Supporting Information

Imidazolium-based ionic liquids containing multipoint hydrogen bond donors as bifunctional organocatalysts for efficient cooperative conversion of CO_2 to cyclic carbonates

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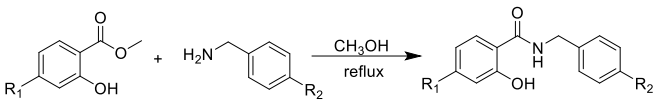
Content

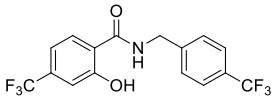
1. Synthesis of Salicylamides 1a-1e.



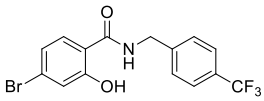
1a: R_1= CF_3; R_2= CF_3;
1b: R_1= Br; R_2= CF_3;
1c: R_1= H; R_2= CF_3;
1d: R_1= OCH_3; R_2= CF_3;
1e: R_1= CF_3; R_2= H;

Scheme S1. Synthetic route for salicylamides **1a-1e**

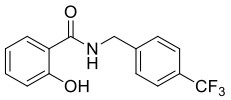
General procedure: Methyl salicylate (50.0 mmol), benzylamine (50.0 mmol) and methanol (50 mL) were added to a round bottom flask and heated to reflux for 5 hours. The mixture was cooled to room temperature and the solvent was removed under reduced pressure to give a solid mixture. The mixture was purified by silica gel column chromatography by using dichloromethane/petroleum ether as the eluent.



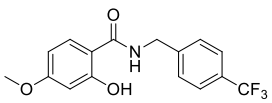
(1a) Yield: 15.43 g, 85%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC) δ 12.28 (s, 1H), 7.64 (s, 1H), 7.62 (s, 1H), 7.46-7.48 (m, 3H), 7.26 (s, 1H), 6.71 (s, 1H), 4.72 (d, *J* = 4.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 ºC) δ 169.04, 161.71, 141.07, 136.05 (q, *J* = 33 Hz), 130.37 (q, *J* = 32 Hz), 128.07, 126.09, 125.90 (q, *J* = 4.0 Hz), 125.29, 124.47, 122.59, 121.76, 116.56, 116.11 (q, *J* = 4.0 Hz), 115.13 (q, *J* = 3.0 Hz), 43.32.



(1b) Yield: 14.92 g, 80%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC) δ 12.30 (s, 1H), 7.63 (d, *J* = 8.0 Hz, 2H), 7.46 (d, *J* = 8.0 Hz, 2H), 7.20-7.22 (m, 2H), 6.97-7.00 (m, 2H), 6.57 (s, 1H), 4.70 (d, *J* = 4.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 ºC) δ 169.44, 162.28, 141.23, 130.39, 130.06, 128.52, 128.03, 126.26, 125.86 (q, *J* = 4.0 Hz), 125.28, 122.58, 122.13, 121.93, 112.75, 43.17.

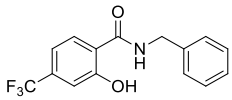


(1c) Yield: 13.13 g, 89%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC) δ 12.14 (s, 1H), 7.62 (d, *J* = 8.0 Hz, 2H), 7.36-7.48 (m, 4H), 7.01 (d, *J* = 8.0 Hz, 1H), 6.85 (t, *J* = 8.0 Hz, 1H), 6.66 (s, 1H), 4.71 (d, *J* = 8.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 ºC) δ 170.01, 161.64, 141.57 (q, *J* = 1.0 Hz), 134.60, 130.26, 129.92, 127.97, 125.80 (q, *J* = 4.0 Hz), 125.33, 125.27, 122.62, 118.79, 118.78, 113.83, 43.08.



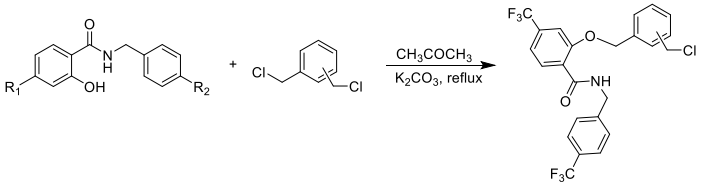
(1d) Yield: 8.45 g, 52%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC) δ 11.63 (s, 1H), 7.18-7.31 (m, 4H), 6.85-6.96 (m, 2H), 6.75 (d, *J* = 4.0 Hz, 1H), 6.45 (s, 1H), 4.55 (d, *J* = 8.0 Hz, 2H), 3.67 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 ºC) δ 169.89, 164.61, 163.96, 141.82,

128.05, 127.92, 127.44, 126.53, 125.76 (q, J = 4.0 Hz), 125.34, 122.64, 107.20, 106.74, 101.60, 77.20, 55.46, 42.96.



(1e) Yield: 12.25 g, 83%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 12.44 (s, 1H), 7.45 (d, J = 8.0 Hz, 1H), 7.34-7.41 (m, 5H), 7.06 (d, J = 8.0 Hz, 1H), 6.61 (s, 1H), 4.66 (d, J = 4.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 168.81, 161.68, 139.90, 135.77 (q, J = 64 Hz), 128.98, 128.07, 127.92, 127.24, 126.11, 124.53, 121.81, 116.82, 115.98 (q, J = 4.0 Hz), 114.98 (q, J = 4.0 Hz), 43.91.

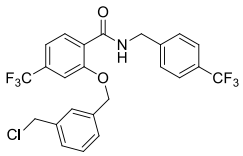
2. Synthesis of Monobranched Substituted Amides 2a-2g.



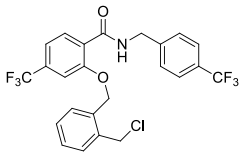
2a: Meta-; R_1= CF_3; R_2= CF_3;
2b: Ortho-; R_1= CF_3; R_2= CF_3;
2c: Para-; R_1= CF_3; R_2= CF_3;
2d: Meta-; R_1= Br; R_2= CF_3;
2e: Meta-; R_1= H; R_2= CF_3;
2f: Meta-; R_1= OCH_3; R_2= CF_3;
2g: Meta-; R_1= CF_3; R_2= H;

Scheme S2. Synthetic route for monobranched substituted amides **2a-2g**

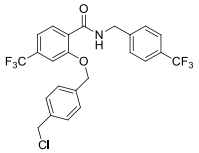
General procedure: Disubstituted benzyl chloride (20.0 mmol), potassium carbonate (40.0 mmol), acetone (30.0 mL) were added to a three necked flask and heated to reflux under stirring. A solution of amide compound 1 (20.0 mmol) in acetone (30.0 mL) was added dropwise to the reaction mixture, and the progress of the reaction was monitored by TLC. When the amount of the produced monosubstituted amide compound no longer increases, the reaction is stopped. After removal of the solvent *in vacuo* , distilled water (50 mL) was added to the residue and extracted with CH_2Cl_2 (3×50 mL). The organic phases were combined and dried over anhydrous sodium sulfate. The resulting solution was concentrated by rotary evaporator and purified by silica gel column chromatography dichloromethane/petroleum ether as the eluent to gave a white solid powder.



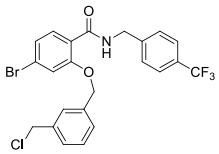
(2a) Yield: 5.21 g, 52%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.39 (d, J = 8.0 Hz, 1H), 8.12 (s, 1H), 7.22-7.47 (m, 10H), 5.17 (s, 2H), 4.60 (d, J = 4.0 Hz, 2H), 4.50 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 163.88, 156.65, 141.95, 138.51, 135.07, 134.78, 134.46, 133.40, 129.73, 129.41, 129.21, 128.31, 128.09, 127.81, 125.54 (q, J = 4.0 Hz), 125.43, 124.73, 124.65, 122.72, 122.02, , 118.55 (q, J = 4.0 Hz), 109.58 (q, J = 4.0 Hz), 71.65, 45.44, 43.54.



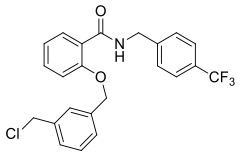
(2b) Yield: 4.221 g, 42%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC) δ 8.37 (d, *J* = 8.0 Hz, 1H), 8.00 (s, 1H), 7.27-7.42 (m, 8H), 7.15 (d, *J* = 8.0 Hz, 2H), 5.28 (s, 2H), 4.56 (s, 2H), 4.53 (d, *J* = 8.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 ºC) δ 163.74, 156.49, 141.77, 136.21, 135.06, 134.73, 134.41, 133.34, 132.84, 130.92, 130.56, 130.05, 129.60, 129.45, 129.28, 127.87, 125.53 (q, *J* = 4.0 Hz), 124.69, 122.70, 122.00, 118.58 (q, *J* = 4.0 Hz), 109.43 (q, *J* = 4.0 Hz), 69.09, 43.53, 43.13.



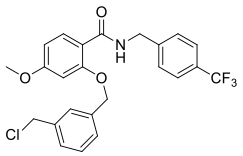
(2c) Yield: 5.81 g, 58%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC) δ 8.39 (d, *J* = 8.0 Hz, 1H), 8.12 (s, 1H), 7.22-7.47 (m, 10H), 5.17 (s, 2H), 4.60 (d, *J* = 4.0 Hz, 2H), 4.50 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 ºC) δ 163.88, 156.65, 141.95, 138.51, 135.07, 134.78, 134.46, 133.40, 129.73, 129.41, 129.21, 128.31, 128.09, 127.81, 125.54 (q, *J* = 4.0 Hz), 125.43, 124.73, 124.65, 122.72, 122.02, , 118.55 (q, *J* = 4.0 Hz), 109.58 (q, *J* = 4.0 Hz), 71.65, 45.44, 43.54.



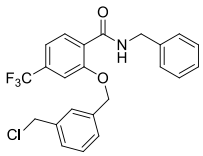
(2d) Yield: 4.39 g, 43%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC) δ 8.14 (d, *J* = 8.0 Hz, 1H), 8.07 (s, 1H), 7.45 (d, *J* = 8.0 Hz, 2H), 7.21-7.39 (m, 8H), 5.11 (s, 1H), 4.57 (d, *J* = 8.0 Hz, 2H), 4.49 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 ºC) δ 164.31, 156.93, 142.09 (q, *J* = 1.0 Hz), 138.40, 135.16, 133.83, 129.56, 129.36, 129.23, 129.20, 128.24, 128.04, 127.77, 127.51, 126.91, 125.48 (q, *J* = 4.0 Hz), 125.15, 122.71, 120.37, 115.98, 71.51, 45.47, 43.42.



(2e) Yield: 4.59 g, 53%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC) δ 8.21 (d, *J* = 8.0 Hz, 1H), 8.17 (s, 1H), 7.37-7.43 (m, 3H), 7.33 (s, 1H), 7.17-7.28 (m, 5H), 7.07 (t, *J* = 8.0 Hz, 1H), 6.99 (d, *J* = 8.0 Hz, 1H), 5.06 (s, 2H), 4.53 (d, *J* = 8.0 Hz, 2H), 4.42 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 ºC) δ 165.17, 156.70, 142.40 (q, *J* = 1.0 Hz), 138.25, 135.87, 133.04, 132.53, 129.42, 129.25, 129.10, 128.92, 128.08, 127.90, 127.73, 125.41 (q, *J* = 4.0 Hz), 122.74, 121.82, 121.33, 112.45, 71.02, 45.55, 43.32.



(2f) Yield: 2.87 g, 31%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.25 (d, *J* = 8.0 Hz, 1H), 8.12 (s, 1H), 7.46 (d, *J* = 8.0 Hz, 2H), 7.39 (s, 1H), 7.24-7.34 (m, 6H), 6.66 (d, *J* = 8.0 Hz, 1H), 6.57 (s, 1H), 5.09 (s, 2H), 4.49 (d, *J* = 4.0 Hz, 2H), 4.49 (s, 2H), 3.86 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 165.07, 163.48, 157.99, 142.65, 138.29, 135.75, 134.18, 129.40, 129.28, 129.08, 128.98, 128.12, 127.94, 127.75, 125.42 (q, *J* = 4.0 Hz), 122.78, 114.29, 105.80, 99.69, 71.04, 55.58, 45.56, 43.27.



(2g) Yield: 4.33 g, 50%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 8.32 (d, *J* = 8.0 Hz, 1H), 7.99 (s, 1H), 7.08-7.33 (m, 11H), 5.09 (s, 2H), 4.50 (d, *J* = 4.0 Hz, 2H), 4.41 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ 163.71, 156.58, 138.41, 137.94, 135.15, 134.54, 134.21, 133.40, 129.45, 129.11, 128.65, 128.09, 127.96, 127.64, 127.33, 125.08, 124.78, 122.06, 118.48 (q, *J* = 4.0 Hz), 109.66 (q, *J* = 4.0 Hz), 71.57, 45.56, 44.03.

3. The Thermal Stability of 3c

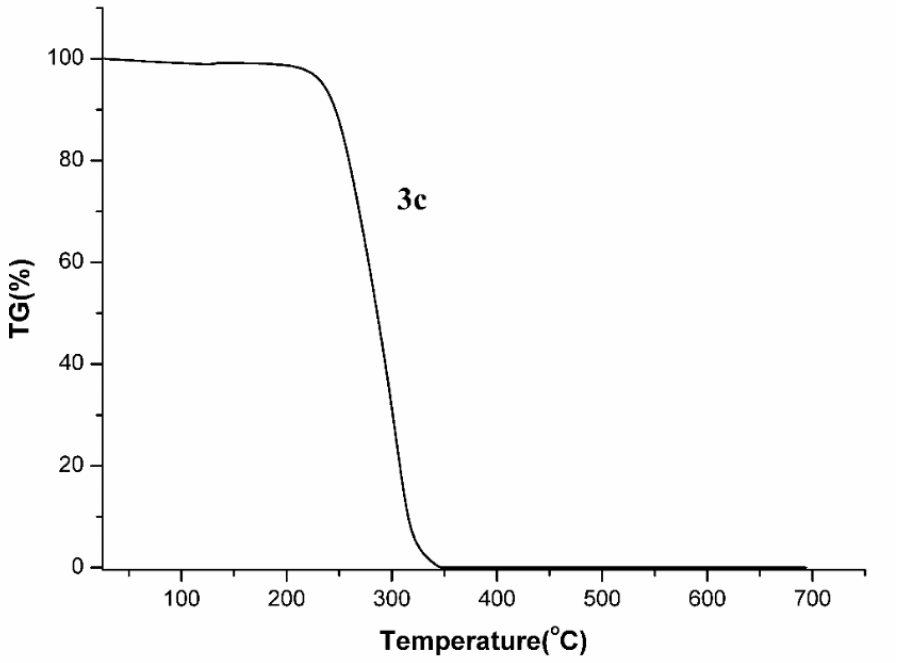
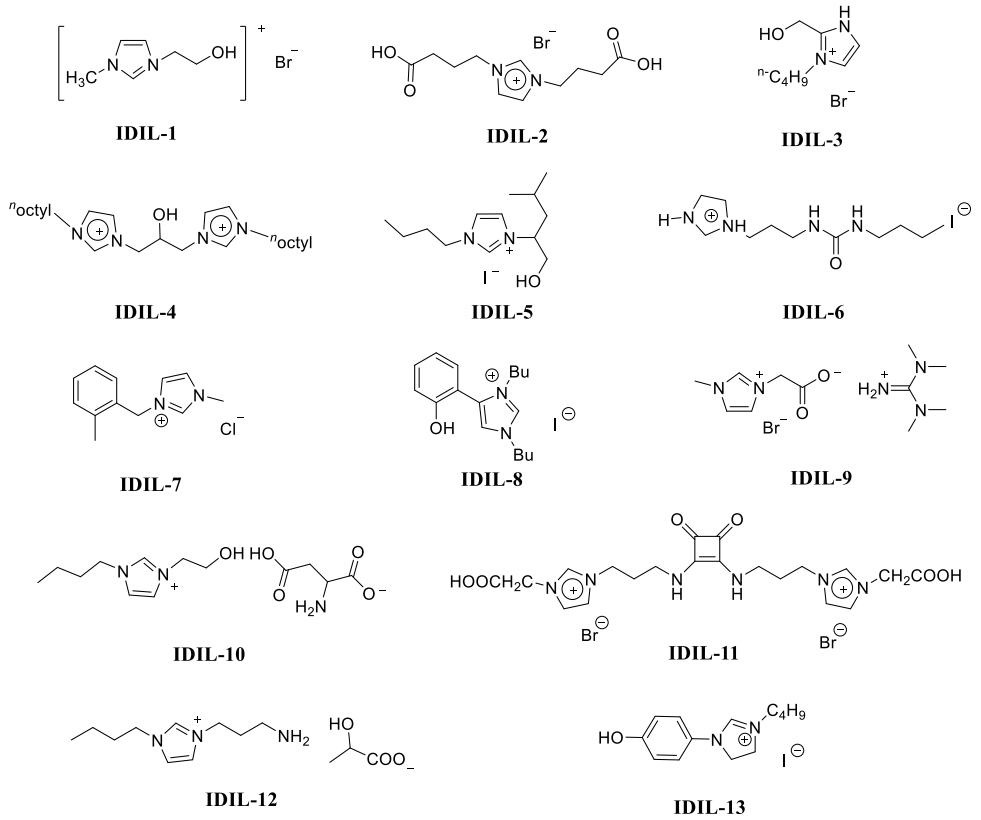


Figure S1. TGA curve of catalyst **3c**.

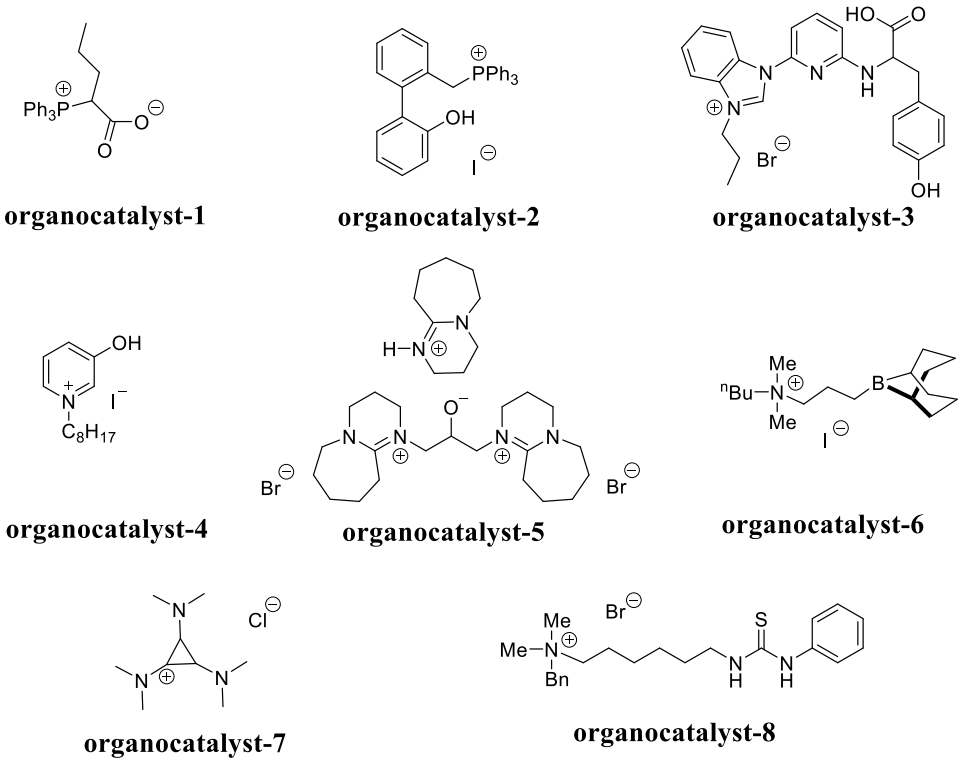
4. Comparison of this Work with Selected Imidazolium-Based Ionic Liquids and Organocatalyst



Scheme S3. Chemical structure of selected imidazolium-based ionic liquids

Table S1. Comparison of this work with selected imidazolium-based ionic liquids

Entry	Catalyst	Epoxide	Epo./Cat.	Condition	TOF(h^{-1})	Ref.
1	**3c** in this work	ECH	1000/1	100 °C, 15 bar, 2 h	315	/
2	**3c** in this work	ECH	500/1	25 °C, 15 bar, 24 h	2.5	/
3	**IDIL-1**	ECH	62.5/1	125 °C, 20 bar, 0.33 h	174	*Tetrahedron Lett.*, **2008**, 49, 3588-3591.
4	**IDIL-2**	ECH	100/1	100 °C, 20 bar, 0.4 h	228	*ChemSusChem*, **2011**, 4, 502-507.
5	**IDIL-3**	ECH	100/1	120 °C, 20 bar, 1 h	98	*RSC Adv*., **2014**, 4, 2360-2367.
6	**IDIL-4**	ECH	20/1	70 °C, 4 bar, 16 h	1.2	*ChemCatChem*, **2015**, 7, 94-98.
7	**IDIL-5**	ECH	50/1	60 °C, 5 bar, 8 h	6.2	*RSC Adv*., **2015**, 5, 45454-45458.
8	**IDIL-6**	ECH	86.3/1	130 °C, 5 bar, 3 h	28.5	*Green Chem*., **2016**, 18, 2851-2863.
9	**IDIL-7**	ECH	400/1	130 °C, 20 bar, 4 h	90.5	*J. CO2 Util*., **2017**, 22, 44-52.
10	**IDIL-8**	ECH	133.3/1	80 °C, 10 bar,1 h	132	*Catal. Sci. Technol.*, **2018**, 8, 1981-1987.
11	**IDIL-9**	ECH	4/1	30 °C, 1 bar, 12 h	0.28	*Green Chem*., **2018**, 20, 2990-2994.
12	**IDIL-10**	ECH	125/1	90 °C, 2.5 bar, 12 h	10.3	*Fuel*, **2018**, 251, 233-241.
13	**IDIL-11**	ECH	33.3/1	100 °C, 15 bar, 3 h	11	*J. CO2 Util.,* **2020**, 37, 39-44.
14	**IDIL-12**	ECH	200/1	80 °C, 5 bar, 12 h	16.2	*Catal. Sci. Technol.*, **2021**,11, 6999-7008.
15	**IDIL-13**	ECH	5/1	RT, 1 bar, 3 h	1.5	*Chem. Catal.*, **2022**, 2, 519-530.



Scheme S4. Chemical structure of selected high-active organocatalysts

Table S2. Comparison of **3c** with selected high-active organocatalysts.

Entry	Catalyst	Epoxide	Epo./Cat.	Condition	TOF(h^{-1})	Ref.
1	**3c** in this work	ECH	1000/1	100 ℃, 15 bar, 2 h	315	/
2	**3c** in this work	ECH	500/1	25 ℃, 15 bar, 24 h	2.5	/
3	**organocatalyst-1**	ECH	20/1	25 ℃, 1 bar, 6 h	3	*ACS Catal.*, **2015**, 5, 6773-6779.
4	**organocatalyst-2**	ECH	100/1	60℃, 1 bar, 24 h	3.5	*Green Chem.*, **2016**, 18, 4611-4615.
5	**organocatalyst-3**	ECH	25/1	RT, 1 bar, 24 h	0.97	*ACS Catal.*, **2018**, 8, 9945-9957.
6	**organocatalyst-4**	ECH	20/1	50℃, 1 bar, 6 h	3.3	*ChemSumChem*, **2018**,11, 4262-4268.
7	**organocatalyst-5**	ECH	16.7/1	30 ℃, 1 bar, 6 h	2.6	*Green Chem.*, **2019**, 21, 3456-2463.
7	**organocatalyst-6**	ECH	5000/1	120 ℃, 20 bar, 8 h	619	*Angew. Chem. Int. Ed.*, **2020**, 59, 23291 -23298.
8	**organocatalyst-7**	ECH	100/1	100 ℃, 1 bar, 3 h	32.3	*J. Org. Chem.*, **2021**, 86, 3422−3432.
9	**organocatalyst-8**	ECH	1000/1	100 ℃, 10 bar, 2 h	205	*J. Org. Chem.*, **2022**, 87, 3145−3155.

5. Crystal Data of Compound 4a

Table S3. Crystallographic and structure refinement data for compound **4a.**

Compound	**4a**
Formula	**$C_{26}H_{25}BrN_3O_2$·Cl·2(H_2O)**
*F*w	562.88
T(K)	123(2)
Crystal system	Triclinic
Space group	*P*$\bar{1}$
a (Å)	8.2791(12)
b (Å)	9.0720(14)
c (Å)	18.780(3)
α (deg)	89.340(2)
β(deg)	83.776(2)
γ(deg)	67.821(2)
V Å^3	1297.8(3)
Z	2
D_{calcd} g.cm^{-3}	1.440
μ (mm^{-1})	1.72
F (000)	580
Index ranges	-7≤*h*≤9 -10≤*k*≤10 -22≤*l*≤10
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GOF	1.02
[*I* >2σ(*I*)]	R_1 = 0.028 wR_2 = 0.078
CCDC number	2181809

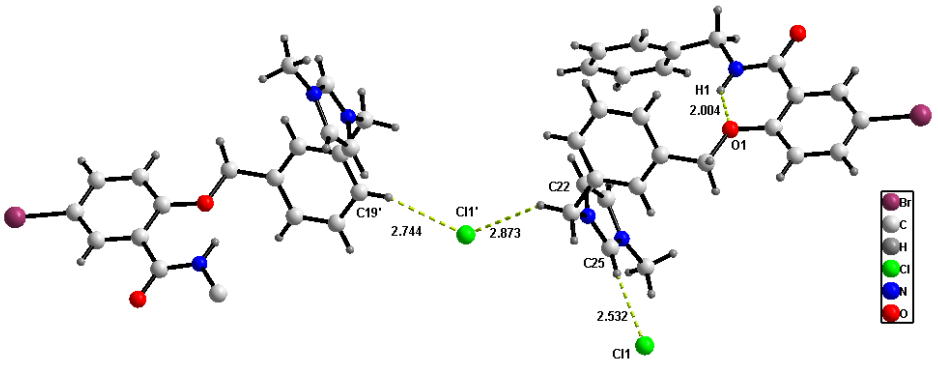

Figure S2. Intramolecular and intermolecular hydrogen bonds in the crystal structure of compound **4a**.

6. Computational Details

To get further understand of the catalytic reaction and the role of HBDs, computational methods are conducted to invesitigated the reaction mechanisms. The calculations were performed using the Gaussian 16 program package.[1] In order to select appropriate functional for our calculation, we conducted calculation with different density functional methods such as B3LYP[2-4], B3LYP-GD3[5,6], M06-2X[7,8] and PBE1PBE[9,10] using 6-311++g**,SDD (SDD only for I) basis sets as well as SMD solvent models.[11-13] Computational results indicate that there is no significant difference amoung these methods in reaction energetics. Considering the formation of multiple hydrogen bonds between the catalyst and the epoxide substrate, it is reasonable that the energy barrier of intermediate **1** (**Int1**) would be lower than that of the reactant. Hence, we selected M06-2X as the functional. Although the energy barrier of **Int1** is also lower than that of the reactant calculated by the B3LYP-GD3 functional, there is a strong cation-π interaction in the structure of the catalyst calculated by this functional, which is different from the obtained crystal structure.

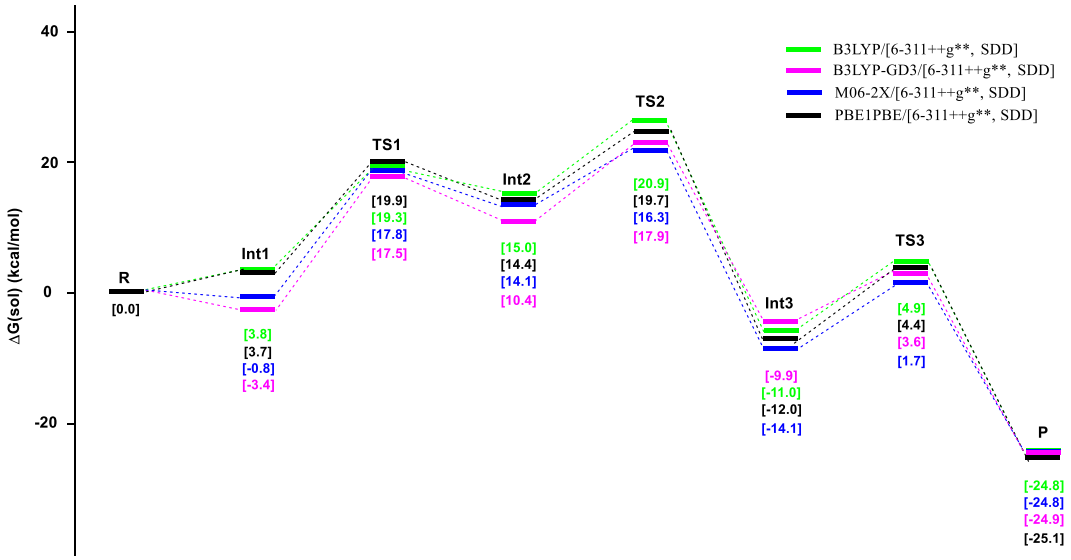

Figure S3. The comparison of energy barrier using different functionals.

All the geometries invloved in the reaction mechanism pathway are full optimized at M06-2X[7,8]/[6-31g**, SDD] level (SDD for iodium and 6-31g** for others). [11-13] All the optimized structures are confirmed to be stational points by vibrational analysis at experimental condition, 298.15 K and 25 atm, at the same level. Whitin this way, the Gibbs free energetics correction of each species in vacuum are avalible. The intrinsic reaction coordinate (IRC)[14] calculations are carried out at the same level for each transition state to verify the right connections with its forward and backward minima. More accurate single point electronic energy and solvation free enegies in PO of the geometries full optimized before are obtained at M06-2X/[6-311++G**,SDD] (SDD for iodium and 6-311++G** for others) level with a self-consistent reaction field (SCRF) with SMD model[11-13]. In SMD model calculation, the dielectric constant of the solvent, PO, is set to $\varepsilon = 16.0$ as reported before[15]. Therefore, for each species, *i*, invloved in the reaction mechanism, the thorough Gibbs free energy in solution G_i^{sol} is calculated as

$G_i^{sol} = E_i + G_i^{corr} + \Delta G_i^{solv}$.

In which, E_i is the single point electronic energy at M06-2X/[6-311++G**,SDD] level for species *i* in vaccum, G_i^{corr} is the Gibbs energy correction with vibrational analyses at M06-2X/ [6-31g**, SDD] level, and ΔG_i^{solv} is the solvation free energy of species *i* in ECH with SMD model at M06-2X/[6-311++G**,SDD] level[11-13].

During the calculation, all depicted three-dimensional (3D) structures were generated using the Gaussview 6 program. To reduce computational costs, propylene oxide are replaced with ECH and **3c'** (R_1 = CF_3, R_2 = CF_3, R_3 = methyl) and **3g'** (R_1 = H, R_2 = CF_3, R_3 = methyl) are used instead of **3c** (R_1 = CF_3, R_2 = CF_3, R_3=butyl) and **3g** (R_1 = H, R_2 = CF_3, R_3 = butyl).

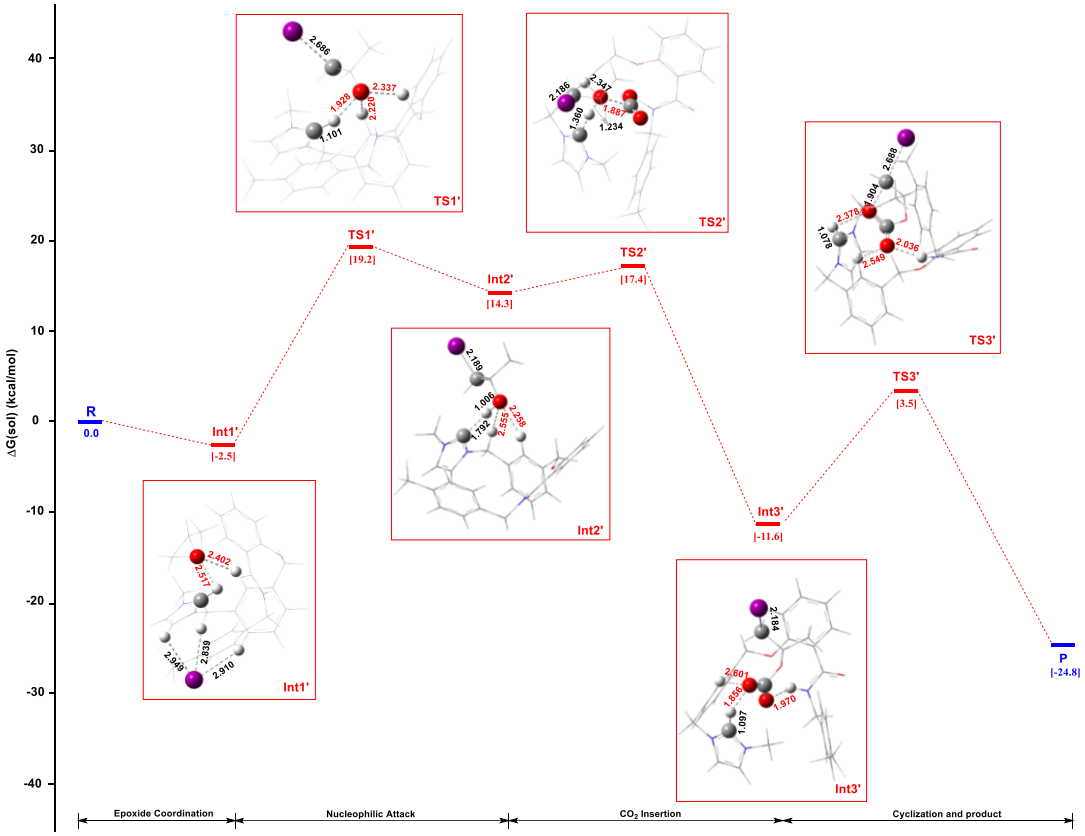

Figure S4. DFT-calculated free energy profiles (M06-2X/[6-31g**, SDD]) and the optimized geometries of key intermediates and transition states for the CO_2/PO coupling catalyzed by **3g'**.The dashed lines depict hydrogen bond interactions are given in angstrom.

Computed energy components of the common small molecules

	$E^{gas[a]}$	$G^{gas[a]}$	$G^{gas-corr[a]}$	$E^{SMD[b]}$	$G^{SMD[c]}$
PO	-193.053412	-192.96132	0.092089	-193.02646	-192.9343738
CO_2	-188.531666	-188.51616	0.015504	-188.50919	-188.4936837
P	-381.604786	-381.49304	0.111746	-381.57932	-381.4675759

[a] Electronic energetics in a. u. which performed via geometries optimization and vibrational analyses at M06-2X/[6-31+g*, SDD] level. [b] Single point electronic energetics in a. u. calculated at M06-2X/6-311++g**, SDD] level in PO with SMD solvent model with the geometries full optimized in a. [c] Gibbs free enenergetics in PO which considered the thermal correction on Gibbs free energetics in vacuum.

Computed energy components of **3c'**

	$E^{gas[a]}$	$G^{gas[a]}$	$G^{gas\text{-}corr[a]}$	$E^{SMD[b]}$	$G^{SMD[c]}$
3c'	-2005.97007	-2005.443	0.527062	-2005.9735	-2005.446411
Int. 1	-2199.03625	-2198.4153	0.620948	-2199.0031	-2198.382113
TS 1	-2198.99073	-2198.3719	0.61886	-2198.9713	-2198.352414
Int. 2	-2199.02504	-2198.4046	0.620472	-2198.9789	-2198.358392
TS 2	-2387.53866	-2386.9059	0.632722	-2387.4812	-2386.848525
Int. 3	-2387.58117	-2386.9421	0.639082	-2387.536	-2386.89687
TS 3	-2387.54429	-2386.906	0.638267	-2387.51	-2386.871777

[a] Electronic energetics in a. u. which performed via geometries optimization and vibrational analyses at M06-2X/[6-31+g*, SDD] level. [b] Single point electronic energetics in a. u. calculated at M06-2X/6-311++g**, SDD] level in PO with SMD solvent model with the geometries full optimized in a. [c] Gibbs free enenergetics in PO which considered the thermal correction on Gibbs free energetics in vacuum.

Computed energy components of **3g'**

	$E^{gas[a]}$	$G^{gas[a]}$	$G^{gas\text{-}corr[a]}$	$E^{SMD[b]}$	$G^{SMD[c]}$
3g'	-1669.02595	-1668.5077	0.518263	-1669.0035	-1668.485286
Int. 1'	-1862.09646	-1861.4844	0.61201	-1862.0356	-1861.423616
TS 1'	-1862.04467	-1861.4347	0.609949	-1861.999	-1861.389046
Int. 2'	-1862.08043	-1861.4688	0.611615	-1862.0085	-1861.396883
TS 2'	-2050.59346	-2049.9697	0.623761	-2050.5094	-2049.885685
Int. 3'	-2050.63271	-2050.0024	0.630321	-2050.5621	-2049.931829
TS 3'	-2050.59784	-2049.9683	0.629561	-2050.5374	-2049.907805

[a] Electronic energetics in a. u. which performed via geometries optimization and vibrational analyses at M06-2X/[6-31+g*, SDD] level. [b] Single point electronic energetics in a. u. calculated at M06-2X/6-311++g**, SDD] level in PO with SMD solvent model with the geometries full optimized in a. [c] Gibbs free enenergetics in PO which considered the thermal correction on Gibbs free energetics in vacuum.

Computed energy components of **4c**

	$E^{gas[a]}$	$G^{gas[a]}$	$G^{gas\text{-}corr[a]}$	$E^{SMD[b]}$	$G^{SMD[c]}$
4c	-434.638189	-434.39549	0.242699	-434.60201	-434.3593078
Int. 1"	-627.696386	-627.35893	0.33746	-627.62346	-627.2860013
TS 1"	-627.640479	-627.30726	0.333221	-627.58212	-627.2489008
Int. 2"	-627.681822	-627.3453	0.336519	-627.6025	-627.26598
TS 2"	-816.194887	-815.84552	0.34937	-816.10036	-815.7509915
Int. 3"	-816.219055	-815.86376	0.355293	-816.14084	-815.7855433
TS 3"	-816.157952	-815.80454	0.353414	-816.07777	-815.7243522

[a] Electronic energetics in a. u. which performed via geometries optimization and vibrational analyses at M06-2X/[6-31+g*, SDD] level. [b] Single point electronic energetics in a. u. calculated at M06-2X/6-311++g**, SDD] level in PO with SMD solvent model with the geometries full optimized in a. [c] Gibbs free enenergetics in PO which considered the thermal correction on Gibbs free energetics in vacuum.

