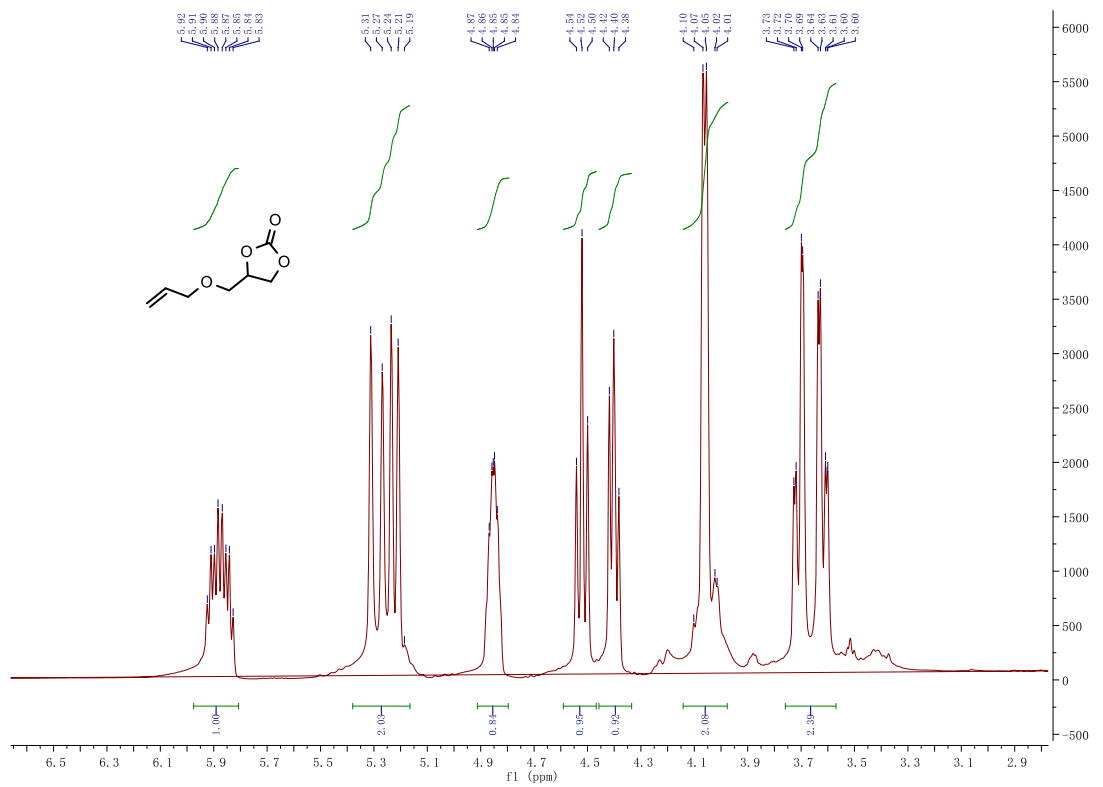
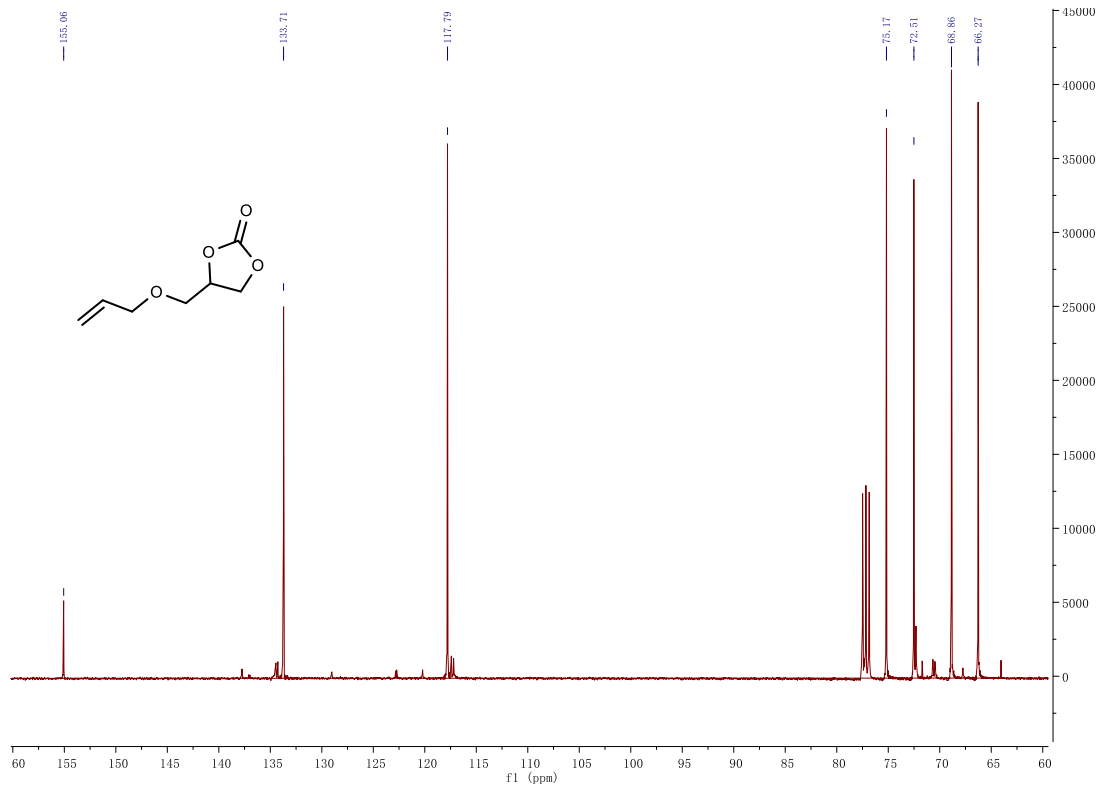


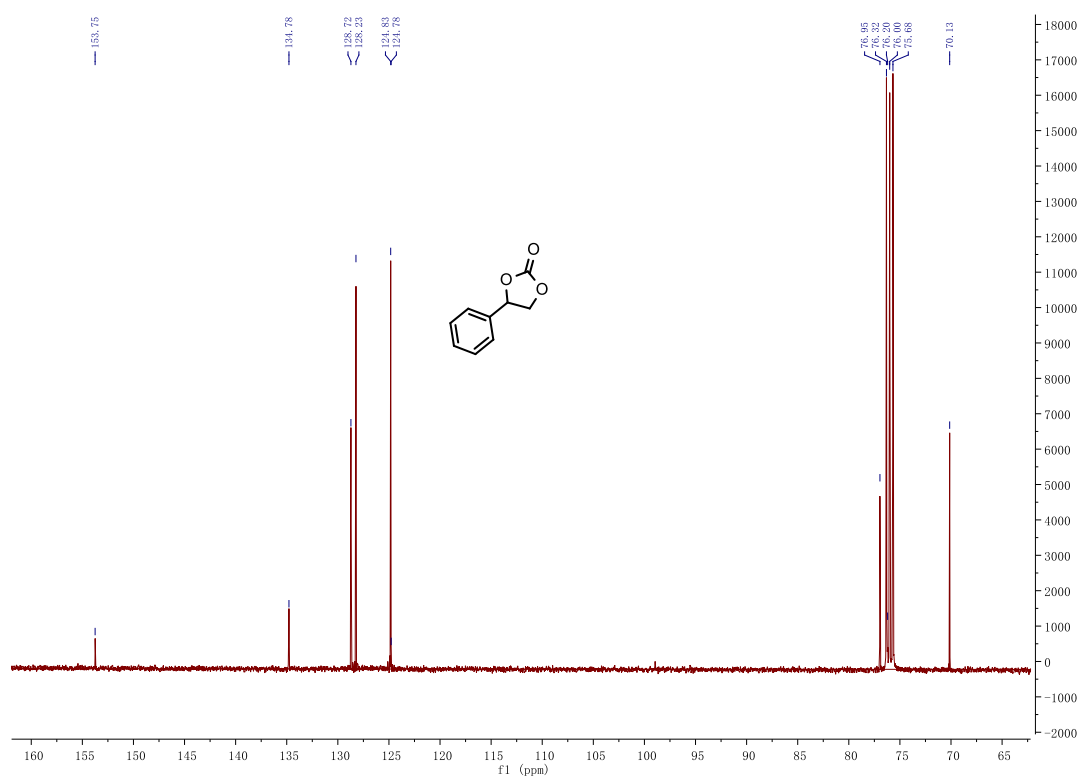
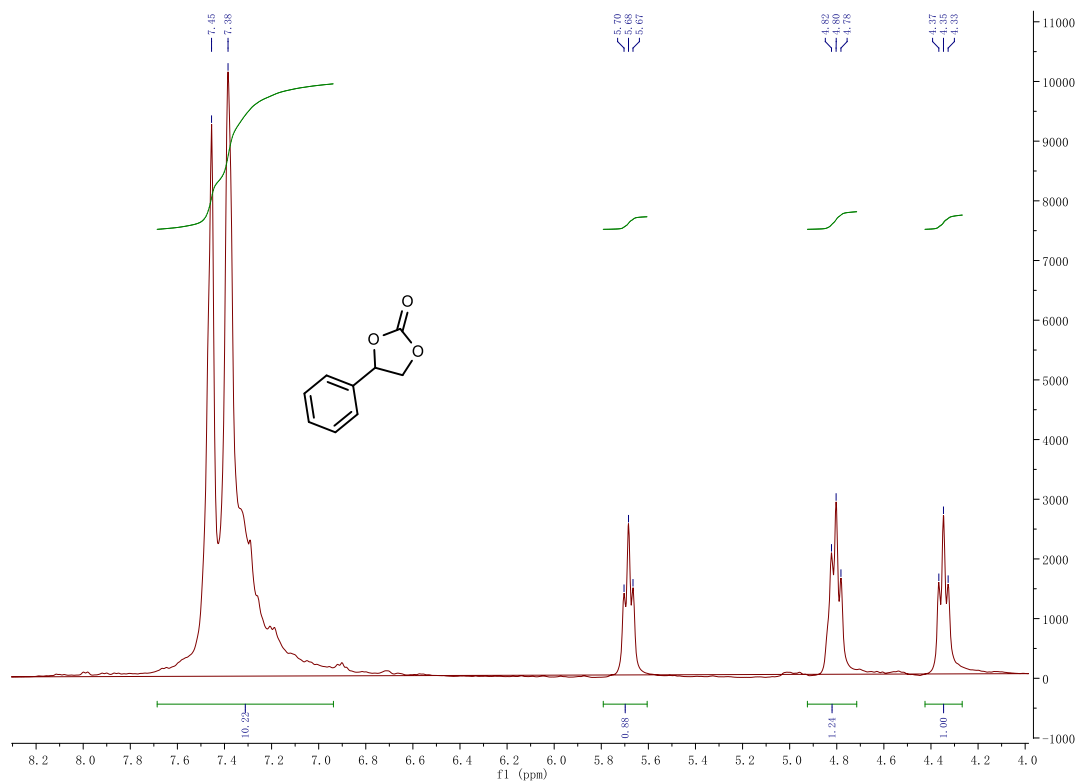






