Supporting information

Promoting Charge Separation in Donor-Acceptor Conjugated Microporous Polymers via Cyanation for Photocatalytic Reductive Dehalogenation of Chlorides

Weijie Zhang[a,c], Jiyong Deng[a], Zhengjun Fang[a], Donghui Lan[a], Yunfeng Liao[a], Xiang Zhou [a], Qingquan Liu[b]*

[a] Hunan Provincial Key Laboratory of Environmental Catalysis & Waste Recycling, School of Chemistry and Chemical Engineering, Hunan Institute of Engineering, Xiangtan 411104, China.
[b]Hunan Provincial Key Lab of Advanced Materials for New Energy Storage and Conversion, Hunan University of Science and Technology, Xiangtan 411201, China, Xiangtan 411201, China.
[c] College of Chemistry and Chemical Engineering, Hunan Provincial Key Laboratory of Efficient and Clean Utilization of Manganese Resources, Central South University, Changsha 410083, China.
E-mail: qqliu@hnust.edu.cn. weijie_zhang@hnie.edu.cn.

Table of Contents

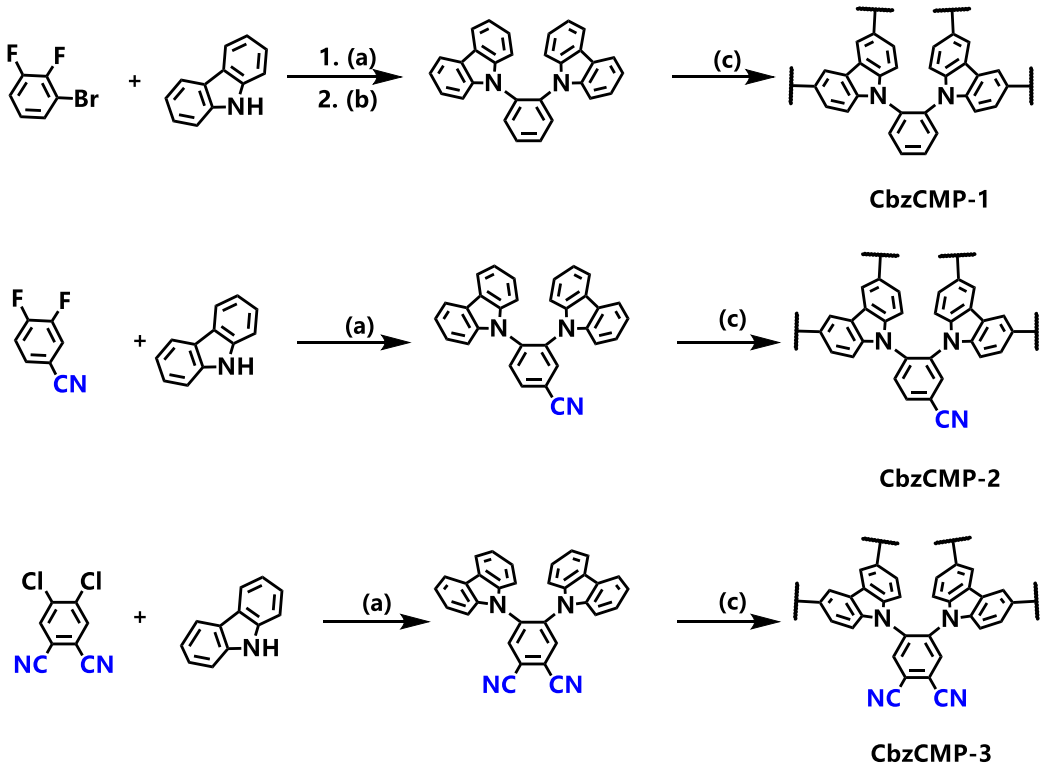
1. Characterizations

The ^{1}H and ^{13}C NMR spectroscopy were measured with the deuterated solvents ($CDCl_3$ and DMSO-d_6) and employed the tetramethyl silane (TMS) as an internal standard (Bruker AM-400 MHz NMR spectrometer). The obtained samples were prepared by dispersing in KBr powder and the corresponding FT-IR spectra were measured in the 400-4000 cm^{-1} region (VARIAN 1000 FT-IR spectrometer). The solid-state ^{13}C/NMR spectra of the polymers were carried out by using an Avance III HD 400 NMR spectrometer. To calculate the surface areas and pore volume of the polymers, Brunauer-Emmett Teller (BET) method was employed at 77 K and the samples were dried at 120 °C in vacuum for 12 hours prior to measurements (Micromeritics ASAP 2020M). The pore-size-distribution of the polymers were acquired by the adsorption branches (non-local density functional theory method, NLDFT). The polymers surface morphologies were carried out at an accelerating voltage of 8.0 kV (FEI SIRION200). The UV-Vis adsorption spectra of the powders in the solid state were obtained on a Scan UV-Vis spectrophotometer (U-4100 spectrometer). The electrochemical impedance spectra (EIS) were performed on an electrochemical workstation at room temperature in the dark (CHI760E). The photocurrent of the polymer was performed on a VersaSTAT 3 electrochemical workstation under irradiation of 300 W Xe lamp. The fluorescence spectra were characterized by using excitation wavelength of 365 nm at room temperature (F97PRO fluorescence spectrometer). The time-correlated fluorescence spectroscopy of solid samples was performed on a FLS-980 fluorescence

lifetime spectrometer. The density functional theory (DFT) calculations were applied to optimize the geometry of monomers and oligomers (B3LYP functional and 6-31G(d) basis set). The molecular configuration optimization and electrostatic potential map was carried out by DFT calculations (Gaussian 09 software package and Gauss View visualization program).

2. Preparation procedures

2.1 Synthesis of intermediates, CbzCMP-1, CbzCMP-2 and CbzCMP-3



Scheme S1. Synthesis routes of **CbzCMP-1**, **CbzCMP-2** and **CbzCMP-3**

2.1.1 Preparation of 9,9'-(3-bromo-1,2-phenylene)bis(9*H*-carbazole)

A mixture of 1-bromo-2,3-difluorobenzene(1.93 g, 0.01mol), K_2CO_3(2.76 g, 0.02 mol) and 9*H*-carbazole (4.01g, 0.024 mol) in DMF (35 mL) was heated to 150 ^oC under N_2 for 24h. After cooling to room temperature, the reaction mixture was concentrated to remove the solvent and the residue was purified by flash column chromatography to obtain as a white solid in 72 % yield. ^1H NMR ($CDCl_3$, 400 MHz): δ 8.03 (d, J = 8.0 Hz, 2H), 7.75-7.62 (m, 6H), 7.08-7.00 (m, 12H) ppm.

2.1.2 Preparation of 1,2-di(9*H*-carbazol-9-yl)benzene

To a mixture of 1-bromo-2,3-difluorobenzene (1.93 g, 0.01mol) in THF under -78 ^{o}C, n-butyllithium (6.00 mL, 2.5 M in hexane) was added dropwise and stirred for 2 h under an N_2 balloon, and then the mixture continued to stir for 14 h at room temperature. NH_4Cl (aq. 2 M) was added the above reaction mixture, which was concentrated under reduced pressure and the resulting residue was treated with water and extracted with EtOAc. The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. The crude product was purified by silica gel column chromatography using petroleum ether/dichloromethane as an eluent to give the desired 1,2-di(9*H*-carbazol-9-yl)benzene as a white solid in 97% yield. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.86-7.78 (m, 6H), 7.19-7.14 (m, 4H), 7.09-7.03 (m, 8H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ 139.9, 134.5, 130.5, 128.9, 125.3, 123.4, 119.9, 119.8, 109.7 ppm.

2.1.3 Preparation of 3,4-di(9*H*-carbazol-9-yl)benzonitrile

A mixture of 3,4-difluorobenzonitrile (1.39 g, 0.01mol), K_2CO_3 (2.76 g, 0.02 mol) and 9*H*-carbazole (4.01g, 0.024 mol) in DMF (50 mL) was heated to 150 ^{o}C under N_2 for 24h. After cooling to room temperature, the reaction mixture was concentrated to remove the solvent and the residue was purified by flash column chromatography to obtain as a white solid in 56 % yield. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.17 (d, J = 4.0 Hz, 2H), 8.01-7.95 (m, 4H), 7.82-7.77 (m ,4H), 7.13-7.05 (m, 12H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ 139.1, 139.0, 138.6, 135.1, 134.4, 131.8, 131.4, 125.8, 125.7, 123.9, 123.8, 120.8, 120.7, 120.1, 117.5, 112.3, 109.4 109.1 ppm.

2.1.4 Preparation of 4,5-di(9*H*-carbazol-9-yl)phthalonitrile

A mixture of 4,5-difluorophthalonitrile (1.64 g, 0.01mol), K_2CO_3 (2.76 g, 0.02 mol) and 9*H*-carbazole (4.01g, 0.024 mol) in DMF (50 mL) was heated to 150 ^{o}C under N_2 for 24 h. After cooling to room temperature, the reaction mixture was concentrated to remove the solvent and the residue was purified by flash column chromatography to obtain as a white solid in 47 % yield. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.33 (s, 2H), 7.80 (d,

J = 4.0 Hz, 4H), 7.15-7.06 (m,12H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ 138.4, 138.2, 135.5, 126.2, 124.3, 121.6, 120.0, 114.7, 114.5, 109.0 ppm.

2.2 The synthetic route of chloroacetophenones[S1-4]

Procedure I. A mixture of bromoacetophenone (300 mg), $PhSO_2Cl$ (8.0 -10.0 equiv.), benzyl triethyl ammonium chloride (0.5 equiv.) and water (5.0 mL) was stirred at rt for 1.5 -3h and then the reaction was stopped and cooled in an ice-bath. Then saturated Na_2CO_3 aq. (10 mL) was added to the reaction mixture with stirring until $PhSO_2Cl$ disappeared. The mixture was then extracted with ethyl acetate, concentrated and purified by silica gel column chromatography using petroleum ether/dichloromethane to give the desired product chloroacetophenones in quantitative yield.

Procedure II. A mixture of benzene derivative (1.0 equiv.), aluminum trichloride (2.0 equiv.), 2-chloroacetyl chloride (1.2 equiv.) in dry $CHCl_3$ was stirred at 50 ^oC for 3h and then the reaction was stopped and cooled in an ice-bath. The mixture was then extracted with ethyl acetate, concentrated and purified by silica gel column chromatography using petroleum ether/dichloromethane to give the desired product chloroacetophenones.

3 Photocatalyst Characterizations

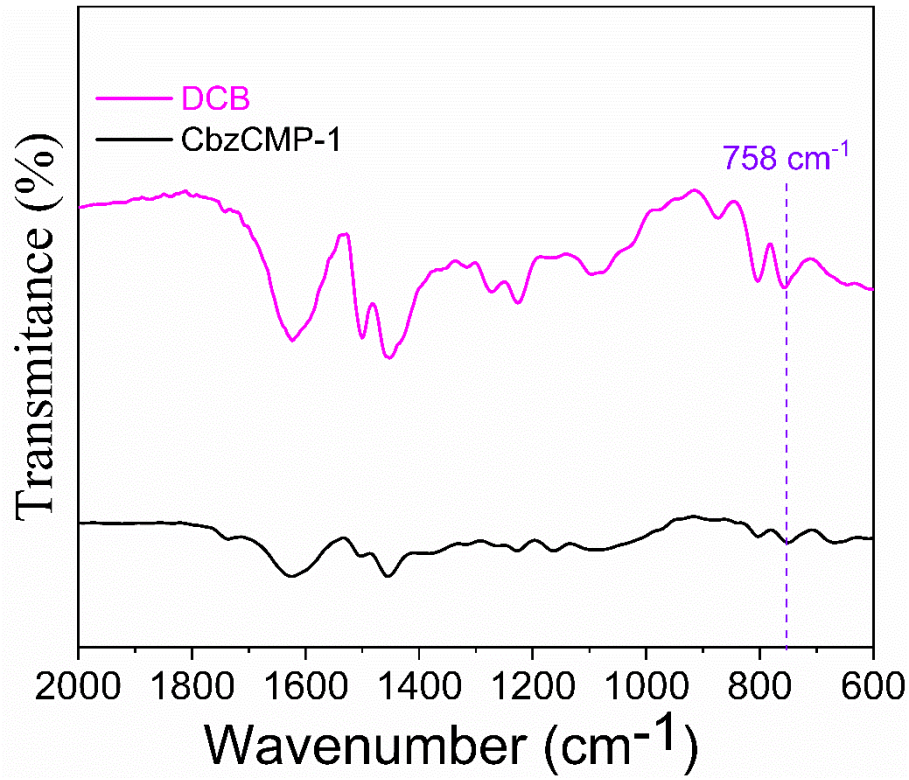


Fig. S1. FT-IR of DCB and CbzCMP-1

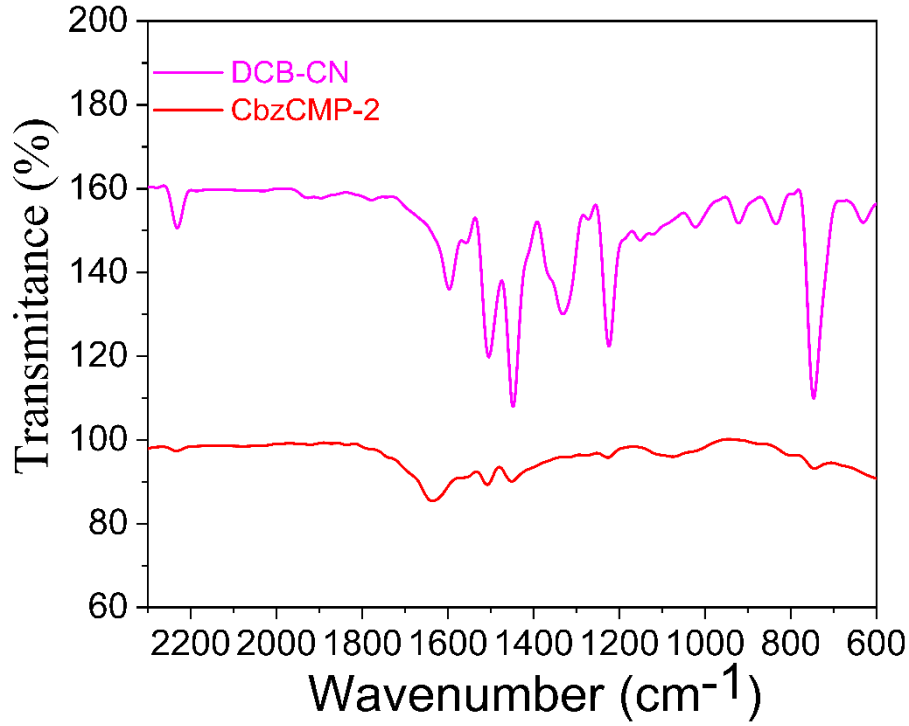


Fig. S2. FT-IR of DCB-CN and CbzCMP-2

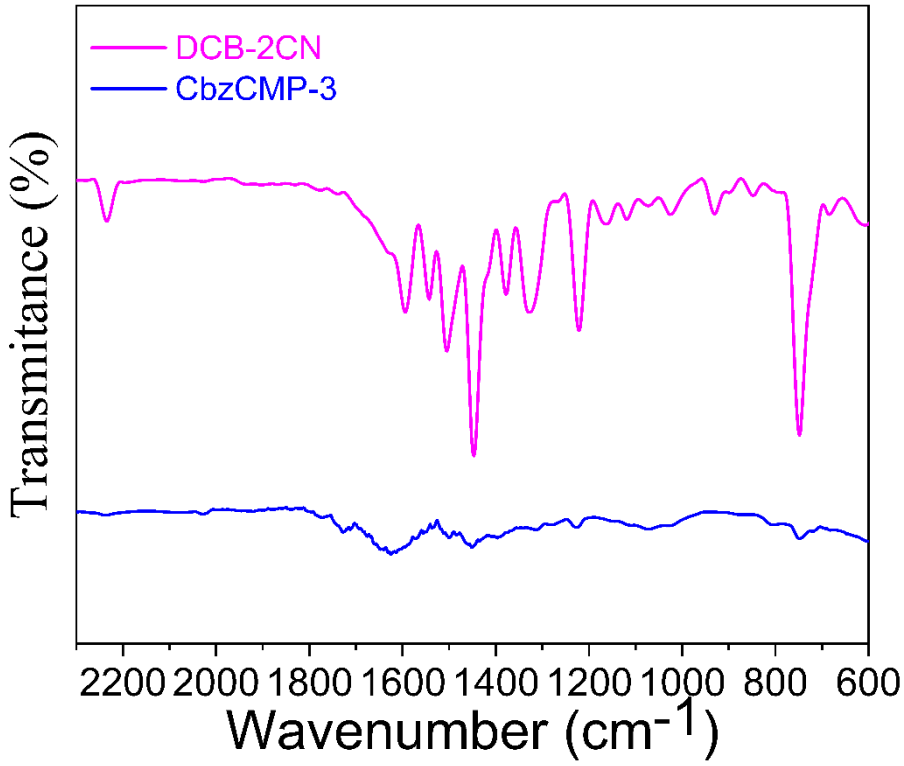


Fig. S3. FT-IR of DCB-2CN and CbzCMP-3

The peak at ~800 cm^{-1} in the CbzCMP-*n* (*n*=1, 2 and 3) and monomer sample is attributed to the vibrational bands of C–H bonds of the bisubstituted carbazole ring , the peak at 850-900 cm^{-1} in the CbzCMP-*n* (*n*=1, 2 and 3) (and ~750 cm^{-1} in monomer sample) is attributed to the vibrational bands of C-H bonds of the bisubstituted phenyl ring connecting with *N* atom in the carbazole moiety, and a newly generated peak at ~900 cm^{-1} in the CMPs is attributed to the vibrational bands of C-H bonds of the trisubstituted carbazole ring, which demonstrates the formation of dimeric carbazole. The signal at ~2225 cm^{-1} hints that the terminal nitriles is well retained in CMPs backbone after polymerization[S5-6].

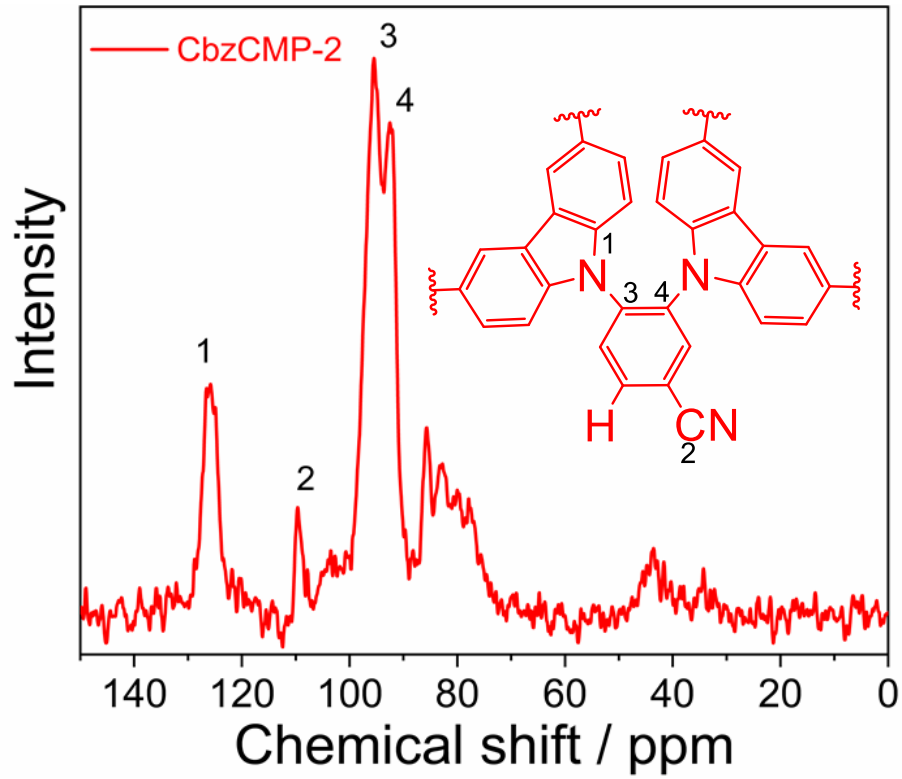


Fig. S4. Solid ^{13}C-NMR spectrum of CbzCMP-2

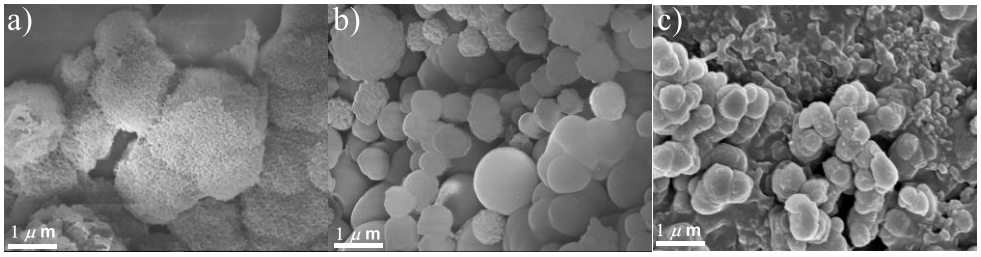


Fig. S5. SEM images of CbzCMP-1 (a), CbzCMP-2 (b), and CbzCMP-3(c).

