Supporting Information

Microwave-assisted Rapid Synthesis of Chiral Oxazolines

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I. Experimental Section

Part 1. General Information

All operations were carried out at room temperature and atmospheric environment. Chlorobenzene was purchased (Energy Chemical, China) and used directly. Deuterated solvents were used as received ($CDCl_3$, C_2D_6SO from Energy Chemical, China). $ZnCl_2$ (Sinopharm Group Co., China), $CoCl_2$ (Energy Chemical, China), $CoBr_2$ (Energy Chemical, China), CoI_2 (Energy Chemical, China) were purchased and used as received. Unless otherwise noted, all other reagents and starting materials were purchased in the analytical purity from commercial sources and used without further purification.

Column chromatography was performed using silica gel 300-400 mesh (purchased from Liangchen Silicon Material CO., Ltd. China) as the solid support. All NMR spectra were recorded on Bruker Avance 500 MHz spectrometer at STP unless otherwise indicated. ^1H NMR and ^{13}C NMR chemical shifts are reported in δ units, parts per million (ppm) relative to the chemical shift of residual solvent. Reference peaks for chloroform in ^1H NMR and ^{13}C NMR spectra were set at 7.26 ppm and 77.16 ppm, respectively. High resolution mass spectra were measured on Bruker MicroTOF II ESI-TOF mass spectrometer. Low resolution mass spectra were measured on Agilent 1260 Infinity II/6125 mass spectrometer. Melting point was recorded on a micro melting point apparatus (X-4, Yuhua Co., Ltd, Gongyi, China).

Part 2. Microwave irradiation experiment and general procedure

1.Microwave Irradiation Experiment:

All microwave irradiation reactions were carried out in a Biotage® Initiator+ microwave reactor, operating with continuous irradiation power from 0 to 400 W and heating up to 300℃ with a cut-off of 30 bar pressure. The microwave reactor was used in the standard configuration as delivered. All reactions were carried out in a Biotage® microwave vial (2-5 mL) and sealed with an aluminum/Teflon® crimp top, which enable to bear maximum internal pressure of 30 bar. The built-in IR sensor of the instrument measures the temperature at all time. After the irradiation period, the reaction vial was cooled down to the ambient temperature by the built-in gas jet cooling before the safety cap was removed[1].

2.General Procedure

General procedure for the reaction of nitrile with β-amino alcohol (Method A): To a flame-dried 2-5 mL microwave vial equipped with a magnetic stir-bar was added with β-amino alcohol (1 mmol, 100 mol %), $CoBr_2$ (21.9 mg,0.1 mmol, 10 mol %), 4A Molecular Sieve (MS, 20% w/w), and nitrile (1 mmol, 100 mol %). Slowly add 2 ml of chlorobenzene along the bottle wall with a dropper. The vial was tightly sealed with aluminum/Teflon® crimp top and was exposed to microwave irradiation at a constant temperature of 200 ℃ for 30 minutes. After completion of the reaction (until no change in pressure was observed), the reaction mixture was cooled to ambient temperature. Subsequently, the reaction mixture was filtered with a Buchner funnel and rinsed three times with a minimum amount of dichloromethane. The solid was recovered after drying in oven. The collected liquid was concentrated in vacuum and then purified by rapid column chromatography.

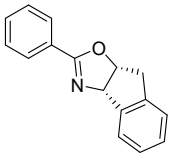
General procedure for the reaction of nitrile with β-amino alcohol (Method B): To a flame-dried 2-5 mL microwave vial equipped with a magnetic stir-bar was charged with β-amino alcohol (1 mmol, 100 mol %), $CoBr_2$ (21.9 mg,0.1 mmol, 10 mol %), 4A MS (20% w/w), nitrile (1 mmol, 100 mol %). The vial was tightly sealed with aluminum/Teflon® crimp top and was exposed to microwave irradiation at a constant temperature of 200 ℃ for 30 minutes. After completion of the reaction (until no change in pressure was observed), the reaction mixture was cooled to ambient temperature. Subsequently, the reaction mixture was filtered with a Buchner funnel and rinsed three

times with a minimum amount of dichloromethane. The solid was recovered after drying in oven. The collected liquid was concentrated in vacuum and then purified by rapid column chromatography.

CAUTION: When method B was used for experimental operation, since there is no solvent, the reactants should be added to the bottom of the microwave vial as smoothly as possible, so as to avoid local overheating caused by the solid adhering to the vial wall, thus causing explosion.

Part 3. Characterization Data of All Compounds

(3a*S*,8a*R*)-2-phenyl-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazole (3).



The title compound was prepared according to the general procedure. After purification in a flash column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was isolated as a white solid. Method A: 188.2 mg (0.80 mmol, 80% yield); Method B: 178.8 mg (0.76 mmol, 76% yield).

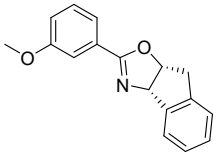
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.01–7.86 (m, 2H), 7.61–7.53 (m, 1H), 7.47–7.41 (m, 1H), 7.40–7.32 (m, 2H), 7.28–7.26 (m, 3H), 5.75 (d, J = 7.9 Hz, 1H), 5.50 (ddd, J = 8.1, 6.9, 1.7 Hz, 1H), 3.51 (dd, J = 17.9, 6.9 Hz, 1H), 3.37 (dd, J = 17.9, 1.7 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 158.7, 136.7, 134.5, 126.0, 123.2, 123.1, 123.0, 122.6, 122.2, 120.4, 120.0, 77.9, 71.7, 34.6.

HRMS (ESI) m/z ([M+H]$^+$) calcd for $C_{16}H_{14}NO$: 236.1070. Found: 236.1098.

M.p.: 142.6-143.6 ºC.

(3a*S*,8a*R*)-2-(3-methoxyphenyl)-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazole (4)



The title compound was prepared according to the general procedure using (1*S*,2*R*)-1-amino-2,3-dihydro-1*H*-inden-2-ol (298.4 mg, 2 mmol, 200 mol %) as the starting amino alcohol. After purification by a flash column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound (209.5 mg, 0.79 mmol, 79% yield) was isolated as a black solid.

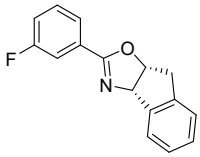
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.60–7.56 (m, 1H), 7.52 (dt, J = 7.6, 1.3 Hz, 1H), 7.47 (dd, J = 2.8, 1.4 Hz, 1H), 7.30–7.26 (m, 4H), 6.99 (ddd, J = 8.3, 2.7, 1.0 Hz, 1H), 5.74 (d, J = 7.8 Hz, 1H), 5.49 (ddd, J = 8.2, 6.9, 1.7 Hz, 1H), 3.82 (s, 3H), 3.54–3.35 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 163.9, 159.3, 141.9, 139.7, 129.2, 129.1, 128.4, 127.4, 125.6, 125.2, 120.8, 118.0, 112.6, 83.1, 76.9, 55.4, 39.8.

HRMS (ESI) m/z ([M+H]$^+$) calcd for $C_{17}H_{16}NO_2$: 266.1176. Found: 266.1176.

M.p.: 104 ºC.

(3a*S*,8a*R*)-2-(3-fluorophenyl)-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazole (5)



The title compound was prepared according to the general procedure. After purification by a flash column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was isolated as a white solid. Method A: 215.3 mg (0.85 mmol, 85% yield); Method B: 202.6 mg (0.80 mmol, 80% yield).

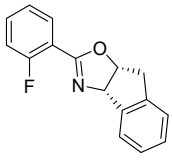
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.72 (dt, J = 7.7, 1.3 Hz, 1H), 7.63 (ddd, J = 9.6, 2.7, 1.5 Hz, 1H), 7.59–7.54 (m, 1H), 7.34 (td, J = 8.0, 5.7 Hz, 1H), 7.31–7.26 (m, 3H), 7.13 (tdd, J = 8.3, 2.6, 0.9 Hz, 1H), 5.75 (d, J = 7.9 Hz, 1H), 5.49 (ddd, J = 8.1, 6.9, 1.7 Hz, 1H), 3.54–-3.34 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 163.5–162.7 (m), 161.4, 141.7, 139.6, 129.8 (d, J = 7.9 Hz), 128.5, 127.5, 125.6, 125.3, 124.0 (d, J = 3.1 Hz), 118.2 (d, J = 21.1 Hz), 115.3 (d, J = 23.4 Hz), 83.4, 77.0, 39.7.

HRMS (ESI) m/z ([M+H]$^+$) calcd for $C_{16}H_{13}FNO$: 254.0976. Found: 254.0975.

M.p.: 162 ºC.

(3a*S*,8a*R*)-2-(2-fluorophenyl)-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazole (6)



The title compound was prepared according to the general procedure A. After purification by a flash column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound (129.2 mg, 0.51 mmol, 51% yield) was isolated as a white solid.

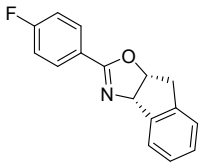
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.85 (td, J = 7.5, 1.9 Hz, 1H), 7.64–7.55 (m, 1H), 7.45–7.36 (m, 1H), 7.31–7.26 (m, 3H), 7.18–7.04 (m, 2H), 5.78 (d, J = 7.9 Hz, 1H), 5.48 (ddd, J = 8.2, 6.8, 1.8 Hz, 1H), 3.56–3.31 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 162.3, 160.9–159.6 (m), 141.7, 139.7, 132.8 (d, J = 8.7 Hz), 131.2 (d, J = 1.9 Hz), 128.5, 127.5, 125.7, 125.3, 123.8 (d, J = 3.8 Hz), 116.6 (d, J = 22.1 Hz), 116.1 (d, J = 10.6 Hz), 82.9, 77.0, 39.8.

HRMS (ESI) m/z ([M+H]$^+$) calcd for $C_{16}H_{13}FNO$: 254.0976. Found: 254.0977.

M.p.: 99.5 ºC.

(3a*S*,8a*R*)-2-(4-fluorophenyl)-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazole (7)



The title compound was prepared according to the general procedure. After purification by a flash column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was isolated as a white solid. Method A: 164.6 mg (0.65 mmol, 65% yield); Method B: 146.9 mg (0.58 mmol, 58% yield).

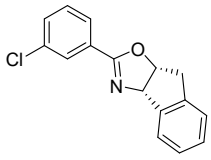
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.93 (dd, J = 8.8, 5.5 Hz, 2H), 7.60–7.53 (m, 1H), 7.31–7.26 (m, 3H), 7.05 (t, J = 8.7 Hz, 2H), 5.73 (d, J = 7.8 Hz, 1H), 5.48 (ddd, J = 8.2, 6.9, 1.7 Hz, 1H), 3.54–3.33 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 165.9, 163.2 (d, J = 27.7 Hz), 141.9, 139.7, 130.6 (d, J = 8.8 Hz), 128.5, 127.5, 125.6, 125.3, 124.1 (d, J = 3.1 Hz), 115.4, 115.2, 83.3, 77.0, 39.8.

HRMS (ESI) m/z ([M+H]$^+$) calcd for $C_{16}H_{13}FNO$: 254.0976. Found: 254.0974.

M.p.: 181.5-182 ºC.

(3a*S*,8a*R*)-2-(3-chlorophenyl)-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazole (8)



The title compound was prepared according to the general procedure. After purification by a flash column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was isolated as a white solid. Method A: 191.5 mg (0.71 mmol, 71% yield); Method B: 188.8 mg (0.70 mmol, 70% yield).

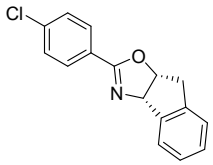
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.93 (t, J = 1.9 Hz, 1H), 7.81 (dt, J = 7.8, 1.3 Hz, 1H), 7.61–7.53 (m, 1H), 7.40 (ddd, J = 8.0, 2.2, 1.1 Hz, 1H), 7.32–7.26 (m, 4H), 5.74 (dd, J = 7.9, 0.8 Hz, 1H), 5.49 (ddd, J = 8.3, 6.9, 1.7 Hz, 1H), 3.56–3.30 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 162.8, 141.7, 139.6, 134.2, 131.2, 129.6, 129.5, 128.5, 128.4, 127.5, 126.4, 125.5, 125.3, 83.4, 77.0, 39.7.

HRMS (ESI) m/z ([M+H]$^+$) calcd for $C_{16}H_{13}ClNO$: 270.0680. Found: 270.0675.

M.p.: 180.5-181.5 ºC.

(3a*S*,8a*R*)-2-(4-chlorophenyl)-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazole (9)



The title compound was prepared according to the general procedure. After purification by a flash column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was isolated as a white solid. Method A: 215.8 mg (0.80 mmol, 80% yield); Method B: 207.7 mg (0.77 mmol, 77% yield).

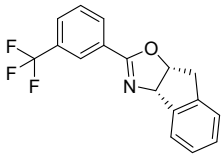
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.90–7.81 (m, 2H), 7.58–7.52 (m, 1H), 7.36–7.32 (m, 2H), 7.30–7.26 (m, 3H), 5.73 (dd, J = 7.9, 0.8 Hz, 1H), 5.48 (ddd, J = 7.9, 6.9, 1.7 Hz, 1H), 3.53–3.33 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 163.1, 141.8, 139.6, 137.4, 129.7, 128.6, 128.5, 127.5, 126.4, 125.6, 125.3, 83.4, 77.0, 39.8.

HRMS (ESI) m/z ([M+H]$^+$) calcd for $C_{16}H_{13}ClNO$: 270.0680. Found: 270.0673.

M.p.: 230.5 ºC.

(3a*S*,8a*R*)-2-(3-(trifluoromethyl)phenyl)-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazole (10)



The title compound was prepared according to the general procedure. After purification by a flash column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was isolated as a white solid. Method A: 248.7 mg (0.82 mmol, 82% yield); Method B: 242.6 mg (0.80 mmol, 80% yield). .

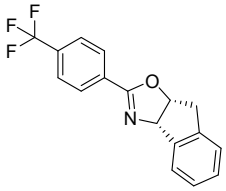
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.21 (d, J = 1.7 Hz, 1H), 8.12 (dd, J = 7.9, 1.4 Hz, 1H), 7.69 (ddt, J = 7.9, 1.8, 0.9 Hz, 1H), 7.61–7.55 (m, 1H), 7.50 (t, J = 7.8 Hz, 1H), 7.32–7.27 (m, 3H), 5.77 (dd, J = 7.9, 0.8 Hz, 1H), 5.52 (ddd, J = 8.1, 6.9, 1.7 Hz, 1H), 3.56–3.37 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 162.7, 141.6, 139.6, 131.5, 130.9, 130.7, 128.7 (d, J = 4.3 Hz), 128.6, 127.7 (q, J = 3.7 Hz), 127.5, 125.6, 125.3 (q, J = 5.6 Hz), 124.8, 122.6, 83.6, 77.1, 39.7.

HRMS (ESI) m/z ([M+H]$^+$) calcd for $C_{17}H_{13}F_3NO$: 304.0944. Found: 304.0949.

M.p.: 172.5 ºC.

(3a*S*,8a*R*)-2-(4-(trifluoromethyl)phenyl)-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazole (11)



The title compound was prepared according to the general procedure A. After purification by a flash column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound (94.1 mg, 0.31 mmol, 31% yield) was isolated as a white solid.

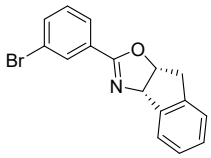
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.07–8.02 (m, 2H), 7.65–7.55 (m, 3H), 7.28 (d, J = 2.3 Hz, 3H), 5.77 (d, J = 7.9 Hz, 1H), 5.52 (ddd, J = 8.2, 6.9, 1.7 Hz, 1H), 3.56–3.35 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 162.8, 141.6, 139.6, 133.0, 132.7, 131.2, 128.7 (d, J = 6.0 Hz), 127.6, 125.6, 125.3, 125.2 (q, J = 3.9 Hz), 122.4, 83.6, 77.1, 39.8.

HRMS (ESI) m/z ([M+H]$^+$) calcd for $C_{17}H_{13}F_3NO$: 304.0944. Found: 304.0938.

M.p.: 188.5 ºC.

(3a*S*,8a*R*)-2-(3-bromophenyl)-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazole (12)



The title compound was prepared according to the general procedure. After purification by a flash column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was isolated as a white solid. Method A: 276.5 mg (0.88 mmol, 88% yield); method B: 263.9 mg (0.84 mmol, 84% yield).

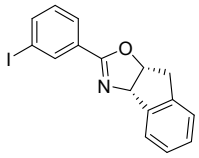
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.09 (t, J = 1.8 Hz, 1H), 7.86 (dt, J = 7.9, 1.3 Hz, 1H), 7.58–7.54 (m, 2H), 7.31–7.27 (m, 3H), 7.23 (t, J = 7.9 Hz, 1H), 5.74 (d, J = 7.8 Hz, 1H), 5.48 (ddd, J = 8.2, 6.9, 1.7 Hz, 1H), 3.53–3.34 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 162.7, 141.7, 139.6, 134.2, 131.34, 129.9, 129.8, 128.6, 127.5, 126.9, 125.6, 125.3, 122.3, 83.4, 77.0, 39.8.

HRMS (ESI) m/z ([M+H]$^+$) calcd for $C_{16}H_{13}BrNO$: 314.0175. Found: 314.0181.

M.p.: 192-193 ºC.

(3a*S*,8a*R*)-2-(3-iodophenyl)-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazole (13)



The title compound was prepared according to the general procedure. After purification by a flash column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was isolated as a white solid. Method A: 339.5 mg (0.94 mmol, 94% yield); Method B: 328.7 mg (0.91 mmol, 91% yield).

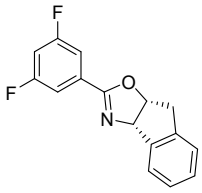
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.29 (t, J = 1.7 Hz, 1H), 7.88 (dt, J = 8.0, 1.4 Hz, 1H), 7.75 (dt, J = 7.9, 1.5 Hz, 1H), 7.58–7.54 (m, 1H), 7.30–7.26 (m, 3H), 7.10 (t, J = 7.9 Hz, 1H), 5.73 (d, J = 7.9 Hz, 1H), 5.48 (ddd, J = 8.3, 7.0, 1.7 Hz, 1H), 3.50 (dd, J = 17.9, 6.9 Hz, 1H), 3.36 (dd, J = 17.9, 1.6 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 162.5, 141.7, 140.1, 139.6, 137.1, 129.9, 129.8, 128.6, 127.5, 127.4, 125.6, 125.3, 93.7, 83.4, 77.0, 39.8.

HRMS (ESI) m/z ([M+H]$^+$) calcd for $C_{16}H_{13}INO$: 362.0036. Found: 362.0031.

M.p.: 197.6 ºC.

(3a*S*,8a*R*)-2-(3,5-difluorophenyl)-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazole(14)



The title compound was prepared according to the general procedure. After purification by a flash column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was isolated as a white solid. Method A: 268.5 mg (0.99 mmol, 99% yield); Method B: 263.1 mg (0.97 mmol, 97% yield).

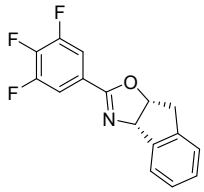
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.56–7.51 (m, 1H), 7.45 (dtd, J = 5.8, 4.6, 2.2 Hz, 2H), 7.30–7.26 (m, 2H), 7.25 (d, J = 5.5 Hz, 1H), 6.86 (tt, J = 8.7, 2.4 Hz, 1H), 5.73 (d, J = 7.8 Hz, 1H), 5.49 (ddd, J = 8.1, 6.9, 1.7 Hz, 1H), 3.52–3.33 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 163.6 (d, J = 12.3 Hz), 162.6–161.0 (m), 141.5, 139.5, 131.0 (t, J = 10.2 Hz), 128.6, 127.6, 125.6, 125.3, 111.5 (d, J = 6.6 Hz), 111.3 (d, J = 6.7 Hz), 106.6 (t, J = 25.3 Hz), 83.7, 77.0, 39.7.

HRMS (ESI) m/z ($[M+H]^+$) calcd for $C_{16}H_{12}F_2NO$: 272.0881. Found: 272.0874.

M.p.: 160.5-161.5 ºC.

(3a*S*,8a*R*)-2-(3,4,5-trifluorophenyl)-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazole (15)



The title compound was prepared according to the general procedure. After purification by a flash column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was isolated as a white solid. Method A: 248.7 mg (0.86 mmol, 86% yield); Method B: 234.3 mg (0.81 mmol, 81% yield).

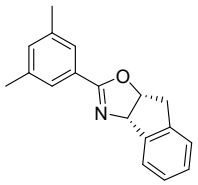
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.62–7.51 (m, 3H), 7.28 (q, J = 2.9 Hz, 3H), 5.74 (d, J = 7.8 Hz, 1H), 5.50 (ddd, J = 8.2, 6.9, 1.7 Hz, 1H), 3.54–3.33 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 161.4 (d, J = 2.6 Hz), 151.9 (dd, J = 10.3, 3.7 Hz), 149.9 (dd, J = 10.3, 3.7 Hz), 142.8 (t, J = 15.4 Hz), 141.4, 140.7 (t, J = 15.2 Hz), 139.5, 128.7, 127.6, 125.5, 125.3, 123.9 (td, J = 8.4, 4.7 Hz), 112.9 (d, J = 5.7 Hz), 112.8 (d, J = 5.7 Hz), 84.0, 77.1, 39.7.

HRMS (ESI) m/z ($[M+H]^+$) calcd for $C_{16}H_{11}F_3NO$: 290.0787. Found: 290.0782.

M.p.: 186.5-187.5 ºC.

(3a*S*,8a*R*)-2-(3,5-dimethylphenyl)-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazole (16)



The title compound was prepared according to the general procedure A. After purification by a flash column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound (134.3 mg, 0.51 mmol, 51% yield)was isolated as a white solid.

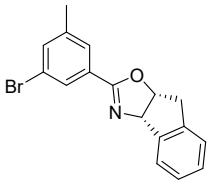
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.60–7.55 (m, 3H), 7.27 (t, J = 3.8 Hz, 1H), 7.25 (d, J = 3.2 Hz, 2H), 7.07 (s, 1H), 5.72 (d, J = 7.9 Hz, 1H), 5.46 (ddd, J = 8.3, 6.9, 1.8 Hz, 1H), 3.52–3.34 (m, 2H), 2.31 (s, 6H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 164.3, 142.0, 139.7, 137.8, 132.9, 128.4, 127.6, 127.4, 126.0, 125.6, 125.2, 83.0, 76.9, 39.8, 21.1.

HRMS (ESI) m/z ($[M+H]^+$) calcd for $C_{18}H_{18}NO$: 264.1383. Found: 264.1384.

M.p.: 166.5-167.5 ºC.

(3a*S*,8a*R*)-2-(3-bromo-5-methylphenyl)-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazole (17)



The title compound was prepared according to the general procedure. After purification by a flash column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was isolated as a white solid. Method A: 265.9 mg (0.81 mmol, 81% yield); Method B: 252.7 mg (0.77 mmol, 77% yield).

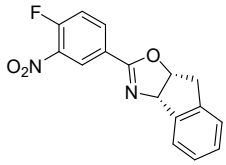
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.87 (t, J = 1.8 Hz, 1H), 7.68 (dt, J = 1.7, 0.9 Hz, 1H), 7.58–7.53 (m, 1H), 7.38 (dq, J = 1.8, 0.9 Hz, 1H), 7.30–7.26 (m, 3H), 5.73 (dd, J = 7.9, 0.8 Hz, 1H), 5.48 (ddd, J = 8.3, 6.9, 1.7 Hz, 1H), 3.53–3.33 (m, 2H), 2.32 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 162.9, 141.7, 140.1, 139.6, 134.8, 129.5, 128.5, 128.4, 127.6, 127.5, 125.5, 125.3, 122.0, 83.4, 77.0, 39.8, 20.9.

HRMS (ESI) m/z ($[M+H]^+$) calcd for $C_{18}H_{15}BrNO$: 328.0332. Found: 328.0324.

M.p.: 208.6 ºC.

(3a*S*,8a*R*)-2-(4-fluoro-3-nitrophenyl)-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazole (18)

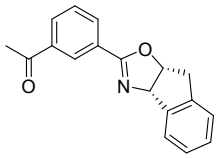


The title compound was prepared according to the general procedure A. After purification by a flash column chromatography (SiO_2: 30% ethyl acetate in petroleum ether), the title compound (259.5 mg, 0.87 mmol, 87% yield) was isolated as a yellow solid.

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.55–8.42 (m, 2H), 7.65–7.60 (m, 1H), 7.52–7.47 (m, 1H), 7.32 (d, J = 5.4 Hz, 1H), 7.21 (s, 1H), 6.89 (d, J = 8.7 Hz, 1H), 5.12 (dd, J = 7.8, 4.8 Hz, 1H), 4.79 (t, J = 4.8 Hz, 1H), 3.32– 3.04(m, 2H).

^{13}C NMR (101 MHz, DMSO-d_6): δ 148.3, 147.0, 141.0 (d, J = 24.7 Hz), 137.9, 136.6, 131.8 (d, J = 46.2 Hz), 130.7, 129.7, 127.9, 126.6, 125.3, 123.6, 120.2, 118.2 (d, J = 12.9 Hz), 116.6, 96.6 (d, J = 32.2 Hz), 71.9, 59.6, 39.7.**M.p.**: 164-166 ºC.

1-(3-((3a*S*,8a*R*)-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazol-2-yl)phenyl)ethan-1-one (19)



The title compound was prepared according to the general procedure A. After purification by a flash column chromatography (SiO_2: 10% ethyl acetate in petroleum ether), the title compound (133.1 mg, 0.48 mmol, 48% yield) was isolated in 48% yield as a white solid.

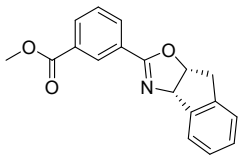
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.47 (t, J = 1.8 Hz, 1H), 8.12 (dt, J = 7.7, 1.5 Hz, 1H), 8.03 (dt, J = 7.9, 1.5 Hz, 1H), 7.60–7.55 (m, 1H), 7.47 (t, J = 7.8 Hz, 1H), 7.31–7.26 (m, 3H), 5.82–5.72 (m, 1H), 5.52 (ddd, J = 8.3, 7.0, 1.7 Hz, 1H), 3.57–3.35 (m, 2H), 2.62 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 197.4, 163.2, 141.7, 139.6, 137.1, 132.7, 130.7, 128.7, 128.6, 128.4, 128.3, 127.5, 125.6, 125.3, 83.5, 77.0, 39.7, 26.7.

HRMS (ESI) m/z ([M+H]$^+$) calcd for $C_{18}H_{16}NO_2$: 278.1176. Found: 278.1175.

M.p.: 119-120 ºC.

methyl 3-((3a*S*,8a*R*)-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazol-2-yl)benzoate (20)



The title compound was prepared according to the general procedure. After purification by a flash column chromatography (SiO_2: 10% ethyl acetate in petroleum ether), the title compound was isolated as a white solid. Method A: 193.6 mg (0.66 mmol, 66% yield); Method B: 173.1 mg, (0.59 mmol, 59% yield).

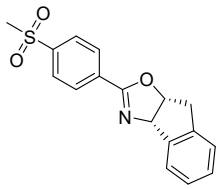
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.57 (t, J = 1.8 Hz, 1H), 8.12 (tt, J = 7.9, 1.4 Hz, 2H), 7.62–7.54 (m, 1H), 7.45 (t, J = 7.8 Hz, 1H), 7.30–7.26 (m, 3H), 5.76 (dd, J = 7.9, 0.9 Hz, 1H), 5.51 (ddd, J = 7.9, 6.9, 1.7 Hz, 1H), 3.92 (s, 3H), 3.55–3.36 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 166.4, 163.2, 141.7, 139.6, 132.6, 132.2, 130.3, 129.4, 128.5, 128.4, 128.2, 127.5, 125.6, 125.3, 83.5, 77.0, 52.2, 39.7.

HRMS (ESI) m/z ([M+H]$^+$) calcd for $C_{18}H_{16}NO_3$: 294.1125. Found: 294.1124.

M.p.: 135-136 ºC.

(3a*S*,8a*R*)-2-(4-(methylsulfonyl)phenyl)-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazole (21)



The title compound was prepared according to the general procedure. After purification by a flash column chromatography (SiO_2: 1% methyl alcohol in dichloromethane), the title compound was isolated as a white solid. Method A: 256.9 mg (0.82 mmol, 82% yield); Method B: 241.3 mg, (0.77 mmol, 77% yield).

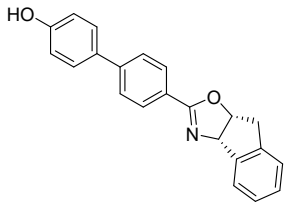
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.14–8.10 (m, 2H), 7.96–7.91 (m, 2H), 7.57–7.53 (m, 1H), 7.28 (d, J = 2.5 Hz, 3H), 5.78 (dd, J = 7.9, 0.8 Hz, 1H), 5.54 (ddd, J = 8.1, 6.9, 1.7 Hz, 1H), 3.56–3.35 (m, 2H), 3.03 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 162.3, 142.6, 141.4, 139.5, 132.9, 129.2, 128.7, 127.5, 127.2, 125.5, 125.3, 83.7, 77.1, 44.3, 39.7.

HRMS (ESI) m/z ([M+H]$^+$) calcd for $C_{17}H_{16}NO_3S$: 314.0845. Found: 314.0838.

M.p.: 244 ºC.

4'-((3a*S*,8a*R*)-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazol-2-yl)-[1,1'-biphenyl]-4-ol (22)



The title compound was prepared according to the general procedure. After purification by a flash column chromatography (SiO_2: 1% methyl alcohol in dichloromethane), the title compound was isolated as a white solid. Method A: 229.2 mg (0.70 mmol, 70% yield); Method B: 199.7 mg, (0.61 mmol, 61% yield).

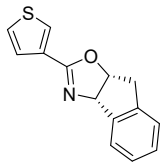
^{1}H NMR (500 MHz, DMSO-d_6): δ 9.69 (s, 1H), 7.88–7.86 (m, 2H), 7.67–7.65 (m, 2H), 7.56–7.54 (m, 2H), 7.48–7.45 (m, 1H), 7.31–7.29 (m, 1H), 7.27–7.25 (m, 2H), 6.88–6.86 (m, 2H), 5.71 (d, J = 7.9 Hz, 1H), 5.54–5.51 (m, 1H), 3.51 (dd, J = 18.1, 6.9 Hz, 1H), 3.27–3.23 (m, 1H).

^{13}C NMR (126 MHz, DMSO-d_6): δ 162.8, 158.2, 143.4, 142.6, 140.3, 130.0, 128.8, 128.7, 128.4, 127.5, 126.2, 125.8, 125.7, 125.6, 116.3, 83.3, 76.7, 39.7.

HRMS (ESI) m/z ([M+H]$^+$) calcd for $C_{22}H_{18}NO_2$: 328.1332. Found: 328.1326.

M.p.: 261-262 ºC.

(3a*S*,8a*R*)-2-(thiophen-3-yl)-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazole (23)



The title compound was prepared according to the general procedure. After purification by a flash column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was isolated as a white solid. Method A: 219.6 mg (0.91 mmol, 91% yield); Method B: 212.4 mg, (0.88 mmol, 88% yield).

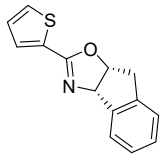
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.86 (dd, J = 3.0, 1.2 Hz, 1H), 7.58–7.54 (m, 1H), 7.50 (dd, J = 5.1, 1.2 Hz, 1H), 7.31–7.26 (m, 3H), 7.25 (s, 1H), 5.71 (d, J = 7.8 Hz, 1H), 5.44 (ddd, J = 8.0, 6.9, 1.8 Hz, 1H), 3.52–3.32 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 160.3, 141.9, 139.7, 130.0, 128.8, 128.5, 127.5, 127.3, 126.0, 125.6, 125.3, 83.0, 76.9, 39.7.

HRMS (ESI) m/z ([M+H]$^+$) calcd for $C_{14}H_{12}NOS$: 242.0634. Found: 242.0634.

M.p.: 147 ºC.

(3a*S*,8a*R*)-2-(thiophen-2-yl)-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazole (24)



The title compound was prepared according to the general procedure. After purification by a flash column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was isolated as a white solid. Method A: 229.2 mg (0.95 mmol, 95% yield); Method B: 219.6 mg, (0.91 mmol, 91% yield).

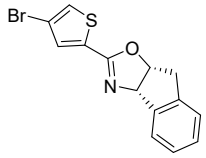
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.60–7.54 (m, 2H), 7.40 (dd, J = 5.0, 1.2 Hz, 1H), 7.27 (d, J = 3.1 Hz, 2H), 7.25 (d, J = 1.3 Hz, 1H), 7.02 (dd, J = 5.0, 3.7 Hz, 1H), 5.71 (d, J = 7.8 Hz, 1H), 5.47 (ddd, J = 8.1, 6.8, 1.8 Hz, 1H), 3.51–3.33 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 159.7, 141.7, 139.6, 130.4, 129.8, 128.5, 127.5, 125.7, 125.3, 83.7, 77.1, 39.6.

HRMS (ESI) m/z ([M+H]$^+$) calcd for $C_{14}H_{12}NOS$: 242.0634. Found: 242.0637.

M.p.: 156.5-157.5 ºC.

(3a*S*,8a*R*)-2-(4-bromothiophen-2-yl)-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazole (25)



The title compound was prepared according to the general procedure. After purification by a flash column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was isolated as a white solid. Method A: 297.8 mg (0.93 mmol, 93% yield); Method B: 281.8 mg, (0.88 mmol, 88% yield).

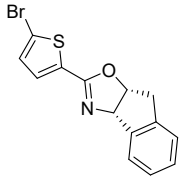
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.56–7.53 (m, 1H), 7.48 (d, J = 1.5 Hz, 1H), 7.30–7.26 (m, 4H), 5.72 (dd, J = 7.8, 0.7 Hz, 1H), 5.48 (ddd, J = 7.8, 6.8, 1.7 Hz, 1H), 3.51–3.33 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 158.5, 141.4, 139.5, 132.5, 131.5, 128.6, 127.5, 126.9, 125.6, 125.3, 110.1, 84.0, 77.1, 39.5.

HRMS (ESI) m/z ([M+H]$^+$) calcd for $C_{14}H_{11}BrNOS$: 319.9739. Found: 319.9738.

M.p.: 162-163 ºC.

(3a*S*,8a*R*)-2-(5-bromothiophen-2-yl)-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazole (26)



The title compound was prepared according to the general procedure. After purification by a flash column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was isolated as a white solid. Method A: 294.6 mg (0.92 mmol, 92% yield); Method B: 281.8 mg, (0.88 mmol, 88% yield).

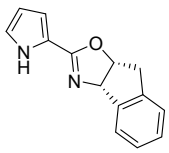
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.55–7.51 (m, 1H), 7.30 (d, J = 3.9 Hz, 1H), 7.29–7.26 (m, 2H), 7.25 (s, 1H), 6.98 (d, J = 3.9 Hz, 1H), 5.68 (d, J = 7.8 Hz, 1H), 5.45 (ddd, J = 7.9, 6.9, 1.7 Hz, 1H), 3.49–3.32 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 158.6, 141.5, 139.5, 131.9, 130.6, 130.5, 128.6, 127.5, 125.6, 125.3, 117.3, 83.8, 77.0, 39.5.