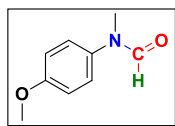






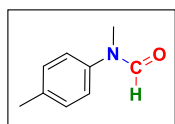
The  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectral copies of various synthesized formamides:

***N*-(4-methoxyphenyl)-*N*-methylformamide:**



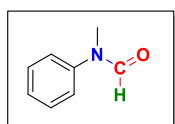
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz, 25  $^\circ\text{C}$ , TMS):  $\delta$  (ppm) = 8.30(s, 1H), 7.05-7.07(d, 2H),  $\delta$  6.89-6.91(d, 2H), 3.78(s, 3H), 3.23(s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 126 MHz, 25  $^\circ\text{C}$ , TMS):  $\delta$  (ppm) = 162.42, 158.24, 135.12, 124.52, 114.70, 55.44, 32.57.

***N*-methyl-*N*-(*p*-tolyl)formamide:**



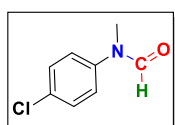
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz, 25  $^\circ\text{C}$ , TMS):  $\delta$  (ppm) = 8.25(s, 1H), 7.04-7.06(d, 2H), 6.88-6.90(d, 2H), 3.13(s, 3H), 2.20(s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 126 MHz, 25  $^\circ\text{C}$ , TMS):  $\delta$  (ppm) = 162.65, 139.50, 136.46, 130.15, 122.51, 32.27, 0.81.

***N*-methyl-*N*-phenylformamide:**



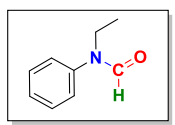
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz, 25  $^\circ\text{C}$ , TMS):  $\delta$  (ppm) = 8.45(s, 1H), 7.37-7.40(t, 2H), 7.23-7.26(t, 1H), 7.13-7.15(d, 2H), 3.29(s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 126 MHz, 25  $^\circ\text{C}$ , TMS):  $\delta$  (ppm) = 162.71, 141.99, 129.65, 126.57, 122.40, 32.23.

***N*-(4-chlorophenyl)-*N*-methylformamide:**



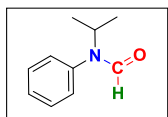
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, 25  $^\circ\text{C}$ , TMS):  $\delta$  (ppm) = 8.38(s, 1H), 7.34-7.37(d, 2H), 7.04-7.06(d, 2H), 3.25(s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 101 MHz, 25  $^\circ\text{C}$ , TMS):  $\delta$  (ppm) = 163.44, 142.05, 135.48, 131.09, 124.89, 33.42.

***N*-(1-Phenylethyl)formamide:**



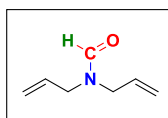
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz, 25  $^\circ\text{C}$ , TMS):  $\delta$  (ppm) = 8.14(s, 1H), 7.22-7.25(t, 2H), 7.11-7.14(t, 1H), 6.96-6.98(d, 2H), 3.66-3.70(m, 2H), 0.96-0.99(t, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 101 MHz, 25  $^\circ\text{C}$ , TMS):  $\delta$  (ppm) = 162.56, 140.49, 129.66, 127.09, 124.28, 40.32, 12.93.

***N*-isopropyl-*N*-phenylformamide:**



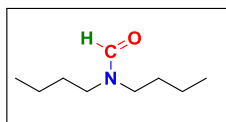
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz, 25 °C, TMS):  $\delta$  (ppm) = 7.99-8.03(s, 1H), 6.99-7.27(m, 5H), 4.61-4.66(m, 1H), 1.04-1.05(d, 6H), 3.66-3.70(m, 2H), 0.96-0.99(t, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 126 MHz, 25 °C, TMS):  $\delta$  (ppm) = 163.13, 137.96, 129.29, 128.80, 128.37, 46.16, 20.77.

***N,N*-diallylformamide:**



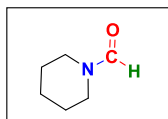
$^1\text{H}$  NMR ( $\text{DMSO-}d_6$ , 400 MHz, 25 °C, TMS):  $\delta$  (ppm) = 8.09(s, 1H), 5.63-5.83(m, 2H), 5.09-5.19(m, 4H), 3.79-3.84(m, 4H);  $^{13}\text{C}$  NMR ( $\text{DMSO-}d_6$ , 101 MHz, 25 °C, TMS):  $\delta$  (ppm) = 164.40, 136.19, 134.60, 119.59, 119.07, 50.51, 45.44.

***N,N*-dibutylformamide:**



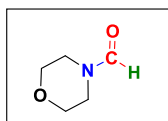
$^1\text{H}$  NMR ( $\text{DMSO-}d_6$ , 400 MHz, 25 °C, TMS):  $\delta$  (ppm) = 8.00(s, 1H), 3.16-3.21(m, 4H), 1.38-1.49(m, 4H), 1.19-1.27(m, 4H); 0.86-0.90(m, 6H);  $^{13}\text{C}$  NMR ( $\text{DMSO-}d_6$ , 101 MHz, 25 °C, TMS):  $\delta$  (ppm) = 164.33, 47.87, 42.61, 32.08, 30.77, 21.39, 20.91, 15.47, 15.34.

***N*-Cyclohexylformamide:**



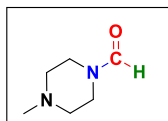
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, 25 °C, TMS):  $\delta$  (ppm) = 7.96(s, 1H), 6.10(s, 1H), 3.75-3.83(m, 1H), 1.56-1.87(m, 4H), 1.11-1.38(m, 6H);  $^{13}\text{C}$  NMR ( $\text{DMSO-}d_6$ , 101 MHz, 25 °C, TMS):  $\delta$  (ppm) = 165.31, 162.10, 52.56, 48.51, 35.83, 34.21, 26.81, 26.37, 26.13.

