

Electronic Supplementary Information (ESI)

Gas uptake, molecular sensing and organocatalytic performances of a multifunctional carbazole-based conjugated microporous polymer

Yuwei Zhang^a, Sigen A^a, Yongcun Zou^b, Xiaolong Luo^b, Zhongping Li^a, Hong Xia^c, Xiaoming Liu^{a*}, Ying Mu^a

^a State Key Laboratory for Supramolecular Structure and Materials, College of Chemistry, Jilin University, Changchun 130012, P. R.China

^b State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, College of Chemistry, Jilin University, Changchun, 130012, P.R.China.

^c State Key Laboratory on Integrated Optoelectronics, College of Electronic Science and Technology, Jilin University, Changchun 130012, P. R.China

Email: xm_liu@jlu.edu.cn

Section 1. TGA Profile

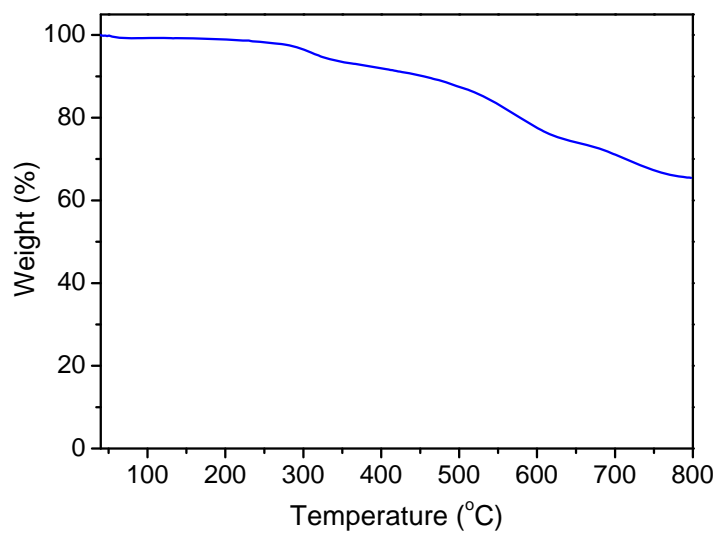


Fig. S1 TGA curve of MFCMP-1 under nitrogen.

Section 2. FT IR Spectra

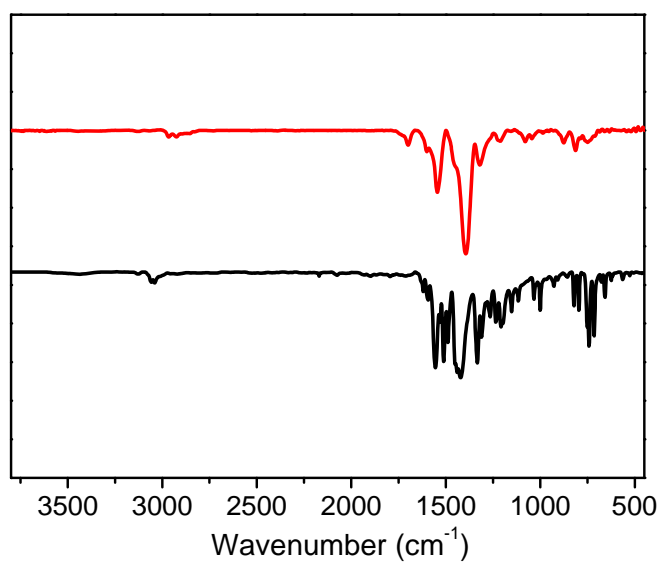


Fig. S2 IR spectra of MFCMP-1 (red line) and its monomer (black line).

Section 3. Powder X-Ray Diffraction

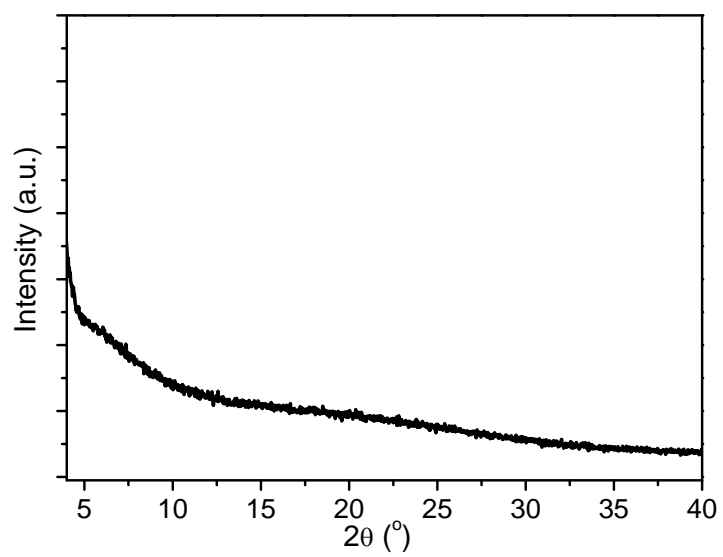


Fig. S3 PXRD curve of MFCMP-1.

Section 4. SEM, DLS and TEM

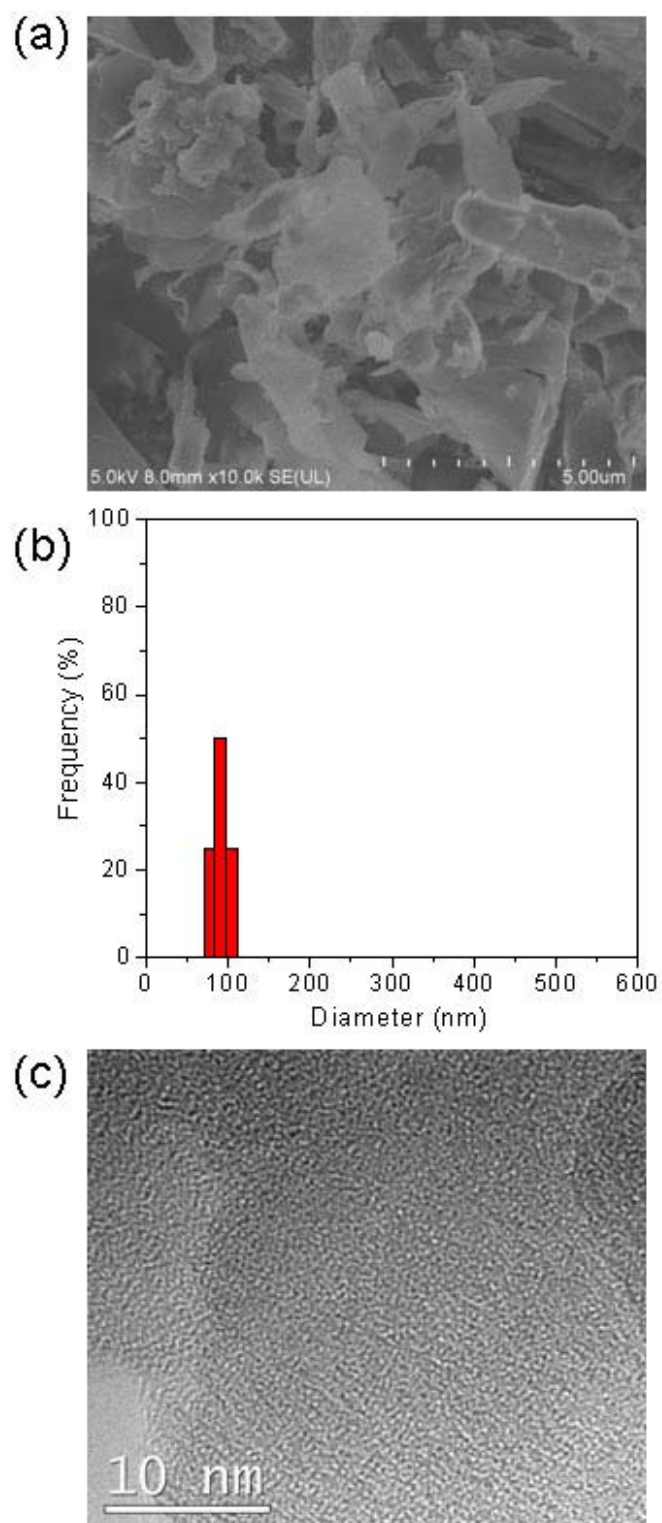


Fig. S4 (a) SEM image, (b) DLS profile and (c) TEM image of MFCMP-1.

Section 5. Uptake of CO₂ at high pressure

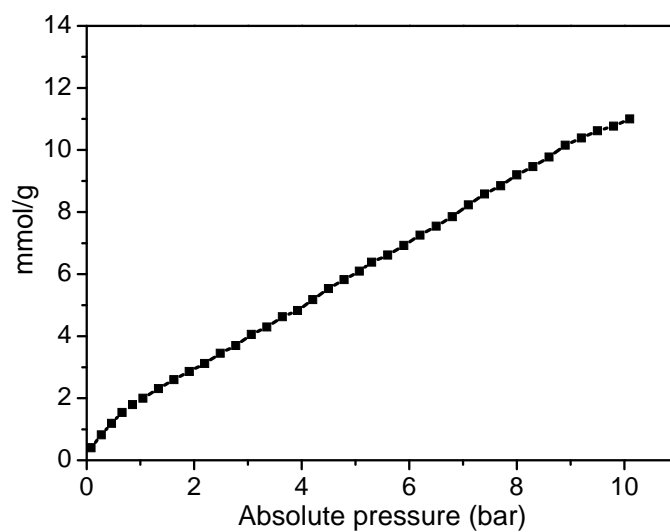


Fig. S5 Adsorption isotherm of MFCMP-1 for CO₂ at 298 K and 10 bar.