HRMS (ESI) m/z ([M+H]$^+$) calcd for $C_{14}H_{11}BrNOS$: 319.9739. Found: 319.9742.

M.p.: 177-178 ºC.

(3a*S*,8a*R*)-2-(1H-pyrrol-2-yl)-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazole (27)



The title compound was prepared according to the general procedure. After purification by a flash column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was isolated as a red brown solid. Method A: 188.4 mg (0.84 mmol, 84% yield); Method B: 174.9 mg, (0.78 mmol, 78% yield).

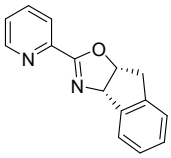
^{1}H NMR (500 MHz, $CDCl_3$): δ 10.94 (s, 1H), 7.39 (d, J = 6.9 Hz, 1H), 7.27 (d, J = 2.8 Hz, 1H), 7.25 (d, J = 2.1 Hz, 1H), 7.19 (ddt, J = 7.9, 5.3, 2.6 Hz, 1H), 6.74 (d, J = 21.4 Hz, 2H), 6.19 (t, J = 2.9 Hz, 1H), 5.73–5.69 (m, 1H), 5.49–5.44 (m, 1H), 3.52–3.35 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 159.2, 141.8, 139.7, 128.5, 127.5, 125.6, 125.3, 122.7, 119.8, 113.3, 109.5, 83.3, 76.0, 39.6.

HRMS (ESI) m/z ([M+H]$^+$) calcd for $C_{14}H_{13}N_2O$: 225.1022. Found: 225.1022.

M.p.: 158.5-159.5 ºC.

(3a*S*,8a*R*)-2-(pyridin-2-yl)-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazole (28)



The title compound was prepared according to the general procedure. After purification by a flash column chromatography (SiO_2: 30% ethyl acetate in petroleum ether), the title compound was isolated as a pale-yellow solid. Method A: 155.9 mg (0.66 mmol, 66% yield); Method B: 125.2 mg, (0.53 mmol, 53% yield).

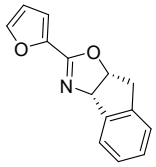
^{1}H NMR (500 MHz, $CDCl_3$): δ 9.12 (dd, J = 2.2, 0.9 Hz, 1H), 8.66 (dd, J = 4.9, 1.8 Hz, 1H), 8.19 (dt, J = 8.0, 1.9 Hz, 1H), 7.59–7.54 (m, 1H), 7.32–7.27 (m, 4H), 5.78–5.74 (m, 1H), 5.51 (ddd, J = 8.2, 6.9, 1.7 Hz, 1H), 3.55–3.35 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 162.0, 151.9, 149.5, 141.6, 139.6, 135.7, 128.6, 127.5, 125.6, 125.3, 124.0, 123.1, 83.5, 77.0, 39.7.

HRMS (ESI) m/z ([M+H]$^+$) calcd for $C_{15}H_{13}N_2O$: 237.1022. Found: 237.1016.

M.p.: 166 ºC.

(3a*S*,8a*R*)-2-(furan-2-yl)-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazole (29)



The title compound was prepared according to the general procedure. After purification by a flash column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was isolated as a pale-yellow solid. Method A: 220.7 mg (0.98 mmol, 98% yield); Method B: 211.7 mg, (0.94 mmol, 94% yield).

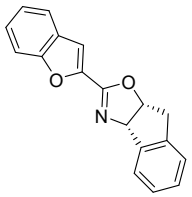
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.60–7.54 (m, 1H), 7.49 (d, J = 1.7 Hz, 1H), 7.27 (d, J = 3.5 Hz, 1H), 7.25 (s, 2H), 6.93 (d, J = 3.5 Hz, 1H), 6.44 (dd, J = 3.5, 1.8 Hz, 1H), 5.73 (d, J = 7.7 Hz, 1H), 5.46 (ddd, J = 8.2, 6.9, 1.7 Hz, 1H), 3.51–3.33 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 156.3, 145.1, 142.9, 141.5, 139.5, 128.5, 127.5, 125.7, 125.2, 114.4, 111.4, 83.5, 76.8, 39.5.

HRMS (ESI) m/z ([M+H]$^+$) calcd for $C_{14}H_{12}NO_2$: 226.0863. Found: 226.0858.

M.p.: 134 ºC.

(3a*S*,8a*R*)-2-(benzofuran-2-yl)-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazole (30)



The title compound was prepared according to the general procedure. After purification by a flash column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was isolated as a white solid. Method A: 269.8 mg (0.98 mmol, 98% yield); Method B: 256.0 mg, (0.93 mmol, 93% yield).

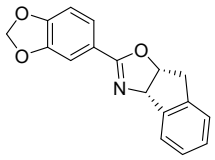
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.64–7.59 (m, 2H), 7.55 (dt, J = 8.4, 0.9 Hz, 1H), 7.36 (ddd, J = 8.5, 7.2, 1.3 Hz, 1H), 7.31–7.27 (m, 4H), 7.26–7.23 (m, 1H), 5.81 (d, J = 7.8 Hz, 1H), 5.53 (ddd, J = 7.9, 6.9, 1.7 Hz, 1H), 3.55–3.38 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 156.8, 155.5, 144.2, 141.3, 139.5, 128.7, 127.6, 127.2, 126.6, 125.8, 125.3, 123.5, 122.1, 112.0, 110.7, 83.8, 77.1, 39.6.

HRMS (ESI) m/z ([M+H]$^+$) calcd for $C_{18}H_{14}NO_2$: 276.1019. Found: 276.1012.

M.p.: 219.5-220.5 ºC.

(3a*S*,8a*R*)-2-(benzo[*d*][1,3]dioxol-5-yl)-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazole(31)



The title compound was prepared according to the general procedure A. After purification by a flash column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound (117.3 mg, 0.42 mmol, 42% yield)was isolated as a white solid.

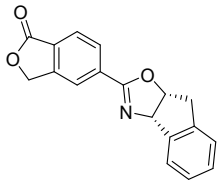
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.54 (dt, J = 4.7, 3.0 Hz, 1H), 7.47 (dd, J = 8.1, 1.7 Hz, 1H), 7.39 (d, J = 1.7 Hz, 1H), 7.27 (d, J = 4.5 Hz, 1H), 7.25 (d, J = 3.3 Hz, 2H), 6.77 (d, J = 8.2 Hz, 1H), 5.96 (q, J = 1.4 Hz, 2H), 5.69 (dd, J = 7.9, 0.8 Hz, 1H), 5.44 (ddd, J = 7.9, 6.9, 1.7 Hz, 1H), 3.50–3.31 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 163.5, 150.1, 147.5, 142.0, 139.7, 128.4, 127.4, 125.5, 125.2, 123.3, 121.8, 108.5, 107.9, 101.4, 83.1, 76.8, 39.7.

HRMS (ESI) m/z ([M+H]$^+$) calcd for $C_{17}H_{14}NO_3$: 280.0968. Found: 280.0969.

M.p.: 243.5 ºC.

5-((3a*S*,8a*R*)-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazol-2-yl)isobenzofuran-1(3*H*)-one (32)



The title compound was prepared according to the general procedure. After purification by a flash column chromatography (SiO_2: 20% ethyl acetate in petroleum ether), the title compound was isolated as a pale-yellow solid. Method A: 279.7 mg (0.96 mmol, 96% yield); Method B: 273.8 mg, (0.94 mmol, 94% yield).

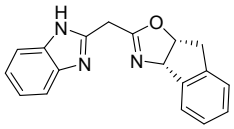
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.10–8.05 (m, 2H), 7.90 (d, J = 7.8 Hz, 1H), 7.57–7.54 (m, 1H), 7.30–7.27 (m, 3H), 5.78 (d, J = 7.8 Hz, 1H), 5.55 (ddd, J = 8.2, 6.9, 1.7 Hz, 1H), 5.29 (d, J = 3.1 Hz, 2H), 3.56–3.36 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 170.2, 162.8, 146.3, 141.4, 139.5, 133.4, 129.2, 128.7, 127.9, 127.6, 125.6, 125.5, 125.4, 122.1, 83.8, 77.1, 69.5, 39.7.

HRMS (ESI) m/z ([M+Na]$^+$) calcd for $C_{18}H_{13}NNaO_3$: 314.0788. Found: 314.0780.

M.p.: 309-310 ºC.

(3a*S*,8a*R*)-2-((1*H*-benzo[*d*]imidazol-2-yl)methyl)-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazole (33)



The title compound was prepared according to the general procedure A. After purification by a flash column chromatography (SiO_2: 5% methyl alcohol in dichloromethane), the title compound (144.7 mg, 0.50 mmol, 50% yield) was isolated as a red brown solid.

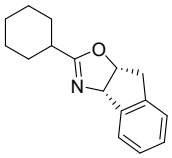
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.51 (dd, J = 6.0, 3.2 Hz, 2H), 7.49–7.45 (m, 1H), 7.28 (d, J = 7.8 Hz, 1H), 7.23 (dd, J = 6.3, 2.4 Hz, 2H), 7.19 (dd, J = 6.0, 3.2 Hz, 2H), 5.60 (dd, J = 7.9, 1.3 Hz, 1H), 5.37 (ddd, J = 8.3, 7.0, 1.7 Hz, 1H), 3.96 (qd, J = 19.1, 1.2 Hz, 2H), 3.47–3.25 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 164.1, 147.8, 141.2, 139.6, 128.8, 127.5, 125.4, 125.3, 122.2, 83.4, 76.3, 39.5, 28.2.

HRMS (ESI) m/z ([M+H]$^+$) calcd for $C_{18}H_{16}N_3O$: 290.1288. Found: 290.1289.

M.p.: 213-215 ºC.

(3a*S*,8a*R*)-2-cyclohexyl-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazole (34)



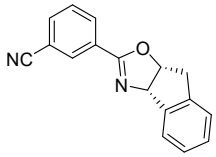
The title compound was prepared according to the general procedure A. After purification by a flash column chromatography (SiO_2: 10% ethyl acetate in petroleum ether), the title compound (55.5 mg, 0.23 mmol, 23% yield) was isolated as a colorless oil.

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.22 (dt, J = 9.5, 2.6 Hz, 4H), 5.34 (dd, J = 8.4, 5.1 Hz, 1H), 4.59 (td, J = 5.2, 2.3 Hz, 1H), 3.15 (dd, J = 16.5, 5.3 Hz, 1H), 2.92 (dd, J = 16.5, 2.3 Hz, 1H), 2.22–2.18 (m, 1H), 1.83–1.65 (m, 4H), 1.42 (s, 2H), 1.40–1.31 (m, 4H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 177.0, 140.8, 139.9, 128.2, 127.2, 125.3, 124.5, 73.7, 57.2, 45.6, 39.7, 31.4, 29.7,25.7.

HRMS (ESI) m/z ([M+H]$^+$) calcd for $C_{16}H_{19}NNaO$: 264.1359. Found: 264.1349.

3-((3a*S*,8a*R*)-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazol-2-yl)benzonitrile (35a)



The title compound was prepared according to the general procedure using (1*S*,2*R*)-1-amino-2,3-dihydro-1*H*-inden-2-ol (447.6 mg, 3 mmol, 300 mol %), benzonitrile (154.7 mg, 1.5 mmol, 150 mol %), chlorobenzene (3 mL). After purification by a flash column chromatography (SiO2: 10% ethyl acetate in petroleum ether), the title compound (105.4 mg, 0.40 mmol, 27% yield) was isolated as a white solid.

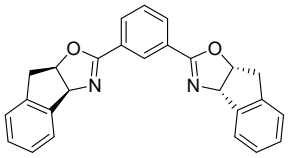
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.21 (d, J = 1.8 Hz, 1H), 8.14 (dt, J = 7.9, 1.6 Hz, 1H), 7.69 (dd, J = 7.7, 1.6 Hz, 1H), 7.57–7.53 (m, 1H), 7.47 (td, J = 7.8, 1.4 Hz, 1H), 7.30–7.26 (m, 3H), 5.76 (d, J = 7.9 Hz, 1H), 5.54–5.49 (m, 1H), 3.55–3.34 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 162.0, 141.4, 139.5, 134.3, 132.4, 131.9, 129.2, 129.1, 128.7, 127.6, 125.5, 125.4, 118.0, 112.6, 83.8, 77.1, 39.7.

HRMS (ESI) m/z ([M+H]$^+$) calcd for $C_{17}H_{13}N_2O$: 261.1022. Found: 261.1017.

M.p.: 218 ºC.

1,3-bis((3a*S*,8a*R*)-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazol-2-yl)benzene (35b)



The title compound was prepared according to the general procedure using (1*S*,2*R*)-1-amino-2,3-dihydro-1*H*-inden-2-ol (447.6 mg, 3 mmol, 300 mol %), benzonitrile (154.7 mg, 1.5 mmol, 150 mol %), chlorobenzene (3 mL). After purification by a flash column chromatography (SiO2: 10% ethyl acetate in petroleum ether), the title compound (394.4 mg, 1.01 mmol, 67% yield) was isolated as a white solid.

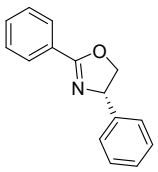
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.45 (s, 1H), 8.02 (dd, J = 7.8, 1.7 Hz, 2H), 7.58–7.55 (m, 2H), 7.38 (t, J = 7.8 Hz, 1H), 7.27 (d, J = 4.5 Hz, 2H), 7.25 (t, J = 2.4 Hz, 4H), 5.73 (d, J = 7.9 Hz, 2H), 5.48 (ddd, J = 8.1, 7.0, 1.7 Hz, 2H), 3.49 (dd, J = 17.9, 6.8 Hz, 2H), 3.36 (dd, J = 17.9, 1.6 Hz, 2H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 163.3, 141.8, 139.7, 131.0, 128.5, 128.3, 128.2, 128.0, 127.5, 125.6, 125.3, 83.3, 77.0, 39.7.

HRMS (ESI) m/z ([M+H]$^+$) calcd for $C_{26}H_{21}N_2O_2$: 393.1598. Found: 393.1595.

M.p.: 313-315 ºC.

(*S*)-2,4-diphenyl-4,5-dihydrooxazole (36)



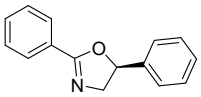
The title compound was prepared according to the general procedure. After purification by a flash column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was isolated as a colorless oil. Method A: 136.2 mg (0.61 mmol, 61% yield); Method B: 140.7 mg, (0.63 mmol, 63% yield).

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.10–8.00 (m, 2H), 7.54–7.27 (m, 8H), 5.37 (dd, J = 10.1, 8.1 Hz, 1H), 4.77 (dd, J = 10.1, 8.4 Hz, 1H), 4.25 (t, J = 8.3 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 164.8, 142.4, 131.6, 128.8, 128.5, 128.4, 127.6, 127.5, 126.8, 74.9, 70.1.

HRMS (ESI) m/z ([M+H]$^+$) calcd for $C_{15}H_{14}NO$: 224.1070. Found: 224.1061.

(*S*)-2,5-diphenyl-4,5-dihydrooxazole (37)



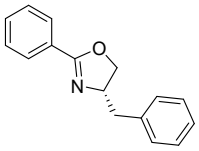
The title compound was prepared according to the general procedure A. After purification by a flash column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound (100.5 mg, 0.45 mmol, 45% yield) was isolated as a colorless oil.

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.07–8.00 (m, 2H), 7.54–7.48 (m, 1H), 7.44 (dd, J = 8.2, 6.6 Hz, 2H), 7.41–7.33 (m, 5H), 5.67 (dd, J = 10.2, 7.9 Hz, 1H), 4.52–3.98 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 164.0, 141.0, 131.5, 128.8, 128.4, 128.3, 127.6, 125.7, 81.0, 63.1.

HRMS (ESI) m/z ([M+H]$^+$) calcd for $C_{15}H_{14}NO$: 224.1070. Found: 224.1064.

(*S*)-4-benzyl-2-phenyl-4,5-dihydrooxazole (38)



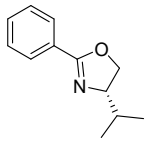
The title compound was prepared according to the general procedure A. After purification by a flash column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound (90.2 mg, 0.38 mmol, 38% yield) was isolated as a colorless oil.

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.00–7.91 (m, 2H), 7.51–7.39 (m, 3H), 7.34–7.29 (m, 2H), 7.27 (d, J = 1.6 Hz, 1H), 7.25 (t, J = 3.9 Hz, 2H), 4.66–4.55 (m, 1H), 4.35 (t, J = 8.9 Hz, 1H), 4.15 (dd, J = 8.5, 7.3 Hz, 1H), 3.29–3.22 (m, 1H), 2.74 (dd, J = 13.7, 8.9 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 164.0, 137.9, 131.4, 129.3, 128.6, 128.5, 128.4, 128.3, 128.2, 127.7, 126.5, 71.8, 67.8, 41.8.

HRMS (ESI) m/z ([M+Na]$^+$) calcd for $C_{16}H_{15}NNaO$: 260.1046. Found: 260.1042.

(*S*)-4-isopropyl-2-phenyl-4,5-dihydrooxazole (40)



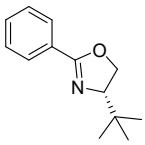
The title compound was prepared according to the general procedure. After purification by a flash column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was isolated as a colorless oil. Method A: 145.7 mg (0.77 mmol, 77% yield); Method B: 138.2 mg, (0.73 mmol, 73% yield).

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.03–7.88 (m, 2H), 7.48–7.36 (m, 3H), 4.43–4.35 (m, 1H), 4.17–4.05 (m, 2H), 1.93–1.82 (m, 1H), 1.03 (dd, J = 6.8, 1.3 Hz, 3H), 0.92 (dd, J = 6.8, 1.3 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 163.4, 131.1, 128.2, 127.9, 72.5, 70.0, 32.8, 18.9, 18.0.

HRMS (ESI) m/z ([M+H]$^+$) calcd for $C_{12}H_{16}NO$: 190.1226. Found: 190.1226.

(*S*)-4-(tert-butyl)-2-phenyl-4,5-dihydrooxazole (41)



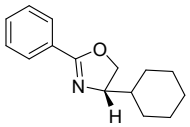
The title compound was prepared according to the general procedure. After purification by a flash column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was isolated as a colorless oil. Method A: 148.4 mg (0.73 mmol, 73% yield); Method B: 142.3 mg, (0.70 mmol, 70% yield).

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.99–7.93 (m, 1H), 7.52–7.37 (m, 3H), 7.18–7.13 (m, 1H), 4.75–4.30 (m, 2H), 4.27–4.00 (m, 1H), 1.02 (s, 6H), 0.95 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 167.4, 163.3, 131.6, 131.1, 128.4, 128.2 (d, J = 2.0 Hz), 128.1, 126.1, 112.3, 69.9, 68.7, 37.1, 25.8, 25.0.

HRMS (ESI) m/z ([M+H]$^+$) calcd for $C_{13}H_{18}NO$: 204.1383. Found: 204.1376.

(*S*)-4-cyclohexyl-2-phenyl-4,5-dihydrooxazole (42)



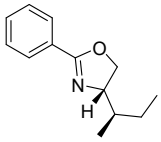
The title compound was prepared according to the general procedure. After purification by a flash column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was isolated as a colorless oil. Method A: 160.5 mg (0.70 mmol, 70% yield); Method B: 126.1 mg, (0.55 mmol, 55% yield).

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.05–7.82 (m, 2H), 7.49–7.33 (m, 3H), 4.38 (dd, J = 9.6, 8.2 Hz, 1H), 4.15 (t, J = 8.0 Hz, 1H), 4.08 (ddd, J = 9.6, 7.9, 6.4 Hz, 1H), 1.98–1.93 (m, 1H), 1.80–1.65 (m, 4H), 1.64–1.49 (m, 2H), 1.29–1.17 (m, 4H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 163.3, 131.1, 128.2, 71.6, 70.3, 42.8, 29.5, 28.7, 26.5, 26.1, 26.0.

HRMS (ESI) m/z ([M+H]$^+$) calcd for $C_{15}H_{20}NO$: 230.1539. Found: 230.1531.

(*S*)-4-((*R*)-sec-butyl)-2-phenyl-4,5-dihydrooxazole (43)



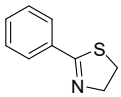
The title compound was prepared according to the general procedure. After purification by a flash column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was isolated as a colorless oil. Method A: 191.1 mg (0.94 mmol, 94% yield); Method B: 176.9 mg, (0.87 mmol, 87% yield).

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.98–7.89 (m, 2H), 7.54–7.33 (m, 3H), 4.33 (dd, J = 9.6, 7.9 Hz, 1H), 4.23–4.17 (m, 1H), 4.10 (t, J = 7.8 Hz, 1H), 1.73–1.53 (m, 2H), 1.24–1.16 (m, 1H), 0.94 (d, J = 7.4 Hz, 3H), 0.83 (d, J = 6.8 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 163.3, 131.1, 128.2, 71.0, 69.4, 39.0, 26.1, 14.2, 11.6.

HRMS (ESI) m/z ([M+H]$^+$) calcd for $C_{13}H_{18}NO$: 204.1383. Found: 204.1381.

2-phenyl-4,5-dihydrothiazole (44)



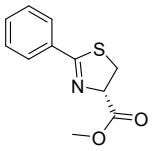
The title compound was prepared according to the general procedure. After purification by a flash column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound was isolated as a light-yellow oil. Method A: 120.8 mg (0.74 mmol, 74% yield); Method B: 117.5 mg, (0.72 mmol, 72% yield).

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.91–7.75 (m, 2H), 7.51–7.34 (m, 3H), 4.45 (t, J = 8.3 Hz, 2H), 3.41 (t, J = 8.3 Hz, 2H).

^{13}C NMR (126 MHz, $CDCl_3$): δ 168.5, 133.2, 131.1, 128.5, 128.3, 65.2, 33.6.

HRMS (ESI) m/z ([M+H]$^+$) calcd for $C_9H_{10}NS$: 164.0528. Found: 164.0522.

methyl (*S*)-2-phenyl-4,5-dihydrothiazole-4-carboxylate (45)



The title compound was prepared according to the general procedure A. After purification by a flash column chromatography (SiO_2: 5% ethyl acetate in petroleum ether), the title compound (79.7 mg, 0.36 mmol, 36% yield) was isolated as a colorless oil

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.90–7.87 (m, 2H), 7.5–7.40 (m, 3H), 5.31 (t, J = 9.0 Hz, 1H), 3.84 (s, 3H), 3.83–3.80 (m, 2H).

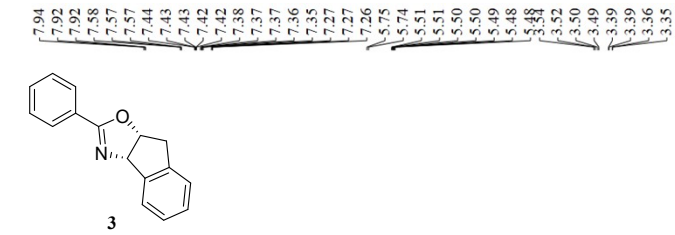
^{13}C NMR (126 MHz, $CDCl_3$): δ 171.2, 132.4, 131.9, 128.72 128.6, 65.7, 52.9, 35.3, 29.7.

HRMS (ESI) m/z ([M+H]$^+$) calcd for $C_{11}H_{12}NO_2S$: 222.0583. Found: 222.0576.

II. Spectral Data for New Compounds

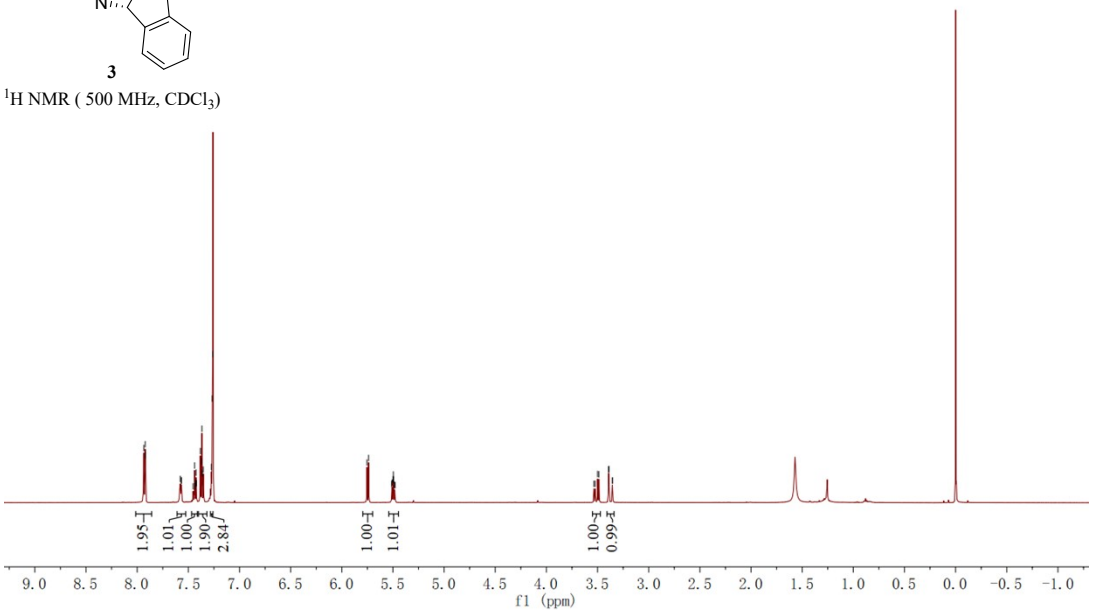
1. NMR and Microwave Data for New Compounds

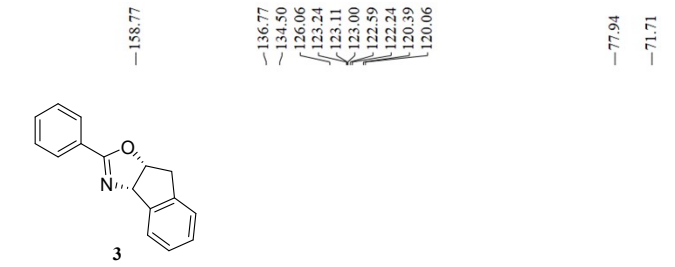
NMR spectra and microwave data of compound 3



3

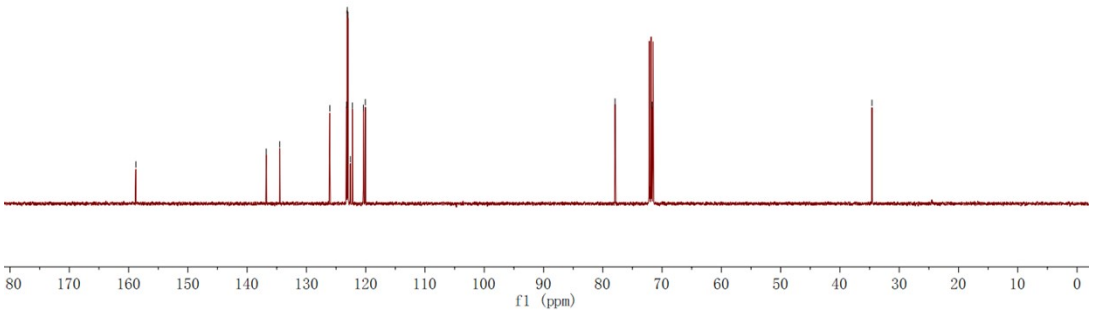
^{1}H NMR (500 MHz, $CDCl_3$)



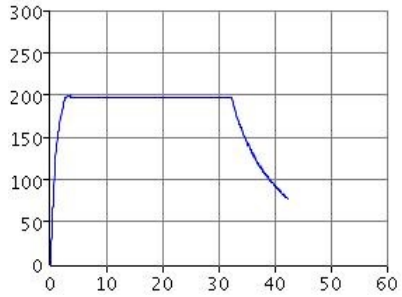


3

^{13}C NMR (126 MHz, $CDCl_3$)

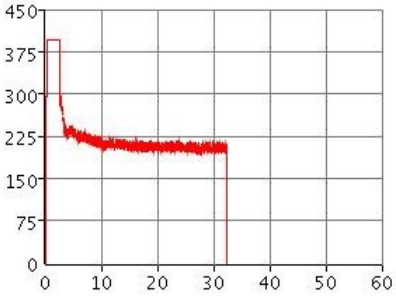


Temperature (℃)

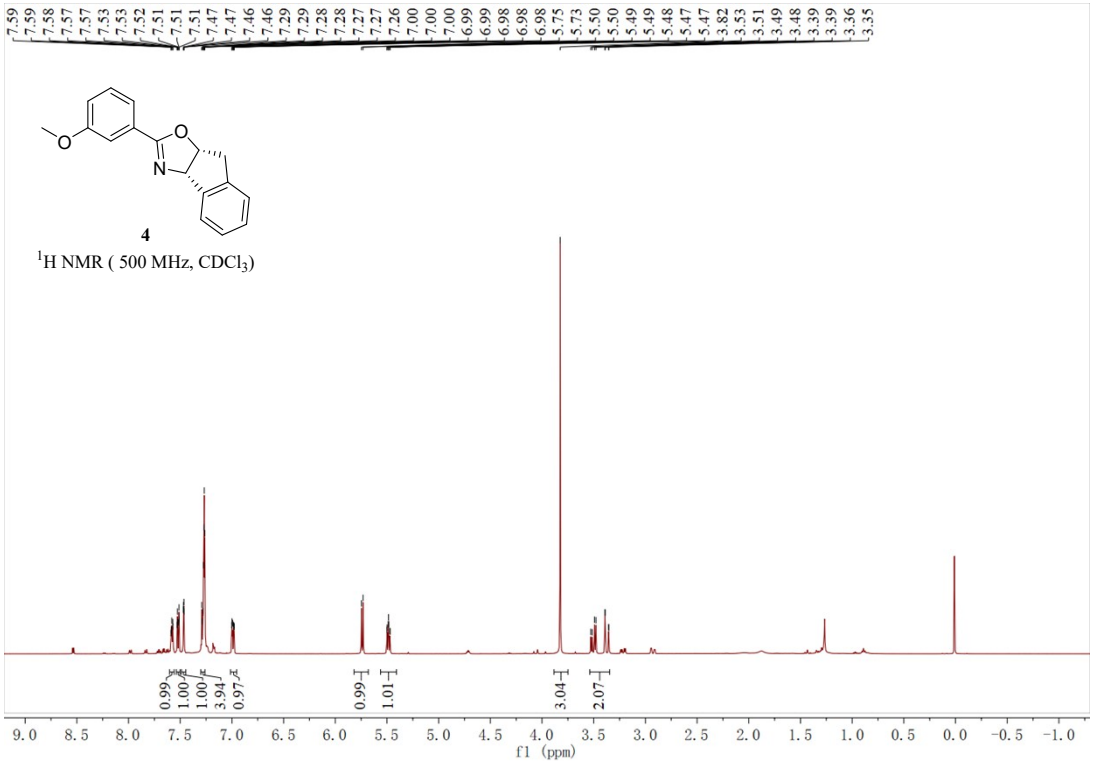


Pressure (bar)

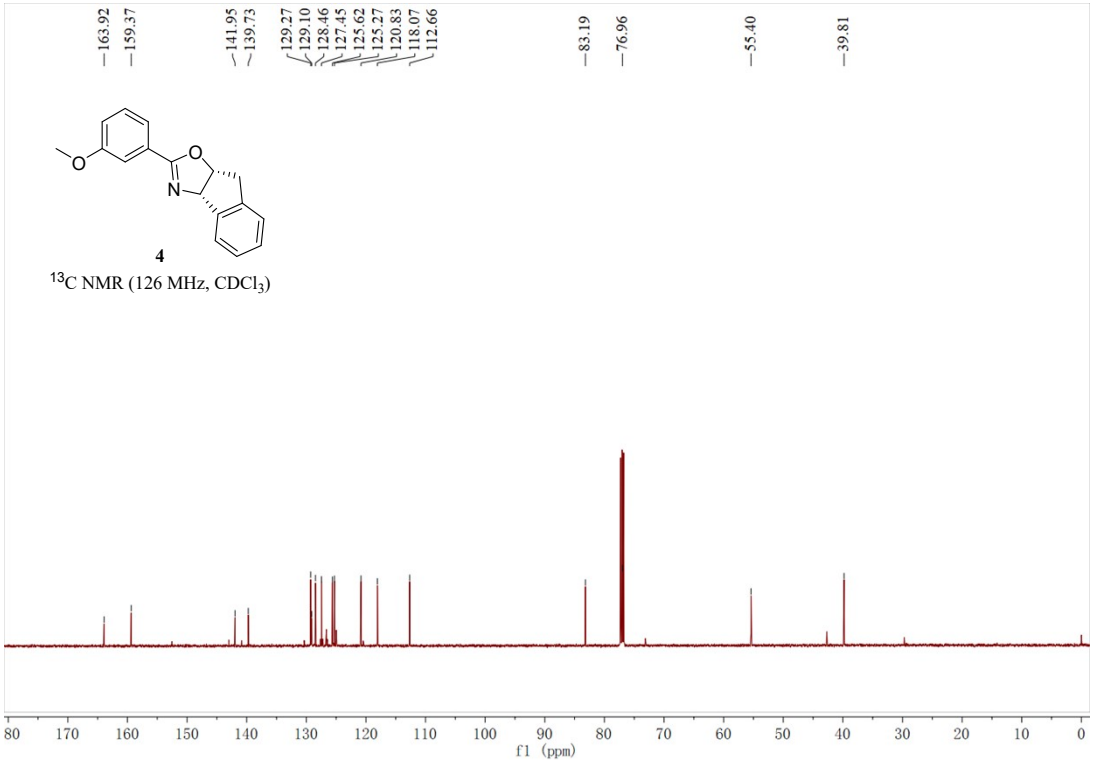
Power (W)



NMR spectra and microwave data of compound 4

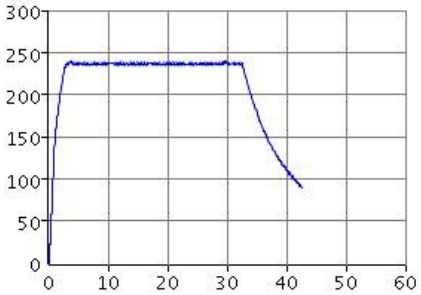


^{1}H NMR (500 MHz, $CDCl_3$)

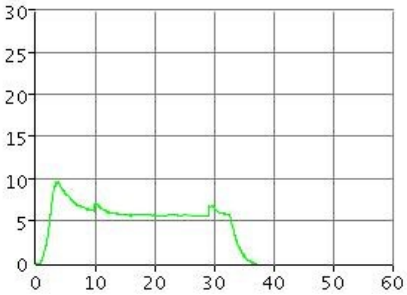


^{13}C NMR (126 MHz, $CDCl_3$)

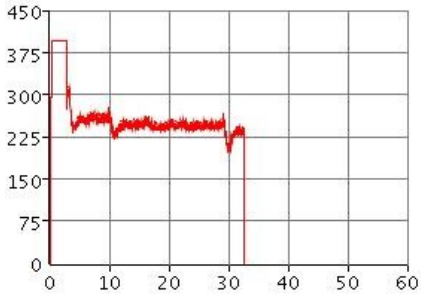
Temperature (°C)