7. pK_a Calculation

The pK_a values of **3c'** and **3g'** in ECH were predicted with the thermodynamical cycle as reported[16,17]. The free energy of acid dissociation in ECH ($\Delta G^{\ominus,soln}$) can be obtained

through Eq. 1. The solvation free energy of a proton ($\Delta G^{\ominus,solv}(H^+)$) was set to -1126.6 kJ mol^{-1}(ca. -269 kcal mol^{-1}). The geometries of each species involved in the thermodynamical cycle were optimized at the B3LYP-D3BJ[1-2]/[6-31g**, SDD] (SDD for iodium and 6-31g** for others) level in vacuum.[11-13] The thermal corrections to Gibbs free energy in vacuum (G_{gas}_correct) were also obtained by frequency analyses at the same level. More accurate single point electronic energy and solvation free enegies in ECH of the geometries full optimized before are obtained at M06-2X/ [6-311++G**, SDD] (SDD for iodium and 6-311++G** for others) level using self-consistent reaction field method (SCRF) with SMD model[11-13]. During the SCRF calculation, the dielectric constant, ε, of ECH is set to 22.6 as reported before[15].

$$G^{\ominus,soln} = \Delta G^{\ominus,gas} + \Delta G^{\ominus,solv}(\mathbf{3}\text{-HI}) + \Delta G^{\ominus,solv}(H) - \Delta G^{\ominus,solv}(\mathbf{3}\text{-I}) \quad (1)$$

$$pK_a = G^{\ominus,soln}/RT\ \ln(10) \quad (2)$$

3c' ($R_1 = CF_3$, $R_2 = CF_3$, R_3 = methyl): **pK_a= 22.98**

	3c'-HI	**3c'**-I	H^+	ΔG^{gas}(au)	$\Delta G^{\circ gas}$(kJ/mol)
E^{gas}(au)	-2006.77672	-2006.216194	0		
G^{gas}(au)	-2006.256736	-2005.711146	-0.01	0.53559	1406.030868
$G^{gas\text{-}correct}$(au)	0.519984	0.505048	-0.01		
E^{SMD}(au)	-2005.982968	-2005.478921			
G^{SMD}(au)	-2005.462984	-2004.973873			
$\Delta G^{\ominus solv}$(au)	0.7937516	0.7372733			
$\Delta G^{\ominus solv}$(kJ/mol)	2083.8	1935.5	-1126.6		
$\Delta G^{\ominus soln}$(kJ/mol)	131.2				

3g' (R_1 = H, $R_2 = CF_3$, R_3 = methyl): **pK_a= 25.32**

	3g'-HI	**3g'**-I	H^+	ΔG^{gas}(au)	$\Delta G^{\circ gas}$(kJ/mol)
E^{gas}(au)	-1669.734716	-1669.167721	0		
G^{gas}(au)	-1669.22306	-1668.671174	-0.01	0.54189	1422.559127
$G^{gas\text{-}correct}$(au)	0.511656	0.496547	-0.01		
E^{SMD}(au)	-1669.010512	-1668.501215			
G^{SMD}(au)	-1668.498856	-1668.004668			
$\Delta G^{\ominus solv}$(au)	0.7242045	0.6665056			
$\Delta G^{\ominus solv}$(kJ/mol)	1901.2	1749.7	-1126.6		
$\Delta G^{\ominus soln}$(kJ/mol)	144.5				

8. Cartesian Coordinates of the Optimized Geometries

PO

C	-1.04201800	0.60938500	-0.05128000	H	0.14630100	-0.29536100	1.55726000
C	0.14896600	-0.05513900	0.49344200	C	1.50067800	0.10703100	-0.14586600
O	-0.81347400	-0.77485300	-0.25883900	H	2.06979500	0.90181800	0.34374800
H	-1.87651300	0.85339000	0.60271100	H	1.38491200	0.35501300	-1.20363200
H	-0.93663800	1.23693000	-0.93492700	H	2.07417800	-0.82063500	-0.07222800

CO_2

C	0.00000000	0.00000000	0.00000000	O	0.00000000	0.00000000	-1.16300300
O	0.00000000	0.00000000	1.16300300				

P

C	0.58081000	1.30572300	0.19275100	C	-1.13022200	-0.16669900	-0.01858700
C	1.08461700	-0.10823300	0.51006900	O	-2.21960700	-0.59382200	-0.23023400
H	1.20573300	1.83126800	-0.53117200	C	1.93095300	-0.71159400	-0.59504500
H	0.45322600	1.91921200	1.08962500	H	2.89480300	-0.19952100	-0.65765100
H	1.58946900	-0.16062600	1.47661600	H	2.10612400	-1.77139600	-0.40301400
O	-0.69375100	1.06121900	-0.39162600	H	1.41784700	-0.60991800	-1.55611700
O	-0.14466000	-0.83292100	0.62768400				

3c'

C	-0.53206900	3.54949300	-0.98475800	H	-2.69700400	-2.48805500	1.09007600
H	-1.59912600	3.74879700	-0.94584300	C	-1.03265700	-2.68217600	-0.26914600
C	0.35714900	4.28680600	-0.21505800	C	-0.62174000	-3.02127700	-1.56090500
H	-0.00347200	5.06852200	0.44570100	H	-1.36899300	-3.17061400	-2.33620500
C	1.72655800	4.02510300	-0.29782100	C	0.72984800	-3.17349400	-1.84918500
C	2.20662200	3.03438800	-1.14877500	H	1.04646400	-3.45109500	-2.84890100
H	3.27233700	2.84221600	-1.21921900	C	1.68721200	-2.97884100	-0.85476100
C	1.30744300	2.29378400	-1.91195600	H	2.74936100	-3.09898200	-1.06584400
H	1.67983000	1.51475300	-2.57104800	C	1.28369400	-2.63733300	0.43627000
C	-0.06180800	2.54553400	-1.83995900	C	-0.07454700	-2.49512800	0.72320500
C	-1.04445000	1.75991600	-2.68414300	H	-0.39704200	-2.24313700	1.73308400
H	-1.60568200	2.44815000	-3.32184200	C	2.32076400	-2.39065400	1.50551400
H	-0.50441500	1.05768600	-3.32487500	H	1.98022400	-2.73045000	2.48673600
C	-3.22190200	1.54909400	-1.60148800	H	3.27238900	-2.87470100	1.25443000
C	-4.23604400	0.68546200	-0.88273700	C	3.62038100	-0.28104800	0.96156800
C	-5.50733600	1.24334900	-0.76147800	H	4.32707300	-0.83210700	0.34068200
H	-5.64983700	2.23464700	-1.17636400	C	3.51530800	1.03120800	1.31276100
C	-6.55015900	0.56358600	-0.14362300	H	4.10296200	1.89108700	1.03765400
C	-6.30910400	-0.70456400	0.36541700	C	1.92272900	-0.07228700	2.35452100
C	-5.05211500	-1.29434100	0.26929000	H	1.07627700	-0.30322300	2.98249400
H	-4.90271000	-2.28932000	0.66927800	C	1.95543600	2.37830400	2.77612400
C	-4.01411400	-0.60206100	-0.35109000	H	1.23230400	2.84638800	2.10614900
C	-2.48656600	-2.43388200	0.01490400	H	2.79567600	3.05355000	2.92896100
H	-3.12912800	-3.15318100	-0.50767000	H	1.48976800	2.15217900	3.73500400

N	2.45203800	1.13988300	2.18277500	C	-7.39462400	-1.44748900	1.09448800
N	2.61719600	-0.94597400	1.62980500	F	-8.61278900	-1.05643000	0.70490300
N	-2.01345400	1.01330400	-1.90252900	F	-7.31477700	-1.24560800	2.41826800
H	-1.78747200	0.08517400	-1.57713900	F	-7.30435800	-2.77096700	0.89605500
O	-2.76209900	-1.11747000	-0.46345300	C	2.68631400	4.85410400	0.50163000
O	-3.51729100	2.69655500	-1.91692300	F	3.12542700	5.92432200	-0.16129900
I	5.57876300	-3.06566700	-0.39952700	F	2.13010700	5.29327200	1.64501500
H	-7.53613300	1.00580500	-0.06628200	F	3.78141800	4.14094200	0.85769200

Int1

C	1.18984200	2.59139500	-1.88733200	H	2.81515700	-2.74603700	1.35799400
H	0.31981000	3.09137500	-2.30196400	C	3.00455900	-0.28107500	2.22841300
C	2.20075100	3.31051000	-1.26511900	H	3.90396200	-0.82525700	2.47472000
H	2.14186600	4.39274700	-1.18912100	C	2.71062200	1.04718700	2.26401400
C	3.29931300	2.63600900	-0.72852100	H	3.29647400	1.89840700	2.57130200
C	3.41881200	1.25539200	-0.84584100	C	0.99958400	-0.00496600	1.34861300
H	4.28232200	0.71946800	-0.45846300	H	0.03958000	-0.18191000	0.87833500
C	2.39945500	0.54016800	-1.47312700	C	0.71608500	2.44390300	1.58029600
H	2.50687600	-0.54005600	-1.55901000	H	1.42697000	3.23897400	1.36123800
C	1.27488300	1.19561800	-1.97775100	H	0.18600100	2.66195600	2.51033800
C	0.16155900	0.42091600	-2.64849000	H	0.01641700	2.34694500	0.74854000
H	-0.12486600	0.92765300	-3.57540400	N	1.45373700	1.19291200	1.71706500
H	0.51365400	-0.58507600	-2.89286400	N	1.91765800	-0.91682900	1.66875700
C	-2.05759600	1.16176500	-1.93236000	N	-1.04109900	0.26496000	-1.83159700
C	-3.40987000	0.79000400	-1.35355100	H	-1.27228200	-0.66464500	-1.51104400
C	-4.32855300	1.83338000	-1.23399100	O	-2.96343200	-1.52523400	-1.23610400
H	-4.00796500	2.81565900	-1.56323600	O	-1.90868600	2.25973400	-2.45392300
C	-5.60350500	1.62424600	-0.72097900	H	-6.30957700	2.44174600	-0.63084000
C	-5.96339200	0.34276900	-0.31556600	C	-7.28302700	0.11983000	0.36578500
C	-5.08516900	-0.72613600	-0.44813200	F	-8.21850300	0.97431900	-0.06034000
H	-5.39392700	-1.72772700	-0.16853600	F	-7.16421700	0.29520800	1.69559900
C	-3.81792600	-0.50490900	-0.98273100	F	-7.74181200	-1.12426000	0.17742800
C	-2.84241000	-2.64355000	-0.34770700	C	4.29722300	3.42526700	0.06031800
H	-3.49918400	-3.45018100	-0.69199000	F	4.66873300	4.55093700	-0.55803900
H	-3.12059000	-2.34164700	0.66750300	F	3.74567200	3.82094000	1.24738500
C	-1.38176800	-3.00396300	-0.43656100	F	5.39074000	2.73147400	0.36682300
C	-0.85527200	-3.43761200	-1.65795800	C	-1.88732600	-0.36789200	2.93767500
H	-1.53024000	-3.66192300	-2.47963800	C	-2.62609700	0.79360700	2.42917600
C	0.52086100	-3.54819200	-1.83011800	O	-2.07602800	-0.17531700	1.53525600
H	0.92451600	-3.88752400	-2.77835000	H	-2.44456000	-1.19830300	3.36796400
C	1.39019100	-3.20520700	-0.79419900	H	-2.09767800	1.74675400	2.40428200
H	2.47042600	-3.24742900	-0.92624500	C	-4.12153400	0.86940500	2.50841000
C	0.87064600	-2.78871300	0.43212800	H	-4.55717300	-0.13202700	2.47468600
C	-0.51257200	-2.70895000	0.60891300	H	-0.86172100	-0.25475600	3.28955200
H	-0.91871300	-2.38073800	1.56352000	H	-4.52169800	1.44602800	1.67243000

C	1.79780300	-2.38782000	1.54711600	I	5.11495000	-2.12736800	-0.04931500
H	1.44059200	-2.75921200	2.51245300	H	-4.42627800	1.35461900	3.43948800

TS1

C	-1.98281300	3.19702300	-0.13808700	H	-2.99485000	-1.97825500	3.38857800
H	-1.10825100	3.62809100	-0.61885200	C	-4.08968600	-1.39484500	1.08672000
C	-3.23729800	3.27172600	-0.73021200	H	-4.82859100	-1.83625100	1.73558300
H	-3.36803000	3.75782800	-1.69193100	C	-4.20444600	-0.83446300	-0.14686000
C	-4.33799900	2.70675300	-0.08581300	H	-5.06298400	-0.65946900	-0.77510400
C	-4.20070800	2.10977000	1.16437000	C	-2.08182300	-0.72275500	0.45484900
H	-5.07099000	1.69603800	1.66286500	H	-0.99555000	-0.56554600	0.39634600
C	-2.94001700	2.03469300	1.74800500	C	-2.58637200	0.14927100	-1.81781700
H	-2.81178500	1.55031300	2.71373500	H	-1.79692700	0.88214400	-1.65460800
C	-1.82230000	2.55360300	1.09229300	H	-3.46960100	0.65043500	-2.21217700
C	-0.44467000	2.43751400	1.70110100	H	-2.24988500	-0.64382600	-2.49565400
H	-0.12531100	3.42450200	2.05240600	N	-2.94507900	-0.43284900	-0.51975600
H	-0.47789300	1.76081000	2.56355600	N	-2.76025600	-1.31743000	1.44322000
C	1.56635200	2.80172200	0.37269700	N	0.56490600	1.96943200	0.77447500
C	2.81478800	2.10735700	-0.10052900	H	0.73562900	0.96642600	0.69968700
C	3.47149700	2.59040400	-1.22776700	O	2.79360700	0.71641600	1.79826800
H	3.06875500	3.47073000	-1.71797900	O	1.46175900	4.01909500	0.36611300
C	4.59985300	1.94417800	-1.72438600	H	5.09978700	2.29906500	-2.61759300
C	5.07310000	0.81568200	-1.06321900	C	6.20882100	0.02092100	-1.64186700
C	4.47555200	0.35301100	0.10586800	F	5.75039300	-1.04123000	-2.32139000
H	4.89355800	-0.49684400	0.63522300	F	7.02204300	-0.45137100	-0.68447000
C	3.35567500	1.01389600	0.59939800	F	6.95212700	0.74529300	-2.48683100
C	2.64349300	-0.64407200	2.20441100	C	-5.65449500	2.64285100	-0.79603800
H	3.50349400	-0.94115700	2.81768600	F	-5.85590700	3.68928600	-1.59957300
H	2.55578500	-1.28768500	1.32464300	F	-5.71592300	1.53690300	-1.58421900
C	1.36109900	-0.66053800	3.00414100	F	-6.68809700	2.55896400	0.04903800
C	1.24801000	0.12868200	4.15252100	C	0.20157700	-2.05806600	-1.39316000
H	2.11435200	0.68100100	4.50471700	C	0.84391300	-0.76256600	-1.60563500
C	0.03390600	0.23018100	4.82421300	O	0.85534300	-0.81447400	-0.20229300
H	-0.04393800	0.84071000	5.71748800	H	-0.81854000	-2.11968500	-1.05193100
C	-1.08928800	-0.43761100	4.33849400	H	0.83847100	-2.91690300	-1.22516600
H	-2.04286100	-0.34580700	4.85239000	H	0.18996600	0.01400900	-2.02645900
C	-0.98558200	-1.23291200	3.19736700	C	2.18850100	-0.77980500	-2.29256200
C	0.24636700	-1.36076700	2.55084700	H	2.84141400	-1.51704900	-1.81542700
H	0.33833400	-1.96382100	1.65143700	H	2.66542400	0.19955500	-2.22786800
C	-2.18940200	-1.95385500	2.65152900	H	2.06087700	-1.04638500	-3.34522800
H	-1.93882300	-2.98410800	2.38244000	I	-0.78351500	-2.95174300	-3.73531100

Int2

C	2.04073800	3.65978100	-1.17336200	H	-2.98516500	0.05576400	3.68822000
H	2.83356700	3.16471900	-1.72668700	C	-2.64213300	2.24467000	2.13736700
C	0.93756900	4.18439100	-1.83310600	H	-2.70692600	2.61659200	3.14798200

H	0.84523800	4.09374400	-2.91028700	C	-2.67949700	2.88893600	0.94614900
C	-0.06088100	4.83198600	-1.10432900	H	-2.78798800	3.93269300	0.69991900
C	0.04423500	4.96030900	0.27661700	C	-2.46328900	0.66683300	0.50182900
H	-0.73421800	5.46868400	0.83613700	H	-2.09911200	-1.04339100	0.08592400
C	1.14895100	4.42496300	0.93153600	C	-2.51846500	2.17958400	-1.45190500
H	1.22793500	4.51098600	2.01153100	H	-1.53013600	2.54936600	-1.73517000
C	2.15292000	3.77477400	0.21640500	H	-3.26832800	2.92534600	-1.72057600
C	3.36401500	3.20251100	0.92360100	H	-2.72023000	1.24615900	-1.97529700
H	4.26617900	3.71060000	0.57279500	N	-2.57030200	1.90985600	-0.02500900
H	3.27379200	3.36457100	2.00164300	N	-2.52232100	0.89948300	1.83927900
C	4.38801700	1.35650200	-0.29748100	N	3.55788900	1.78536700	0.68498600
C	4.59727100	-0.13269600	-0.46646700	H	3.02738100	1.10942400	1.21488600
C	5.52632800	-0.48961900	-1.44309600	O	3.05597700	-0.79298000	1.20608300
H	6.00480600	0.31977800	-1.98242000	O	4.97674800	2.13994200	-1.03467600
C	5.83032500	-1.81685200	-1.71585900	H	6.56138100	-2.07833500	-2.47174800
C	5.18250800	-2.80997300	-0.99363200	C	5.44415400	-4.25629000	-1.31103100
C	4.24782300	-2.49570000	-0.01298500	F	6.69873800	-4.44926500	-1.73737000
H	3.76875500	-3.29563300	0.53644700	F	4.62603800	-4.69977600	-2.27603100
C	3.95386400	-1.15897800	0.25584600	F	5.25112400	-5.04229300	-0.24105000
C	2.30770100	-1.79409500	1.89661000	C	-1.23031700	5.44242700	-1.81674600
H	2.99596300	-2.42282600	2.47585000	F	-1.03872800	6.73709900	-2.09549900
H	1.77216800	-2.42053700	1.17416000	F	-1.49178500	4.82182600	-2.97713000
C	1.34419400	-1.06428400	2.79057800	F	-2.35632700	5.37409400	-1.07203900
C	1.81402000	-0.39982200	3.92736100	C	-4.27612700	-2.46026000	0.14174400
H	2.86929000	-0.45301100	4.18233500	C	-2.99265600	-2.61204400	-0.67558600
C	0.93424600	0.31861600	4.72788300	O	-1.95901300	-2.03895700	0.08774800
H	1.29666800	0.82458100	5.61668500	H	-4.44893900	-1.41442900	0.39412100
C	-0.41760700	0.38193200	4.39100100	H	-4.24245300	-3.07079900	1.04464700
H	-1.10717200	0.93951400	5.02031100	H	-3.12214500	-2.07166600	-1.62697900
C	-0.89277000	-0.27110600	3.25629400	C	-2.62592000	-4.05826800	-0.95520300
C	-0.00546500	-0.99876100	2.45921900	H	-2.51157500	-4.59432000	-0.00779800
H	-0.38139600	-1.51737600	1.57854100	H	-1.67222200	-4.09249900	-1.48543200
C	-2.33935900	-0.15823200	2.83171900	H	-3.38628800	-4.55992000	-1.55689100
H	-2.66417800	-1.08843700	2.36027900	I	-6.07753000	-3.08035600	-0.93556500

TS2

C	2.06874300	2.07223800	-0.95708700	H	-1.57894300	3.63967200	3.03731200
H	2.19241200	1.02719700	-1.22065400	C	-1.67093100	3.52809800	0.82072600
C	1.26113100	2.89201500	-1.74215000	H	-1.54933300	4.50975300	0.39163400
H	0.77269600	2.48531900	-2.62124300	C	-1.94576600	1.29650300	0.79309700
C	1.10224100	4.23117400	-1.40088300	H	-1.85393100	0.00225900	0.32210800
C	1.73702700	4.75385500	-0.27293600	C	-2.03071300	2.41027700	-1.41093000
H	1.60974200	5.80157400	-0.01691000	H	-1.71566300	3.37379100	-1.80558300
C	2.53831400	3.92989900	0.50200300	H	-3.08776400	2.25638200	-1.63947400
H	3.04130700	4.33363600	1.37685800	H	-1.43366100	1.61234700	-1.85365000

C	2.72157700	2.58524400	0.16137600	N	-1.84097000	2.40577600	0.03797100
C	3.66548900	1.73471600	0.99104200	N	-1.86547400	1.73311500	2.06502700
H	4.69610000	1.98069300	0.71792400	N	3.50822300	0.31686000	0.80113900
H	3.53112000	1.97546900	2.05164600	H	2.68998000	-0.14862300	1.16948400
C	4.32820600	-0.37458800	-0.03296800	O	2.74334100	-2.08835900	1.71437500
C	4.00502300	-1.83292300	-0.26647600	O	5.26775600	0.14760800	-0.61641000
C	4.55843800	-2.39770100	-1.41341400	H	4.73185000	-4.14429500	-2.66904300
H	5.19530500	-1.76285000	-2.01934800	C	3.13011300	-5.88992200	-1.34831500
C	4.30114800	-3.71571000	-1.77190500	F	1.99139900	-5.93324800	-2.05680600
C	3.47985100	-4.48264100	-0.95500600	F	2.94861300	-6.67475800	-0.27439700
C	2.93152100	-3.95877000	0.21145300	F	4.08478000	-6.44917000	-2.10291900
H	2.32258600	-4.58736800	0.85050300	C	0.25470600	5.15022200	-2.22348700
C	3.19999800	-2.63753700	0.56135400	F	0.90992000	6.25590500	-2.59118300
C	1.55056800	-2.59542200	2.30690900	F	-0.21726800	4.56322000	-3.33114700
H	1.78760200	-3.48492700	2.90542300	F	-0.83221600	5.57701800	-1.52691700
H	0.82887800	-2.85770200	1.52668300	C	-3.91958000	-1.42944300	-0.37014100
C	1.01905900	-1.47608900	3.16330300	C	-2.60433200	-1.35043400	-1.14258600
C	1.79804600	-0.96450000	4.20525500	O	-1.61377200	-1.08496900	-0.16500200
H	2.76202800	-1.41615800	4.42132200	H	-4.07243600	-0.54277500	0.24414800
C	1.35133100	0.12398600	4.94545400	H	-3.96583000	-2.32600600	0.24751400
H	1.95708500	0.51603700	5.75568900	H	-2.65431300	-0.51710400	-1.86032900
C	0.12407200	0.71298400	4.64466700	C	-2.26346900	-2.63544500	-1.87784800
H	-0.22618700	1.56580900	5.22098100	H	-2.18205800	-3.45648000	-1.15909000
C	-0.65652800	0.20889100	3.60744900	H	-1.30811200	-2.52078600	-2.39303000
C	-0.20706200	-0.88852700	2.87139700	H	-3.02719900	-2.88487700	-2.61773600
H	-0.79840900	-1.26925000	2.04073900	I	-5.66945900	-1.49961800	-1.67583400
C	-1.96817800	0.85325500	3.23524500	C	0.05071800	-0.63307600	-0.87158700
H	-2.71248000	0.09226000	2.98923300	O	0.79975000	-0.86833600	0.02233500
H	-2.35915400	1.45580600	4.05882300	O	-0.15428700	-0.22250300	-1.97168200
C	-1.68194800	3.10048700	2.10931500				

Int3

C	-2.03737600	1.65854700	1.56549600	H	-4.99041300	-4.22317300	-1.57518900
H	-0.96916300	1.49682600	1.46385600	C	-4.93631100	-2.02414800	-1.25377400
C	-2.66222900	2.68017500	0.85710500	H	-5.84892100	-1.70175300	-0.77966200
H	-2.08165400	3.34137100	0.22112500	C	-2.93256200	-1.80263000	-2.14744300
C	-4.04142900	2.84778200	0.95341100	H	-1.97950400	-1.33371400	-2.42153700
C	-4.79716300	2.00935500	1.77106900	C	-3.85029000	0.27145100	-1.20010900
H	-5.86935700	2.15658100	1.85046300	H	-3.68036800	0.32285100	-0.12463100
C	-4.16560300	0.98958000	2.47236700	H	-4.76652000	0.79003600	-1.48118300
H	-4.75142000	0.32841400	3.10631300	H	-2.99076400	0.70269800	-1.71404200
C	-2.78426500	0.79598800	2.36903800	N	-3.93394900	-1.13834600	-1.58257300
C	-2.13649400	-0.35269700	3.12183600	N	-3.27073800	-3.09207800	-2.21190900
H	-2.14655600	-0.13916300	4.19441700	N	-0.76953600	-0.59536100	2.74224100
H	-2.72894800	-1.25886400	2.95073100	H	-0.60955100	-0.89163600	1.77785300

C	0.24302900	-0.16455200	3.52967600	O	1.18602500	-2.02235900	1.47503900
C	1.63746000	-0.22789100	2.94878100	O	0.07116800	0.32566100	4.63938400
C	2.54463300	0.68051700	3.48564100	H	4.52632300	1.54104400	3.39148000
H	2.19305700	1.29938900	4.30366900	C	5.54496400	0.17382800	1.25299200
C	3.83728100	0.81089600	2.98472500	F	6.13913700	-1.00348100	1.00277200
C	4.21819400	-0.00403200	1.93019900	F	6.39271400	0.91288800	1.97590300
C	3.35251300	-0.95990300	1.40207900	F	5.39202400	0.78575900	0.06355200
H	3.70364700	-1.59229900	0.59616200	C	-4.73466300	3.85394600	0.08842000
C	2.06210500	-1.08555300	1.91386300	F	-5.85421900	4.32484400	0.65510700
C	1.51802900	-2.73267200	0.29286000	F	-3.95261600	4.89853500	-0.20663200
H	2.46017300	-3.27747300	0.44205900	F	-5.10556300	3.30401900	-1.09032100
H	1.64939000	-2.02339100	-0.53572500	C	2.29544000	0.60743500	-1.67927100
C	0.41185800	-3.70810100	-0.00339000	C	1.22903500	1.35899500	-0.89085500
C	0.15569400	-4.76922500	0.86729500	O	0.48392200	0.39894000	-0.13514700
H	0.75908300	-4.87946700	1.76374600	H	1.83902200	-0.18705400	-2.26516100
C	-0.86837200	-5.66995100	0.59679700	H	3.09416200	0.24317200	-1.03316600
H	-1.05946700	-6.49517300	1.27443700	H	0.55183700	1.85346200	-1.59362700
C	-1.65539300	-5.50738800	-0.54162400	C	1.80867900	2.33746100	0.11335400
H	-2.46539700	-6.20273900	-0.74816800	H	2.46720000	1.81109400	0.81049600
C	-1.40780000	-4.44874600	-1.41181500	H	1.00624900	2.80964500	0.68599300
C	-0.36728700	-3.55934900	-1.14422900	H	2.38229500	3.11671400	-0.39280900
H	-0.18305700	-2.71483000	-1.80710100	I	3.28314000	1.88915500	-3.14473500
C	-2.32797300	-4.16430100	-2.57315300	C	-0.52531400	-0.28874800	-0.80179600
H	-1.77639800	-3.82470600	-3.45271600	O	-1.26299300	-0.95454300	-0.05070200
H	-2.92105600	-5.03756400	-2.85273600	O	-0.57438900	-0.18167400	-2.05077900
C	-4.51738300	-3.25712100	-1.64362000				

TS3

C	2.36632000	-2.00316100	-0.70371700	H	3.77028500	2.88031300	2.99948400
H	1.33877300	-2.29466800	-0.51444600	C	4.03486100	2.12100600	0.92654700
C	2.81524400	-1.86132800	-2.01497100	H	4.84526500	1.41090400	0.88987000
H	2.14180900	-2.04184300	-2.85167700	C	2.34714900	3.28425500	0.14138200
C	4.13209500	-1.47103700	-2.25183300	H	1.56297900	3.62360700	-0.51666400
C	5.00666800	-1.25383500	-1.18972900	C	3.41894700	1.73940000	-1.48024500
H	6.03558700	-0.97117400	-1.38854800	H	3.04125600	0.72357700	-1.35407200
C	4.54508600	-1.39442400	0.11489500	H	4.46429300	1.71880900	-1.78634500
H	5.22623000	-1.23492600	0.94863800	H	2.81773600	2.26182400	-2.22123300
C	3.21836500	-1.75192700	0.37478500	N	3.30354000	2.42808200	-0.19640900
C	2.75356400	-1.90010700	1.81495400	N	2.46746900	3.57347000	1.43596800
H	3.09277500	-2.86600800	2.20075500	N	1.32403000	-1.84053600	1.97814700
H	3.21225400	-1.10841800	2.41672700	H	0.88883900	-0.93020500	1.86318500
C	0.58725300	-2.97532800	1.90914000	O	-1.03399700	-0.62253900	2.62662000
C	-0.90919200	-2.82265100	1.74689800	O	1.09185700	-4.09070100	1.89188800
C	-1.55074100	-3.92636000	1.19223000	H	-3.38892200	-4.76828700	0.42876300
H	-0.94070900	-4.80105400	0.99659400	C	-5.07570400	-2.64014300	0.76246300

C	-2.90730700	-3.90954000	0.88006000	F	-5.80991100	-2.12181700	1.76090700
C	-3.62938400	-2.75839800	1.14720800	F	-5.61248100	-3.81868400	0.43248500
C	-3.02828100	-1.64539000	1.73292900	F	-5.22817400	-1.81772000	-0.28959600
H	-3.63653300	-0.77298700	1.93652600	C	4.55886600	-1.13423700	-3.64807900
C	-1.66974100	-1.67079700	2.03803700	F	5.88970600	-1.20691200	-3.80137600
C	-1.73448100	0.61067900	2.70893300	F	3.99165900	-1.91679300	-4.56315500
H	-2.63805600	0.48400500	3.31942600	F	4.20816500	0.14060600	-3.94378300
H	-2.03274500	0.93024200	1.70084600	C	0.00320800	0.39794300	-2.49182500
C	-0.81495700	1.61660400	3.34629900	C	-0.87130800	-0.40922300	-1.53913700
C	-0.51253000	1.53059600	4.70767900	O	-0.25190400	-0.36372400	-0.23712800
H	-0.98185700	0.75707100	5.30879500	H	1.03304400	0.11722100	-2.66003300
C	0.38951600	2.41499900	5.28775400	H	-0.40140400	1.22194000	-3.05732500
H	0.61215900	2.34840800	6.34715200	H	-0.86706400	-1.46270100	-1.81475300
C	1.02498800	3.37488900	4.50118200	C	-2.28503700	0.13511900	-1.47347200
H	1.75130900	4.05101000	4.94588800	H	-2.26018000	1.18404600	-1.16007500
C	0.73264600	3.46244000	3.14245800	H	-2.88531900	-0.44313900	-0.76832000
C	-0.20741300	2.60142100	2.57875800	H	-2.74575900	0.06768700	-2.46198700
H	-0.42367300	2.66455000	1.51491300	I	-0.46304900	-1.07933400	-4.69741600
C	1.51858100	4.37156400	2.23256600	C	0.54149400	0.72385100	-0.07838900
H	0.87748500	4.89724700	1.52094100	O	1.21432600	0.82056900	0.94622000
H	2.09193200	5.11341000	2.79370700	O	0.49882000	1.54677000	-1.06499000
C	3.51045500	2.83732400	1.95431600				

3g'

C	-2.32803100	2.78856400	-0.87314500	H	2.70457800	-2.65849000	-0.96513800
H	-3.39725000	2.68038100	-0.71493800	C	1.30444800	-2.51092700	0.65870700
C	-1.61717300	3.81182400	-0.26135200	C	-0.00558300	-2.73829200	1.08165400
H	-2.11964600	4.51578900	0.39422600	H	-0.29784300	-2.50540900	2.10525700
C	-0.24614200	3.93936900	-0.49596700	C	2.31215600	-1.88973300	1.59536700
C	0.41124500	3.05230200	-1.34275900	H	2.16481400	-2.22023100	2.62651500
H	1.47425900	3.16196900	-1.53175000	H	3.33890000	-2.10918700	1.27813400
C	-0.30768000	2.02433100	-1.94750200	C	2.89386000	0.43997200	0.77709300
H	0.20524600	1.32616400	-2.60284800	H	3.67034100	0.05433500	0.11651500
C	-1.67641100	1.88554500	-1.72221300	C	2.44828900	1.69699100	1.05644800
C	-2.46975300	0.78332200	-2.39404000	H	2.73534300	2.65820000	0.66373800
H	-3.26597700	1.22826100	-2.99710200	C	1.34367400	0.29216800	2.33929800
H	-1.81596900	0.20790300	-3.05517100	H	0.65996100	-0.10836100	3.07158400
C	-4.37597100	0.06725200	-1.04690800	C	0.71029700	2.68201300	2.60515600
C	-5.02558800	-0.98495800	-0.17956000	H	-0.17409200	2.87013700	1.99419600
C	-6.38553700	-0.79488400	0.06752600	H	1.33368400	3.57441200	2.62339600
H	-6.84251400	0.08769100	-0.36589400	H	0.41787500	2.42062200	3.62183900
C	-7.12364500	-1.69395200	0.82746500	N	1.48357600	1.58294400	2.03399900
C	-6.49162400	-2.81179900	1.35821800	N	2.19084900	-0.41476900	1.59572600
C	-5.13390100	-3.02747200	1.13812300	N	-3.09867300	-0.13232900	-1.46123200
H	-4.65637400	-3.90237900	1.56123600	H	-2.58963100	-0.93581900	-1.12436800

C	-4.39931800	-2.11888000	0.37564100	O	-3.06462700	-2.27059300	0.14511000
C	-2.38401100	-3.42102700	0.63738500	O	-5.01066300	1.06223100	-1.38287600
H	-2.83858200	-4.32565400	0.21438200	I	5.47019400	-1.79743500	-0.57041300
H	-2.46806400	-3.46358900	1.73048800	H	-8.18036300	-1.52471900	0.99987900
C	-0.95128000	-3.27070100	0.20988200	C	0.50955000	5.06924000	0.13565500
C	-0.57370500	-3.58211900	-1.09878300	F	0.55471100	6.15905900	-0.63159800
H	-1.31017900	-3.99942300	-1.78081600	F	-0.03214500	5.43246100	1.31244700
C	0.73327500	-3.36681600	-1.52214500	F	1.79319900	4.72367200	0.39565400
H	1.02765700	-3.62305500	-2.53431500	H	-7.05057600	-3.52850600	1.95120000
C	1.67594200	-2.82762900	-0.64828100				

Int1'

C	1.02540900	3.23204400	-1.74956200	H	-0.66881500	-2.48847300	1.56329700
H	0.41897900	4.08328900	-2.04128600	H	0.94083700	-2.76194600	0.80790900
C	2.14327500	3.40618600	-0.94514800	C	1.58439500	-0.53986100	1.97790300
H	2.43725100	4.39959900	-0.61802300	H	2.29865900	-1.31821800	2.20590200
C	2.87180800	2.29317200	-0.52547900	C	1.59135500	0.79723100	2.22241200
C	2.53075700	1.01129600	-0.94725000	H	2.30352700	1.42027600	2.73811700
H	3.10786900	0.14154800	-0.63525600	C	-0.15943400	0.35224800	0.95974400
C	1.41216400	0.85255700	-1.76360700	H	-1.06655000	0.45879100	0.38403400
H	1.13220700	-0.14537300	-2.09005400	C	0.09685400	2.73848500	1.61007900
C	0.63955400	1.94991700	-2.14764300	H	1.00487500	3.34051200	1.62648400
C	-0.62079400	1.75362100	-2.96666600	H	-0.49828300	2.92970800	2.50574600
H	-0.90962800	2.70331900	-3.42858300	H	-0.47772100	2.97164100	0.71109400
H	-0.44233800	1.02162000	-3.75825800	N	0.49239300	1.33258000	1.58020400
C	-2.32464100	2.04566500	-1.25253200	N	0.47744900	-0.79443600	1.19458200
C	-3.46094300	1.48105800	-0.43266800	N	-1.73599200	1.24964200	-2.17235900
C	-3.69258300	2.12703000	0.78749200	H	-2.18232800	0.38173100	-2.43018100
H	-3.07033700	2.98462500	1.01986500	O	-4.15773200	-0.16866600	-2.02546200
C	-4.68852400	1.70656300	1.65536900	O	-1.89518200	3.17186500	-1.00937800
C	-5.49308000	0.62649100	1.29724400	H	-4.84847400	2.22367700	2.59548100
C	-5.30016500	-0.01534100	0.08090300	C	3.99131600	2.51609300	0.44602900
H	-5.96535300	-0.81581500	-0.22497900	F	4.93651400	3.32913900	-0.03852800
C	-4.28712600	0.40303100	-0.78684300	F	3.51650600	3.12812700	1.56919300
C	-4.03349700	-1.60014000	-2.09014700	F	4.57010700	1.38554400	0.84068500
H	-4.42972200	-1.88448200	-3.06670400	C	-1.85411800	-0.87237600	3.57119100
H	-4.64368800	-2.06917900	-1.31294300	C	-3.28005700	-1.04445300	3.25997200
C	-2.58571600	-1.98374500	-1.95207200	O	-2.37119800	-0.55803100	2.28057900
C	-1.80883600	-2.25761500	-3.07842900	H	-1.21112400	-1.75081800	3.61767900
H	-2.27717400	-2.28314700	-4.05930200	H	-3.96615400	-0.28067200	3.62525700
C	-0.44447400	-2.51195200	-2.94618200	C	-3.87656200	-2.39354400	2.97591900
H	0.15382500	-2.74697400	-3.82035400	H	-3.10412200	-3.08618900	2.63028600
C	0.15599200	-2.47404800	-1.69125800	H	-1.52263200	-0.01671200	4.15525000
H	1.22095200	-2.67146200	-1.57041500	H	-4.63763000	-2.30536600	2.19423500
C	-0.61333200	-2.18012700	-0.56030600	I	3.66474500	-2.73179900	0.00829200

C	-1.98167200	-1.95067500	-0.69219400	H	-4.34663600	-2.81021700	3.87003900
H	-2.57581700	-1.73104800	0.19451300	H	-6.29350600	0.29659700	1.95296700
C	0.03523400	-2.14658000	0.79934100				

TS1'