Section 6. Adsorption Selectivity

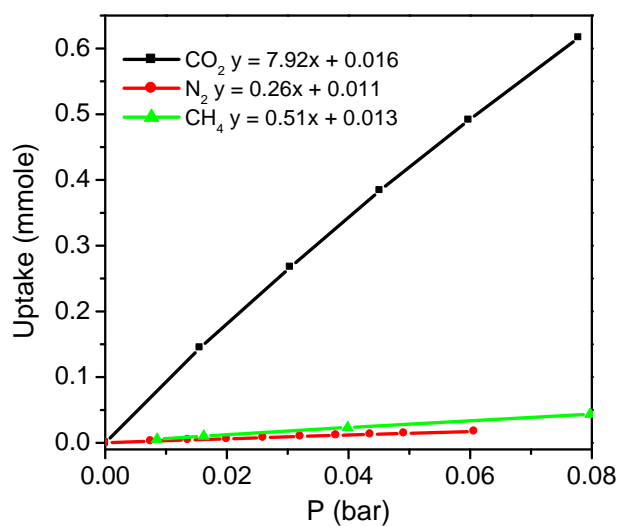


Fig. S6 CO₂/N₂ and CO₂/CH₄ initial slope selectivity studies for MFCMP-1.

Section 7. Stability of Water Vapor

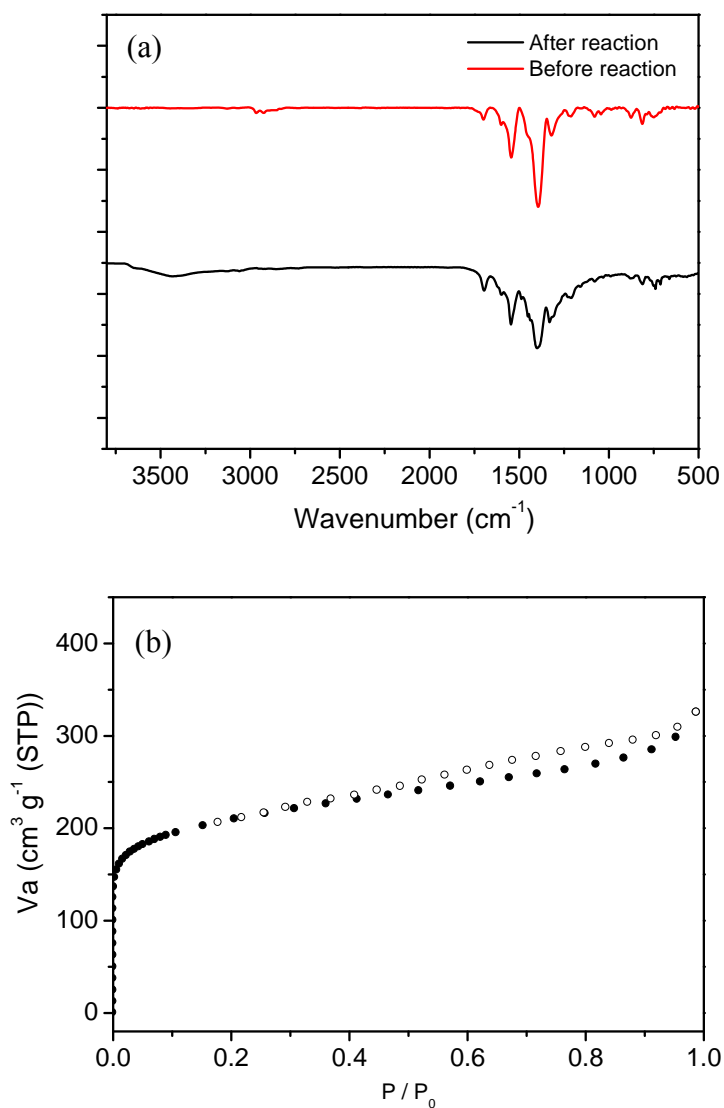


Fig. S7 (a) IR spectra of MFCMP-1 samples fresh (red line) and after reaction 5h in boiling water (black line) (b) Nitrogen adsorption/desorption isotherms (●: adsorption, ○: desorption) of MFCMP-1 samples after reaction 5h in boiling water, the surface area is $768 \text{ m}^2 \text{ g}^{-1}$.

Section 8. FT IR Spectra

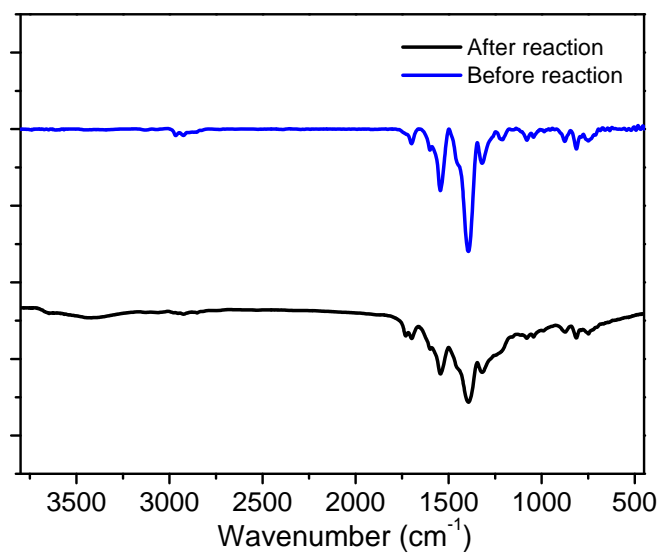
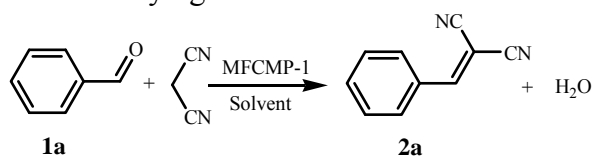


Fig. S8 IR spectra of MFCMP-1 samples fresh (red line) and after six-time catalytic reaction (black line). It is evident that the structure of MFCMP-1 was maintained after catalytic reactions.

Section 9. Catalytic Data

Table S1. The Knoevenagel condensation of benzaldehyde with malononitrile catalyzed by MFCMP-1 in varying solvent ^{a)}



Entry	Solvent	Amount (mL)	Time (h)	Yield (%) ^b
1	Dioxane	0.8	4	8
2	THF	0.8	4	7
3	Toluene	0.8	4	5
4	EtOAc	0.8	4	4
5	DMF	0.8	4	5
6	H ₂ O	0.8	4	48
7	Methanol	0.8	4	41
8	Ethanol	0.8	4	65
9	Ethanol/H ₂ O	0.4 /0.4	4	76
10	MeOH/H ₂ O	0.4 /0.4	4	79
11	DMF/H ₂ O	0.4 /0.4	4	91
12	Dioxane/H ₂ O	0.4 /0.4	4	99
13	Dioxane/H ₂ O	0.4 /0.4	2	91
14	Dioxane/H ₂ O	0.4 /0.4	1	82
15	Dioxane/H ₂ O	0.4 /0.4	30min	68
16	Dioxane/H ₂ O	0.4 /0.4	10min	32
17 ^{c)}	Dioxane/H ₂ O	0.4 /0.4	2	98
18 ^{d)}	Dioxane/H ₂ O	0.4 /0.4	10min	22
19 ^{d)}	Dioxane/H ₂ O	0.4 /0.4	30min	30
20 ^{d)}	Dioxane/H ₂ O	0.4 /0.4	1	39
21 ^{d)}	Dioxane/H ₂ O	0.4 /0.4	2	59
22 ^{d)}	Dioxane/H ₂ O	0.4 /0.4	4	76
23 ^{d)}	Dioxane/H ₂ O	0.4 /0.4	7	95

^{a)} Reaction conditions: benzaldehyde (0.2 mmol), malononitrile (0.2 mmol), MFCMP-1 (1.0 mol % of the substrate), 25 °C; ^{b)} Determined by GC using undecane as internal standard; ^{c)} malononitrile (0.3 mmol); ^{d)} MFCMP-1 0.5 mol % of the substrate.

Section 10. Sorption Isotherms

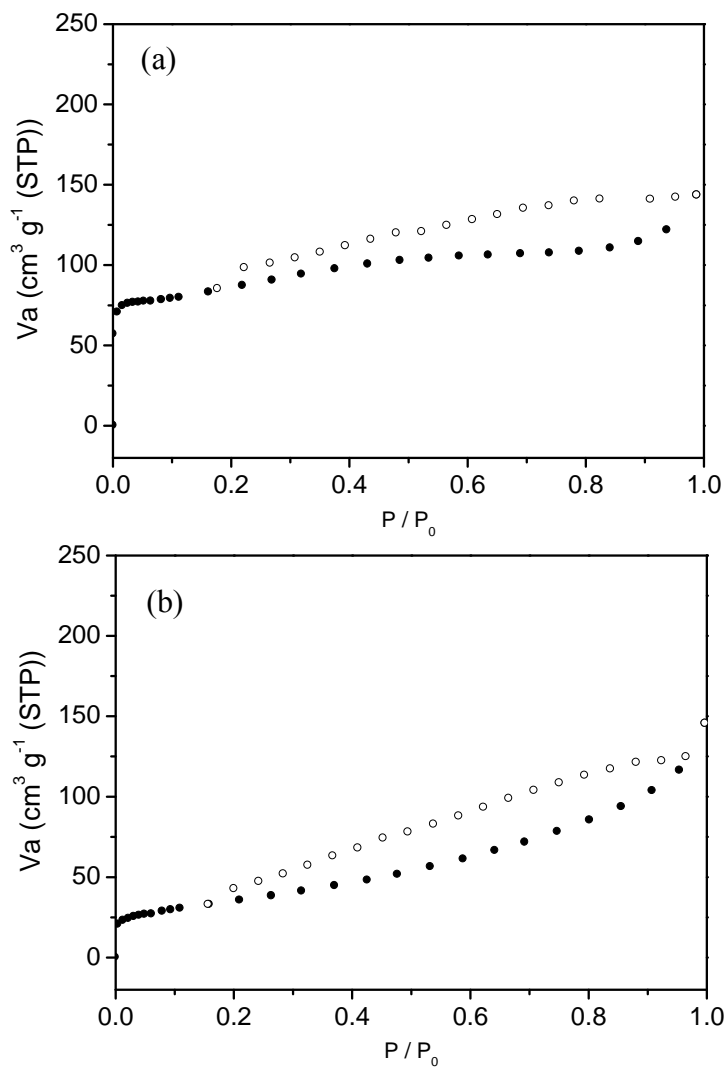
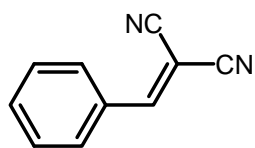