Pressure (bar)Pressure (bar)

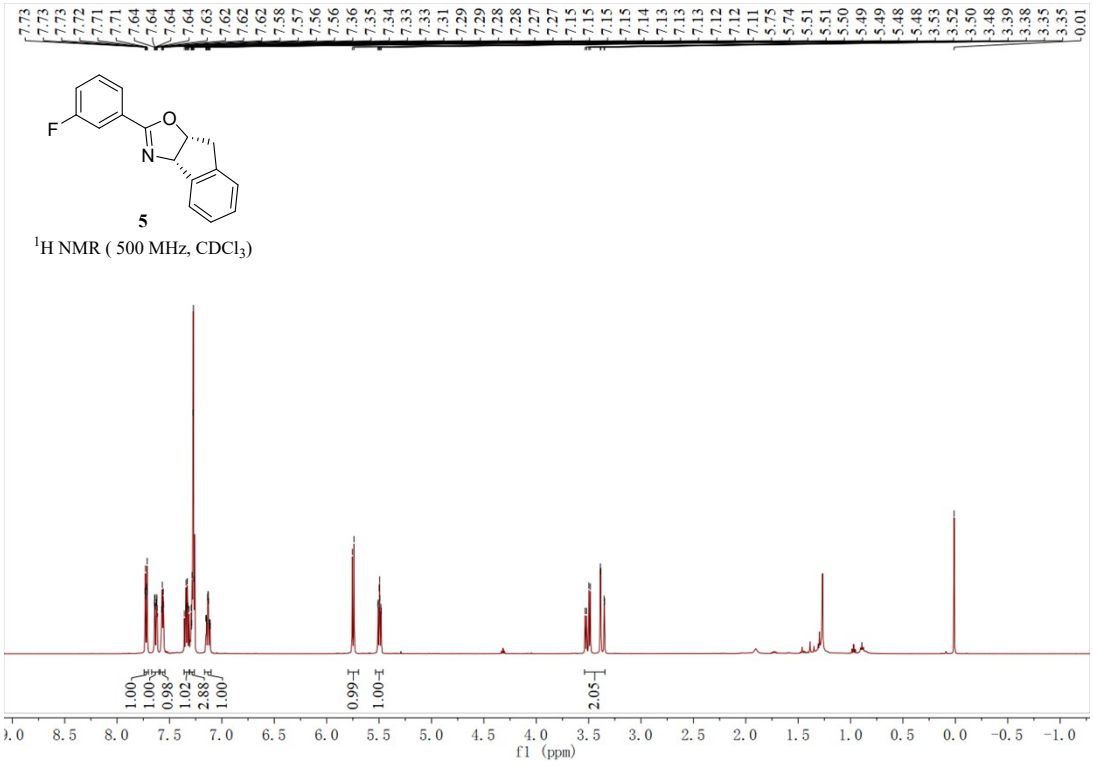


Power (W)Power (W)

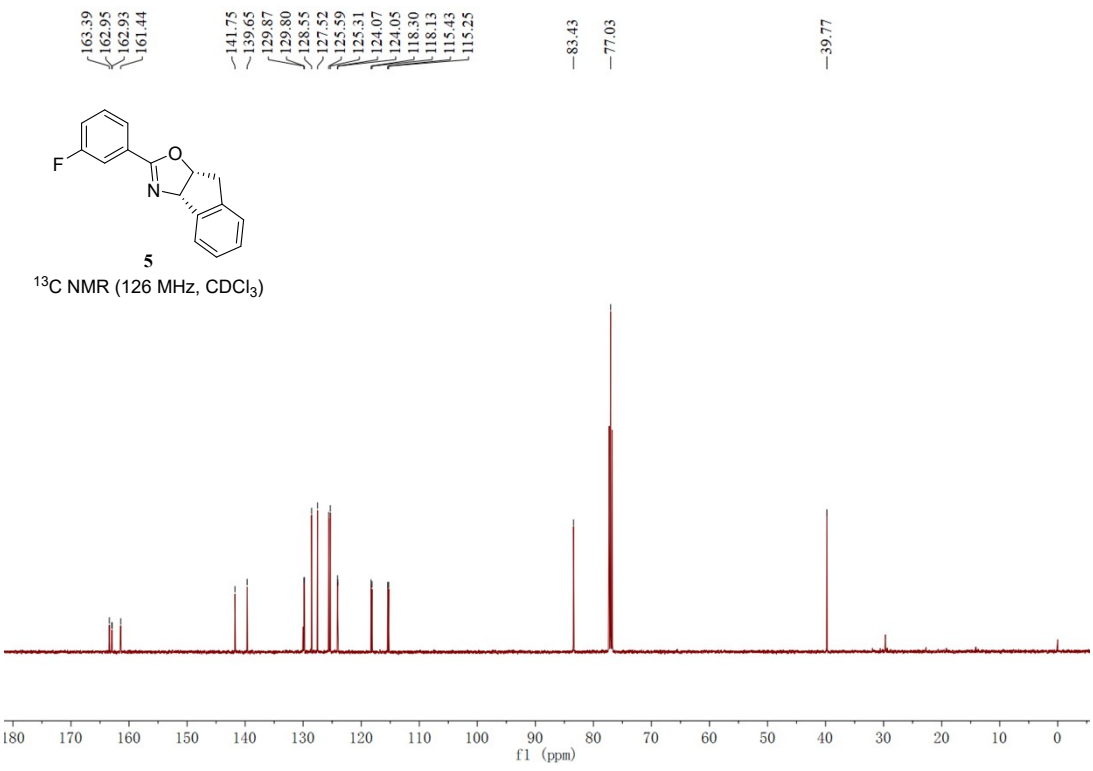


)minTime (Time

NMR spectra and microwave data of compound 5

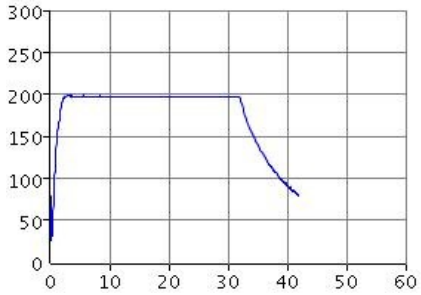


^{1}H NMR (500 MHz, $CDCl_3$)

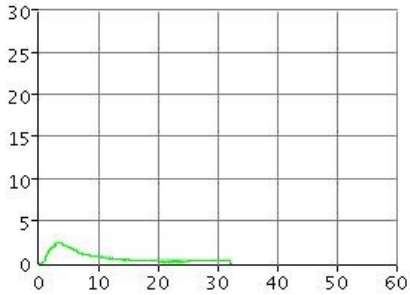


^{13}C NMR (126 MHz, $CDCl_3$)

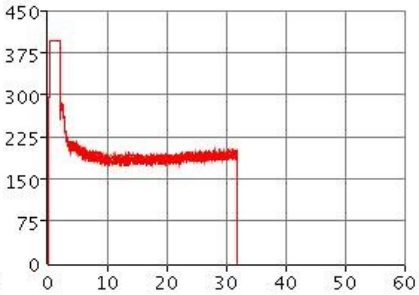
Temperature (°C)



Pressure (bar)

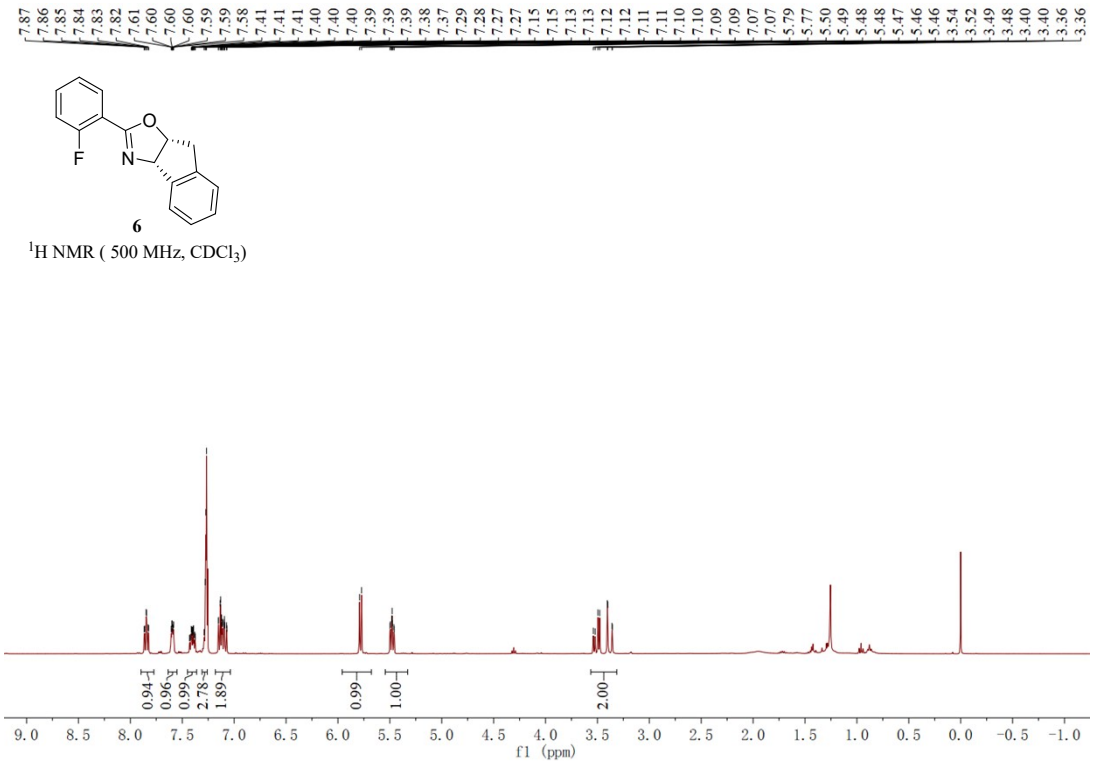


Power (W)

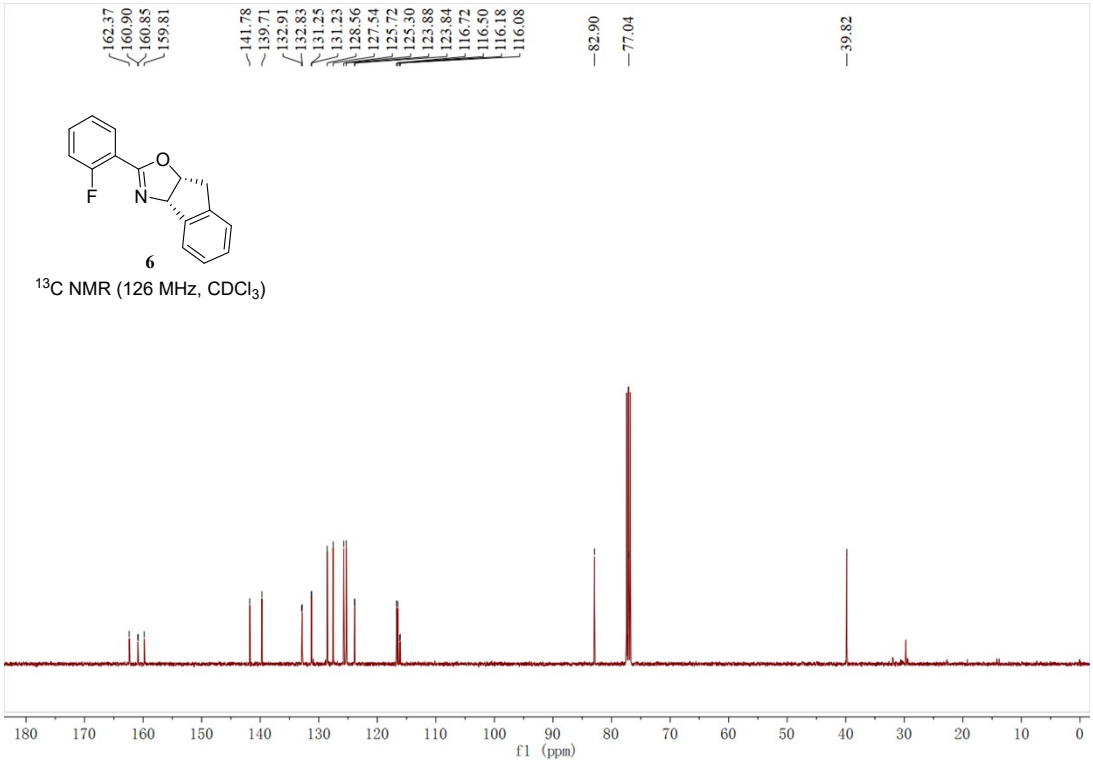


Time (min)

NMR spectra and microwave data of compound 6

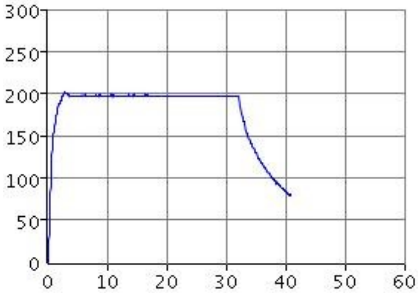


^{1}H NMR (500 MHz, $CDCl_3$)

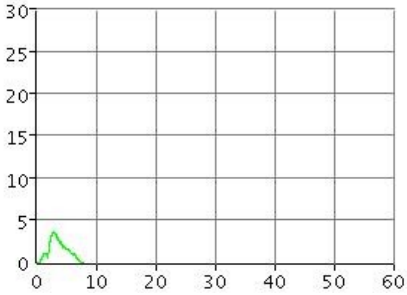


^{13}C NMR (126 MHz, $CDCl_3$)

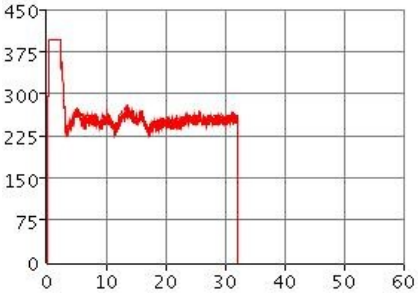
Temperature (°C)



Pressure (bar)

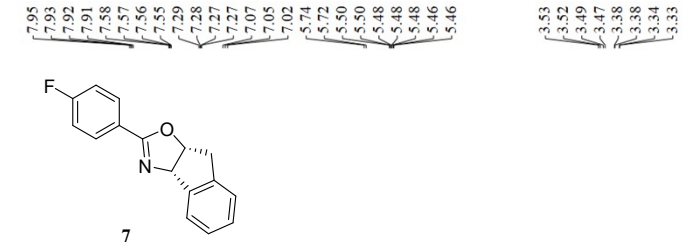


Power (W)



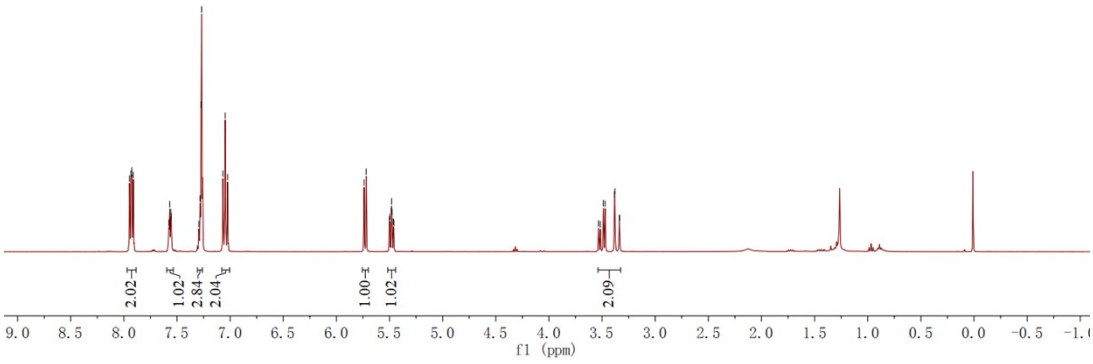
Time (min)

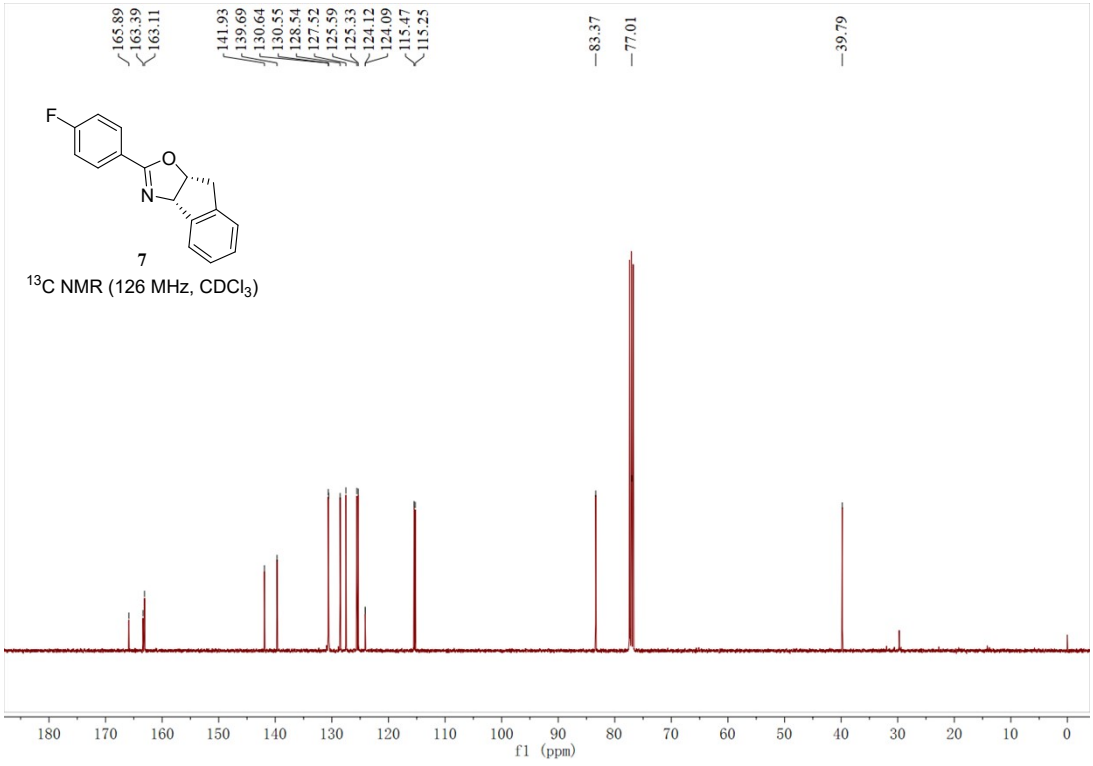
NMR spectra and microwave data of compound 7



7

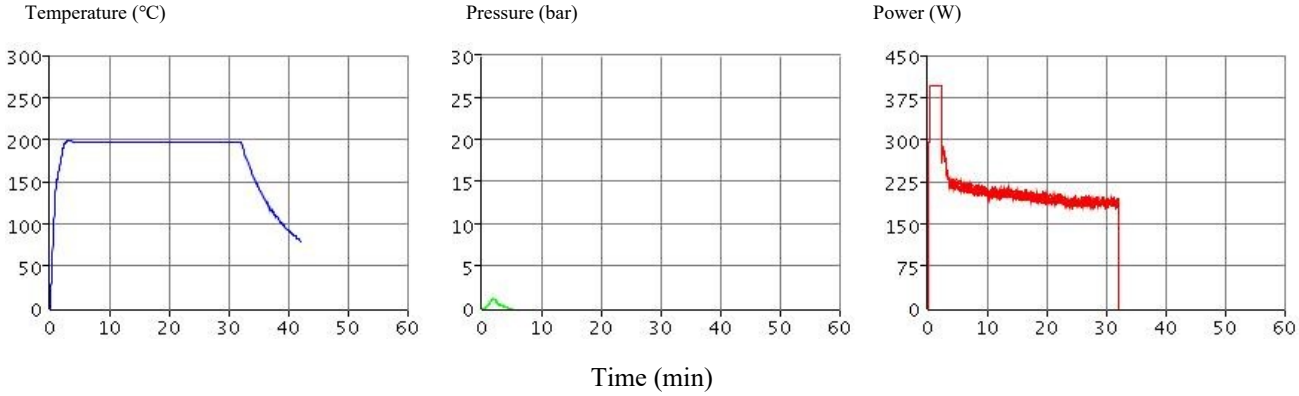
^{1}H NMR (500 MHz, $CDCl_3$)



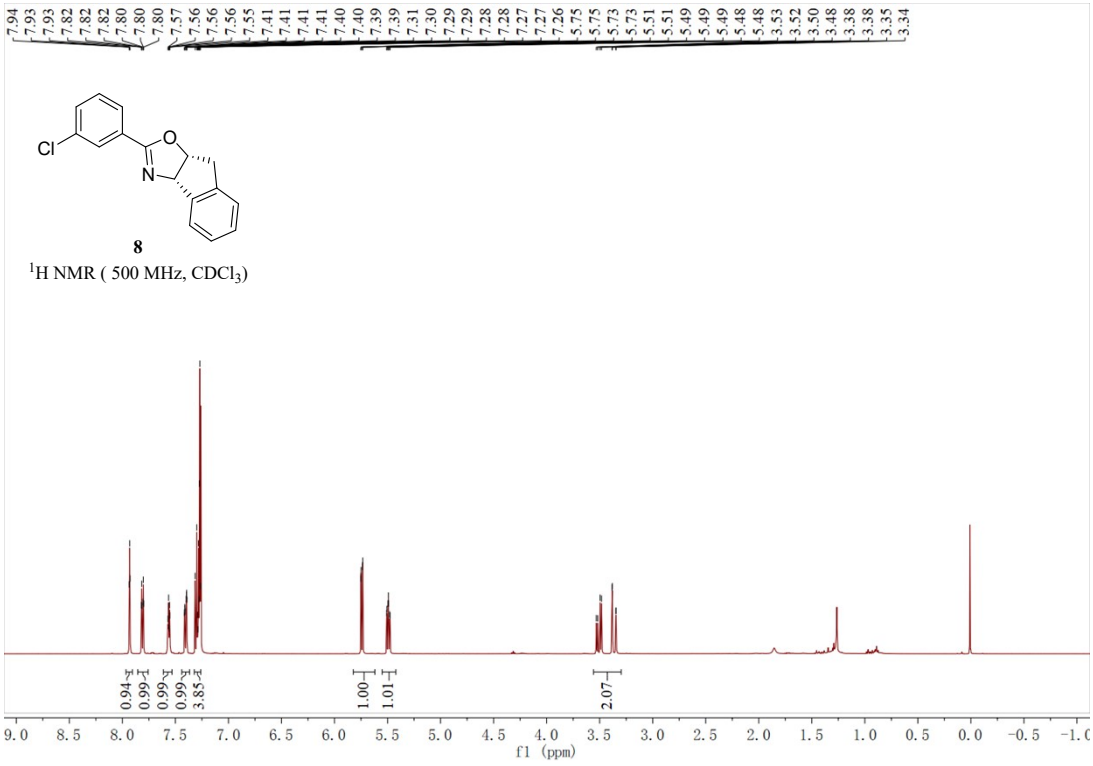


7

^{13}C NMR (126 MHz, $CDCl_3$)

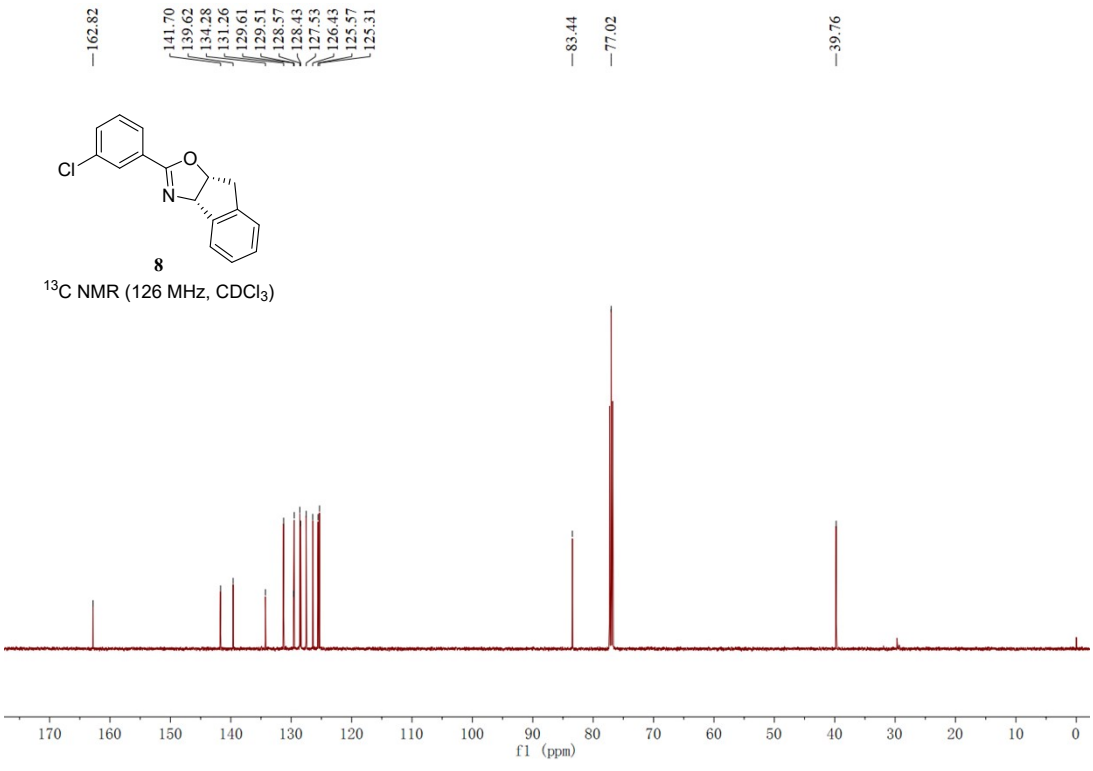

Temperature (°C)
Pressure (bar)
Power (W)
300
250
200
150
100
50
0
30
25
20
15
10
5
0
450
375
300
225
150
75
0
0 10 20 30 40 50 60
Time (min)

NMR spectra and microwave data of compound 8



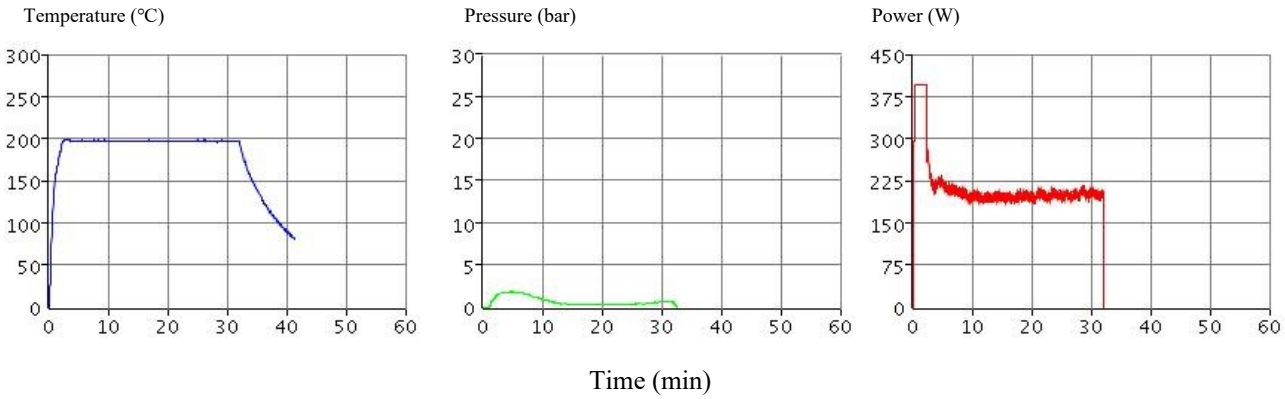
8

^{1}H NMR (500 MHz, $CDCl_3$)

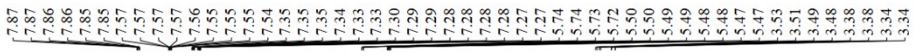


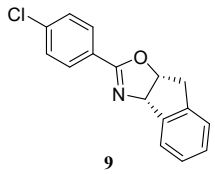
8

^{13}C NMR (126 MHz, $CDCl_3$)


Temperature (°C)
300
250
200
150
100
50
0
0 10 20 30 40 50 60
Pressure (bar)
30
25
20
15
10
5
0
0 10 20 30 40 50 60
Power (W)
450
375
300
225
150
75
0
0 10 20 30 40 50 60
Time (min)

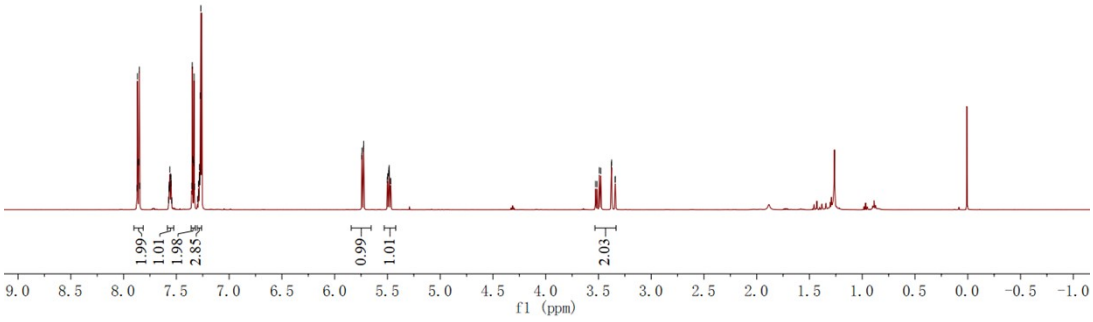
NMR spectra and microwave data of compound 9

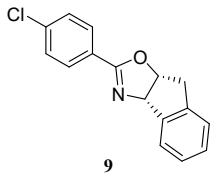




9

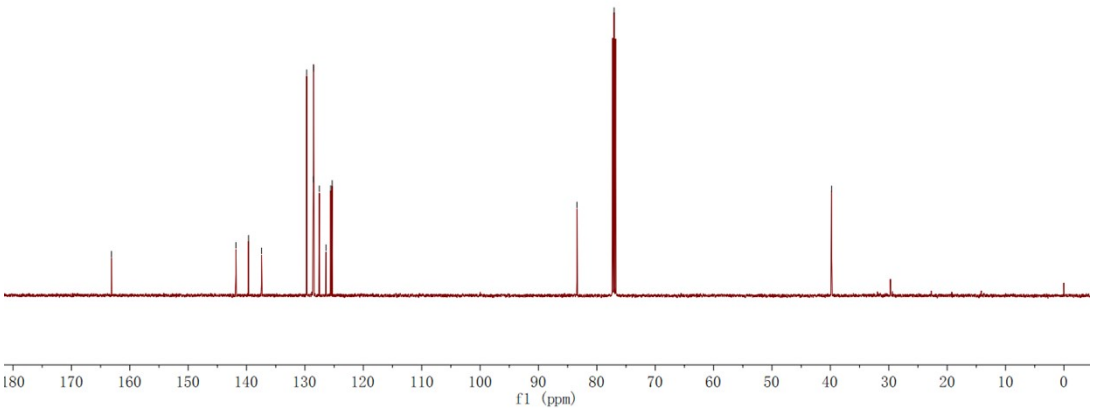
^{1}H NMR (500 MHz, $CDCl_3$)

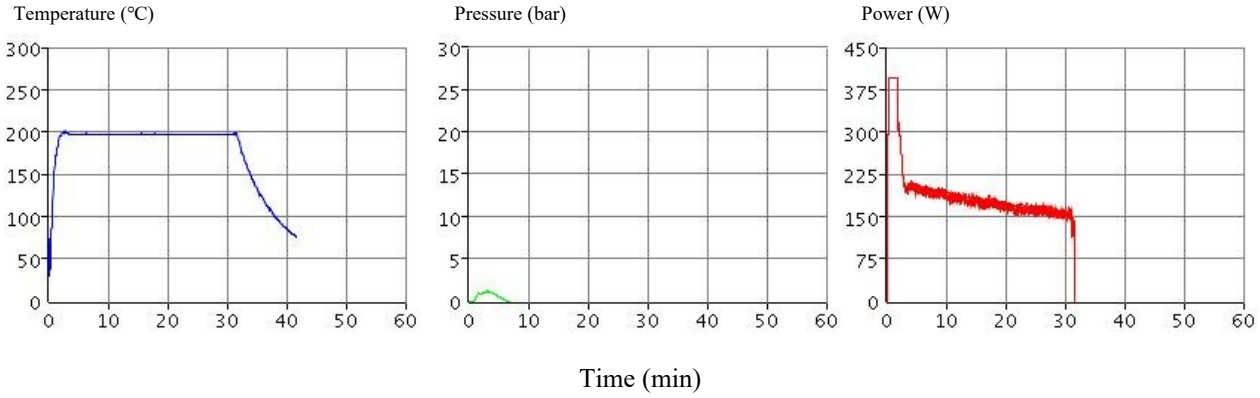




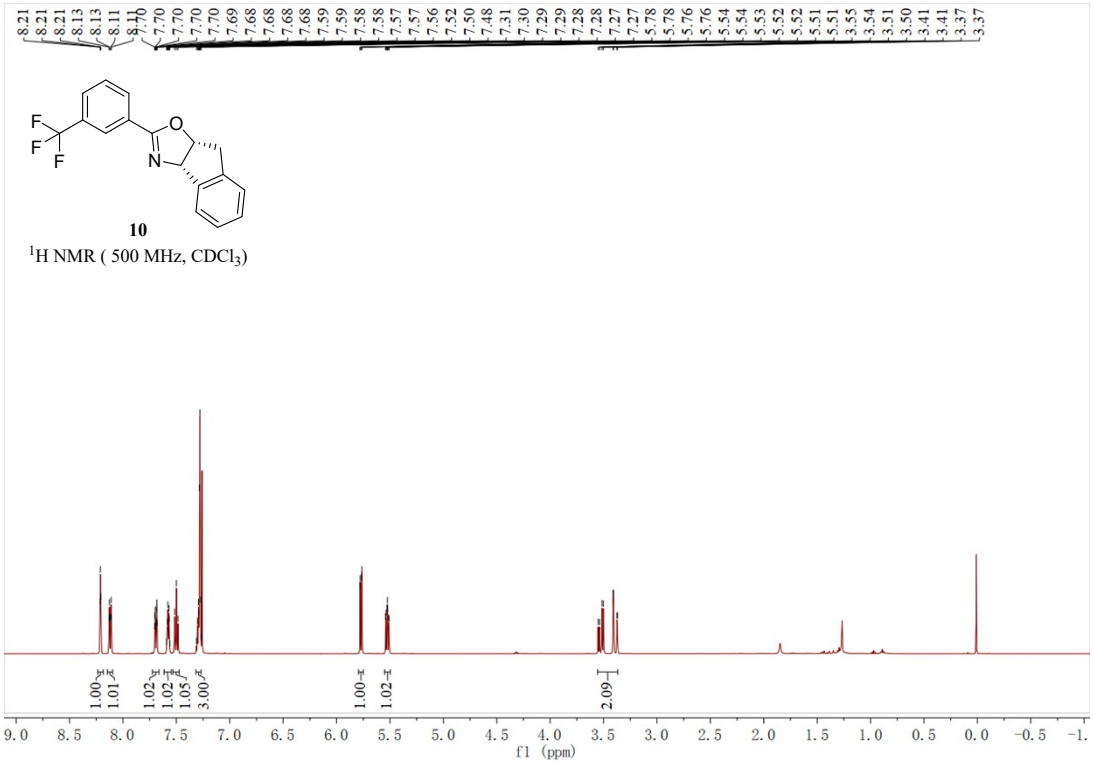
9

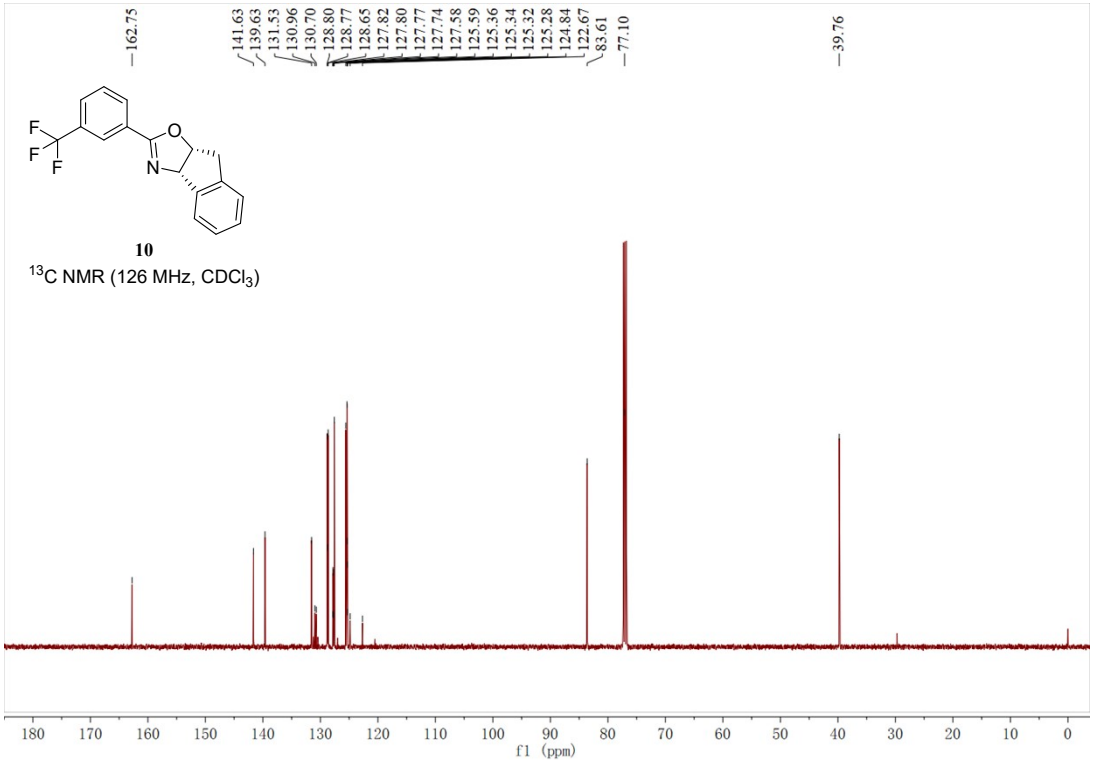
^{13}C NMR (126 MHz, $CDCl_3$)