***Morpholine-4*-carbaldehyde:**



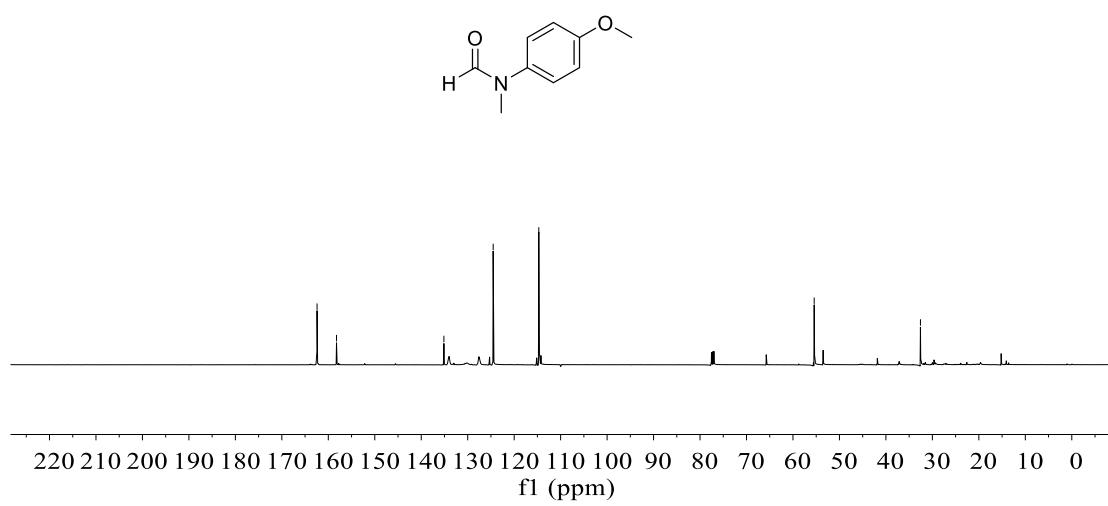
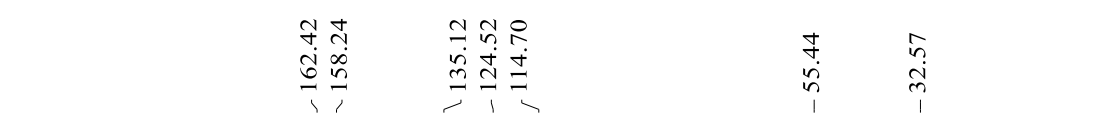
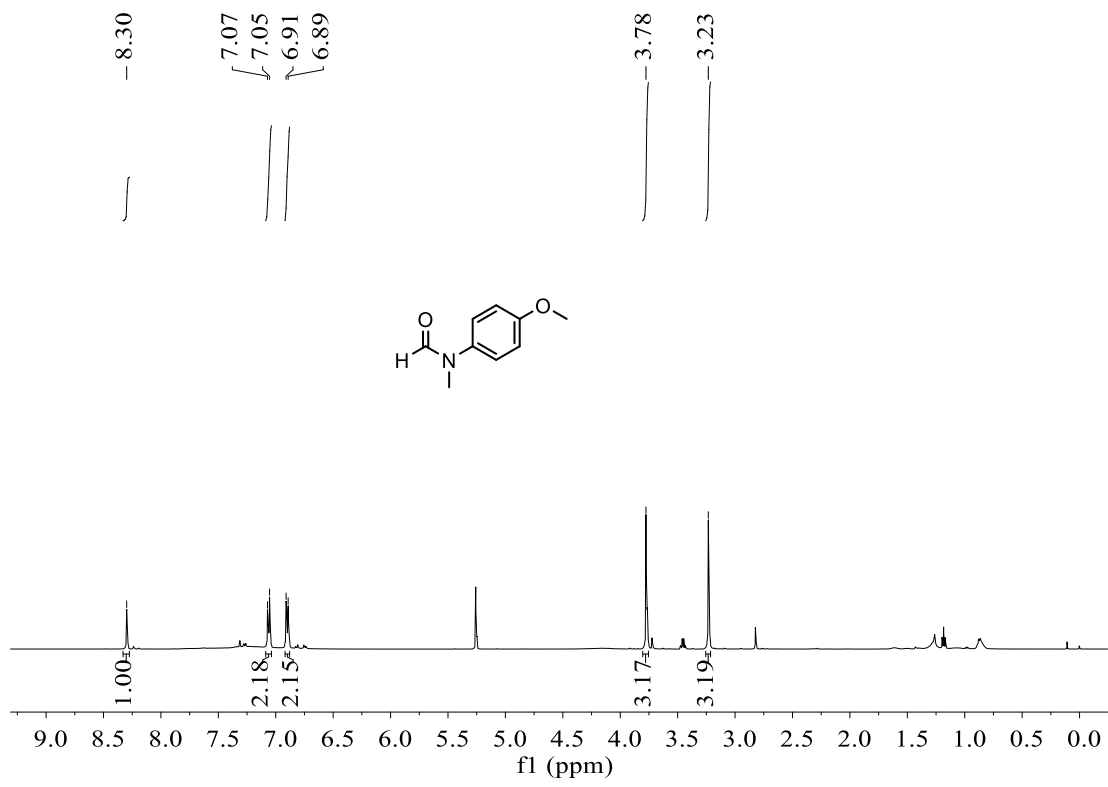
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, 25 °C, TMS):  $\delta$  (ppm) = 7.87(s, 1H), 3.48-3.52(m, 4H), 3.39-3.42(t, 2H), 3.19-3.21(t, 2H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 101 MHz, 25 °C, TMS):  $\delta$  (ppm) = 159.94, 66.12, 65.30, 44.72, 39.54 .

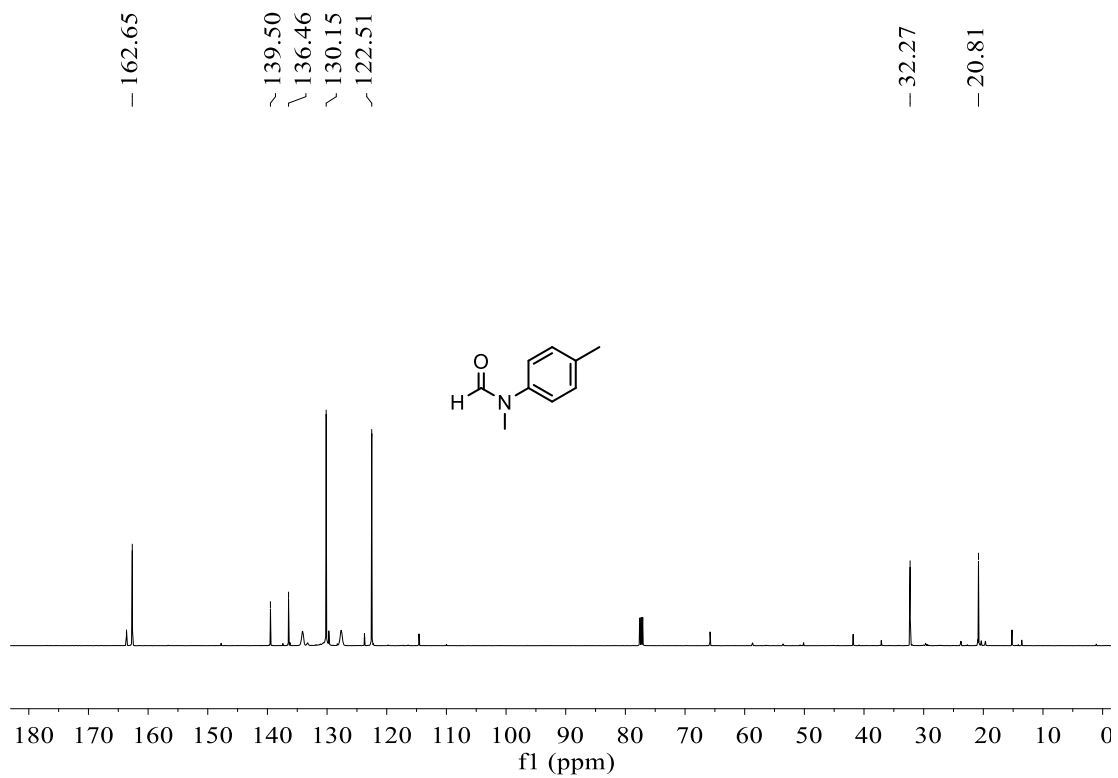
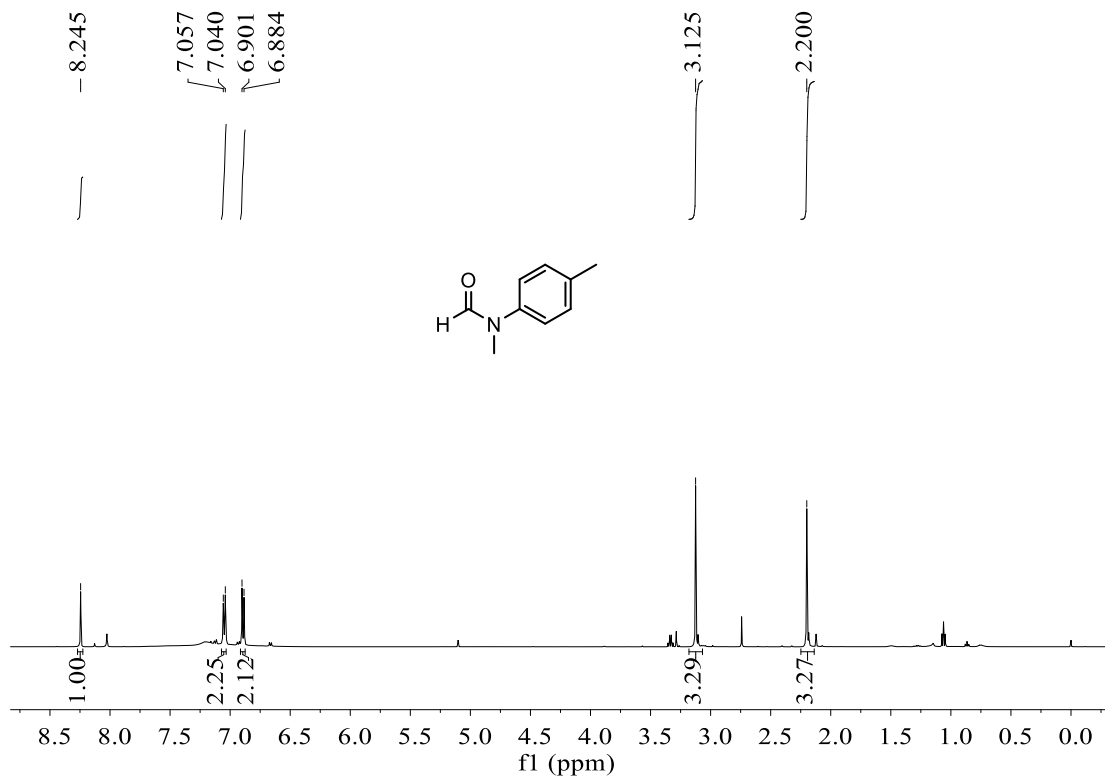
***4*-methylpiperazine-1-carbaldehyde:**