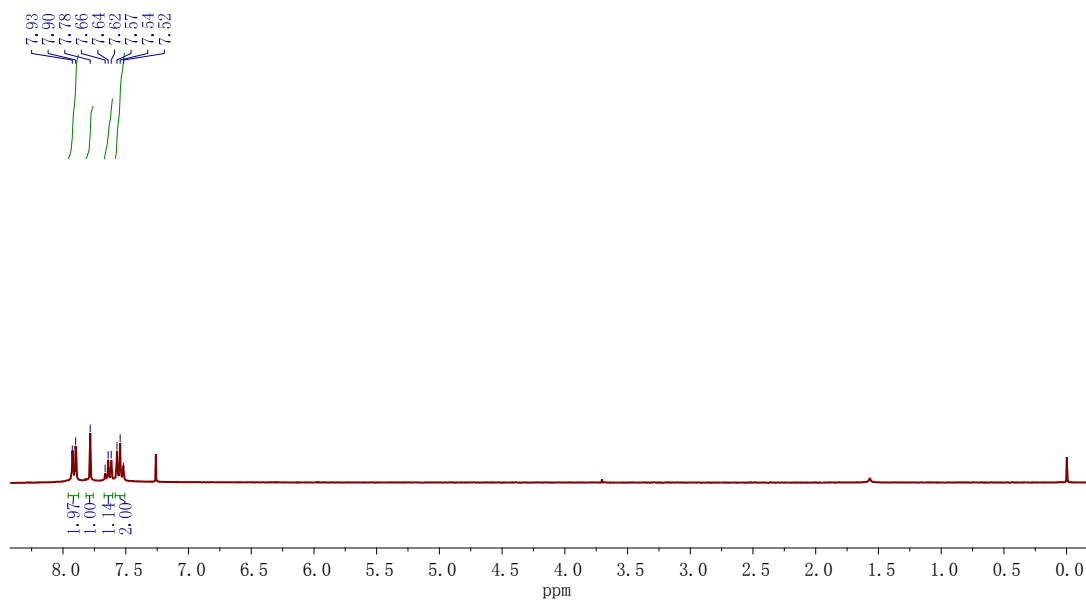
Fig. S9 Nitrogen adsorption (●) and desorption (○) isotherm profiles of MFCMP-1 prepared in $\text{CH}_3\text{CN}/\text{CHCl}_3$ (a) and CH_3CN (b).

Section 11. The Characterization of Products

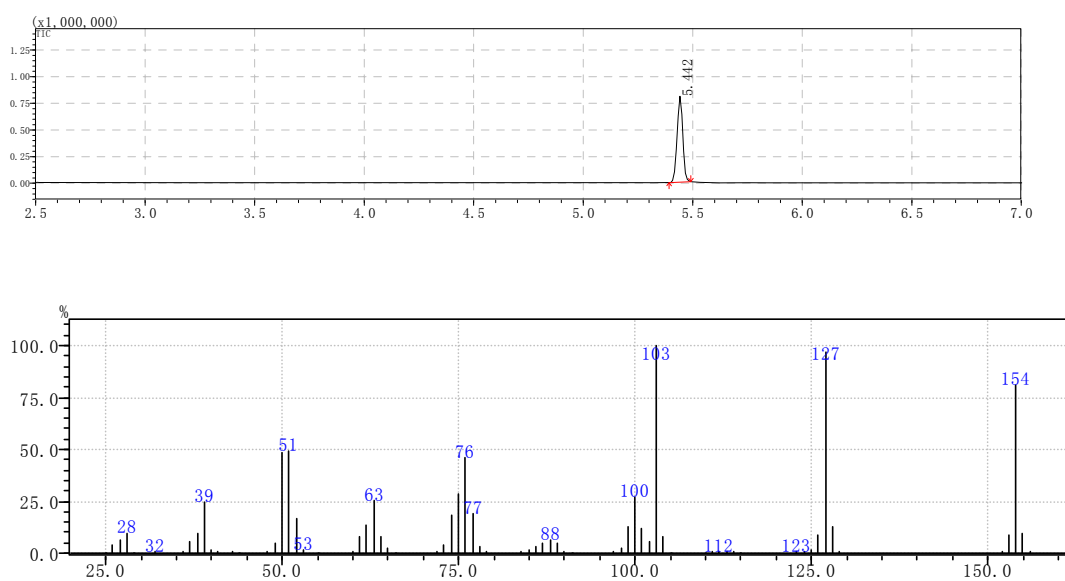


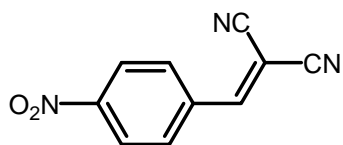
2a: White solid; m.p. 83-84 °C (lit.,² 84 °C); ¹H NMR (300MHz, CDCl₃) δ 7.54 (t, *J* = 9.0 Hz, *J* = 6.0 Hz, 2H), 7.64 (t, *J* = 6.0 Hz, 1H), 7.78 (s, 1H), 7.92 (d, *J* = 9.0 Hz, 2H) ppm. GC-MS retention time 5.442 min., *m/z* (EI) 154 (M⁺, 81), 127 (98), 103 (100).

¹H-NMR spectrum of 2a



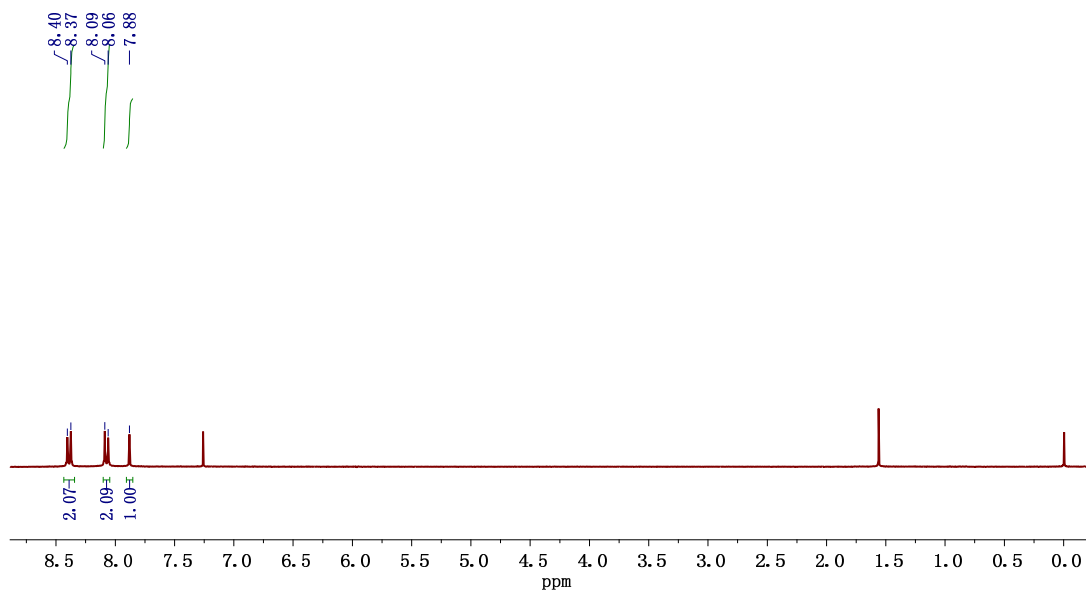
GC-MS spectra of 2a



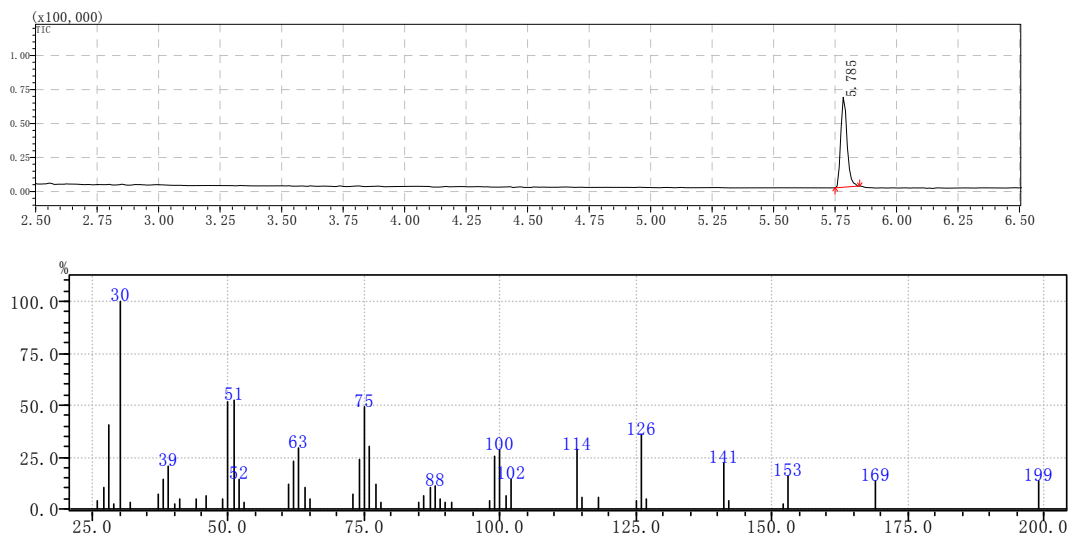


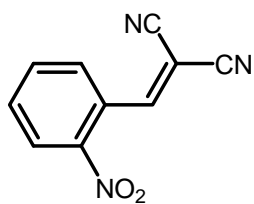
2b: Pale solid; m.p. 164-166 °C (lit.,³ 167-168 °C); ¹H NMR (300MHz, CDCl₃) δ 7.88 (s, 1H), 8.08 (d, *J* = 9.0 Hz, 2H), 8.39 (d, *J* = 9.0 Hz, 2H) ppm. GC-MS retention time 5.785 min., *m/z* (EI) 199 (M⁺, 13), 153 (16), 141 (23), 126 (35), 114 (28), 100 (29), 75 (49), 63 (29).