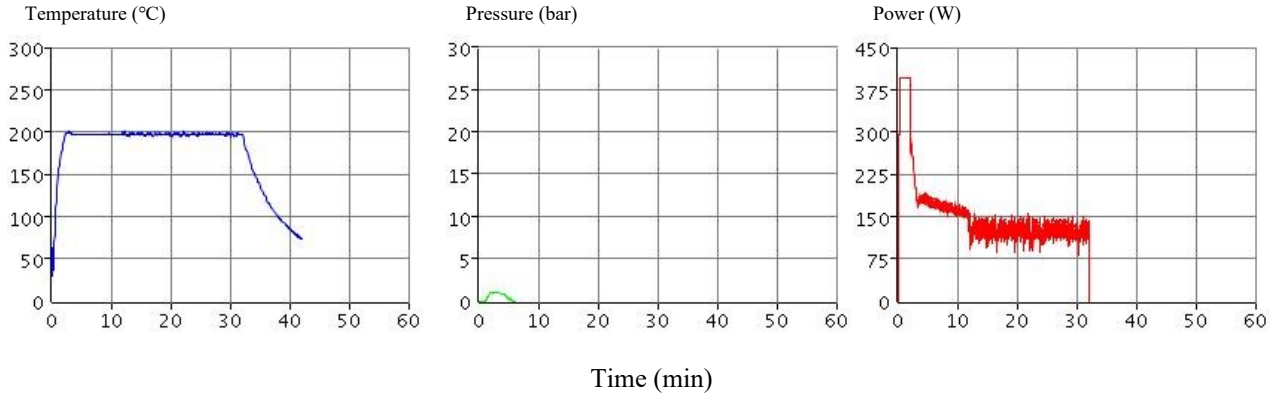



Temperature (°C)
Pressure (bar)
Power (W)
300
250
200
150
100
50
0
30
25
20
15
10
5
0
450
375
300
225
150
75
0
0 10 20 30 40 50 60
Time (min)

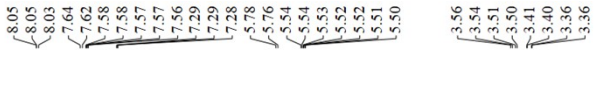
NMR spectra and microwave data of compound 10

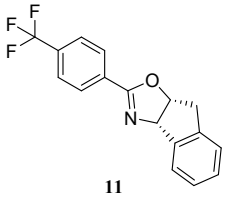





Temperature (°C)
300
250
200
150
100
50
0
0 10 20 30 40 50 60
Pressure (bar)
30
25
20
15
10
5
0
0 10 20 30 40 50 60
Power (W)
450
375
300
225
150
75
0
0 10 20 30 40 50 60
Time (min)

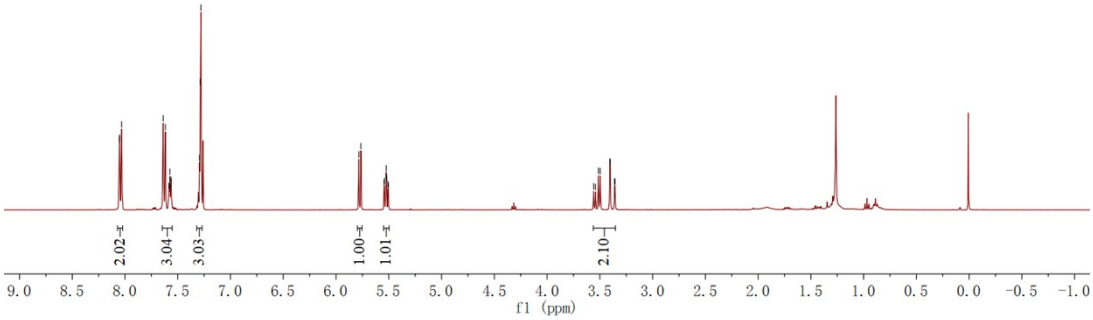
NMR spectra and microwave data of compound 11

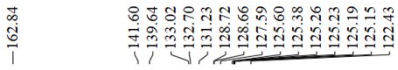


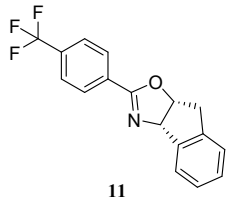


11

^{1}H NMR (500 MHz, $CDCl_3$)

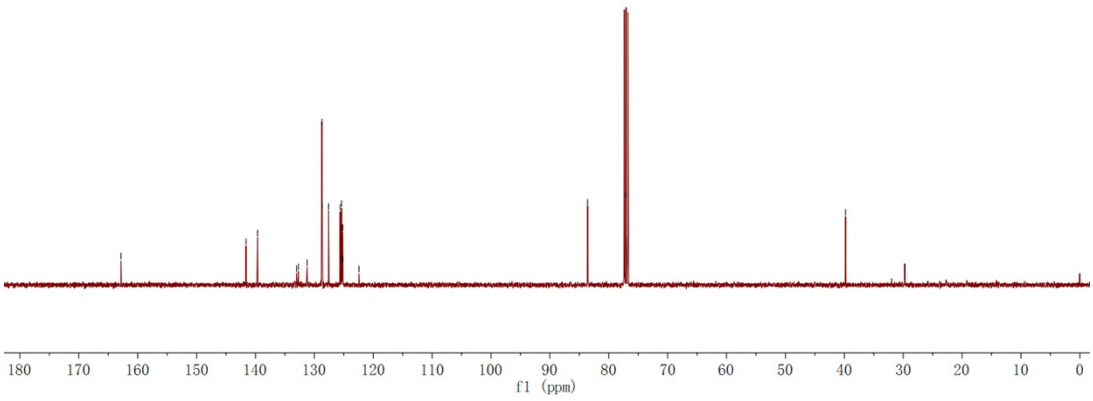


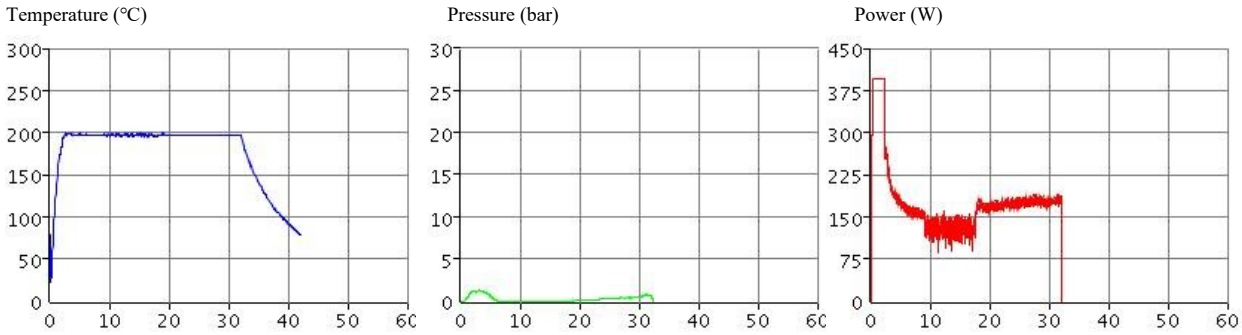




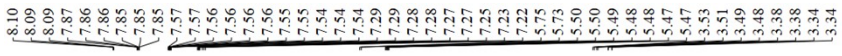
11

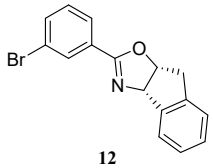
^{13}C NMR (126 MHz, $CDCl_3$)




Temperature (°C)
Pressure (bar)
Power (W)
300
250
200
150
100
50
0
30
25
20
15
10
5
0
450
375
300
225
150
75
0
0 10 20 30 40 50 60
Time (min)

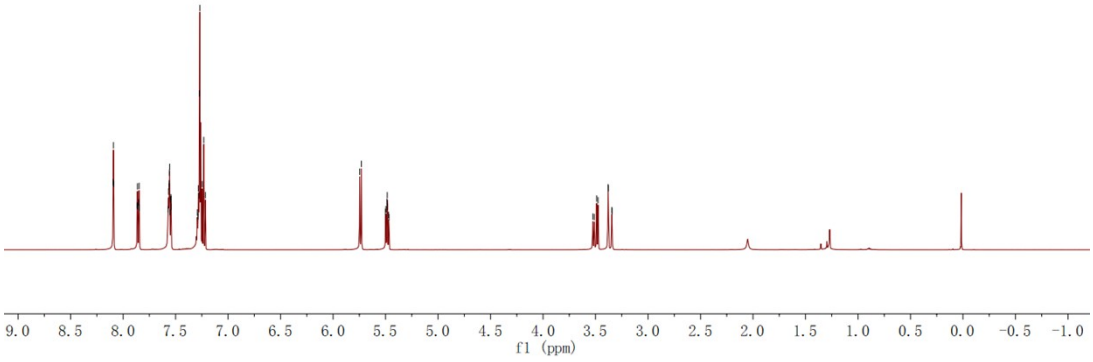
NMR spectra and microwave data of compound 12

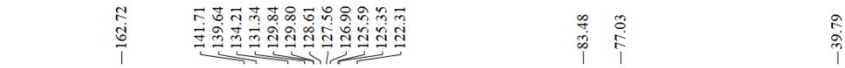


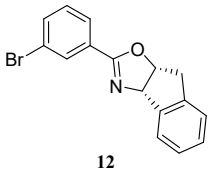


12

^{1}H NMR (500 MHz, $CDCl_3$)

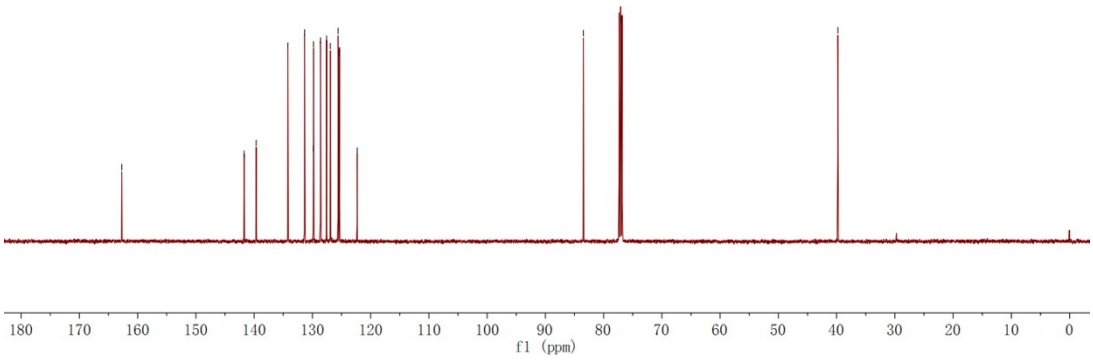


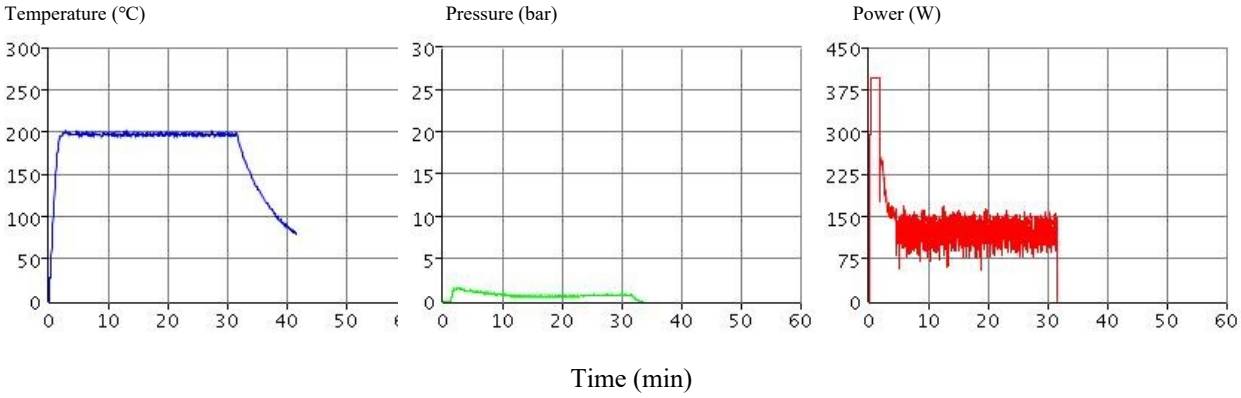




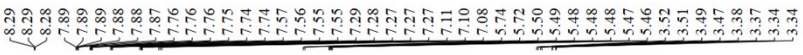
12

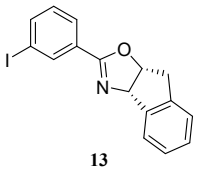
^{13}C NMR (126 MHz, $CDCl_3$)




Temperature (°C)
Pressure (bar)
Power (W)
300
250
200
150
100
50
0
30
25
20
15
10
5
0
450
375
300
225
150
75
0
0 10 20 30 40 50 60
Time (min)

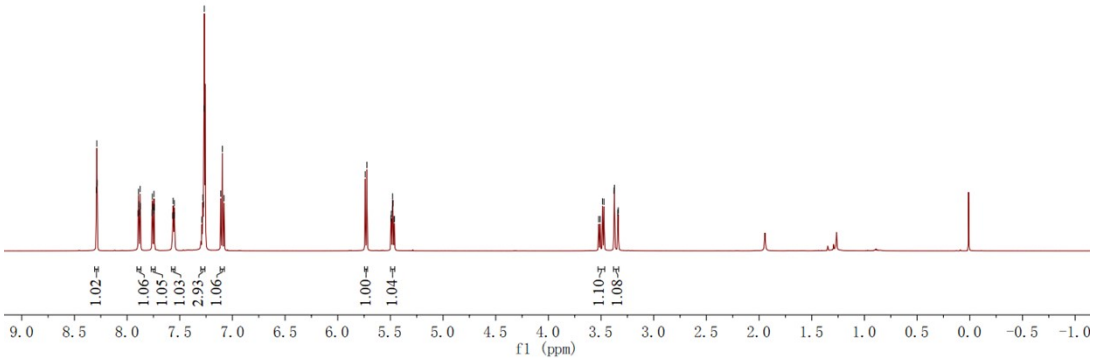
NMR spectra and microwave data of compound 13

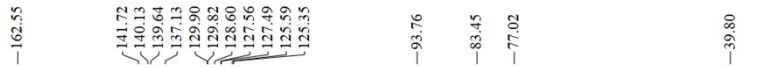


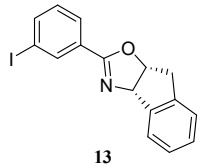


13

^{1}H NMR (500 MHz, $CDCl_3$)

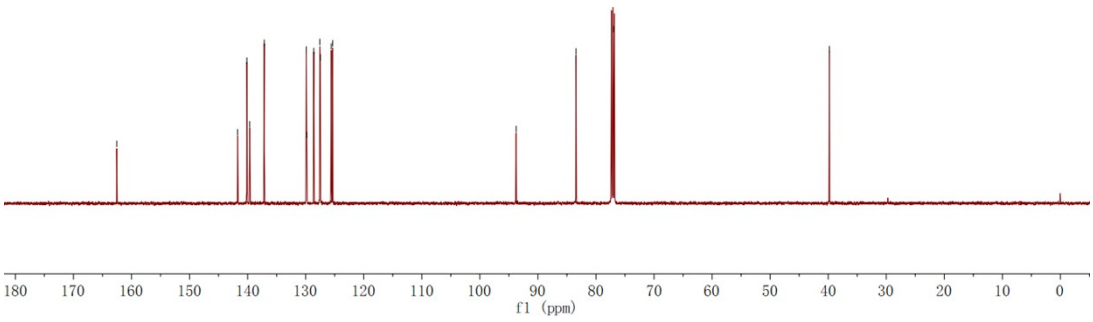


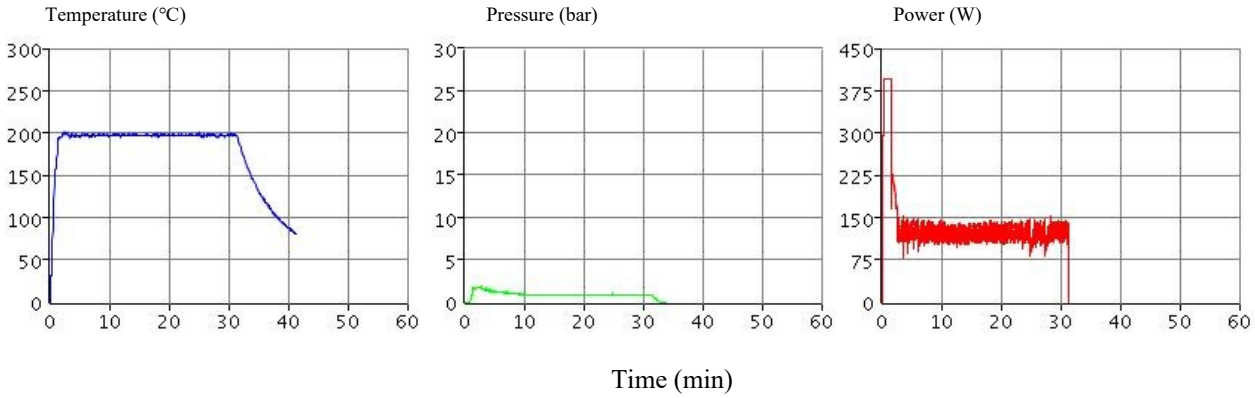




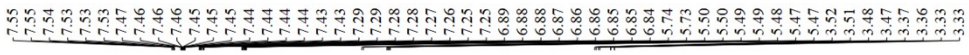
13

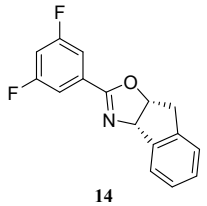
^{13}C NMR (126 MHz, $CDCl_3$)




Temperature (°C)
Pressure (bar)
Power (W)
300
250
200
150
100
50
0
30
25
20
15
10
5
0
450
375
300
225
150
75
0
0 10 20 30 40 50 60
Time (min)

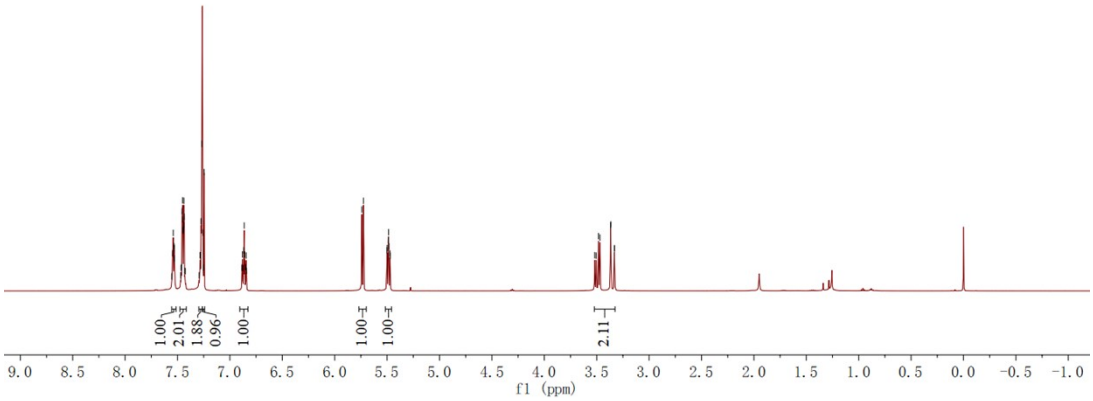
NMR spectra and microwave data of compound 14

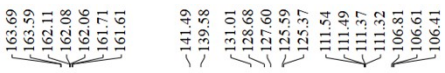


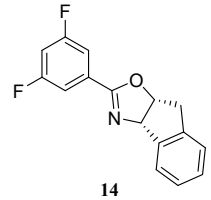


14

^{1}H NMR (500 MHz, $CDCl_3$)

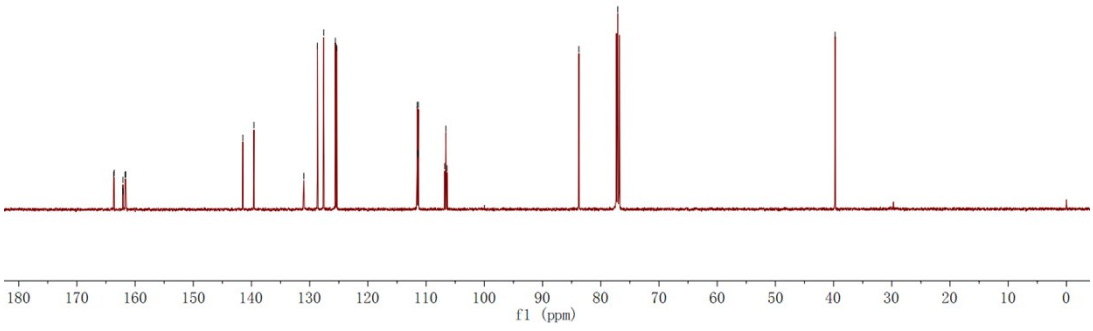


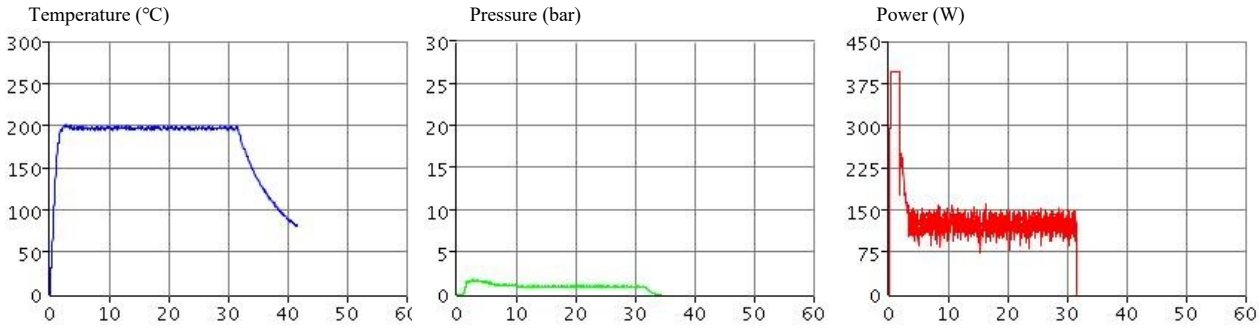




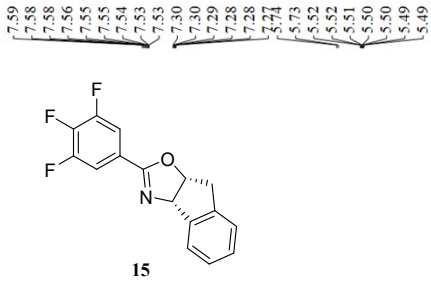
14

^{13}C NMR (126 MHz, $CDCl_3$)



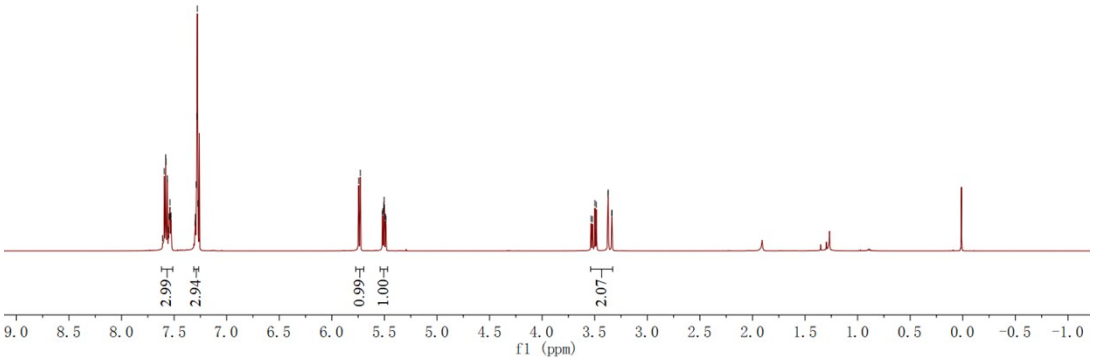

Temperature (°C)
Pressure (bar)
Power (W)
Time (min)

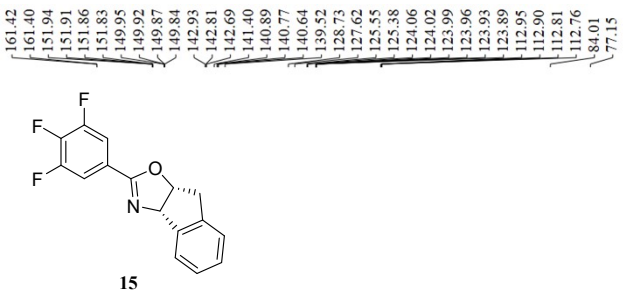
NMR spectra and microwave data of compound 15



15

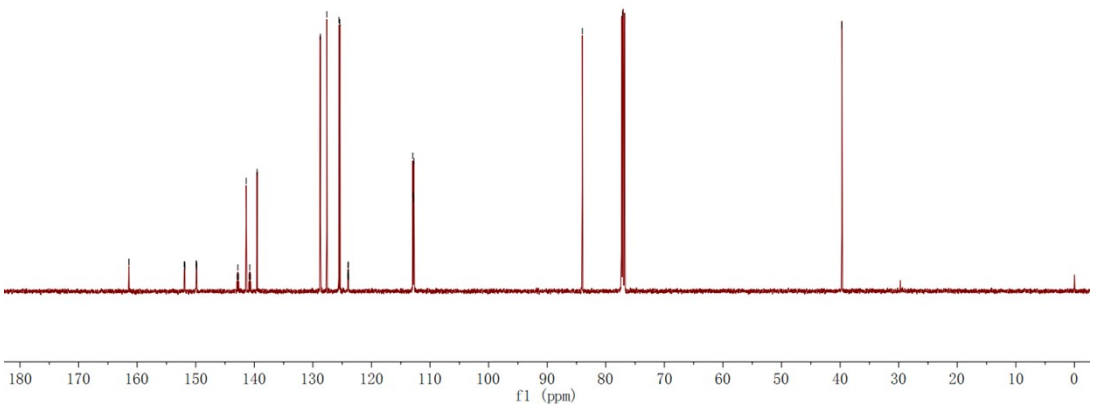
^{1}H NMR (500 MHz, $CDCl_3$)

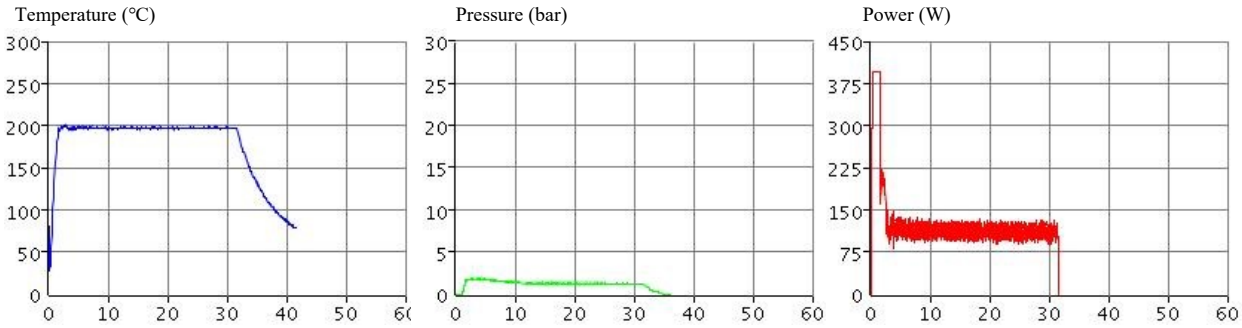




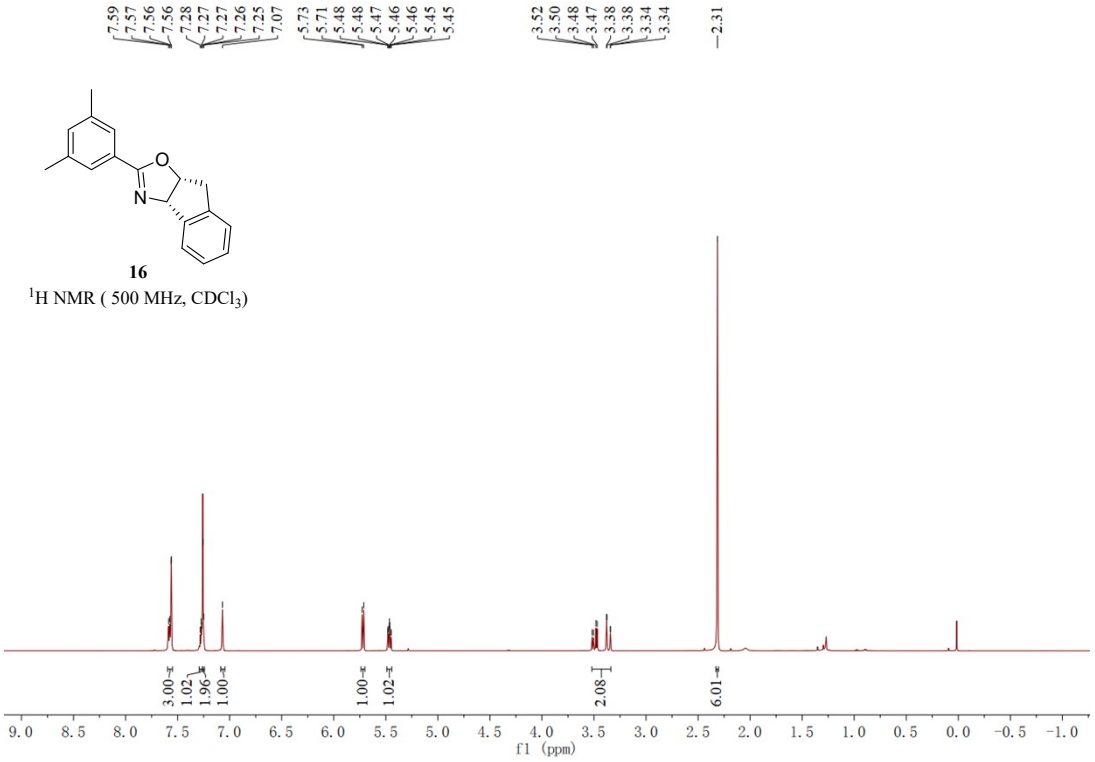
15

^{13}C NMR (126 MHz, $CDCl_3$)



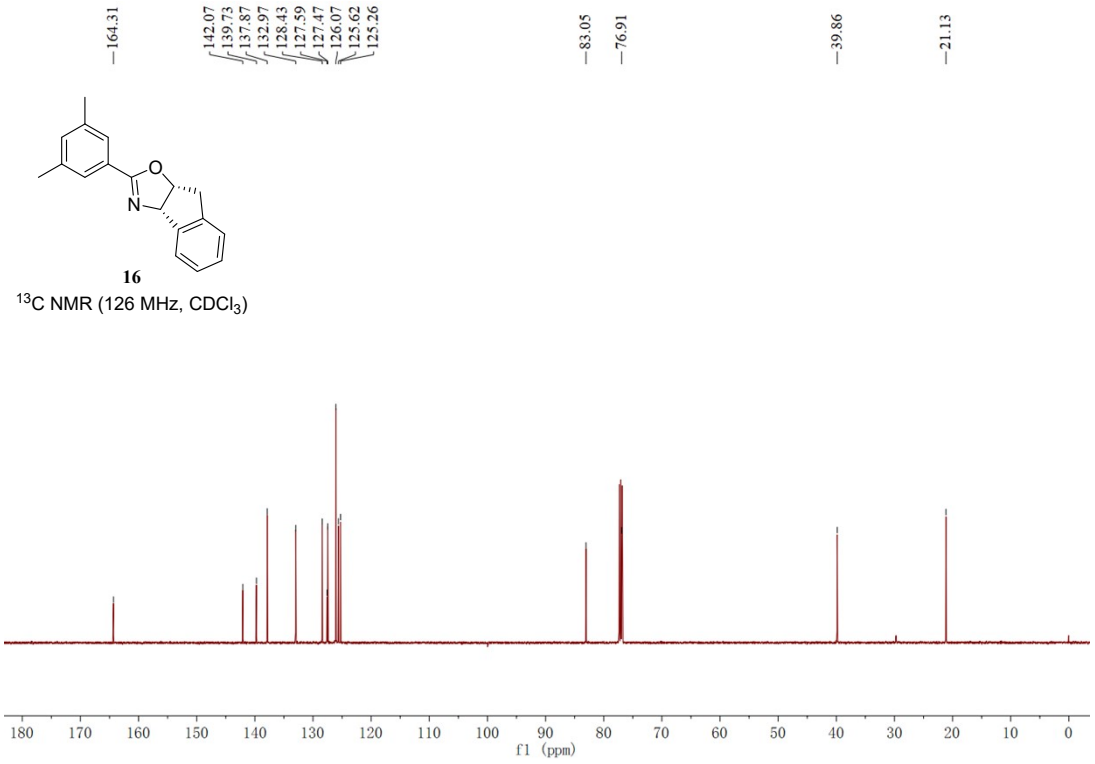

Temperature (°C)
Pressure (bar)
Power (W)
300
250
200
150
100
50
0
30
25
20
15
10
5
0
450
375
300
225
150
75
0
0 10 20 30 40 50 60
Time (min)