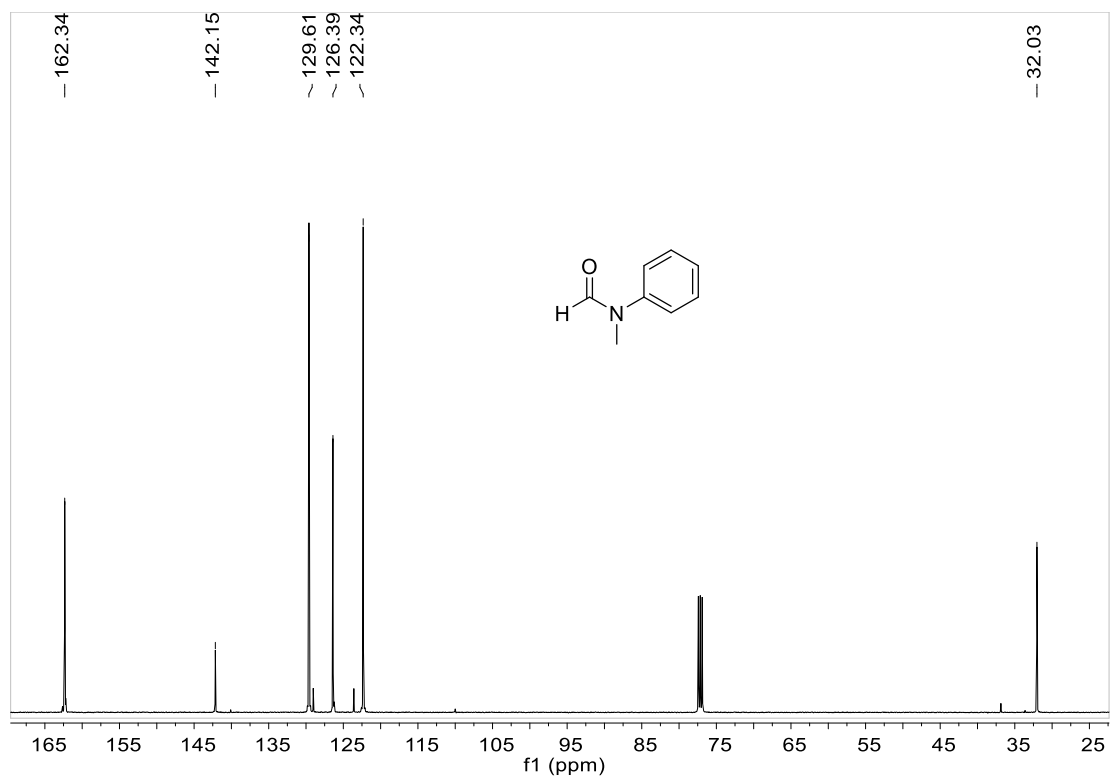
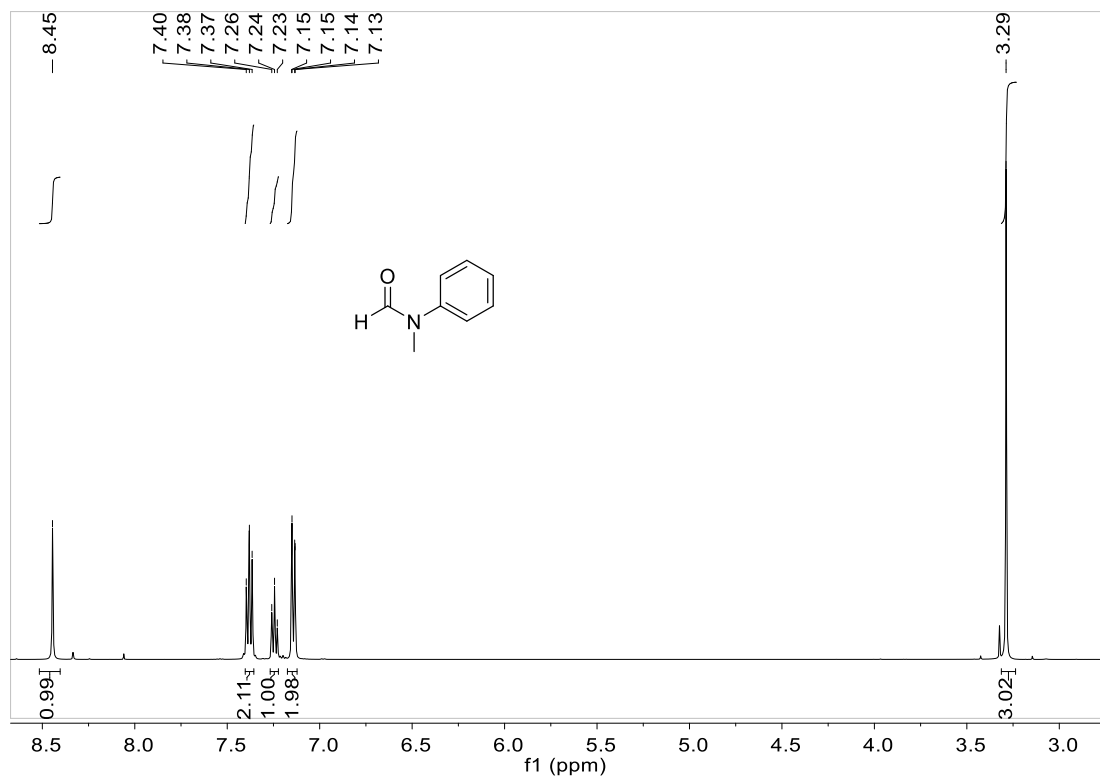


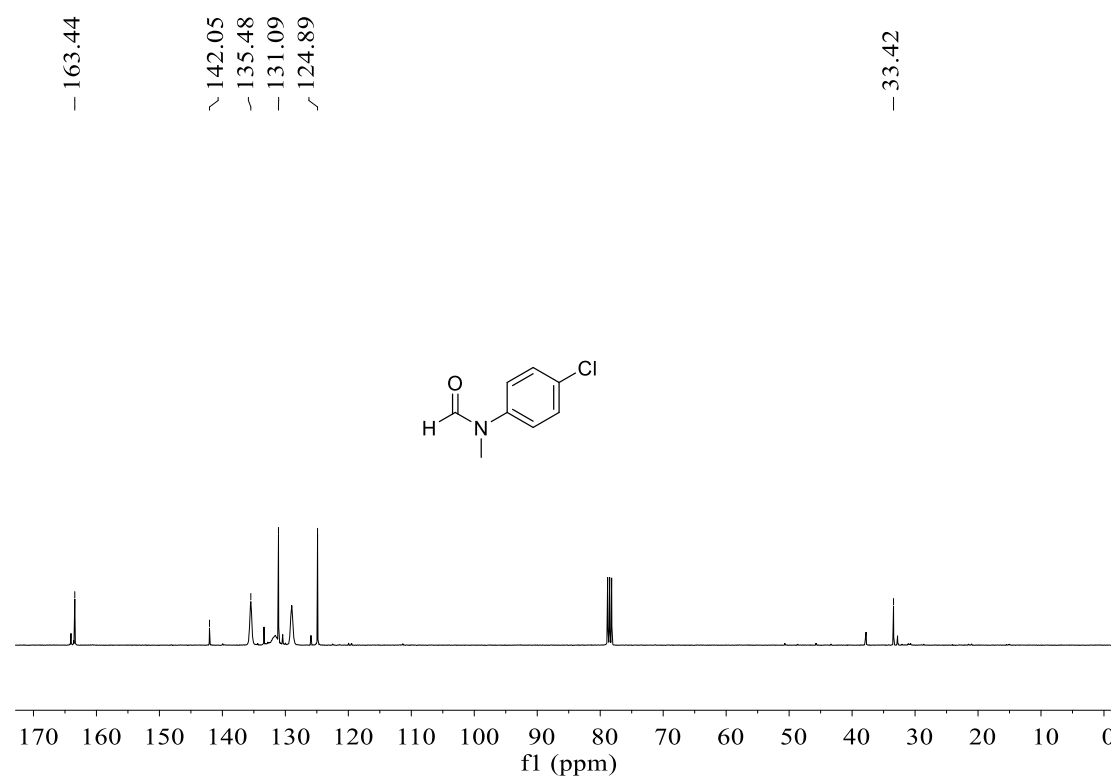
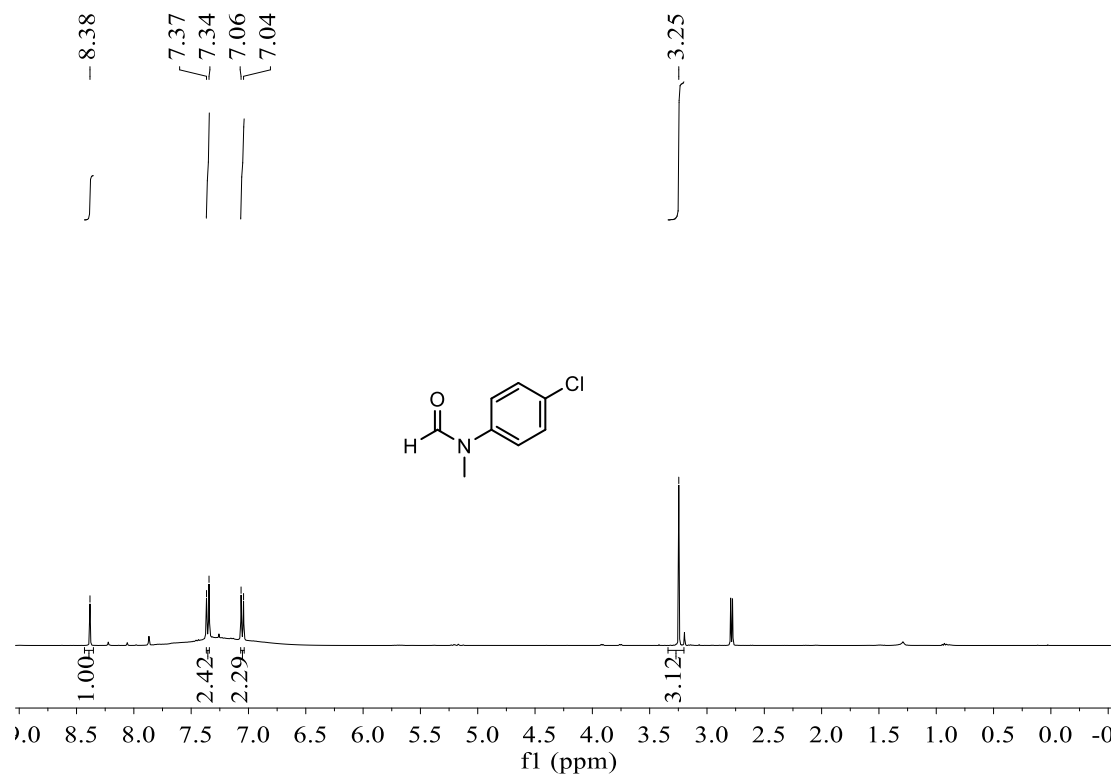
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz, 25 °C, TMS):  $\delta$  (ppm) = 7.94(s, 1H), 3.48-3.50(t, 2H), 3.30-3.33(t, 2H), 2.24-2.36(m, 4H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 101 MHz, 25 °C, TMS):  $\delta$  (ppm) = 162.03, 56.48, 55.32, 47.17, 46.56, 40.90.