C	2.25572400	-1.50880300	-2.30353300	H	1.69121500	-0.13782800	4.21135700
H	1.39178100	-1.49292600	-2.96350800	H	2.96577500	-1.35187300	4.00735200
C	3.44465700	-0.88351500	-2.65699700	C	3.88012200	0.35338100	2.24743500
H	3.53376300	-0.35558900	-3.60131100	H	4.62833300	0.18005800	3.00370800
C	4.53161200	-0.92488100	-1.78321500	C	3.92980900	1.06051800	1.08689000
C	4.45297300	-1.62616900	-0.58324900	H	4.73446600	1.59807900	0.61129500
H	5.31504600	-1.66843300	0.07411400	C	1.90504800	0.19496100	1.26861600
C	3.25668400	-2.24473200	-0.23385200	H	0.84001900	-0.00020900	1.07082300
H	3.17021400	-2.77453800	0.71259100	C	2.26698200	1.62583300	-0.72991400
C	2.14601100	-2.16784300	-1.07551800	H	1.58165800	0.96362700	-1.25838900
C	0.82915200	-2.79298900	-0.68004700	H	3.15410000	1.79105200	-1.34034900
H	0.65985700	-3.68280400	-1.29613200	H	1.77915600	2.57615200	-0.48404700
H	0.86955900	-3.10603600	0.37008100	N	2.69126700	0.95342900	0.50315900
C	-1.22564300	-2.19153800	-1.84193900	N	2.61075800	-0.17645400	2.34304800
C	-2.60871700	-1.66017200	-1.59273400	N	-0.31158200	-1.91954900	-0.86573800
C	-3.32500200	-1.11508900	-2.65645700	H	-0.63296600	-1.36212800	-0.07529900
H	-2.85239900	-1.09635300	-3.63342900	O	-2.56309200	-2.47461300	0.62041100
C	-4.60211300	-0.59838600	-2.46190300	O	-0.94008100	-2.80622600	-2.85976900
C	-5.17450900	-0.64365900	-1.19191600	H	-5.14546300	-0.15837700	-3.29053700
C	-4.49568900	-1.23094700	-0.12800600	C	5.74994100	-0.10977500	-2.08602100
H	-4.95888300	-1.30842200	0.85034900	F	5.99642400	-0.02021700	-3.39487100
C	-3.22184200	-1.75743100	-0.33243900	F	5.59208100	1.16386700	-1.63776200
C	-2.54911100	-2.02260600	1.97300000	F	6.84721800	-0.58523400	-1.48557600
H	-3.37084300	-2.49210400	2.52920000	C	-0.67138000	2.13677300	1.18675700
H	-2.63709900	-0.93274200	2.00451900	C	-1.20540500	1.44801100	0.01263600
C	-1.20375300	-2.46232700	2.50508200	O	-1.04500300	0.35619100	0.87975300
C	-0.86882300	-3.81977000	2.50834800	H	0.37342700	2.06325600	1.44066400
H	-1.61381900	-4.55052500	2.20731300	H	-1.36160300	2.38946500	1.98069500
C	0.41129600	-4.23231200	2.86402500	H	-0.53802700	1.43713600	-0.86089000
H	0.66088600	-5.28801200	2.86829400	C	-2.62295200	1.78795600	-0.38043200
C	1.38194800	-3.28736400	3.19352400	H	-3.26705600	1.74021400	0.50324100
H	2.38851900	-3.60651600	3.45197300	H	-2.99807500	1.08145000	-1.12249800
C	1.05688100	-1.93105300	3.19922400	H	-2.65876300	2.79955200	-0.79384200
C	-0.24283400	-1.52773600	2.88218600	I	-0.12249400	4.69046300	0.55970100
H	-0.50543000	-0.47333800	2.86669800	H	-6.16665100	-0.23521700	-1.02899400
C	2.09615700	-0.89327500	3.53179900				

Int2'

C	3.63734700	1.98161000	-1.05647300	H	-2.50241400	-0.92066500	2.19285900
H	4.08779900	1.30455000	-1.77645100	H	-2.22335700	-0.05005100	3.72271400
C	2.85447700	3.04737200	-1.47960200	C	-0.98540400	2.03918300	2.52224400

H	2.66861100	3.20892100	-2.53622100	H	-0.82221900	2.18215800	3.57899600
C	2.30075000	3.91589200	-0.53821300	C	-0.78284000	2.86638500	1.46869300
C	2.53477700	3.72602900	0.81977100	H	-0.41329300	3.87739500	1.41251100
H	2.10476600	4.40870800	1.54567500	C	-1.62633700	0.92033400	0.64268400
C	3.31389200	2.65130400	1.23629300	H	-2.09039400	-0.64932300	-0.08775900
H	3.48689000	2.49129400	2.29674600	C	-1.07826800	2.67318700	-1.01185200
C	3.87033300	1.77391000	0.30722200	H	-0.04598600	2.61459500	-1.36509700
C	4.73094800	0.61053800	0.75568200	H	-1.40858700	3.71251400	-1.04825000
H	5.75168300	0.75163800	0.39004500	H	-1.71484000	2.05942900	-1.64757800
H	4.75829200	0.57202100	1.84871700	N	-1.18016100	2.16388100	0.34522100
C	4.80393100	-1.19895100	-0.87815500	N	-1.50792300	0.87209600	1.99528700
C	4.33665500	-2.56392900	-1.32426000	N	4.27819700	-0.67239900	0.25763600
C	4.97544100	-3.06635100	-2.45857800	H	3.52638900	-1.15771000	0.72472800
H	5.73722800	-2.43878000	-2.90723200	O	2.72338800	-2.84665900	0.38851800
C	4.65288000	-4.30776900	-2.99179000	O	5.64888000	-0.59586100	-1.53255500
C	3.66334900	-5.06950700	-2.38241200	H	5.16605400	-4.67391800	-3.87369000
C	3.00415300	-4.59756300	-1.25121700	C	1.49176700	5.09428700	-0.98935600
H	2.23385700	-5.20310800	-0.79081600	F	2.22387700	6.21073500	-1.08326000
C	3.33686900	-3.35123900	-0.71784400	F	0.92761100	4.88864100	-2.18921000
C	1.63268100	-3.55274400	0.97331000	F	0.48824100	5.36778500	-0.12534300
H	1.98524400	-4.52472700	1.34232800	C	-4.67323100	-0.95497500	0.00404700
H	0.85086700	-3.71919500	0.22315400	C	-3.62556600	-1.45909600	-0.98931500
C	1.12147100	-2.69413100	2.09722200	O	-2.42047900	-1.58115500	-0.27431400
C	1.87716800	-2.55359700	3.26510300	H	-4.34445600	-0.02613600	0.46931300
H	2.81013000	-3.10153700	3.36860400	H	-4.89074800	-1.70707000	0.76315200
C	1.43472000	-1.72204700	4.28662700	H	-3.52804300	-0.71503800	-1.79613500
H	2.01597300	-1.62222200	5.19745200	C	-3.96314100	-2.81495700	-1.58286100
C	0.23833300	-1.02003000	4.14165400	H	-4.07516100	-3.54739900	-0.77726700
H	-0.11084500	-0.37251800	4.94246100	H	-3.14471800	-3.13889400	-2.22874300
C	-0.51672700	-1.14757000	2.97842500	H	-4.88609900	-2.78417100	-2.16532900
C	-0.07160400	-1.99213300	1.95806900	I	-6.59395600	-0.46438300	-0.92419500
H	-0.66948800	-2.09825100	1.05407500	H	3.39284800	-6.04090000	-2.78379600
C	-1.77698200	-0.34000900	2.76709300				

TS2'

C	-0.21485200	2.87680500	-1.24808500	H	-2.56018900	0.21464800	4.46730300
H	0.58024300	2.17296100	-1.47044100	C	-3.38002700	1.55062300	2.34327400
C	-1.42472400	2.79420200	-1.93362400	H	-3.60506100	2.15137900	3.20982400
H	-1.56162300	2.03587800	-2.69720200	C	-3.77209300	1.66644800	1.04836500
C	-2.44251800	3.69753700	-1.64442600	H	-4.39935900	2.38824300	0.55023100
C	-2.26230200	4.67651200	-0.66583900	C	-2.42322000	-0.12462600	1.19192000
H	-3.06166100	5.37923300	-0.44951400	H	-1.51801900	-1.05980900	0.79906600
C	-1.05486900	4.74994600	0.01106100	C	-3.43393400	0.27334500	-1.02705500
H	-0.90644500	5.51498000	0.76878600	H	-3.90073600	1.12035800	-1.52469700
C	-0.01581700	3.85949200	-0.28075300	H	-4.10902800	-0.58451600	-1.06717900

C	1.31658300	4.01926000	0.42803900	H	-2.48992300	0.02743700	-1.51428400
H	1.85981700	4.85226000	-0.02856300	N	-3.17775000	0.62486200	0.36805400
H	1.13732700	4.26940000	1.47990600	N	-2.56610800	0.43781300	2.40686100
C	3.16384900	2.79092300	-0.57999300	N	2.17377000	2.86703800	0.35063900
C	3.92903300	1.49346700	-0.67266200	H	1.94968000	2.03945700	0.88561600
C	4.62203500	1.28281800	-1.86436300	O	3.36379100	0.75693700	1.50191200
H	4.58234800	2.07527000	-2.60379100	O	3.40840500	3.71127400	-1.34871400
C	5.32233900	0.10529300	-2.09890900	H	5.84421300	-0.04183600	-3.03782900
C	5.34076900	-0.88234900	-1.11984600	C	-3.75261000	3.65517700	-2.36605900
C	4.67828200	-0.68974200	0.08877200	F	-4.07488100	4.83316900	-2.90996600
H	4.71575400	-1.45218700	0.85858700	F	-3.77783600	2.73311900	-3.33768400
C	3.98114600	0.49596600	0.31738600	F	-4.77266000	3.34523900	-1.52171600
C	2.89900800	-0.32480000	2.30041800	C	-2.06186300	-3.60821200	0.55951400
H	3.72730100	-0.72297400	2.90207000	C	-1.23529600	-2.78886000	-0.43030600
H	2.49610200	-1.11753100	1.66174700	O	-0.62256700	-1.77776100	0.34376900
C	1.81394700	0.25447400	3.17090100	H	-2.72803100	-2.97251500	1.14159200
C	2.10369000	1.31947200	4.02900800	H	-1.42504600	-4.19153200	1.22426800
H	3.12402300	1.68590100	4.09625800	H	-1.90878000	-2.33818200	-1.17656100
C	1.09260400	1.91721000	4.77245500	C	-0.17120400	-3.60910300	-1.14072600
H	1.32264100	2.74128500	5.43967300	H	0.51377900	-4.03477600	-0.40095900
C	-0.21886900	1.45877700	4.65752900	H	0.39472100	-2.96557500	-1.81664500
H	-1.01219700	1.92704100	5.23510000	H	-0.61450900	-4.41961900	-1.72373800
C	-0.51474800	0.39987200	3.80295100	I	-3.39276600	-5.04091400	-0.41788800
C	0.50498800	-0.20304200	3.06477400	C	0.20429200	-0.42253200	-0.67693400
H	0.27460700	-1.01052800	2.37206100	O	0.96406400	0.06295100	0.09609200
C	-1.93188500	-0.08300500	3.62420700	O	-0.31619300	-0.46017900	-1.74754900
H	-1.95928600	-1.17259000	3.54863800	H	5.87997700	-1.80938100	-1.28726700

Int3'

C	1.83626300	-1.59243900	1.41571700	H	1.69461600	5.15664200	-2.98730000
H	0.75423300	-1.51622200	1.44218000	C	3.55209100	3.49914600	-1.98839800
C	2.45494400	-2.56423100	0.63617500	H	3.95312300	4.49894200	-1.95319700
H	1.86002300	-3.27499600	0.07068400	C	4.10686000	2.29885100	-1.67378900
C	3.84546900	-2.61852300	0.56936100	H	5.08930800	2.04438000	-1.31101200
C	4.62073500	-1.71607400	1.29475900	C	2.03847300	1.92921200	-2.34195500
H	5.70316500	-1.77445400	1.24685500	H	1.09918800	1.39002400	-2.51457800
C	3.99405900	-0.74654300	2.06862700	C	3.21407600	-0.07502500	-1.54066600
H	4.59395200	-0.03548300	2.63149200	H	3.16776700	-0.14631000	-0.45393300
C	2.59923900	-0.66641000	2.12843100	H	4.13110300	-0.51801400	-1.92815100
C	1.95119300	0.43039600	2.95454800	H	2.33889800	-0.56885900	-1.96383000
H	2.10954600	0.22540700	4.01715000	N	3.14616300	1.33980300	-1.90761300
H	2.44190400	1.38051700	2.71398700	N	2.26574400	3.24196200	-2.41739800
C	-0.33827300	0.02111500	3.63025400	N	0.53403100	0.56119300	2.74571700
C	-1.80052200	0.01824800	3.25160400	H	0.23392800	0.86887900	1.82104200
C	-2.58092700	-0.93321500	3.90647200	O	-1.65236300	1.84119600	1.75034800

H	-2.08071600	-1.54857500	4.64631500	O	0.01863300	-0.50003800	4.68126100
C	-3.93303600	-1.09491200	3.62214700	H	-4.51519000	-1.85111400	4.13665700
C	-4.52096900	-0.28018800	2.66272100	C	4.50689400	-3.57099800	-0.37685500
C	-3.77231800	0.69813300	2.01069800	F	5.74525900	-3.90115000	0.01593300
H	-4.25815700	1.33172000	1.27903800	F	3.81008500	-4.70299600	-0.53159800
C	-2.41629500	0.86315500	2.30858900	F	4.62954100	-3.02374500	-1.60786500
C	-2.17634800	2.54037500	0.63633500	C	-2.89782300	-0.77270300	-1.25153900
H	-3.11931200	3.03113100	0.91304600	C	-1.72238400	-1.48829900	-0.59747400
H	-2.37502600	1.83600000	-0.18299100	O	-0.92979500	-0.49180300	0.05276900
C	-1.17543800	3.58411200	0.21880500	H	-2.53647300	-0.00752000	-1.93448400
C	-0.88699200	4.65501300	1.06731000	H	-3.57823800	-0.36839800	-0.50200200
H	-1.38694400	4.71946400	2.02949800	H	-1.12102400	-1.96803700	-1.37595900
C	0.03726100	5.62323200	0.69168500	C	-2.13651600	-2.47146800	0.48163700
H	0.25256600	6.45544600	1.35337500	H	-2.72765500	-1.96054700	1.24772300
C	0.69324300	5.51984500	-0.53335300	H	-1.24990100	-2.89697200	0.95885000
H	1.42530900	6.26915800	-0.82495900	H	-2.72896700	-3.28582400	0.05941200
C	0.41520700	4.45147500	-1.38220700	I	-4.10569600	-2.10624700	-2.49004300
C	-0.52602700	3.49266200	-1.00642900	C	-0.05569600	0.24813000	-0.73679400
H	-0.72933700	2.64103600	-1.65469800	O	0.72246600	0.96903500	-0.08504100
C	1.20769400	4.23971500	-2.64840400	O	-0.15138100	0.12597800	-1.98241700
H	0.58111700	3.86098200	-3.45910800	H	-5.57175000	-0.39267000	2.41457500

TS3'

C	1.59381500	0.48155300	-1.90368500	H	0.38945900	-5.98979800	2.53134200
H	0.61327800	0.92570200	-1.77164600	C	1.70139600	-4.67883900	0.41531500
C	2.72660100	1.15301100	-1.44813100	H	1.30734400	-5.54906400	-0.08373800
H	2.63467100	2.12197500	-0.96016600	C	2.61747900	-3.75597800	0.02365600
C	3.98249200	0.57115100	-1.61073800	H	3.18625100	-3.65480400	-0.88661400
C	4.11311900	-0.65967500	-2.25020200	C	1.88536700	-3.17400800	2.00916500
H	5.09911300	-1.09153500	-2.39065600	H	1.68545100	-2.58003200	2.88661800
C	2.97412400	-1.32364000	-2.69268900	C	3.45499400	-1.57287000	0.94705600
H	3.07058000	-2.28180300	-3.19986400	H	2.92078000	-0.92667600	0.24865200
C	1.70170400	-0.77247600	-2.50960200	H	4.46605800	-1.76273300	0.58861400
C	0.48222700	-1.52934000	-3.01186900	H	3.48366300	-1.10432900	1.92850600
H	0.40459000	-1.39454900	-4.09488100	N	2.72714000	-2.83659900	1.04005900
H	0.62281400	-2.59567800	-2.80578700	N	1.27034400	-4.30525300	1.66963200
C	-1.46710300	-0.09398100	-2.99397900	N	-0.76176000	-1.10381700	-2.42642100
C	-2.58794000	0.51810900	-2.18644600	H	-0.93726000	-1.38103500	-1.46665700
C	-2.98632600	1.78660300	-2.60735100	O	-2.84783600	-1.30312500	-0.68588900
H	-2.50104300	2.18068300	-3.49343600	O	-1.17638800	0.36911700	-4.09049200
C	-3.94719800	2.52044800	-1.92087300	H	-4.22806600	3.51001600	-2.26284500
C	-4.52878700	1.97220200	-0.78580400	C	5.17763100	1.19732400	-0.96026800
C	-4.16697500	0.69870800	-0.35118000	F	6.32258200	0.85807700	-1.57202900
H	-4.63949400	0.29179000	0.53389800	F	5.10602200	2.52613300	-0.91992100
C	-3.20607400	-0.03692300	-1.04876800	F	5.28768200	0.76768700	0.32046600

C	-3.27505200	-1.77628000	0.58071800	C	1.04505900	1.29140800	1.79927900
H	-4.37181200	-1.77926000	0.62890100	C	-0.31595100	1.41099400	1.12407500
H	-2.89055900	-1.11600300	1.37069700	O	-0.52270500	0.22008800	0.34050500
C	-2.75365600	-3.17938900	0.74111400	H	1.94120300	1.18151900	1.20527200
C	-3.30836600	-4.22025100	-0.00835000	H	1.14567700	1.35842400	2.87045800
H	-4.14211300	-4.01008400	-0.67221300	H	-0.31590000	2.22589600	0.40172600
C	-2.79351800	-5.50806700	0.08028900	C	-1.43641400	1.57297600	2.13265600
H	-3.23580700	-6.31240600	-0.49748600	H	-1.41776100	0.73642800	2.83920800
C	-1.69262400	-5.76074700	0.89762000	H	-2.39846600	1.59211800	1.61583500
H	-1.27015300	-6.76138300	0.95028800	H	-1.30525300	2.50903000	2.68070500
C	-1.12972500	-4.72738000	1.64218000	I	1.65949700	3.90860100	1.78147400
C	-1.68096100	-3.44802400	1.58126900	C	0.18744300	-0.83740900	0.80389600
H	-1.23043200	-2.64068300	2.15446900	O	0.17265700	-1.88656200	0.16414300
C	0.15548900	-4.93015200	2.40327300	O	0.82264900	-0.59712400	1.89627100
H	0.12908400	-4.46102900	3.38970100	H	-5.27342600	2.52903500	-0.22583600

4c

C	-3.44010000	1.83523900	0.73097500	N	-1.63604200	-0.97116200	-0.53307800
H	-2.59195200	2.51851600	0.76566900	C	0.37936500	-2.18849800	0.23575300
H	-3.85400400	1.71745600	1.73272300	H	0.54037900	-1.37114000	0.94849400
C	-3.70367900	-0.61624500	0.13327500	H	-0.21438800	-2.96828300	0.73092100
H	-4.74687400	-0.65915800	0.40120000	C	1.73723500	-2.73348100	-0.20078600
C	-2.86284900	-1.56915700	-0.35274600	H	1.59857100	-3.53391400	-0.93906500
H	-3.03002000	-2.60813400	-0.58720400	H	2.28672100	-1.92356500	-0.69447000
C	-1.71628300	0.30433300	-0.16086700	C	2.54581600	-3.24642400	0.98665500
H	-0.85795000	0.99279400	-0.15553800	H	3.51359700	-3.63774600	0.66526900
C	-0.38251000	-1.62374600	-0.95572200	H	2.73031900	-2.43587700	1.69720000
H	0.22156000	-0.85354900	-1.44352300	H	2.01522900	-4.04706200	1.51222400
H	-0.65128900	-2.39422100	-1.68341400	H	-4.20068000	2.22619600	0.05431100
N	-2.96425100	0.54298100	0.24630300	I	1.58680900	1.52835500	-0.06597300

Int1"

C	1.33651900	3.19971000	-0.03570400	H	5.63609000	-0.21707200	0.59306800
C	0.20785100	3.70017400	0.53206500	H	5.59775400	-1.81607300	-0.16304900
N	1.03335500	1.93518300	-0.48892100	H	4.49030000	-1.44330600	1.16303600
C	-0.23969700	1.66414300	-0.20201000	C	-2.12655900	2.81047900	0.93128800
N	-0.76253700	2.72864800	0.41283400	H	-2.12894100	2.56560800	1.99448600
H	2.31712600	3.62894000	-0.16183500	H	-2.74285700	2.10117200	0.38008400
H	0.00895200	4.65010400	1.00072400	C	-3.49078100	-0.88718500	-0.17858800
H	-0.75754700	0.72640500	-0.38817300	C	-3.02467100	-0.87965600	-1.56853800
C	1.98370400	0.99609600	-1.10769600	O	-2.87662200	0.27827300	-0.74224600
C	3.05751200	0.56245300	-0.11869300	H	-3.75269600	-0.76967200	-2.37024300
H	2.40653000	1.48613700	-1.98990000	H	-2.09191300	-1.38706600	-1.80365900
H	1.40039000	0.12425400	-1.41322000	C	-4.94816900	-0.74502100	0.15979400
C	3.92868900	-0.53867300	-0.71852000	H	-2.84954400	-1.39861100	0.53831200
H	2.55364800	0.17328500	0.77275200	H	-5.47478500	-0.21026800	-0.63497000

H	3.67493700	1.42132400	0.17803700	H	-5.07758700	-0.19296400	1.09526400
C	4.97666500	-1.03113700	0.27443900	H	-5.40603000	-1.72955300	0.28526100
H	4.41436100	-0.17459500	-1.63335100	H	-2.49509400	3.82539000	0.78138400
H	3.27482200	-1.37147500	-1.00202100	I	0.15383000	-1.84855200	0.40455800

TS1"

C	-3.67661000	1.31880400	-0.68713000	C	0.89793300	4.17590900	0.92226000
C	-4.60858000	0.40189200	-0.31752700	H	0.10583100	4.78990700	1.36401000
N	-2.44022400	0.72296700	-0.53827200	H	1.68319900	4.84419400	0.56215300
H	-3.78177700	2.33066200	-1.04490100	H	1.32788800	3.54684500	1.70696400
N	-3.91400800	-0.72992000	0.05171500	H	-5.13639500	-2.41175500	-0.22339900
H	-5.68494100	0.45470300	-0.29031600	H	-5.01998600	-1.82388200	1.45926200
C	-2.59855700	-0.52526900	-0.08571300	C	0.37743000	-1.32543000	1.18901800
C	-4.47104700	-1.99128000	0.53174400	H	-0.21548300	-0.42723100	1.29303800
H	-1.84177800	-1.36193500	0.22562600	H	0.73571800	-1.78942500	2.09773000
C	-1.15769600	1.39374400	-0.80916800	C	1.13764200	-3.32792200	-0.19197600
C	-0.78751300	2.41122000	0.26466900	H	2.09781200	-2.96060500	-0.56194200
H	-1.25134900	1.87449900	-1.78788700	H	0.71865300	-4.03716100	-0.91026600
H	-0.38398300	0.62323100	-0.88232000	H	1.29438800	-3.84796100	0.75666900
H	-1.66257900	3.02458700	0.51765500	H	0.01915000	-1.61835900	-0.92255300
C	0.36035000	3.30365500	-0.20668500	O	-0.99472200	-2.49085100	0.70855100
H	-0.48524100	1.87928100	1.17511800	C	0.18000700	-2.17922500	0.01692200
H	0.01178400	3.92573800	-1.04137100	H	-3.63628800	-2.67073500	0.71222200
H	1.16930000	2.66852000	-0.58328200	I	2.51460400	0.19801500	0.82395800

Int2"

C	2.72978800	1.96894600	-1.20892600	C	5.49015500	-2.83126300	-0.09814700
C	2.30794900	3.10217100	-0.59862100	H	6.26990000	-2.26410000	-0.61584500
N	2.19155000	0.92034400	-0.48504700	H	5.66153200	-3.89257200	-0.29286900
H	3.34647300	1.82165500	-2.08197700	H	5.61308200	-2.66218800	0.97568400
N	1.53731400	2.69526300	0.47673000	H	0.14079300	4.21651400	0.86167600
H	2.47883700	4.14066100	-0.83520900	H	1.59854500	4.25014000	1.88686200
C	1.45212900	1.34466300	0.57290900	C	-1.32661100	-0.76834000	0.00729500
C	0.87082600	3.60167000	1.39334500	H	-0.67074400	-0.07305000	-0.51550500
H	0.69300400	-0.03657600	1.52265500	H	-1.14895500	-1.78974300	-0.33026800
C	2.45044900	-0.49052400	-0.75279300	C	-1.95592400	-1.66326700	2.30529500
C	3.84158700	-0.91544700	-0.29431100	H	-3.02942700	-1.53625500	2.15138500
H	2.32319200	-0.67102900	-1.82627100	H	-1.73164700	-1.55811000	3.36846500
H	1.68542500	-1.05509200	-0.21215900	H	-1.66848900	-2.67246700	1.99441600
H	4.60055100	-0.30626000	-0.80298400	H	-1.44246900	0.37419500	1.81937000
C	4.10212300	-2.39618300	-0.55979000	O	0.21438100	-0.87186500	1.78552900
H	3.93031100	-0.70379600	0.77793600	C	-1.14689300	-0.64521700	1.52123500
H	3.98799400	-2.59943100	-1.63203400	H	0.35918100	2.99580000	2.13952400
H	3.33709300	-2.99181700	-0.04789500	I	-3.34046700	-0.24837800	-0.68407400

TS2"

C	3.58669000	1.14406800	-1.34944800	H	1.84622800	-3.21232100	2.44392500

C	3.33021100	2.45918000	-1.12960500	H	2.45014900	-4.73213800	1.76883500
N	2.41730900	0.46213500	-1.07745000	H	1.33824000	4.48108200	-1.12491200
H	4.48125500	0.63909200	-1.67701200	H	1.77879300	4.15567400	0.58109700
N	2.01555100	2.54010200	-0.72436600	C	-2.62304700	0.01196200	0.76864400
H	3.95691800	3.33052500	-1.22954500	H	-3.57038900	-0.37500000	0.39369300
C	1.46473800	1.32021600	-0.68797400	H	-2.66500600	0.19686600	1.84004400
C	1.30694200	3.75031500	-0.31490600	C	-3.14485700	2.35329600	0.23667300
H	0.34807300	1.19876700	-0.28347900	H	-4.16061000	2.07214800	-0.05982400
C	2.26699800	-0.99277500	-1.05946800	H	-2.84437000	3.23292800	-0.33856100
C	2.58697300	-1.56761800	0.31532800	H	-3.14037600	2.61992700	1.29764000
H	2.92359800	-1.40434900	-1.83200000	H	-2.15273300	0.96499400	-1.08169000
H	1.23222700	-1.21519100	-1.33162500	O	-0.86299700	1.63701300	0.36971800
H	3.61835000	-1.31189400	0.58987100	C	-2.11861200	1.23342900	-0.00558800
C	2.39214700	-3.08139700	0.35204400	C	-0.18788000	1.75261700	2.41370300
H	1.92806200	-1.08539900	1.04765600	O	-1.18435300	1.60178600	3.01285600
H	3.09314600	-3.55954200	-0.34371600	O	0.94400500	1.93709000	2.15154900
H	1.38448300	-3.32284900	-0.01031200	H	0.28044900	3.45284800	-0.08679000
C	2.57791000	-3.64732100	1.75670300	I	-1.23326600	-1.68383200	0.59072800
H	3.57681300	-3.42034700	2.14173500				

Int3"

C	1.69246500	2.17204700	-0.58631100	H	6.63162600	-2.37582700	-0.99993200
C	0.91826200	2.92803500	0.23786000	H	6.35046800	-1.48305700	0.49926100
N	1.80185800	0.92904100	-0.00277600	H	0.14017400	3.10761100	3.11863800
H	2.14802900	2.39891100	-1.53655800	H	-0.65815200	1.50995300	2.84744600
N	0.57832900	2.13020200	1.30841300	C	-1.95815900	-1.44138500	-1.08671300
H	0.56896100	3.94366000	0.14780300	H	-2.55383900	-1.73549800	-1.94999100
C	1.12579400	0.92678400	1.14425400	H	-0.91337600	-1.71087400	-1.19400800
C	-0.34887500	2.45571200	2.39335000	C	-2.32976900	-3.50736200	0.23260500
H	0.96479100	0.09003200	1.82684500	H	-2.76317100	-3.98974200	-0.64858400
C	2.47161500	-0.25483700	-0.55198900	H	-2.80727700	-3.91952600	1.12442700
C	3.96990700	-0.24240700	-0.27459300	H	-1.25900400	-3.71200000	0.27411600
H	2.26774000	-0.26585000	-1.62721900	H	-3.63503500	-1.79241800	0.18264400
H	1.96503300	-1.11282800	-0.09793800	O	-2.12562700	-1.37463300	1.39211400
H	4.41951300	0.66693000	-0.69487200	C	-2.55820400	-1.99479100	0.20124600
C	4.65543400	-1.47665200	-0.85745400	C	-0.76250500	-1.26540400	1.65297900
H	4.13088500	-0.20492500	0.80959400	O	0.04357700	-1.71898300	0.81019200
H	4.47979500	-1.51207500	-1.93967200	O	-0.51163600	-0.66033200	2.71332100
H	4.19046300	-2.37616900	-0.43804800	H	-1.21805900	2.95473600	1.96337200
C	6.15541800	-1.48836400	-0.57715400	I	-1.94700200	0.75236900	-1.14512300
H	6.64138600	-0.60797700	-1.00875400				

TS3"

C	-3.27726300	0.44528200	-1.65815500	H	-2.22590300	-3.50385100	-0.48668700
C	-3.15619300	-0.77461400	-2.24297400	C	1.78532700	-0.79760200	0.20906500
N	-2.95113100	0.28499000	-0.32797500	H	2.58182800	-0.66729700	-0.51378200

H	-3.53506500	1.40632900	-2.07095500	H	0.62730200	3.03731200	3.48393200
N	-2.76478900	-1.65314000	-1.25798800	H	1.12351200	2.37061500	1.92422600
H	-3.27703500	-1.08353100	-3.26804300	H	-2.97591600	-3.54791200	-2.11356400
C	-2.63963900	-0.99324400	-0.11102200	H	1.34700200	0.13017800	0.56521700
C	-2.28475700	-3.01694000	-1.45883400	C	3.34678400	-1.28270300	2.03750200
H	-2.31194000	-1.43102600	0.83453700	H	4.21770100	-1.23966700	1.38035500
C	-2.75795700	1.34712500	0.66846700	H	3.56099300	-1.96372700	2.86335000
C	-1.35122400	1.26023500	1.25384600	H	3.15722300	-0.28836800	2.45051100
H	-3.52493400	1.25224100	1.44277000	H	2.32041600	-2.76854000	0.83677100
H	-2.91296200	2.29573400	0.14827700	O	1.05829800	-1.88260200	2.21262100
H	-1.25073800	0.31011400	1.79242400	C	2.11650500	-1.78795900	1.28356400
C	-1.02665400	2.40344100	2.20973400	C	-0.14966300	-1.99173400	1.55653000
H	-0.64178600	1.24106900	0.41597500	O	-0.04577500	-1.90498100	0.29475500
H	-1.73594900	2.39655600	3.04615300	O	-1.16975100	-2.10641200	2.23710200
H	-1.14755900	3.36709400	1.69989400	H	-1.28250800	-2.96017100	-1.88985800
C	0.39979700	2.27047000	2.74002700	I	0.54763800	-0.30662500	-2.25474300
H	0.54792600	1.28910200	3.20299400				

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9. ^{1}H-, ^{13}C-NMR spectra for the Synthesized Compounds

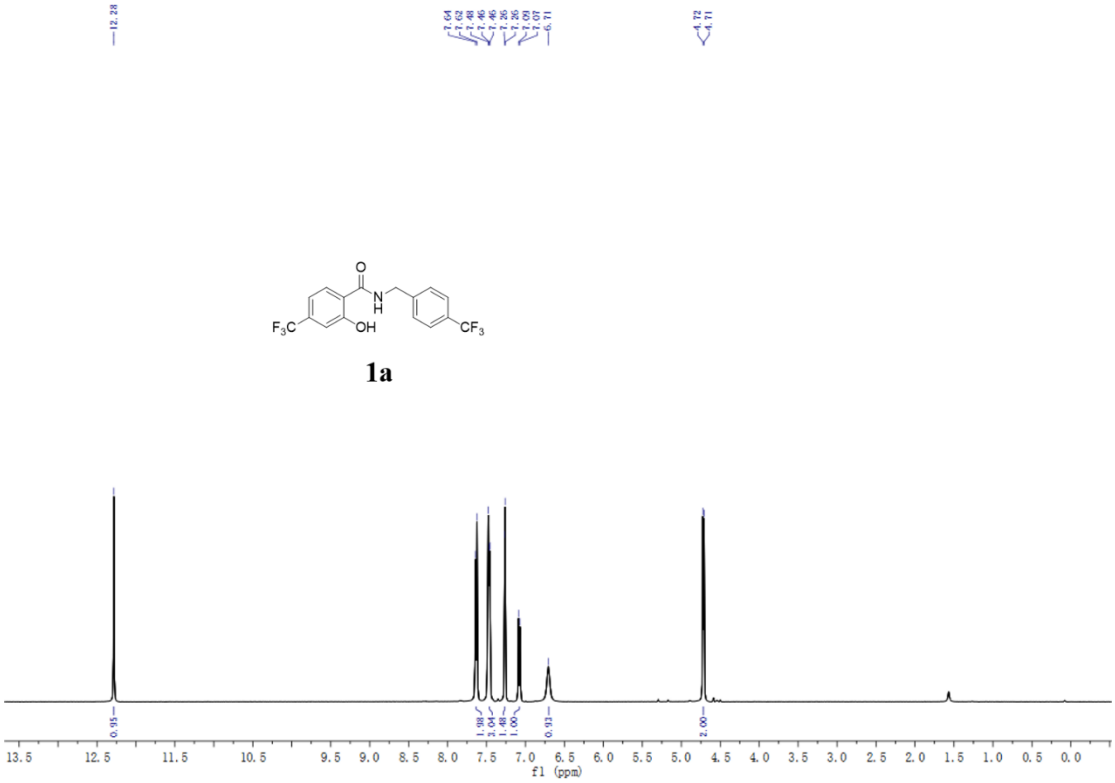

Figure S5. ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) spectra of catalyst **1a**.

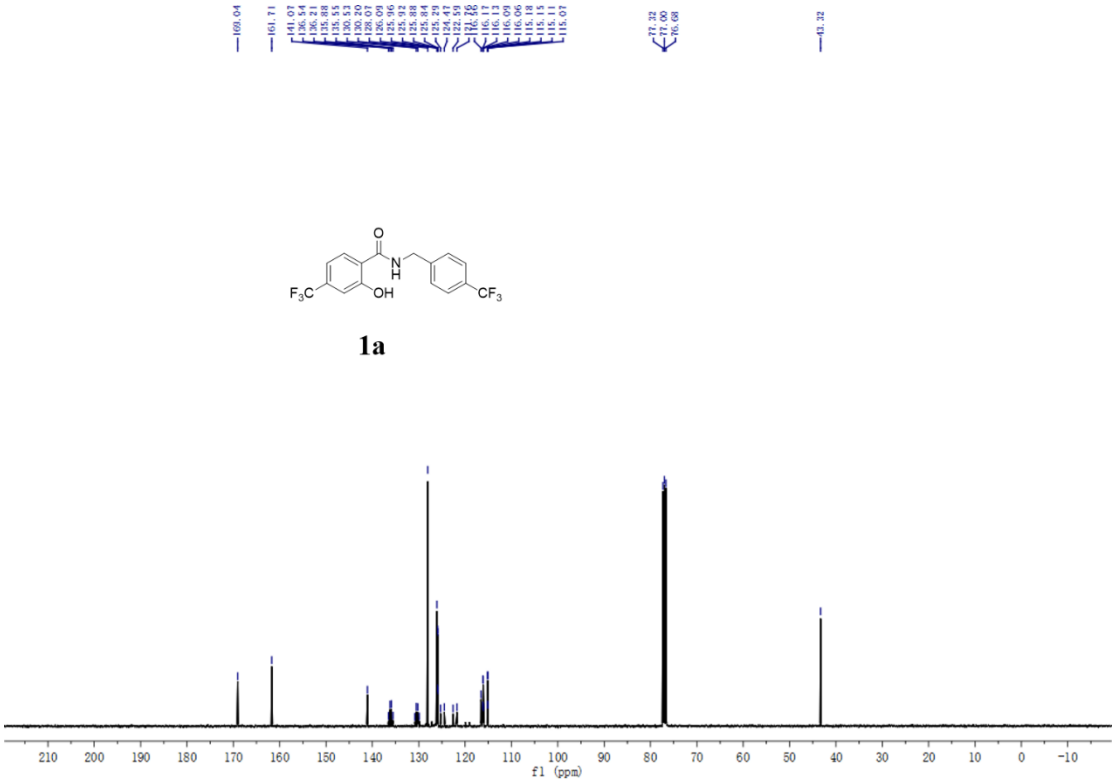

Figure S6. ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) spectra of catalyst **1a**.

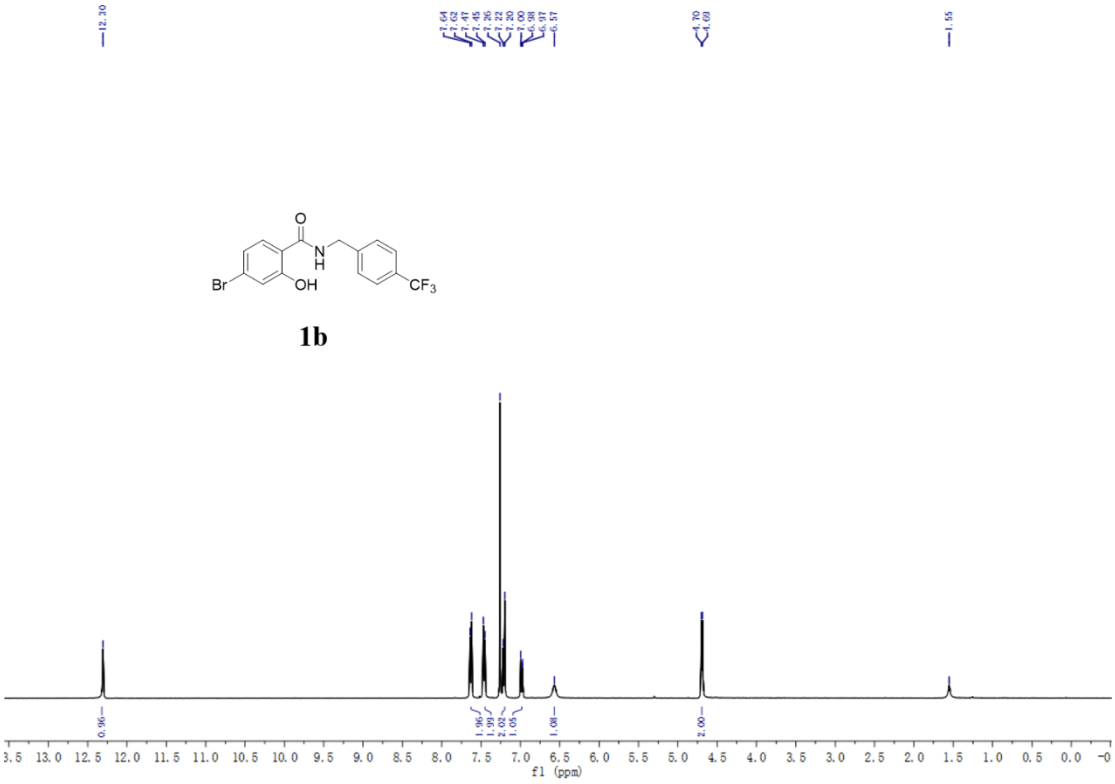

Figure S7. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ^{o}C) spectra of catalyst **1b**.