NMR spectra and microwave data of compound 16



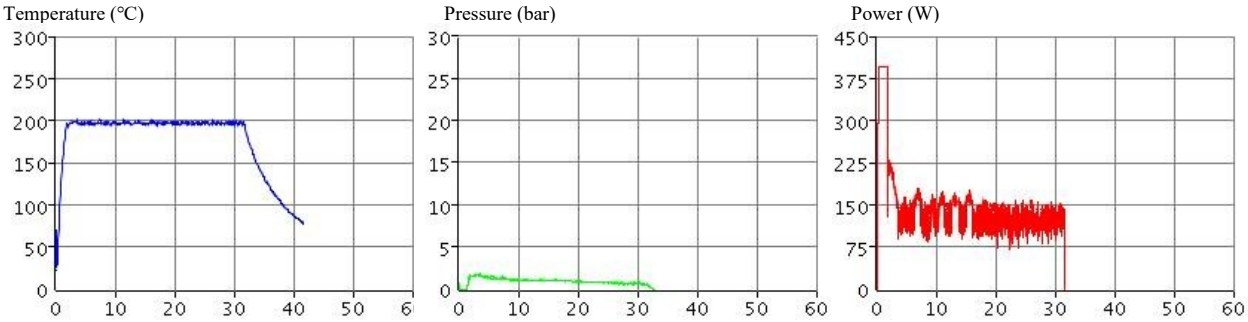
16

^{1}H NMR (500 MHz, $CDCl_3$)

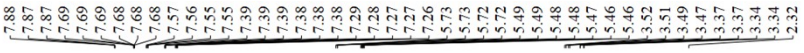


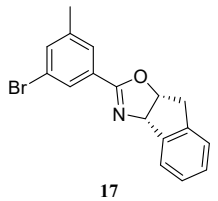
16

^{13}C NMR (126 MHz, $CDCl_3$)


Temperature (°C)
300
250
200
150
100
50
0
0 10 20 30 40 50 6
Pressure (bar)
30
25
20
15
10
5
0
0 10 20 30 40 50 60
Power (W)
450
375
300
225
150
75
0
0 10 20 30 40 50 60
Time (min)

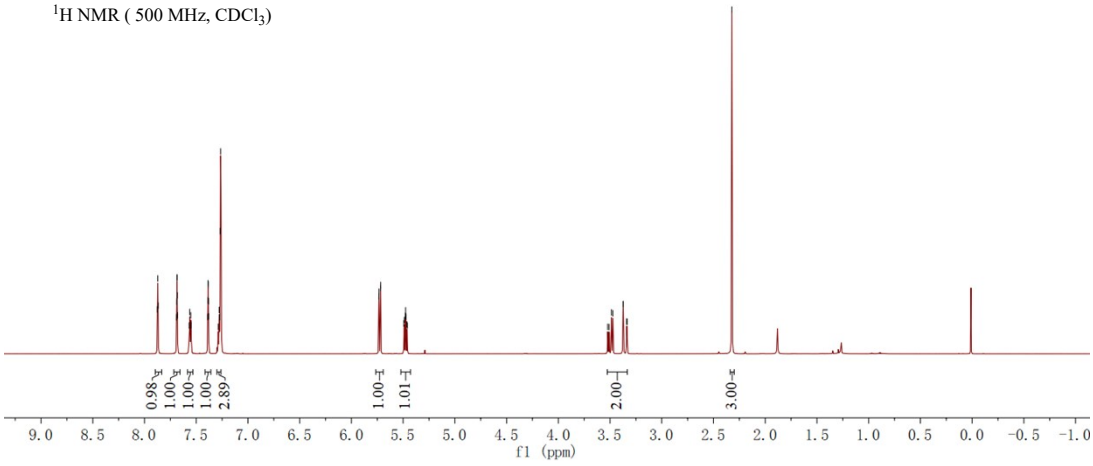
NMR spectra and microwave data of compound 17

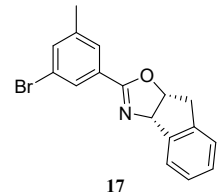




17

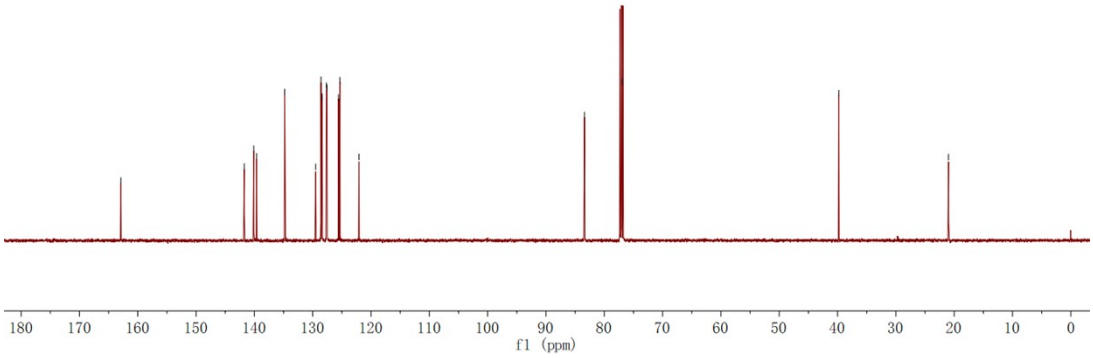
^{1}H NMR (500 MHz, $CDCl_3$)

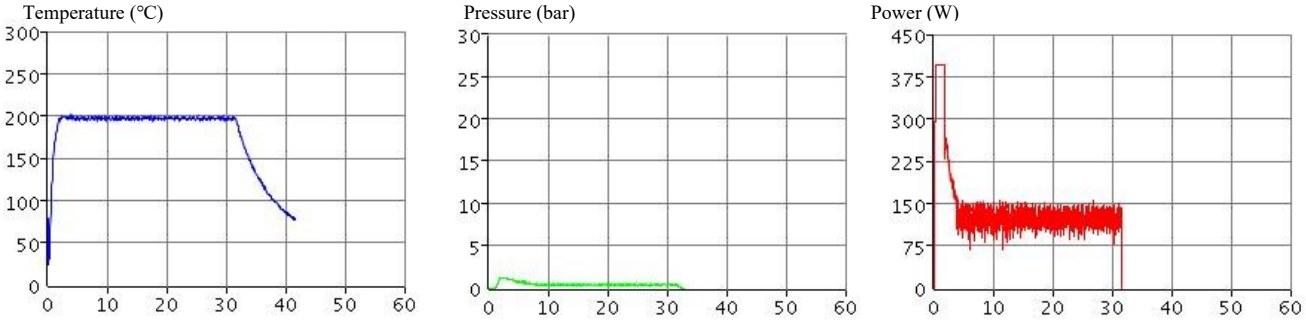




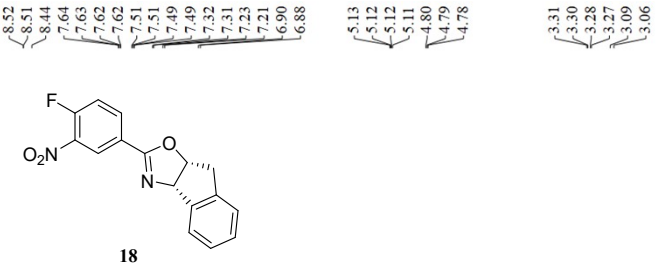
17

^{13}C NMR (126 MHz, $CDCl_3$)



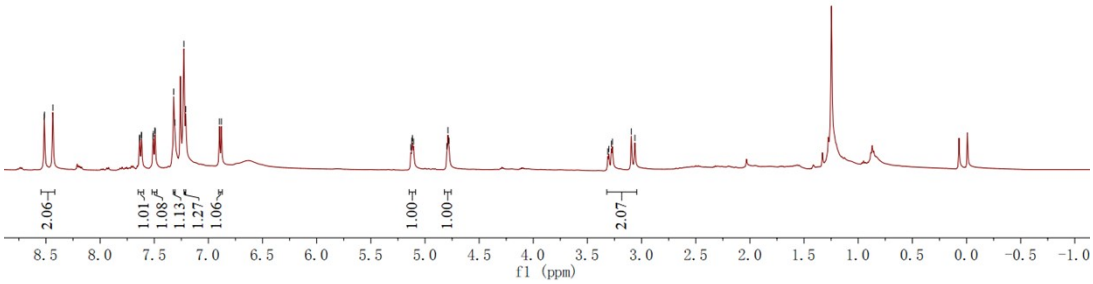

Temperature (°C)
300
250
200
150
100
50
0
0 10 20 30 40 50 60
Pressure (bar)
30
25
20
15
10
5
0
0 10 20 30 40 50 60
Power (W)
450
375
300
225
150
75
0
0 10 20 30 40 50 60
Time (min)

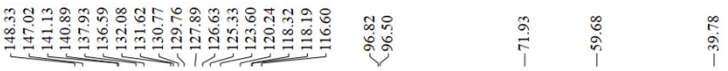
NMR spectra and microwave data of compound 18

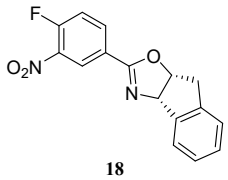


18

^{1}H NMR (500 MHz, $CDCl_3$)

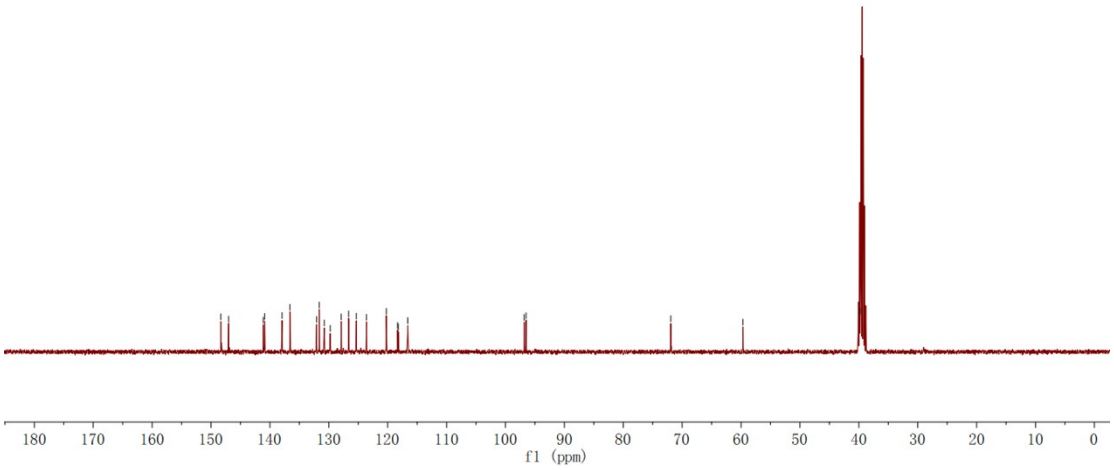


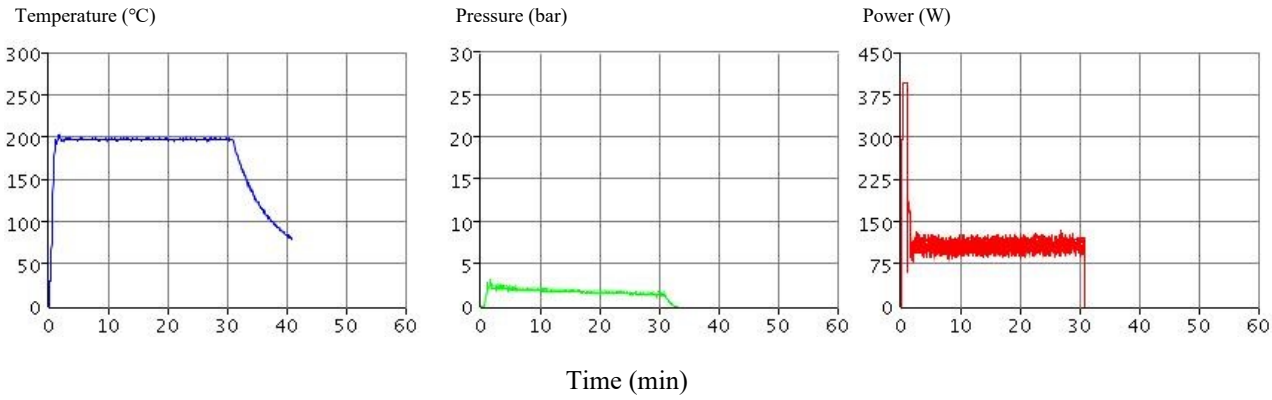




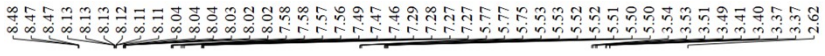
18

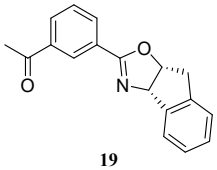
^{13}C NMR (101 MHz, DMSO-d6)




Temperature (°C)
Pressure (bar)
Power (W)
300
250
200
150
100
50
0
30
25
20
15
10
5
0
450
375
300
225
150
75
0
0 10 20 30 40 50 60
Time (min)

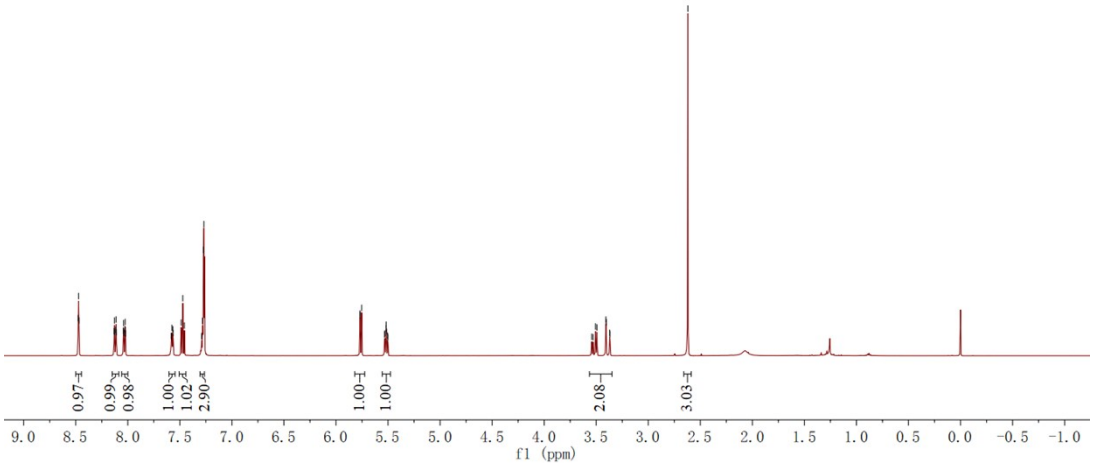
NMR spectra and microwave data of compound 19

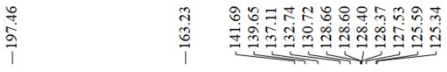


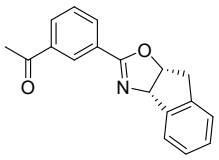


19

^{1}H NMR (500 MHz, $CDCl_3$)

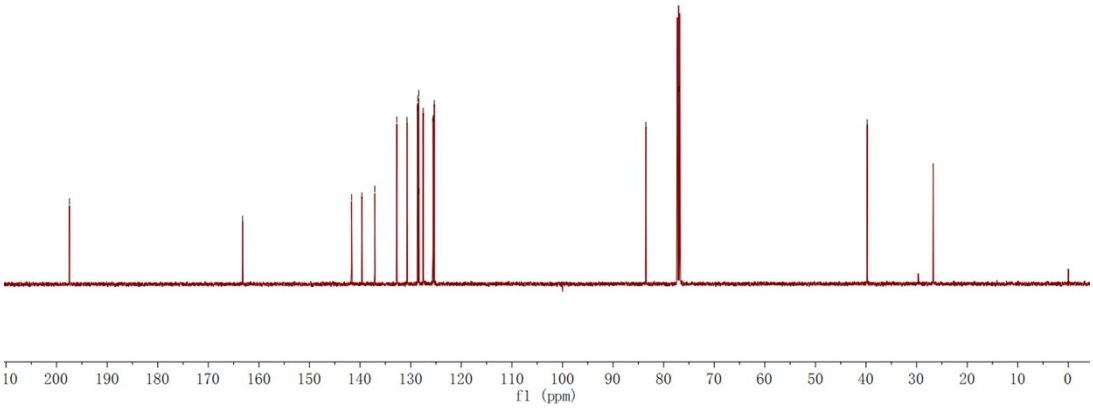


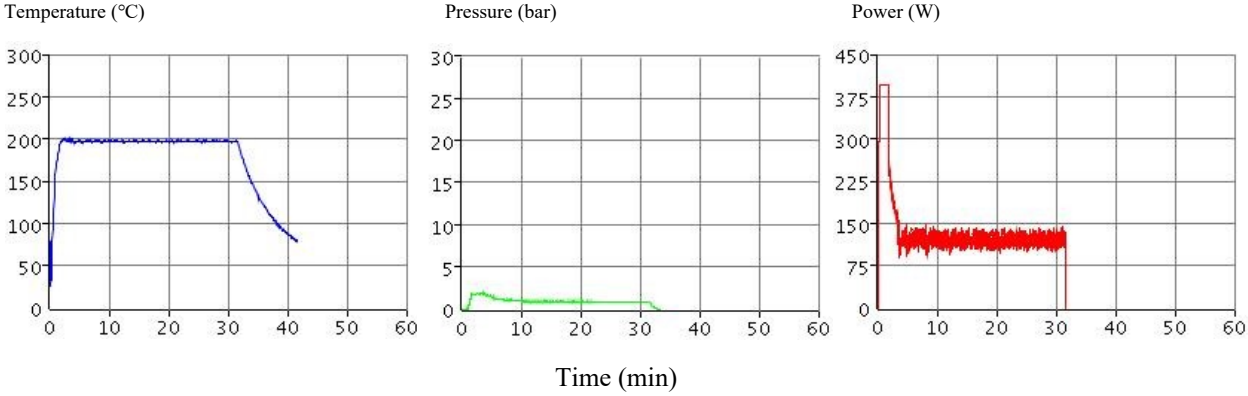




19

^{13}C NMR (126 MHz, $CDCl_3$)




Temperature (°C)
Pressure (bar)
Power (W)
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150
100
50
0
30
25
20
15
10
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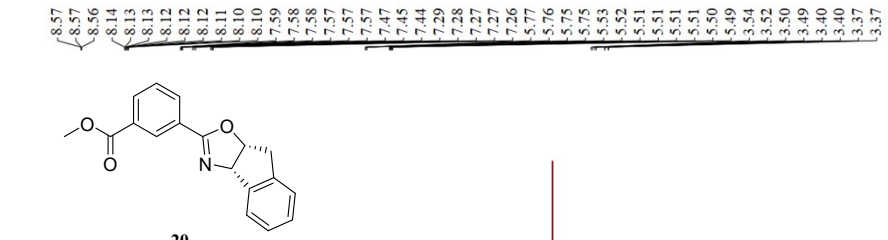
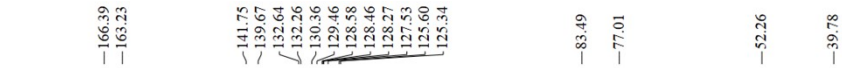
0
450
375
300
225
150
75
0
0 10 20 30 40 50 60
Time (min)

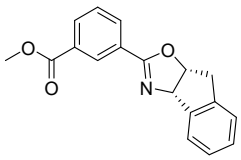
NMR spectra and microwave data of compound 20



20

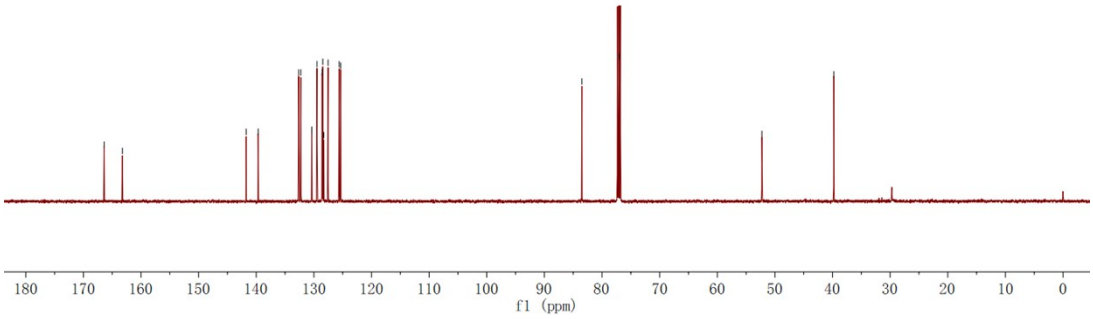
^{1}H NMR (500 MHz, $CDCl_3$)

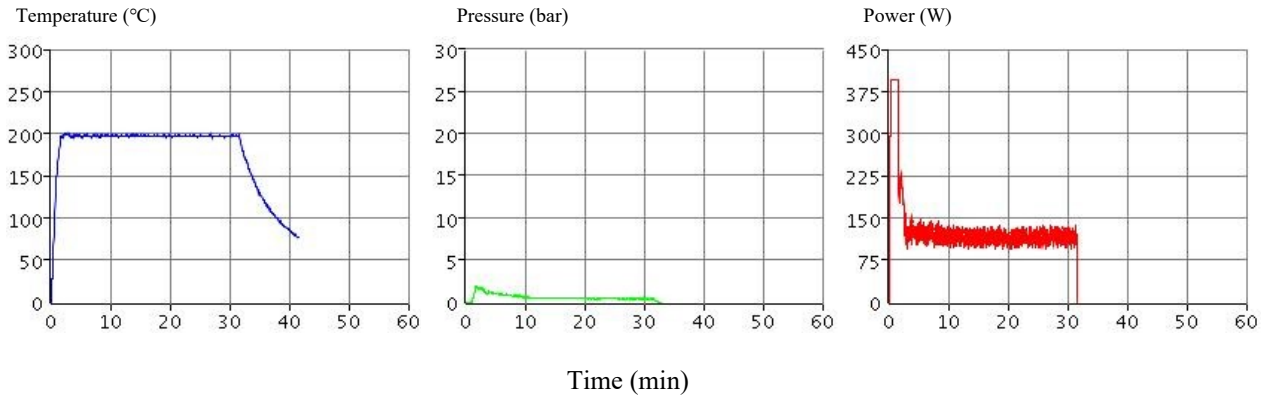




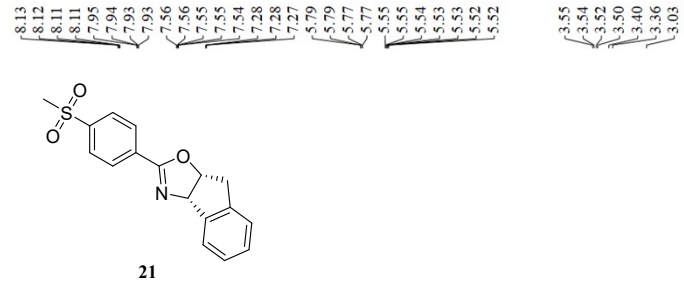
20

^{13}C NMR (126 MHz, $CDCl_3$)



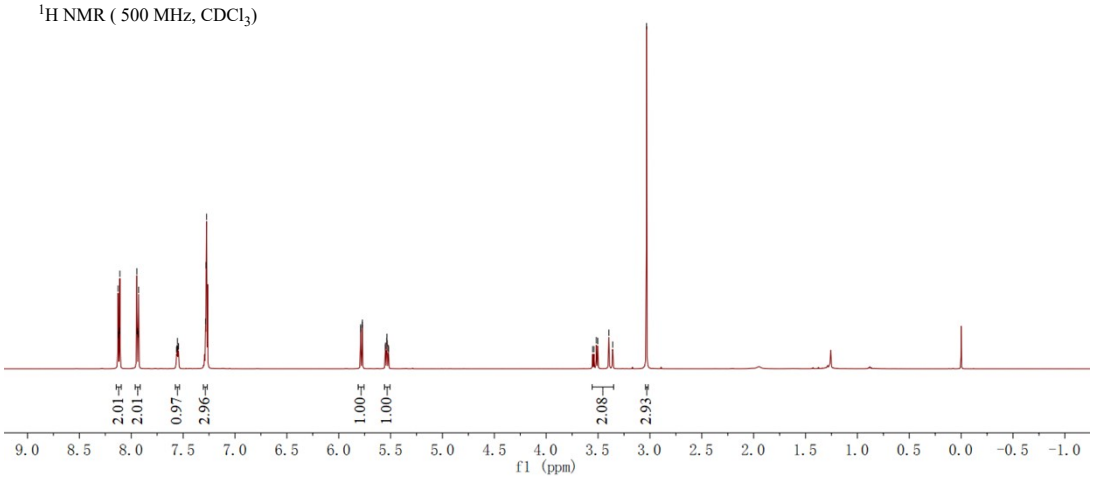

Temperature (°C)
300
250
200
150
100
50
0
0 10 20 30 40 50 60
Pressure (bar)
30
25
20
15
10
5
0
0 10 20 30 40 50 60
Power (W)
450
375
300
225
150
75
0
0 10 20 30 40 50 60
Time (min)

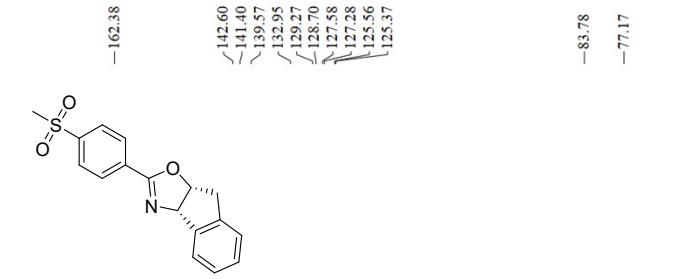
NMR spectra and microwave data of compound 21



21

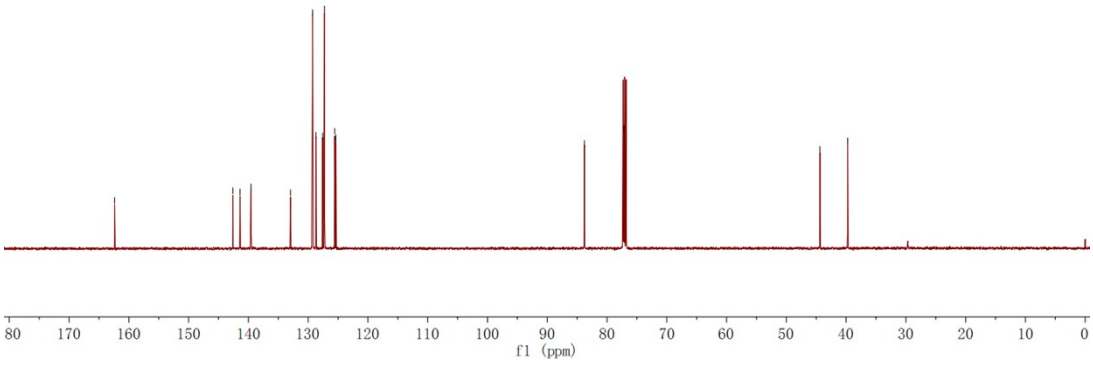
^{1}H NMR (500 MHz, $CDCl_3$)

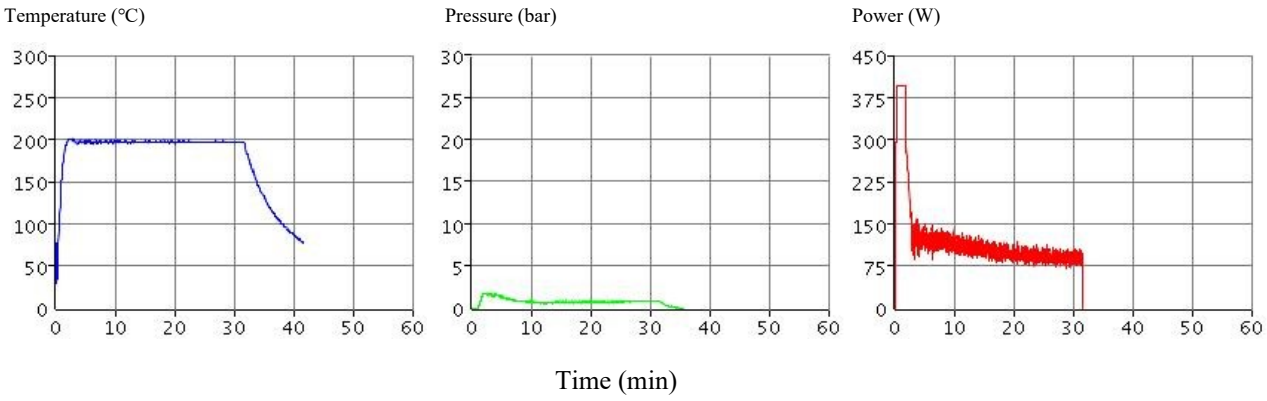




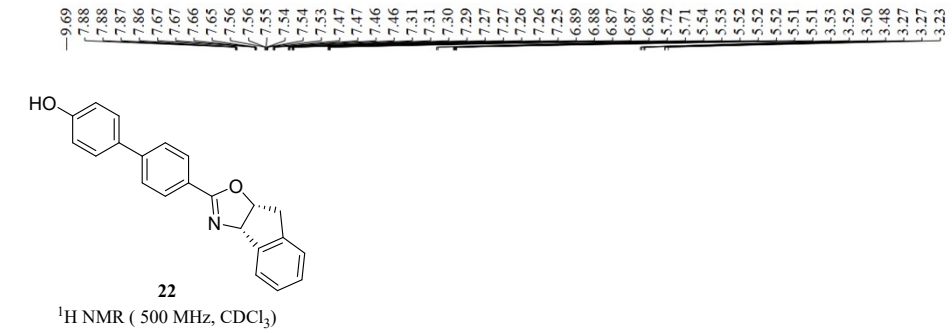
21

^{13}C NMR (126 MHz, $CDCl_3$)



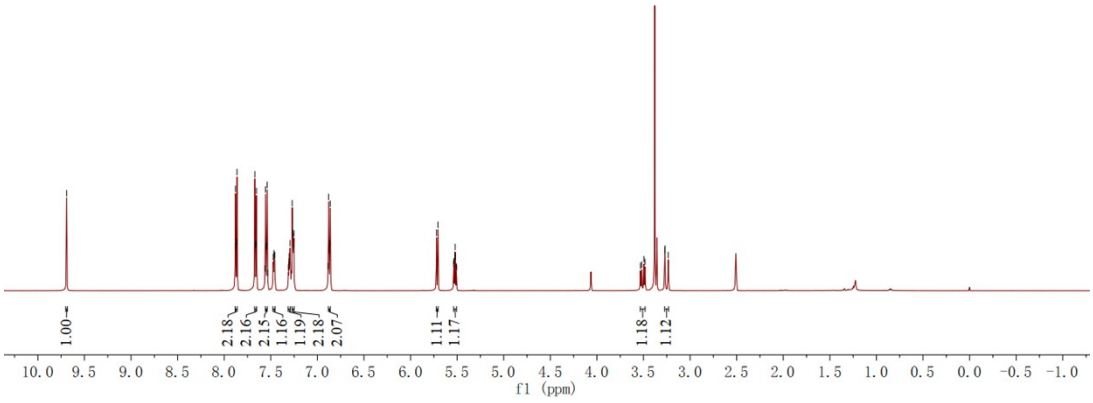

Temperature (°C)
300
250
200
150
100
50
0
0 10 20 30 40 50 60
Pressure (bar)
30
25
20
15
10
5
0
0 10 20 30 40 50 60
Power (W)
450
375
300
225
150
75
0
0 10 20 30 40 50 60
Time (min)

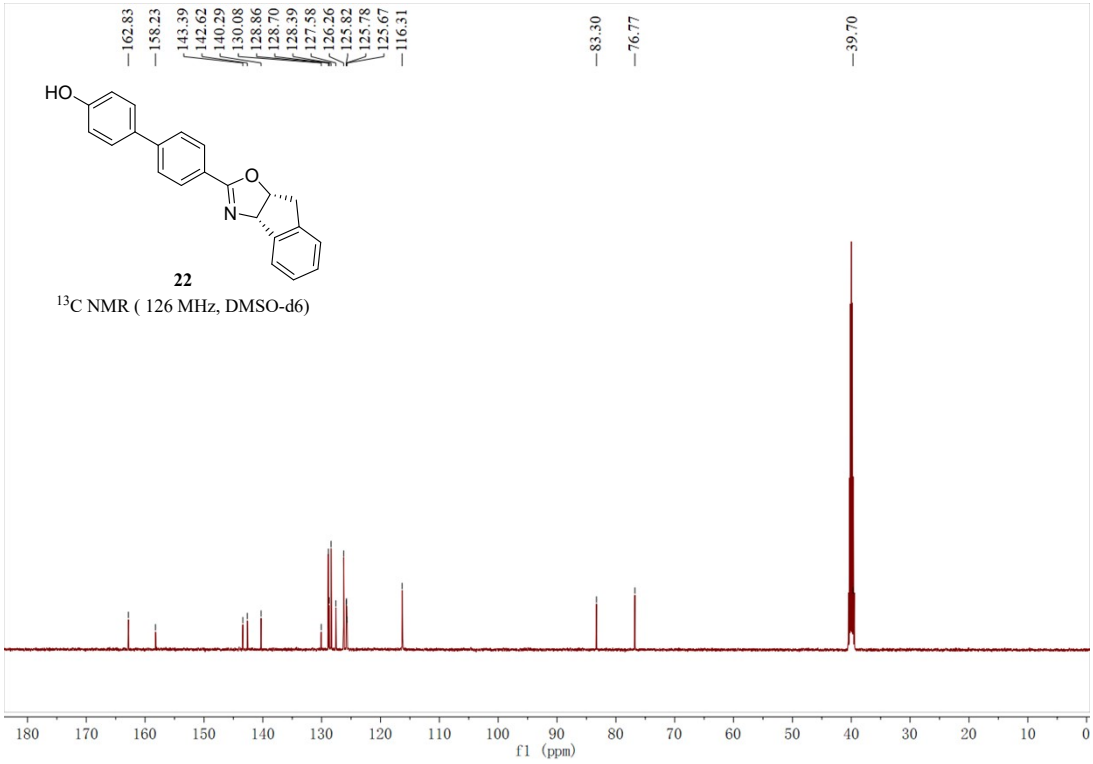
NMR spectra and microwave data of compound 22