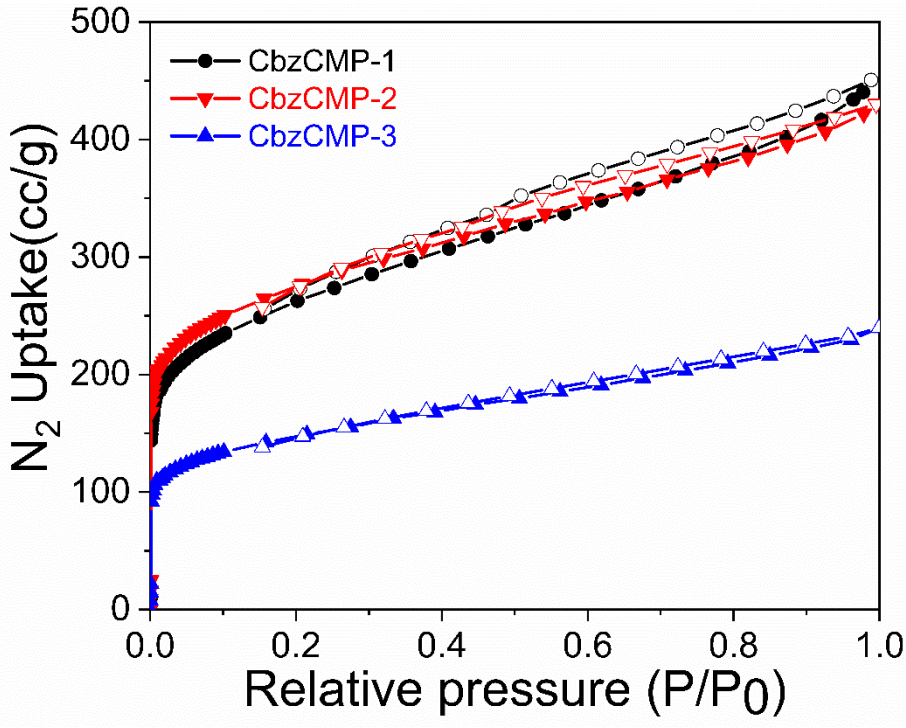


Fig. S6. Nitrogen sorption isotherms of CbzCMP-1, CbzCMP-2 and CbzCMP-3 at 77 K

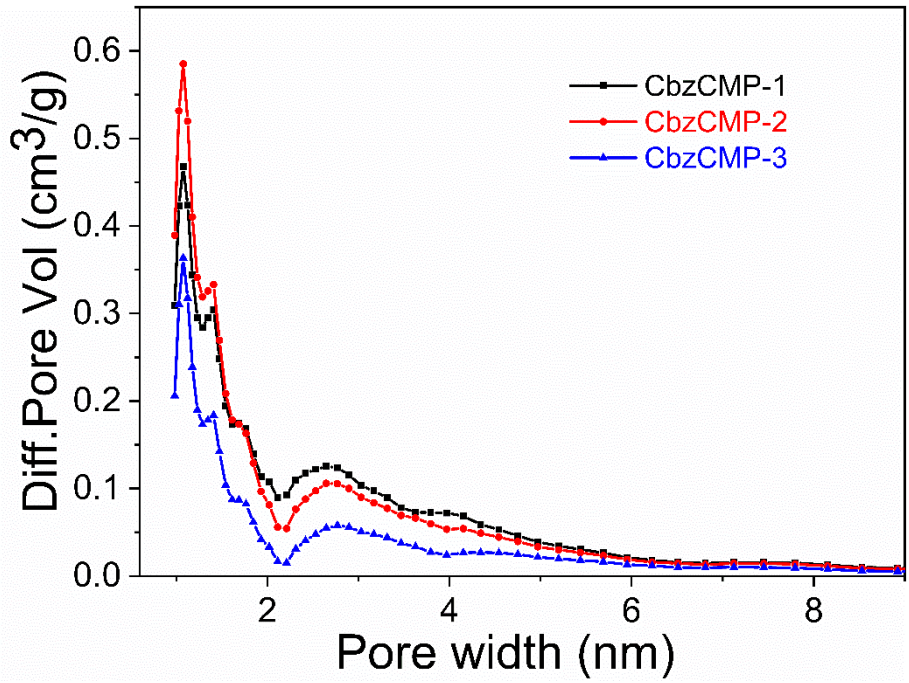


Fig. S7. Pore size distributions of CbzCMP-1, CbzCMP-2 and CbzCMP-3

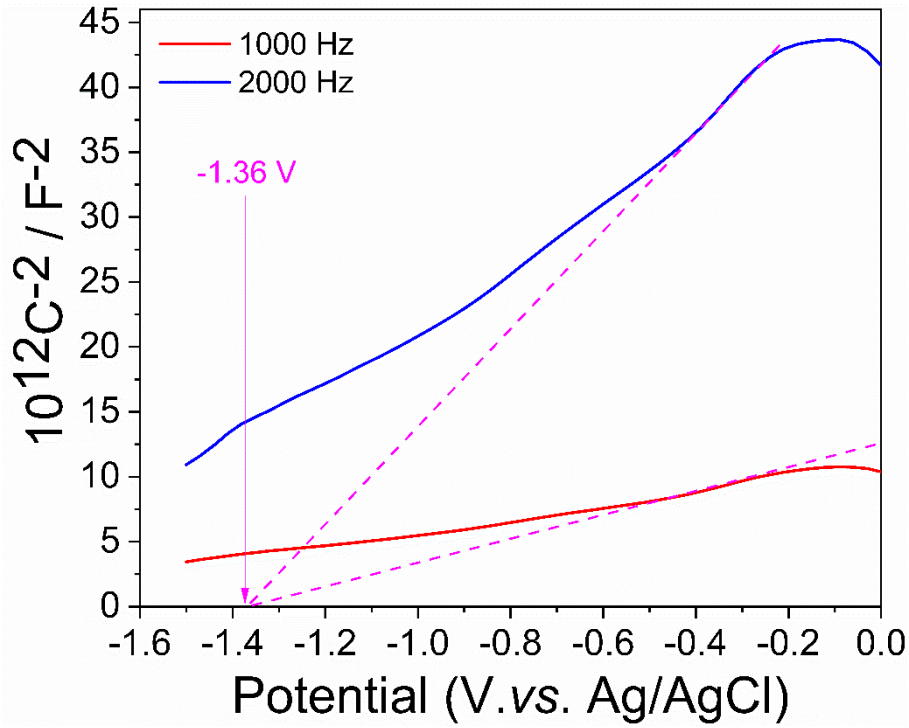


Fig. S8. Mott-Schottky plots for CbzCMP-1in 0.2 M Na_2SO_4 aqueous solution at 1000 and 2000 Hz

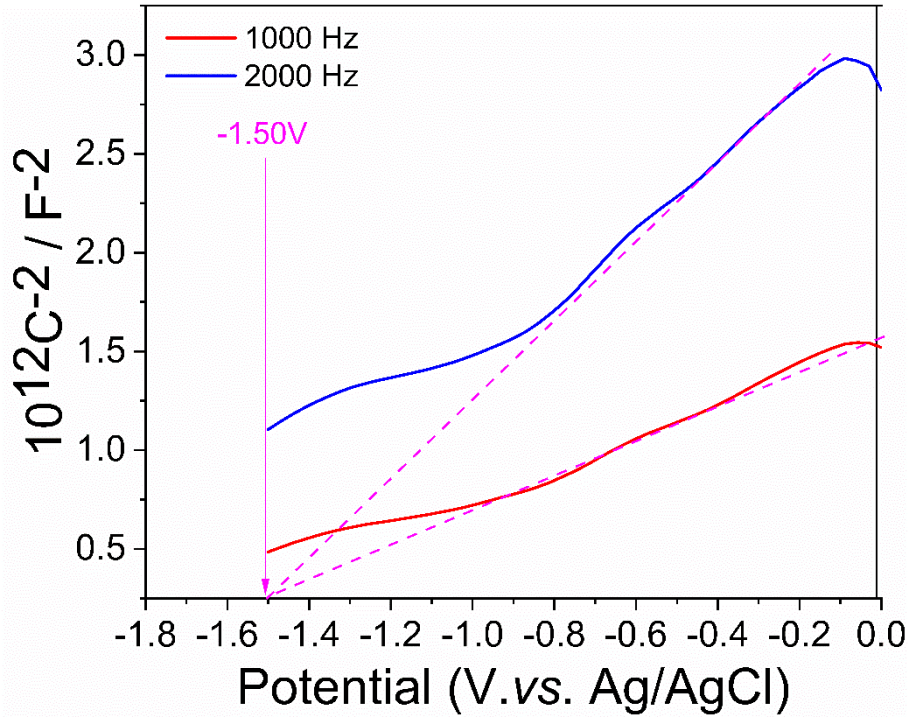


Fig. S9. Mott-Schottky plots for CbzCMP-2 in 0.2 M Na_2SO_4 aqueous solution at 1000 and 2000 Hz

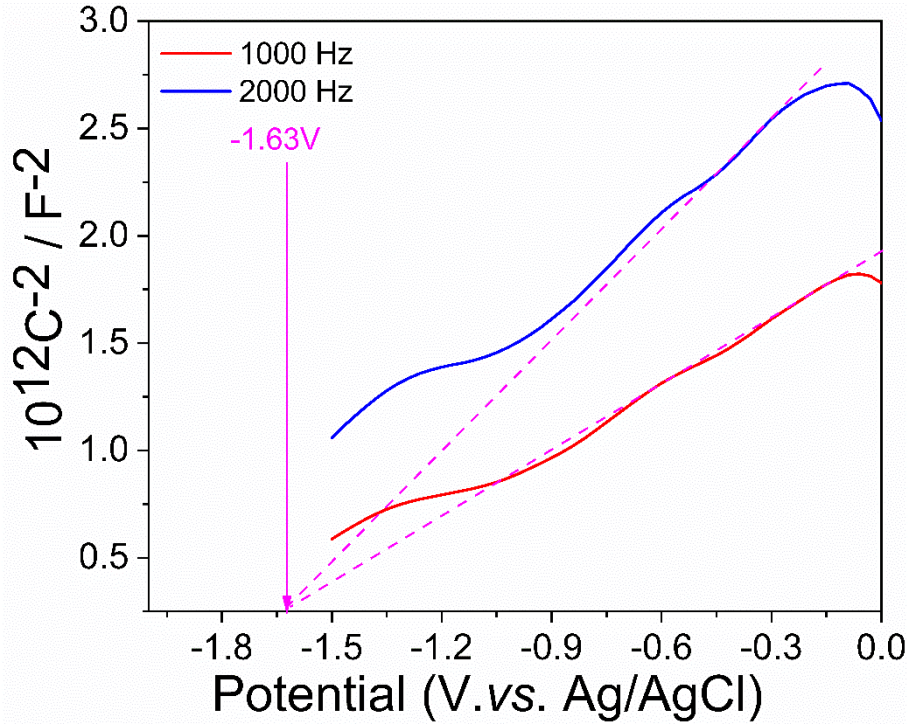


Fig. S10. Mott-Schottky plots for CbzCMP-3 in 0.2 M Na_2SO_4 aqueous solution at 1000 and 2000 Hz

Table S1. Porosity data and electrochemical properties of CbzCMP-*n* (*n*=1, 2 and 3)

Polymers	BET (m^2/g)	V_{total} (cm^3/g^{-1})	V_{micro} (cm^3/g^{-1})	V_{micro}/V_{total}	Eg (eV)	LUMO (V *vs* NHE)	HOMO (V *vs* NHE)
CbzCMP-1	949	0.70	0.36	51%	2.10	-1.36	0.74
CbzCMP-2	997	0.67	0.36	54%	2.02	-1.30	0.72
CbzCMP-3	537	0.37	0.21	57%	1.90	-1.43	0.56

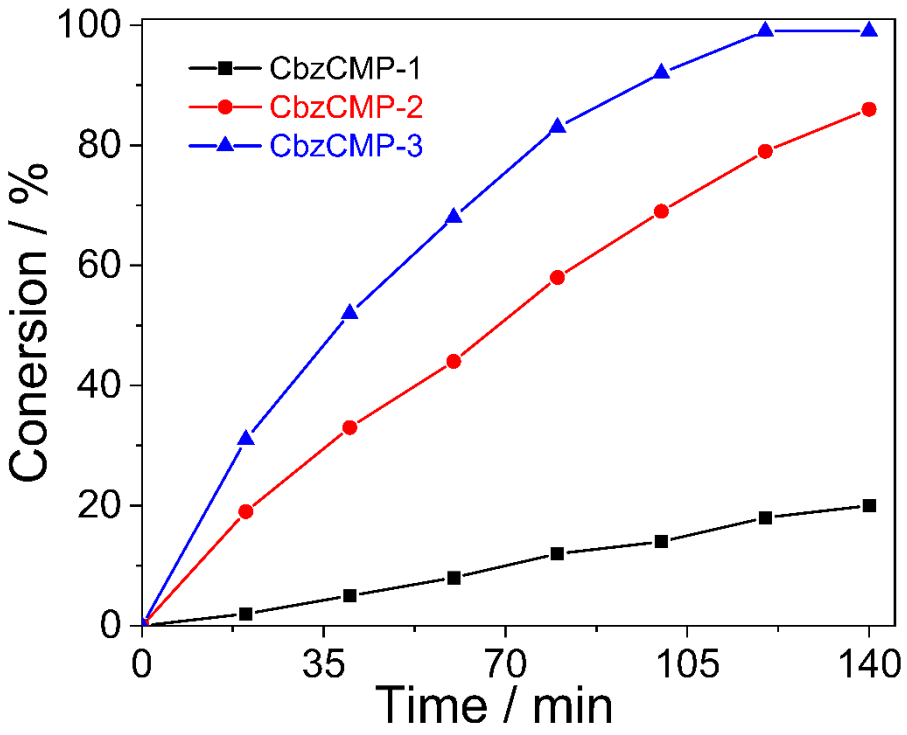


Fig. S11. The time course of 2-chloro-1-phenylethan-1-one conversion catalyzed by CbzCMP-*n* (*n*=1, 2 and 3)

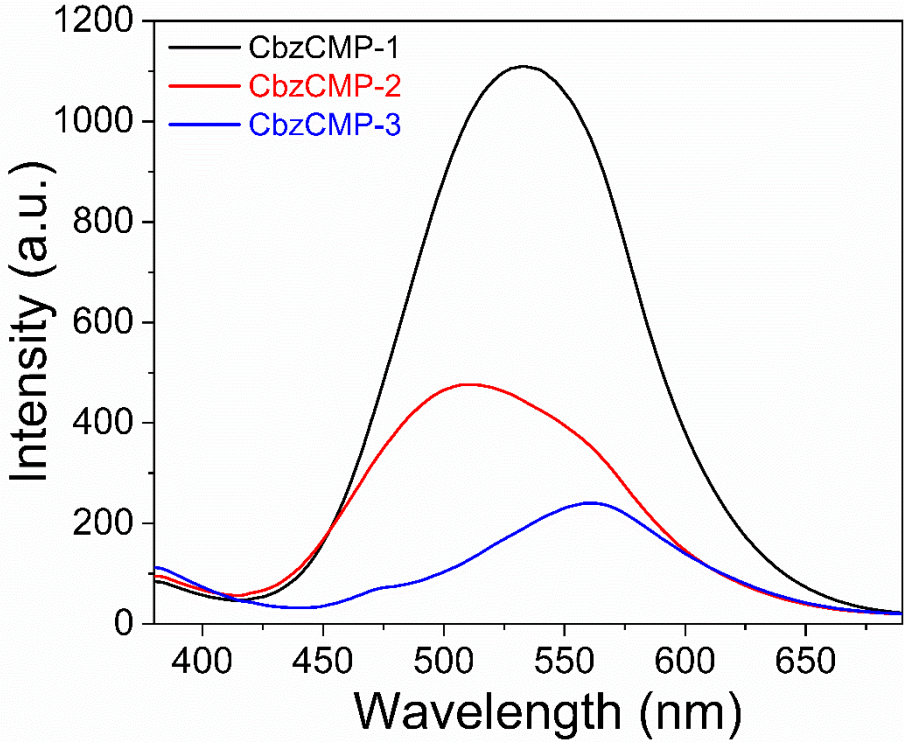


Fig. S12. PL spectra of CbzCMP-*n* (*n*=1, 2 and 3)

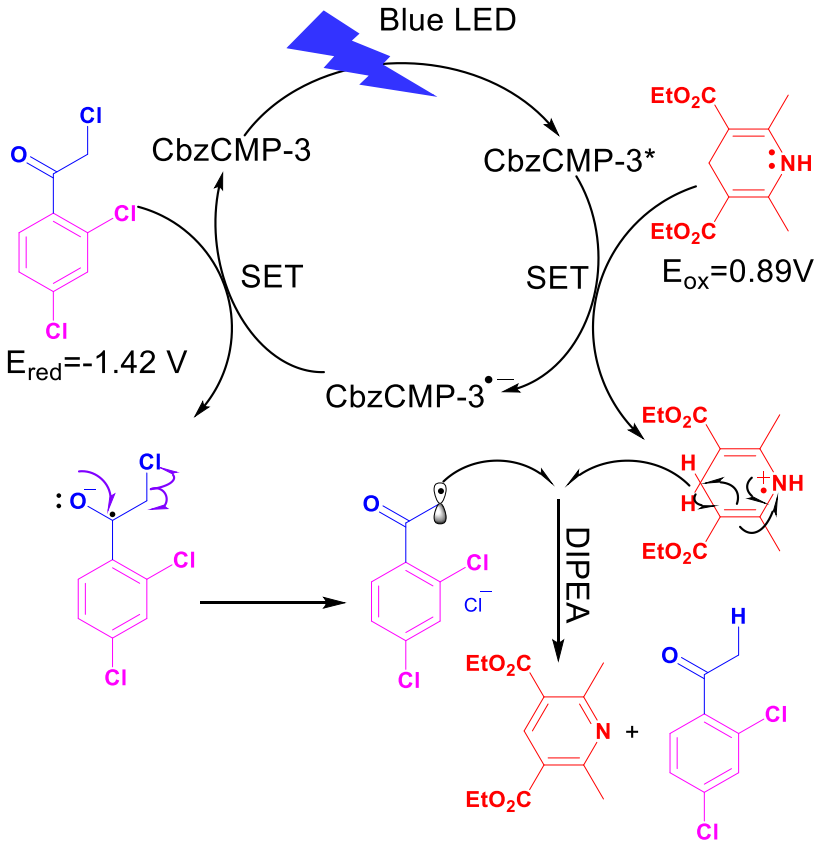


Fig. S13. Possible mechanism for photocatalytic reductive dehalogenation of chlorides catalyzed by CbzCMP-3 under light