¹H-NMR spectrum of 2b



GC-MS spectra of 2b

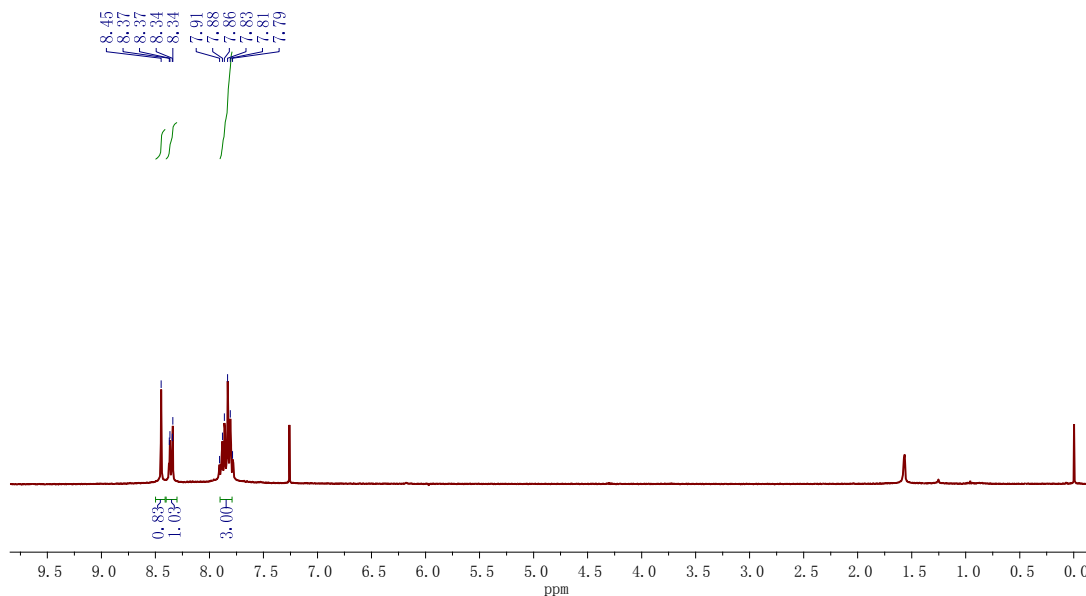




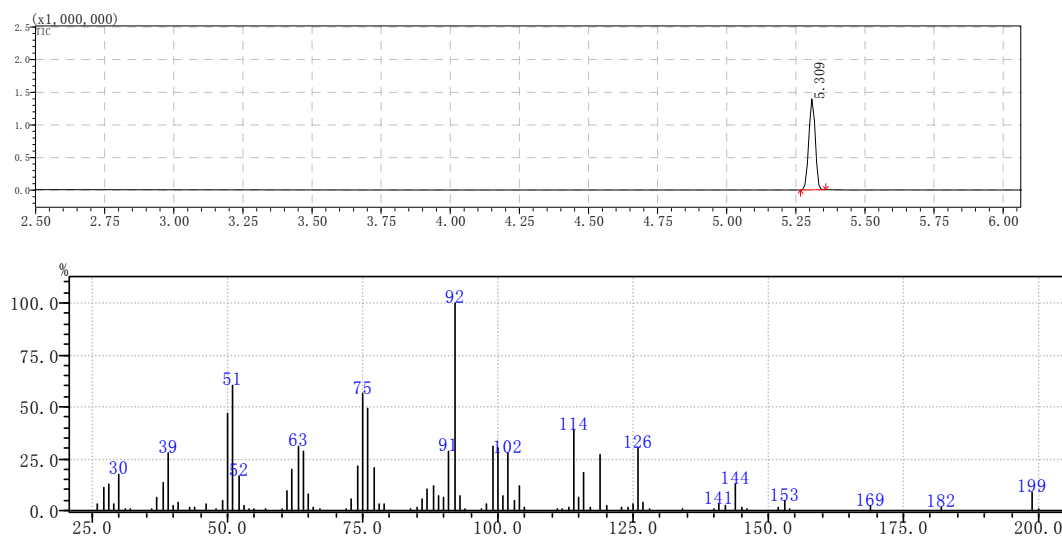
2c: White solid; m.p. 135-136 °C (lit.,⁴ 136-138 °C); ¹H NMR

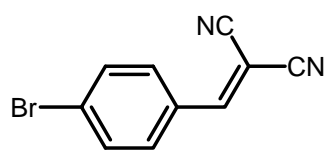
(300MHz, CDCl₃) δ 7.81–7.88 (m, 5H), 8.35 (d, *J* = 9.0 Hz, 1H), 8.45 (s, 1H) ppm. GC-MS retention time 5.309 min., m/z (EI) 199 (M⁺, 16), 144 (18), 126 (39), 114 (47), 92 (100), 75 (53), 51 (50).

¹H-NMR spectrum of 2c



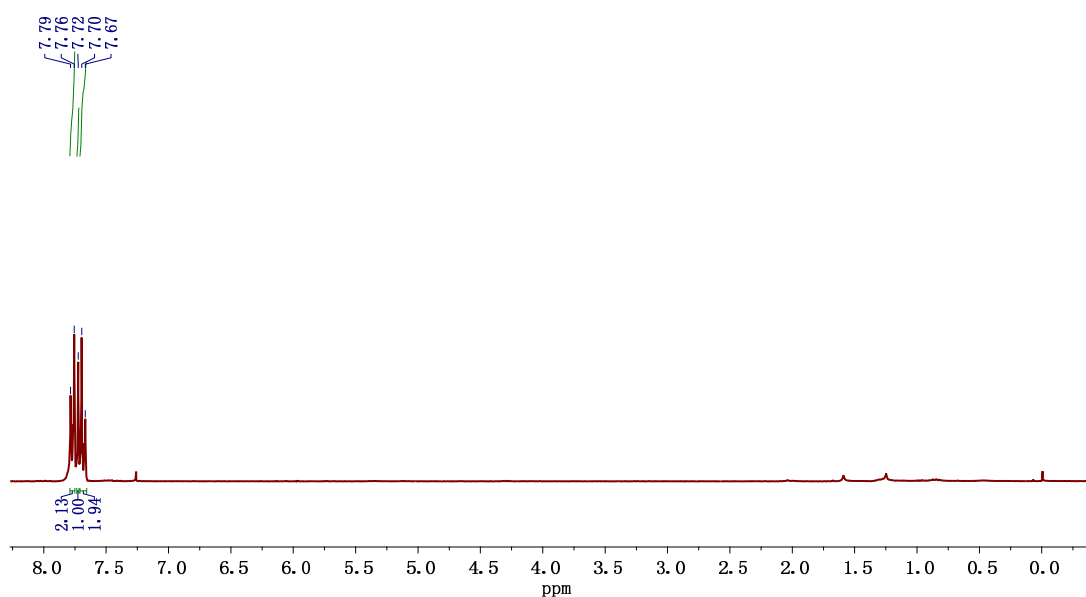
GC-MS spectra of 2c



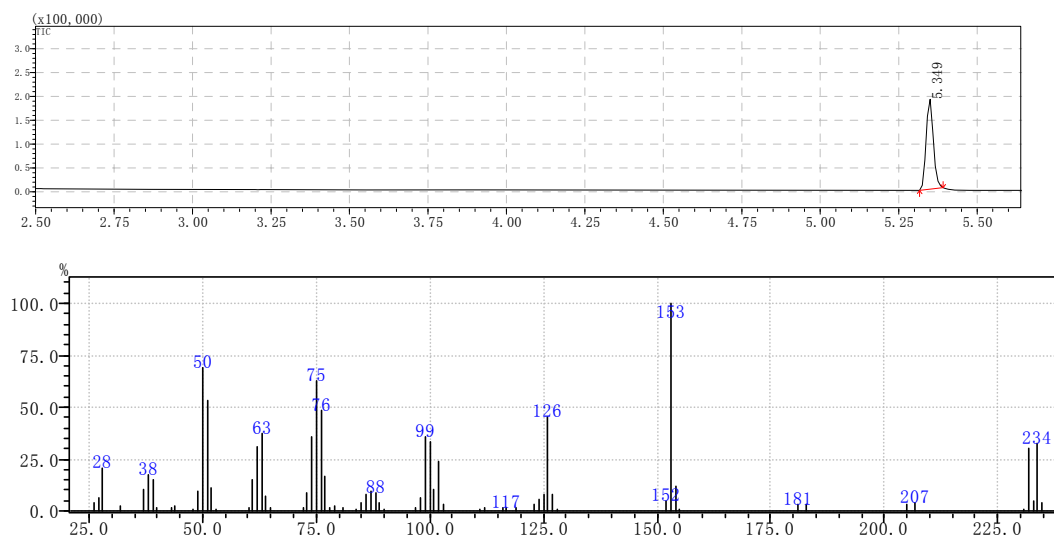


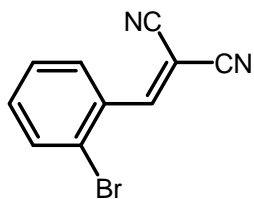
2d: White solid; m.p. 155-157 °C (lit.,⁵ 159-161 °C); ¹H NMR (300MHz, CDCl₃) δ 7.69 (d, *J* = 9.0 Hz, 2H), 7.72 (s, 1H), 7.78 (d, *J* = 9.0 Hz, 2H) ppm. GC-MS retention time 5.349 min., m/z (EI) 234 (M⁺, 32), 153 (100), 126 (45), 99 (36), 75 (63), 63 (38), 50 (69).