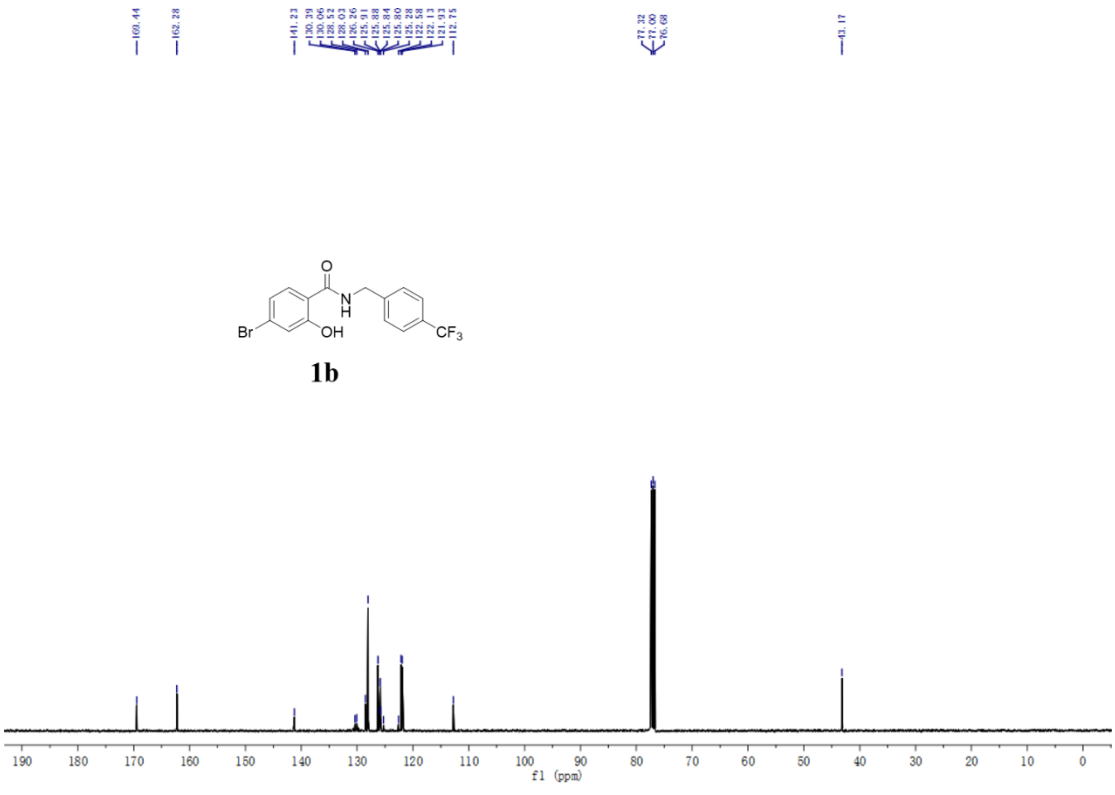

Figure S8. ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) spectra of catalyst **1b**.

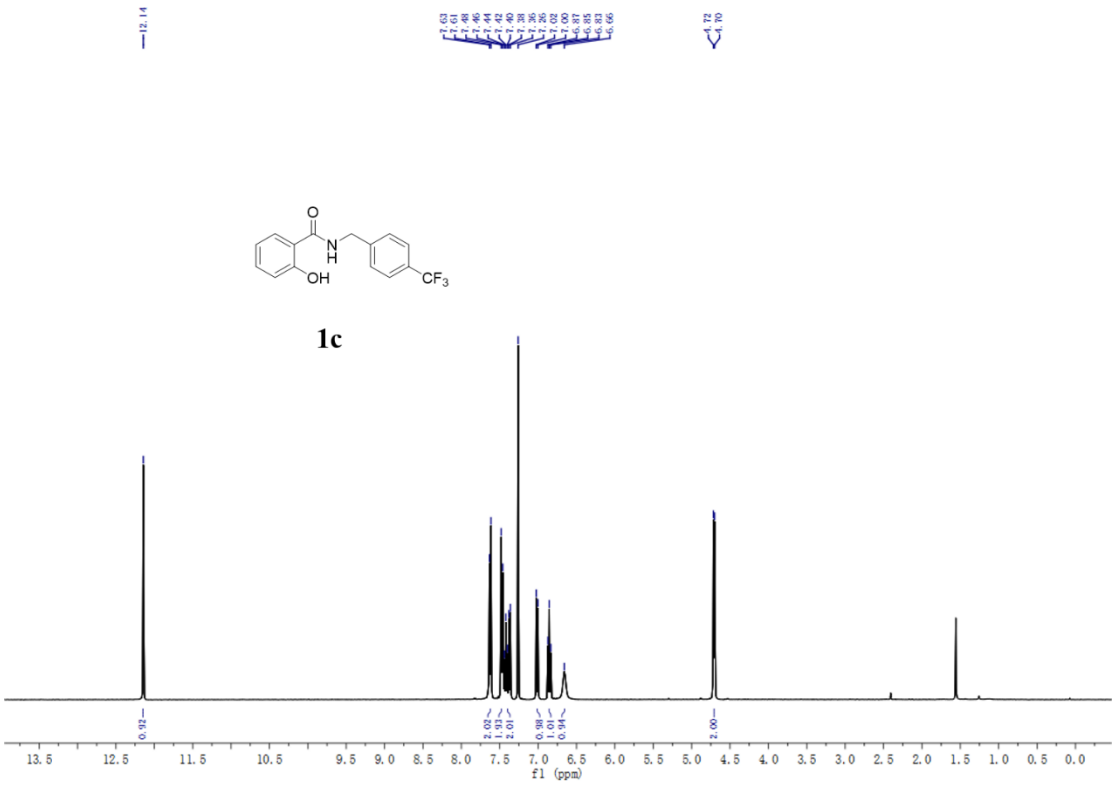

Figure S9. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ^{o}C) spectra of catalyst **1c**.

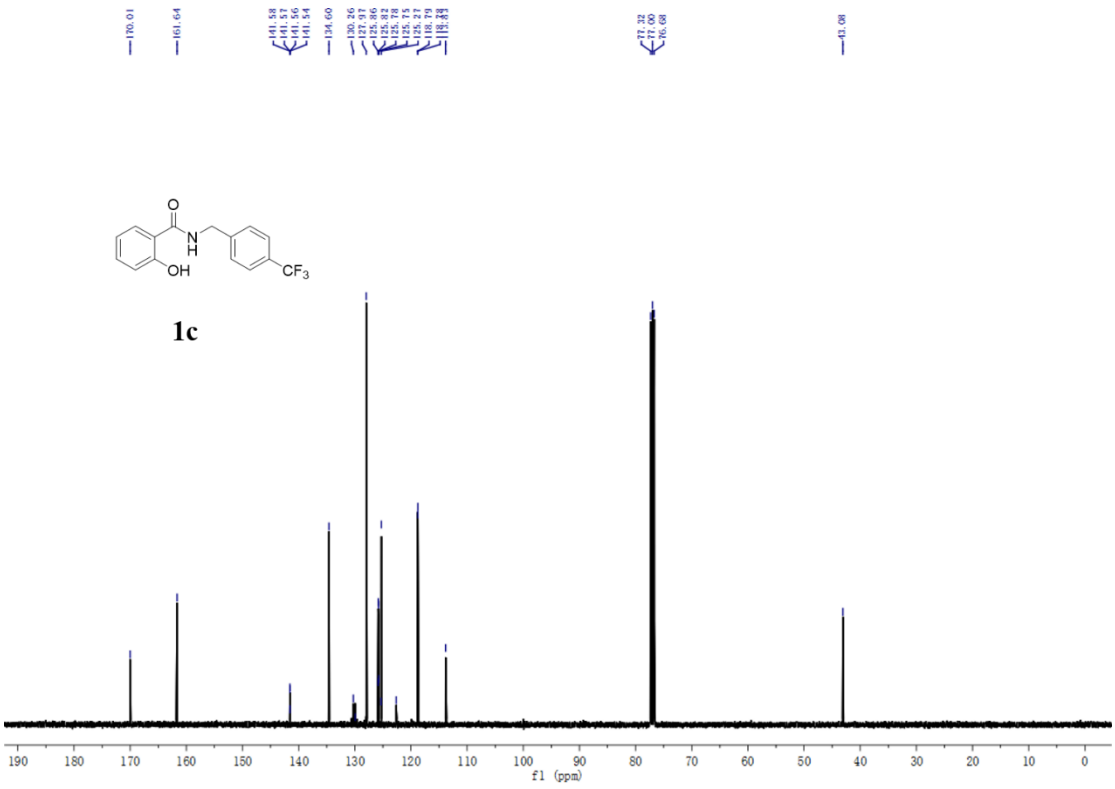

Figure S10. ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) spectra of catalyst **1c**.

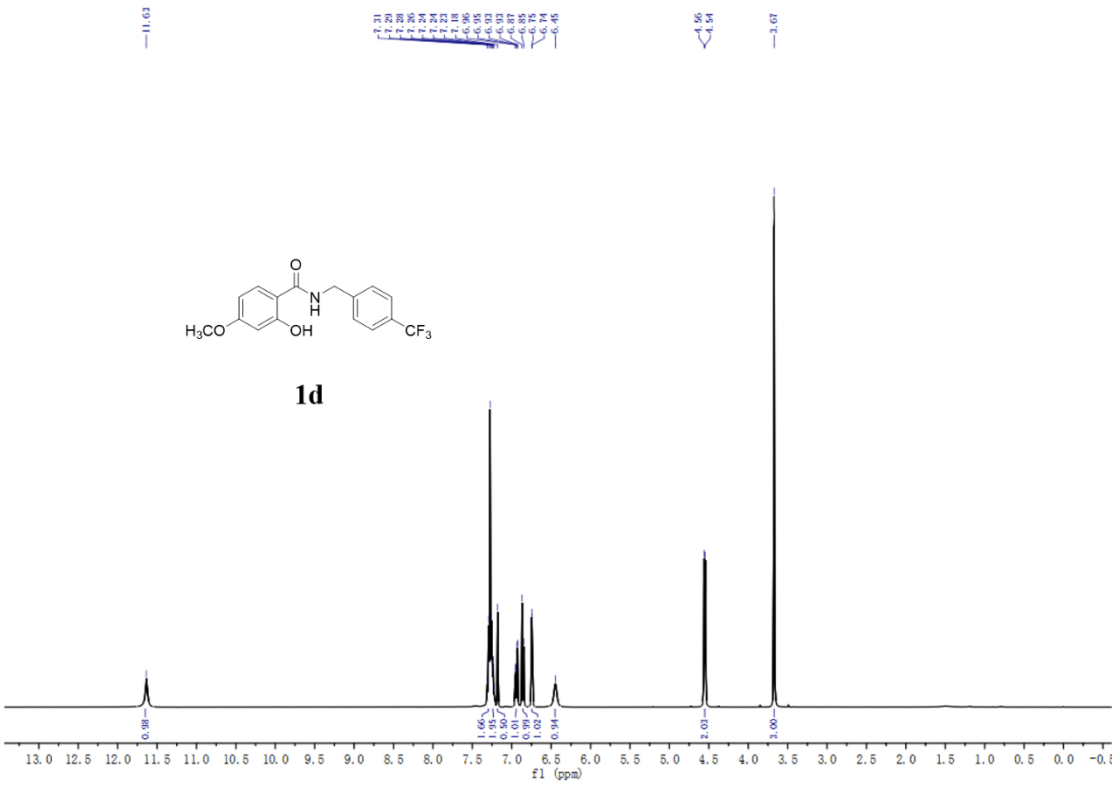

Figure S11. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ^{o}C) spectra of catalyst **1d**.

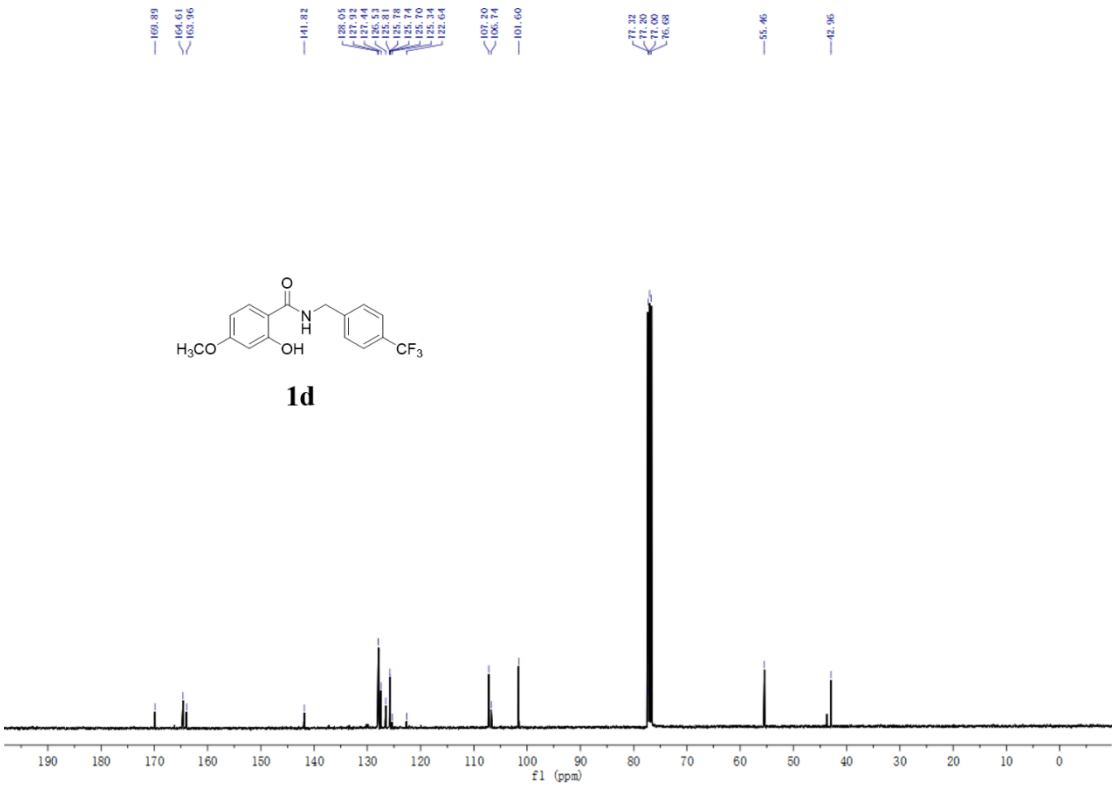

Figure S12. ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) spectra of catalyst **1d**.

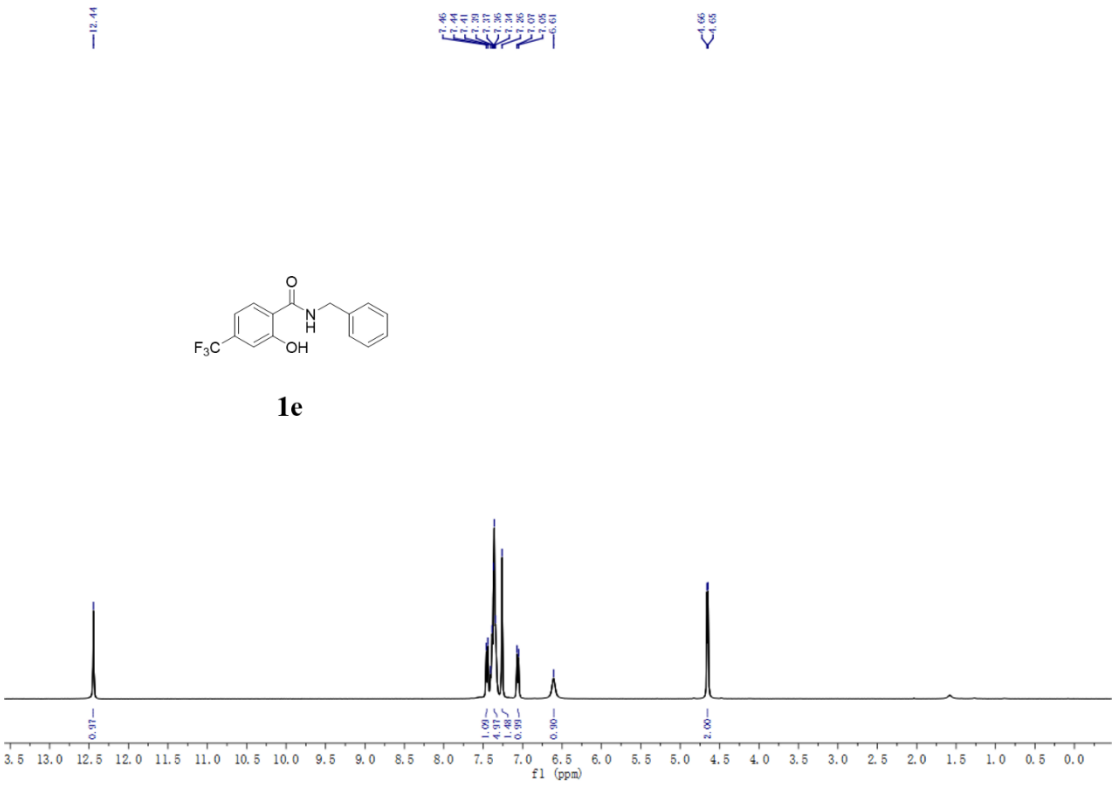

Figure S13. ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) spectra of catalyst **1e**.

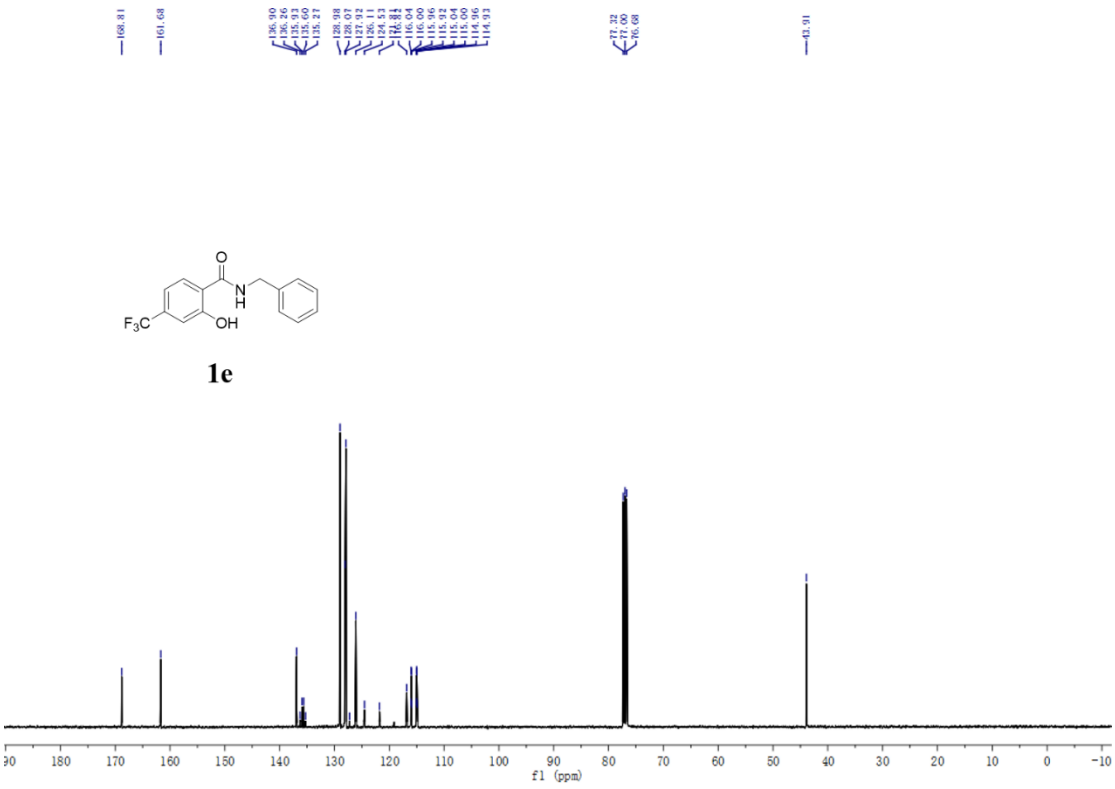

Figure S14. ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) spectra of catalyst **1e**.

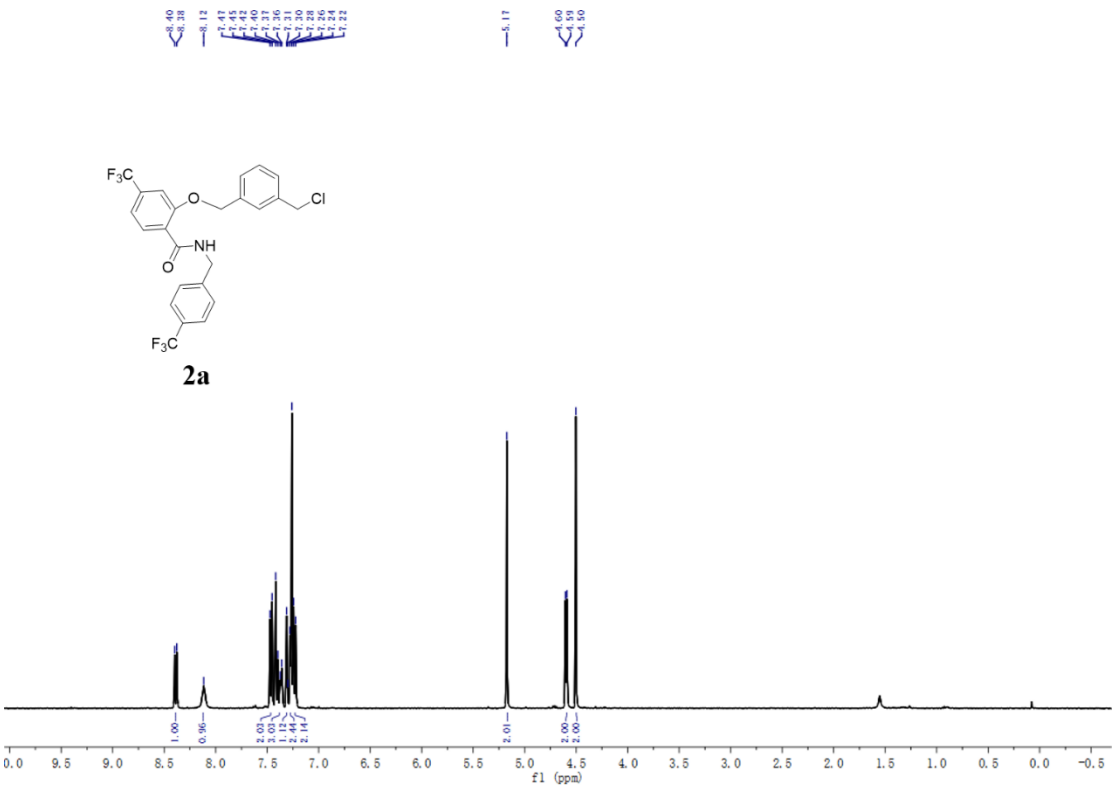

Figure S15. ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) spectra of catalyst **2a**.

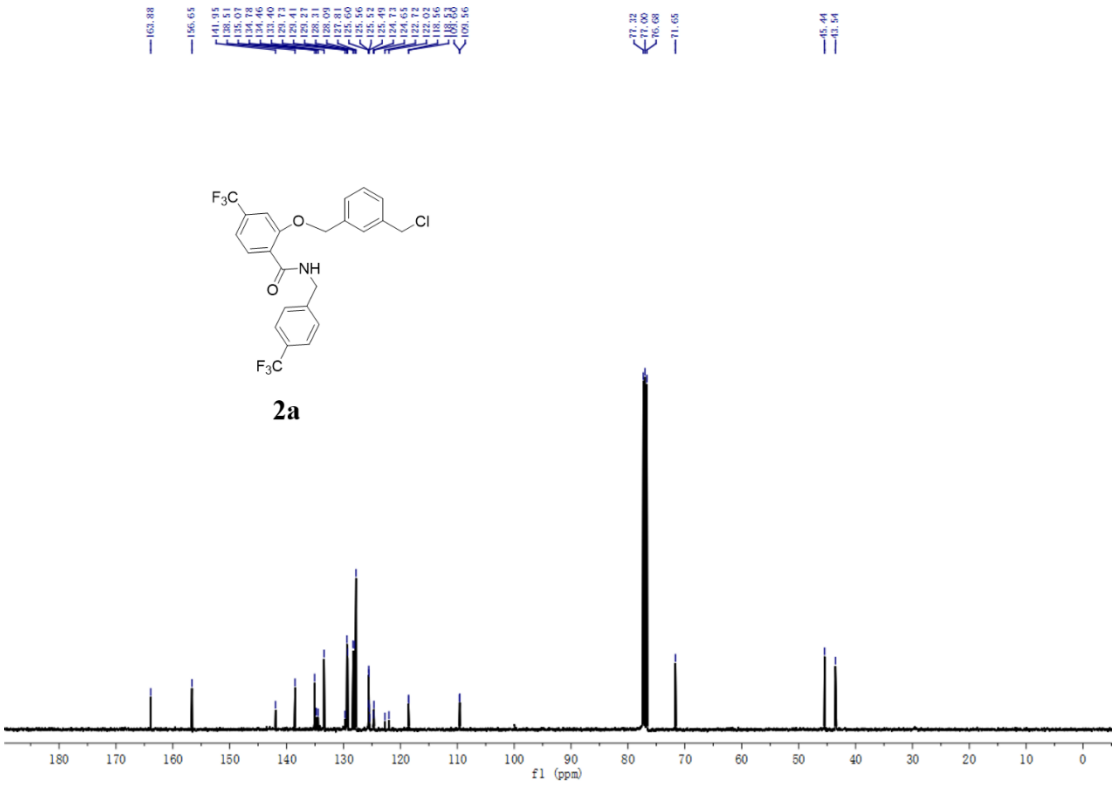

Figure S16. ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) spectra of catalyst **2a**.

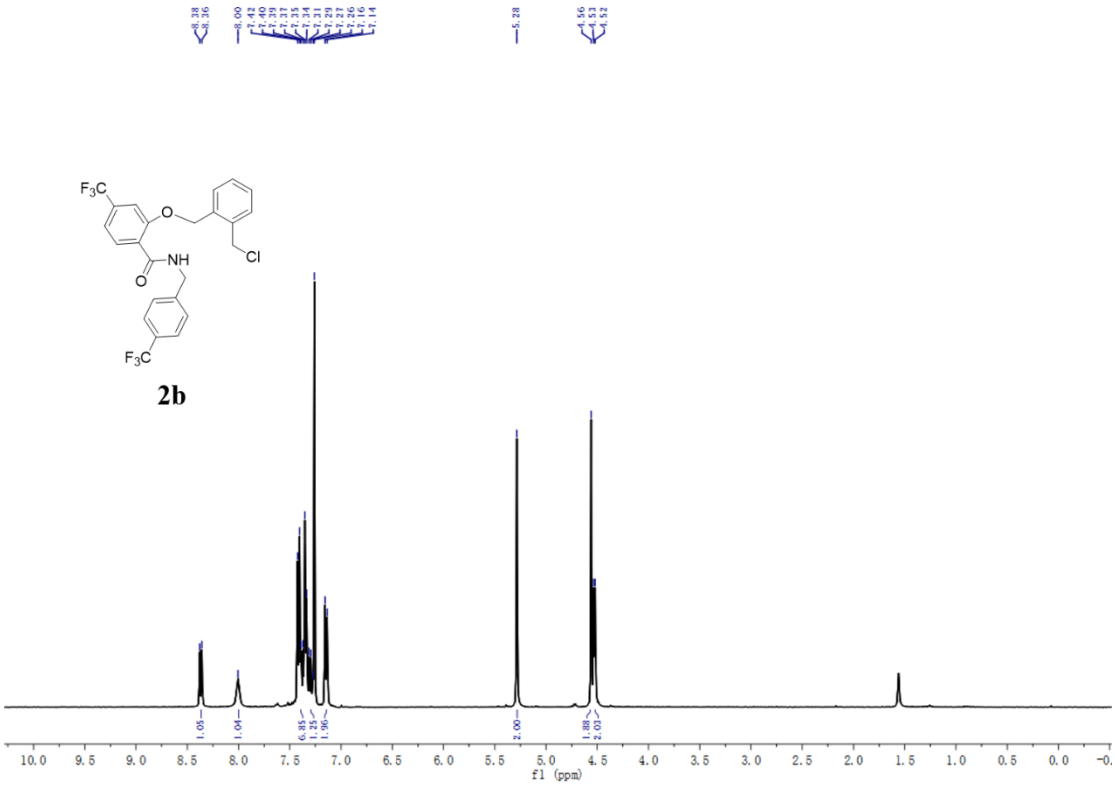

Figure S17. ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) spectra of catalyst **2b**.

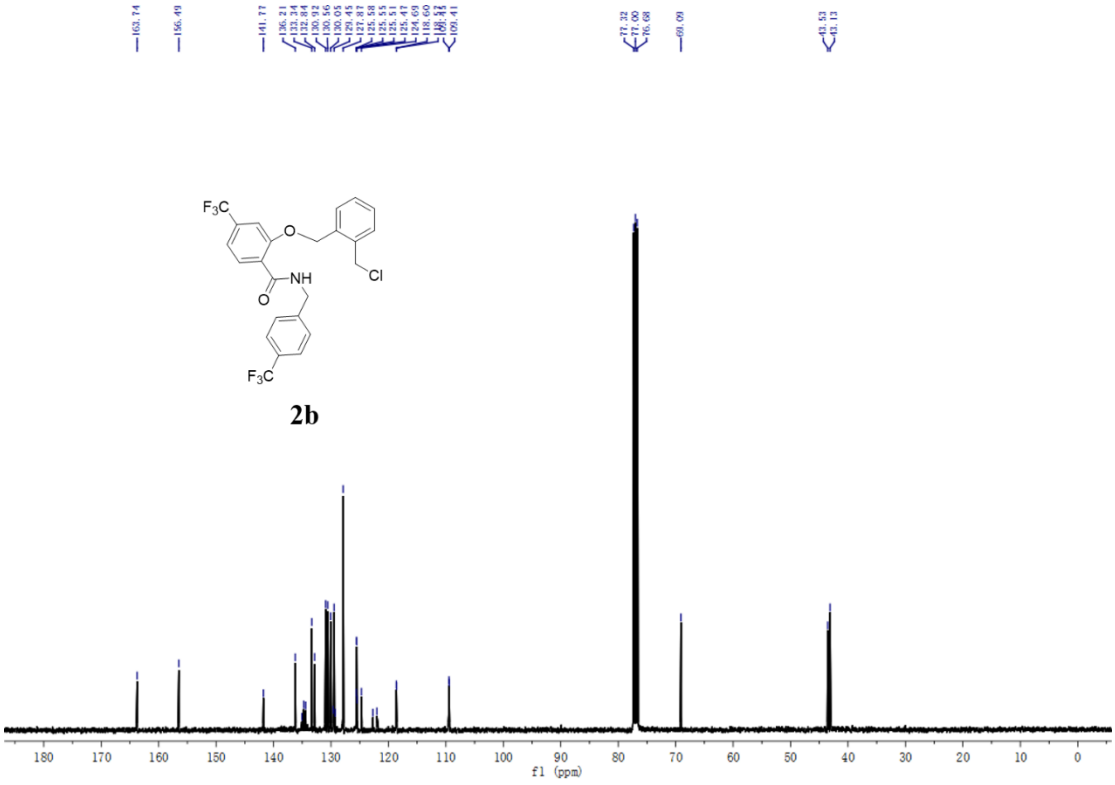

Figure S18. ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) spectra of catalyst **2b**.

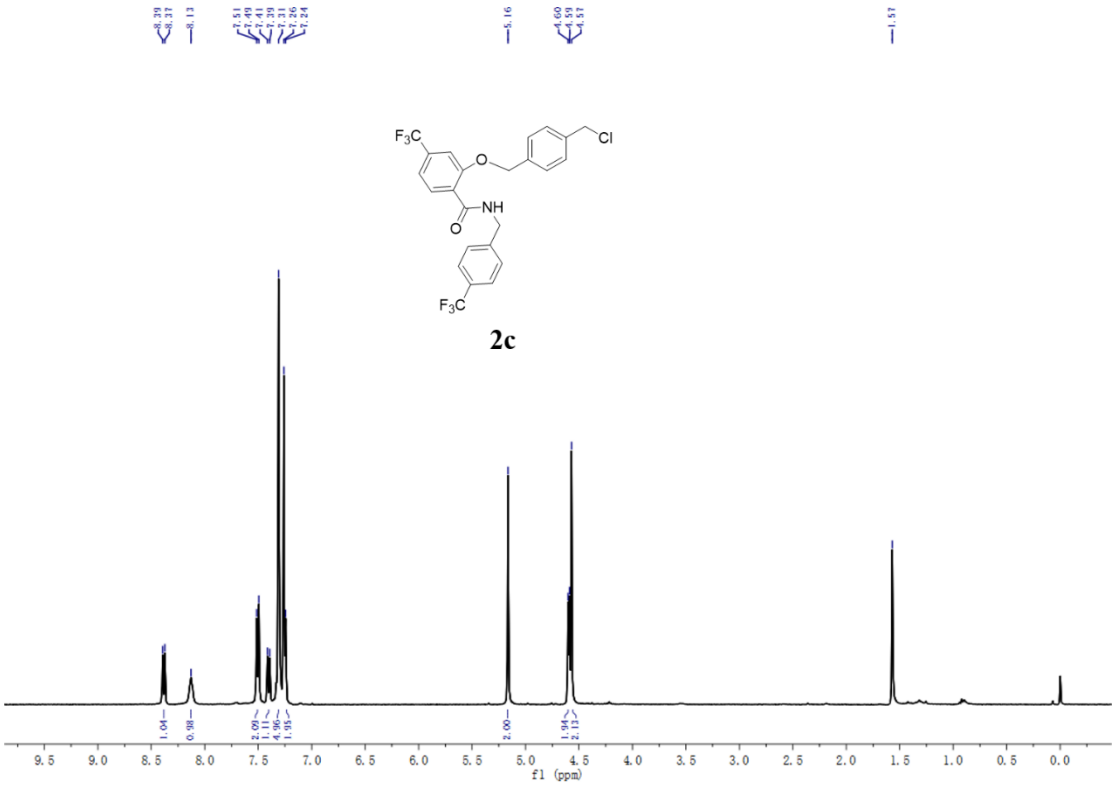

Figure S19. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC) spectra of catalyst **2c**.

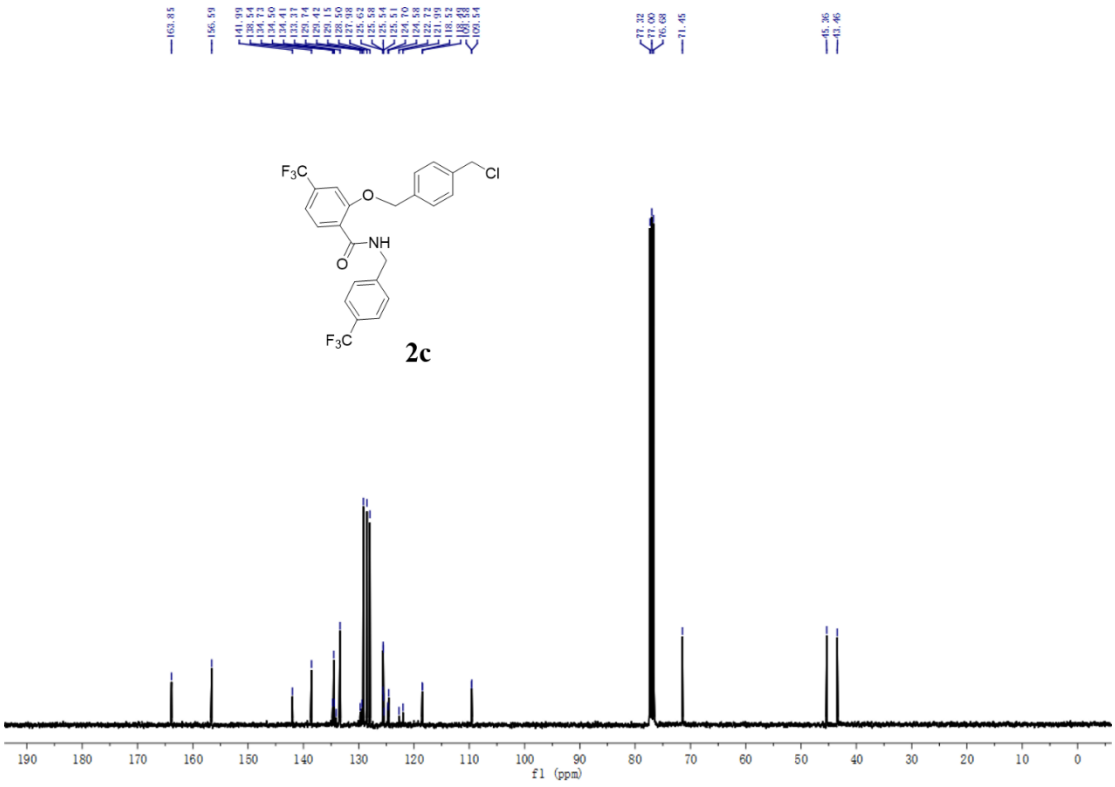

Figure S20. ^{13}C NMR (100 MHz, $CDCl_3$, 25 ºC) spectra of catalyst **2c**.