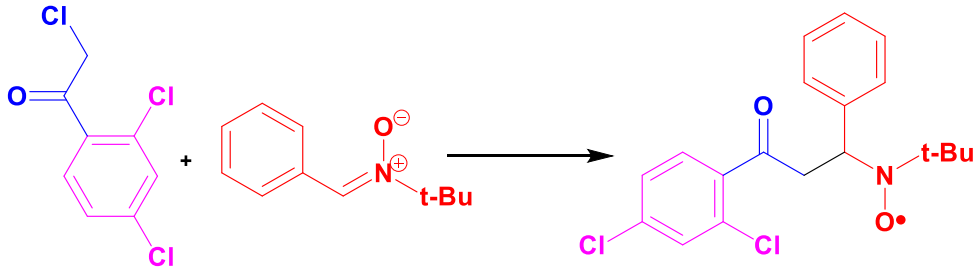


Fig.S14. The spin trapping of free radical photoinduced by CbzCMP-3 under light

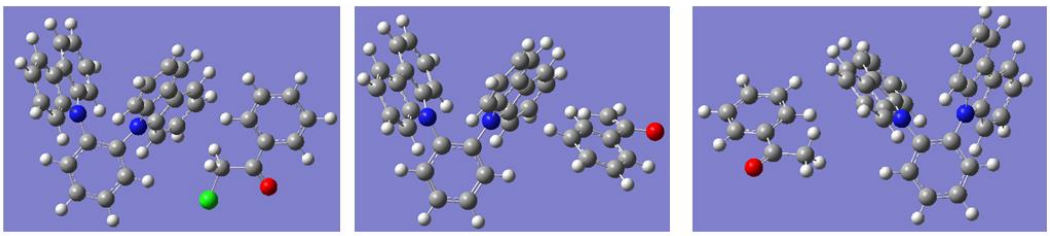


Fig. S15. Binding site locations of 2-chloro-1-phenylethan-1-one, α-carbonyl radicals and acetophenone in CbzCMP-1

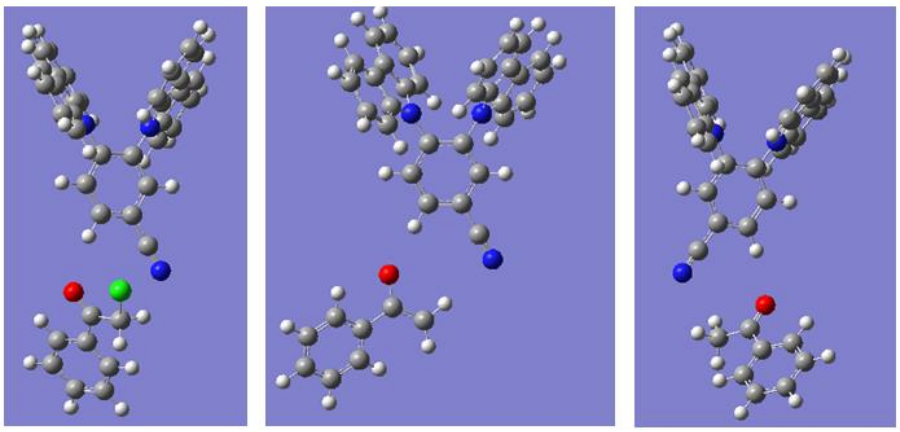


Fig.e S16. Binding site locations of 2-chloro-1-phenylethan-1-one, α-carbonyl radicals and acetophenone in CbzCMP-2

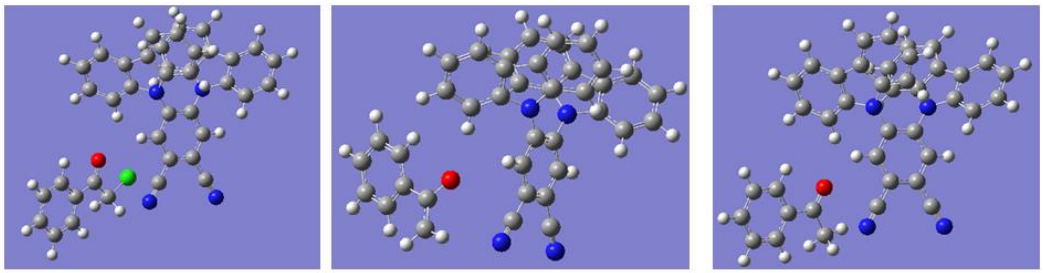


Fig. S17. Binding site locations of 2-chloro-1-phenylethan-1-one, α-carbonyl radicals and acetophenone in CbzCMP-3

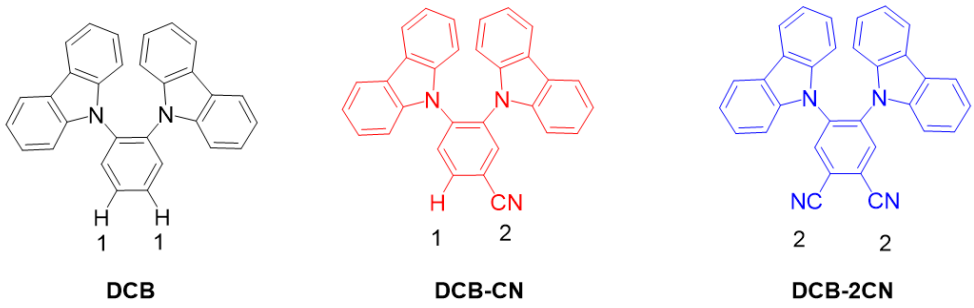


Fig. S18. Two possible binding sites on the molecular unit (DCB, DCB-CN and DCB-2CN)

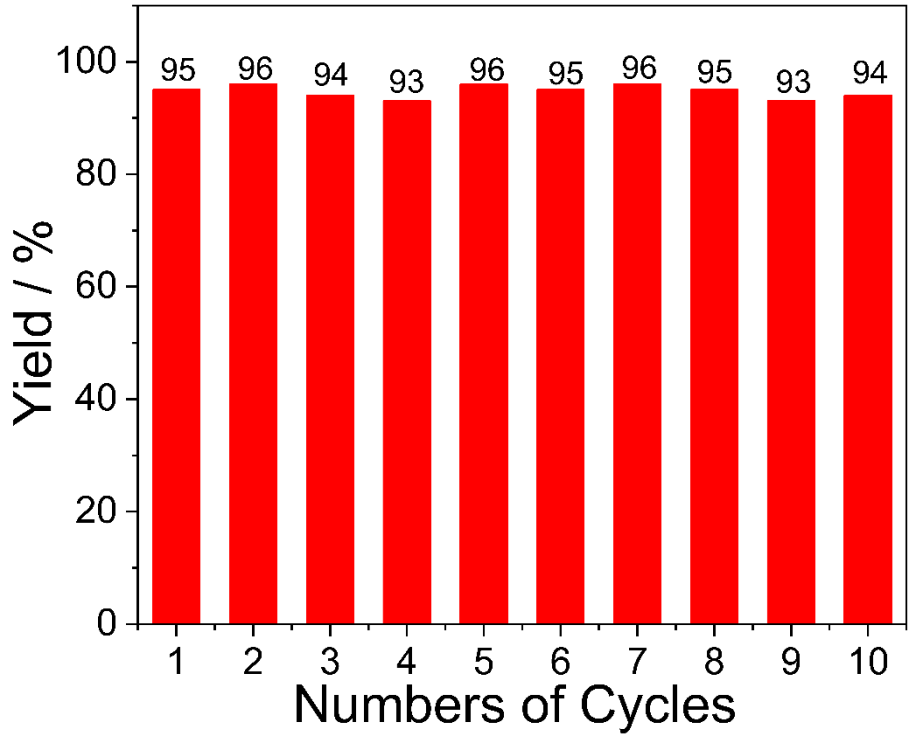


Fig. S19. Recyclability tests of CbzCMP-3 in reductive dehalogenation of 2-chloro-1-phenylethan-1-one

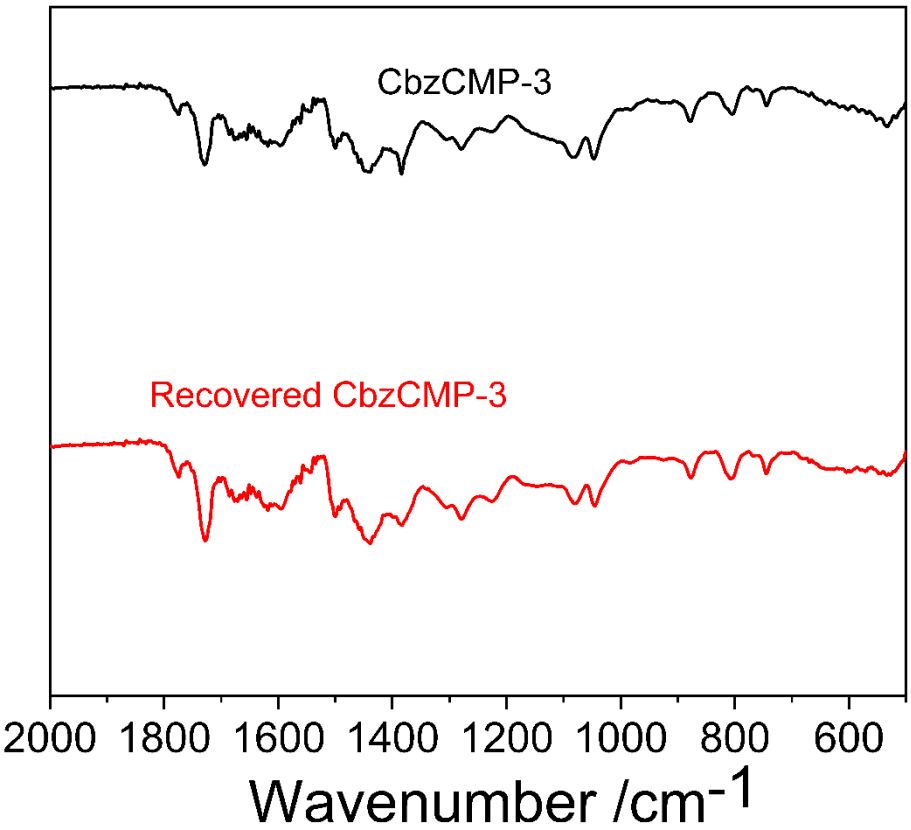


Fig. S20. FT-IR spectra of CbzCMP-3 and recovered CbzCMP-3 after ten cycles

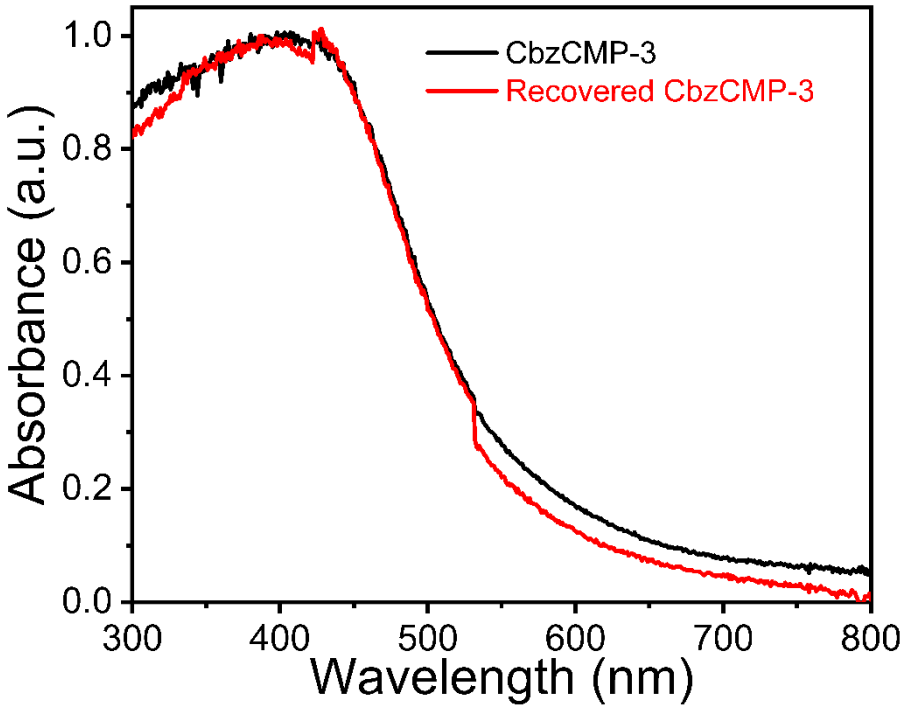


Fig.S21. UV/vis DRS spectra of CbzCMP-3 and recovered CbzCMP-3 after ten cycles

References

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S2. Q. L. Wei, S. S. Zhang, J. Gao, W. hua Li, L. Z. Xu and Z. G. Yu, Bioorganic Med. Chem., 2006, 14, 7146–7153.

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S4. Y. Wang, G. L. V. Damu, J. S. Lv, R. X. Geng, D. C. Yang and C. H. Zhou, Bioorganic Med. Chem. Lett., 2012, 22, 5363–5366.

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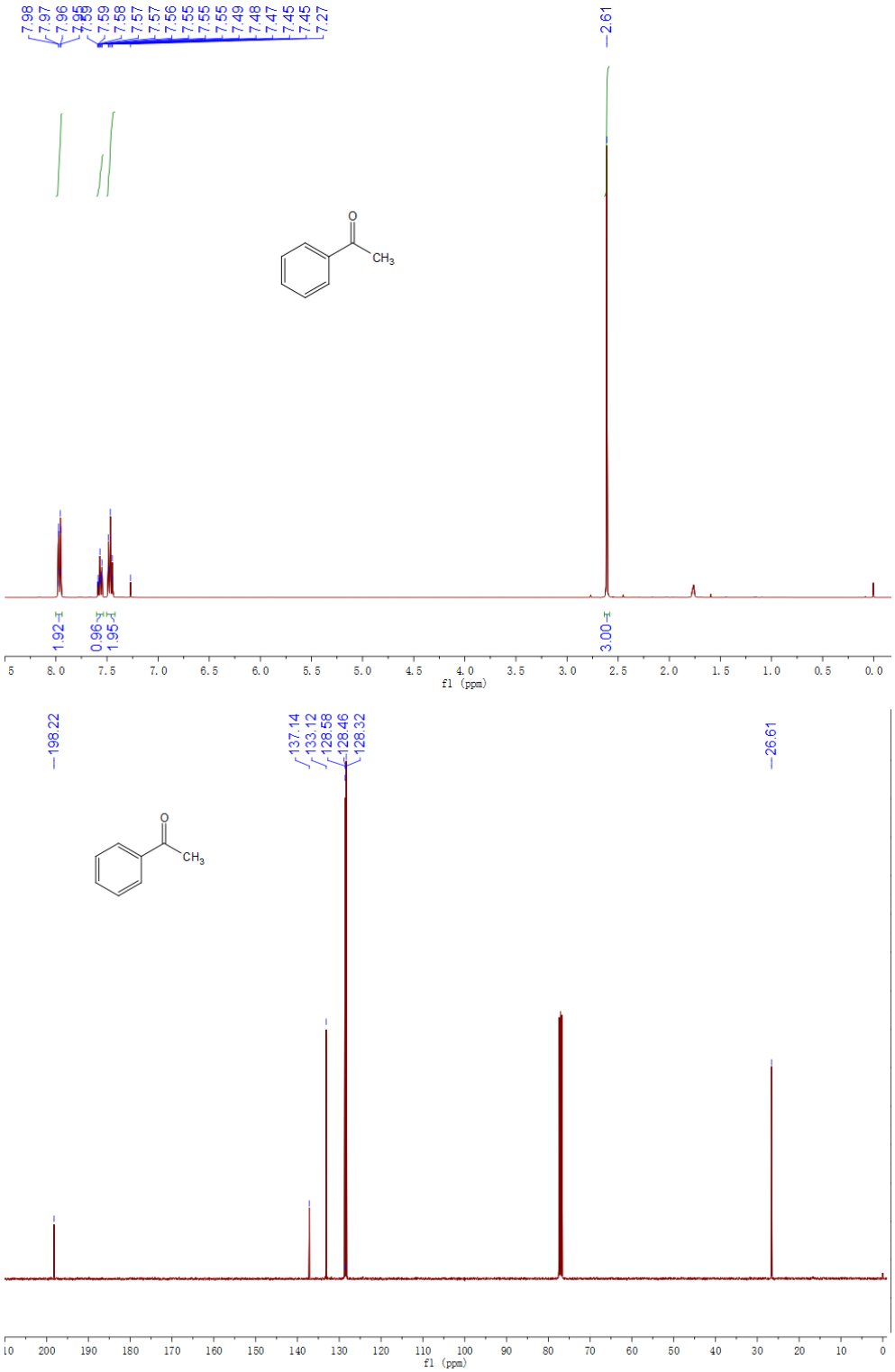
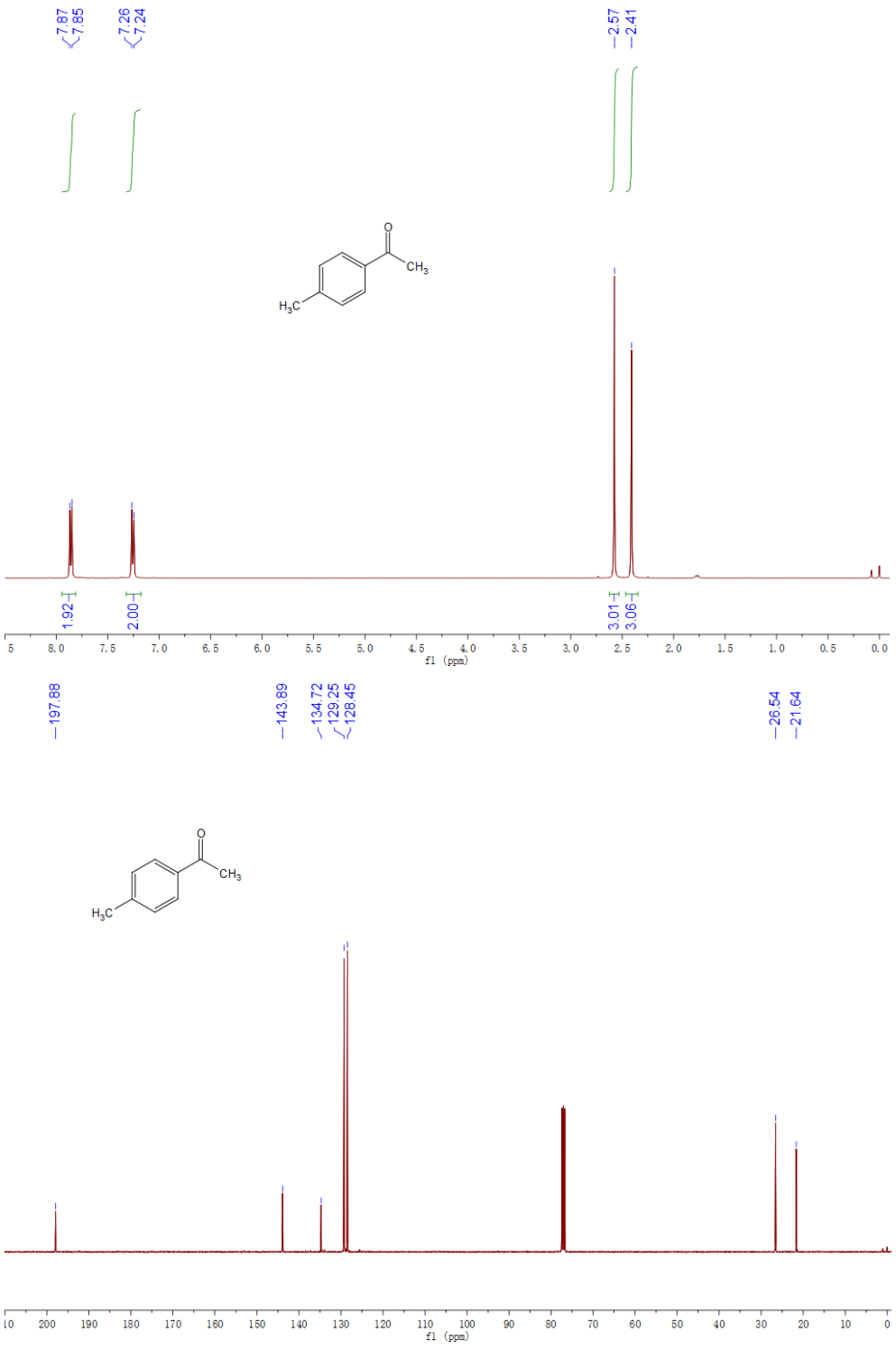
S6. C. Gu, N. Huang, J. Gao, F. Xu, Y. Xu and D. Jiang, *Angew. Chemie Int. Ed.*, 2014, **53**, 4850–4855.