¹H-NMR spectrum of 2d



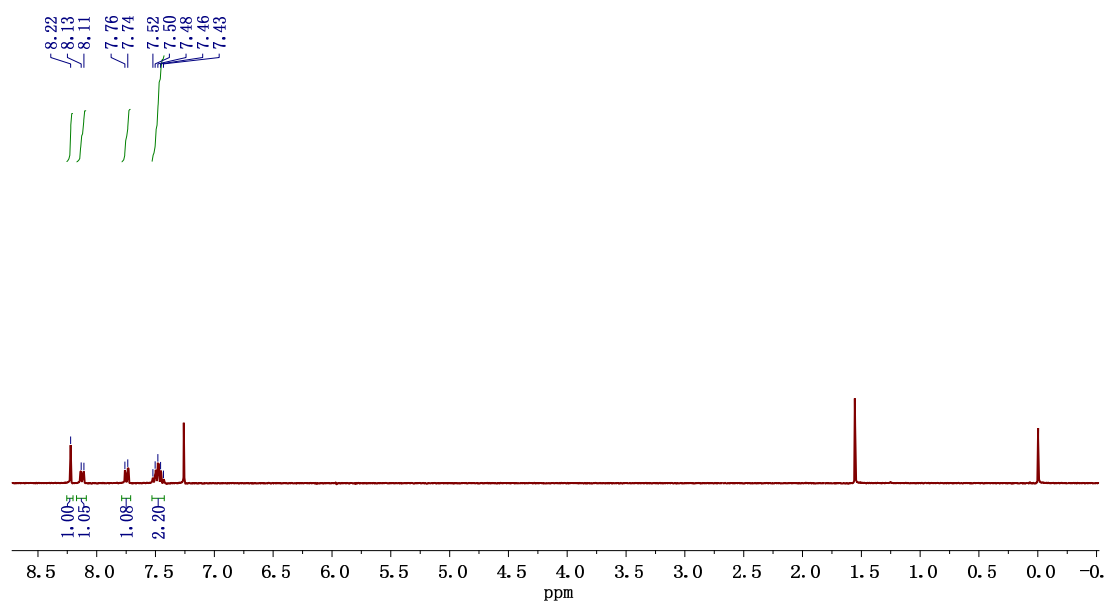
GC-MS spectra of 2d



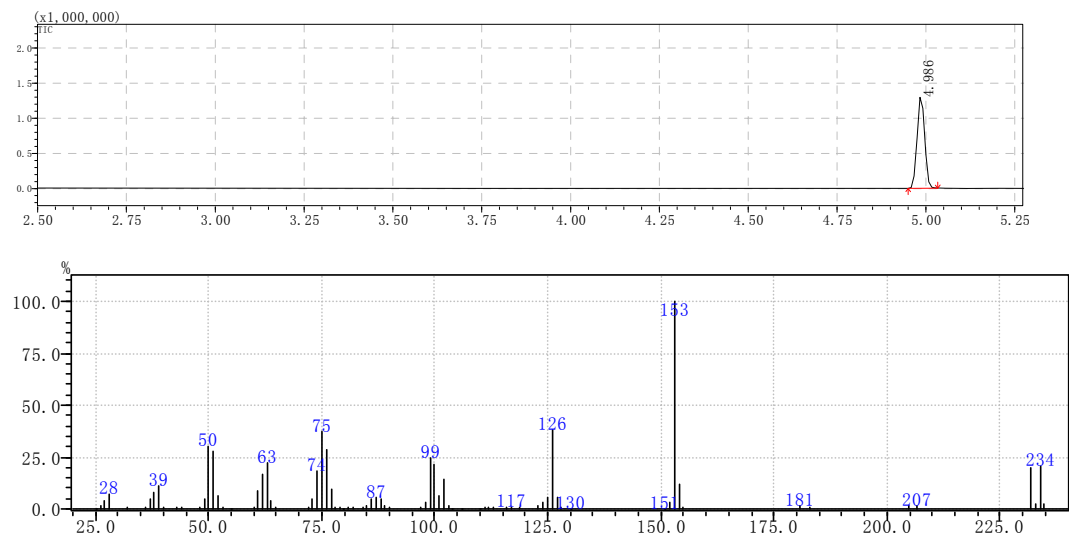


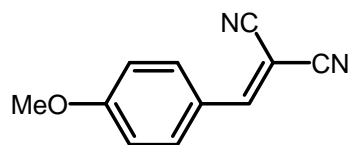
2e: White solid; m.p. 90-92 °C (lit.,⁵ 92-93 °C); ¹H NMR (300MHz, CDCl₃) δ 7.48 (m, 2H), 7.75 (d, *J* = 6.0 Hz, 1H), 8.12 (d, *J* = 6.0 Hz, 1H), 8.22 (s, 1H) ppm. GC-MS retention time 4.986 min., *m/z* (EI) 234 (M⁺, 21), 153 (100), 126 (38), 99 (24), 75 (37), 63 (22), 50 (30).

¹H-NMR spectrum of **2e**



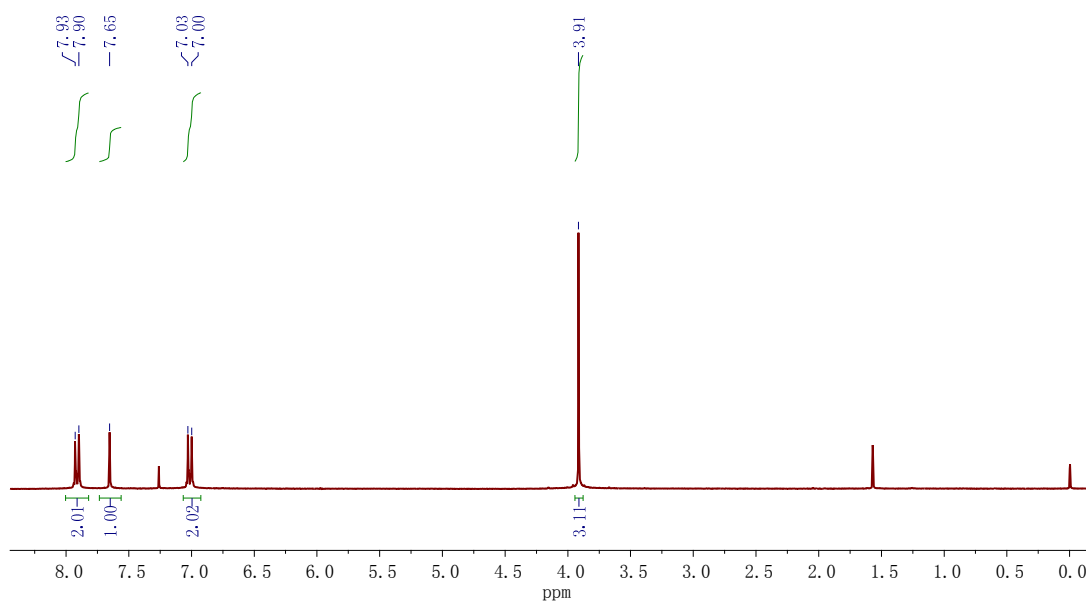
GC-MS spectra of **2e**



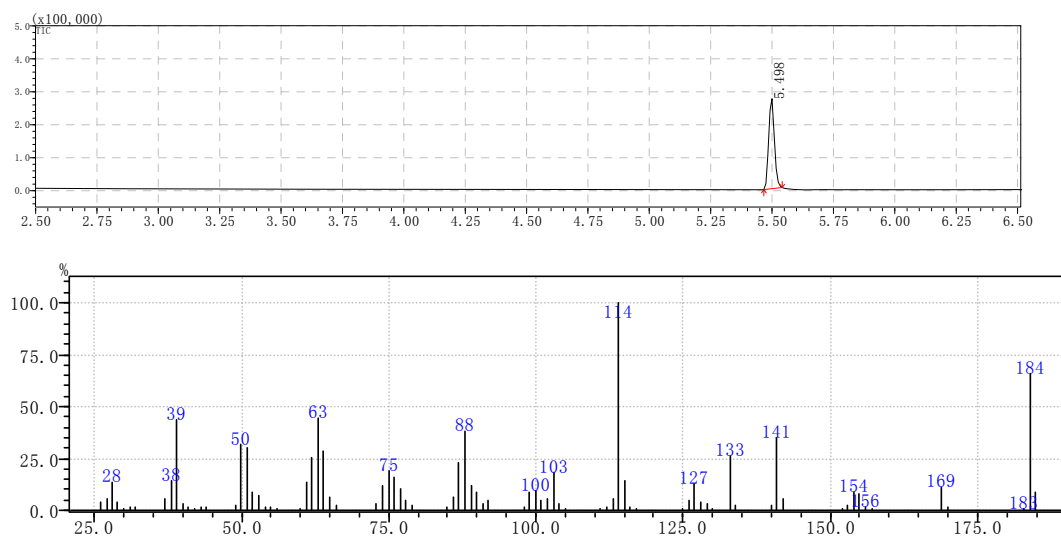


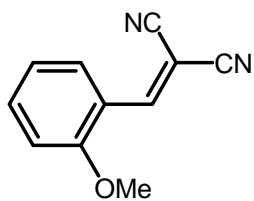
2f: Yellow solid; m.p. 114-115 °C (lit.,² 116 °C); ¹H NMR (300MHz, CDCl₃) δ 3.91 (s, 3H), 7.02 (d, *J* = 9.0 Hz, 2H), 7.65 (s, 1H), 7.92 (d, *J* = 9.0 Hz, 2H) ppm. GC-MS retention time 5.498 min., m/z (EI) 184 (M⁺, 66), 141 (35), 133 (26), 114 (100), 88 (38), 64 (28).