22

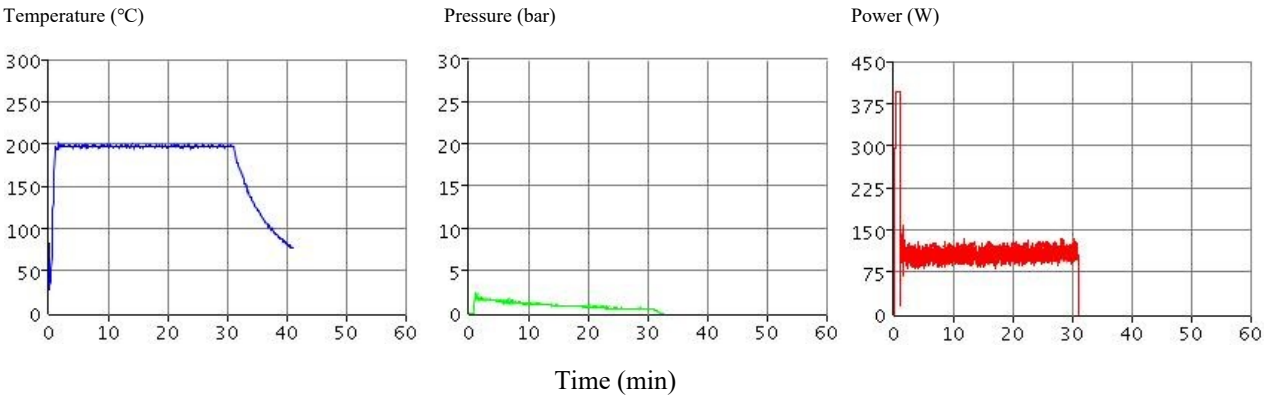
^{1}H NMR (500 MHz, $CDCl_3$)



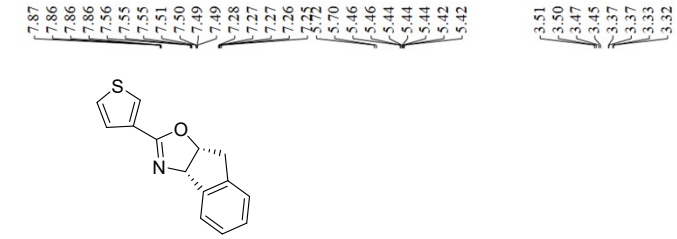


22

^{13}C NMR (126 MHz, DMSO-d6)

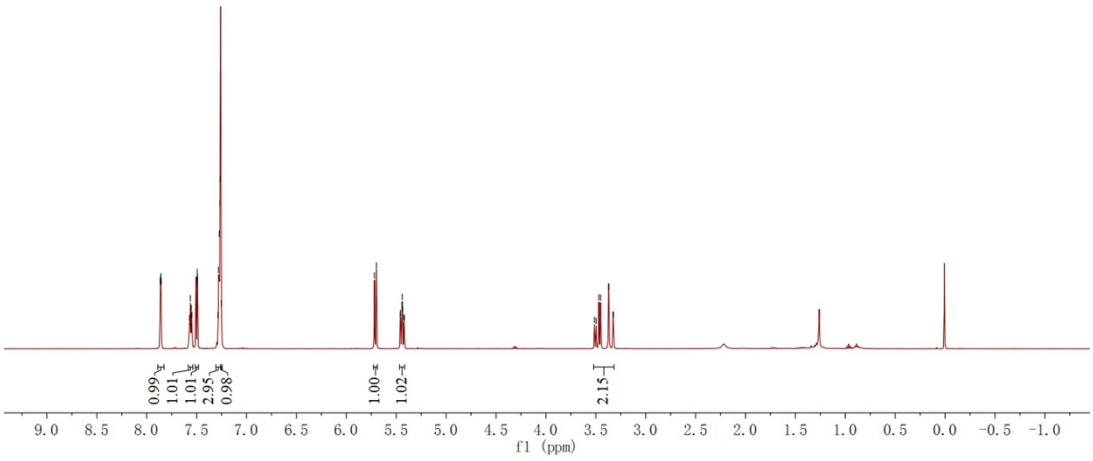

Temperature (°C)
Pressure (bar)
Power (W)
300
250
200
150
100
50
0
30
25
20
15
10
5
0
450
375
300
225
150
75
0
0 10 20 30 40 50 60
Time (min)

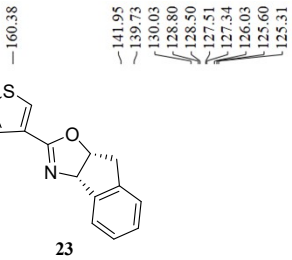
NMR spectra and microwave data of compound 23



23

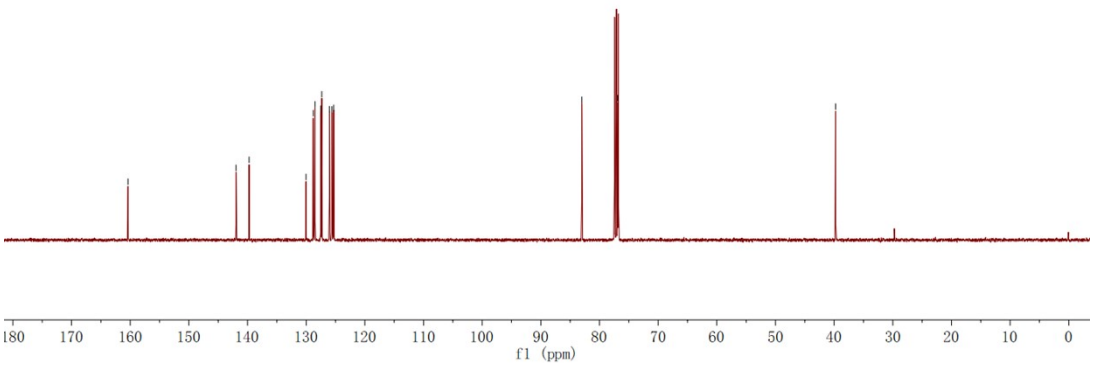
^{1}H NMR (500 MHz, $CDCl_3$)



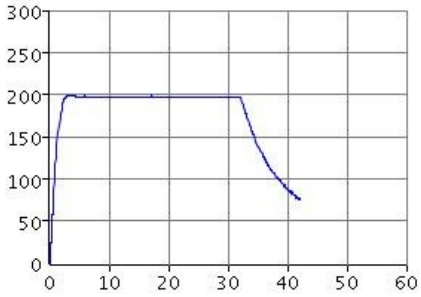


23

^{13}C NMR (126 MHz, $CDCl_3$)

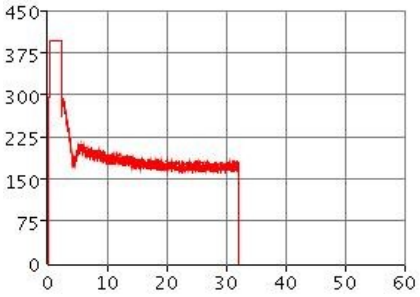


Temperature (°C)



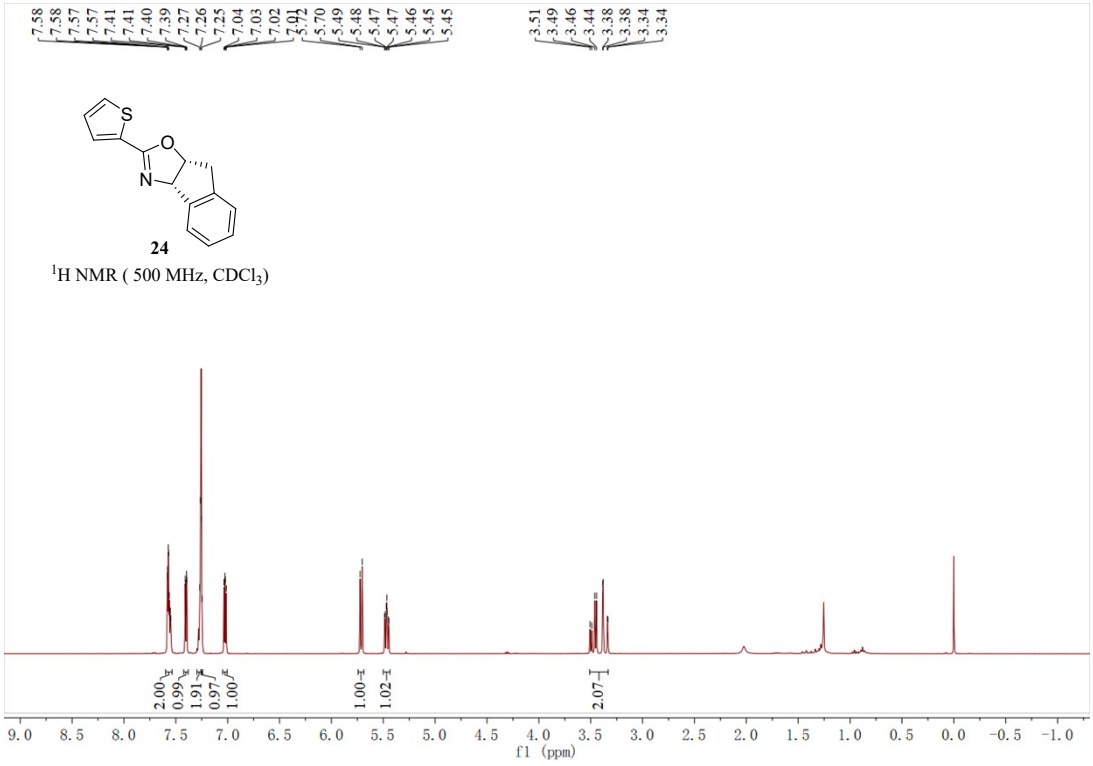
Pressure (bar)

Power (W)

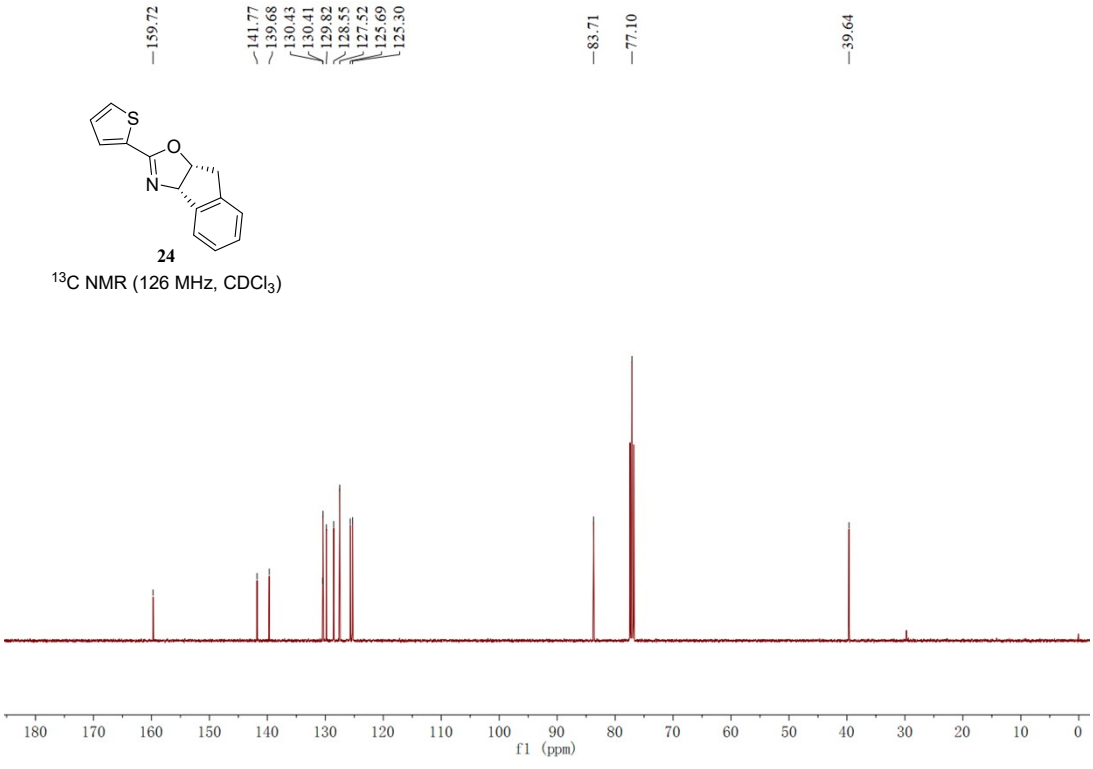


Time (min)

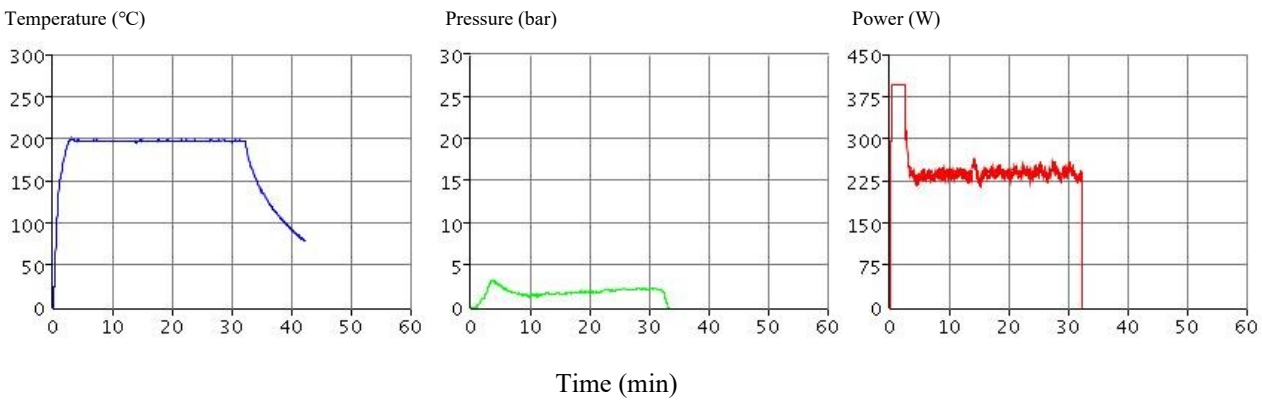
NMR spectra and microwave data of compound 24



^{1}H NMR (500 MHz, $CDCl_3$)



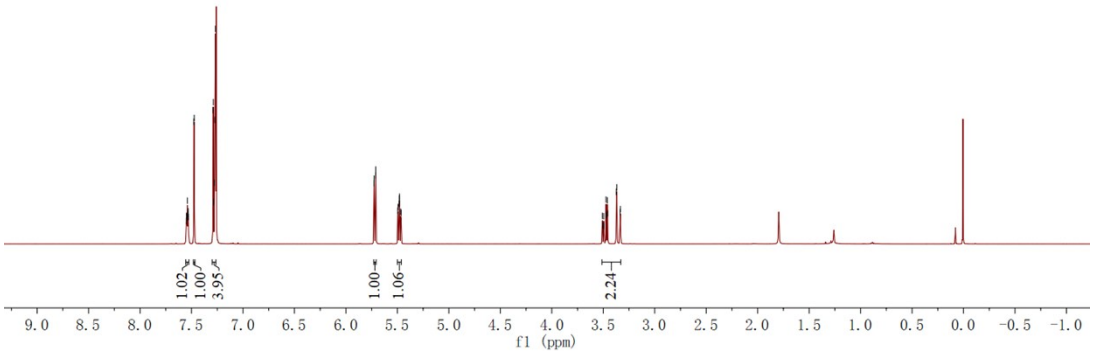
^{13}C NMR (126 MHz, $CDCl_3$)

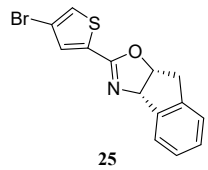

Temperature (°C)
Pressure (bar)
Power (W)
300
250
200
150
100
50
0
30
25
20
15
10
5
0
450
375
300
225
150
75
0
0 10 20 30 40 50 60
Time (min)

NMR spectra and microwave data of compound 25

25

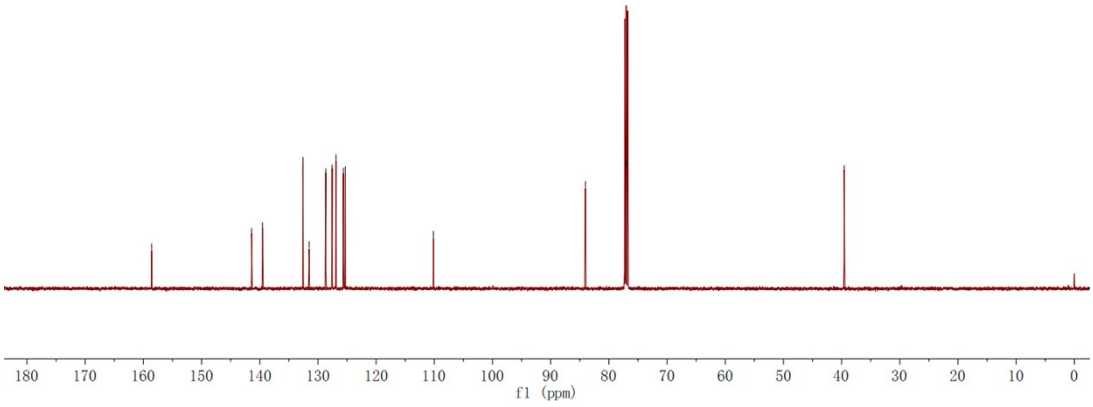
^{1}H NMR (500 MHz, $CDCl_3$)

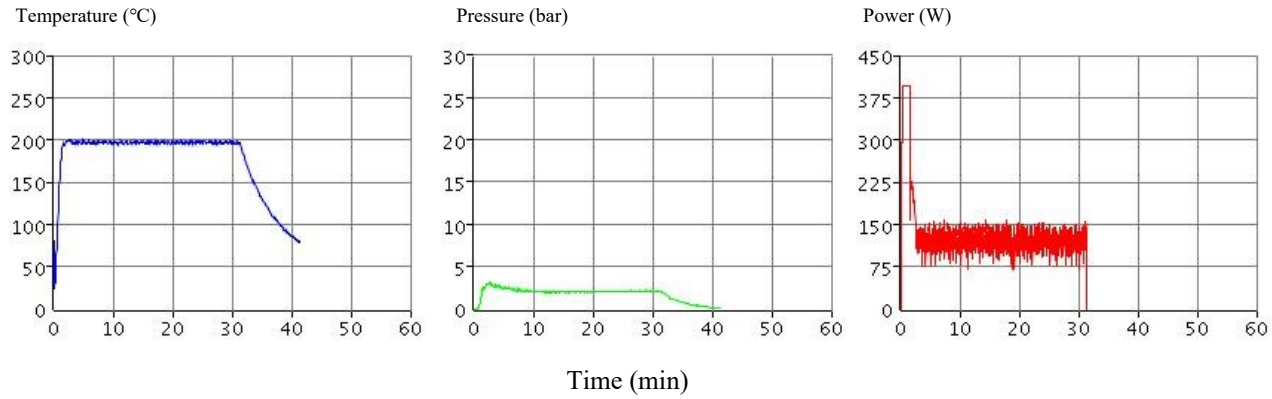




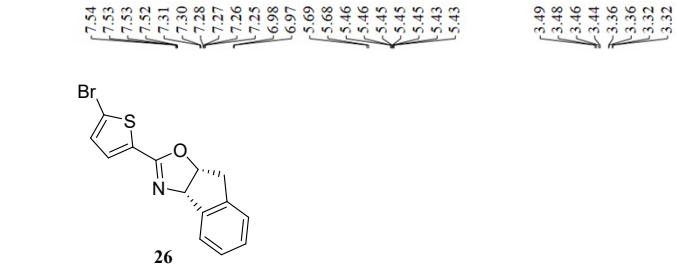
25

^{13}C NMR (126 MHz, $CDCl_3$)



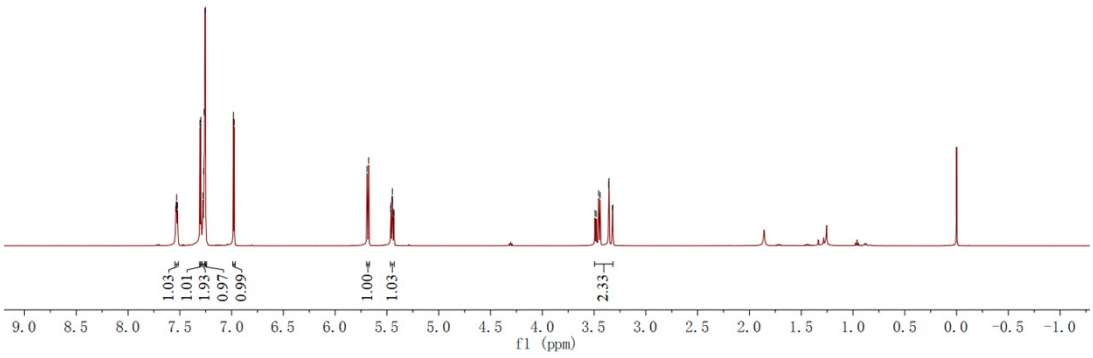

Temperature (°C)
Pressure (bar)
Power (W)
300
250
200
150
100
50
0
30
25
20
15
10
5
0
450
375
300
225
150
75
0
0 10 20 30 40 50 60
Time (min)

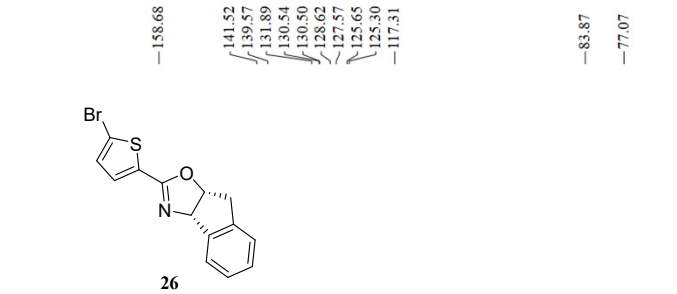
NMR spectra and microwave data of compound 26



26

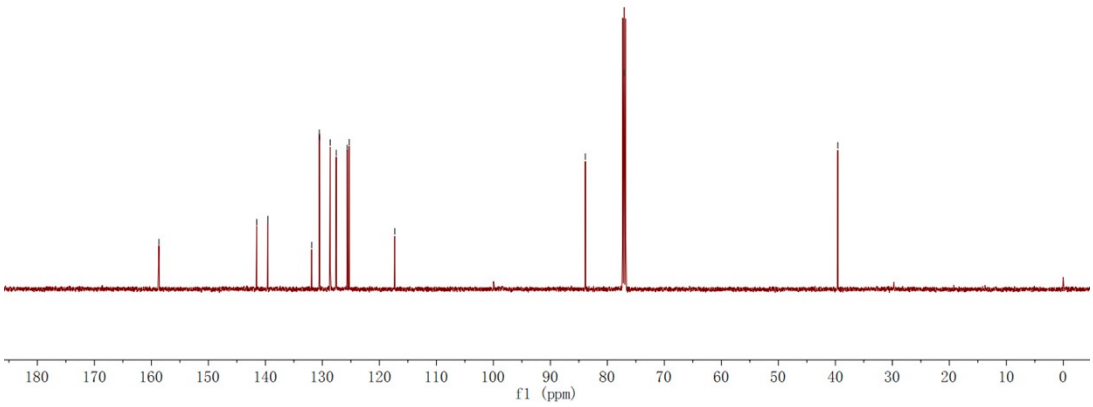
^{1}H NMR (500 MHz, $CDCl_3$)

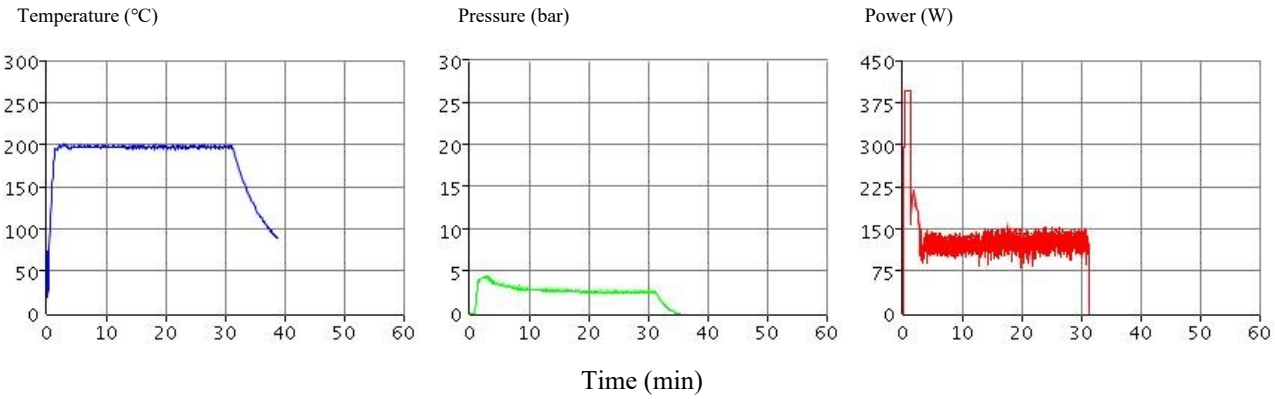




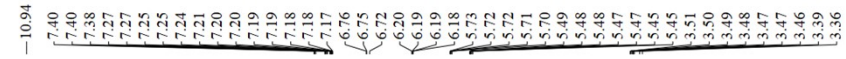
26

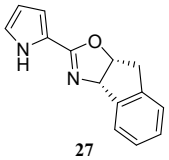
^{13}C NMR (126 MHz, $CDCl_3$)




Temperature (°C)
Pressure (bar)
Power (W)
300
250
200
150
100
50
0
30
25
20
15
10
5
0
450
375
300
225
150
75
0
0 10 20 30 40 50 60
Time (min)

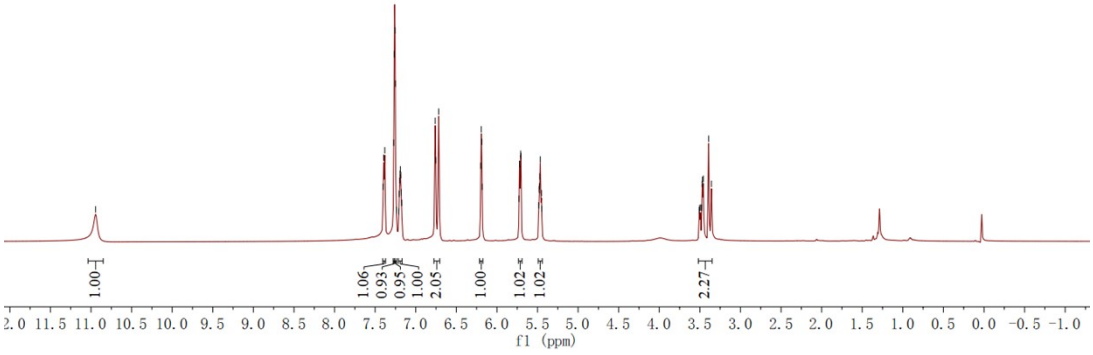
NMR spectra and microwave data of compound 27

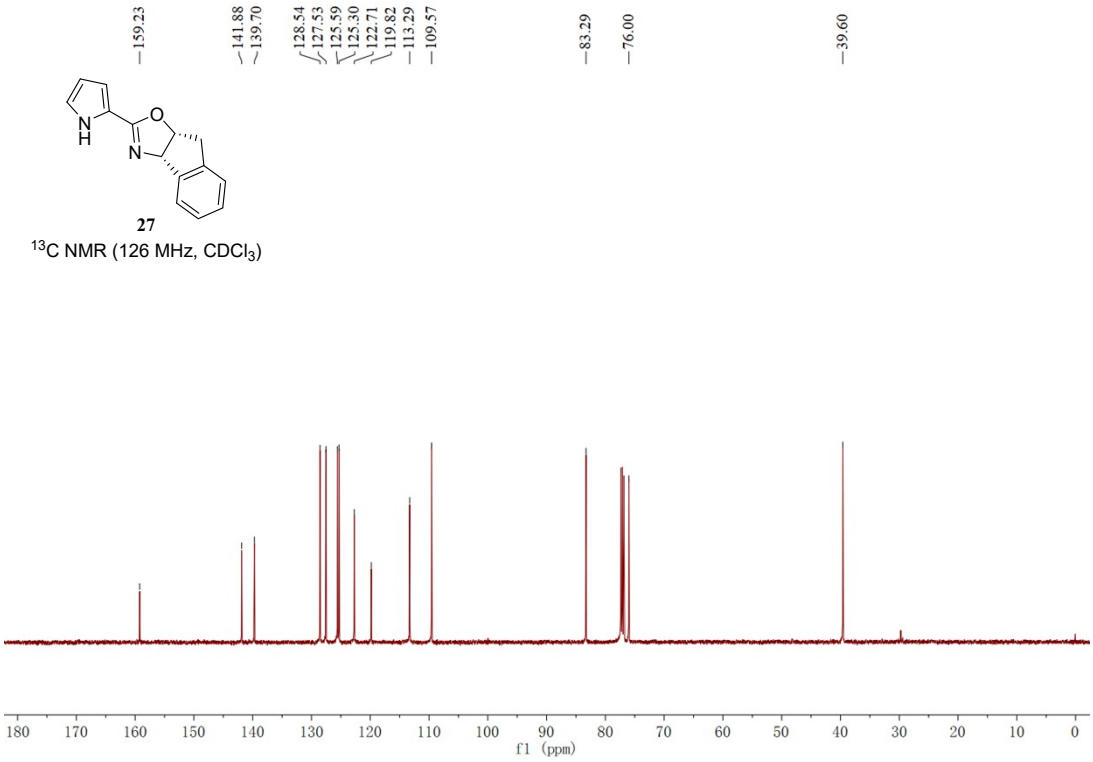




27

^{1}H NMR (500 MHz, $CDCl_3$)

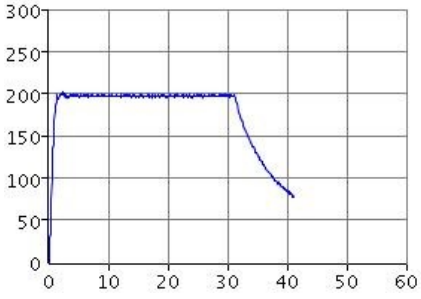




27

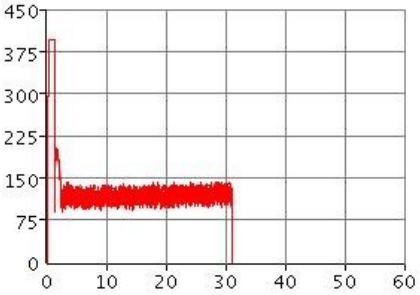
^{13}C NMR (126 MHz, $CDCl_3$)

Temperature (°C)



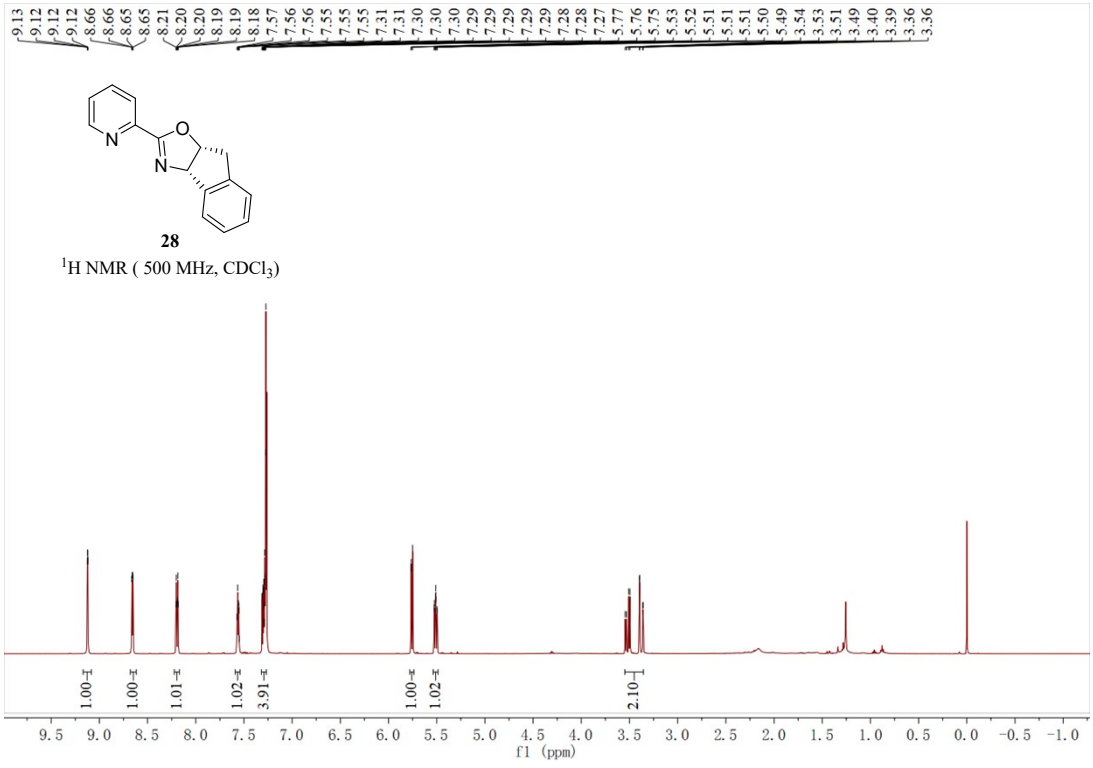
Pressure (bar)