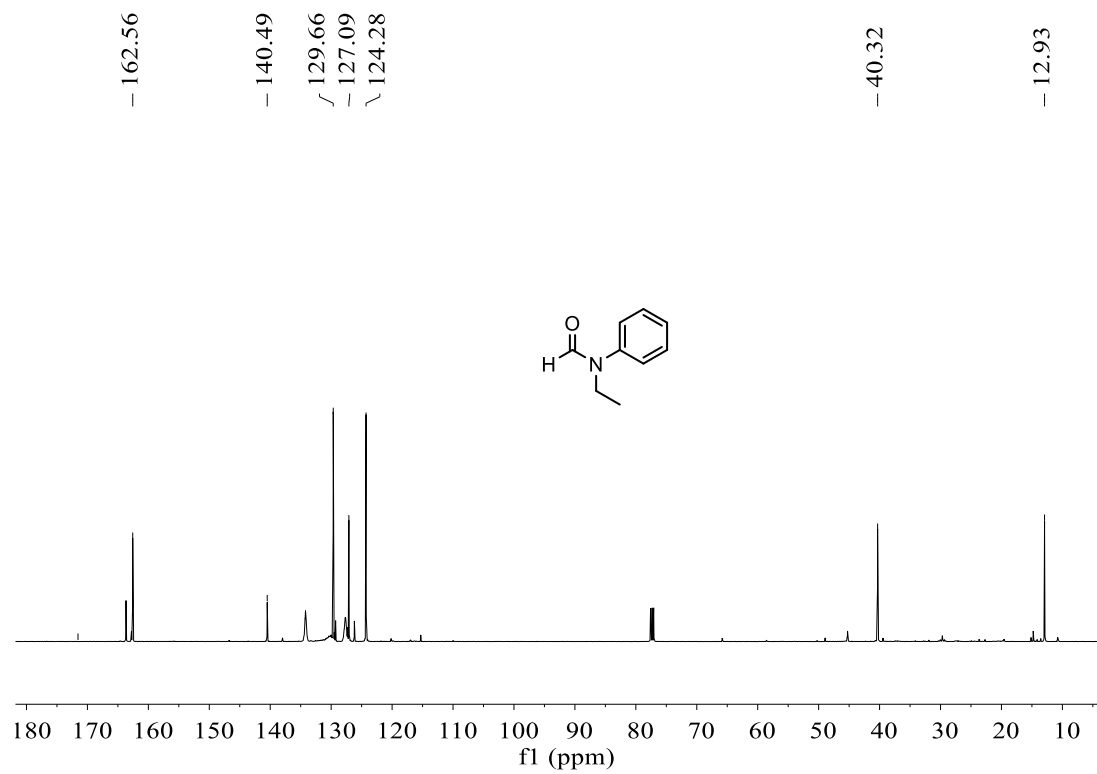
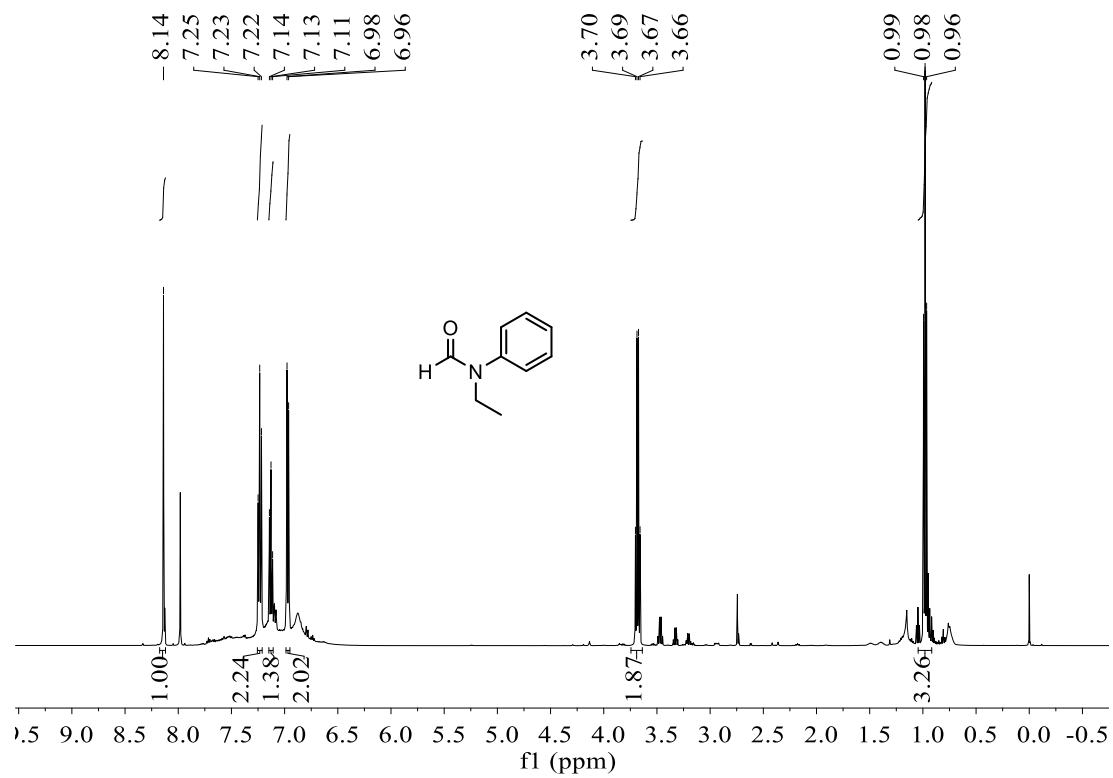


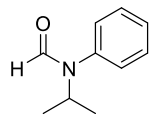
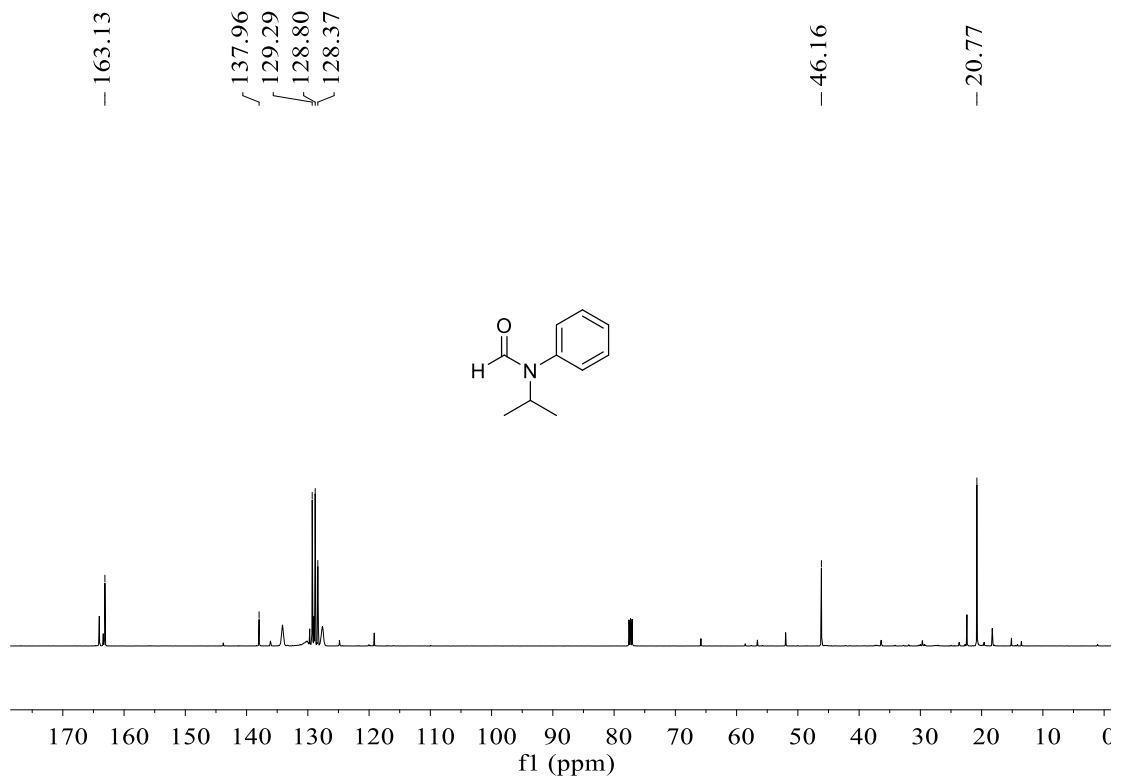
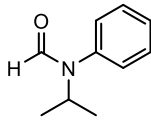
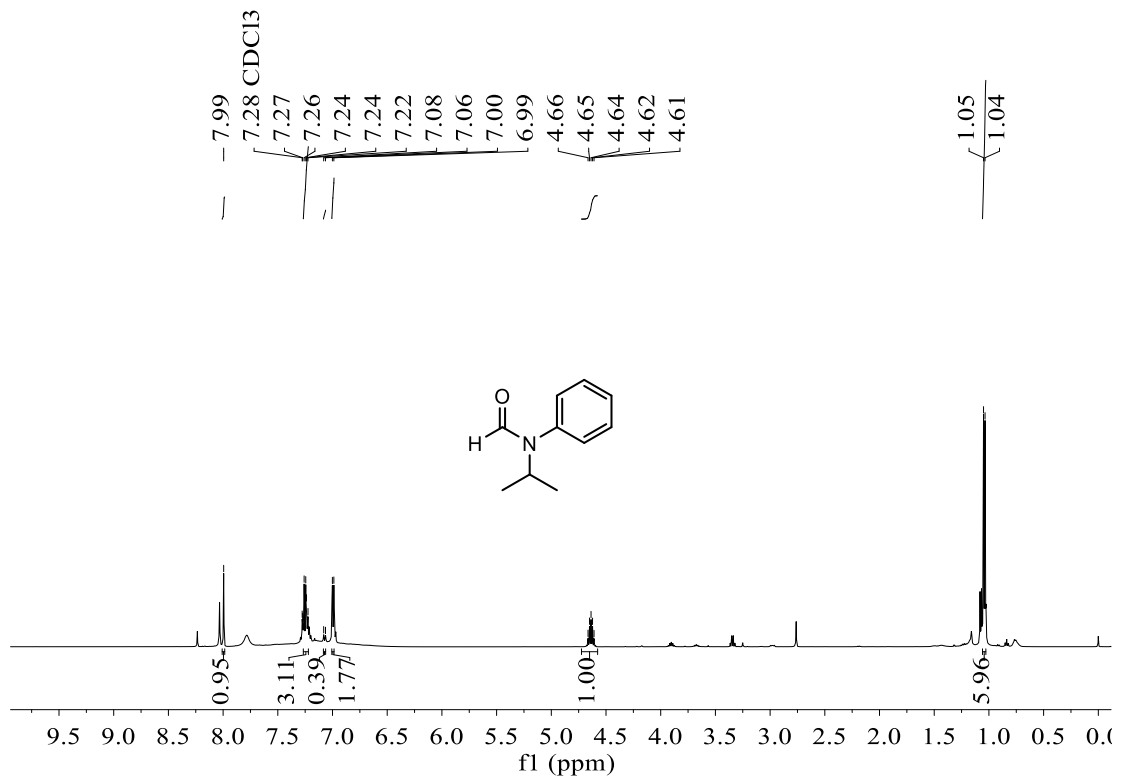