¹H-NMR spectrum of **2f**



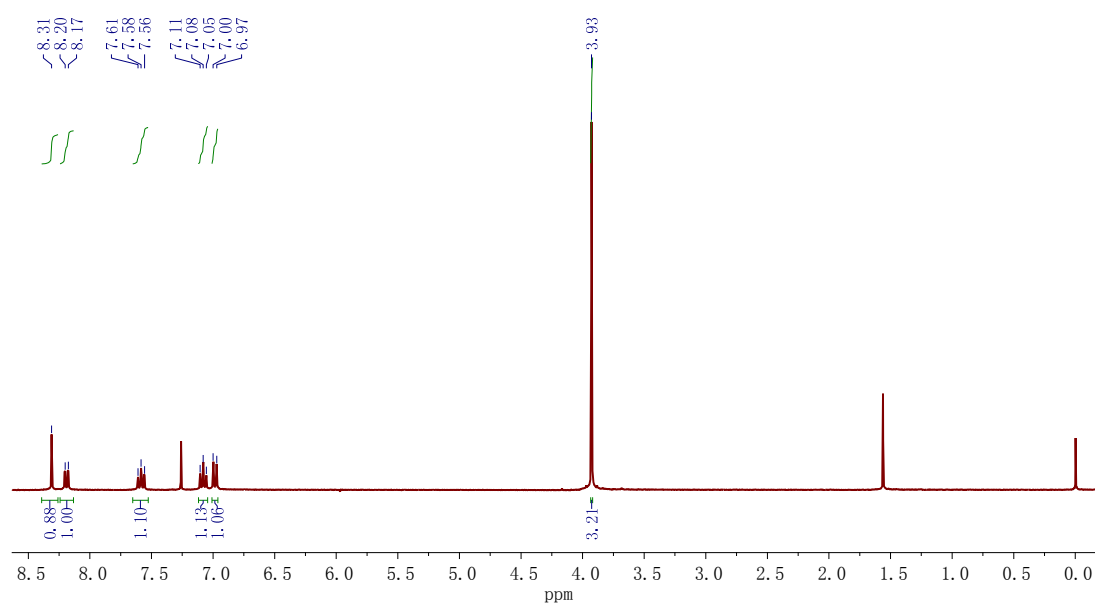
GC-MS spectra of **2f**



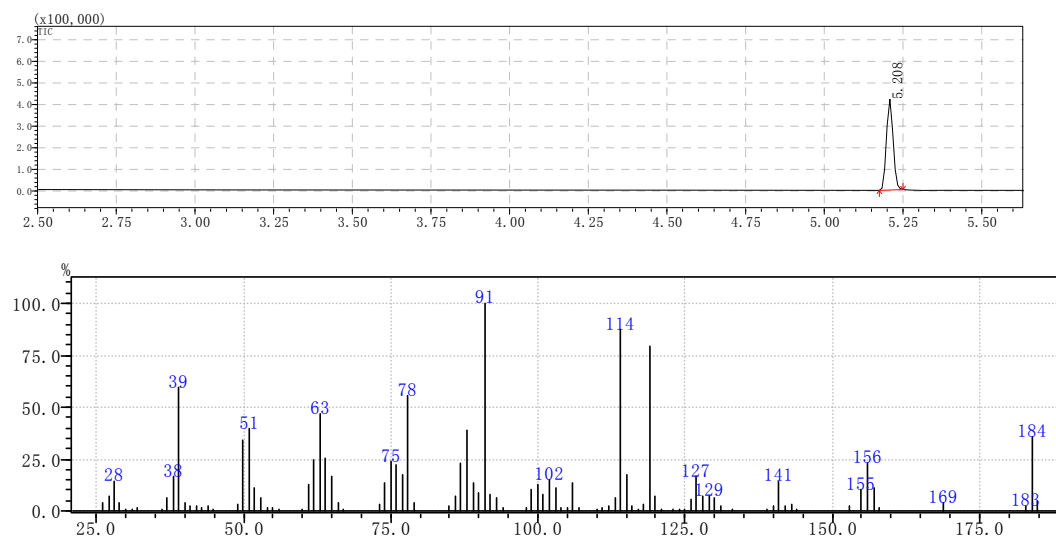


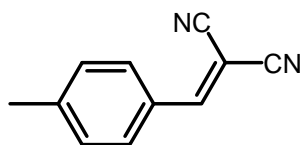
2g: Pale yellow solid; m.p. 79-80 °C (lit.,⁶ 79-80 °C); ¹H NMR (300MHz, CDCl₃) δ 3.93 (s, 3H), 6.99 (d, *J* = 9.0 Hz, 1H), 7.08 (t, *J* = 9.0 Hz, 1H), 7.58 (t, *J* = 9.0 Hz, 1H), 8.19 (d, *J* = 9.0 Hz, 1H), 8.31 (s, 1H) ppm. GC-MS retention time 5.208 min., m/z (EI) 184 (M⁺, 36), 119 (79), 114 (87), 91 (100), 88 (39), 78 (56), 63 (47), 51 (40).

¹H-NMR spectrum of **2g**



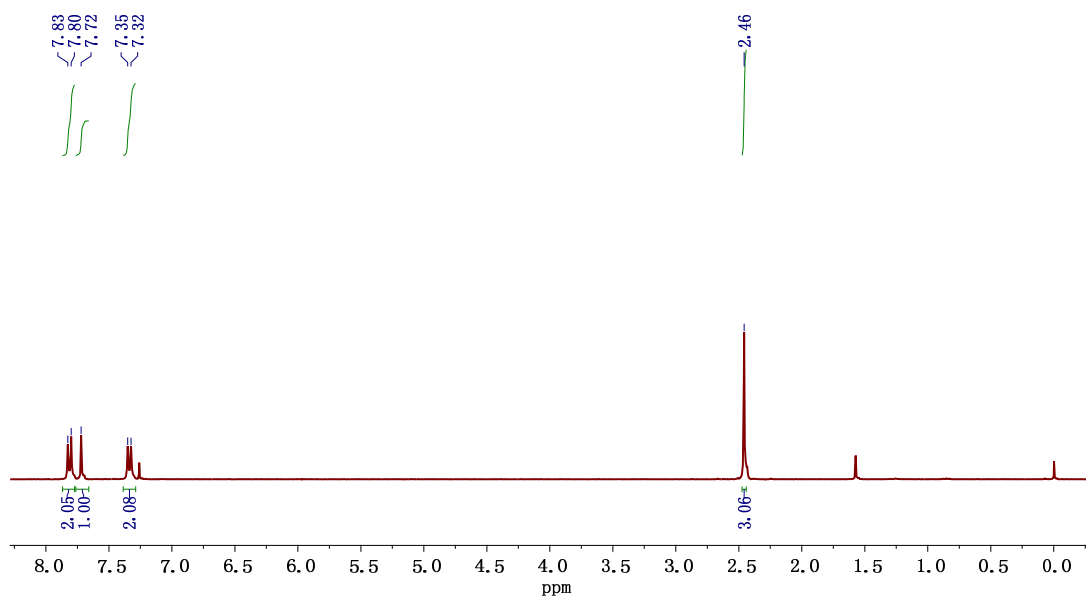
GC-MS spectra of **2g**



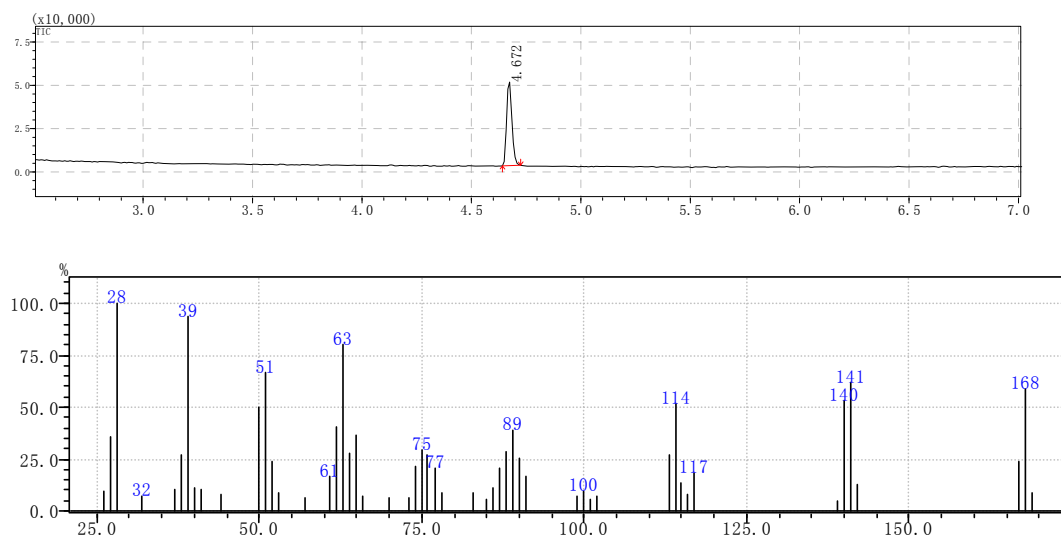


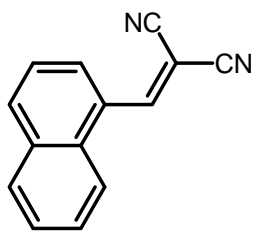
2h: White solid; m.p. 130-131 °C (lit.,³ 132-134 °C); ¹H NMR (300MHz, CDCl₃) δ 2.46 (s, 3H), 7.34 (d, *J* = 9.0 Hz, 2H), 7.72 (s, 1H), 7.82 (d, *J* = 9.0 Hz, 2H) ppm. GC-MS retention time 4.672 min., *m/z* (EI) 168 (M⁺, 59), 141 (63), 114 (51), 63 (75), 51 (63).