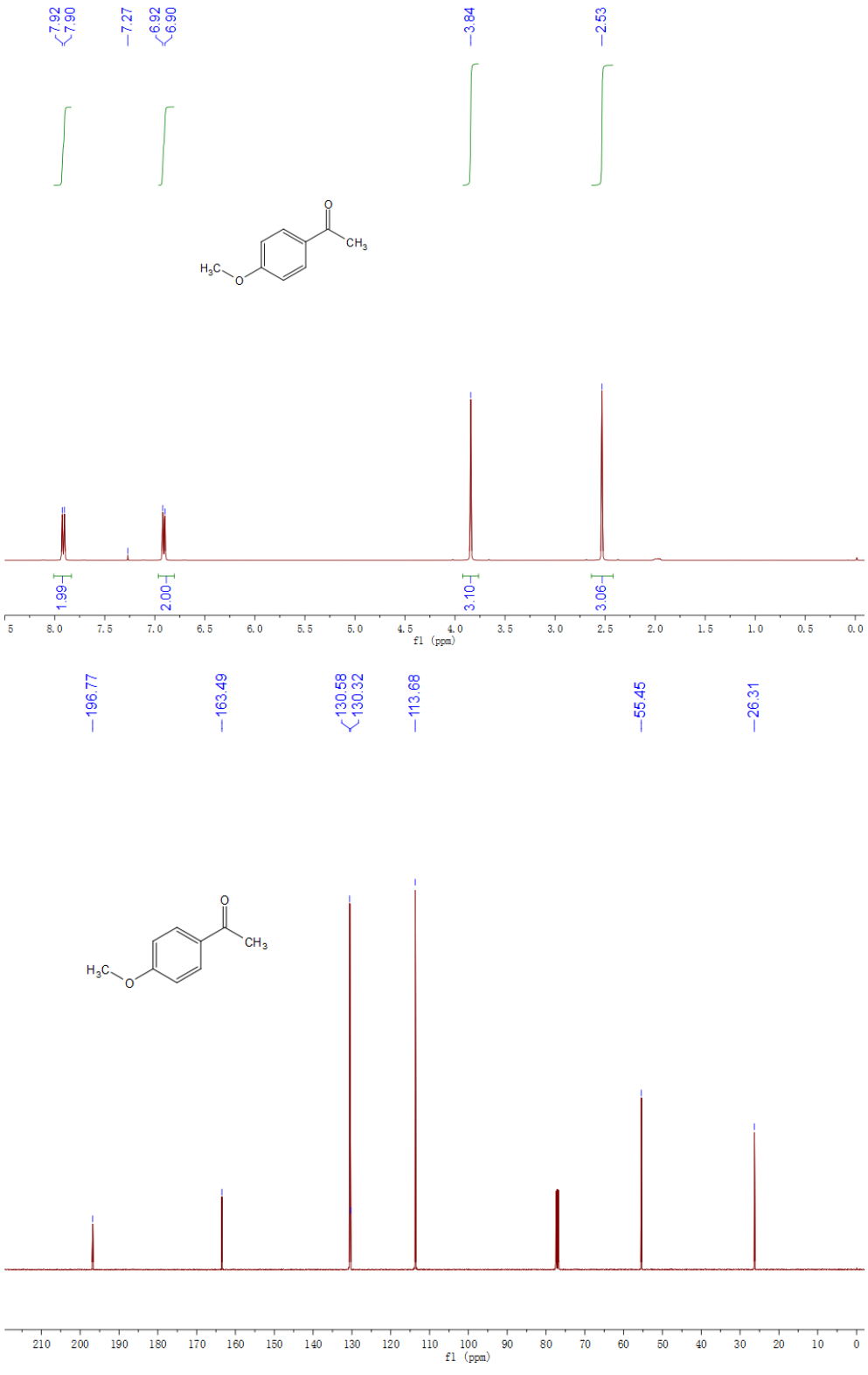
4. ^{1}HNMR and ^{13}CNMR spectra



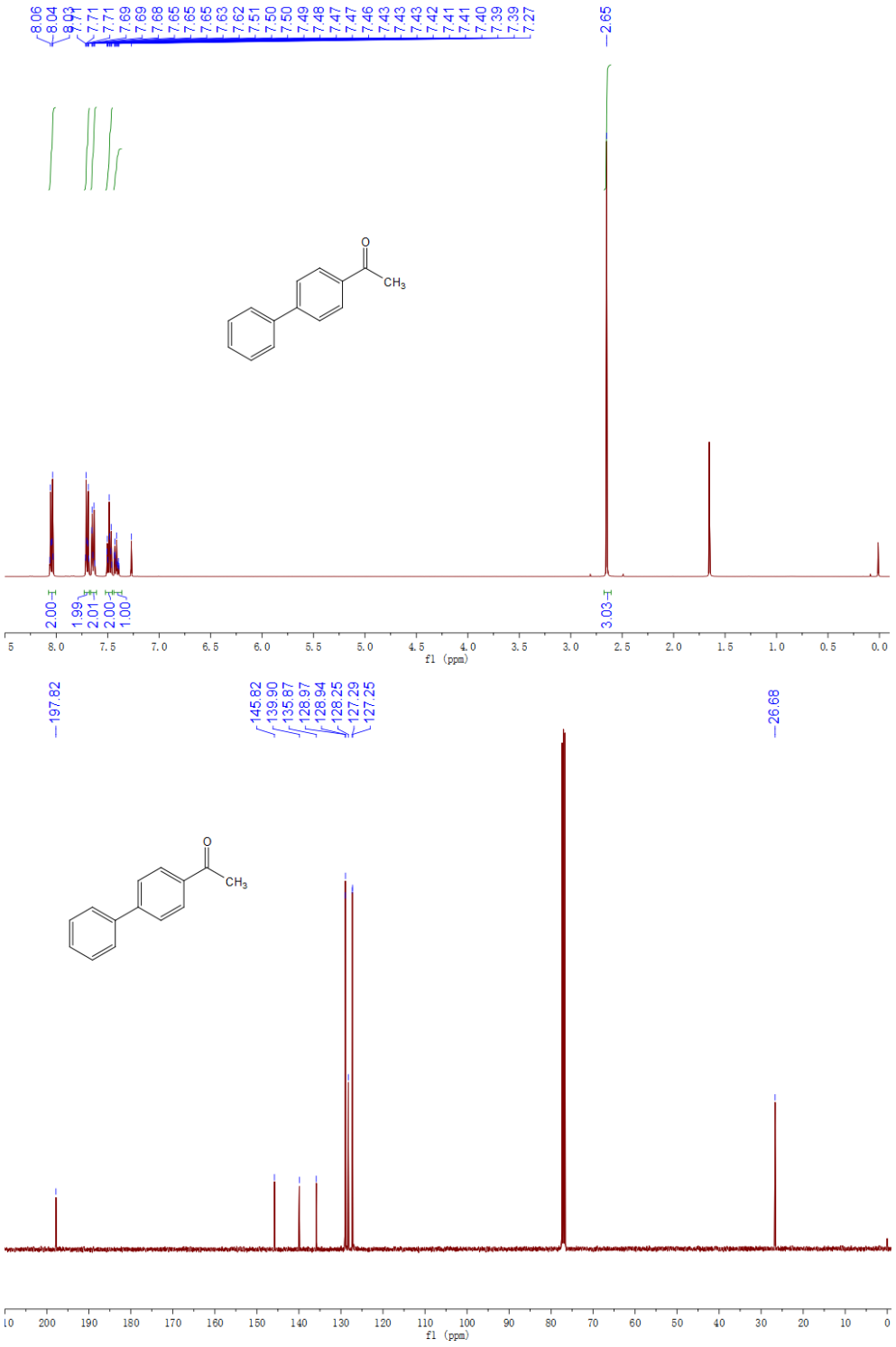
Acetophenone: ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.98-7.95 (m, 2H), 7.59-7.55 (m, 1H), 7.49-7.450 (m, 2H), 2.61 (s, 3H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ 198.2, 137.1, 133.1, 128.6, 128.3, 26.6 ppm.



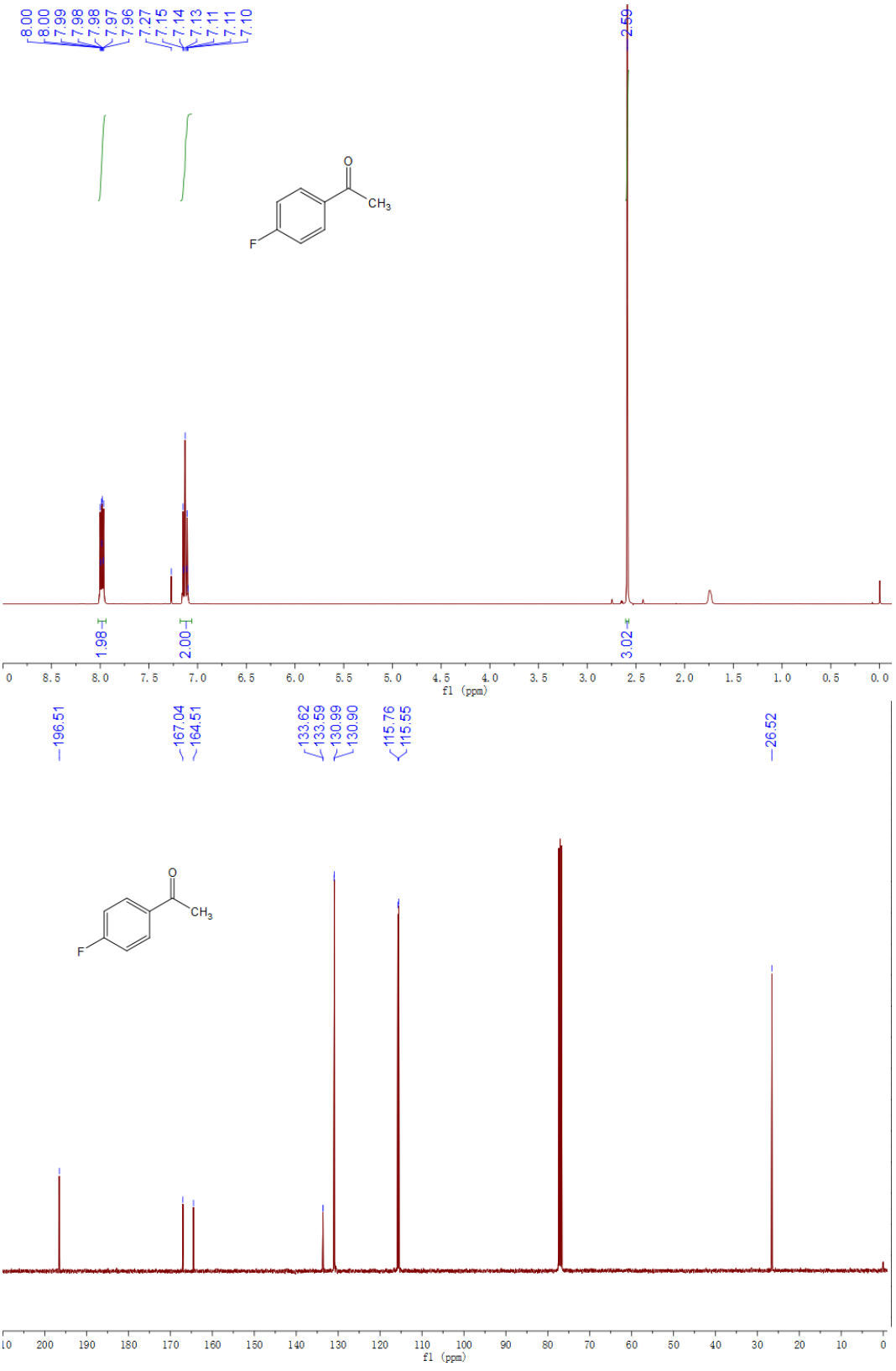
1-(p-tolyl)ethan-1-one: ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.86 (d, J = 8 Hz, 2H), 7.25 (d, J = 8 Hz, 2H), 2.57 (s, 3H), 2.41 (s, 3H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ 197.9, 143.9, 134.7, 129.2, 128.4, 26.5, 21.6 ppm.



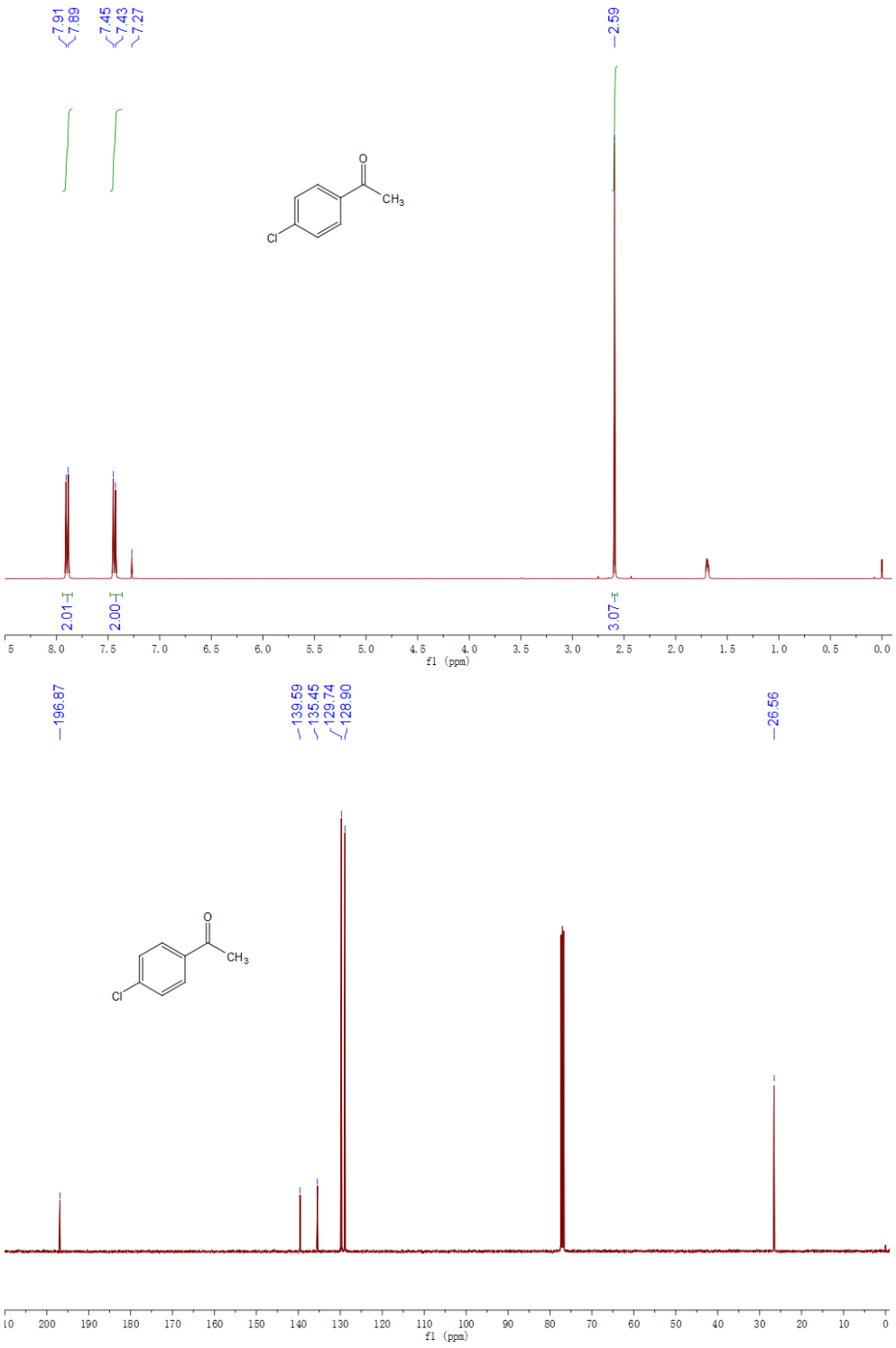
4-Methoxyacetophenone: ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.91 (d, J = 8 Hz, 2H), 6.91 (d, J = 8 Hz, 2H), 3.84 (s, 3H), 2.53 (s, 3H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ 196.8, 163.5, 130.6, 130.3, 113.7, 55.4, 26.3 ppm.



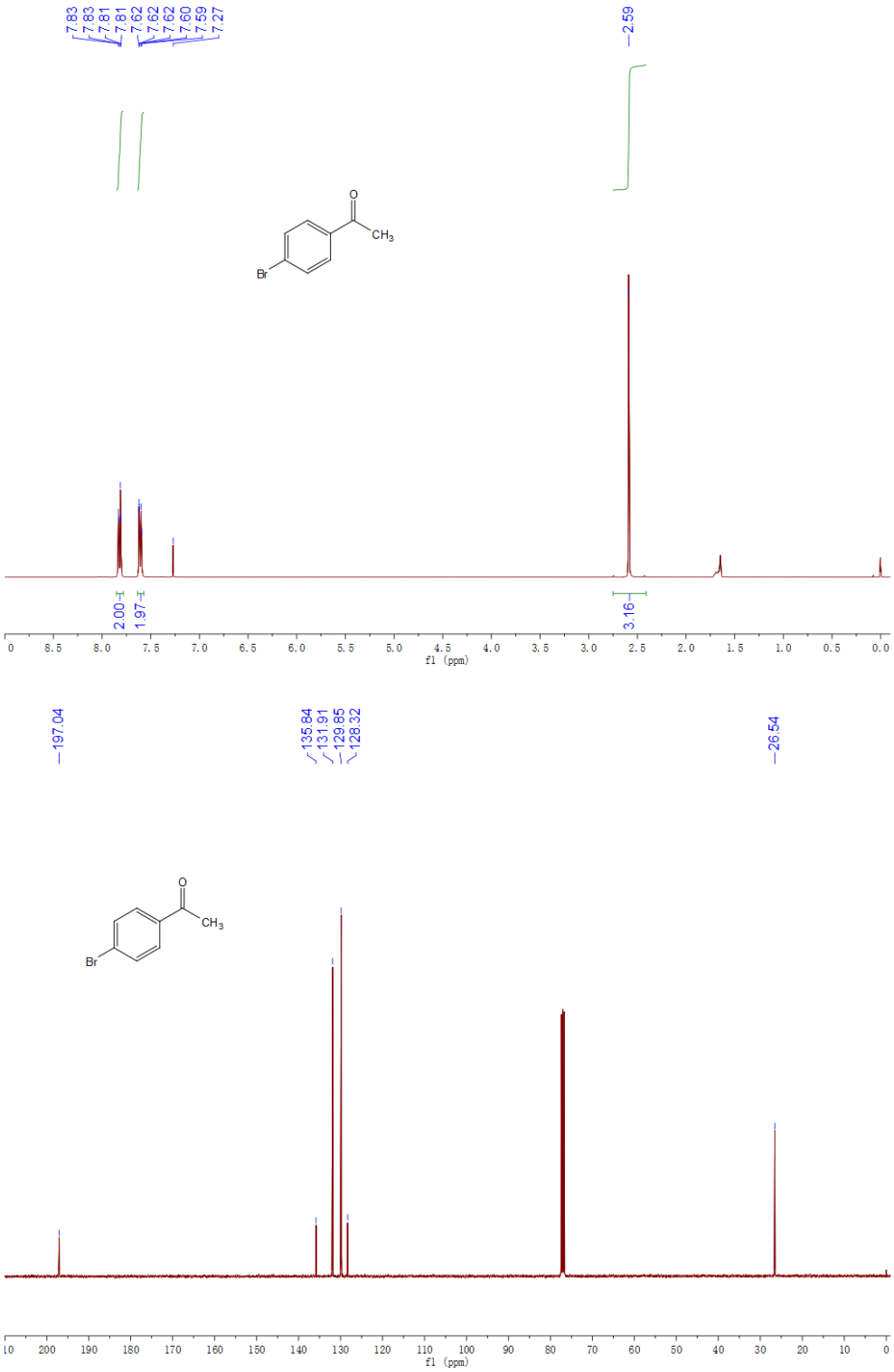
1-([1,1'-biphenyl]-4-yl)ethan-1-one: ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.06-8.03 (m , 2H),7.71-7.68 (m, 2H), 7.65-7.62 (m, 2H), 7.51-7.46 (m, 2H), 7.43-7.39 (m, 1H), 2.65 (s, 3H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ 197.8, 145.8, 139.9, 135.9, 128.97,128.94, 128.3, 127.3,127.2 26.7 ppm.