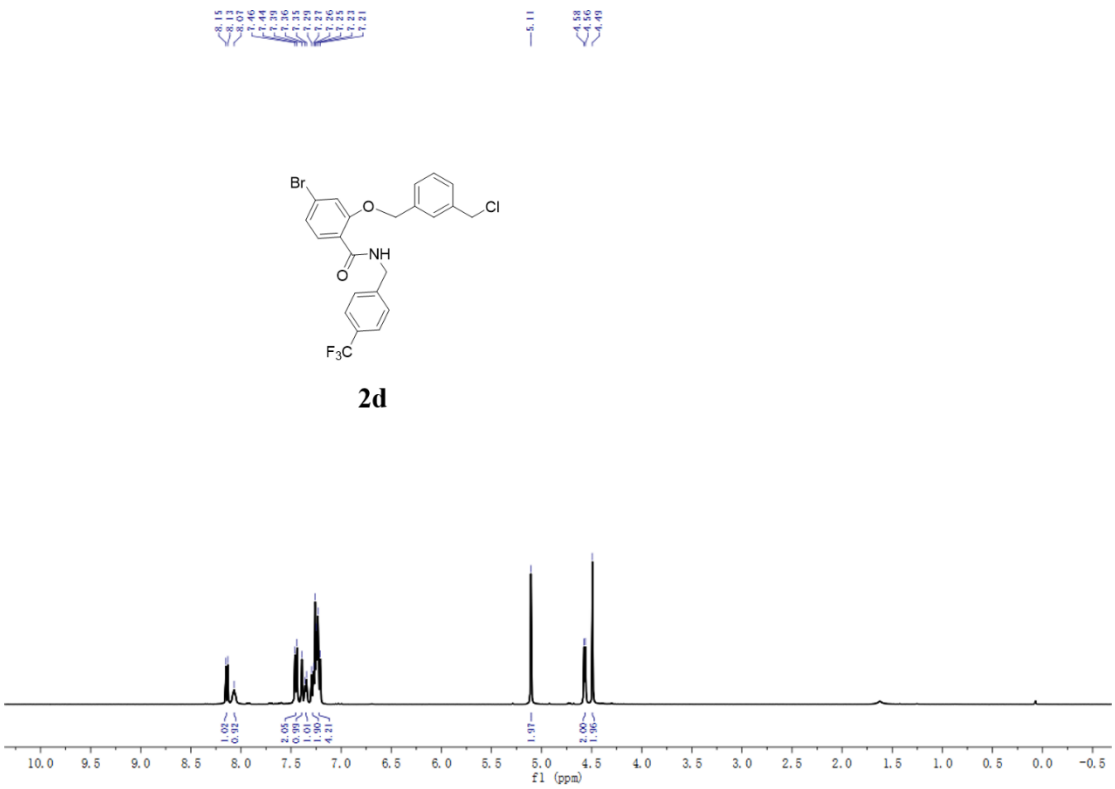

Figure S21. ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) spectra of catalyst **2d**.

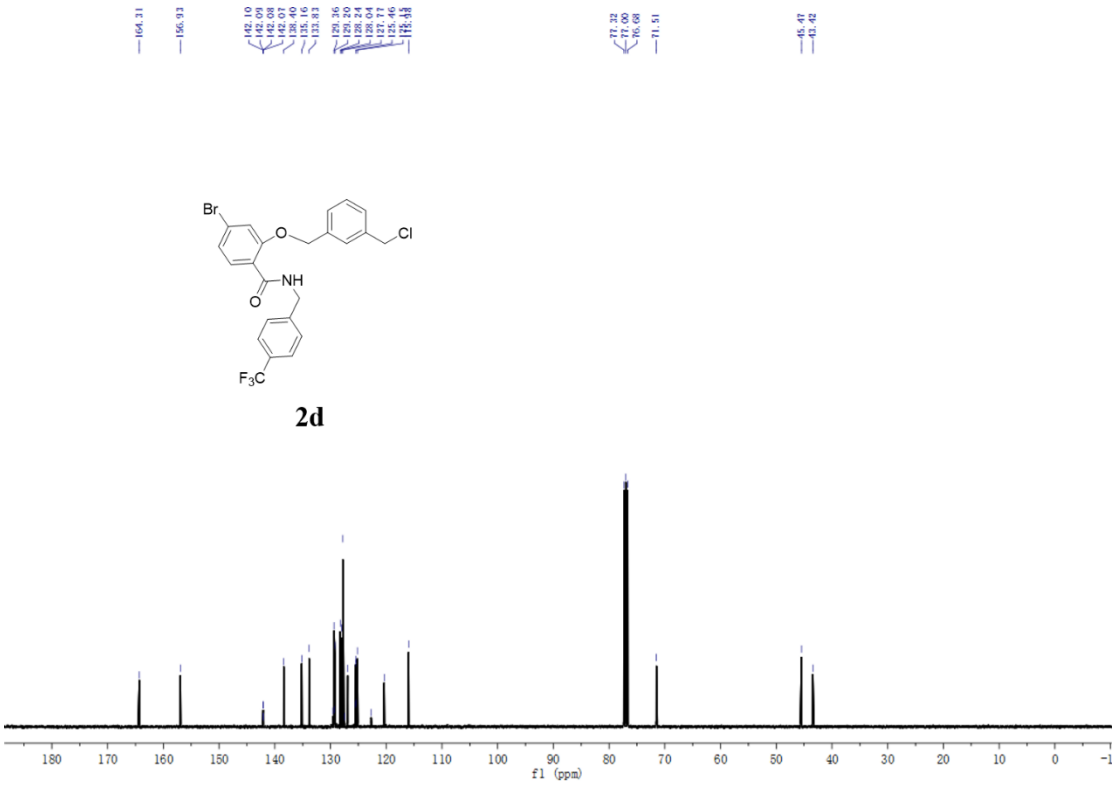

Figure S22. ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) spectra of catalyst **2d**.

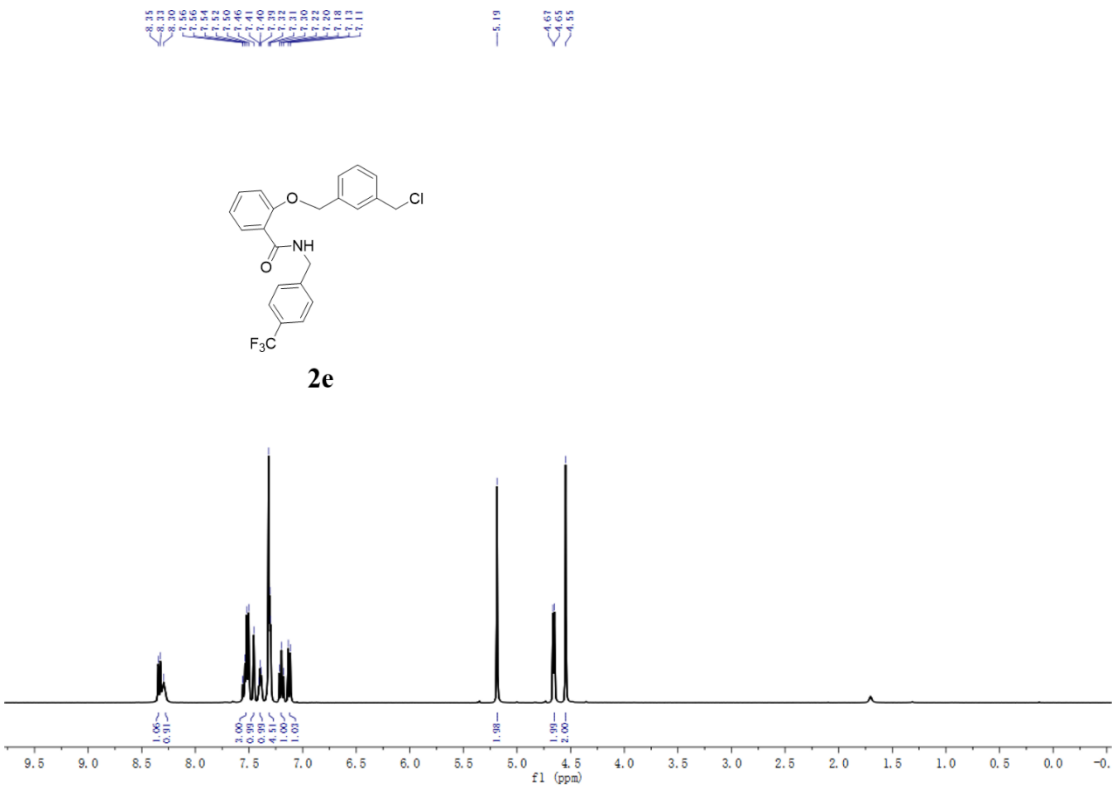

Figure S23. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC) spectra of catalyst **2e**.

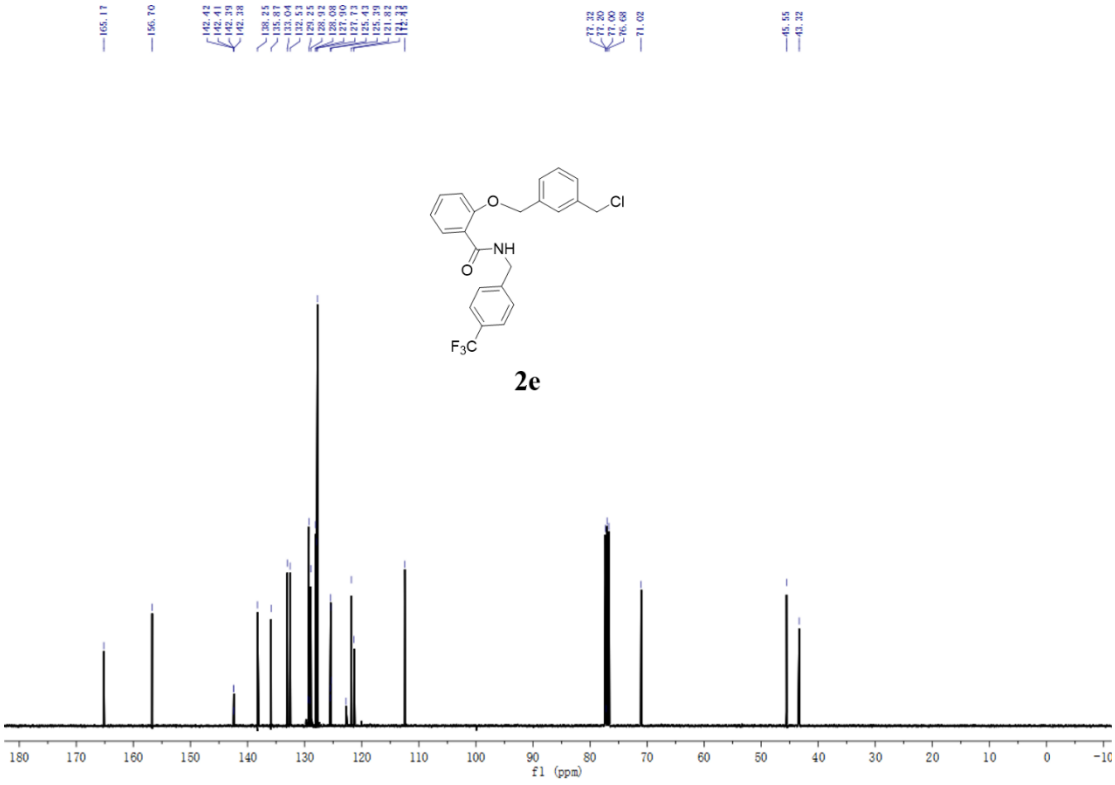

Figure S24. ^{13}C NMR (100 MHz, $CDCl_3$, 25 ºC) spectra of catalyst **2e**.

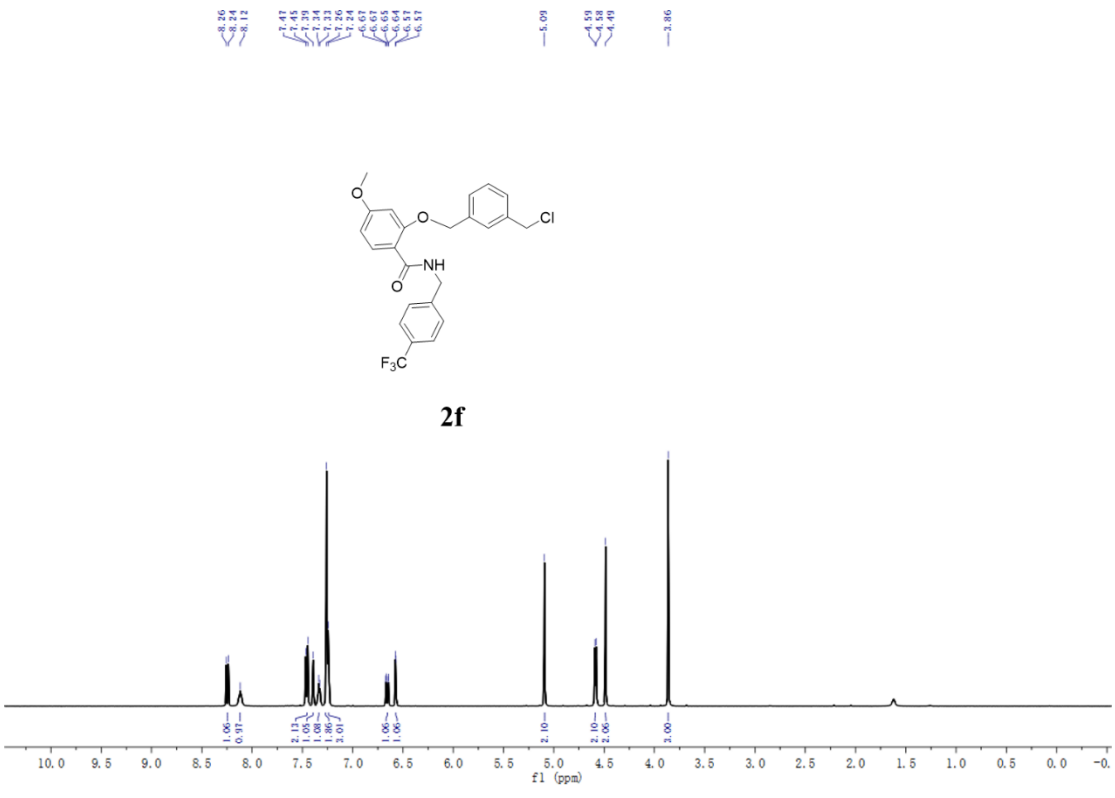

Figure S25. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ^{o}C) spectra of catalyst **2f**.

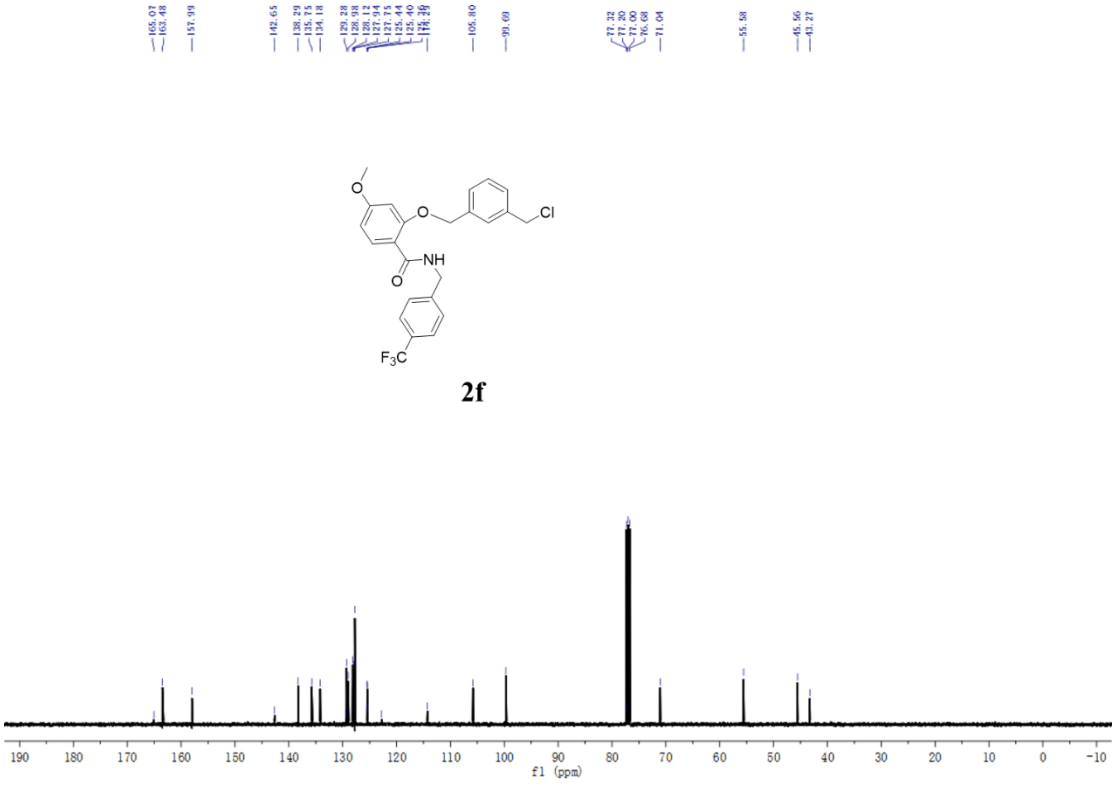

Figure S26. ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) spectra of catalyst **2f**.

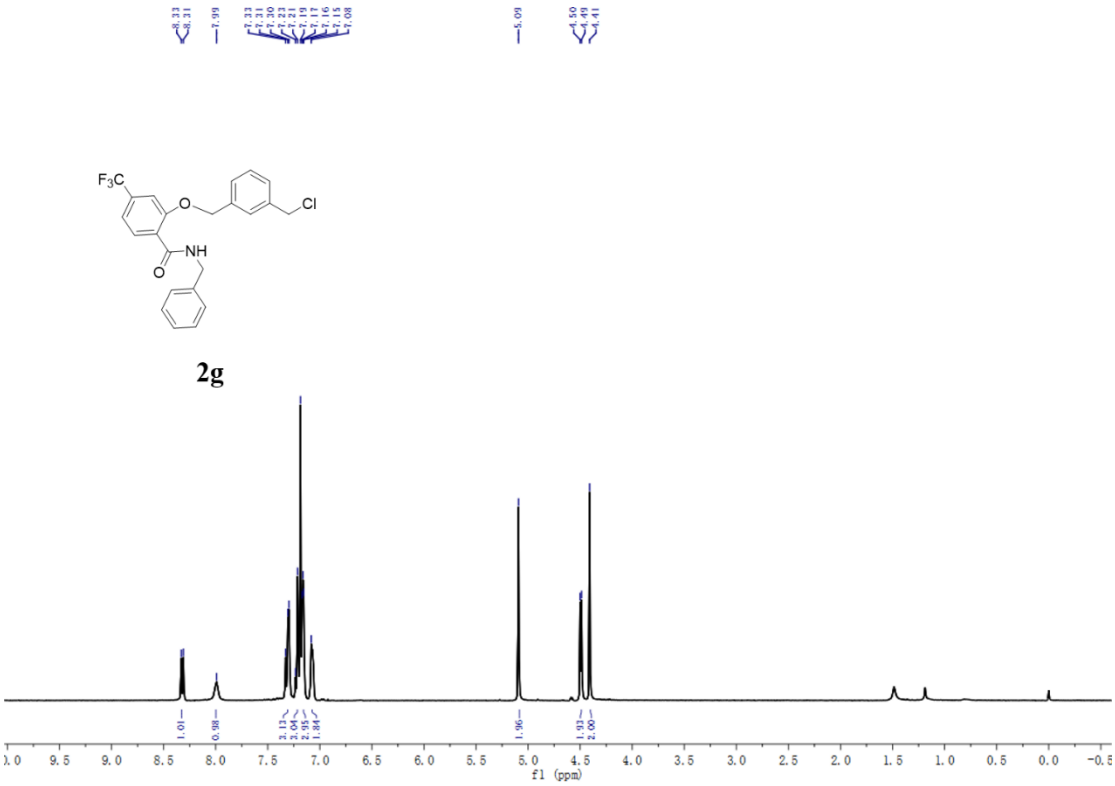

Figure S27. ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) spectra of catalyst **2g**.

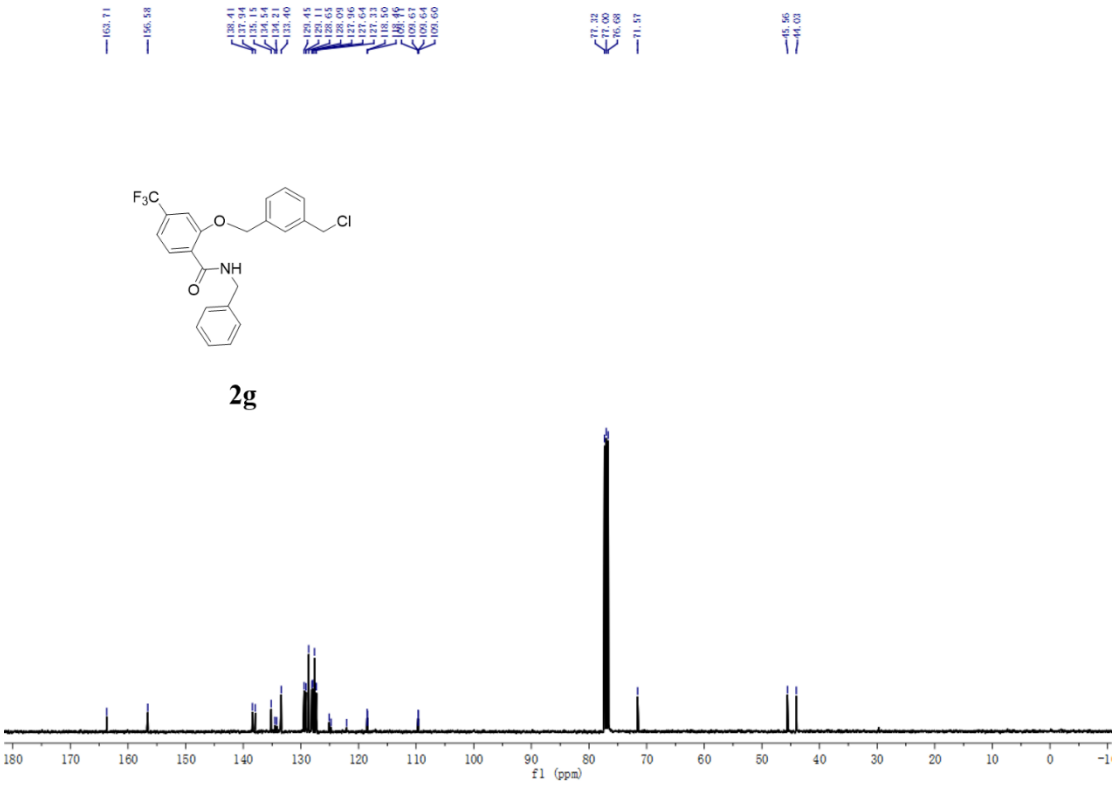

Figure S28. ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) spectra of catalyst **2g**.

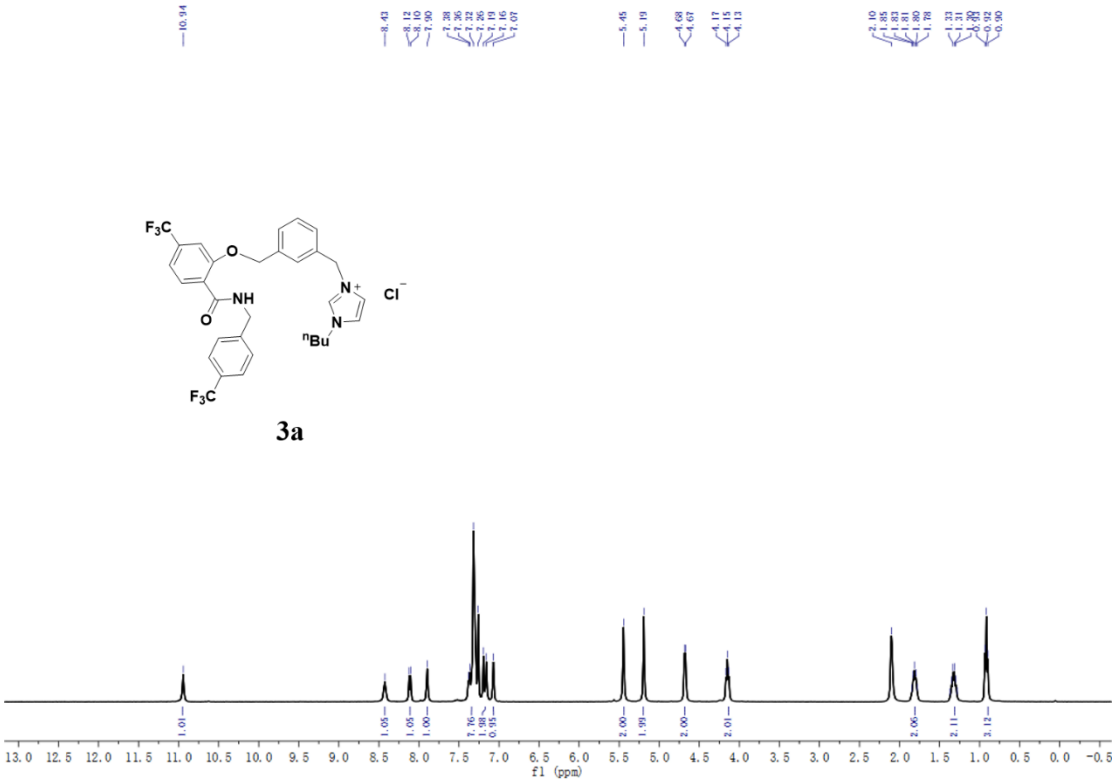

Figure S29. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC) spectra of catalyst **3a**.

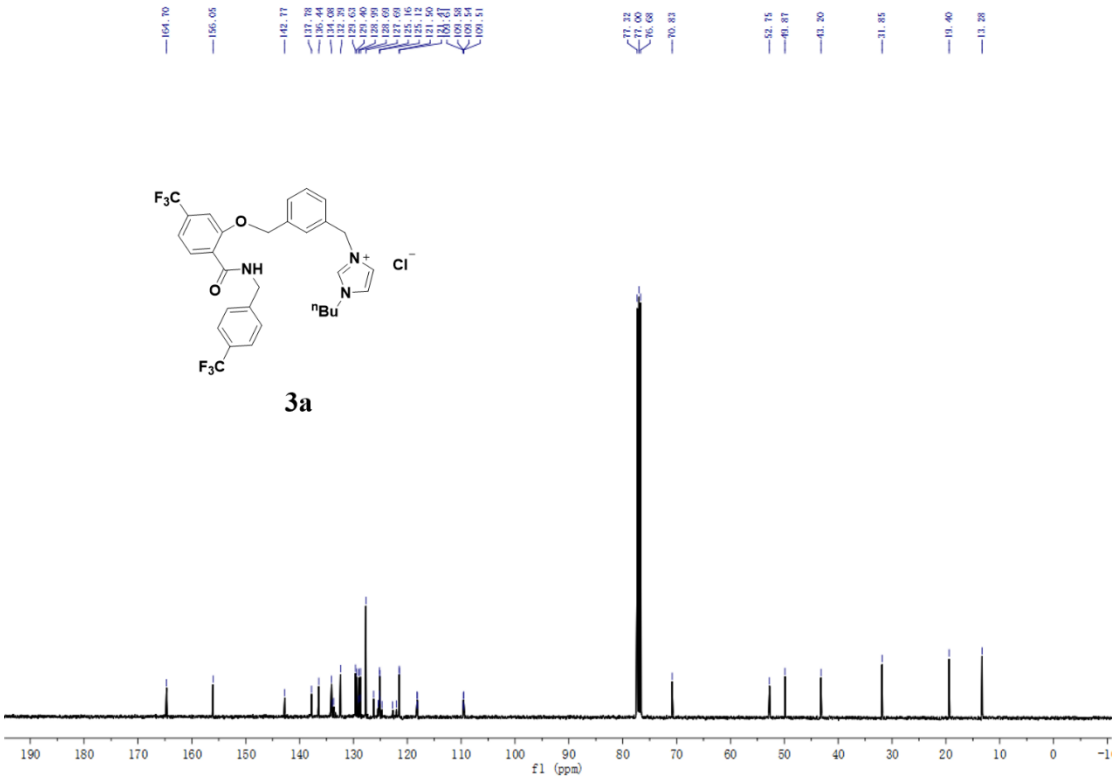

Figure S30. ^{13}C NMR (100 MHz, $CDCl_3$, 25 ºC) spectra of catalyst **3a**.

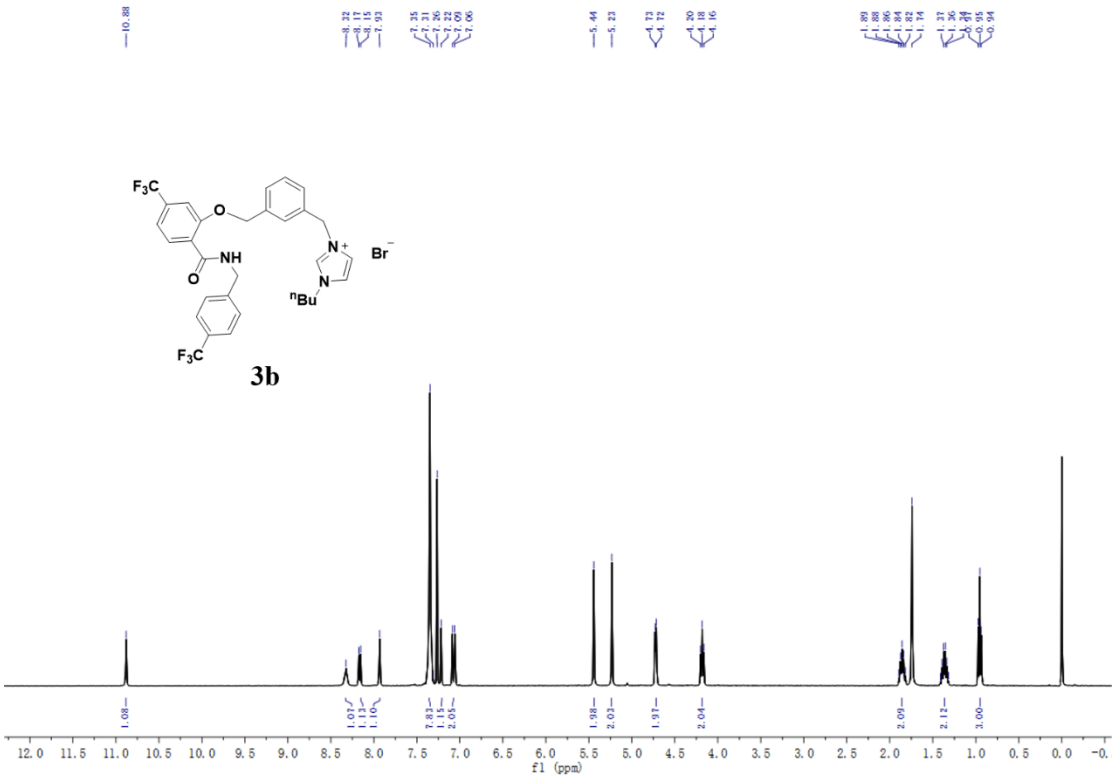

Figure S31. ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) spectra of catalyst **3b**.

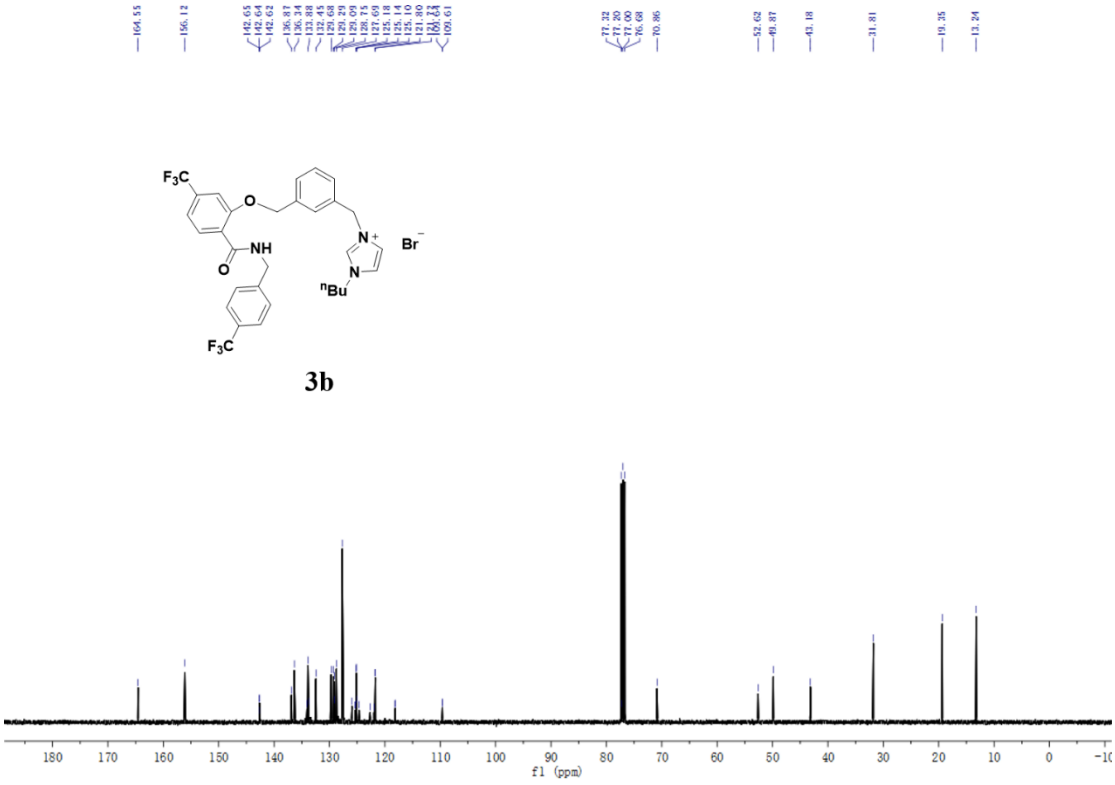

Figure S32. ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) spectra of catalyst **3b**.

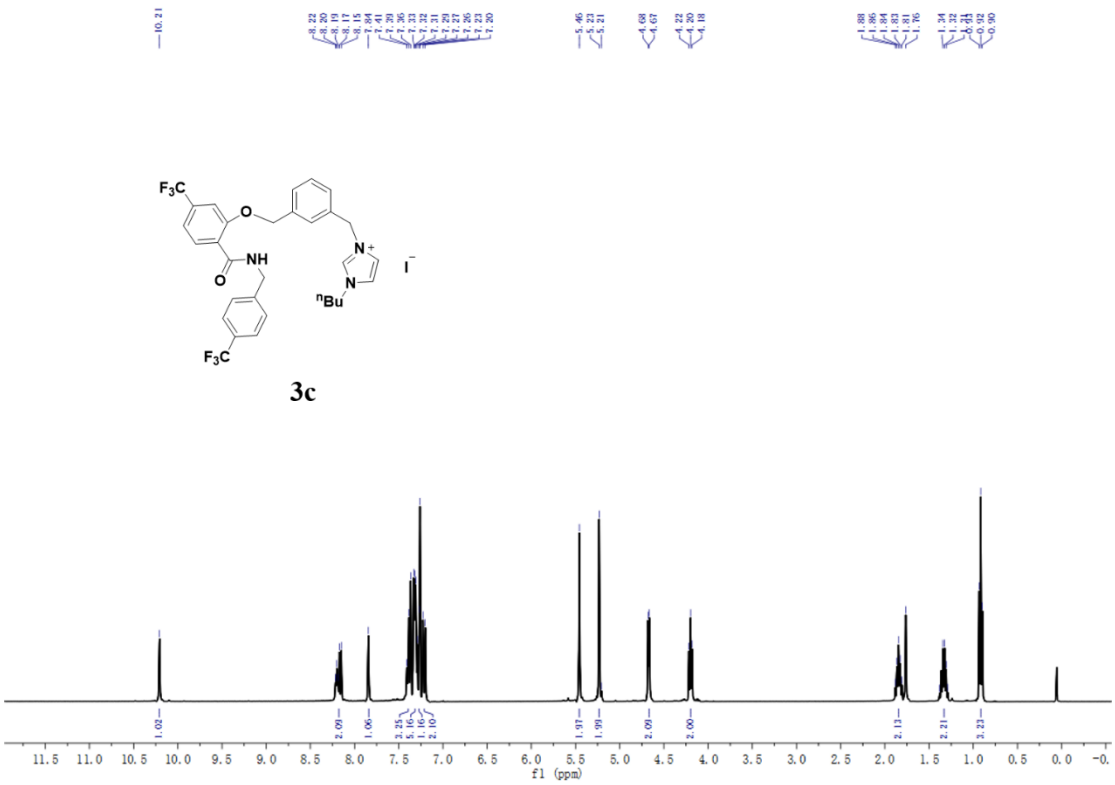

Figure S33. ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) spectra of catalyst **3c**.

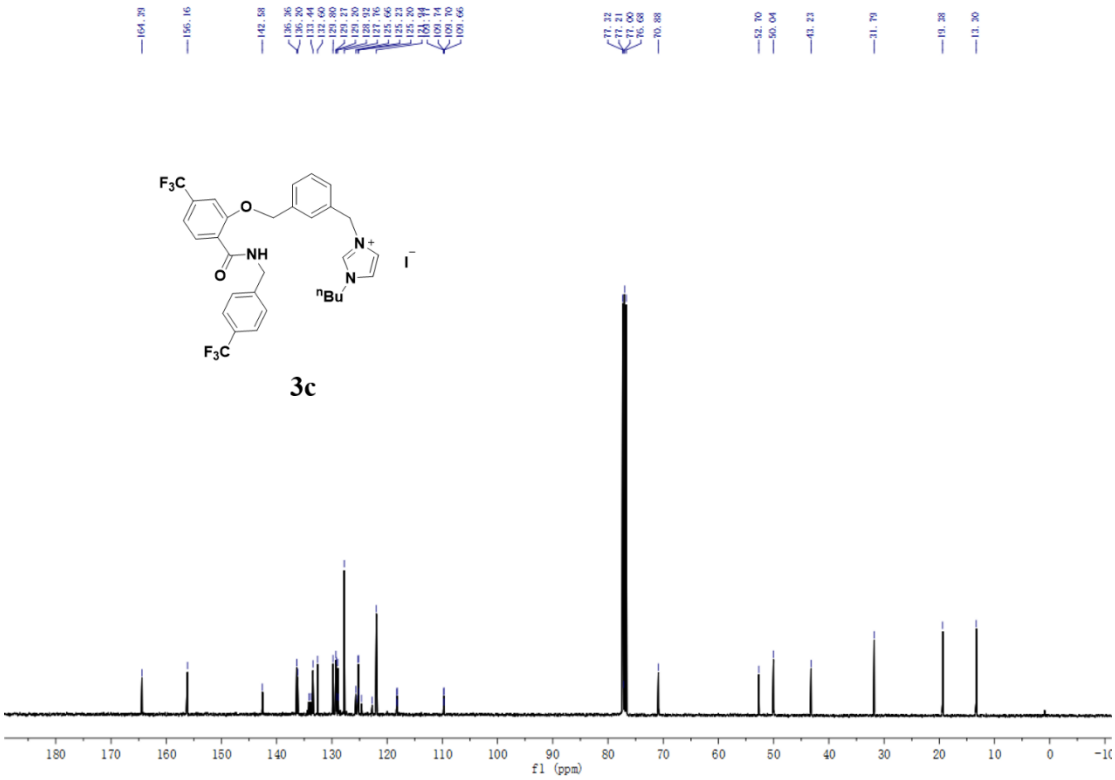

Figure S34. ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) spectra of catalyst **3c**.