¹H-NMR spectrum of **2h**



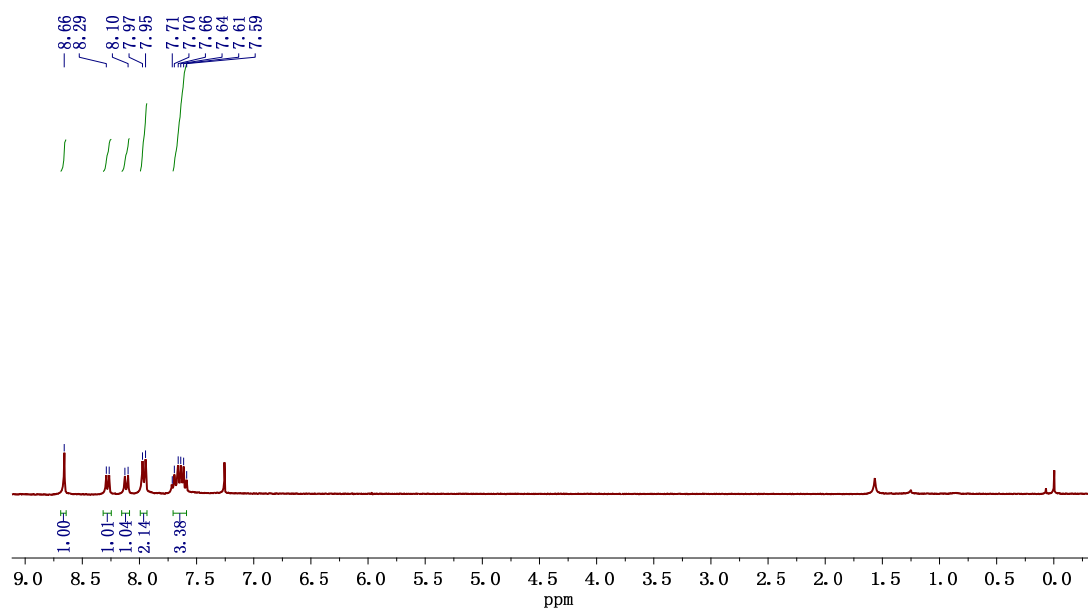
GC-MS spectra of **2h**



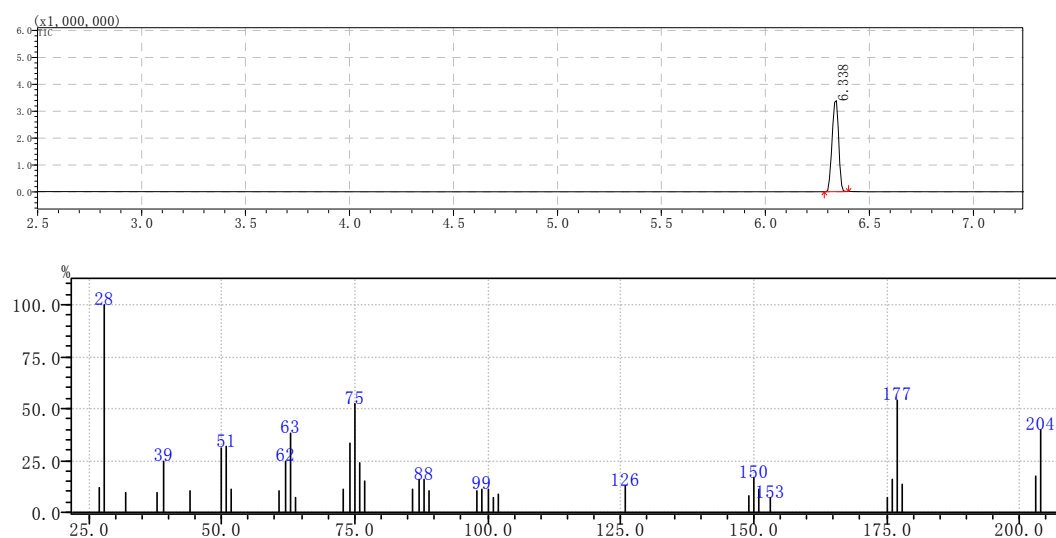


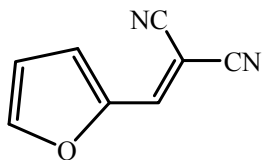
2i: Bright orange solid; m.p. 164-165 °C (lit.,⁸ 168-169 °C); ¹H NMR (300MHz, CDCl₃) δ 7.59–7.71 (m, 3H), 7.96 (d, *J* = 6.0 Hz, 2H), 8.12 (d, 6.0 Hz, 1H), 8.28 (d, 6.0 Hz, 1H), 8.66 (s, 1H) ppm. GC-MS retention time 6.338 min., *m/z* (EI) 204 (M⁺, 40), 177 (54), 150 (17), 126 (13), 75 (52), 63 (38), 51 (32).

¹H-NMR spectrum of **2i**



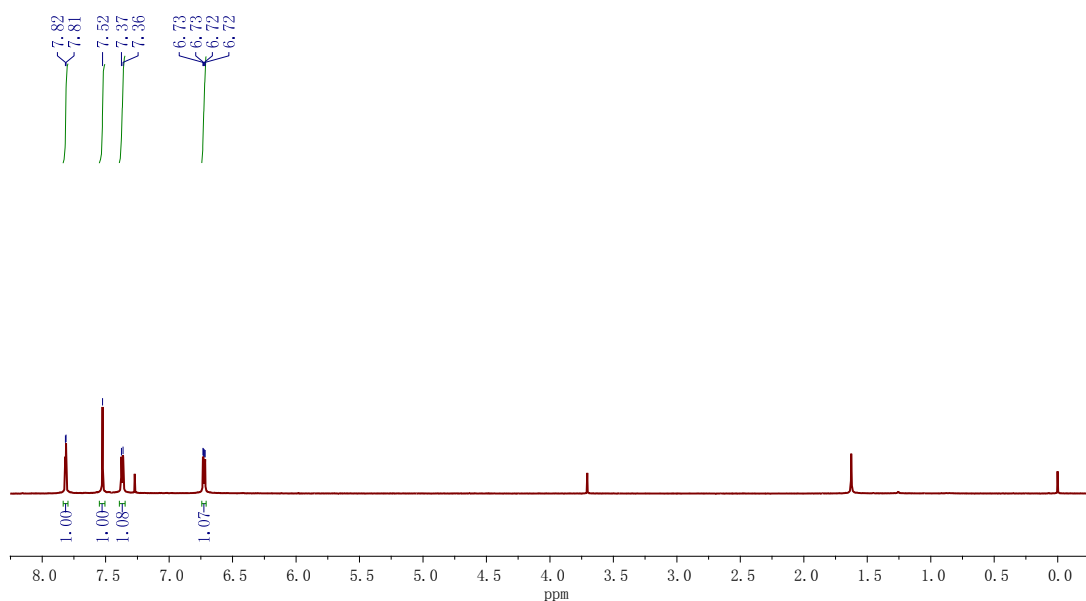
GC-MS spectra of **2i**



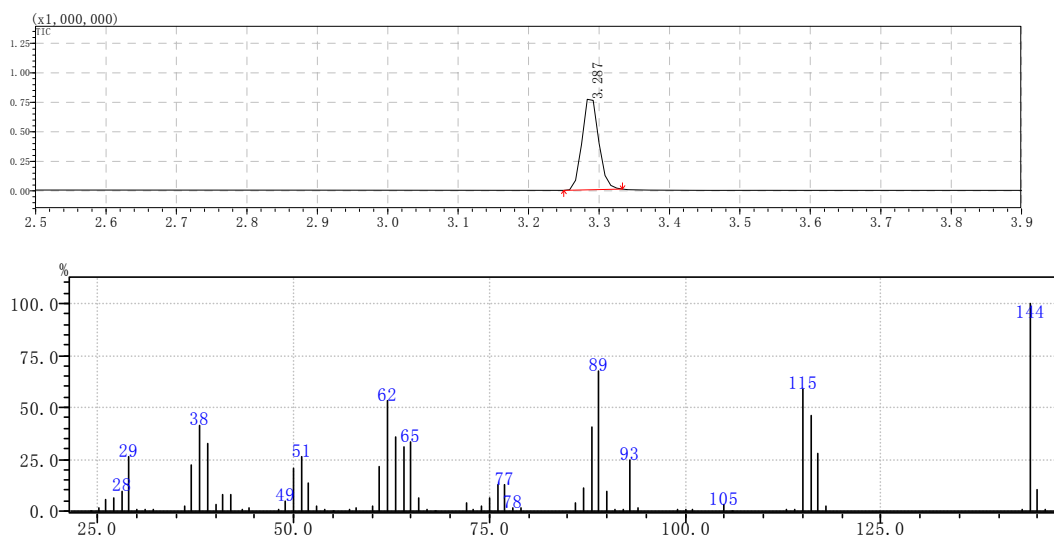


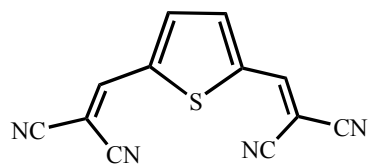
2j: Light pink solid; m.p. 70-71 °C (lit.,⁹ 72-73 °C); ¹H NMR (300MHz, CDCl₃) δ 6.72 (dd, 1H), 7.36 (d, *J* = 3.0 Hz, 1H), 7.52 (s, 1H), 7.81 (d, 3.0 Hz, 1H) ppm. GC-MS retention time 3.287 min., m/z (EI) 144 (M⁺, 100), 115 (59), 89 (68), 62 (53).