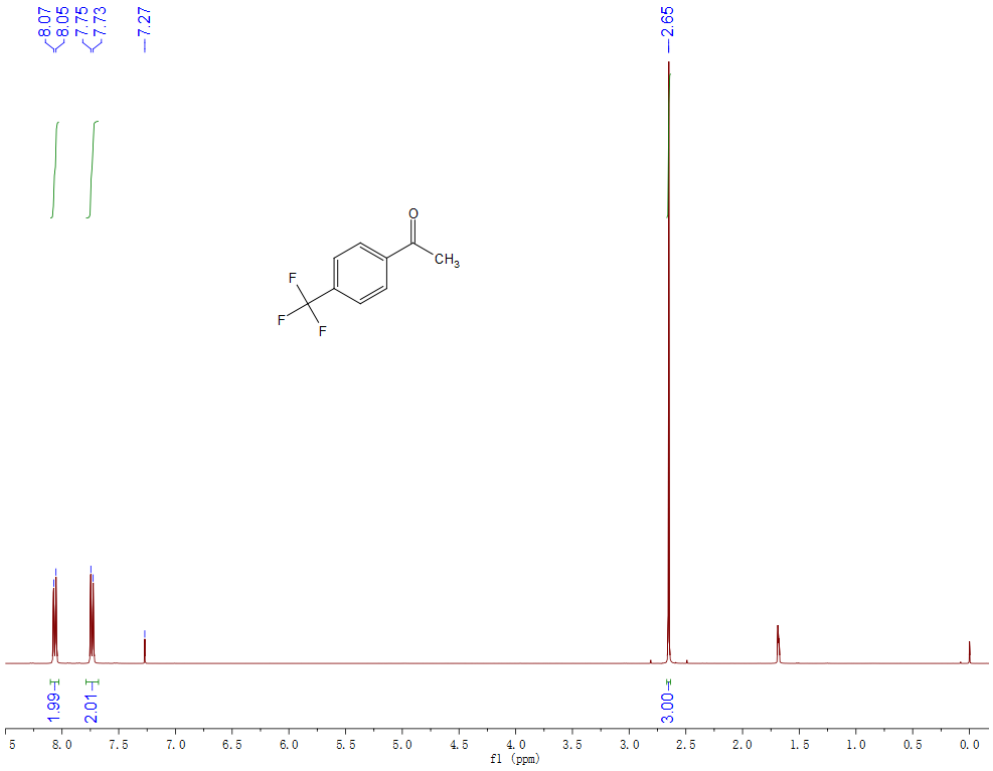
4-Fluoroacetophenone: ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.00-7.96 (m, 2H), 7.15–7.10 (m, 2H), 2.59 (s, 3H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ 196.5, 167.0,164.5, 133.6, 133.5, 130.99, 130.90, 115.8,115.6, 26.5 ppm.

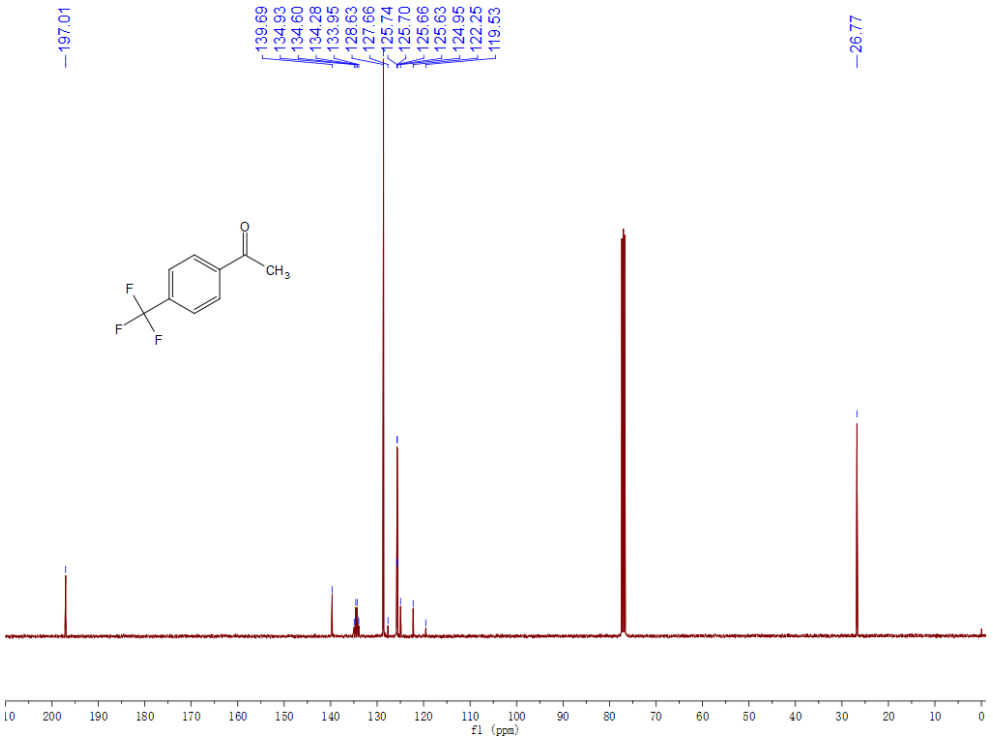


4-Chloroacetophenone: ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.90 (d, J = 8 Hz, 2H), 7.44 (d, J = 8 Hz, 2H), 2.59 (s, 3H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ 196.8, 139.6, 135.5, 129.7, 128.9, 25.6 ppm.

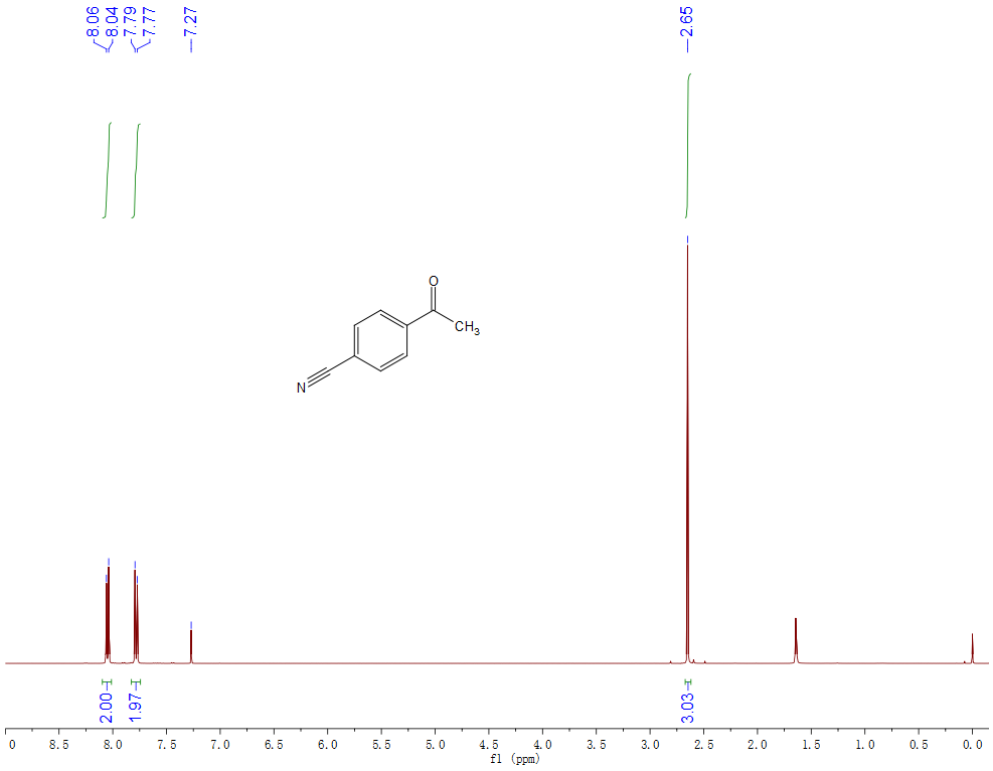


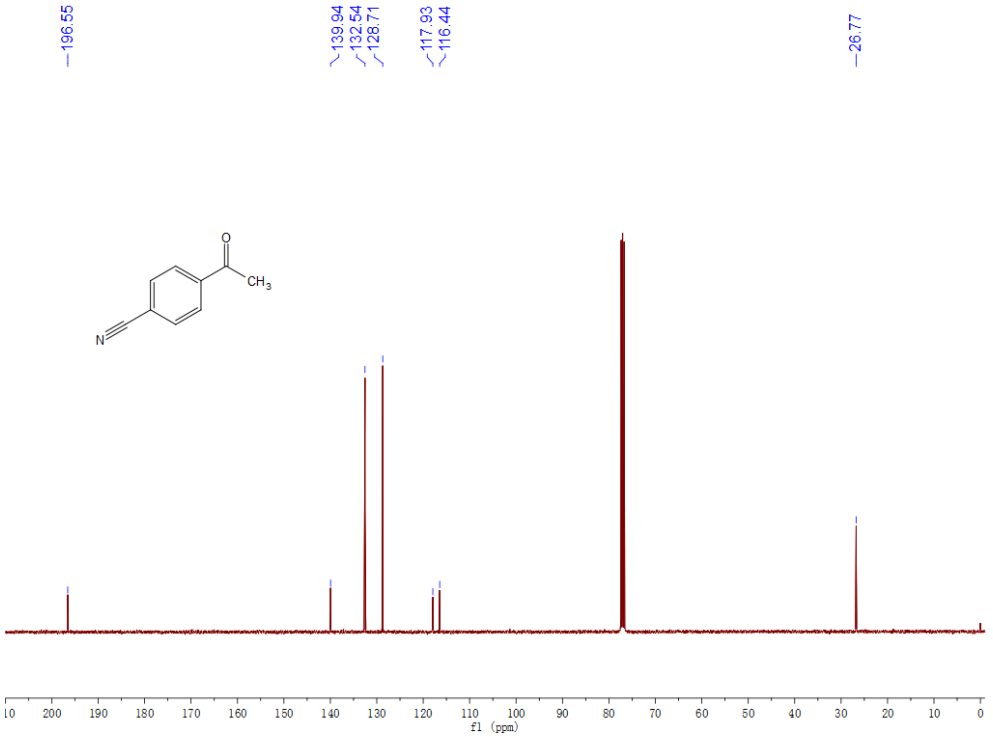
4-Bromoacetophenone: ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.82 (d, J = 8 Hz, 2H), 7.61(d, J = 8 Hz, 2H), 2.57 (s, 3H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ 197.0, 135.8, 131.9, 129.8, 128.3, 26.5 ppm.



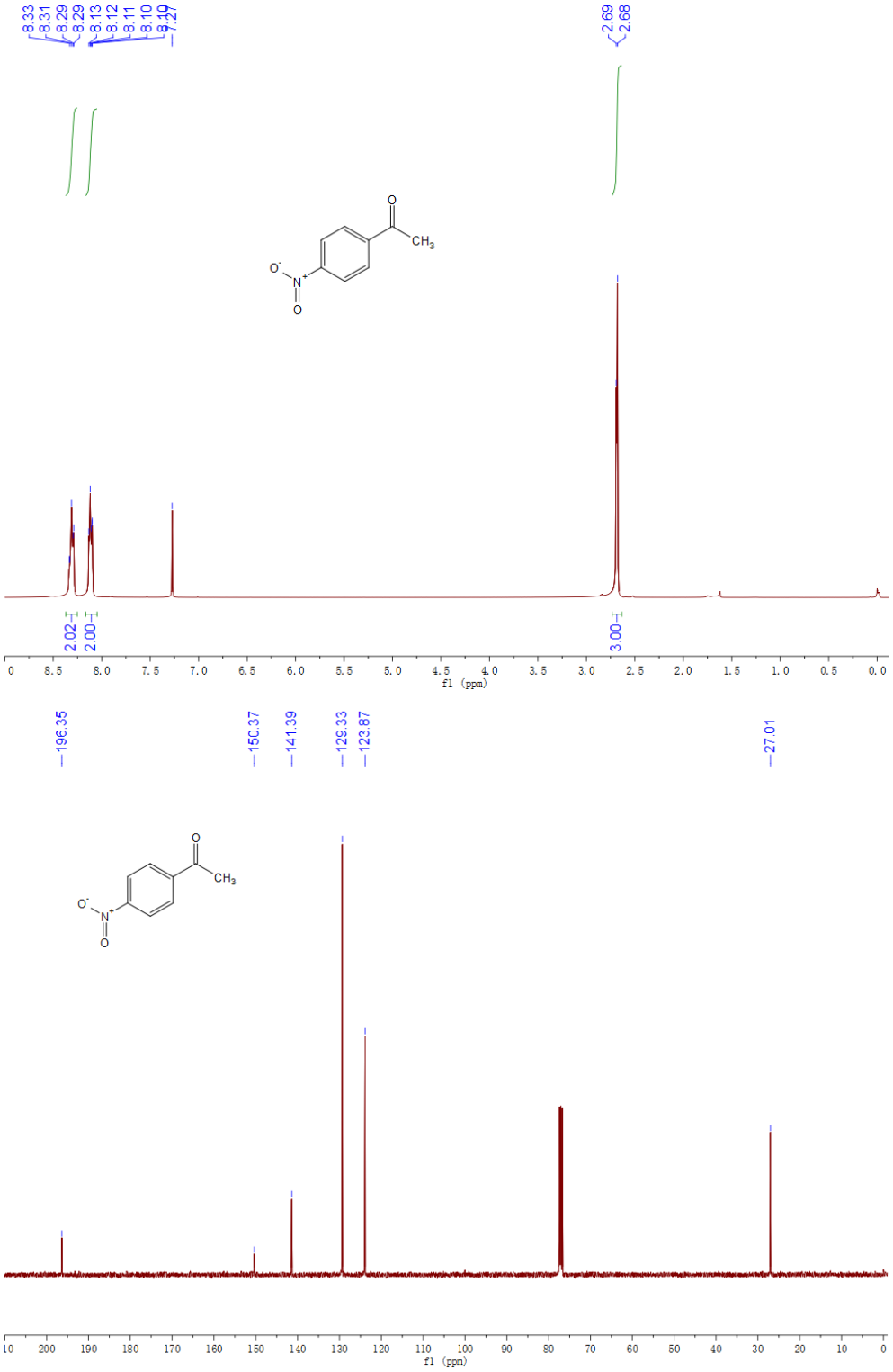


1-(4-(trifluoromethyl)phenyl)ethan-1-one: ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.06 (d, J = 8 Hz, 2H), 7.74(d, J = 8 Hz, 2H), 2.65 (s, 3H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ 197.0, 139.7, 134.9-133.9 (m), 128.6, 127.7, 125.7-14.9(m), 124.9,122.2, 119.5, 26.8 ppm.

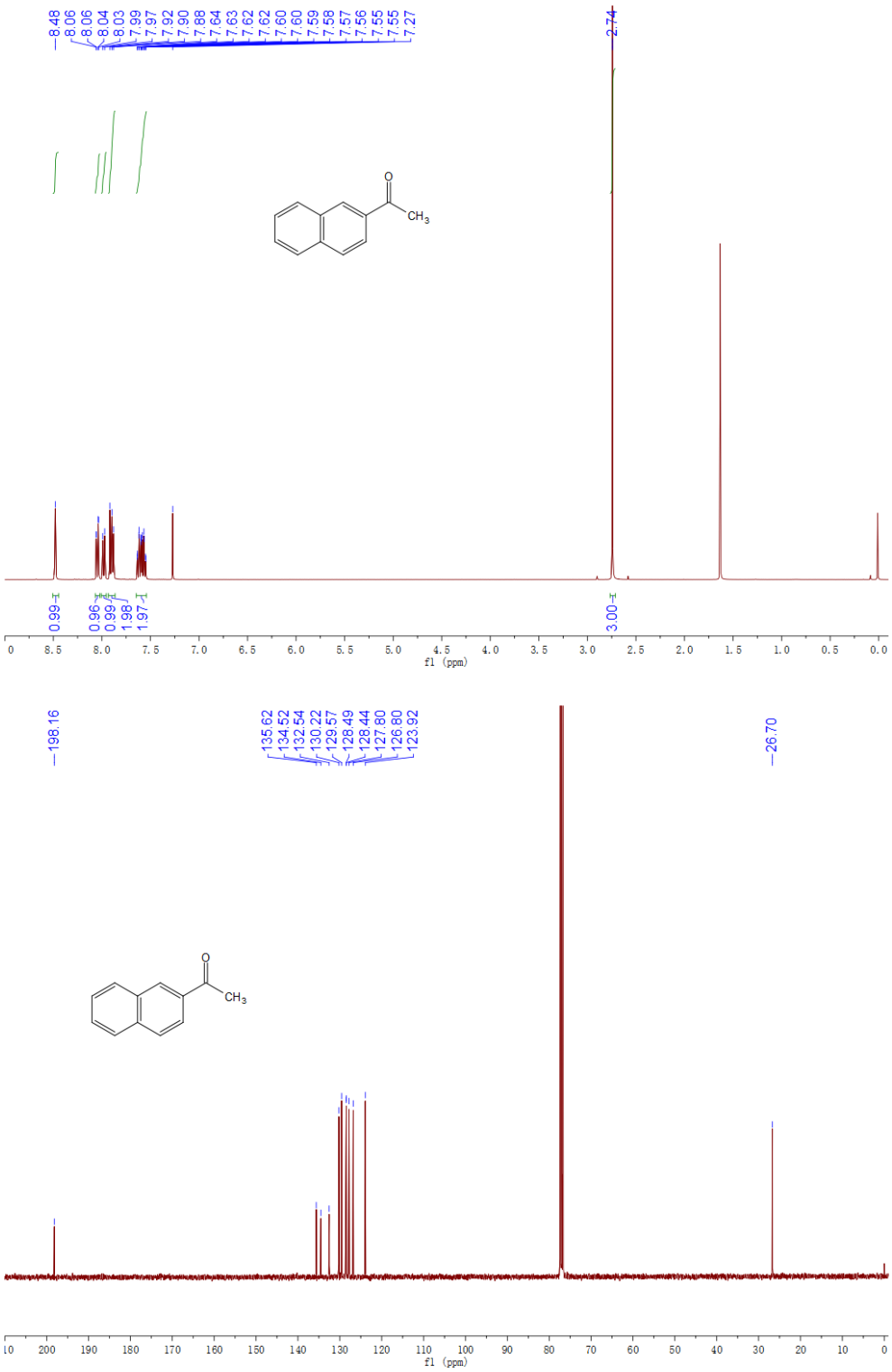




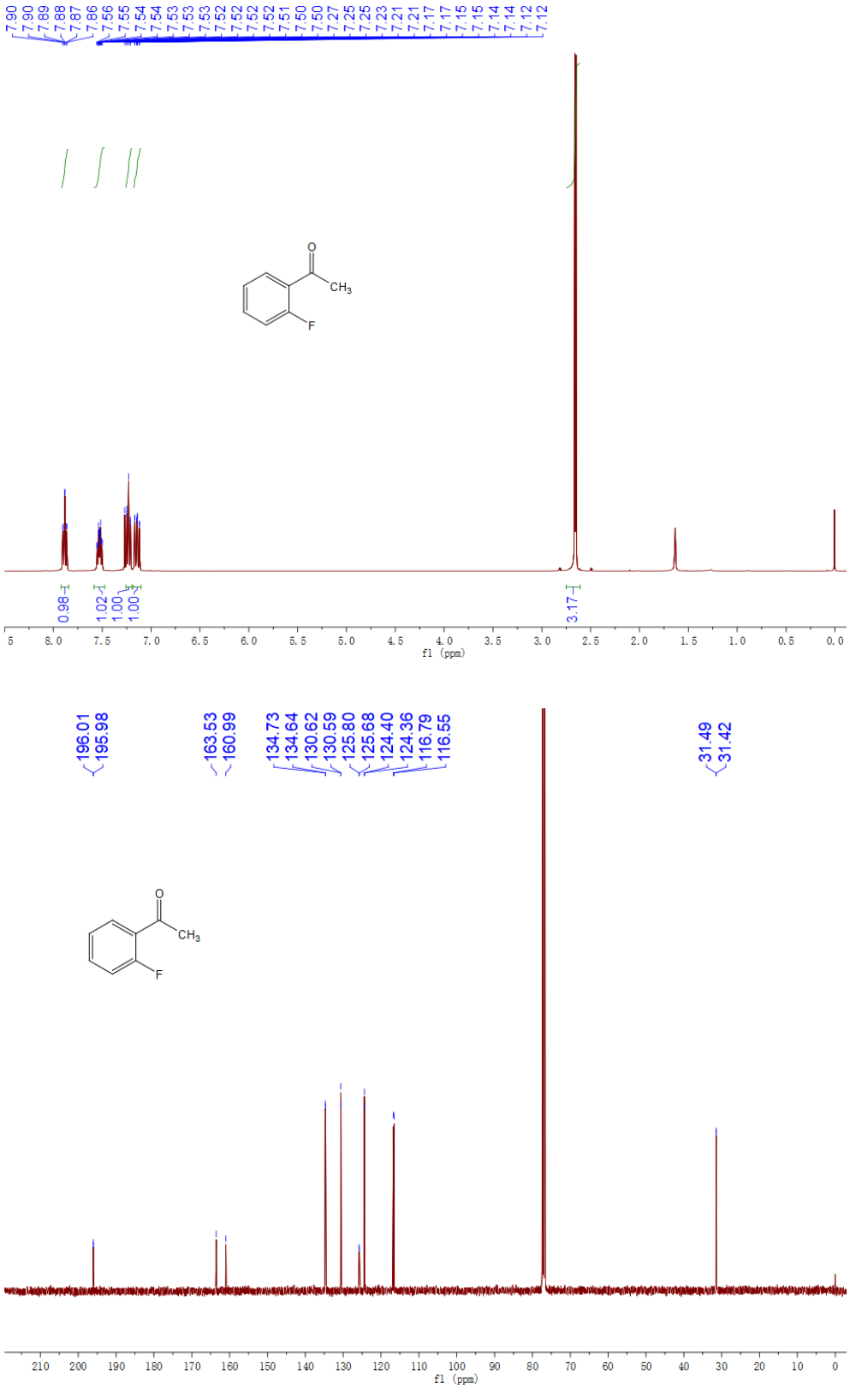
4-Acetylbenzonitrile: ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.05 (d, J = 8 Hz, 2H), 7.78 (d, J = 8 Hz, 2H), 2.65 (s, 3H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ 196.6, 139.9, 132.5, 128.7, 117.9, 116.4, 26.8 ppm.