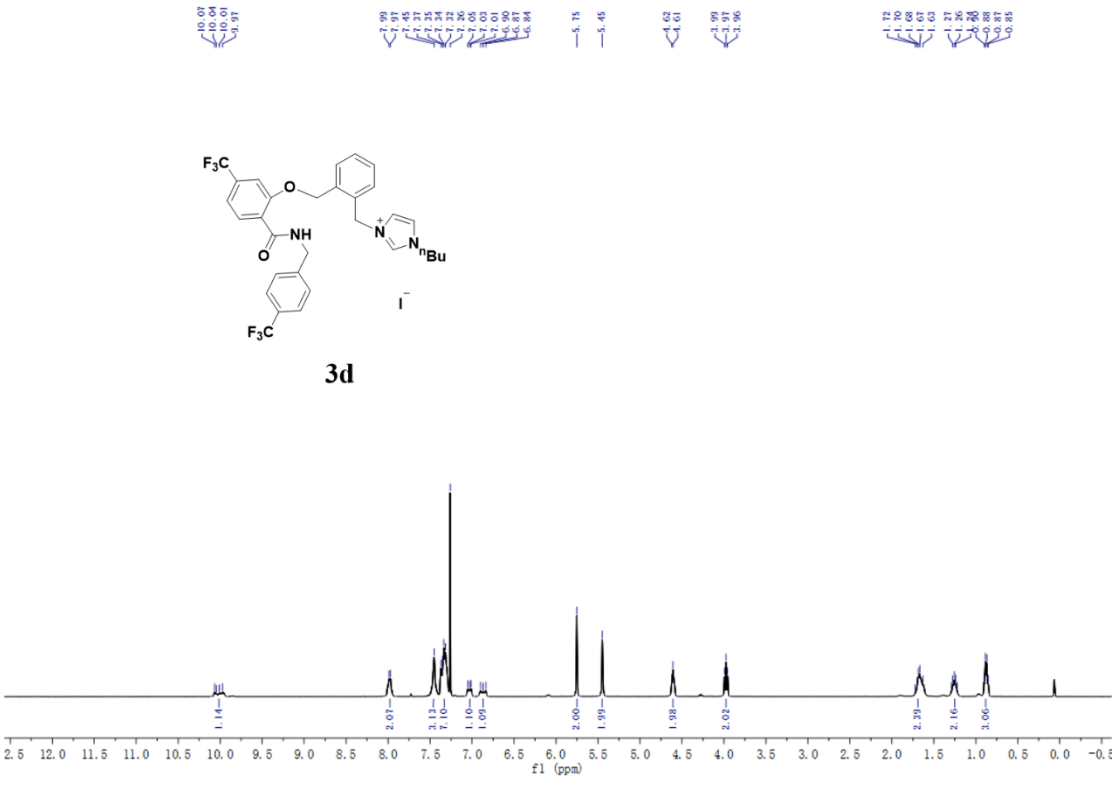

Figure S35. ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) spectra of catalyst **3d**.

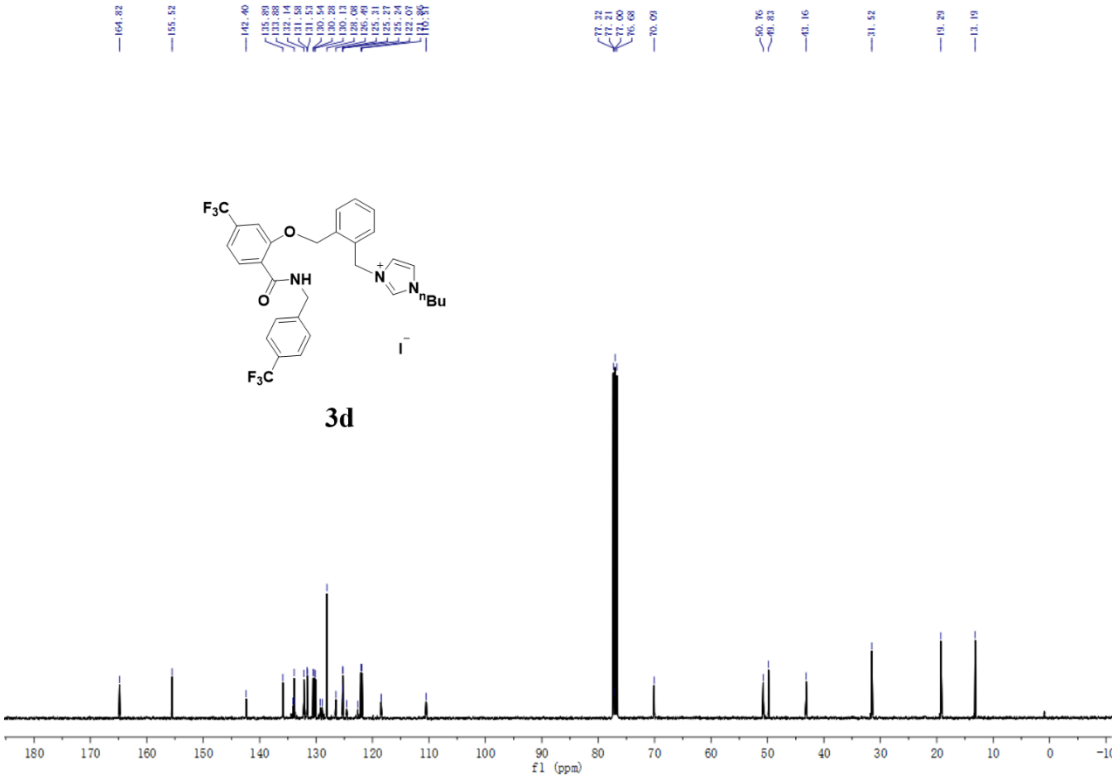

Figure S36. ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) spectra of catalyst **3d**.

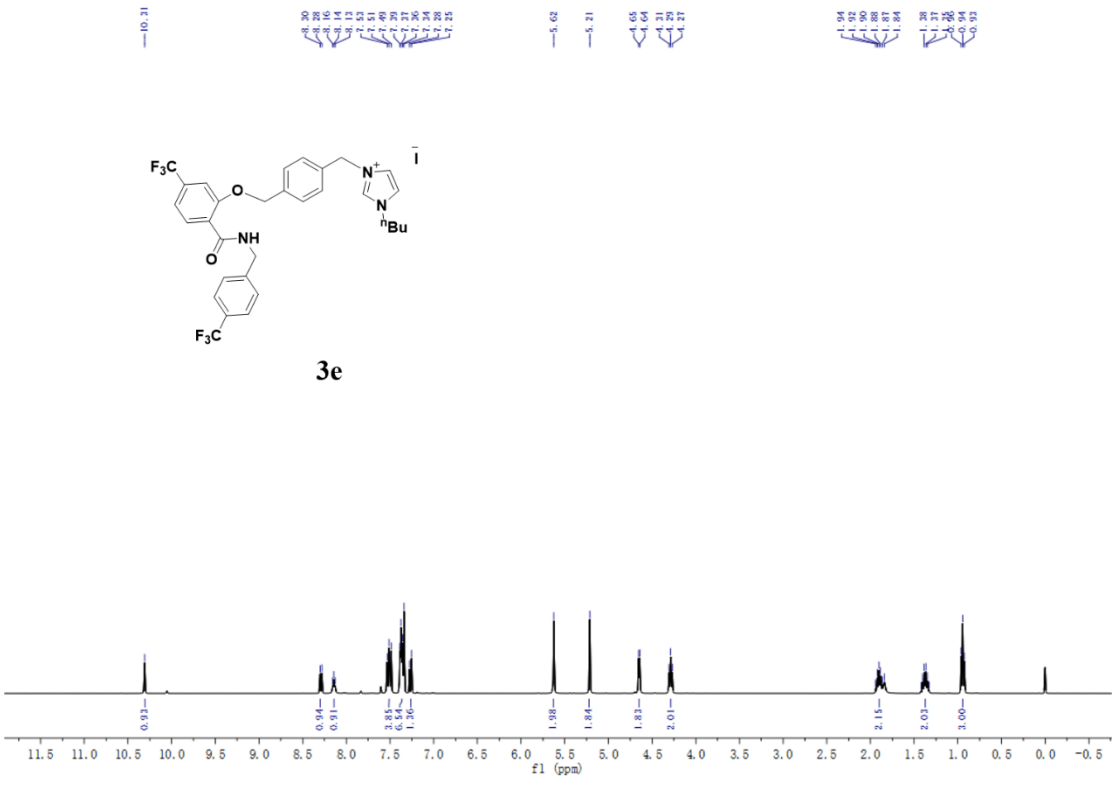

Figure S37. ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) spectra of catalyst **3e**.

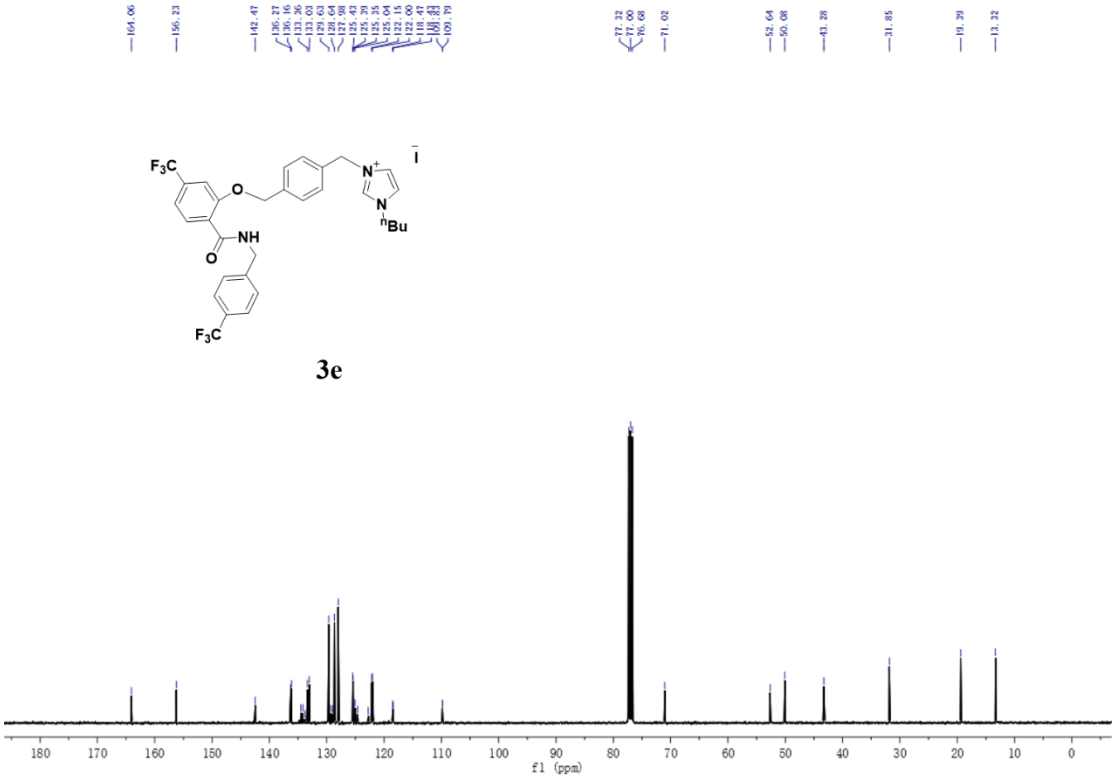

Figure S38. ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) spectra of catalyst **3e**.

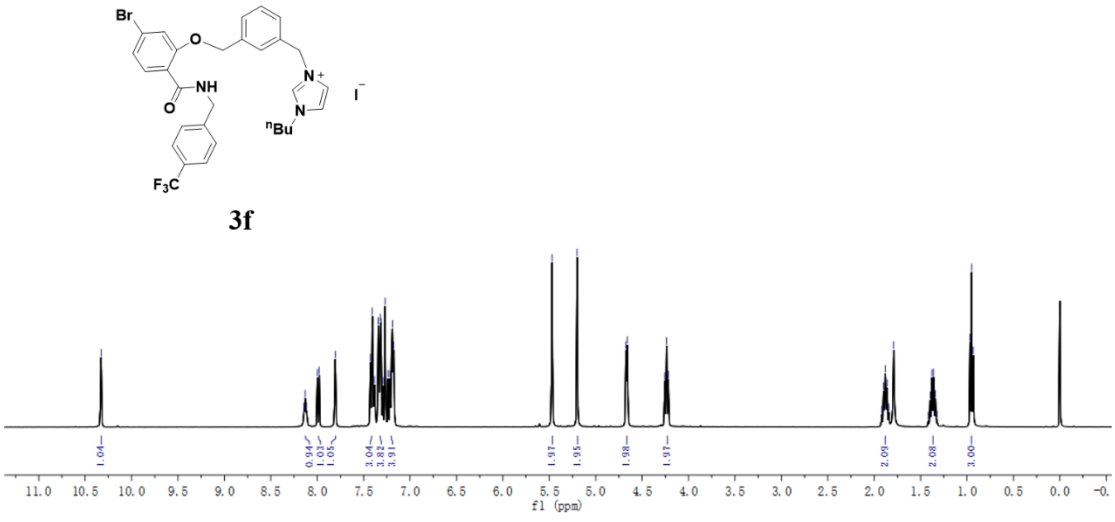

Figure S39. ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) spectra of catalyst **3f**.

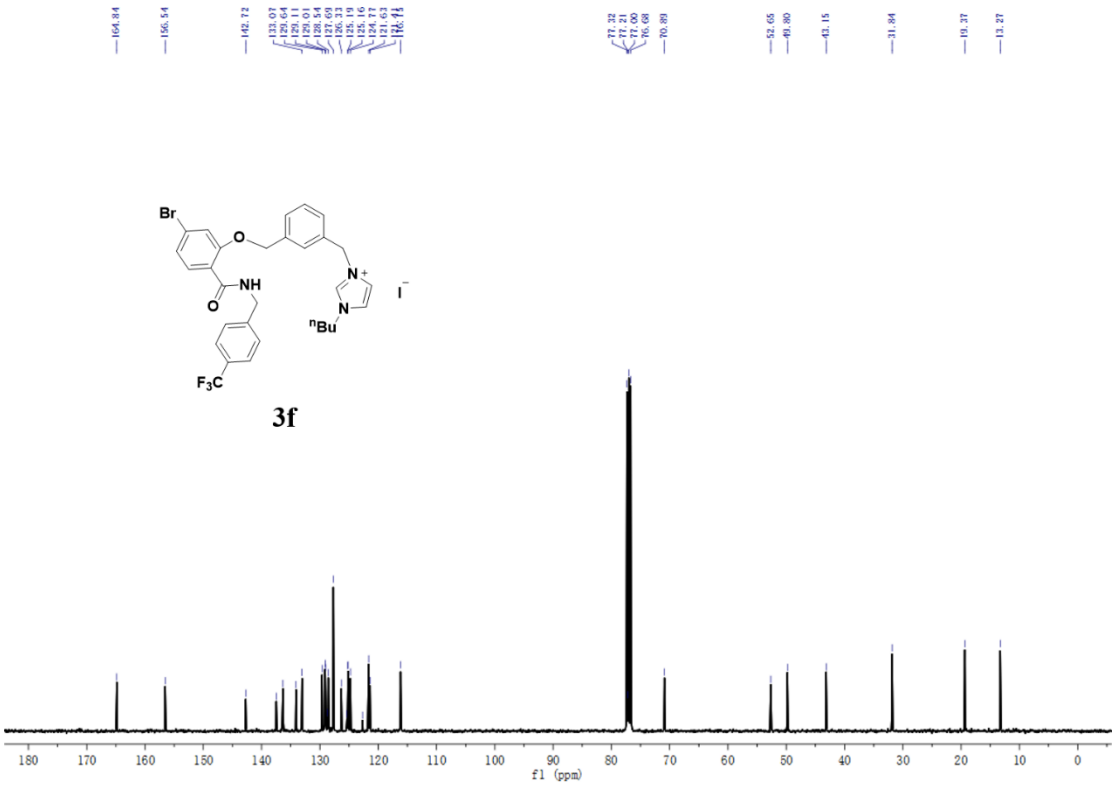

Figure S40. ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) spectra of catalyst **3f**.

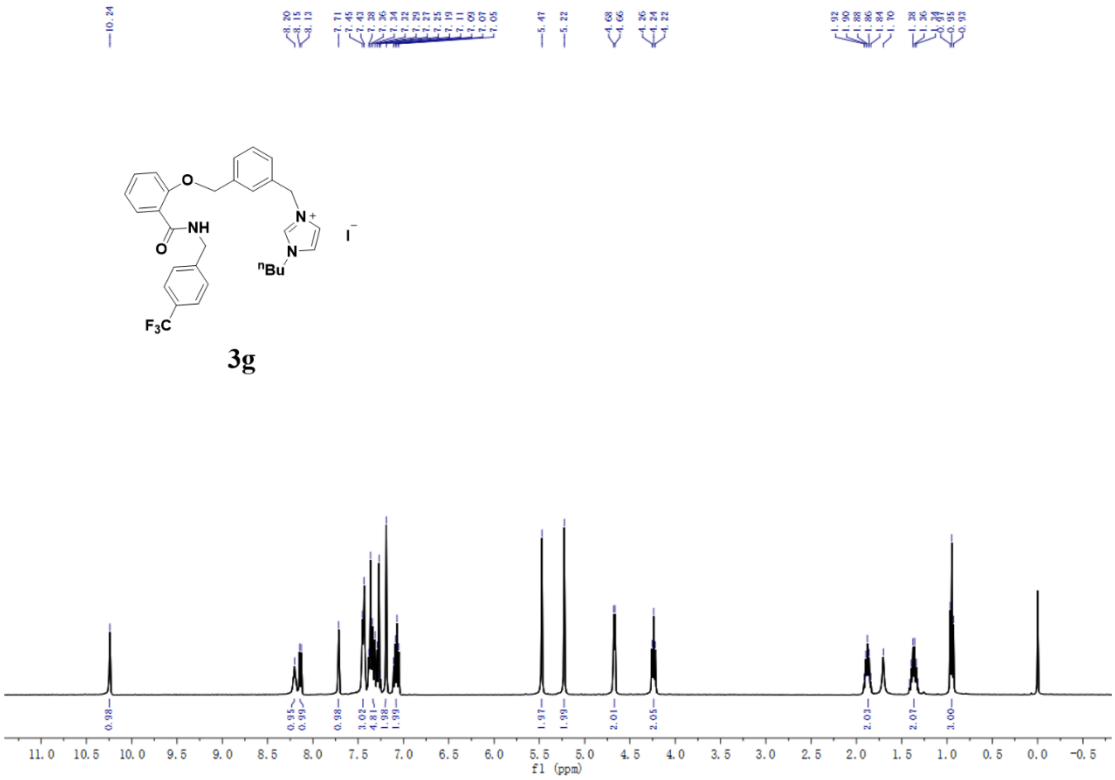

Figure S41. ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) spectra of catalyst **3g**.

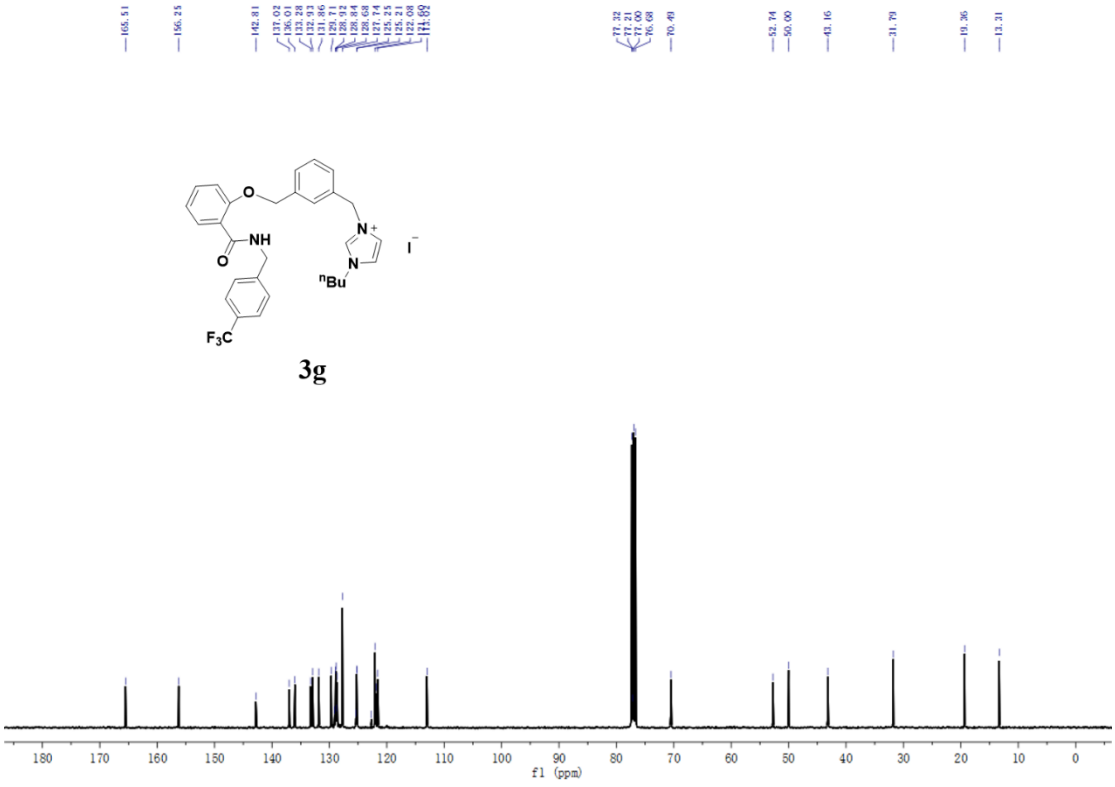

Figure S42. ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) spectra of catalyst **3g**.

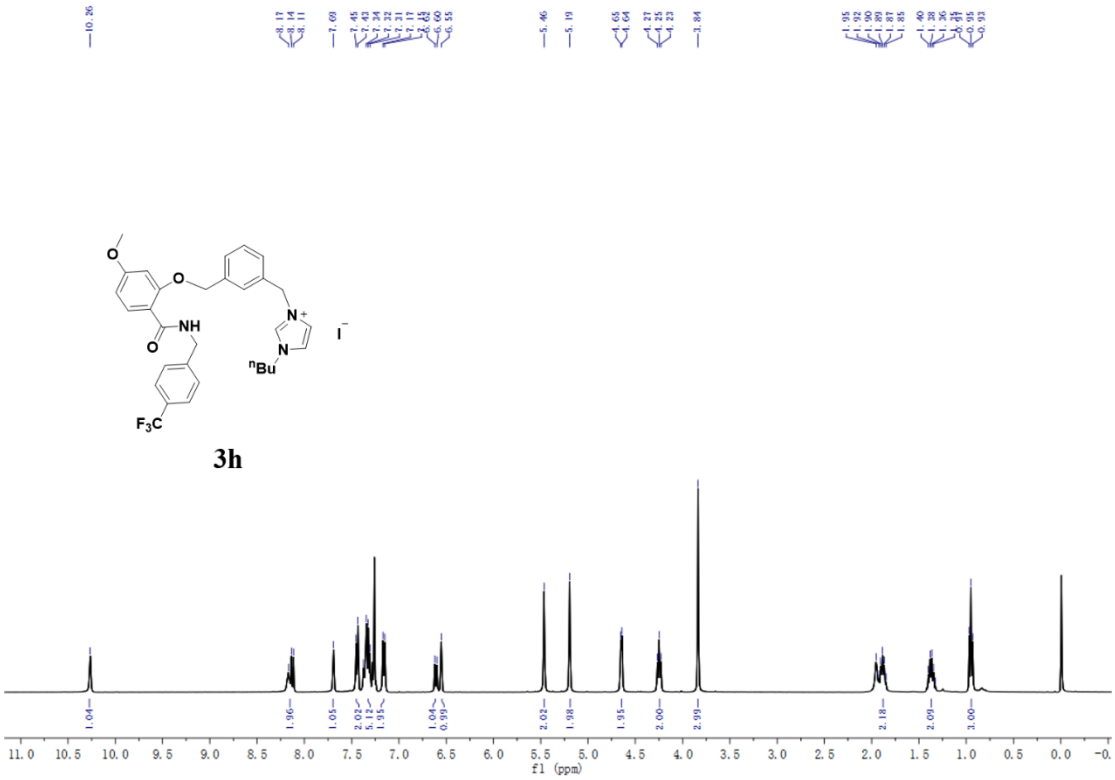

Figure S43. ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) spectra of catalyst **3h**.

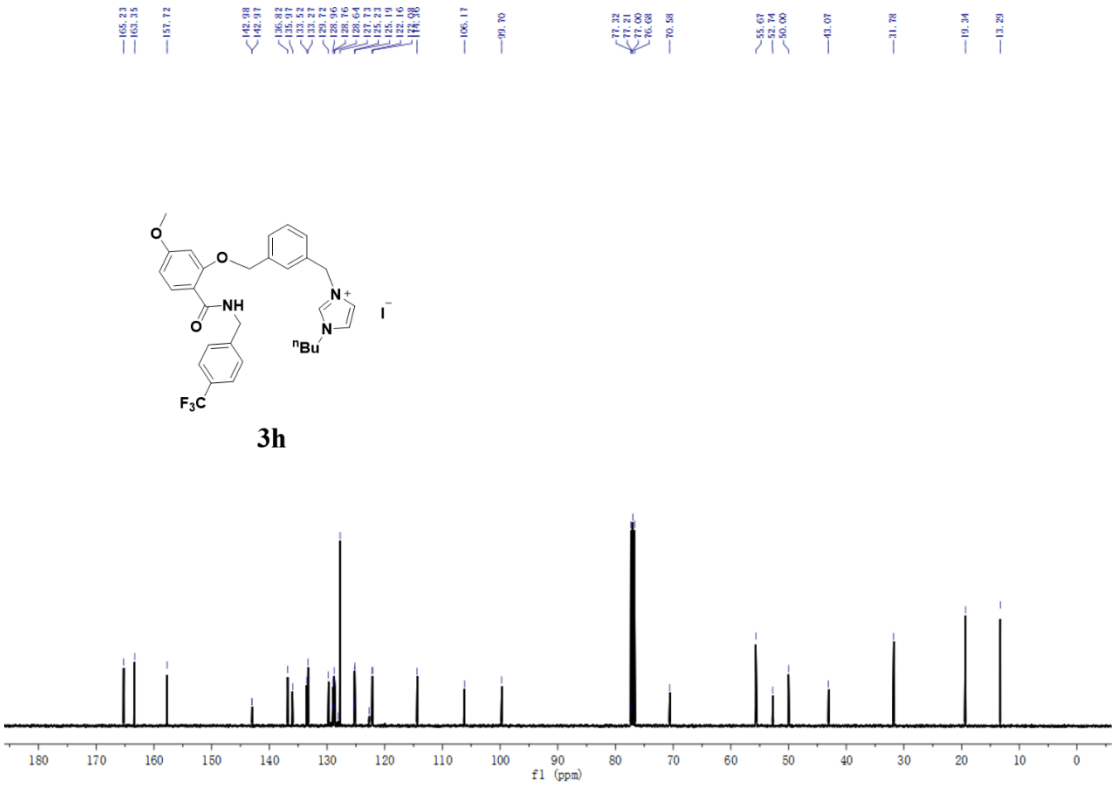

Figure S44. ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) spectra of catalyst **3h**.

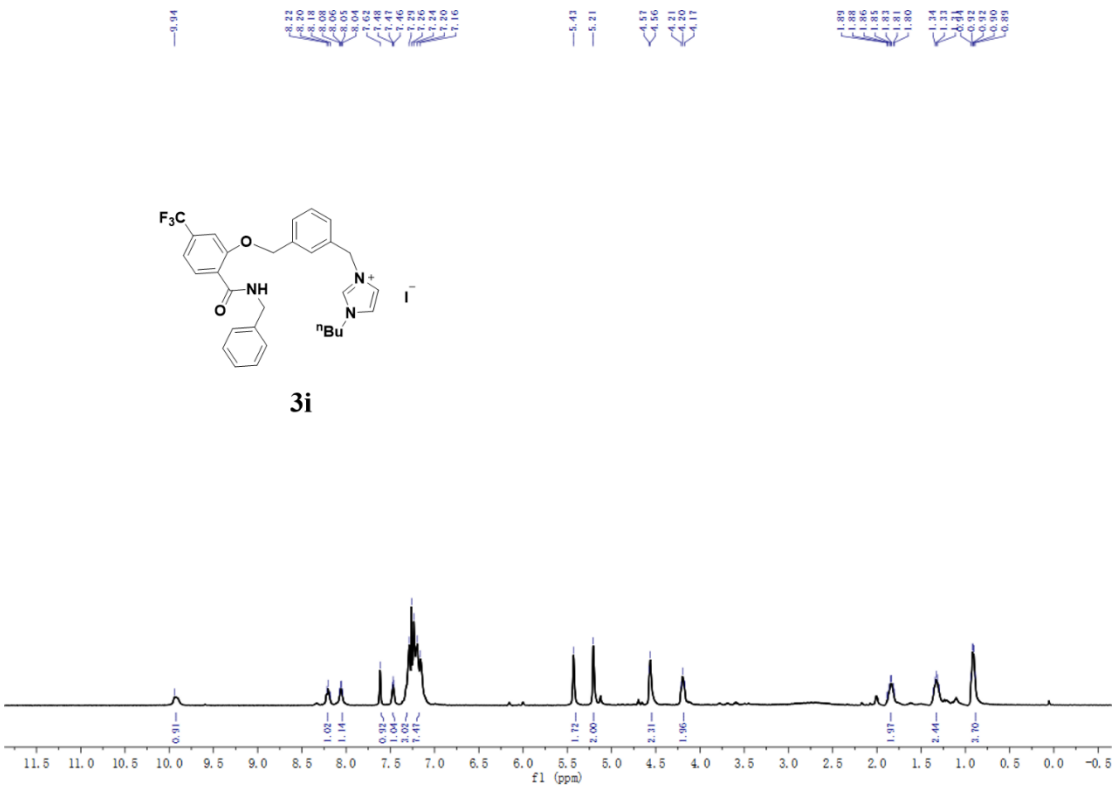

Figure S45. ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) spectra of catalyst **3i**.

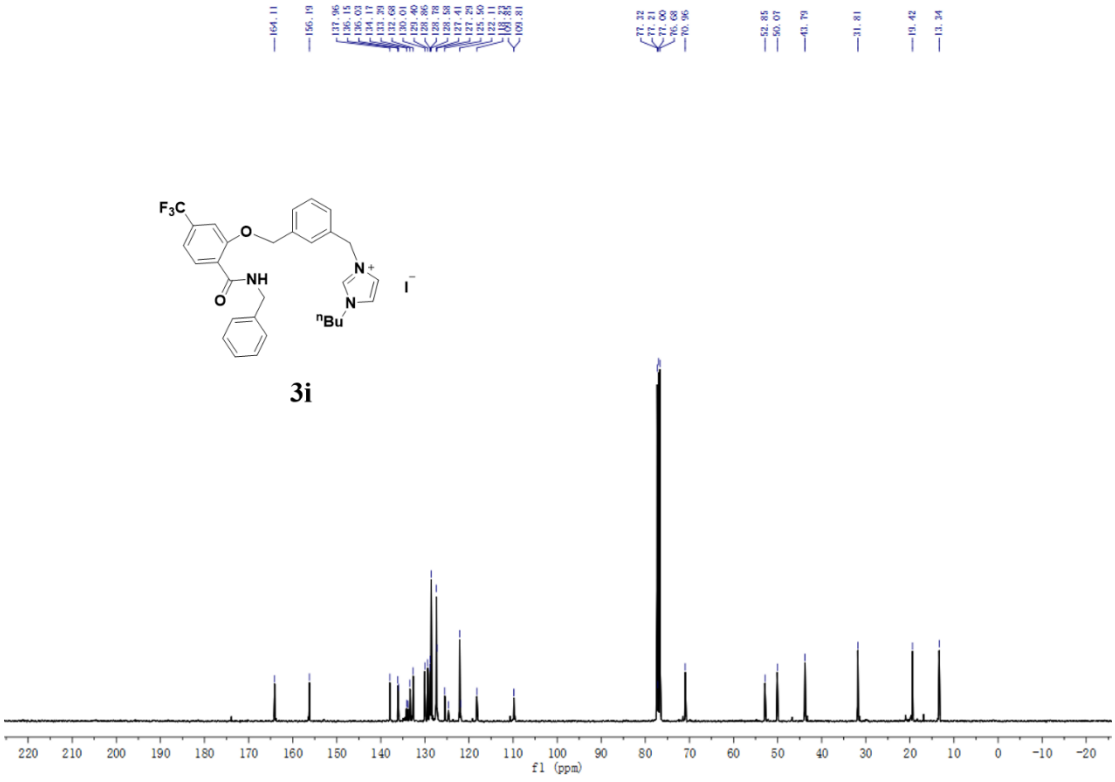

Figure S46. ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) spectra of catalyst **3i**.

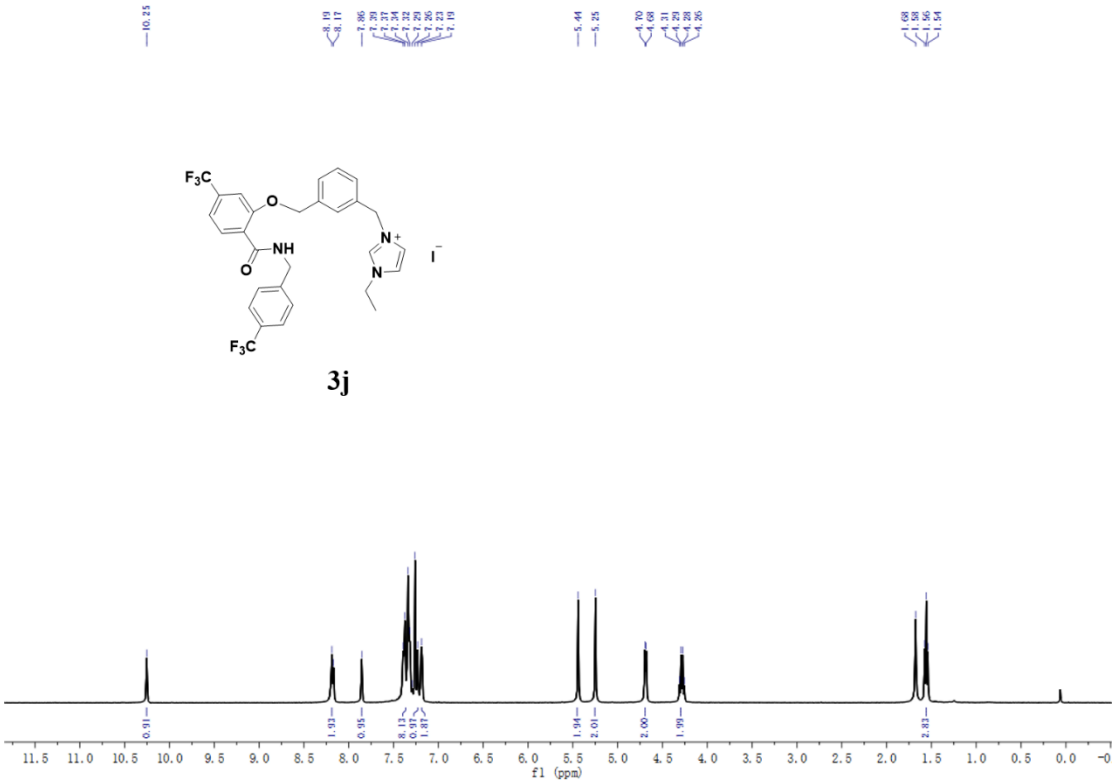

Figure S47. ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) spectra of catalyst **3j**.

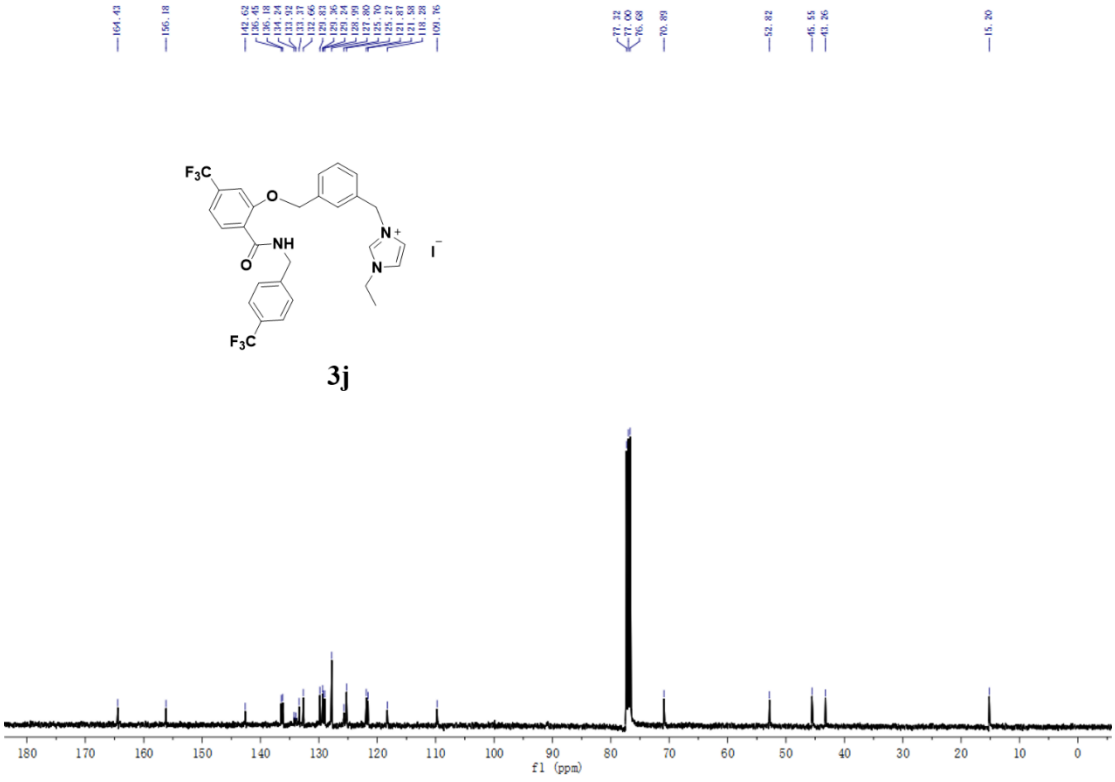

Figure S48. ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) spectra of catalyst **3j**.