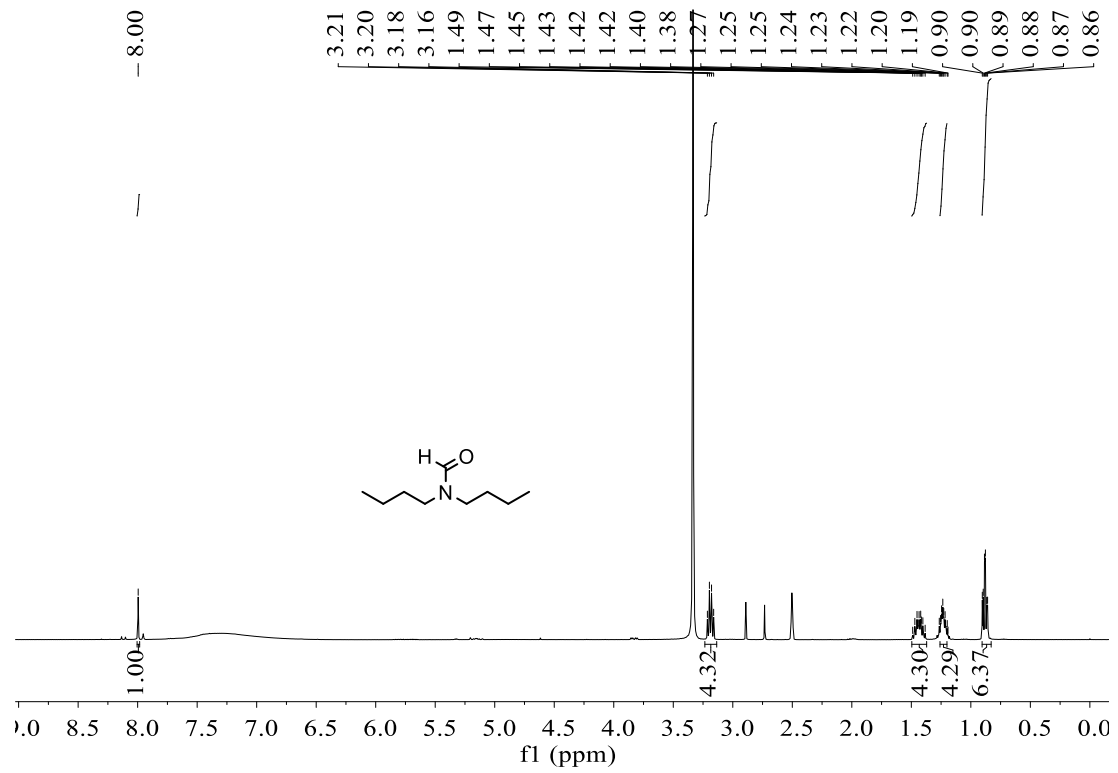
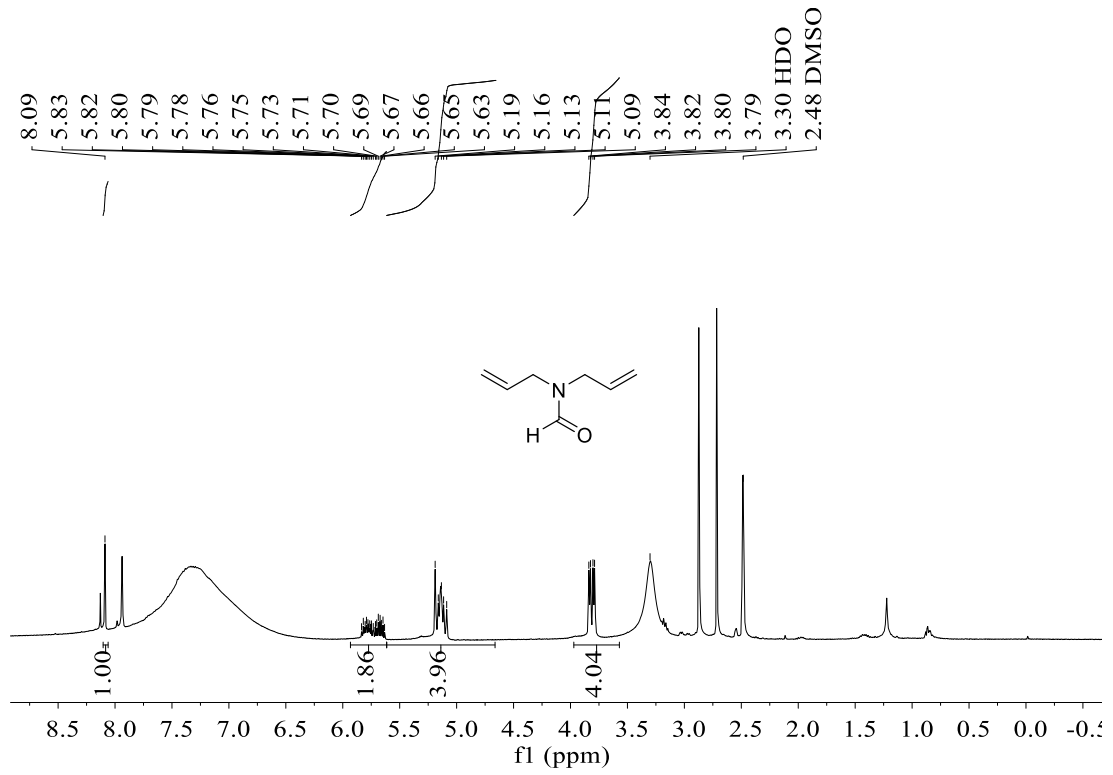