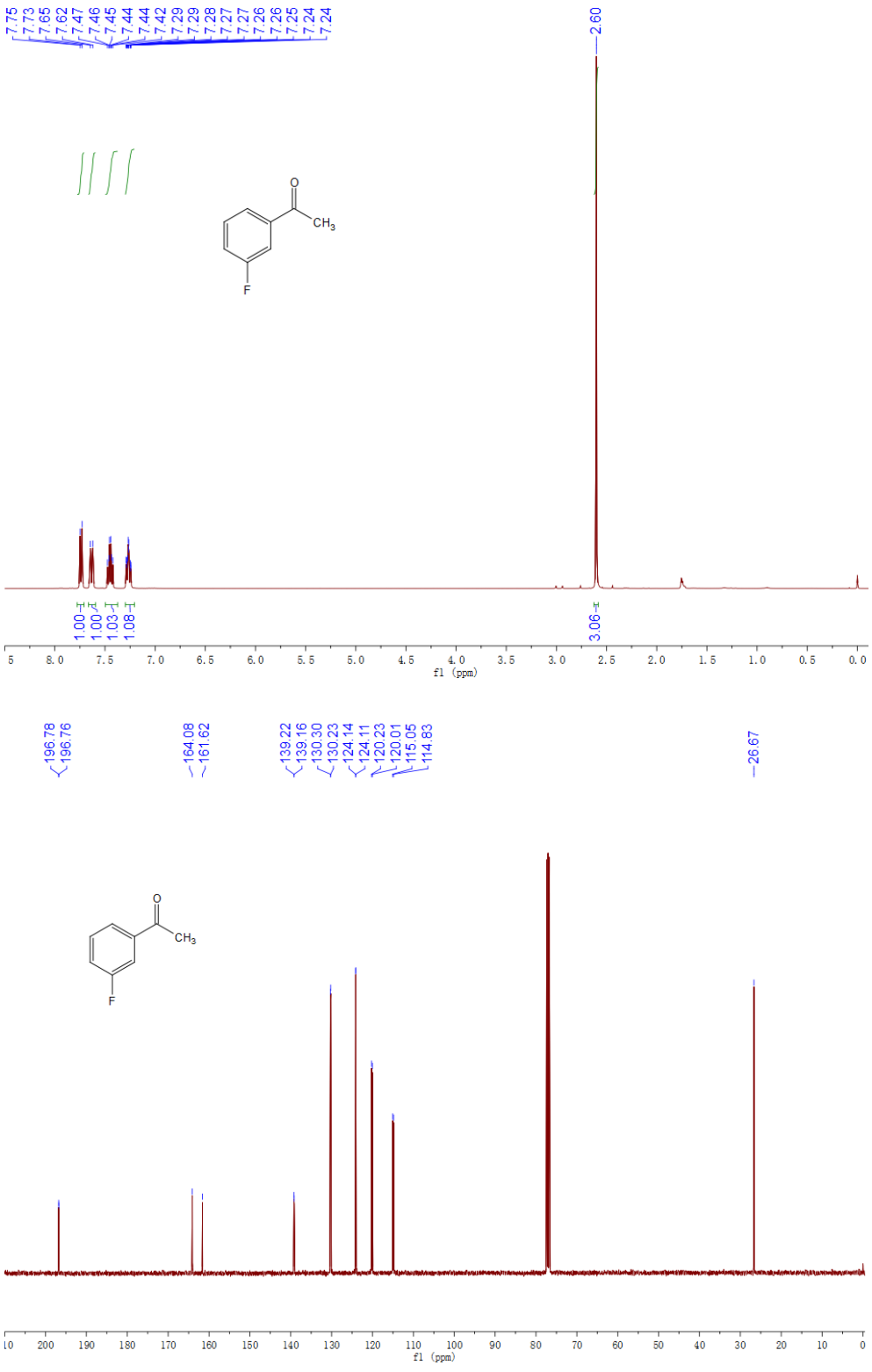
4-Nitroacetophenone: ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.31-8.29 (m, 2H), 8.13-8.10 (m, 2H), 2.68 (s, 3H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ 196.3, 150.4, 141.4, 129.3, 123.9, 27.0 ppm.



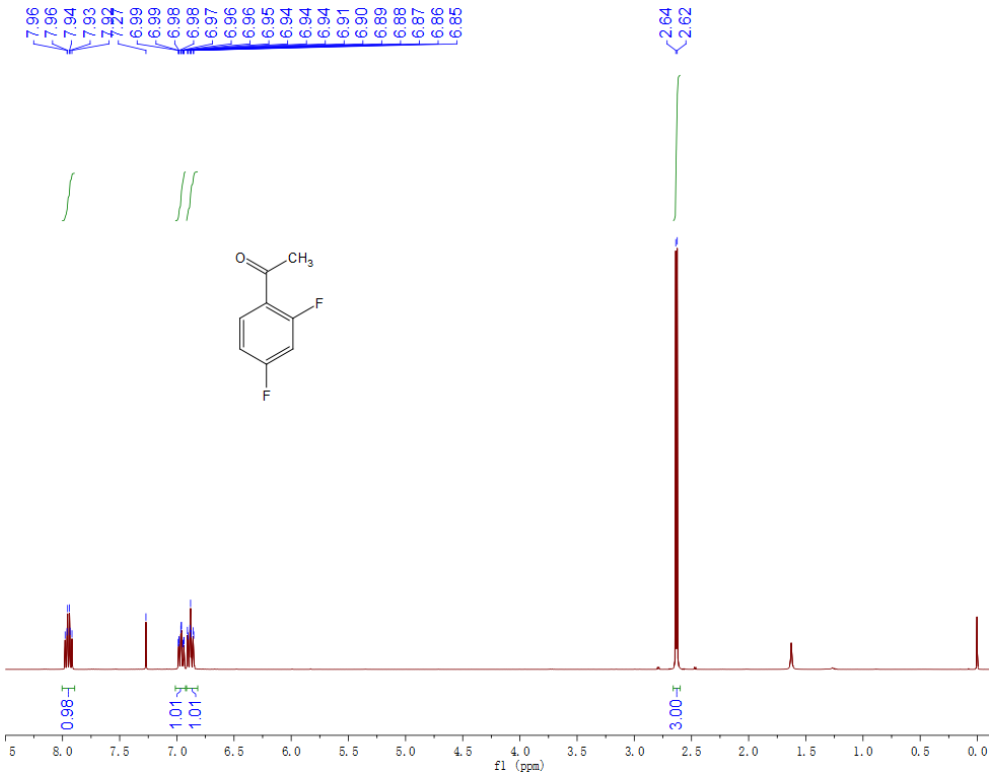
1-(naphthalen-2-yl)ethan-1-one: ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.48 (s, 1H), 8.06-8.03 (dd, J = 8 Hz, 2H), 7.98 (d, J = 8 Hz, 1H), 7.92-7.88(t, J = 8 Hz, 2H), 7.64-7.55 (m, 2H) 2.74 (s, 3H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ 198.2, 135.6, 134.5, 132.5, 130.2, 129.6, 128.5, 128.4, 127.8, 126.8, 123.9, 26.7 ppm.



1-(2-fluorophenyl)ethan-1-one: ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.90-7.86 (m, 1H), 7.56-7.50 (m, 1H), 7.25-7.21 (m, 1H), 7.17-7.14 (m , 1H), 2.65 (d, 3H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ 196.0, 195.9,163.5,161.0, 134.7, 134.6, 130.6, 130.5, 125.8, 125.7, 124.4, 124.3, 116.8, 116.5, 31.5, 31.4.



1-(3-fluorophenyl)ethan-1-one: ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.75-7.73 (d, J = 8 Hz, 1H), 7.65-7.62 (d, J = 12 Hz, 1H), 7.47-7.42 (m, 1H), 7.29-7.24(m , 1H), 2.60 (d, 3H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ 196.78, 196.76, 164.08, 161.62, 139.22, 139.16, 130.30, 130.23,124.14,124.11,120.23, 120.01, 115.05, 114.83, 26.67.


7.96
7.96
7.94
7.93
7.92
7.91
6.99
6.99
6.98
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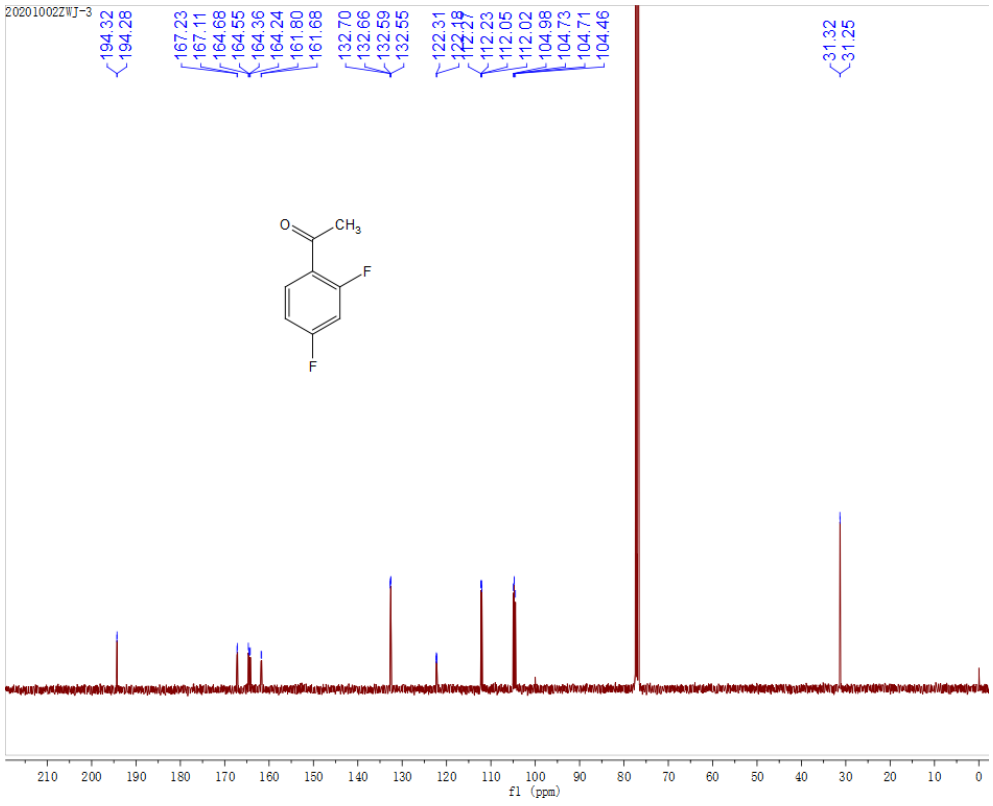
6.91
6.90
6.89
6.88
6.87
6.86
6.85
2.64
2.62
O
CH3
F
F
0.98
1.01
1.01
3.00
f1 (ppm)


20201002ZWJ-3
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167.11
164.68
164.55
164.36
164.24
161.80
161.68
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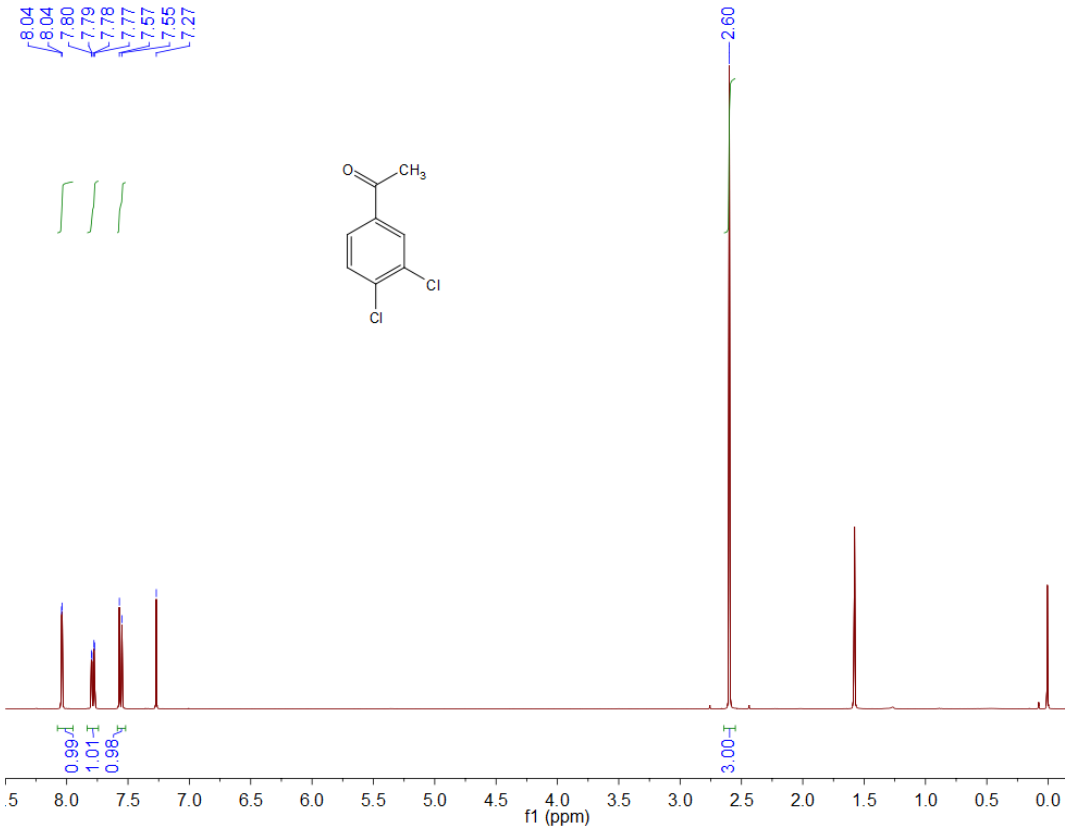
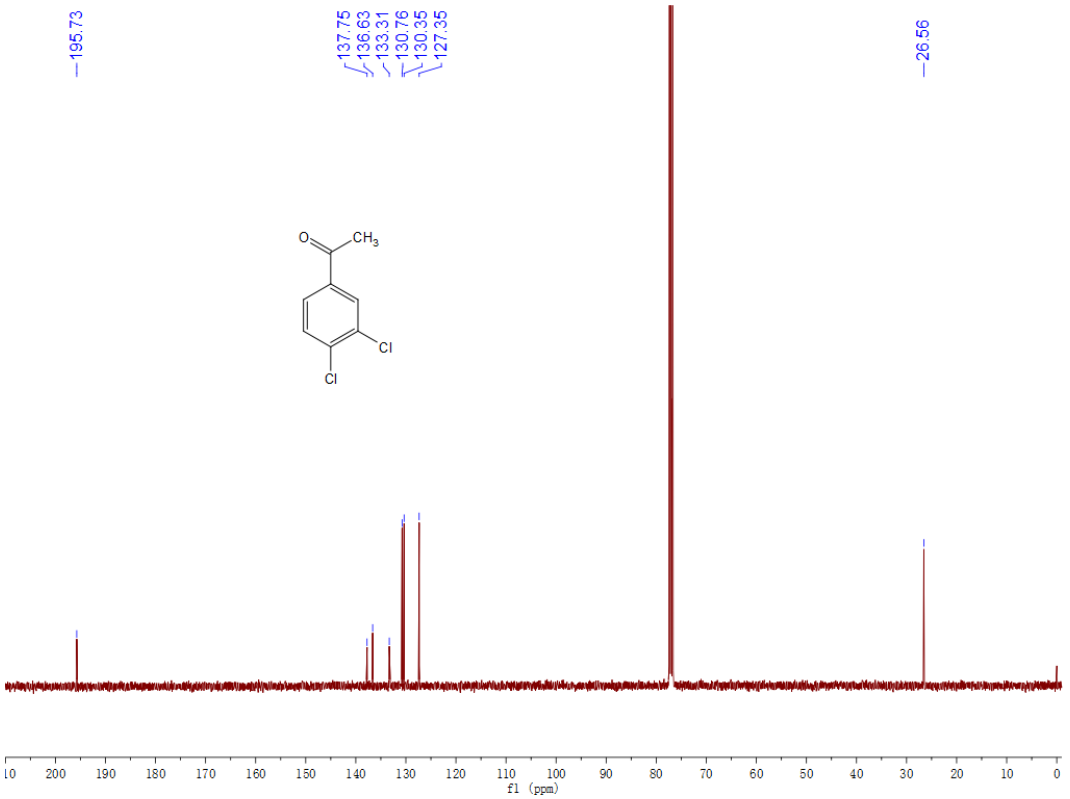
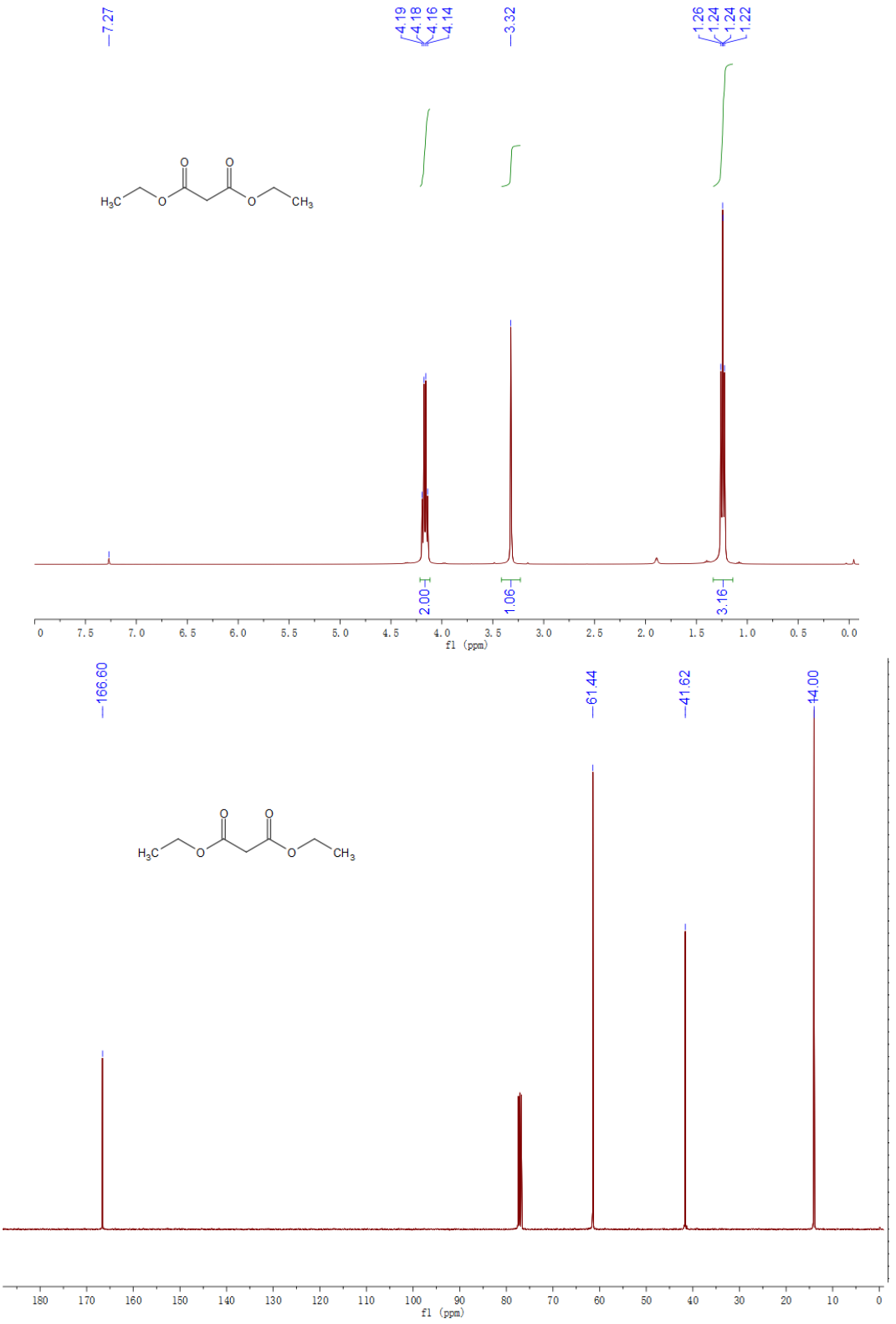
132.66
132.59
132.55
122.31
122.18
122.27
112.23
112.05
112.02
104.98
104.73
104.71
104.46
31.32
31.25
O
CH3
F
F
f1 (ppm)