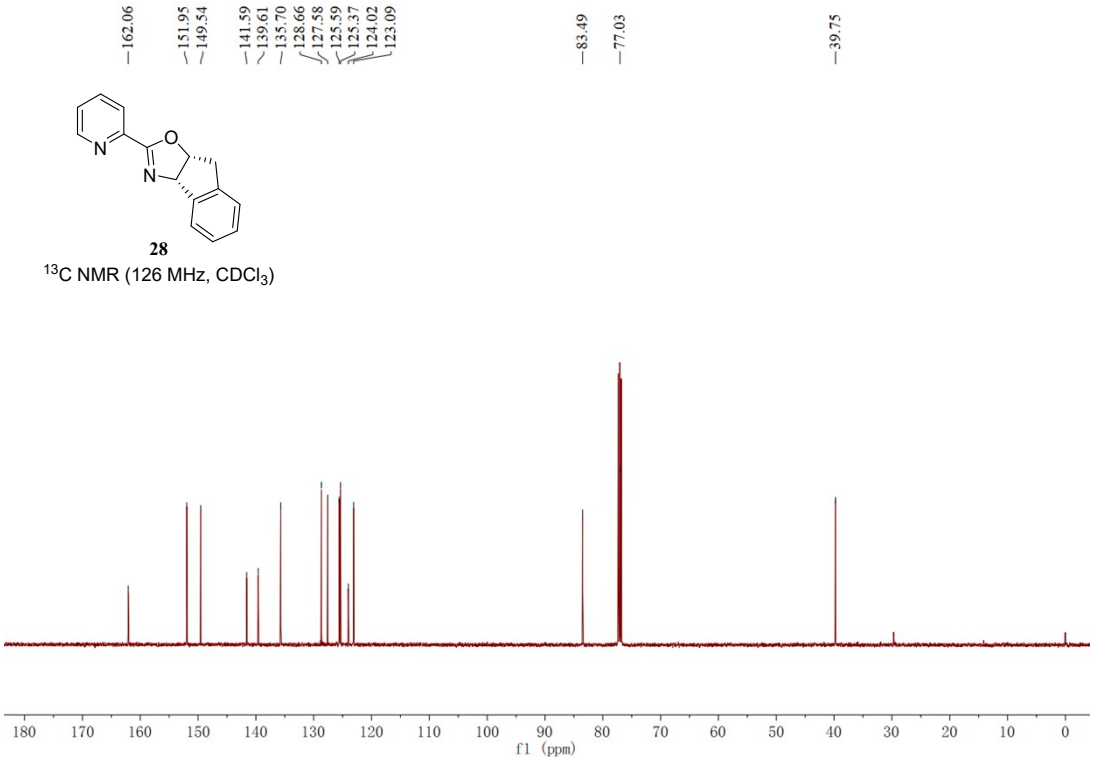
Power (W)

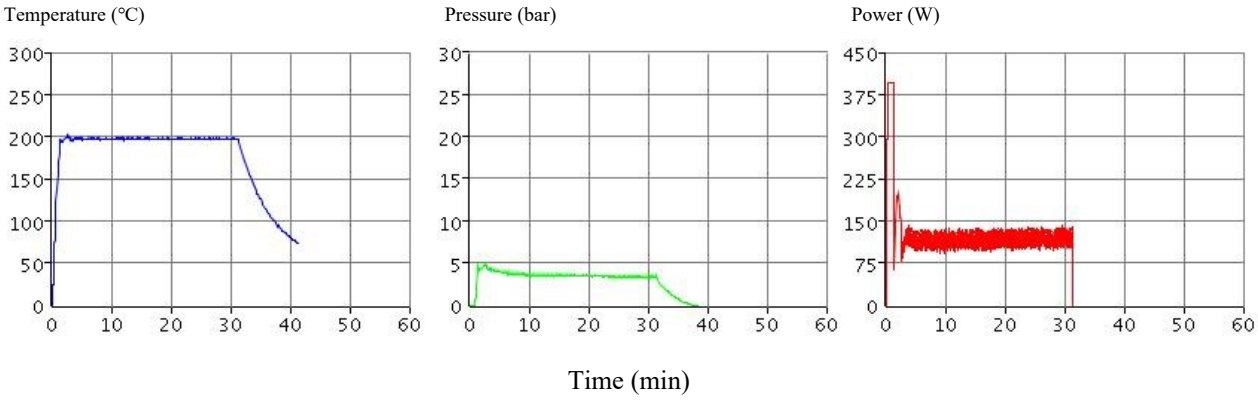


Time (min)

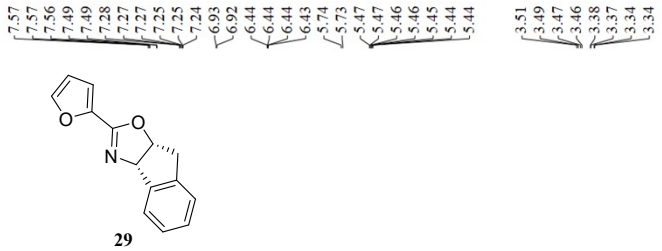
NMR spectra and microwave data of compound 28





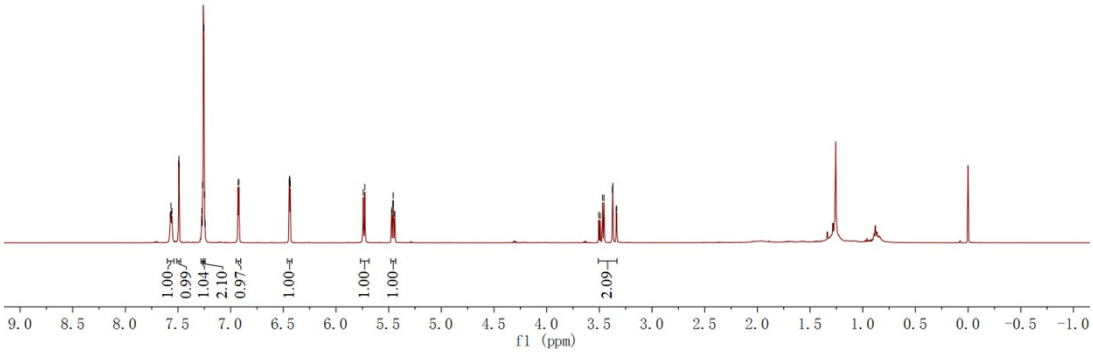

Temperature (°C)
Pressure (bar)
Power (W)
300
250
200
150
100
50
0
30
25
20
15
10
5
0
450
375
300
225
150
75
0
0 10 20 30 40 50 60
Time (min)

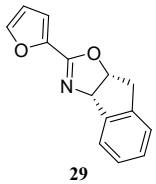
NMR spectra and microwave data of compound 29



29

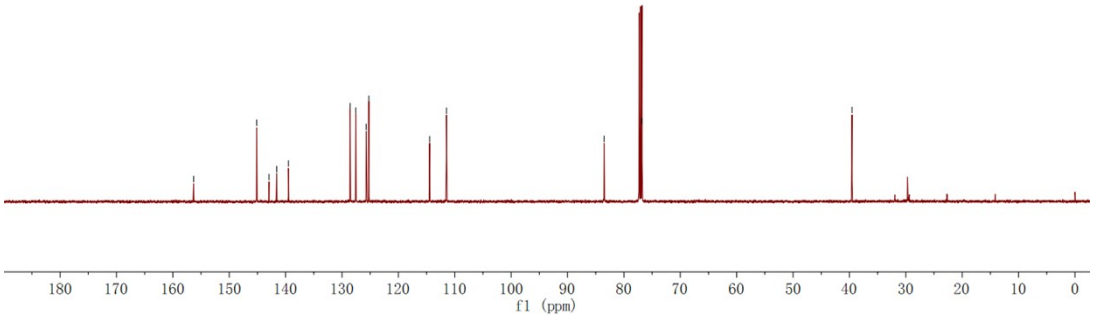
^{1}H NMR (500 MHz, $CDCl_3$)

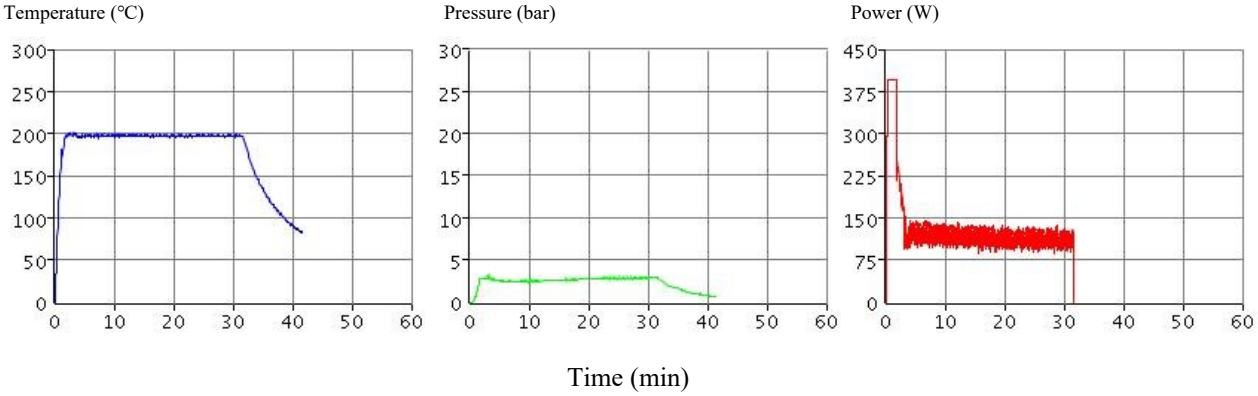




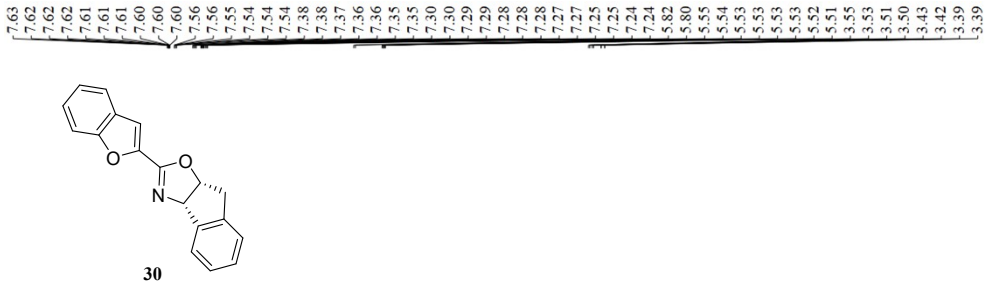
29

^{13}C NMR (126 MHz, $CDCl_3$)



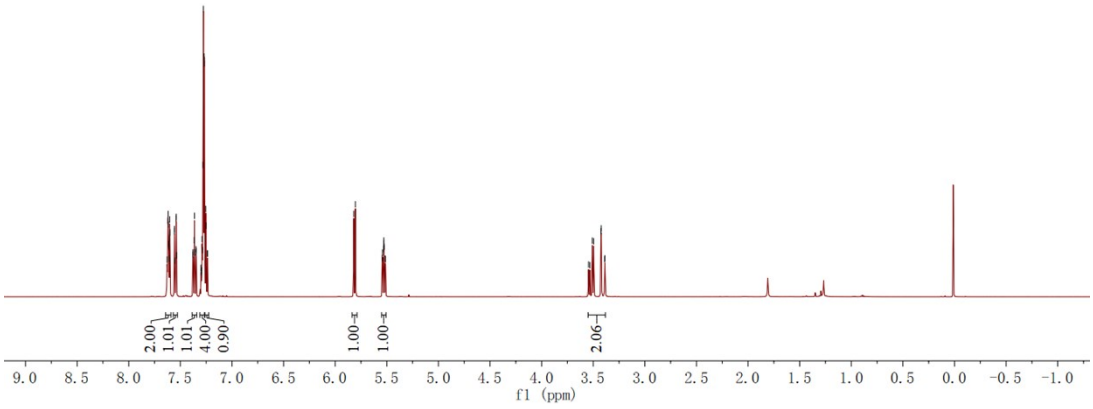

Temperature (°C)
Pressure (bar)
Power (W)
300
250
200
150
100
50
0
30
25
20
15
10
5
0
450
375
300
225
150
75
0
0 10 20 30 40 50 60
Time (min)

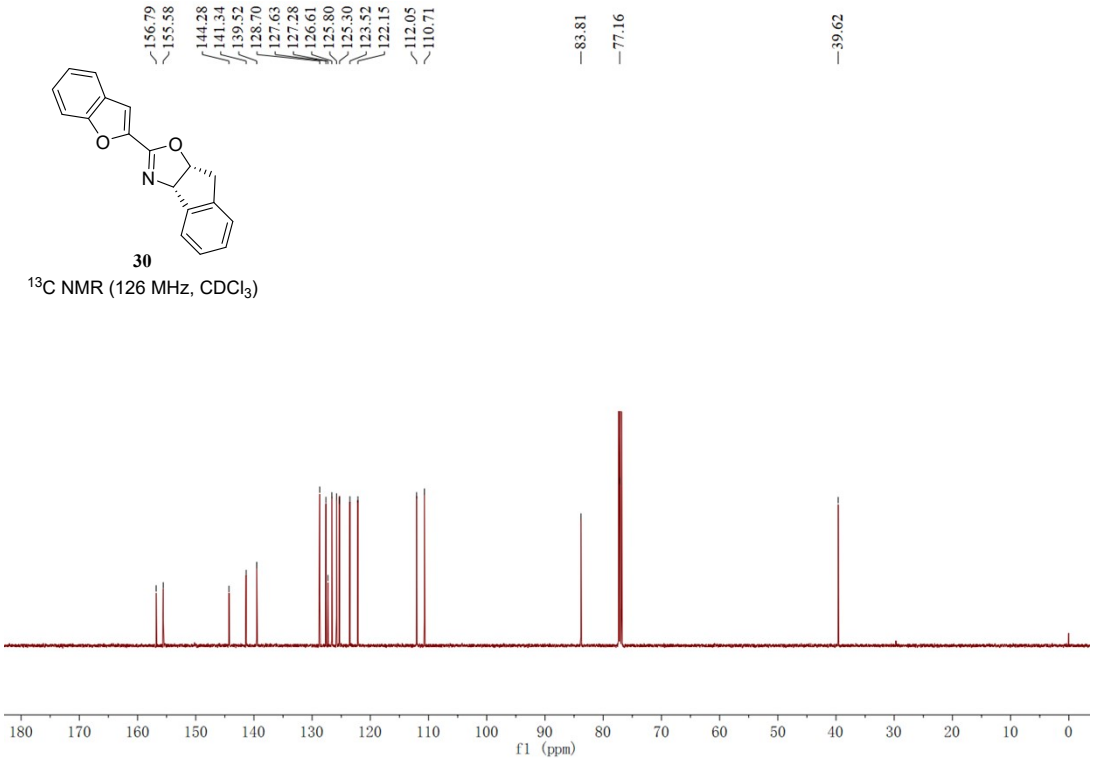
NMR spectra and microwave data of compound 30



30

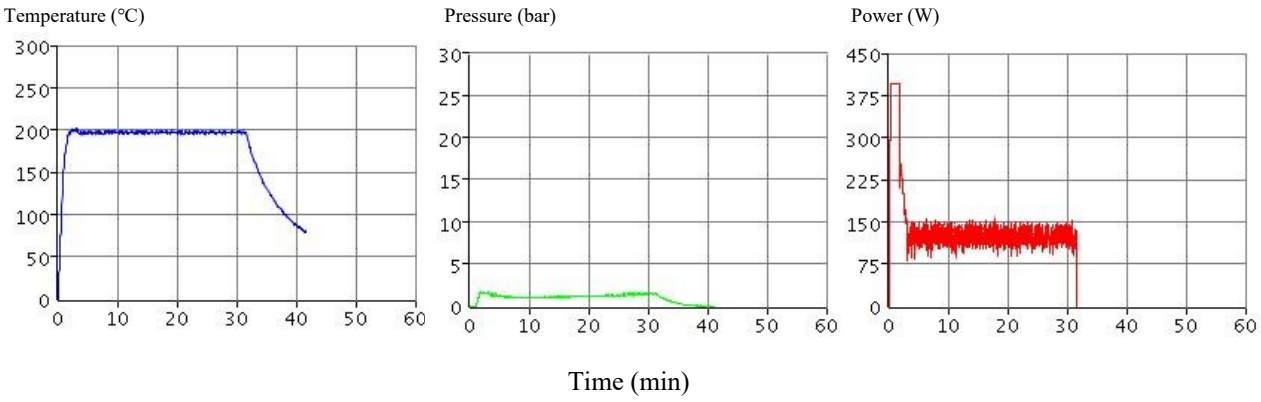
^{1}H NMR (500 MHz, $CDCl_3$)



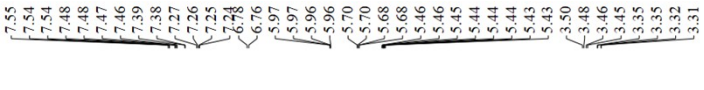


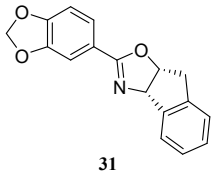
30

^{13}C NMR (126 MHz, $CDCl_3$)


Temperature (°C)
Pressure (bar)
Power (W)
300
250
200
150
100
50
0
30
25
20
15
10
5
0
450
375
300
225
150
75
0
0 10 20 30 40 50 60
Time (min)

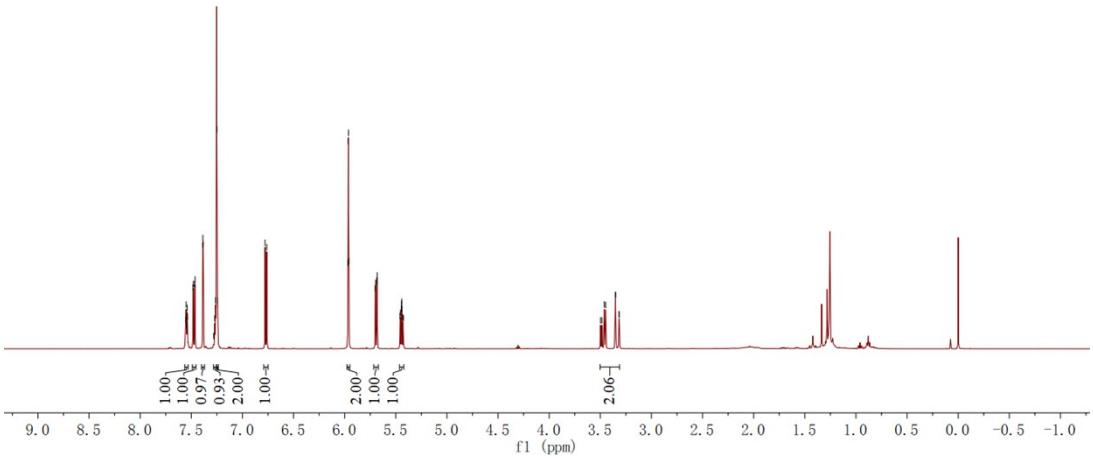
NMR spectra and microwave data of compound 31

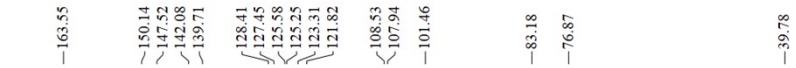


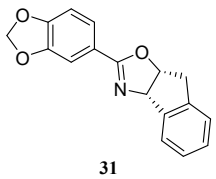


31

^{1}H NMR (500 MHz, $CDCl_3$)

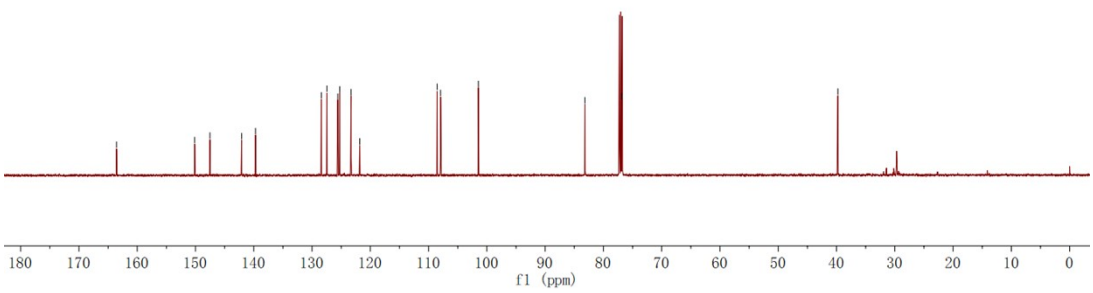


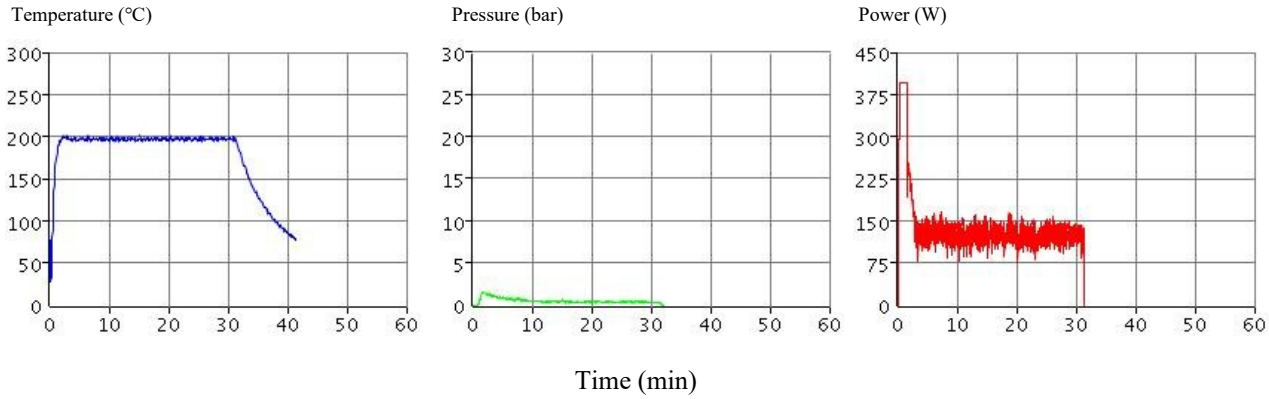




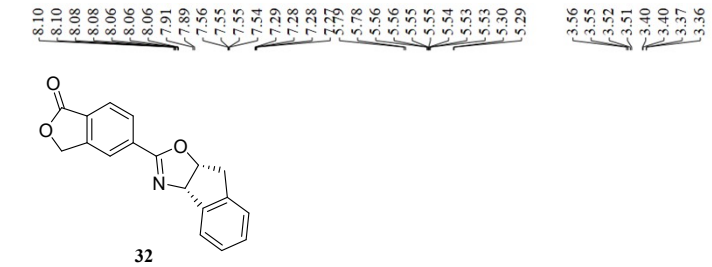
31

^{13}C NMR (126 MHz, $CDCl_3$)



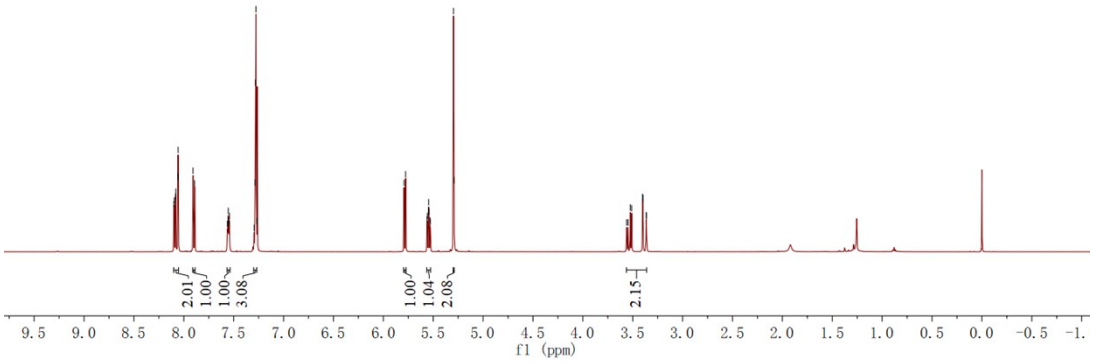

Temperature (°C)
Pressure (bar)
Power (W)
300
250
200
150
100
50
0
30
25
20
15
10
5
0
450
375
300
225
150
75
0
0 10 20 30 40 50 60
Time (min)

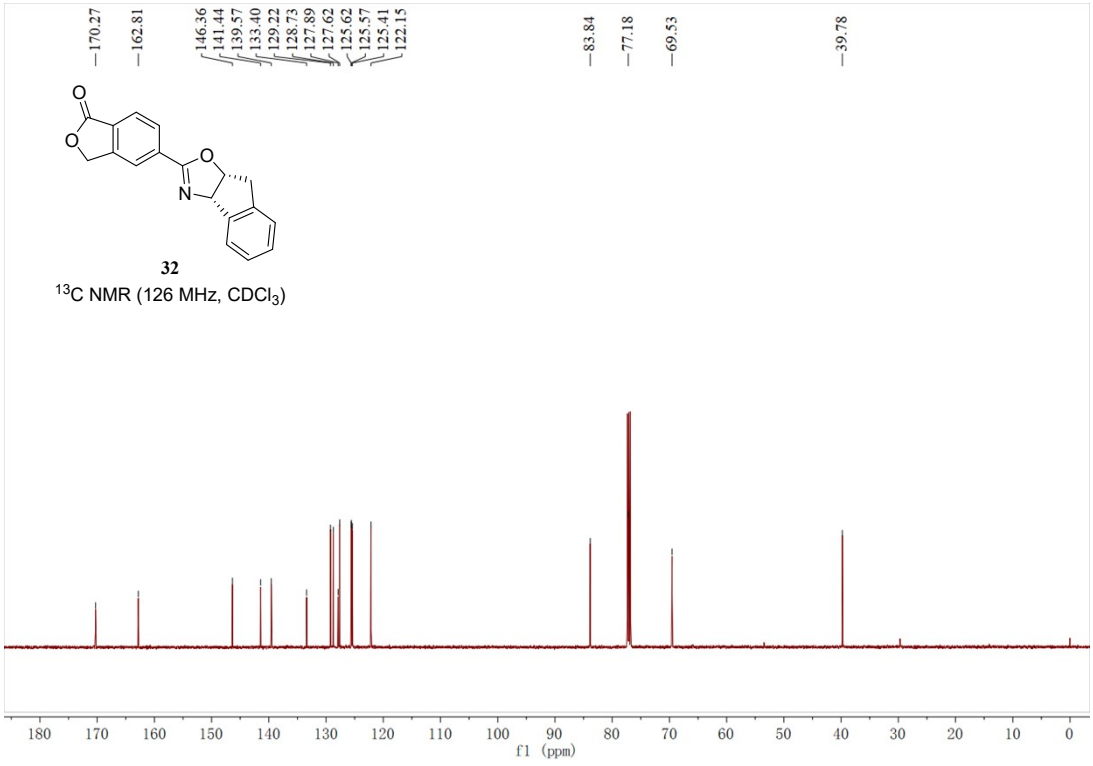
NMR spectra and microwave data of compound 32



32

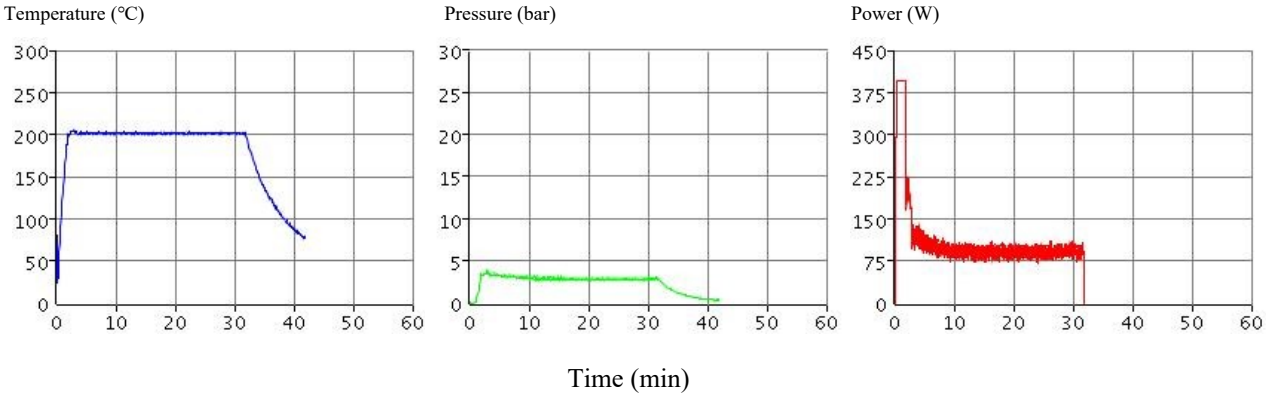
^{1}H NMR (500 MHz, $CDCl_3$)



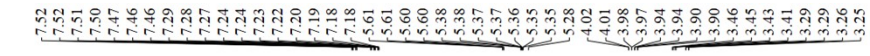


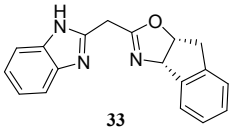
32

^{13}C NMR (126 MHz, $CDCl_3$)


Temperature (°C)
300
250
200
150
100
50
0
Pressure (bar)
30
25
20
15
10
5
0
Power (W)
450
375
300
225
150
75
0
0 10 20 30 40 50 60
Time (min)

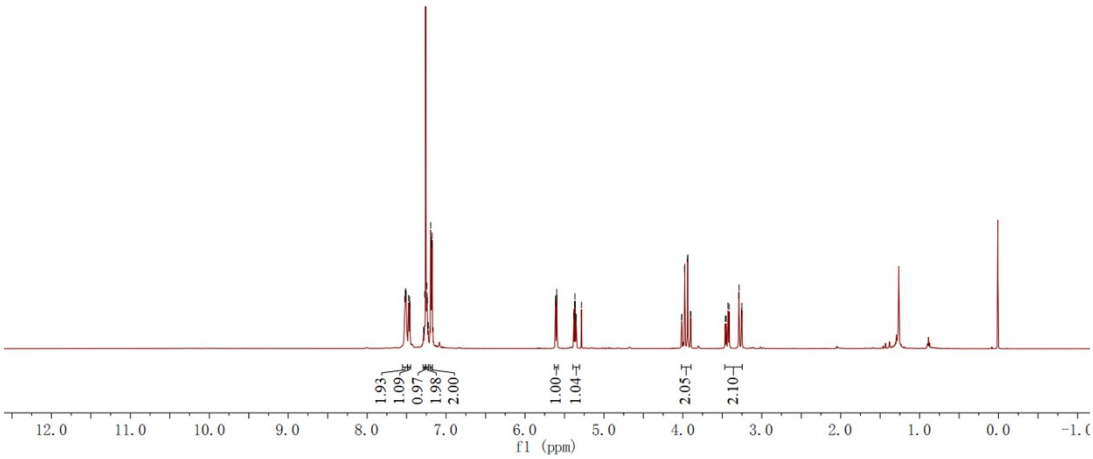
NMR spectra and microwave data of compound 33

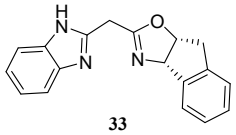




33

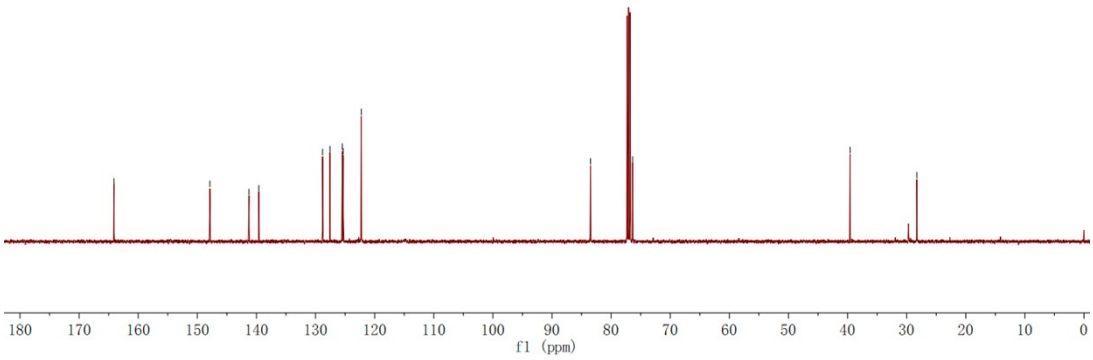
^{1}H NMR (500 MHz, $CDCl_3$)

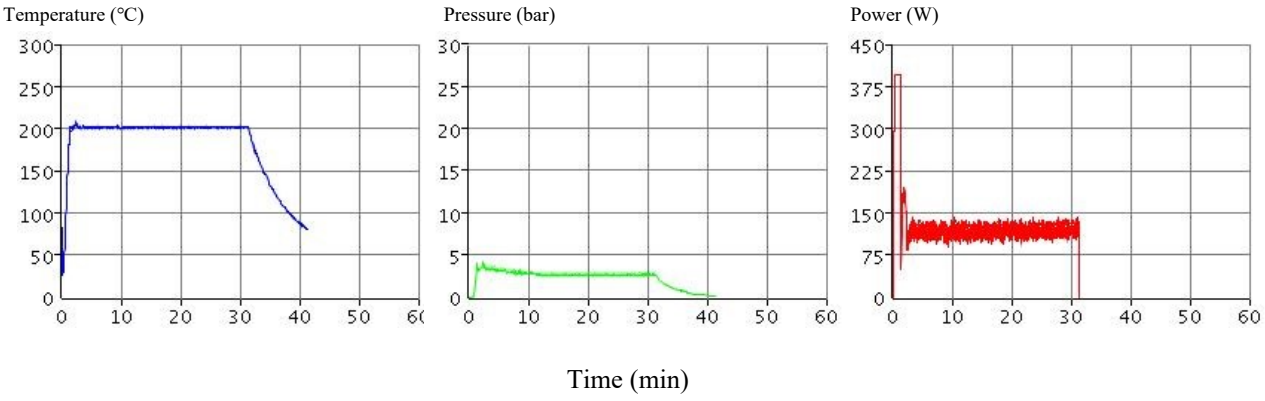




33

^{13}C NMR (126 MHz, $CDCl_3$)

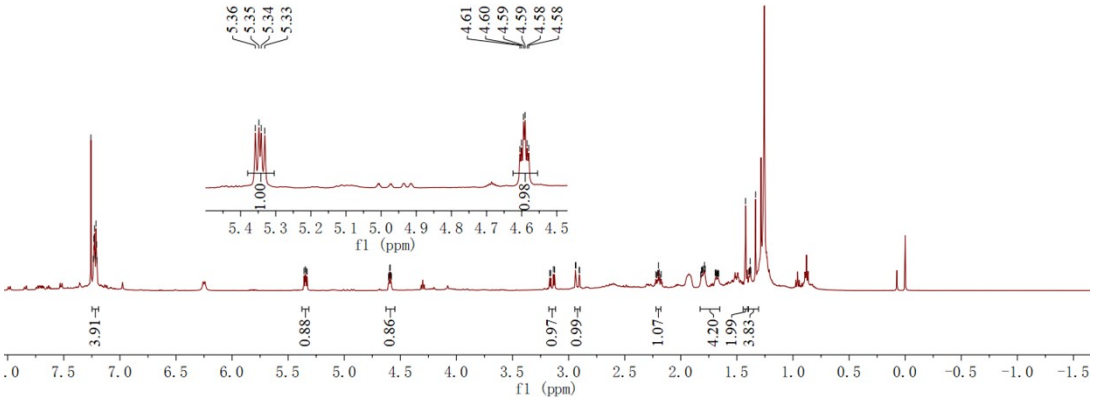


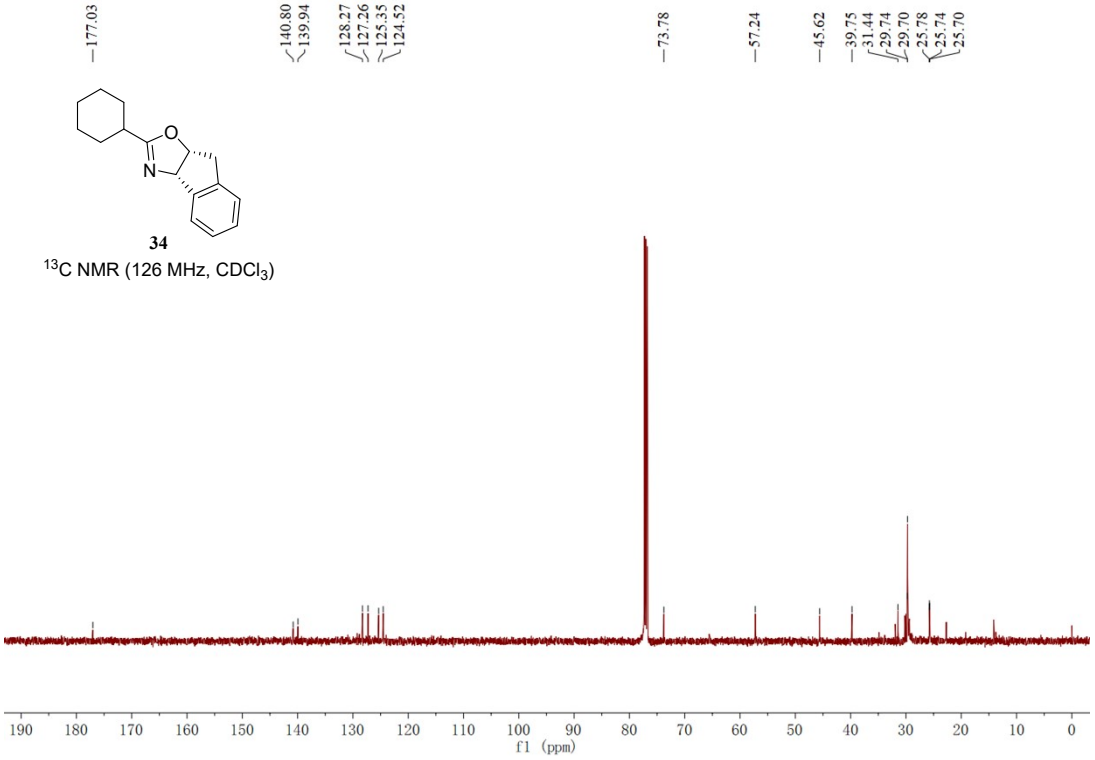

Temperature (°C)
300
250
200
150
100
50
0
0 10 20 30 40 50 60
Pressure (bar)
30
25
20
15
10
5
0
0 10 20 30 40 50 60
Power (W)
450
375
300
225
150
75
0
0 10 20 30 40 50 60
Time (min)