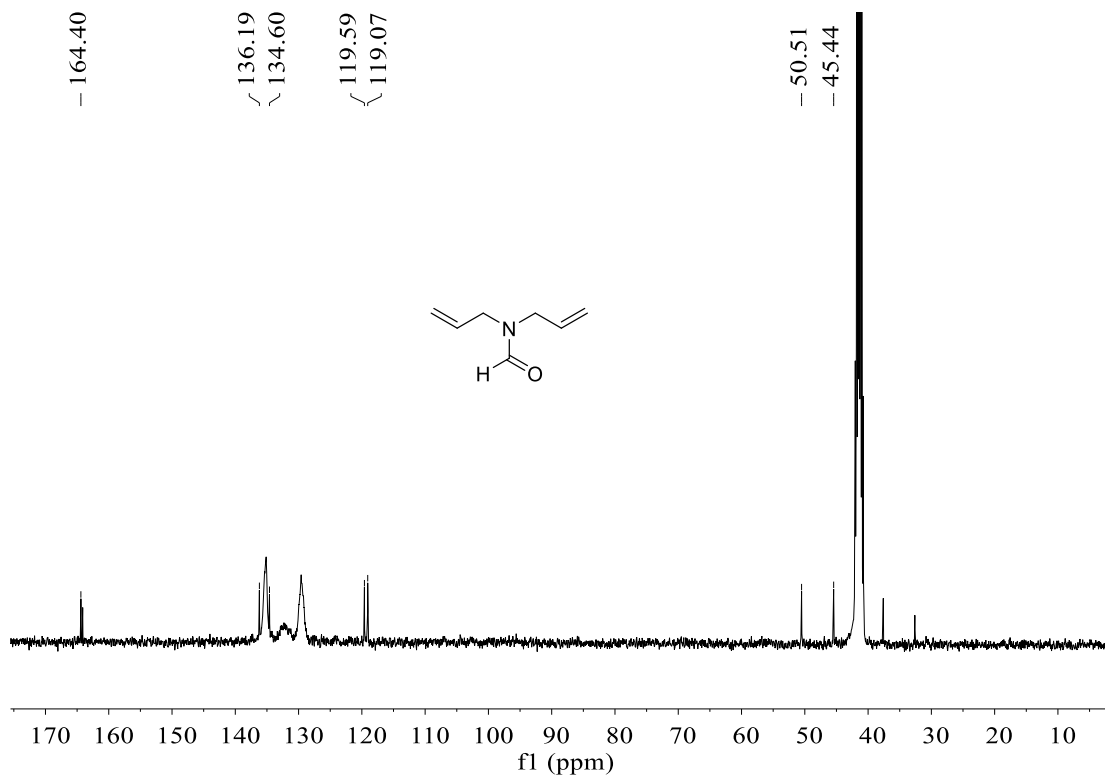
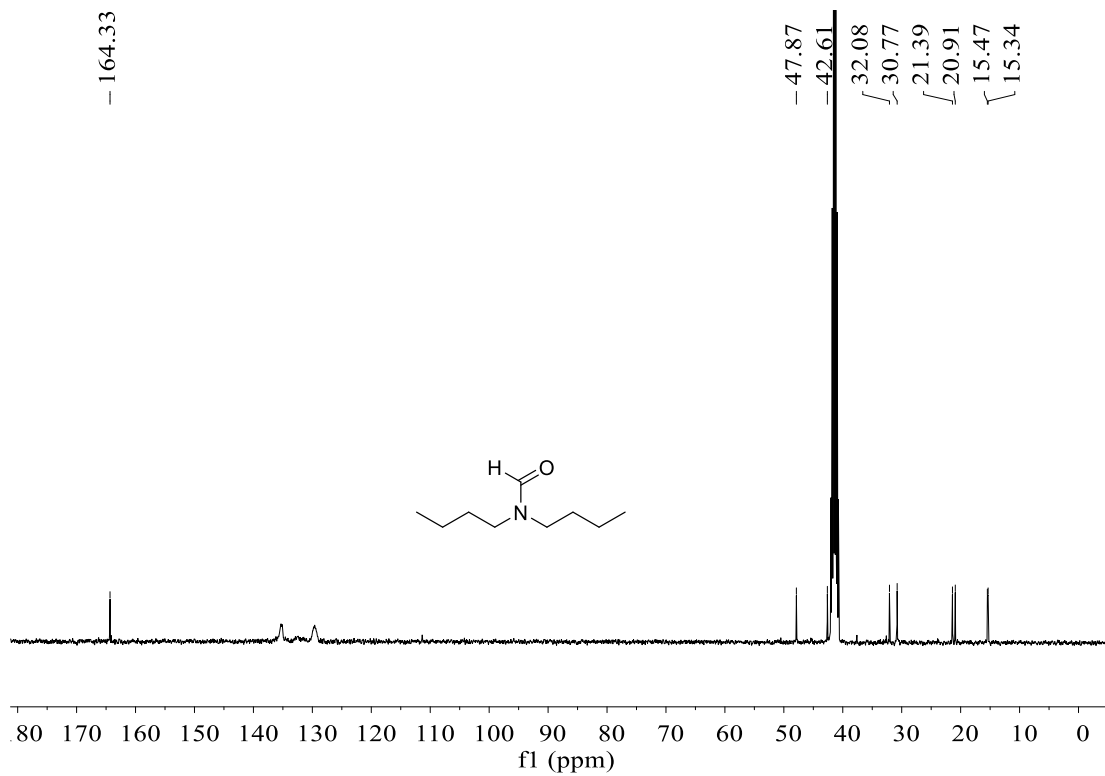




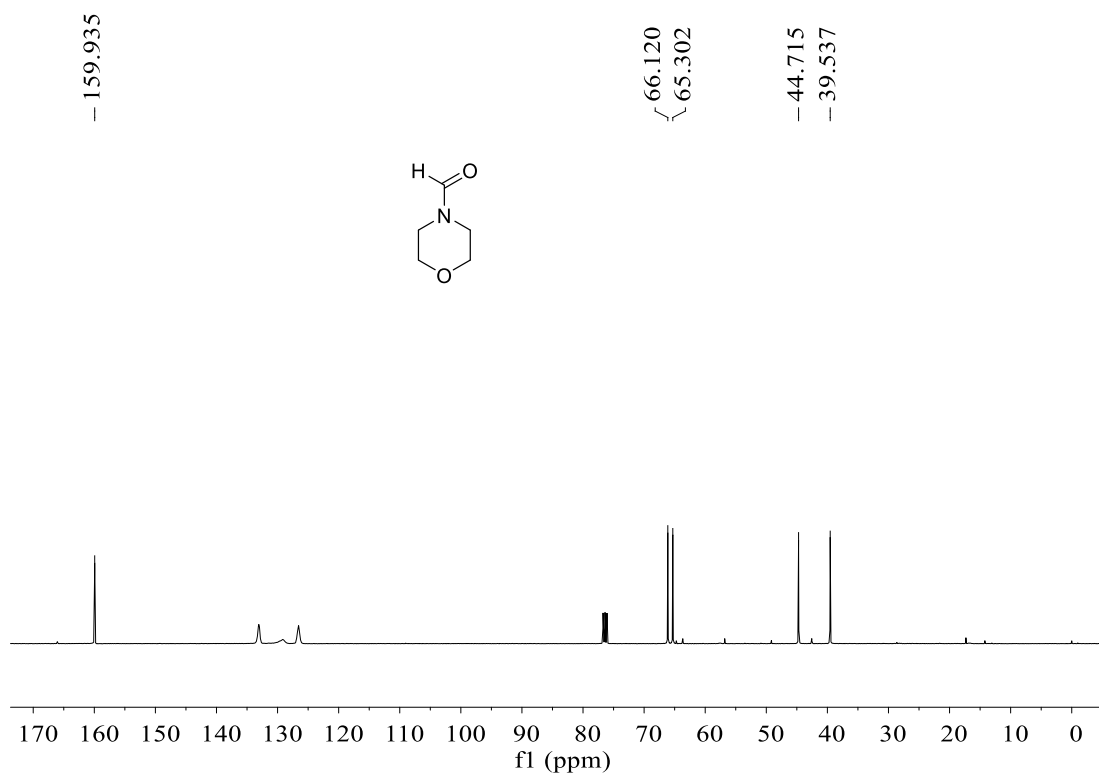
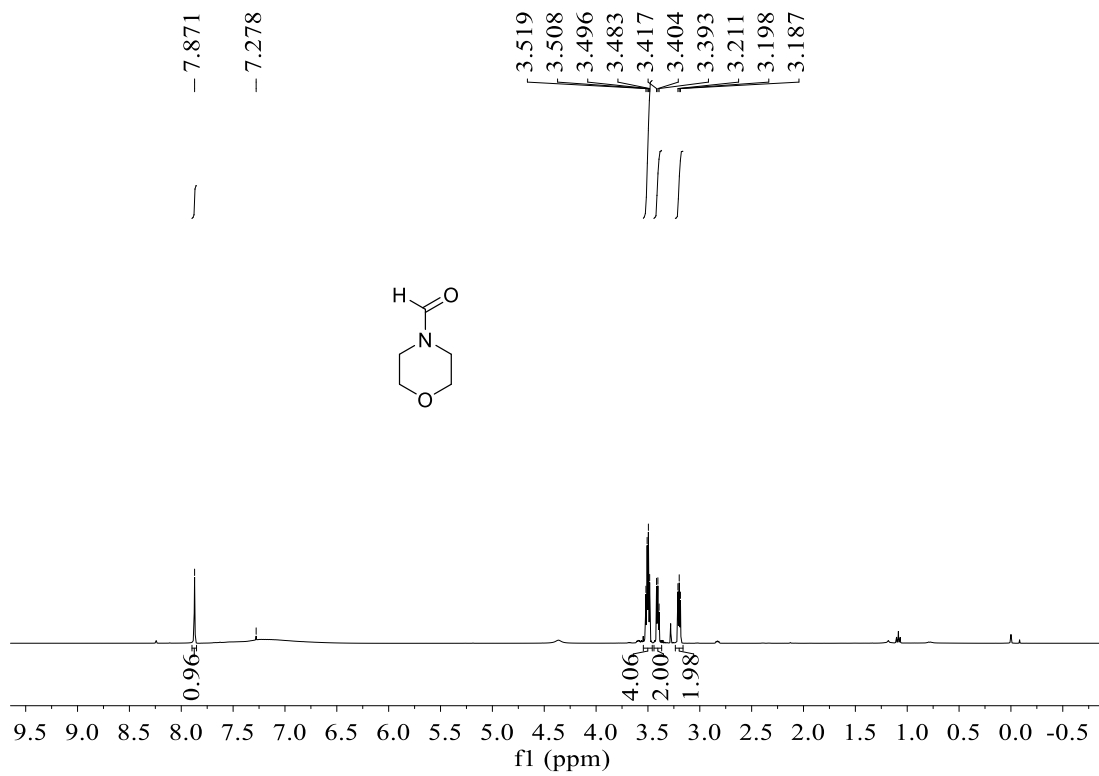