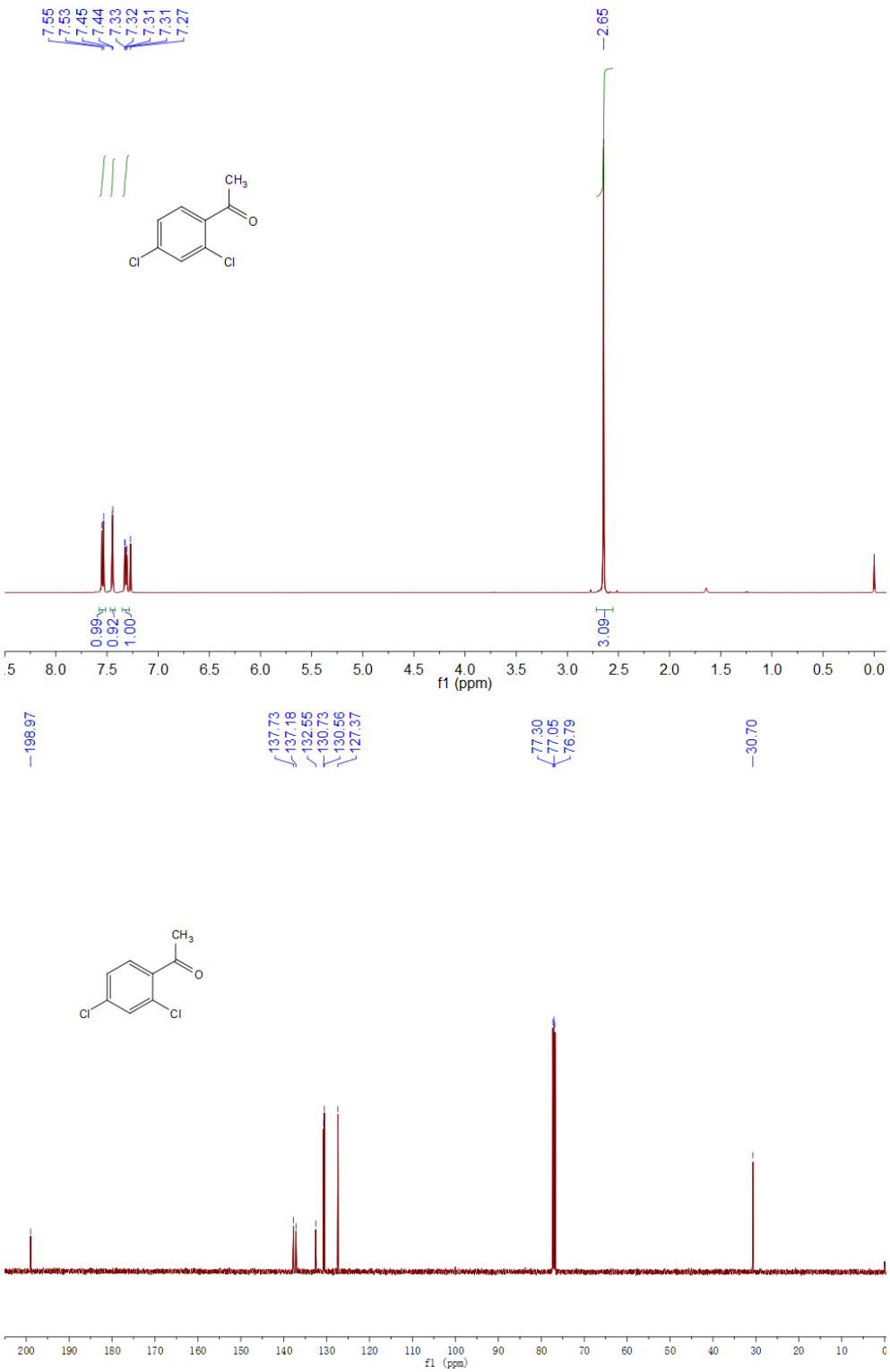




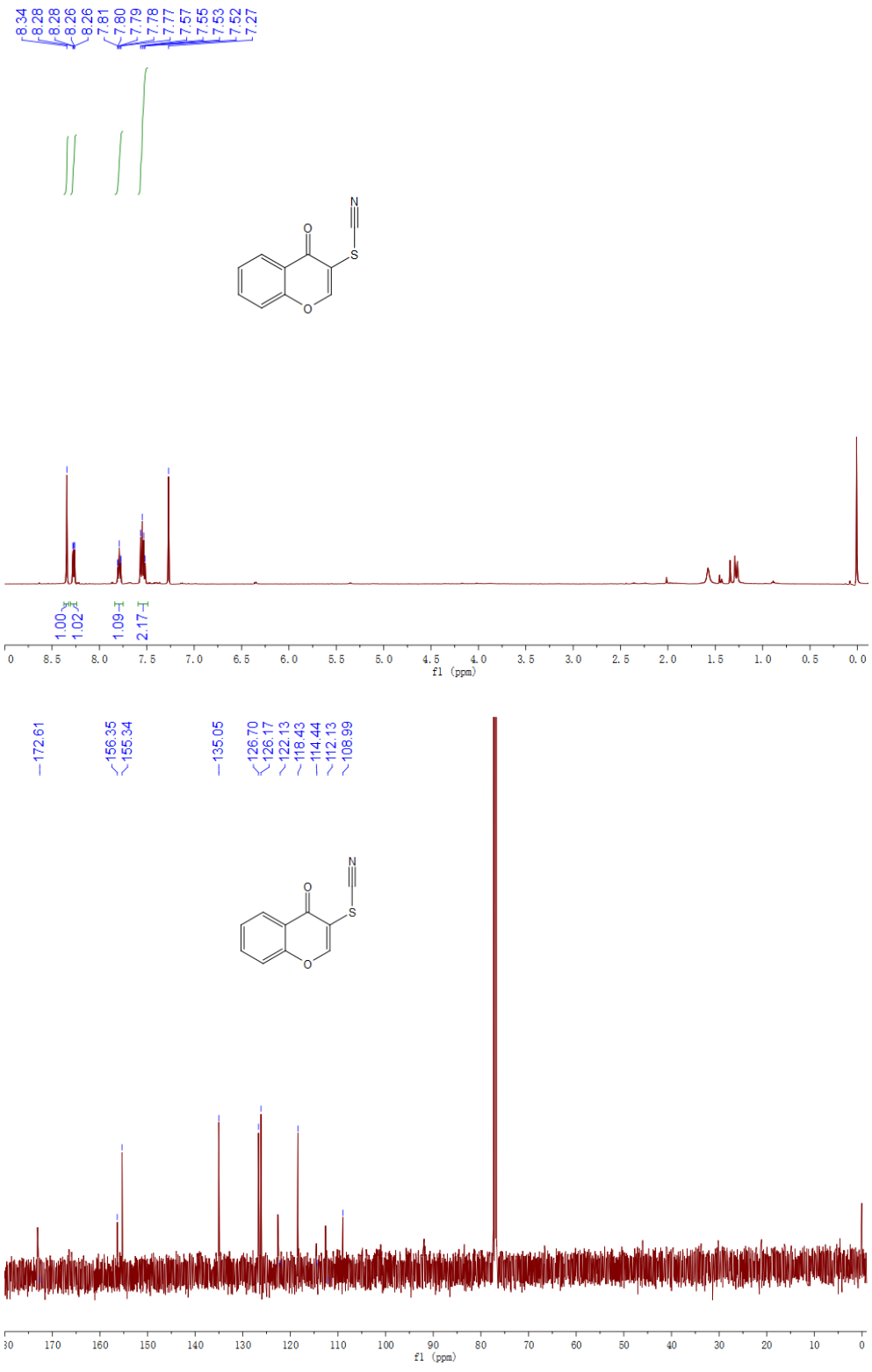
1-(3,4-dichlorophenyl)ethan-1-one: ^{1}H NMR ($CDCl_3$, 400 MHz): *δ* 8.04 (d, 1H), 7.80-7.77 (dd, *J*=4.0 Hz, 1H), 7.56 (d, d, *J*=4.0 Hz, 1H), 2.60 (s, 3H), ^{13}C NMR ($CDCl_3$, 100 MHz): *δ* 195.7, 137.8, 136.6, 133.3, 130.8, 130.3, 127.3, 26.6.



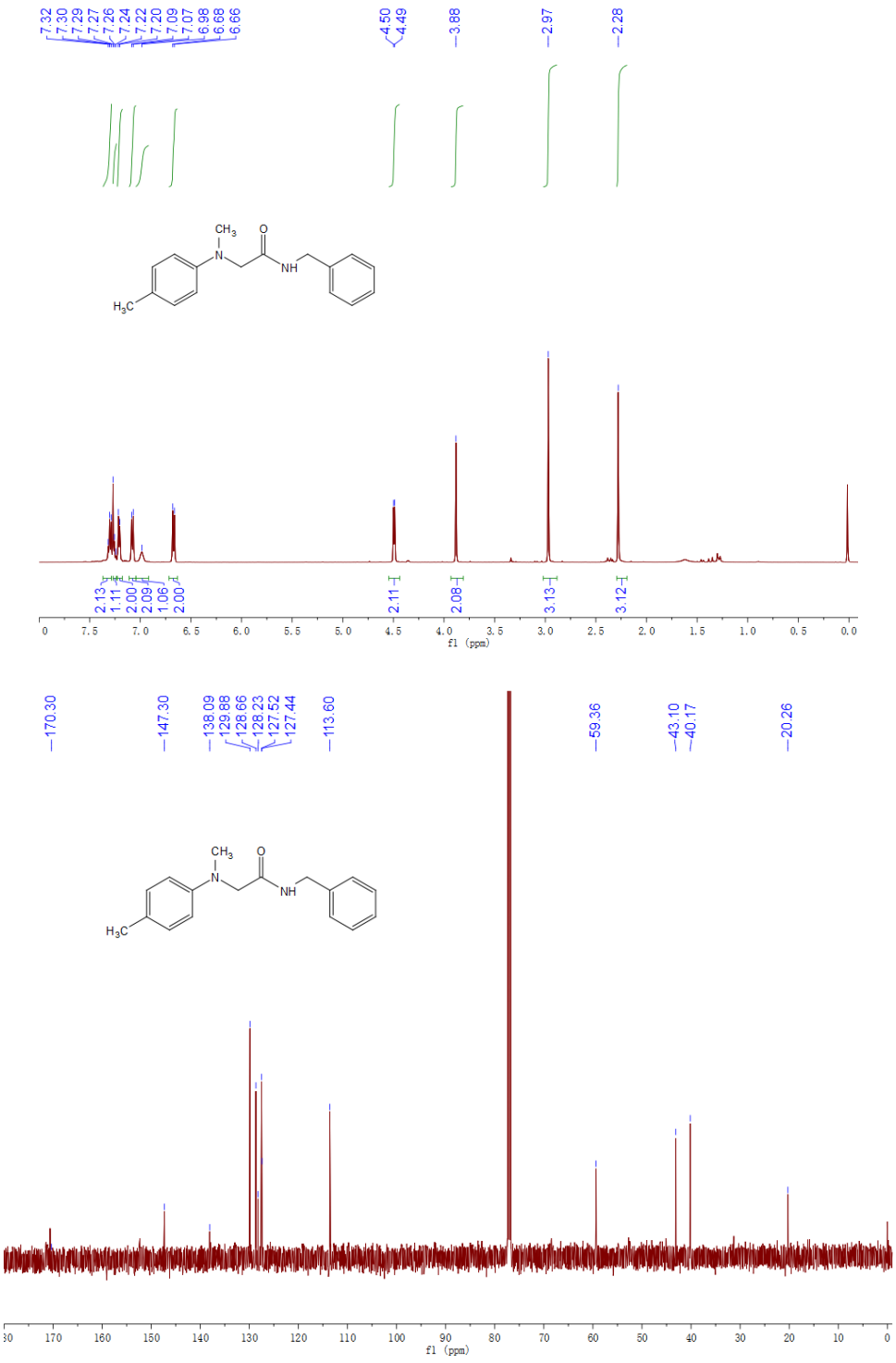
Diethyl malonate: ^{1}H NMR ($CDCl_3$, 400 MHz): δ 4.18-4.14 (q, 2H), 3.32 (s, 1H), 1.26-1.22(q, 3H), 2.60 (s, 3H), ^{13}C NMR ($CDCl_3$, 100 MHz): δ 166.6, 61.4, 41.6, 14.0.



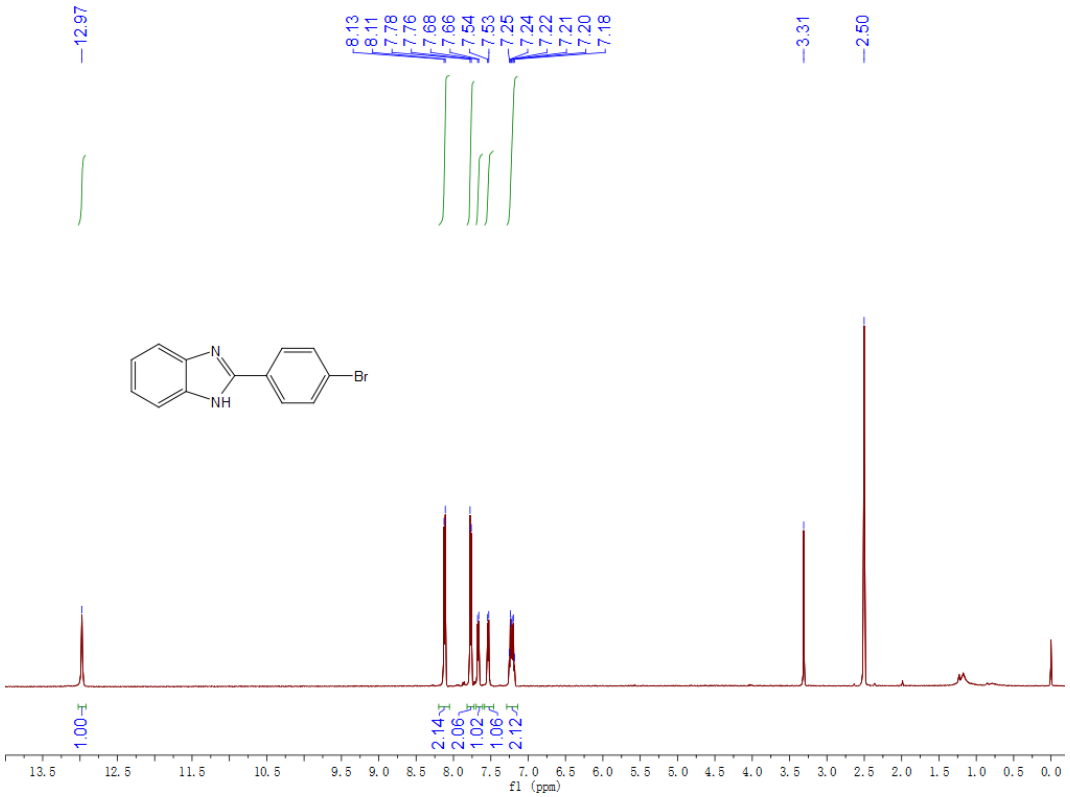
1-(2,4-dichlorophenyl)ethan-1-one: ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.54 (d, J=8.0 Hz 1H), 7.45 (d, J=4.0 Hz, 1H), 7.33-7,31 (dd, J=4.0 Hz, 1H), 2.65 (s, 3H), ^{13}C NMR ($CDCl_3$, 100 MHz): δ 198.9, 137.7,137.2,132.5, 130.7, 130.6,127.4, 30.7

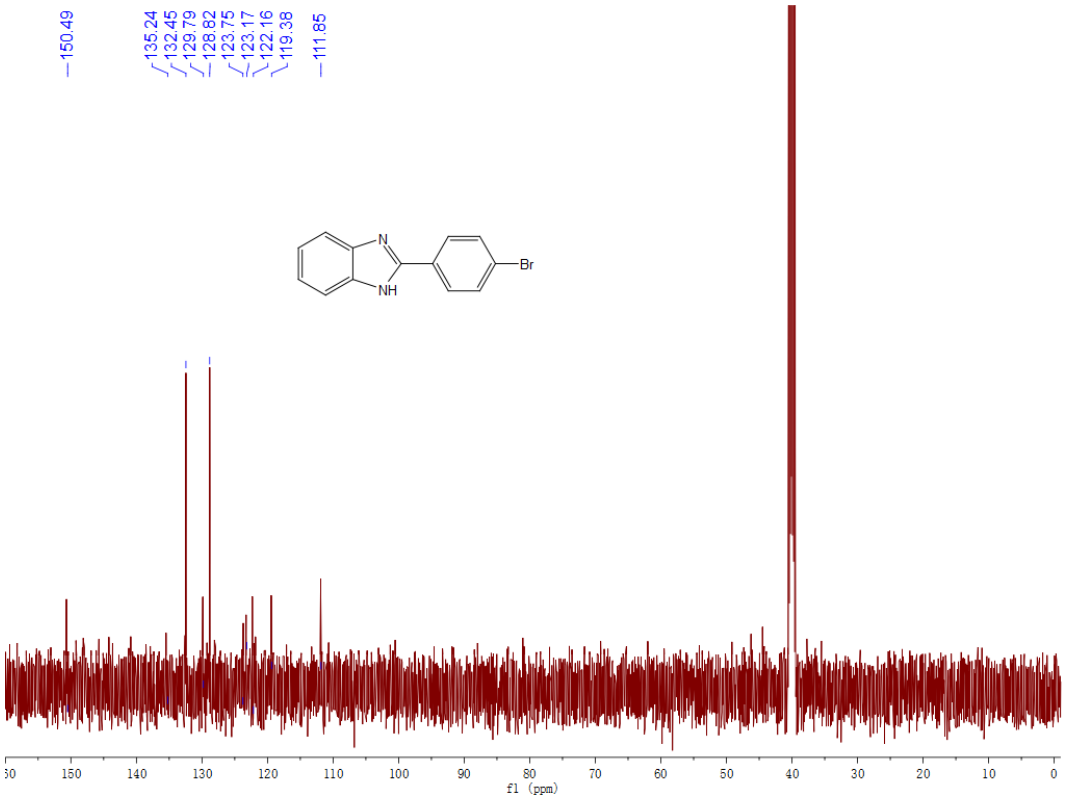


3-thiocyanato-4H-chromen-4-one: ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.34 (s, 1H), 8.28-8.26 (m, 1H), 7.81-7.77 (m, 2H), 7.57-7.52 (m, 1H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ 172.6, 156.3, 155.3, 135.0, 126.7, 126.2, 122.1,118.4, 114.4,112.1, 109.0.