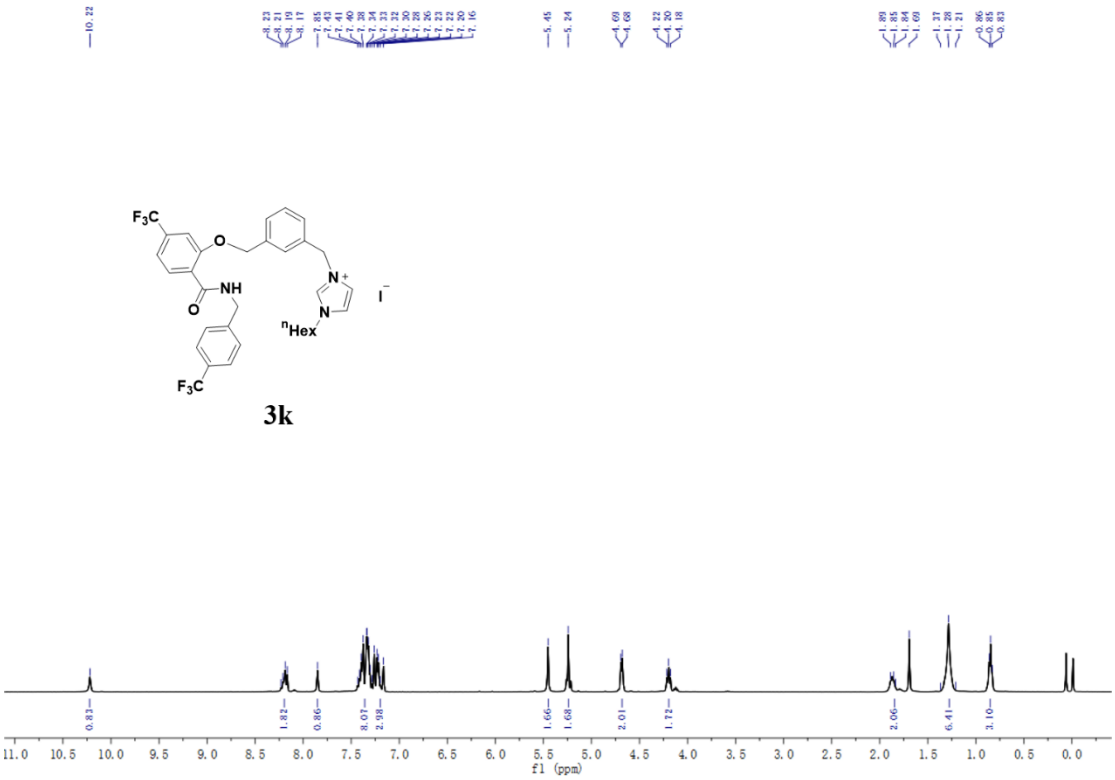

Figure S49. ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) spectra of catalyst **3k**.

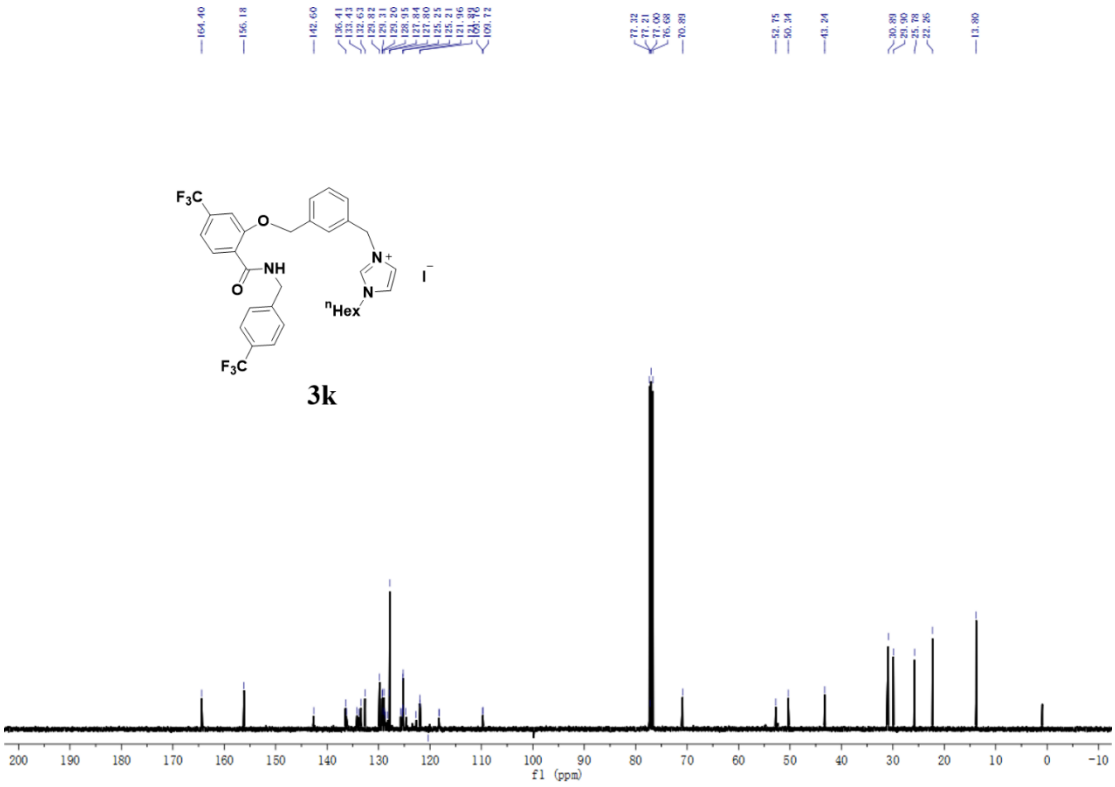

Figure S50. ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) spectra of catalyst **3j**.

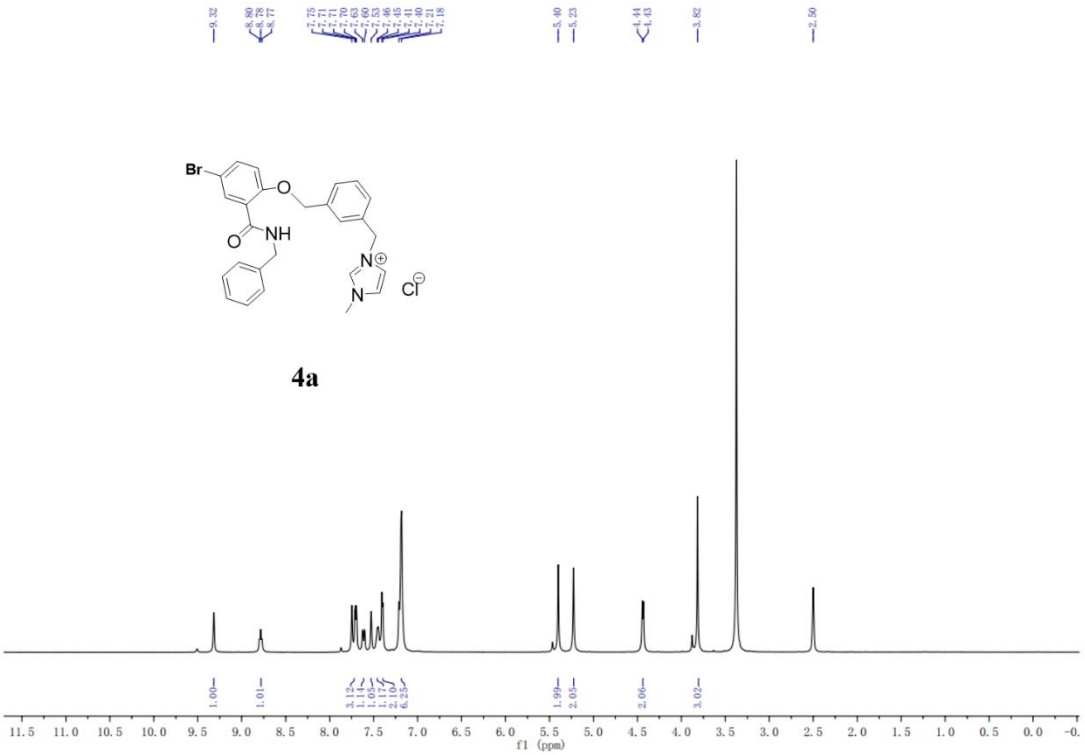

Figure S51. ^{1}H NMR (400 MHz, DMSO-d_6, 25 °C) spectra of catalyst **4a**.

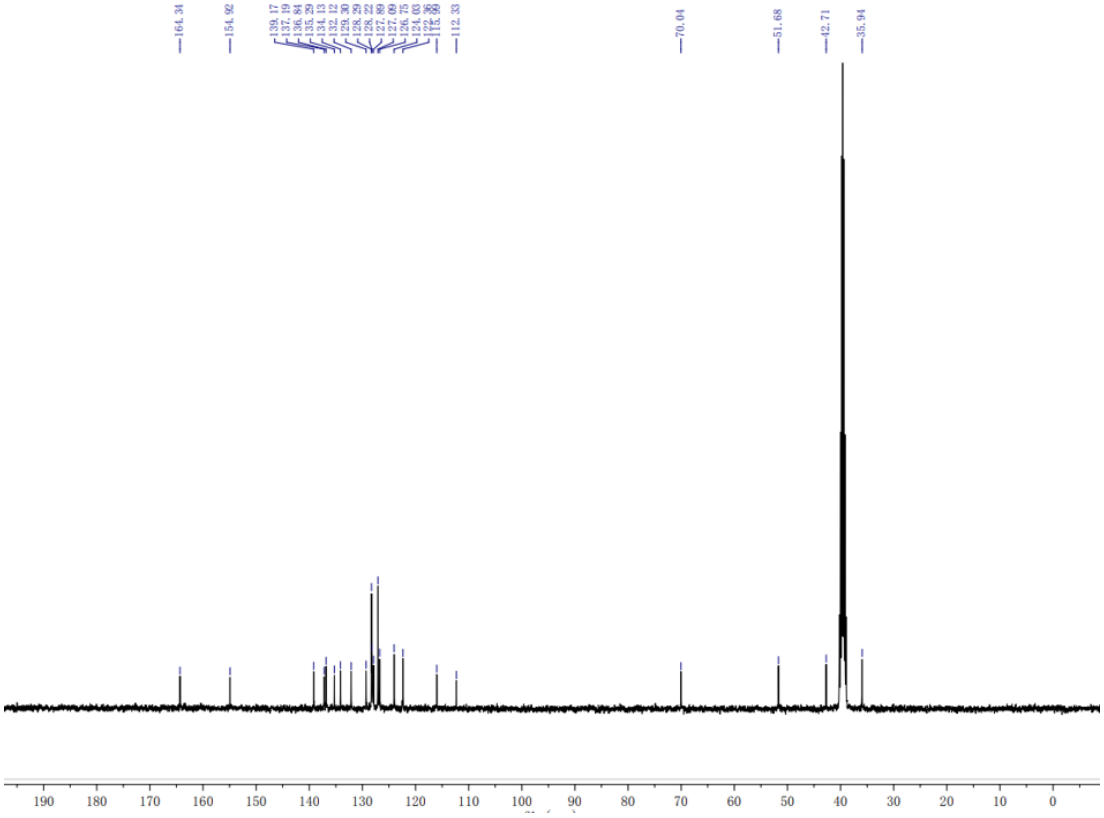

Figure S52. ^{13}C NMR (100 MHz, DMSO-d_6, 25 °C) spectra of catalyst **4a**.

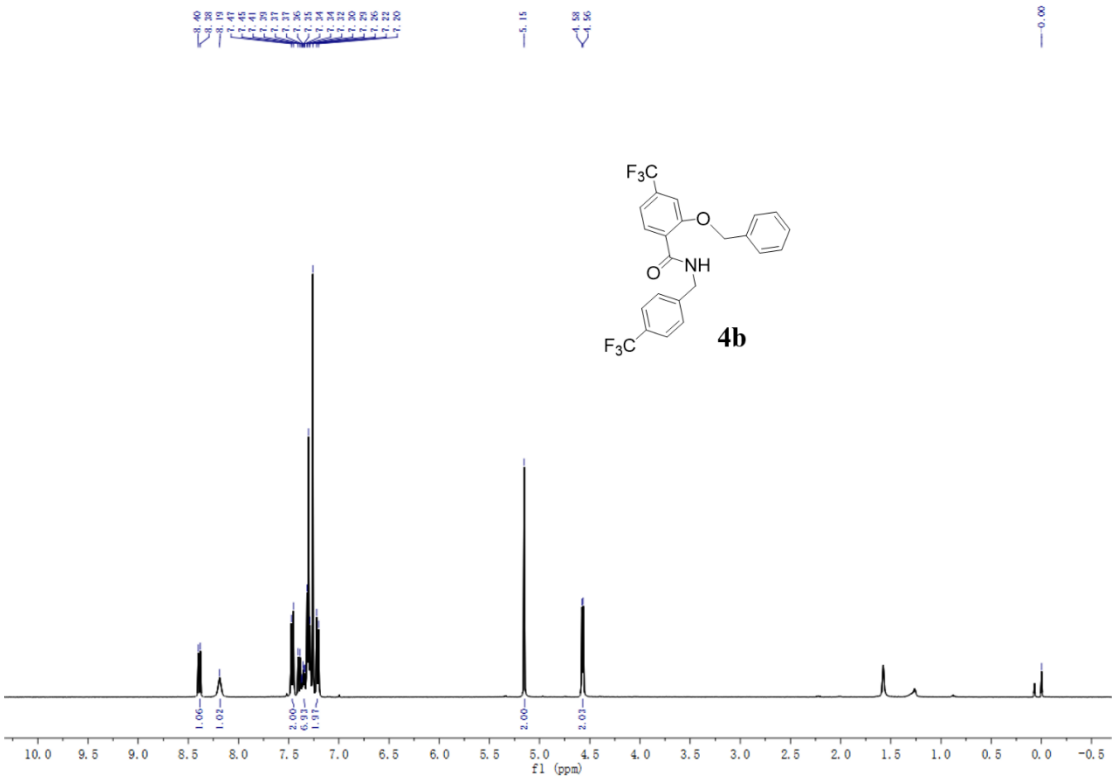

Figure S53. ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) spectra of catalyst **4b**.

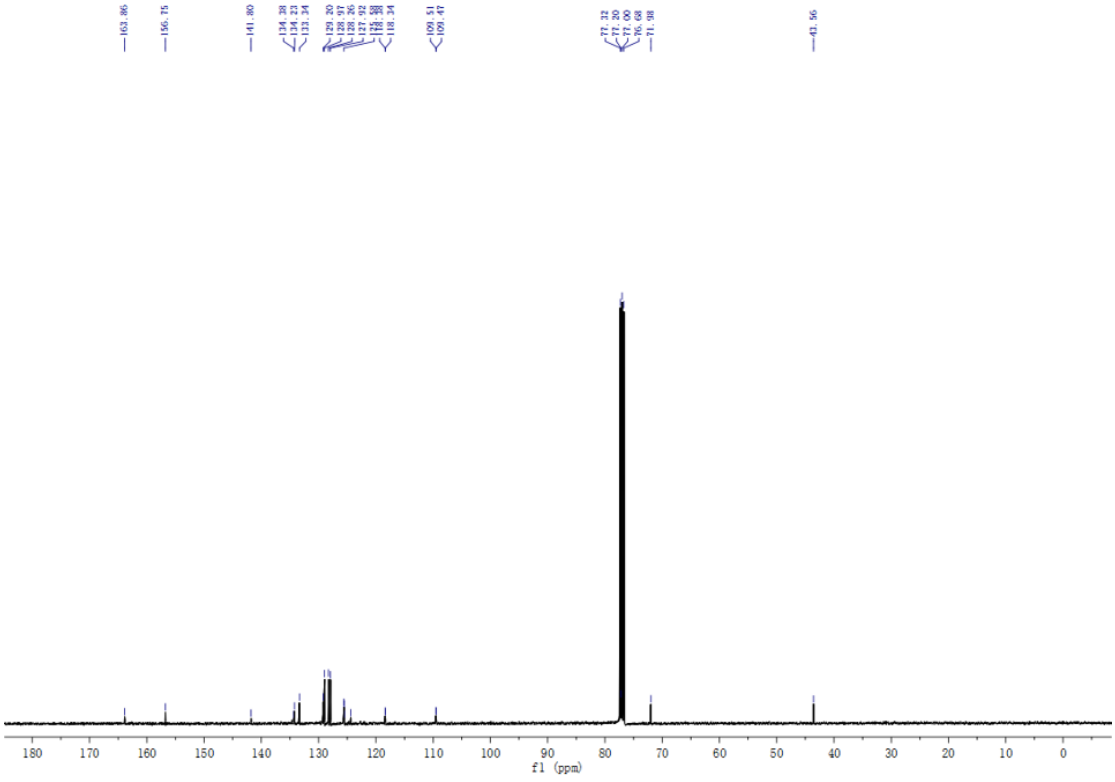

Figure S54. ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) spectra of catalyst **4b**.

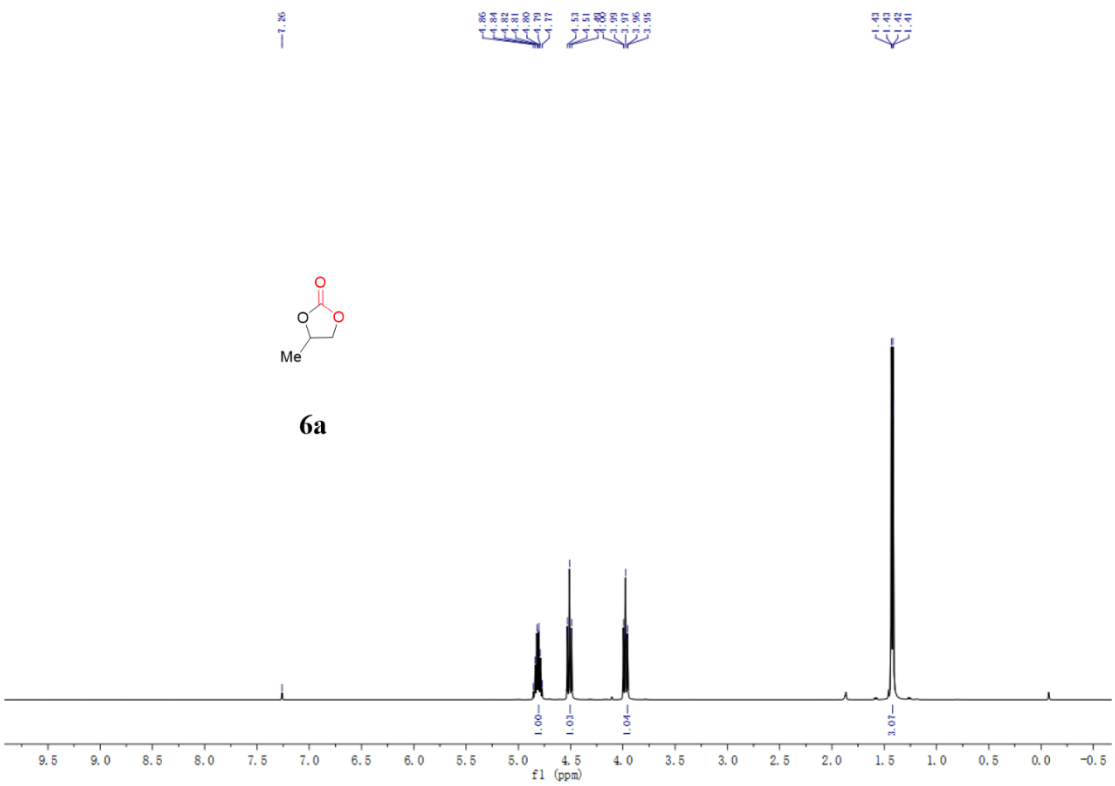

Figure S55. ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) spectra of catalyst **6a**.

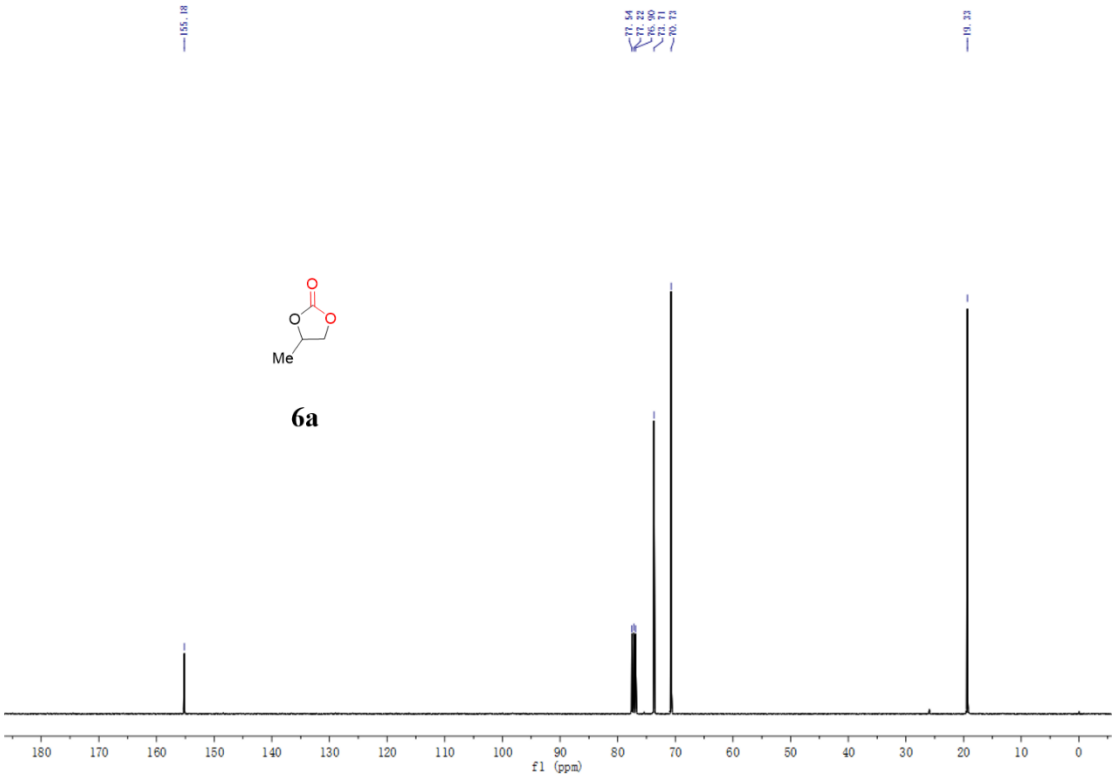

Figure S56. ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) spectra of catalyst **6a**.

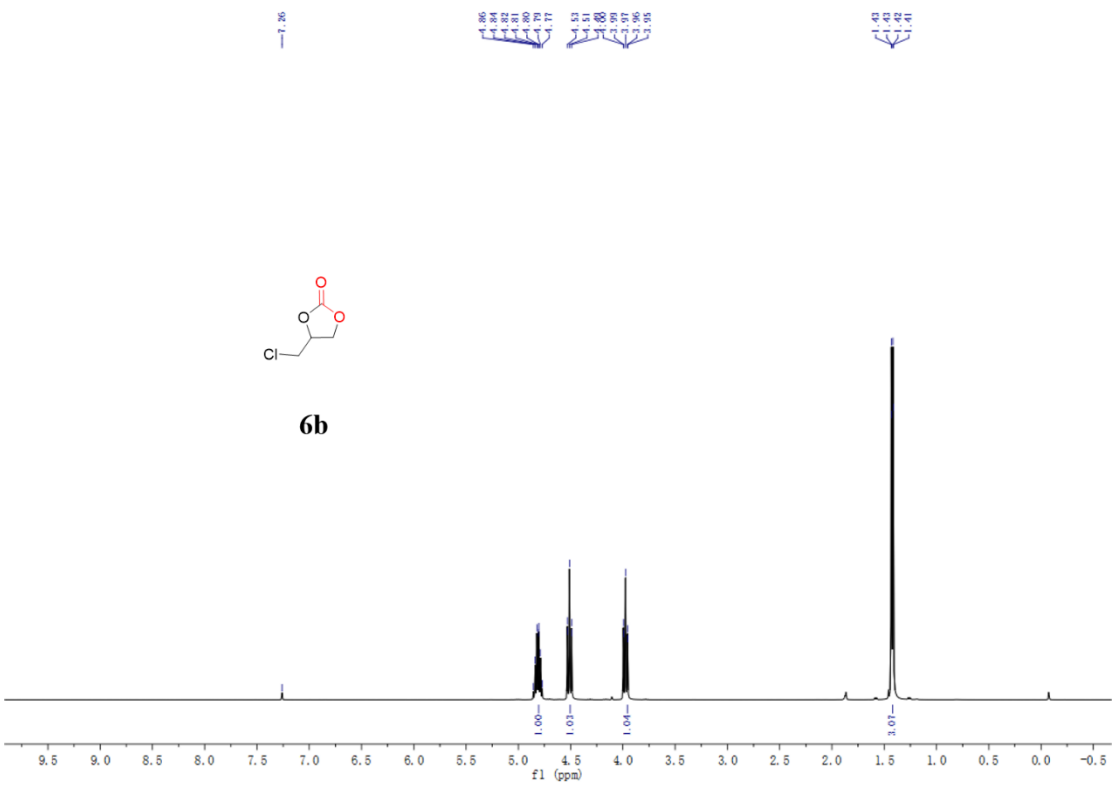

Figure S57. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ^{o}C) spectra of catalyst **6b**.

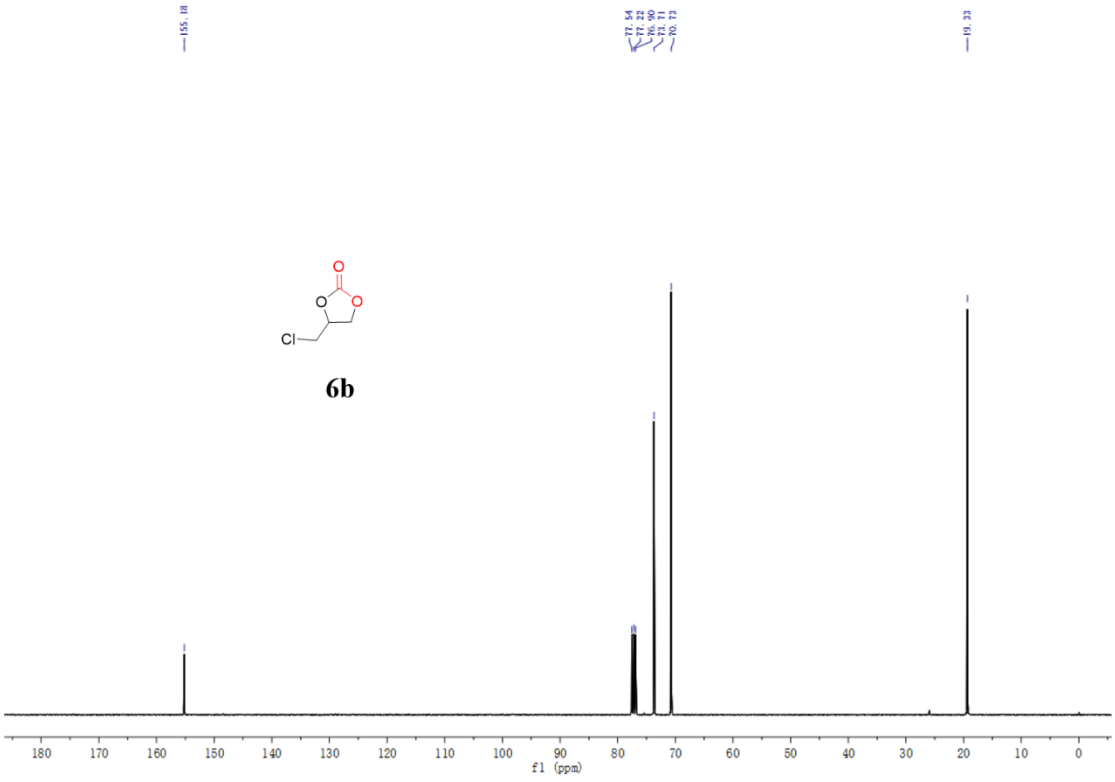

Figure S58. ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) spectra of catalyst **6b**.

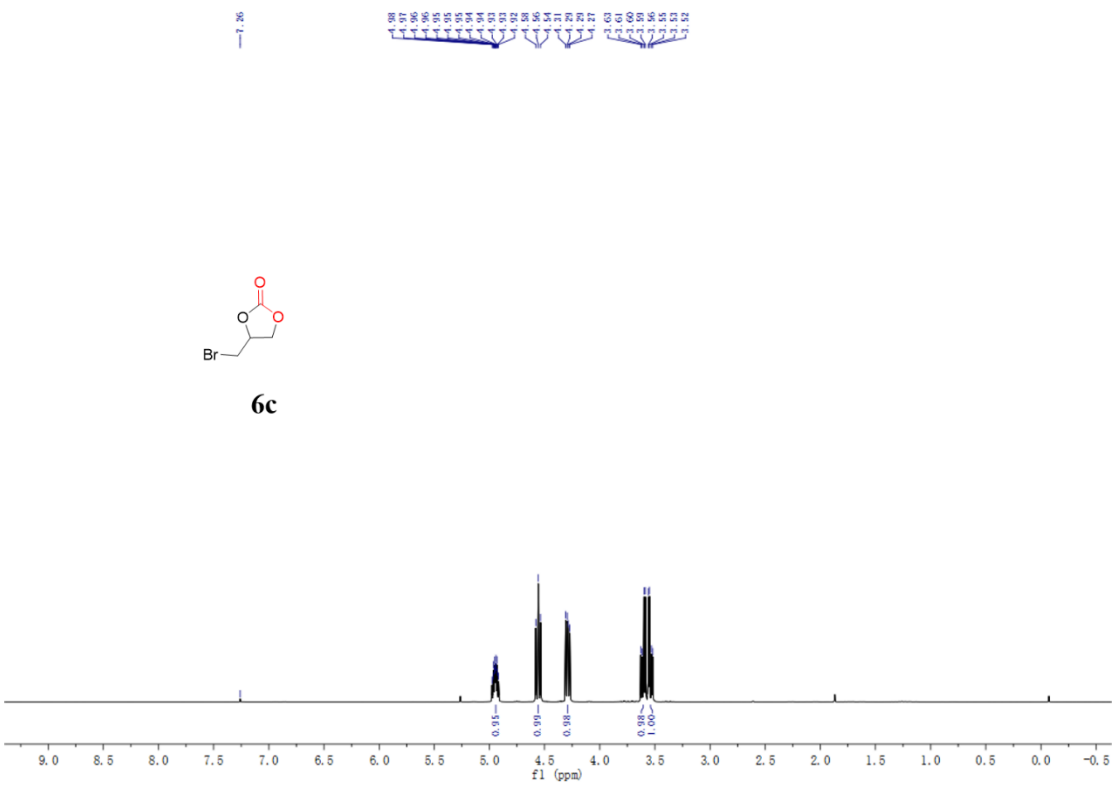

Figure S59. ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) spectra of catalyst **6c**.

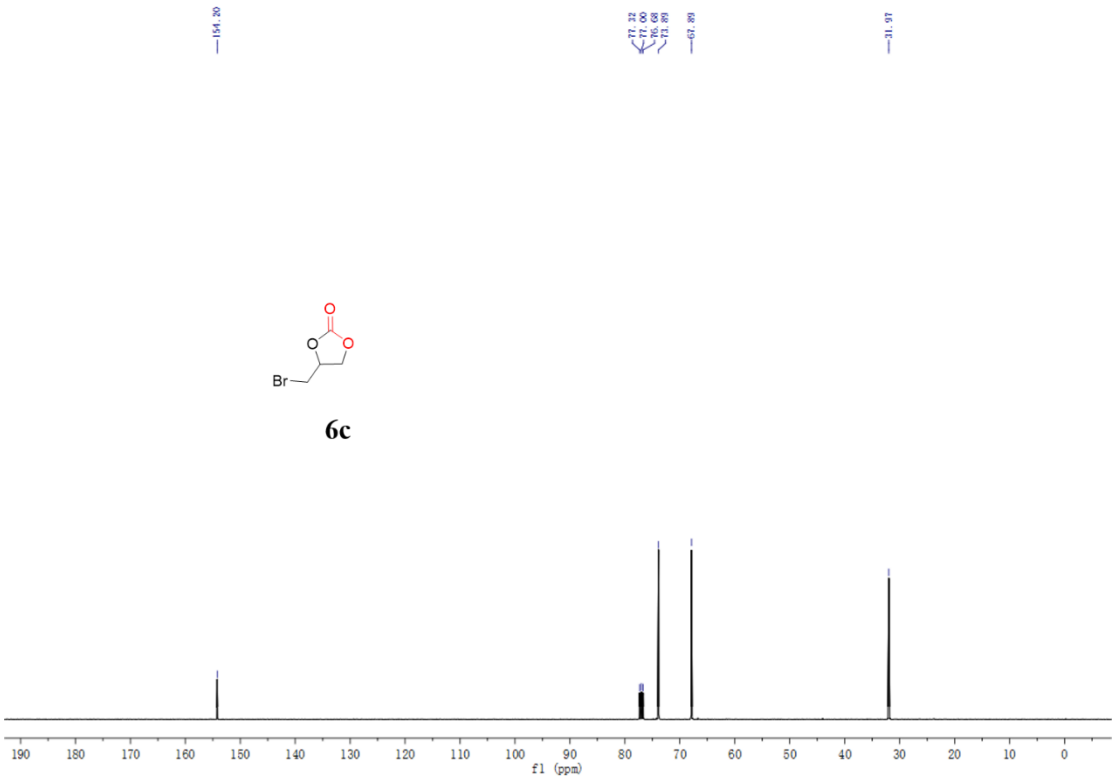

Figure S60. ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) spectra of catalyst **6c**.

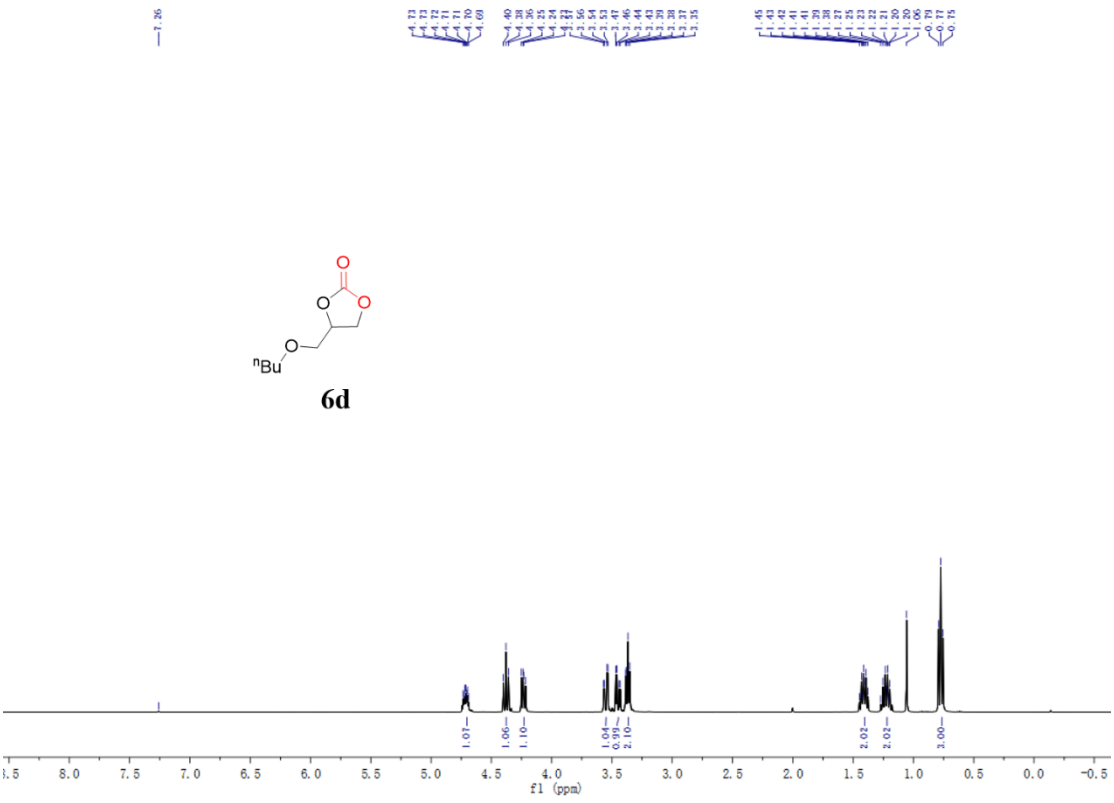

Figure S61. ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) spectra of catalyst **6d**.

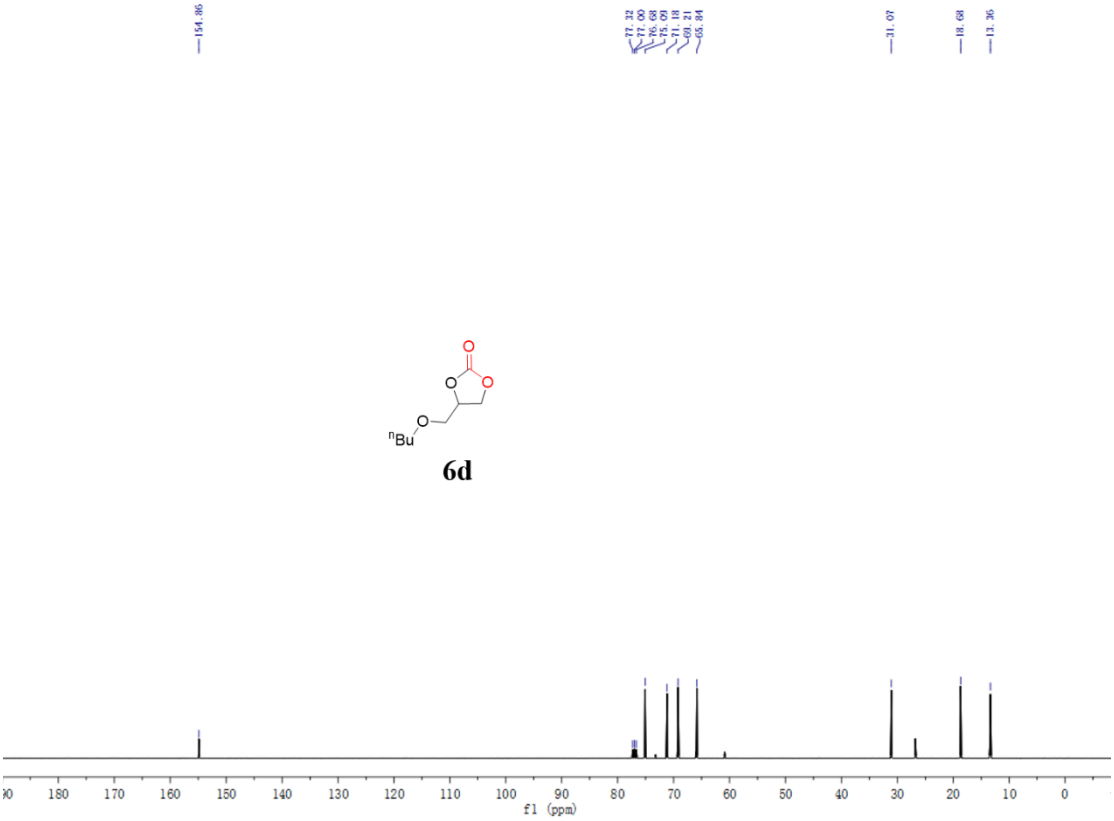

Figure S62. ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) spectra of catalyst **6d**.