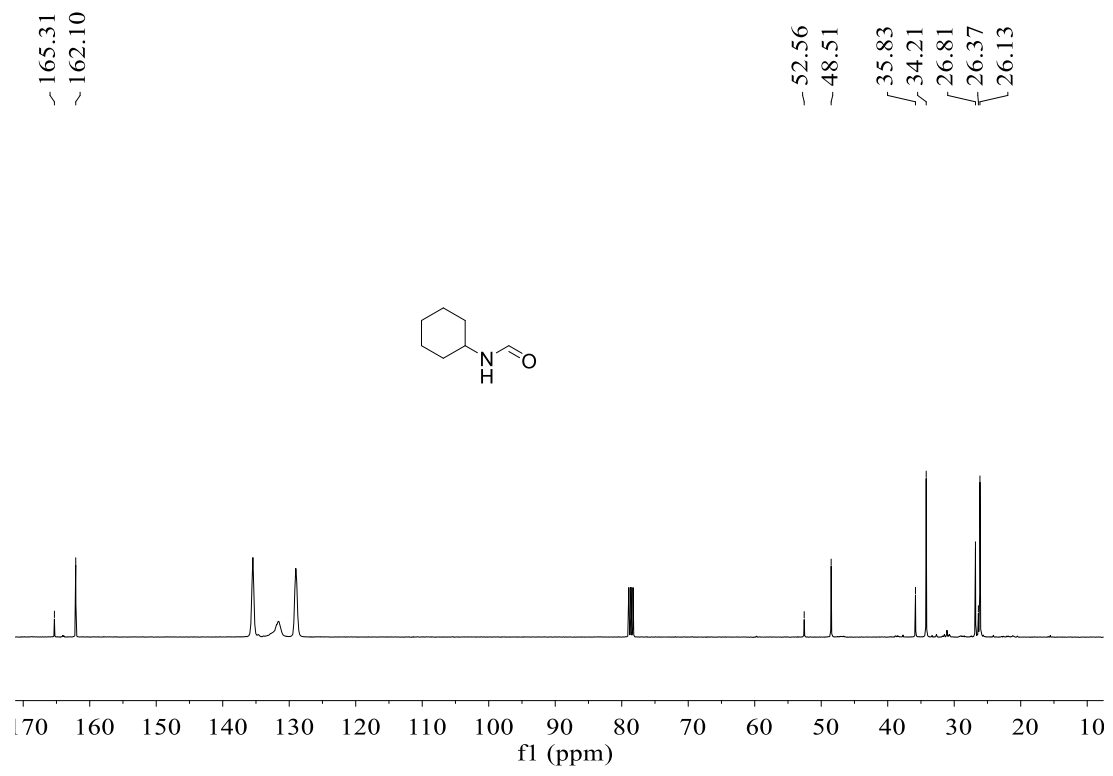
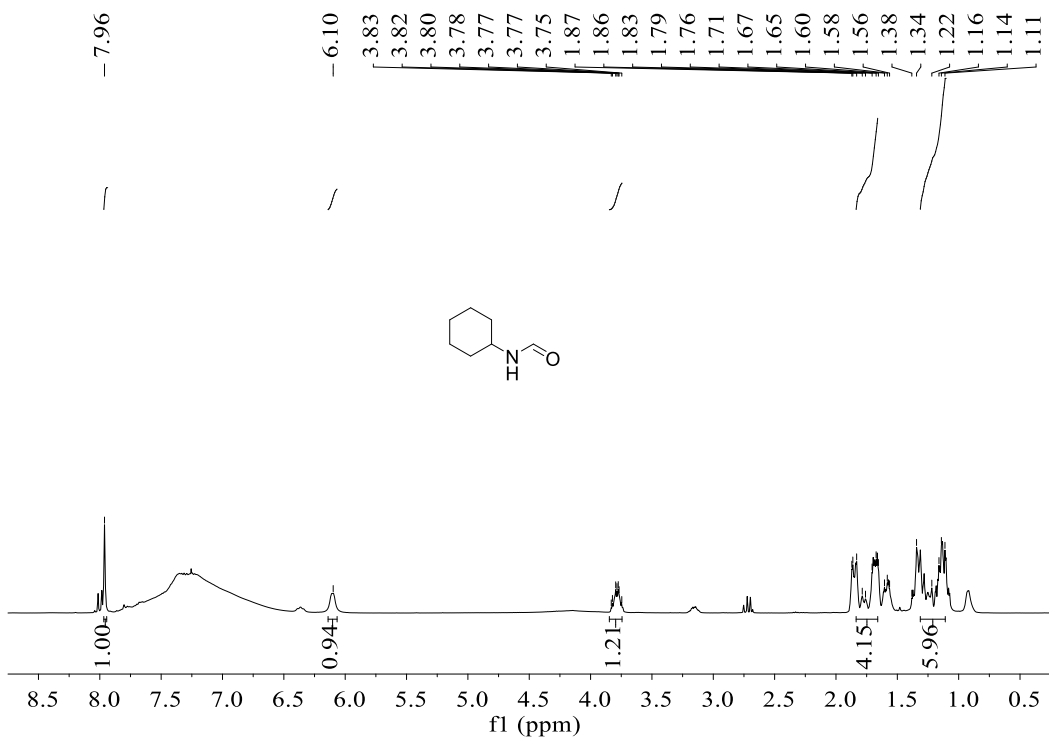


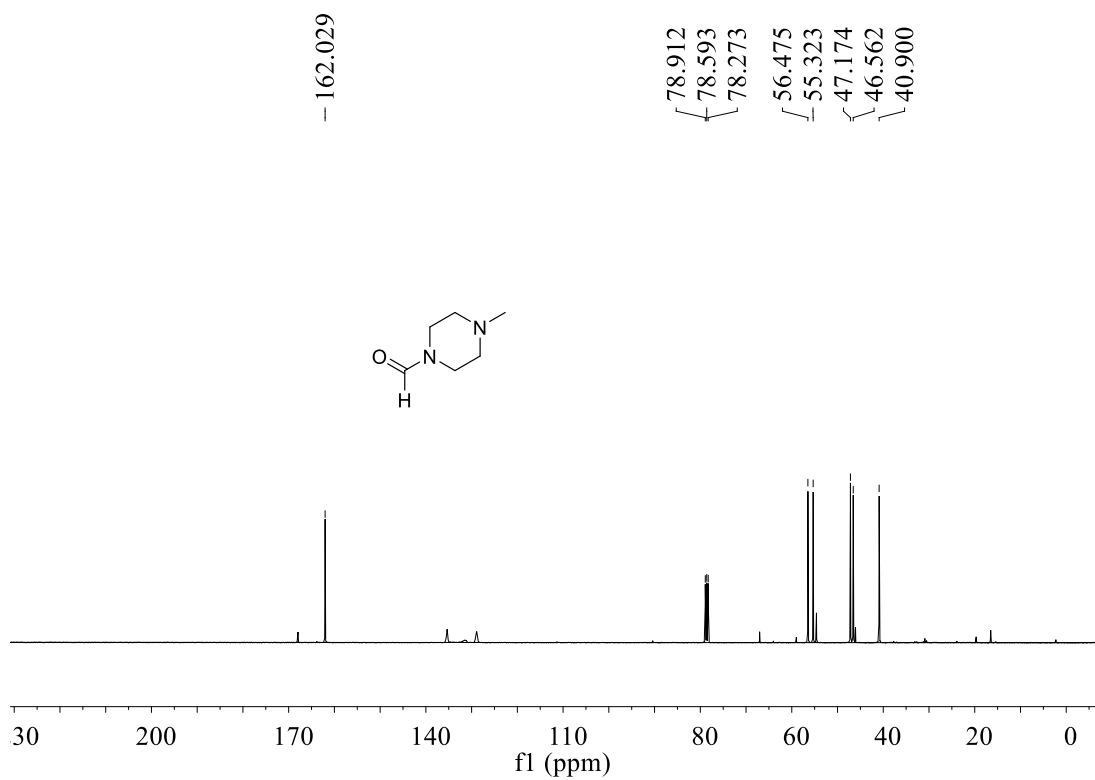
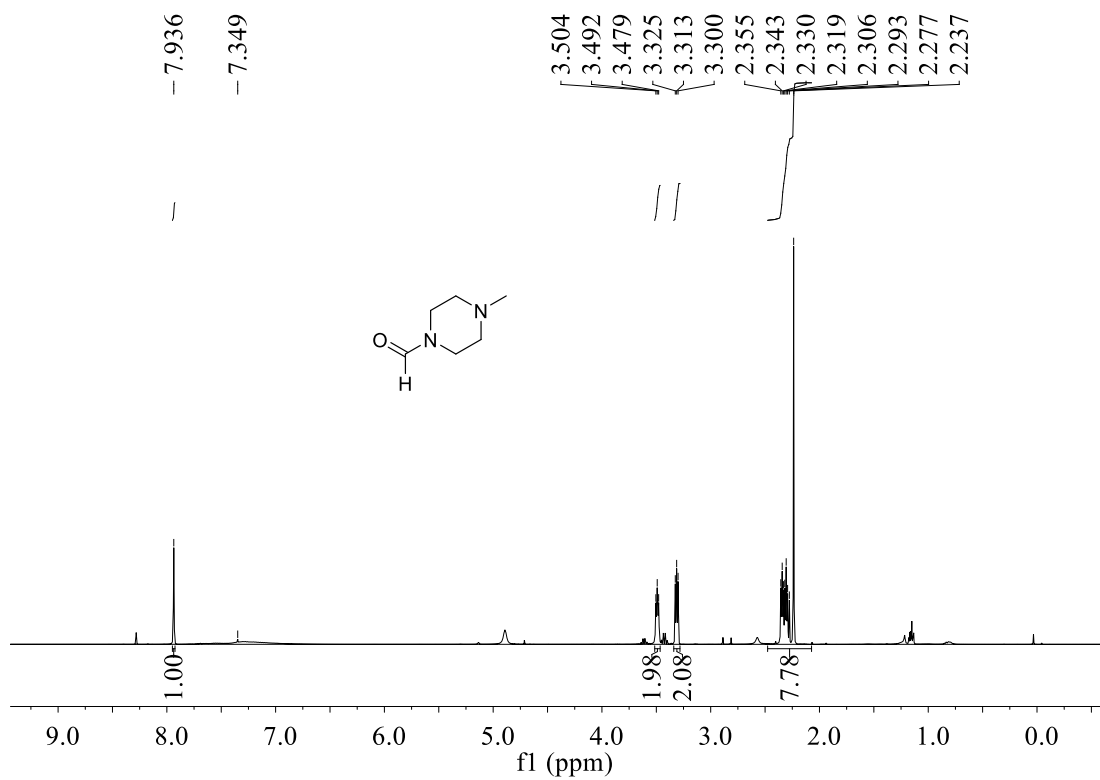












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