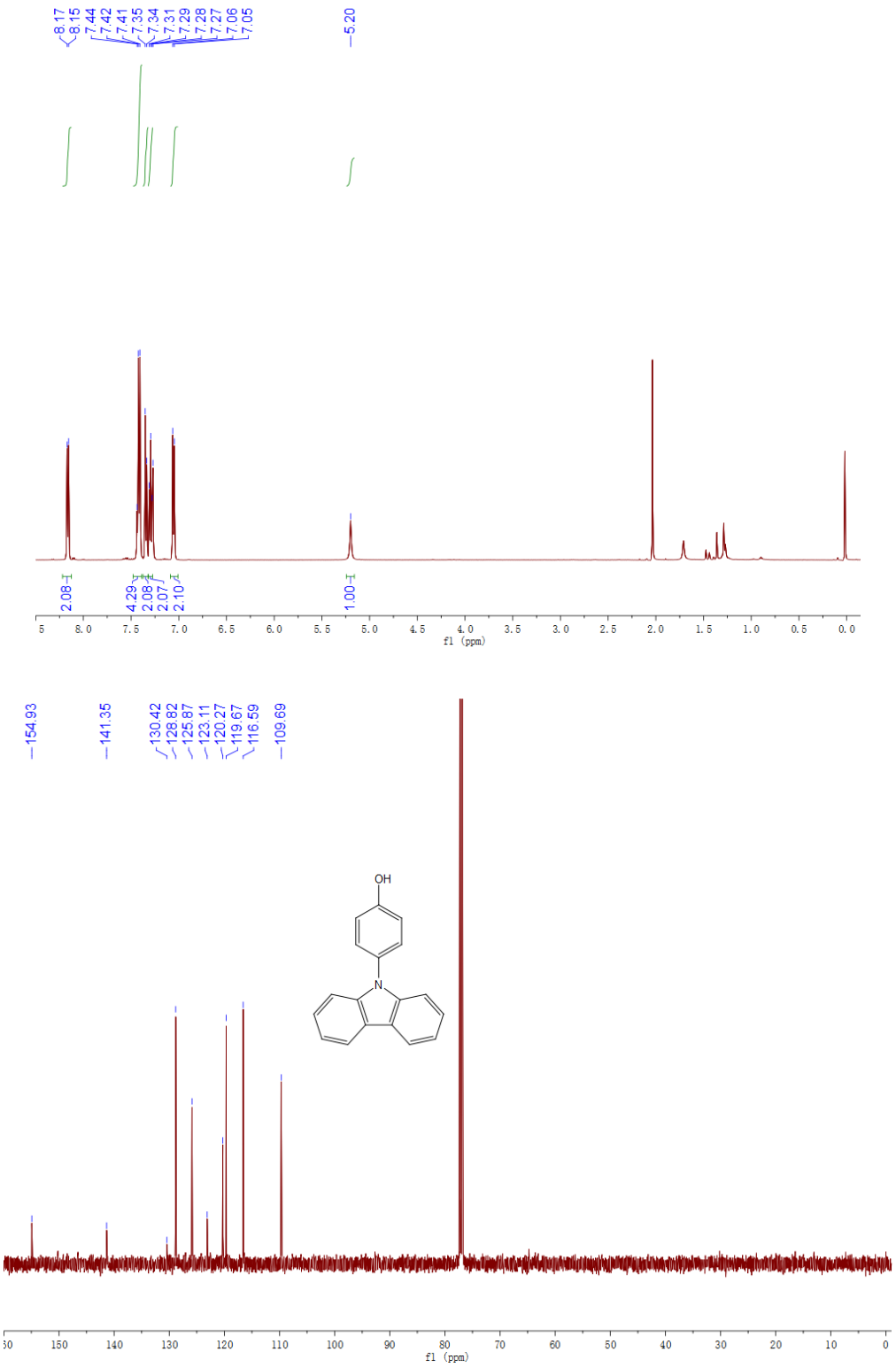


***N*-benzyl-2-(methyl(p-tolyl)amino)acetamide:** ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.32-7.24 (m, 3H), 7.21 (d, J = 8.0 Hz, 2H), 7.08 (m, J = 8.0 Hz, 2H), 6.98 (s, 1H), 6.67(d, J = 8.0 Hz, 2H), 4.50 (d, 2H) , 3.88 (s, 2H), 2.97 (s, 3H), 2.28 (s, 3H)ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ 169.2, 166.3, 142.9., 137.1, 131.2, 130.8, 127.4, 127.2, 126.9, 99.9, 61.7, 42.6, 21.1, 14.1.

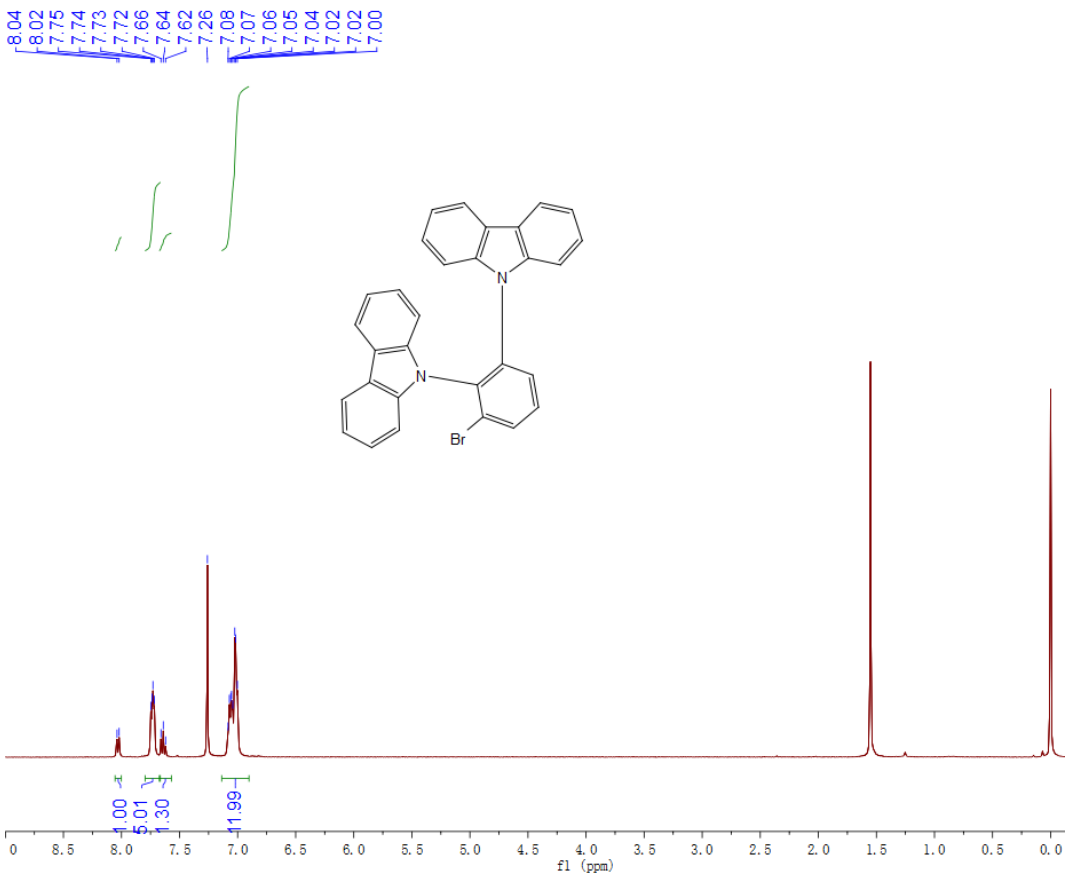




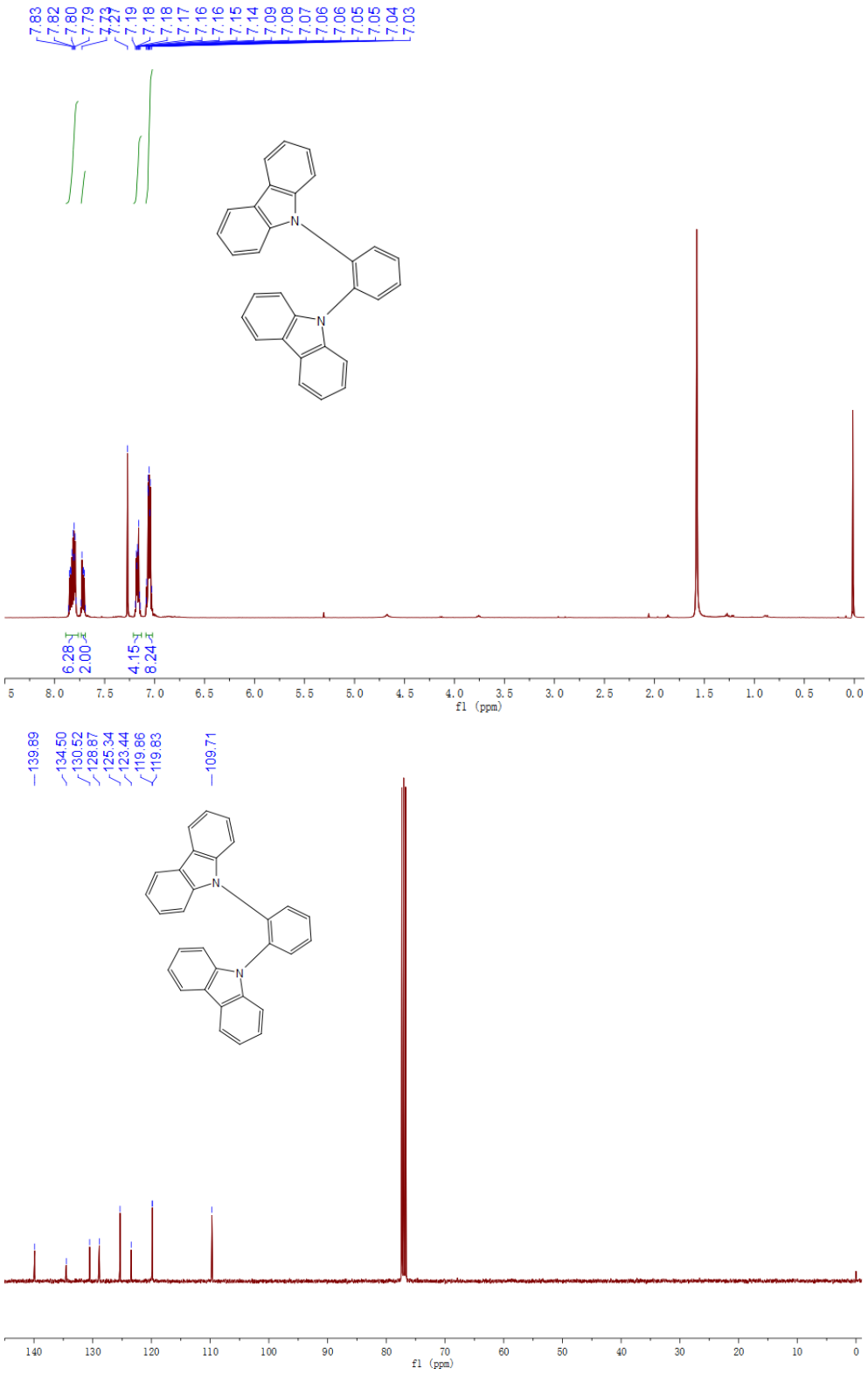
2-(4-bromophenyl)-1H-benzo[d]imidazole: ^{1}H NMR (DMSO, 400 MHz): δ12.8 (s, 1H), 8.12 (d, *J* = 8.0 Hz, 2H), 7.77 (d, *J* = 8.0 Hz, 2H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.54(d, *J* = 4.0 Hz, 1H), 7.25-7.18 (m, 2H) ppm. ^{13}C NMR (DMSO, 100 MHz): δ 150.5, 135.2, 132.4, 129.8, 128.8, 123.7, 123.2, 122.2, 119.4, 111.9.



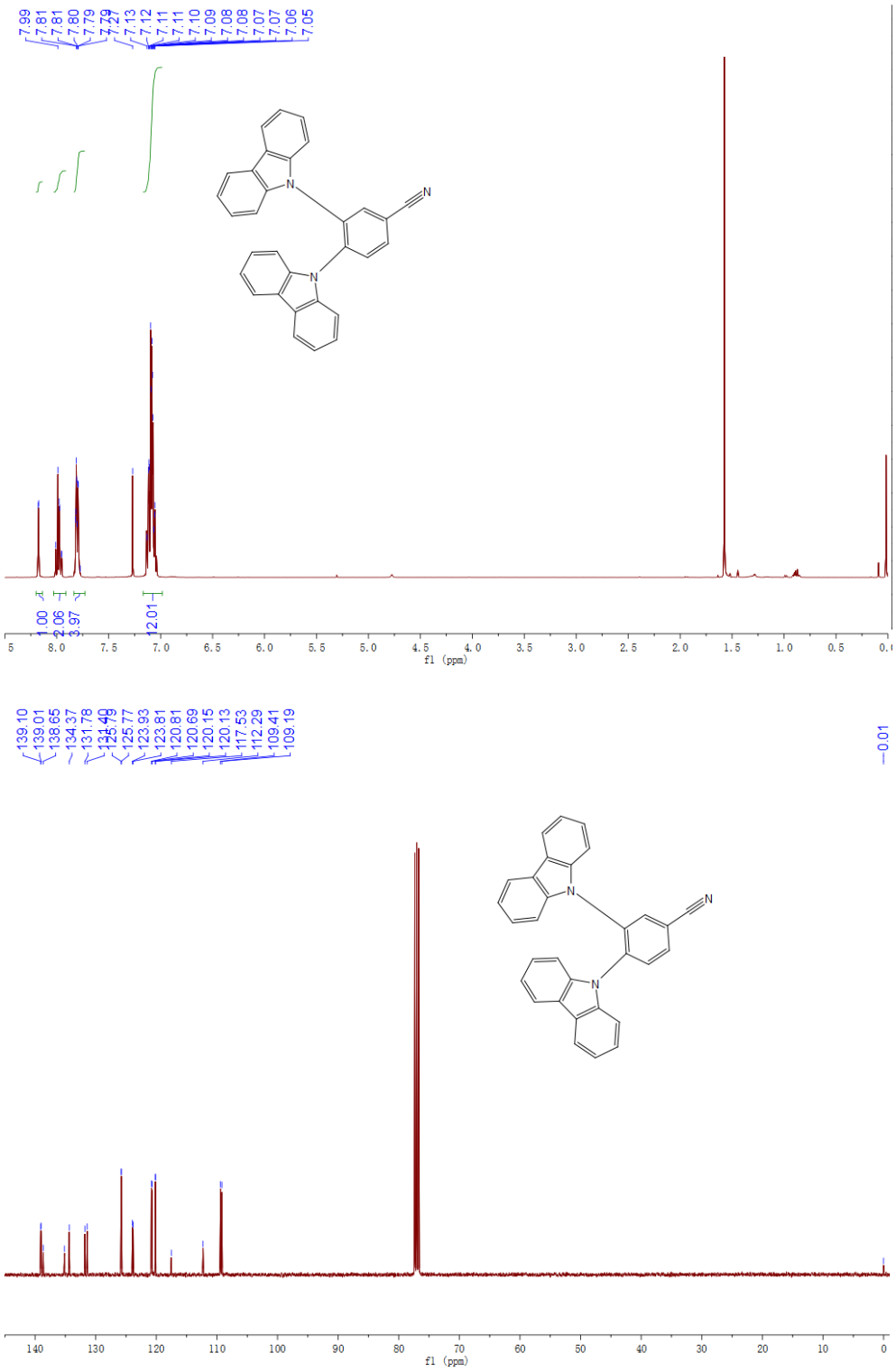
4-(9H-carbazol-9-yl)phenol: ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.16 (d, J = 4.0 Hz, 2H), 7.42 (t, J = 4.0 Hz, 4H), 7.34 (d, J = 8.0 Hz, 2H), 7.29 (d, J = 8.0 Hz, 2H), 7.06 (d, J = 8.0 Hz, 2H), 5.20 (s, 1H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ 154.9, 141.3, 130.4, 128.8, 125.9, 123.1, 120.3, 119.7, 116.6, 107.7.



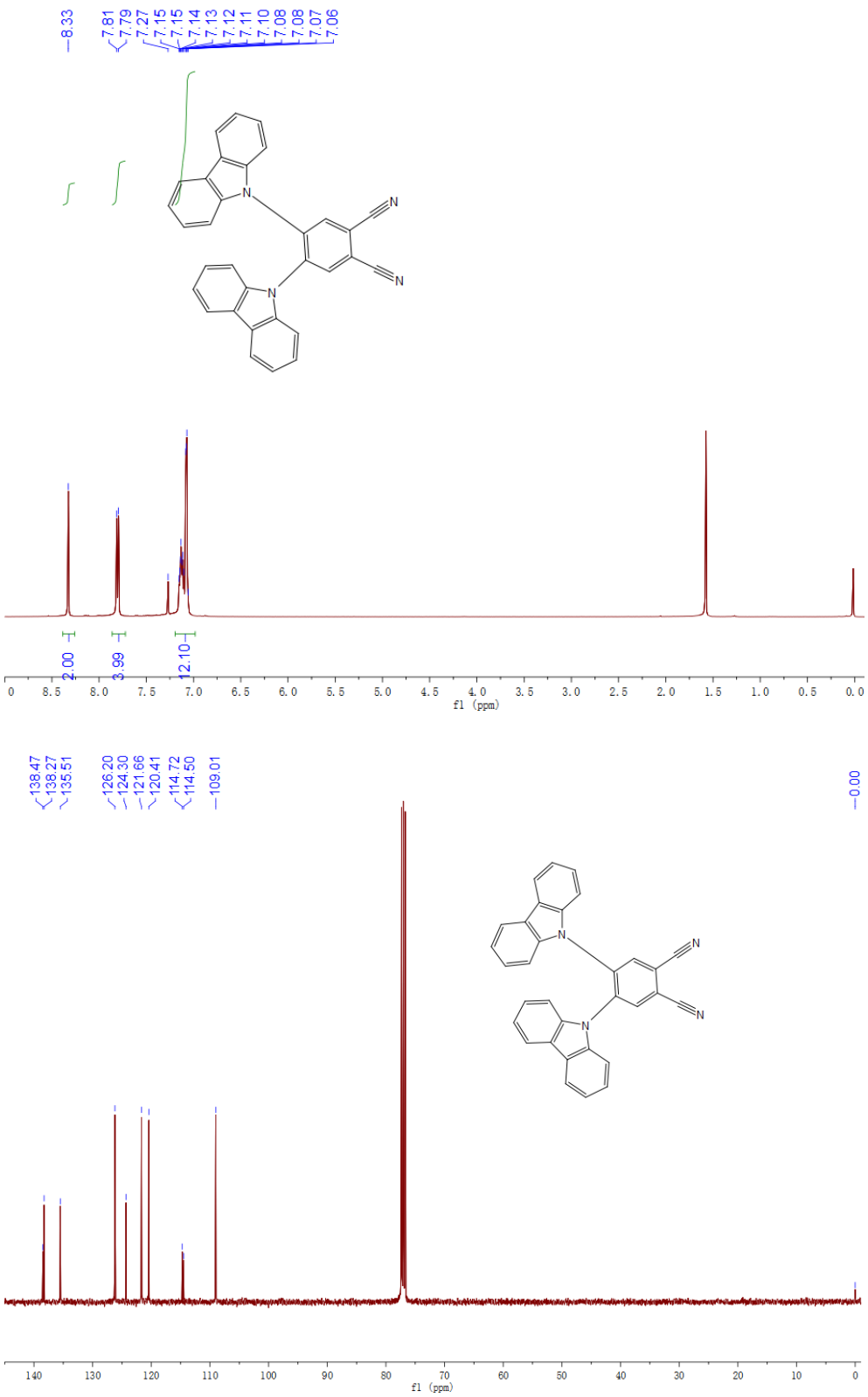
9,9'-(3-bromo-1,2-phenylene)bis(9H-carbazole): ^{1}H NMR ($CDCl_3$, 400 MHz): *δ* 8.03 (d, *J* = 8.0 Hz, 2H), 7.75-7.62 (m, 6H), 7.08-7.00 (m, *12*H) ppm.



1,2-di(9H-carbazol-9-yl)benzene: ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.86-7.78 (m, 6H), 7.19-7.14 (m, 4H), 7.09-7.03 (m ,8H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ 139.9, 134.5, 130.5, 128.9, 125.3, 123.4, 119.9, 119.8, 109.7 ppm.



3,4-di(9H-carbazol-9-yl)benzonitrile: ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.17 (d, J = 4.0 Hz, 2H), 8.01-7.95 (m , 4H), 7.82-7.77 (m ,4H), 7.13-7.05 (m, 12H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ 139.1, 139.0, 138.6, 135.1, 134.4, 131.8, 131.4, 125.8, 125.7, 123.9, 123.8, 120.8, 120.7, 120.1, 117.5, 112.3, 109.4 109.1 ppm.



4,5-di(9H-carbazol-9-yl)phthalonitrile: ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.33 (s, 2H), 7.80 (d , J = 4.0 Hz, 4H), 7.15-7.06 (m ,12H) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz): δ 138.4, 138.2, 135.5, 126.2, 124.3, 121.6, 120.0, 114.7, 114.5, 109.0 ppm.