¹H-NMR spectrum of **2j**



GC-MS spectra of **2j**

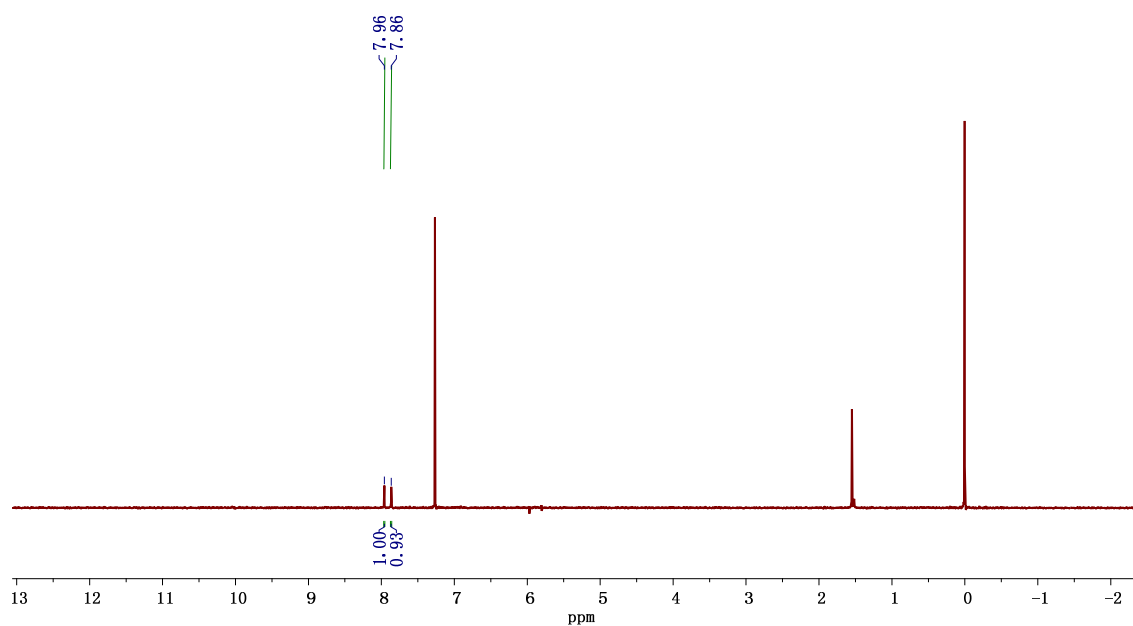




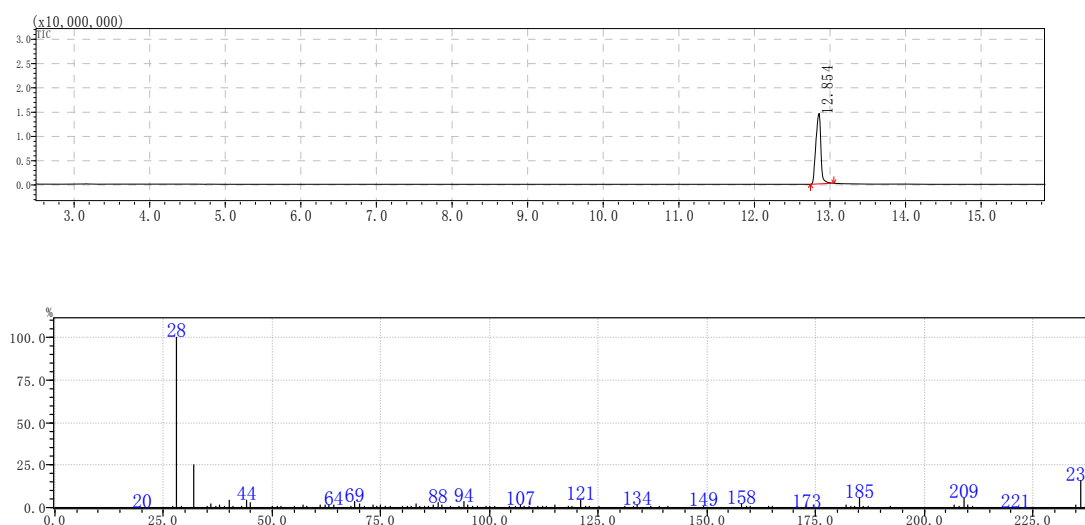
2k: Bright yellow solid; m.p. 299-301 °C; ^1H

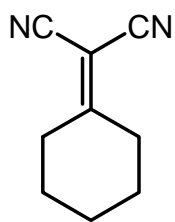
NMR (300 MHz, CDCl_3) δ 7.86 (s, 2H), 7.96 (s, 2H) ppm. GC-MS retention time 12.854 min., m/z (EI) 237(M+, 15), 209 (6), 185 (6), 121(4), 94 (5).

^1H -NMR spectrum of **2k**



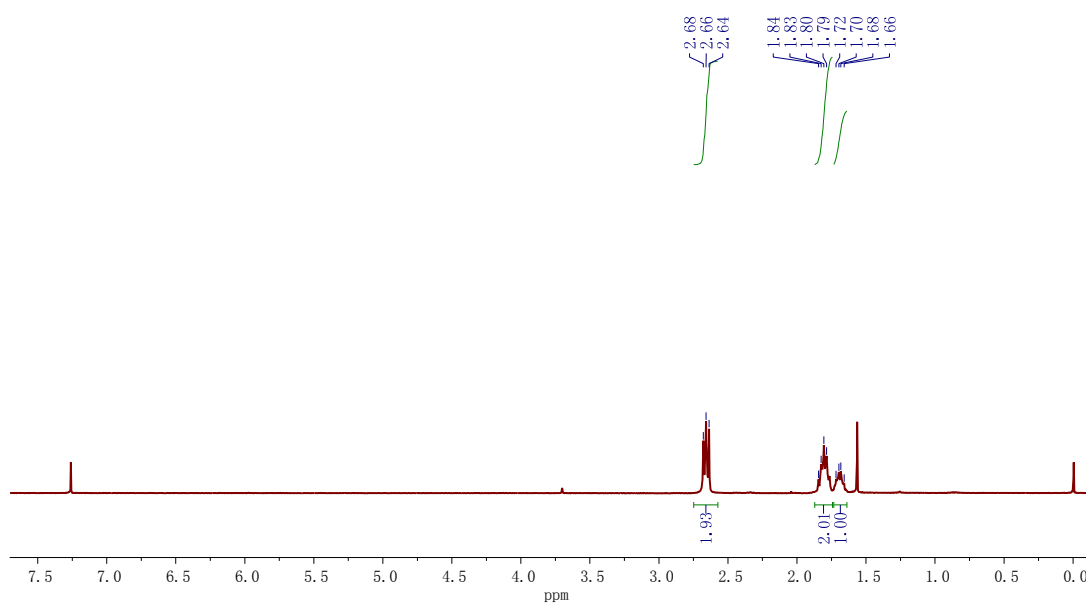
GC-MS spectra of **2k**



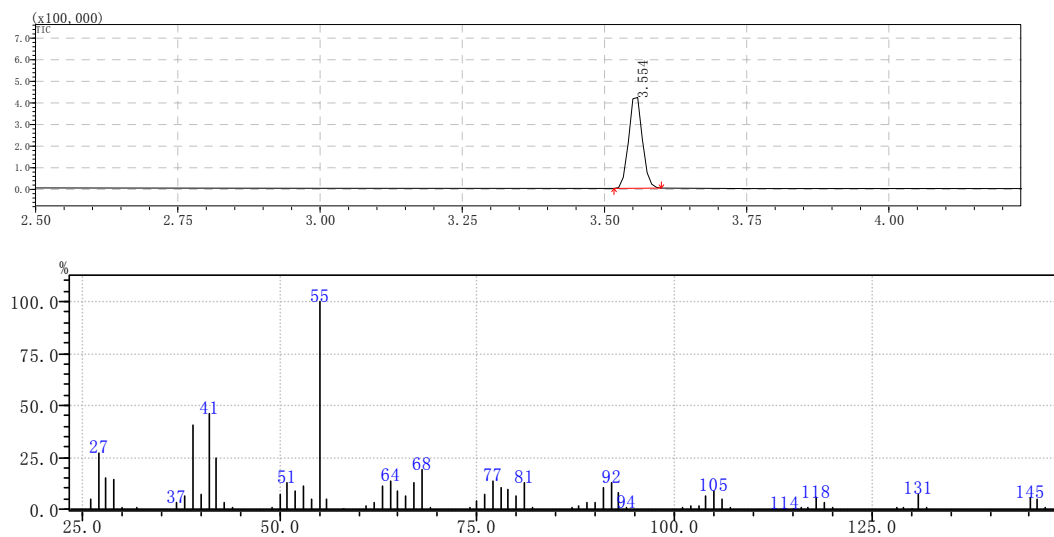


2I: Light yellow oil; ^1H NMR (300MHz, CDCl_3) δ 1.68 (t, 2H), 1.83 (t, 4H), 2.66 (t, $J = 6.0$ Hz, 4H) ppm. GC-MS retention time 3.554 min., m/z (EI) 146 (M^+ , 5.01), 92 (13), 81 (13), 68 (19), 55 (100).

^1H -NMR spectrum of 2I



GC-MS spectra of 2I



Section 12. References

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