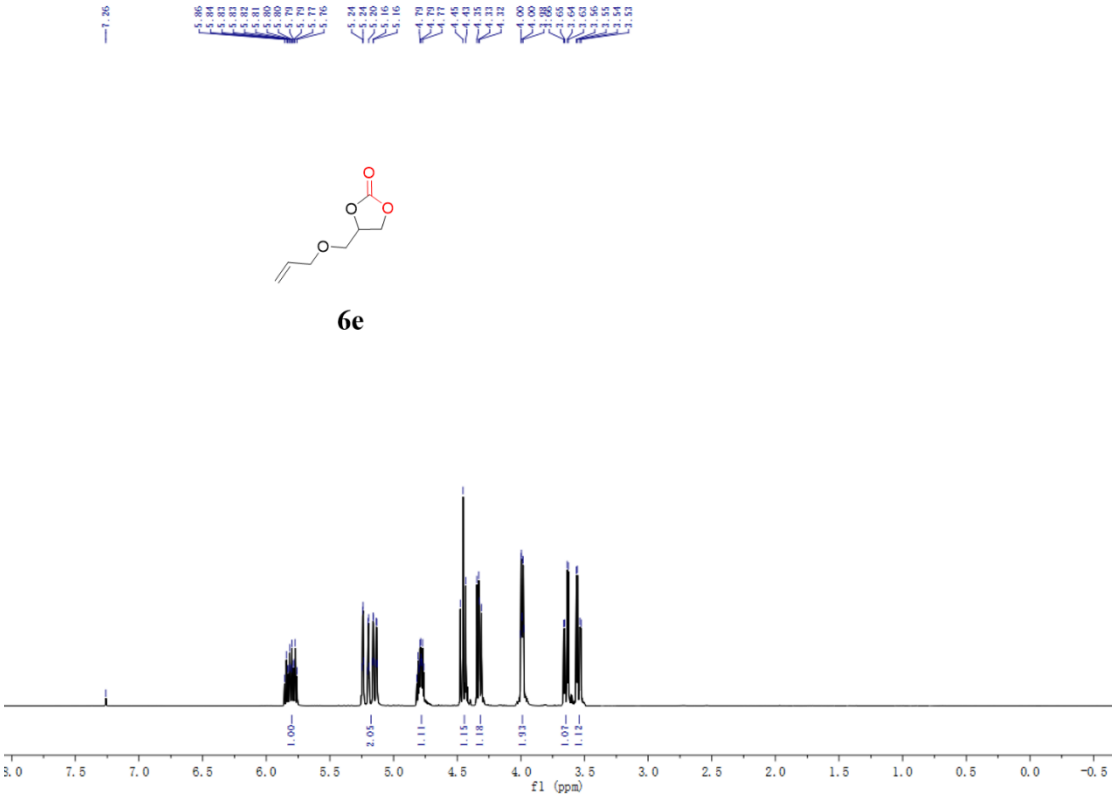

Figure S63. ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) spectra of catalyst **6e**.

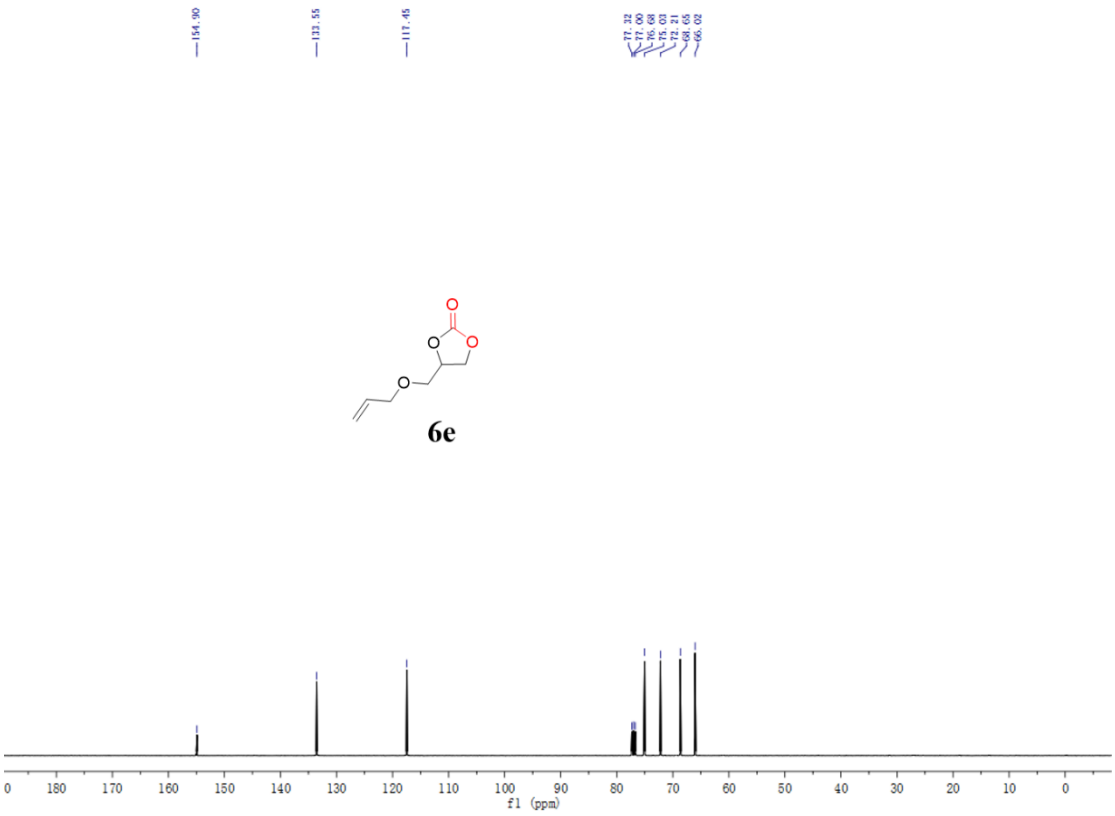

Figure S64. ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) spectra of catalyst **6e**.

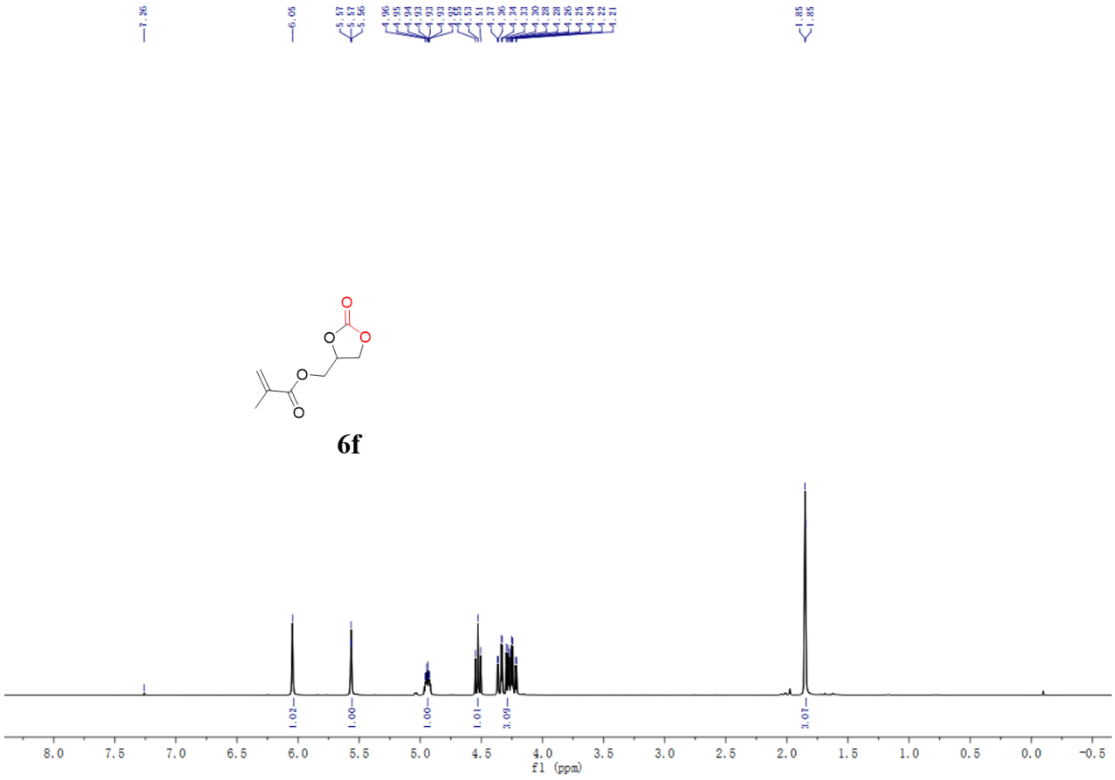

Figure S65. ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) spectra of catalyst **6f**.

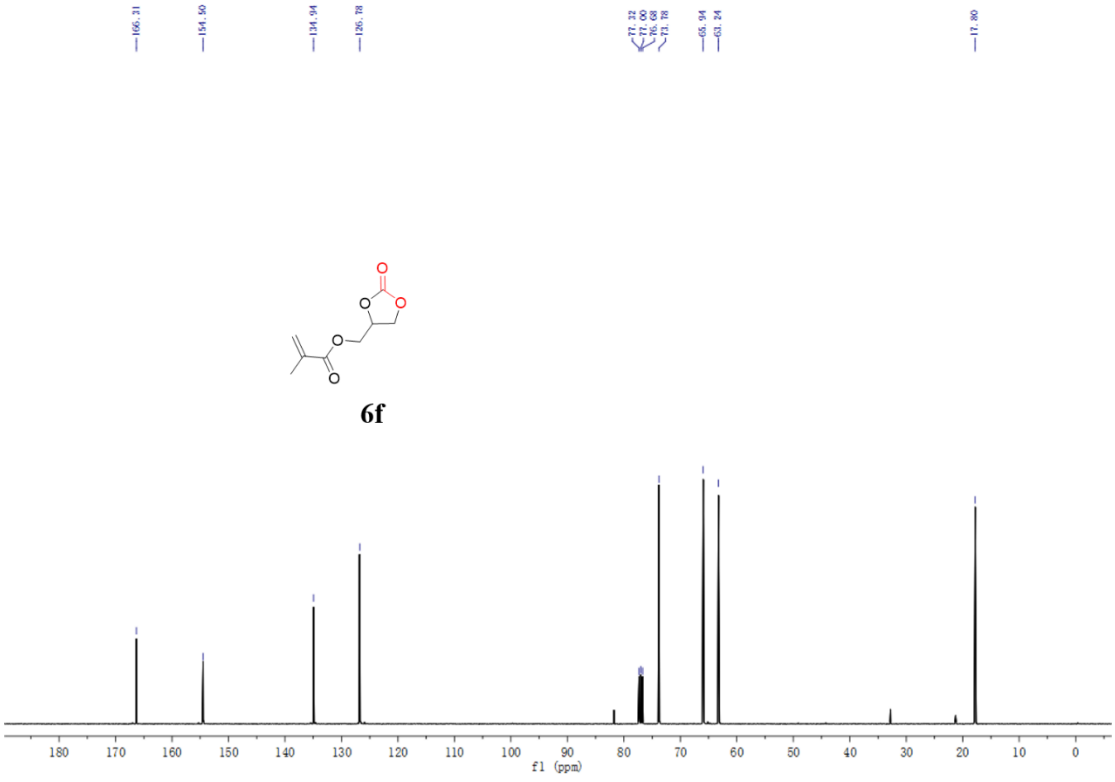

Figure S66. ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) spectra of catalyst **6f**.

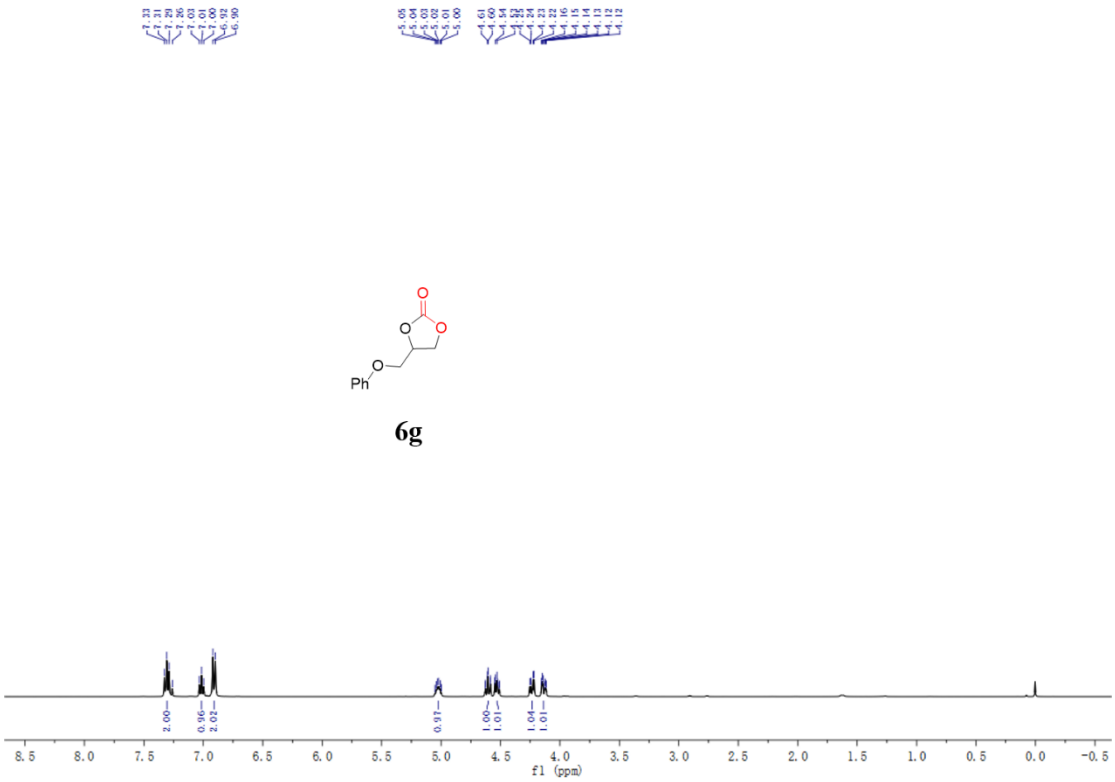

Figure S67. ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) spectra of catalyst **6g**.

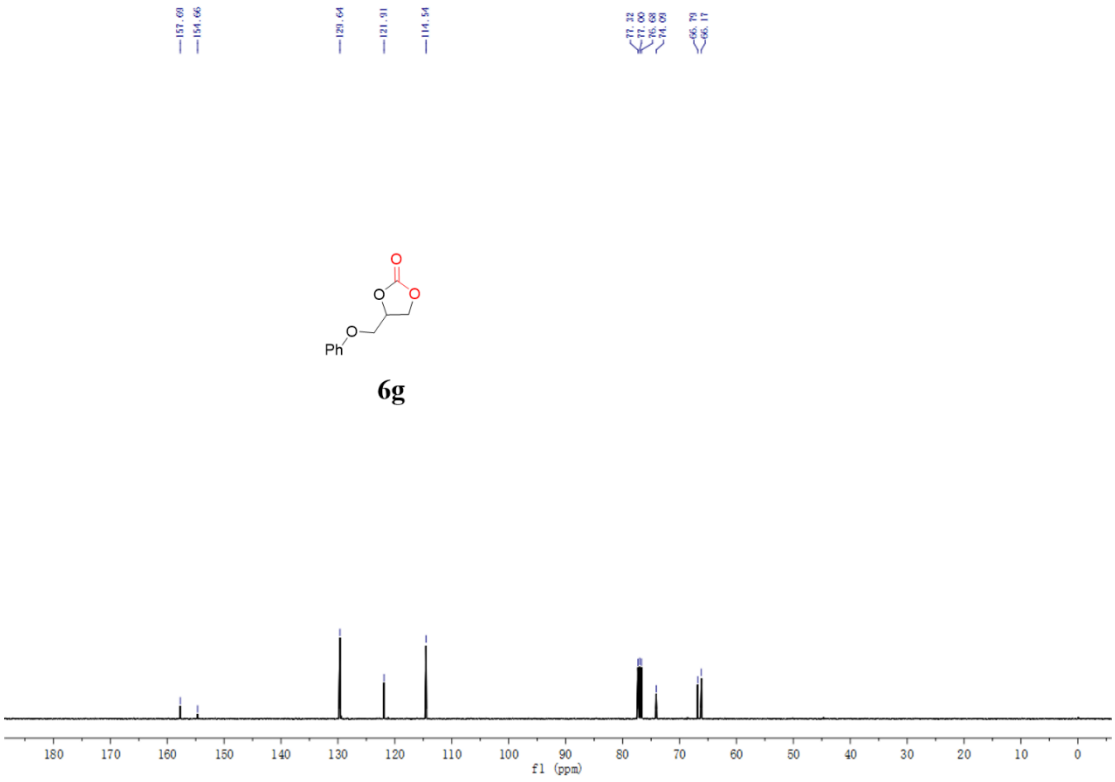

Figure S68. ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) spectra of catalyst **6g**.

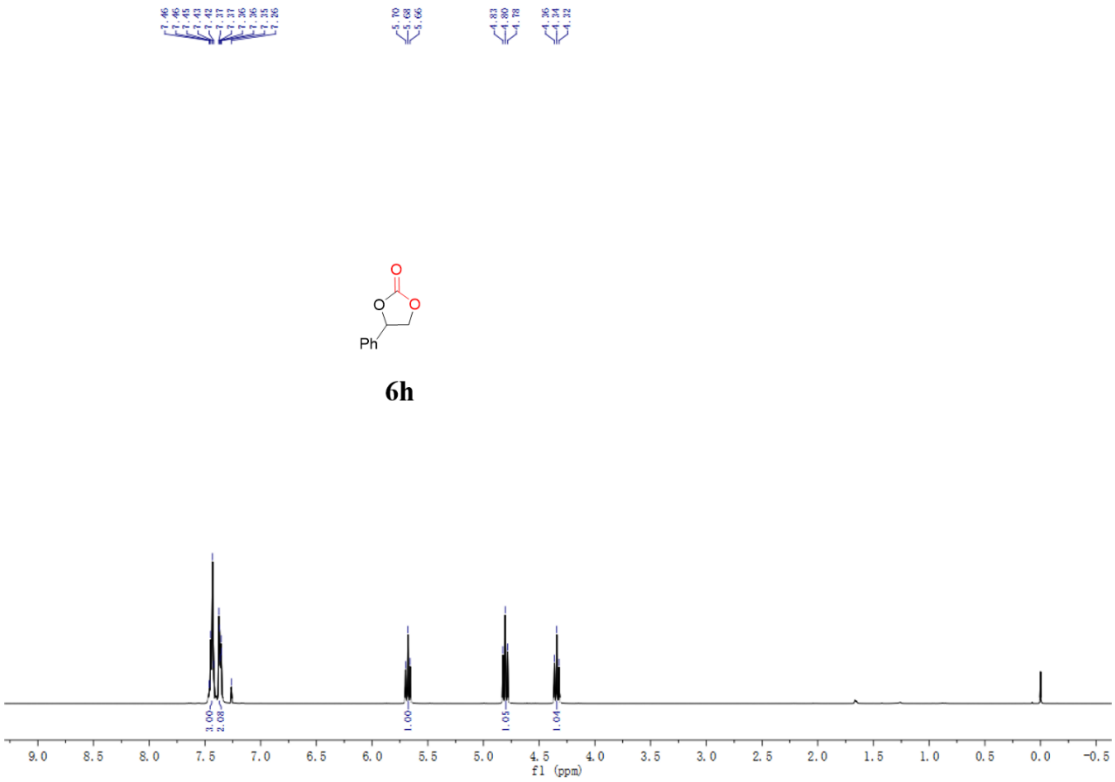

Figure S69. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ^{o}C) spectra of catalyst **6h**.

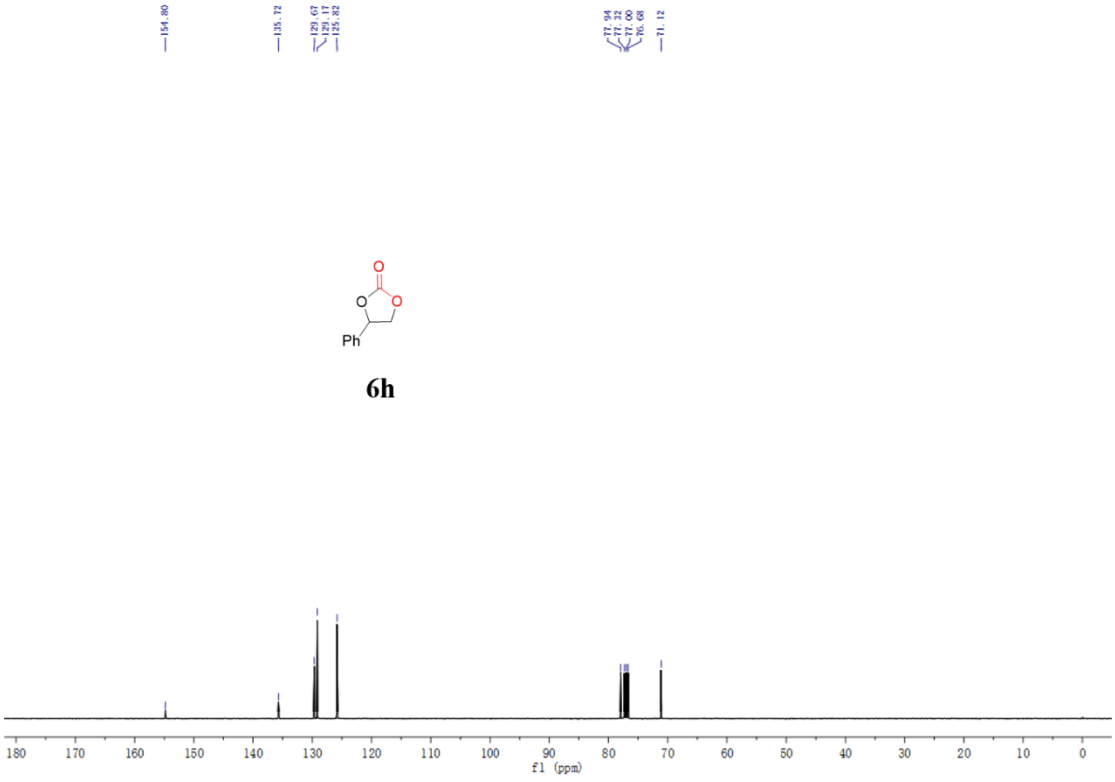

Figure S70. ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) spectra of catalyst **6h**.

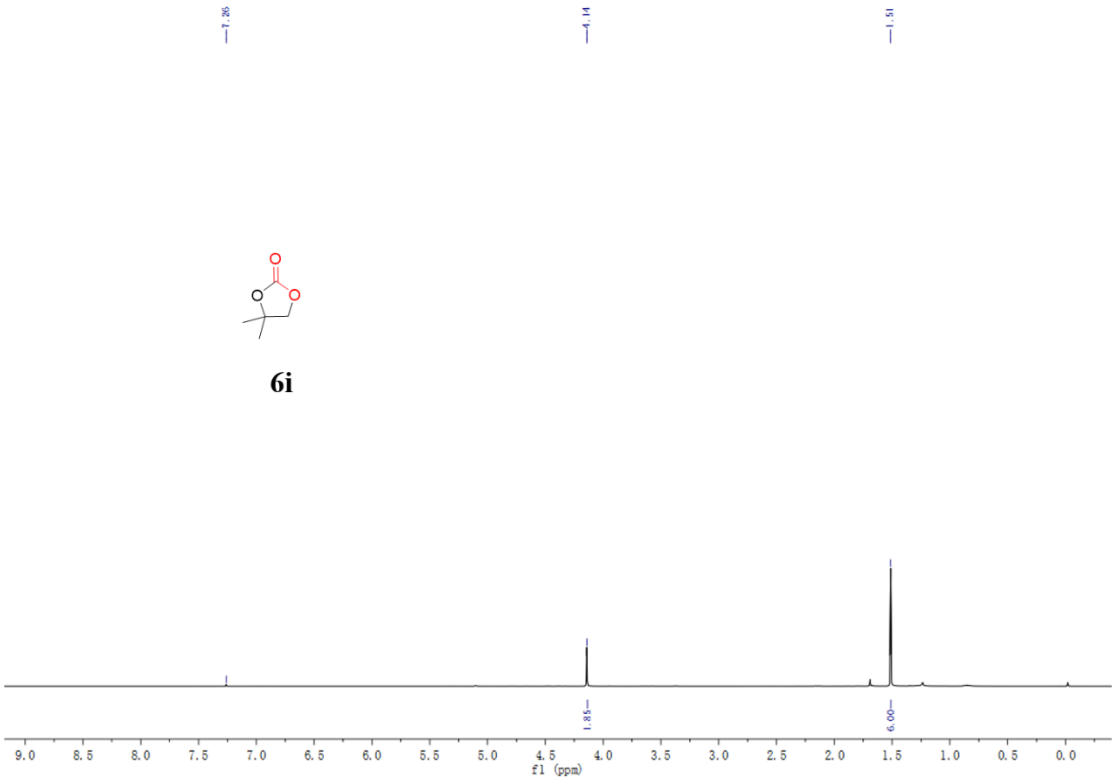

Figure S71. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ^{o}C) spectra of catalyst **6i**.

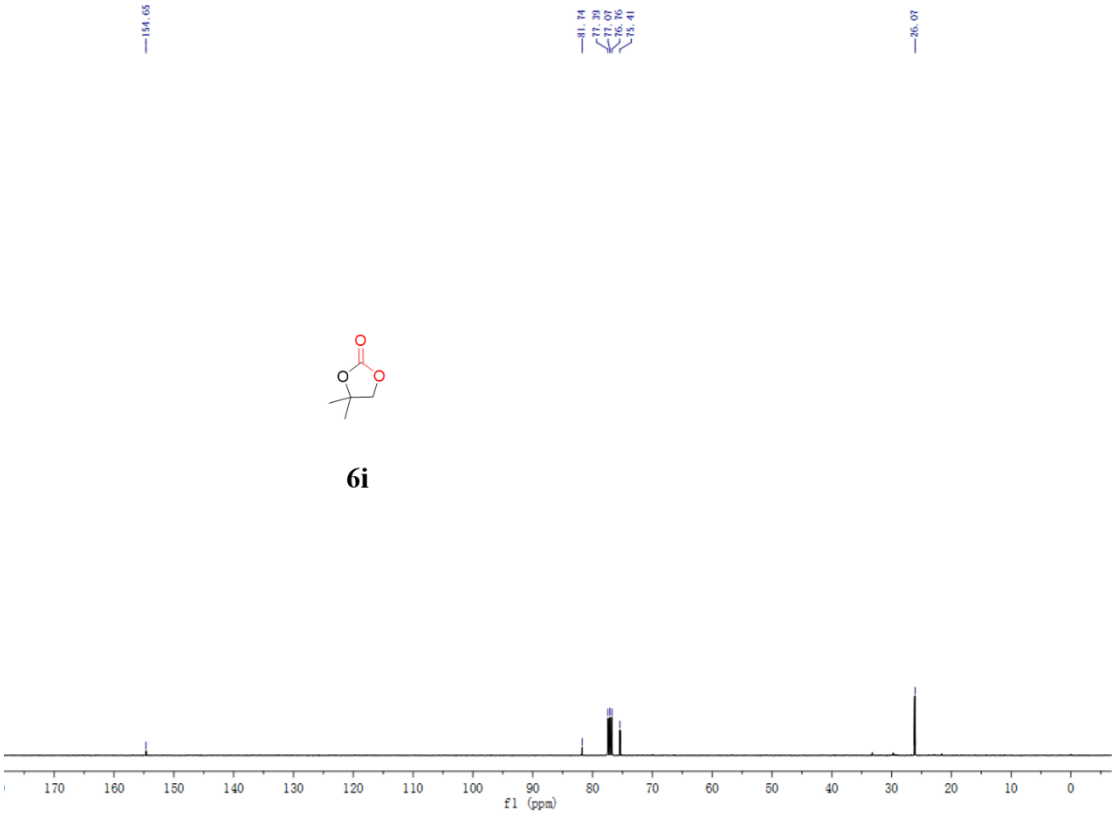

Figure S72. ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) spectra of catalyst **6i**.

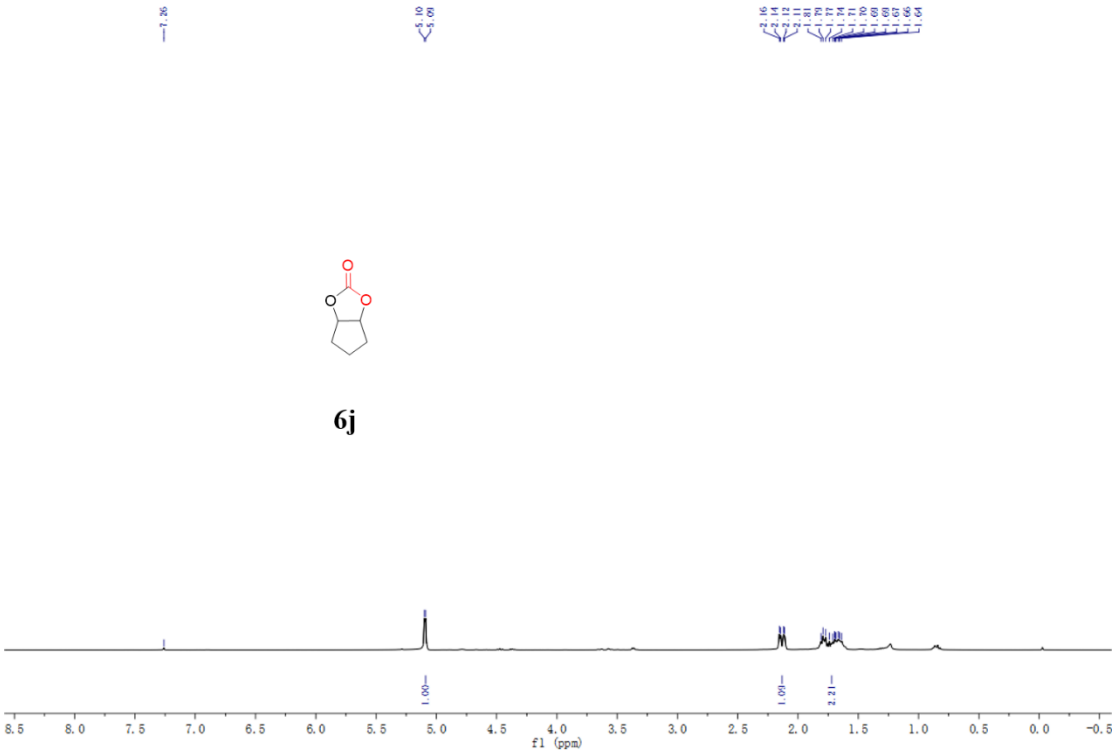

Figure S73. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ^{o}C) spectra of catalyst **6j**.

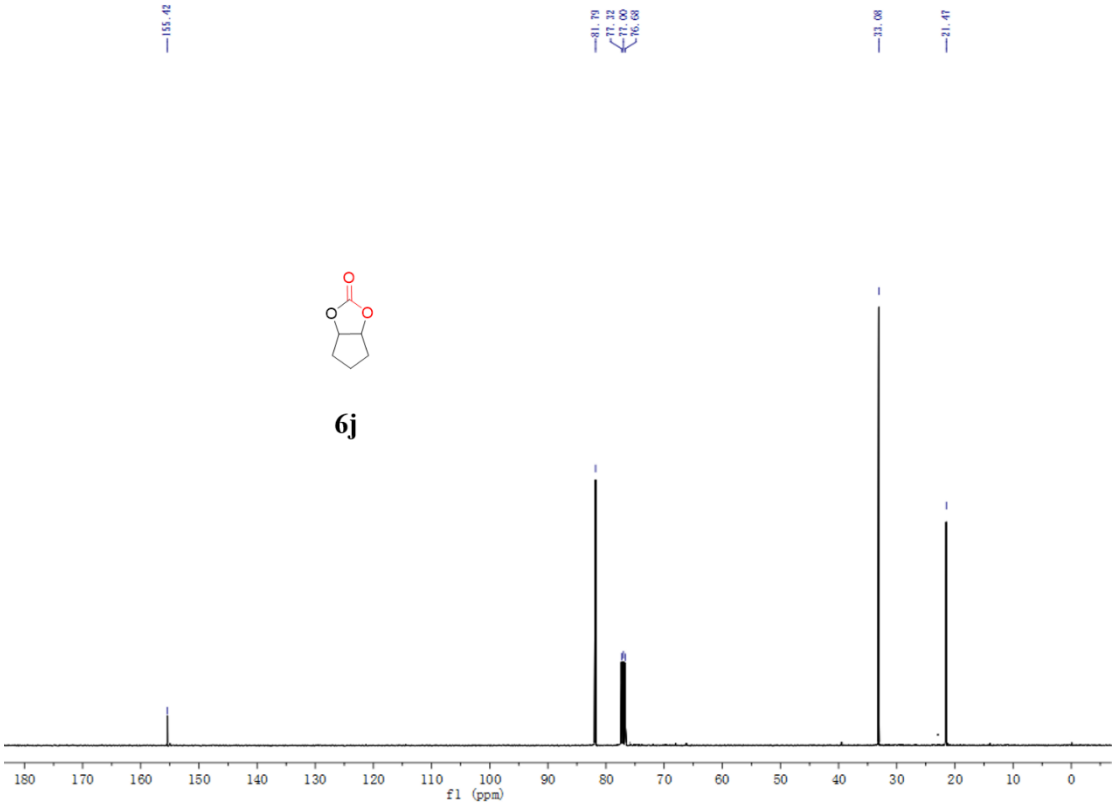

Figure S74. ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C) spectra of catalyst **6j**.

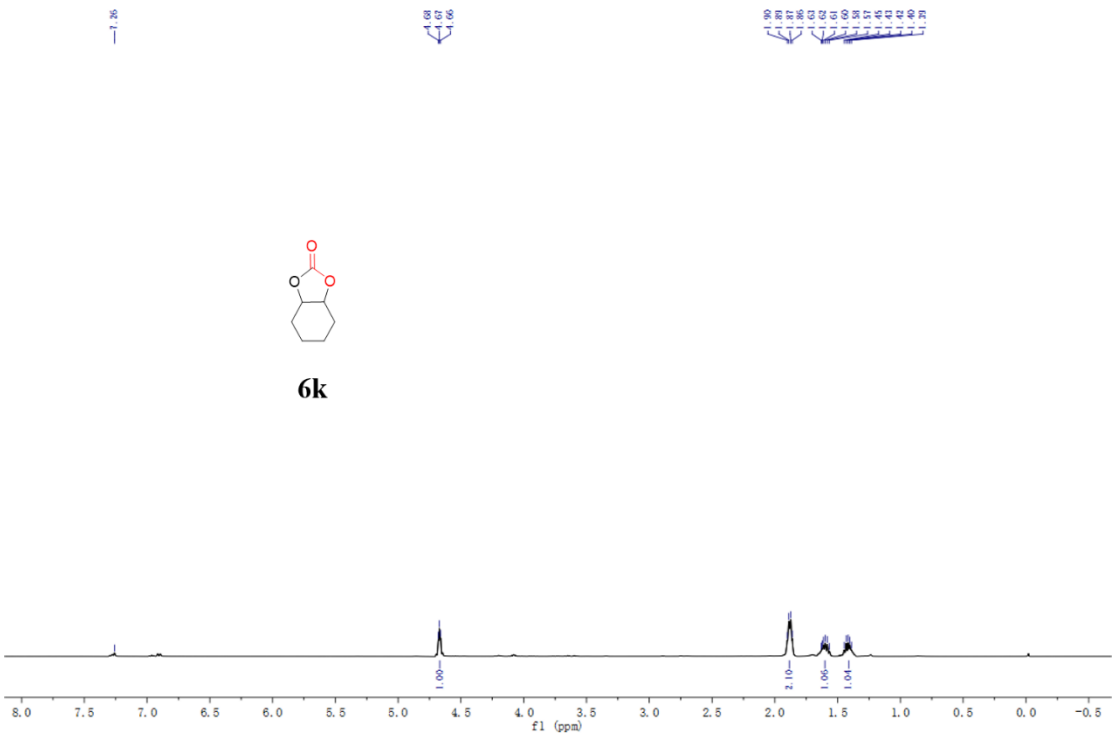

Figure S75. ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) spectra of catalyst **6k**.

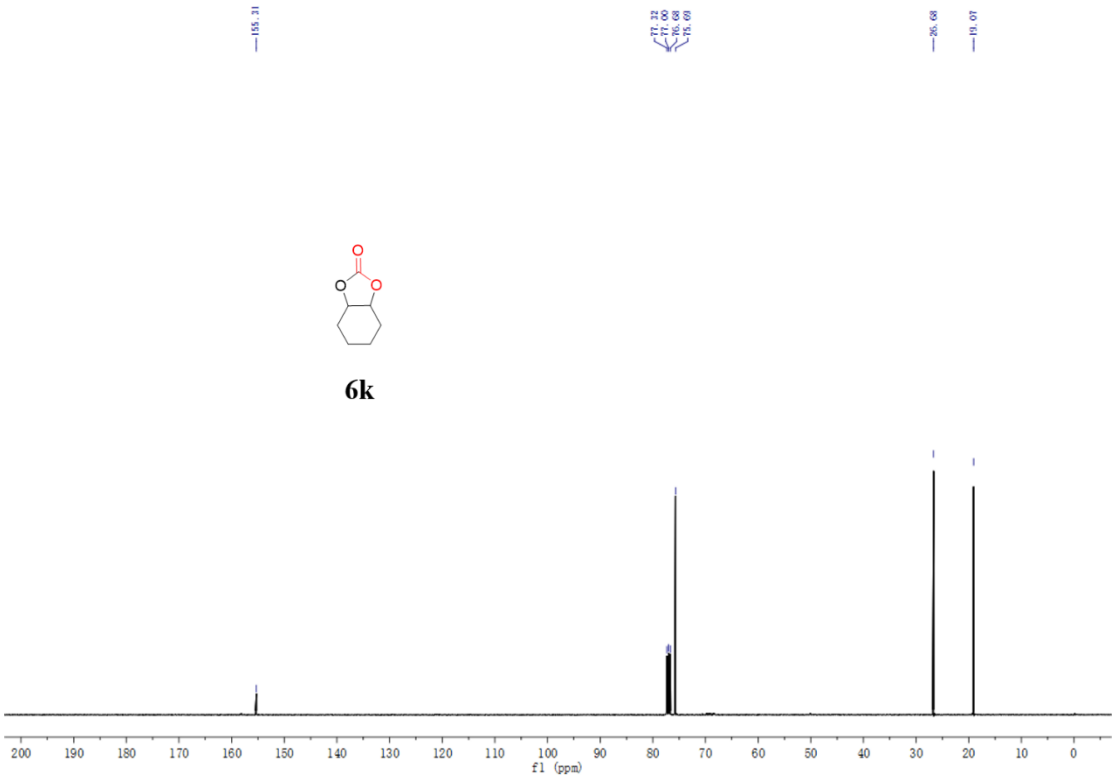

Figure S76. ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) spectra of catalyst **6k**.