NMR spectra and microwave data of compound 34

34

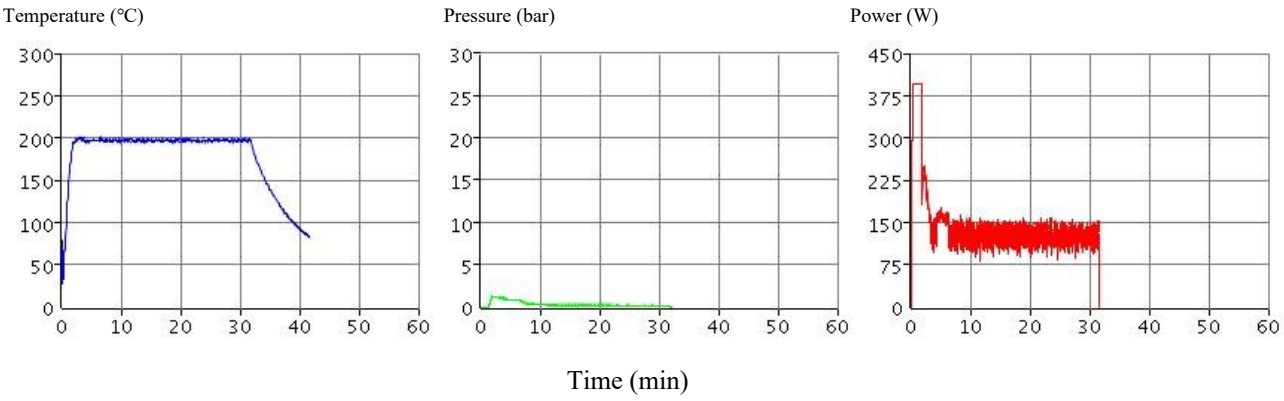
^{1}H NMR (500 MHz, $CDCl_3$)



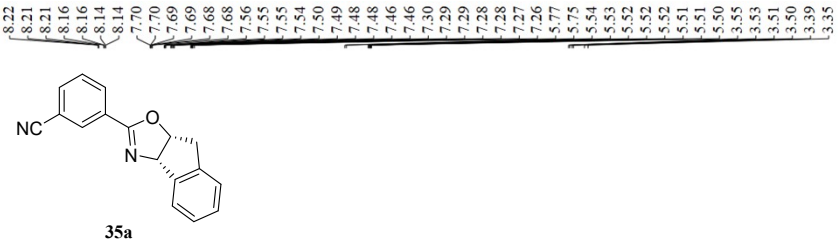


34

^{13}C NMR (126 MHz, $CDCl_3$)

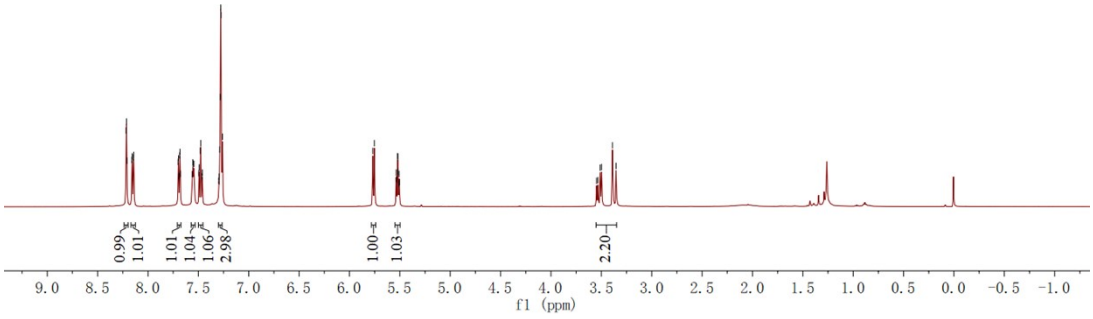

Temperature (°C)
300
250
200
150
100
50
0
Pressure (bar)
30
25
20
15
10
5
0
Power (W)
450
375
300
225
150
75
0
0 10 20 30 40 50 60
Time (min)

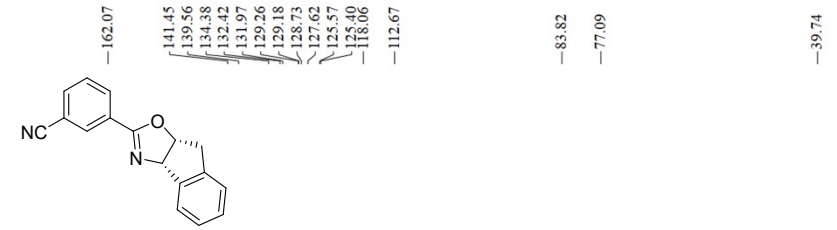
NMR spectra and microwave data of compound 35a, 35b



35a

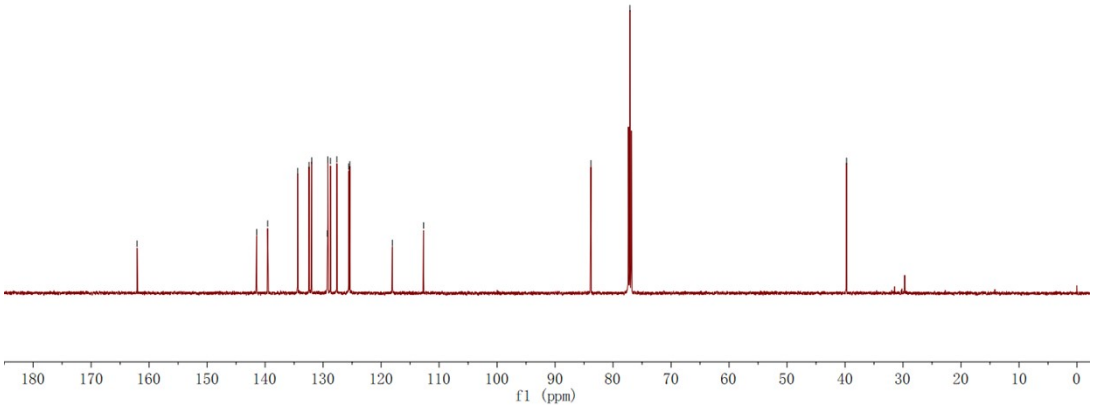
^{1}H NMR (500 MHz, $CDCl_3$)

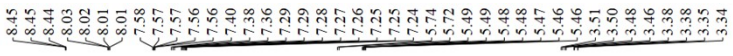


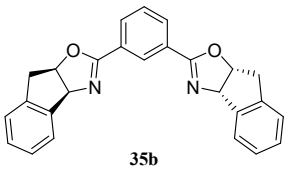


35a

^{13}C NMR (126 MHz, $CDCl_3$)

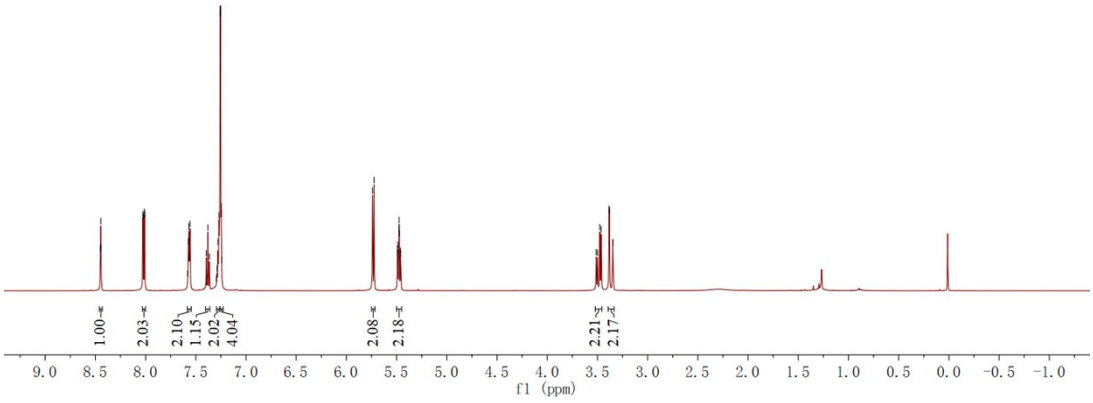


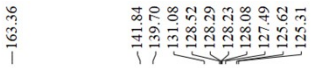


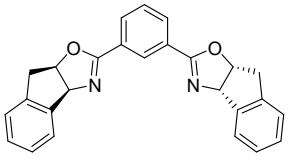


35b

^{1}H NMR (500 MHz, $CDCl_3$)

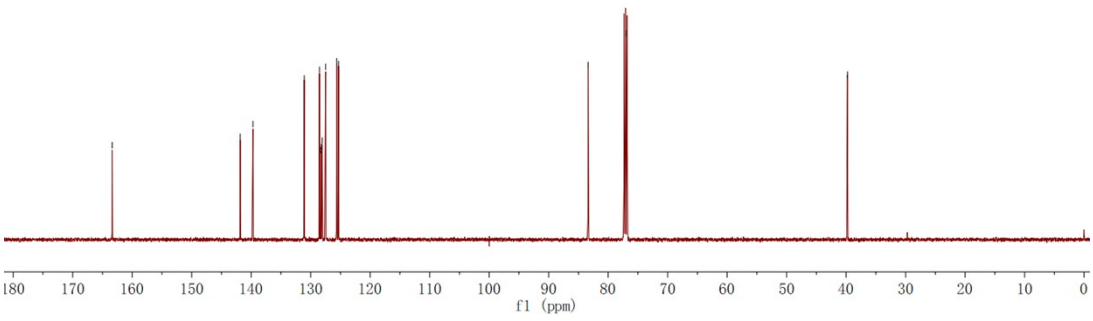


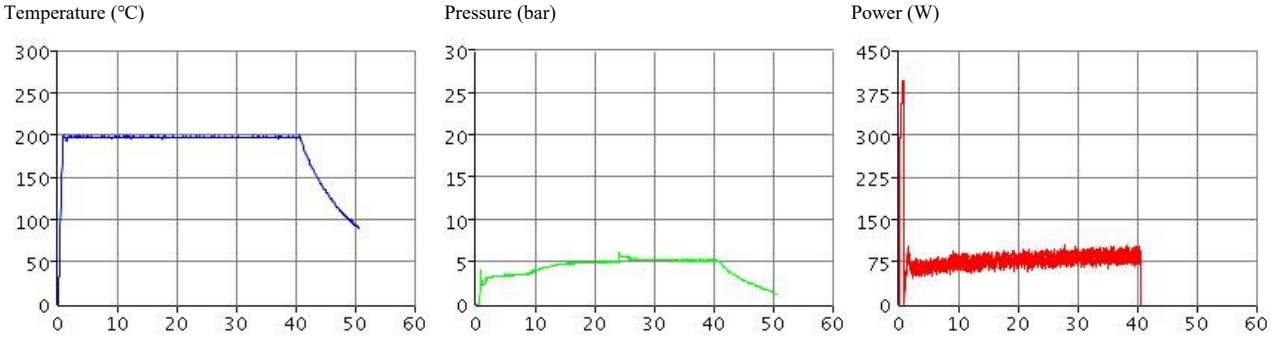




35b

^{13}C NMR (126 MHz, $CDCl_3$)

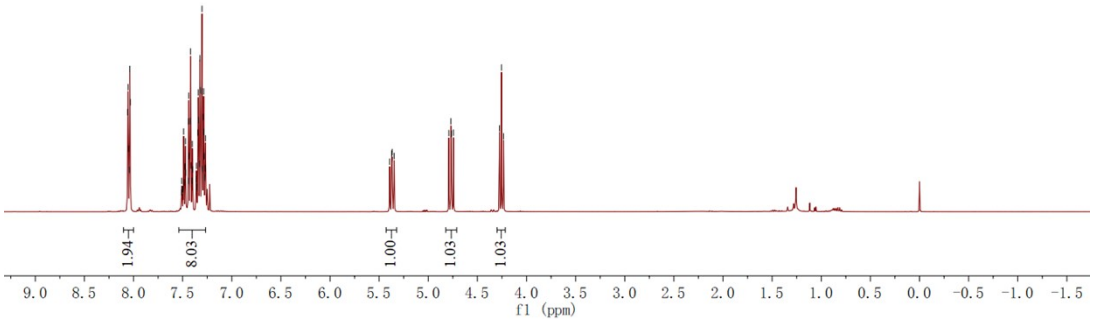


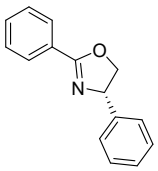

Temperature (°C)
Pressure (bar)
Power (W)
300
250
200
150
100
50
0
30
25
20
15
10
5
0
450
375
300
225
150
75
0
0 10 20 30 40 50 60
Time (min)

NMR spectra and microwave data of compound 36

36

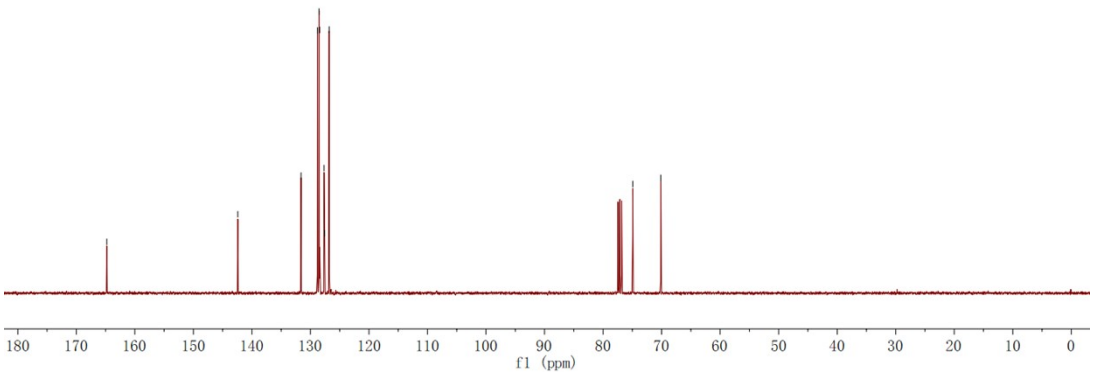
^{1}H NMR (500 MHz, $CDCl_3$)

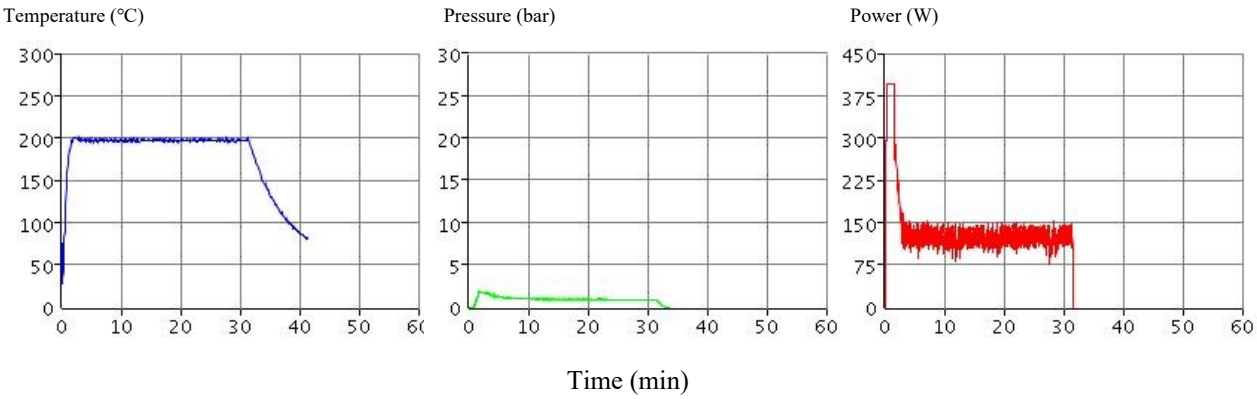




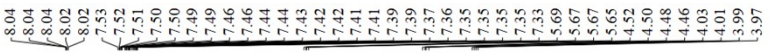
36

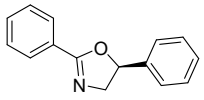
^{1}H NMR (500 MHz, $CDCl_3$)




Temperature (°C)
Pressure (bar)
Power (W)
300
250
200
150
100
50
0
30
25
20
15
10
5
0
450
375
300
225
150
75
0
0 10 20 30 40 50 60
Time (min)

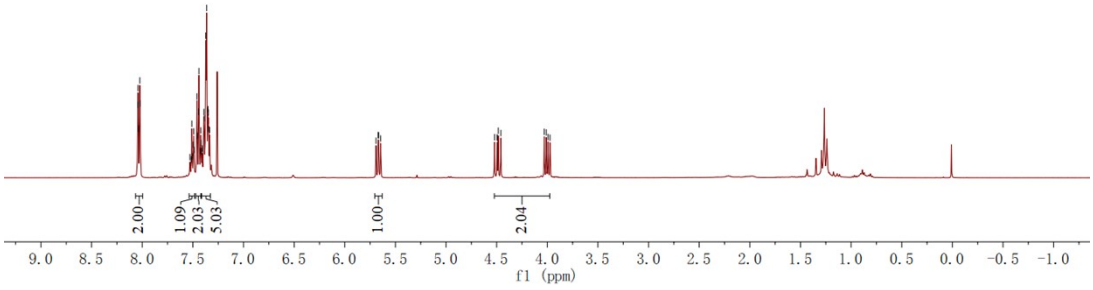
NMR spectra and microwave data of compound 37

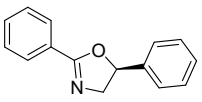




37

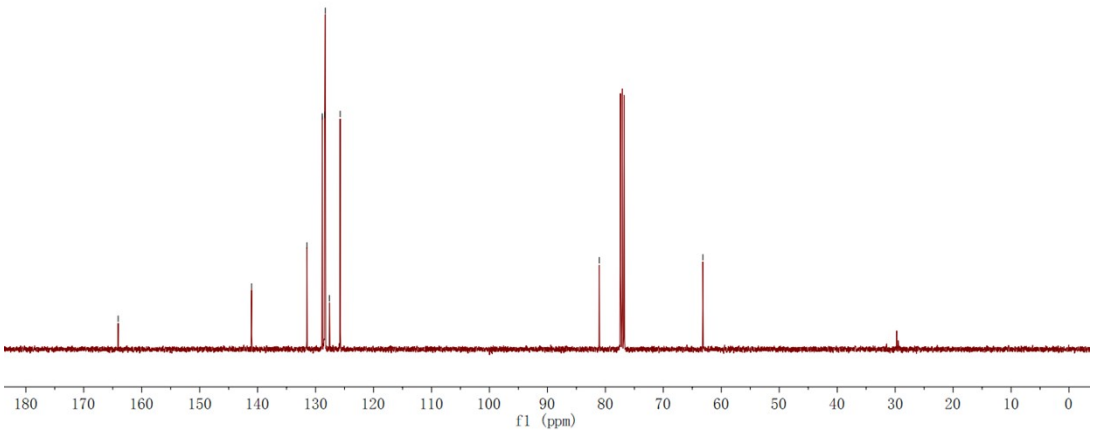
^{1}H NMR (500 MHz, $CDCl_3$)

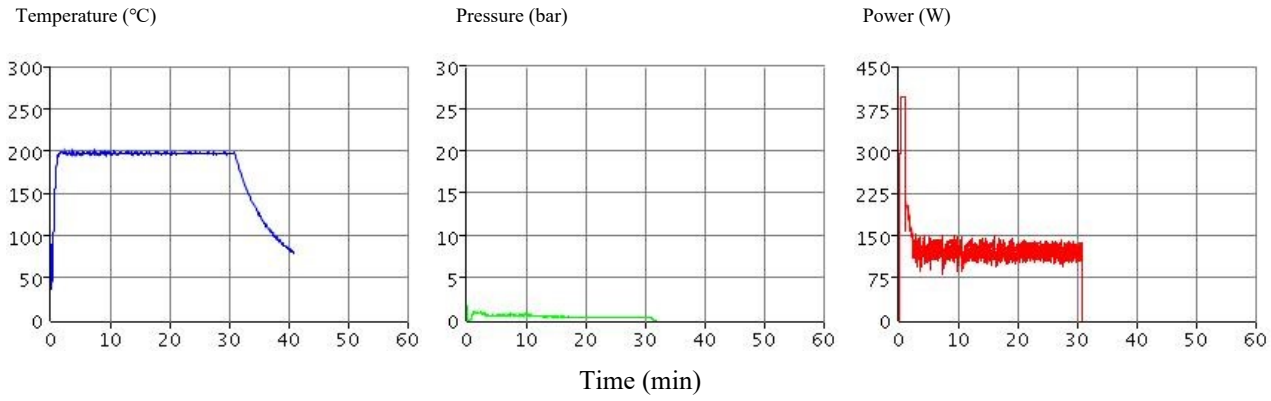




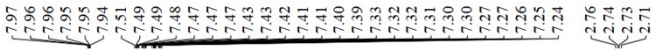
37

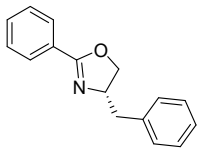
^{13}C NMR (126 MHz, $CDCl_3$)




Temperature (°C)
Pressure (bar)
Power (W)
300
250
200
150
100
50
0
30
25
20
15
10
5
0
450
375
300
225
150
75
0
0 10 20 30 40 50 60
Time (min)

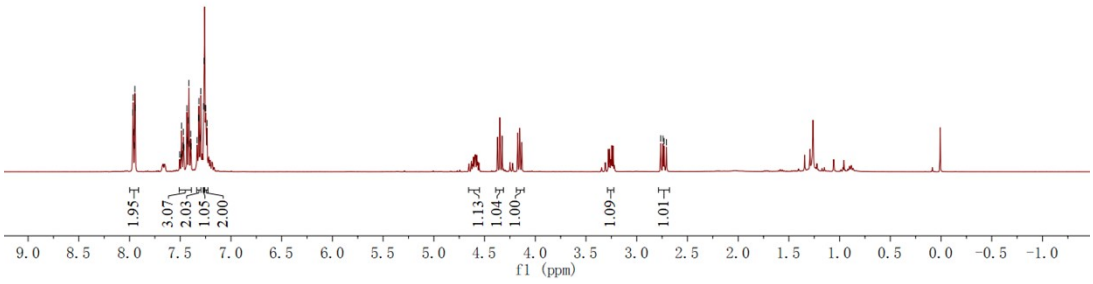
NMR spectra and microwave data of compound 38

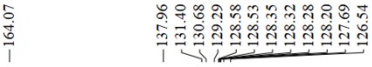


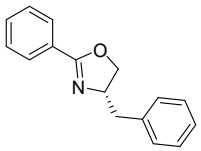


38

^{1}H NMR (500 MHz, $CDCl_3$)

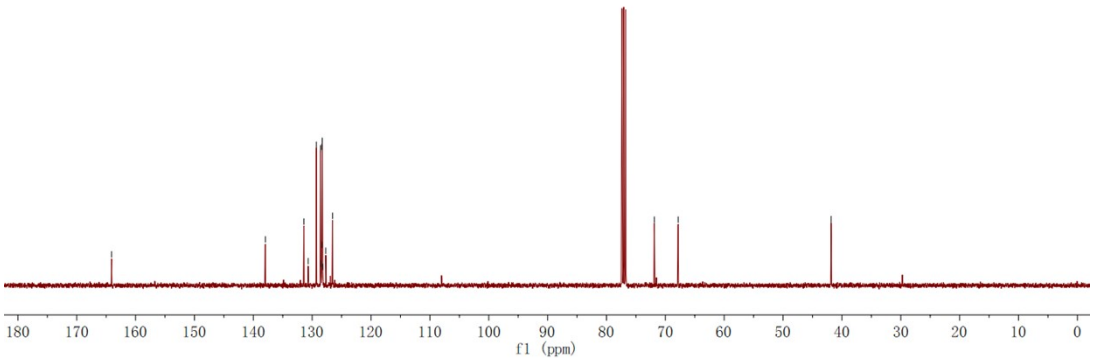


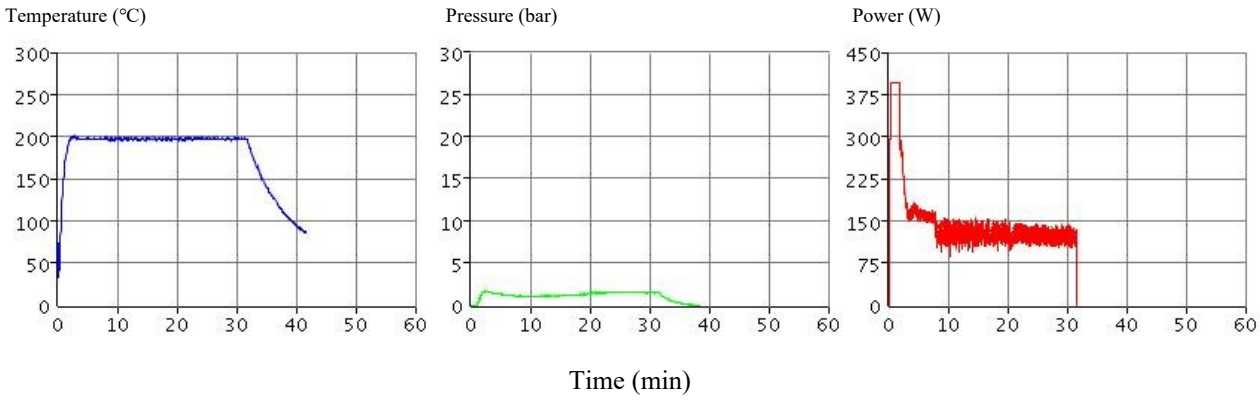




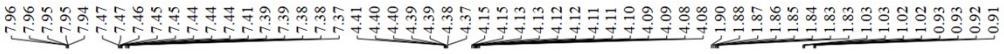
38

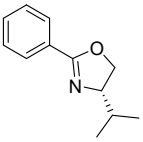
^{13}C NMR (126 MHz, $CDCl_3$)




Temperature (°C)
Pressure (bar)
Power (W)
300
250
200
150
100
50
0
30
25
20
15
10
5
0
450
375
300
225
150
75
0
0 10 20 30 40 50 60
Time (min)

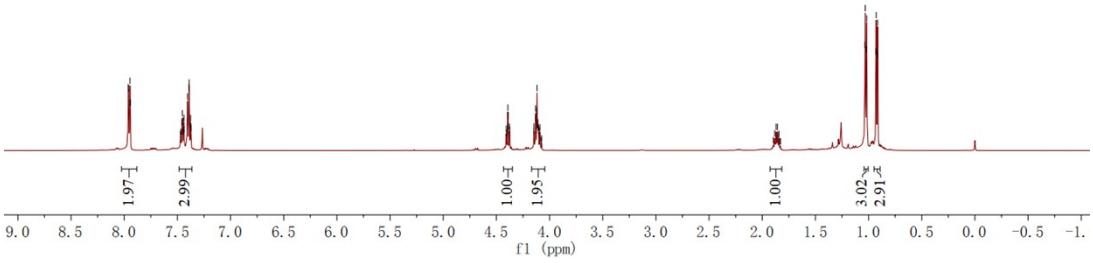
NMR spectra and microwave data of compound 40

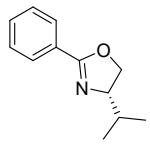




40

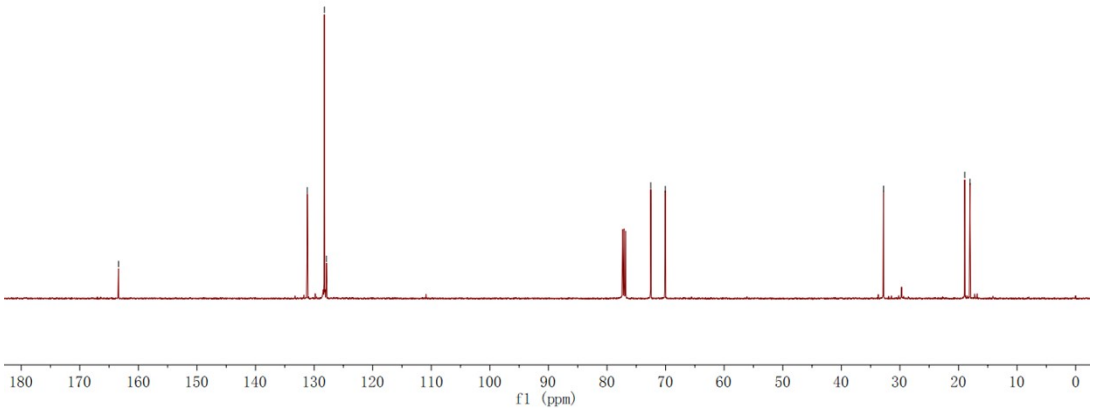
^{1}H NMR (500 MHz, $CDCl_3$)

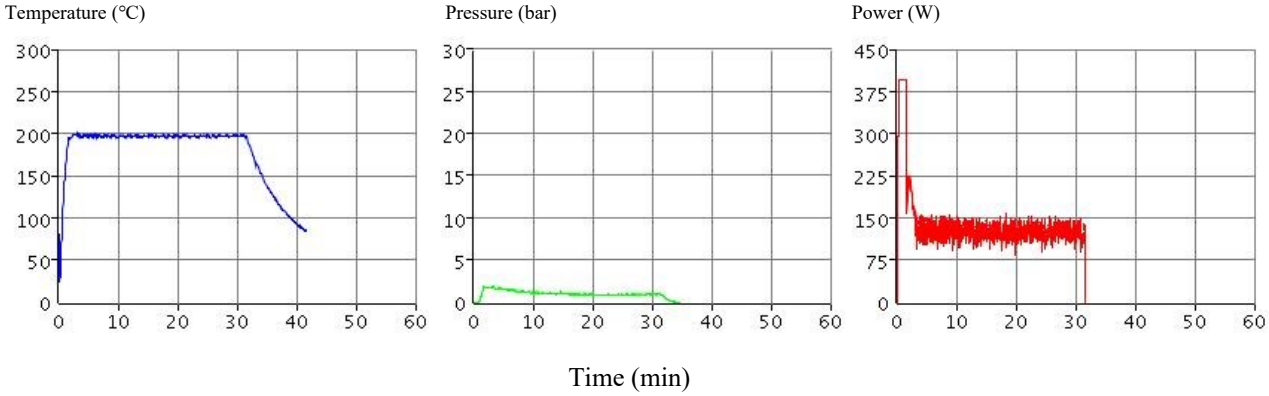




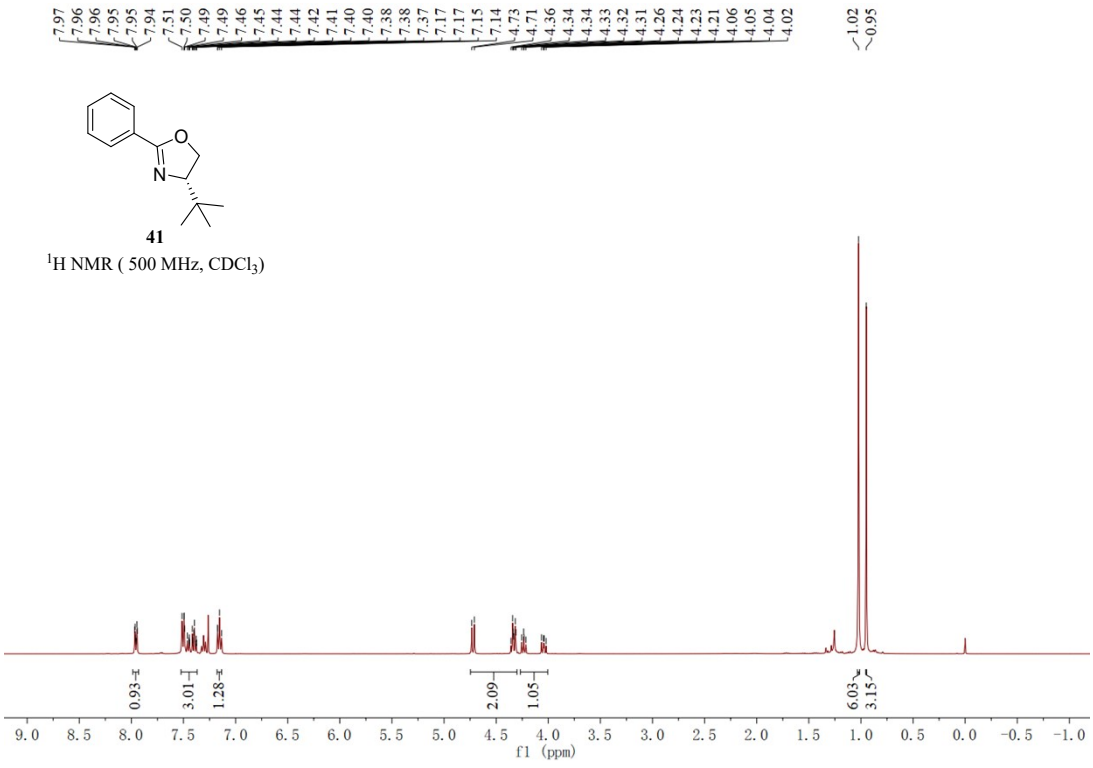
40

^{13}C NMR (126 MHz, $CDCl_3$)



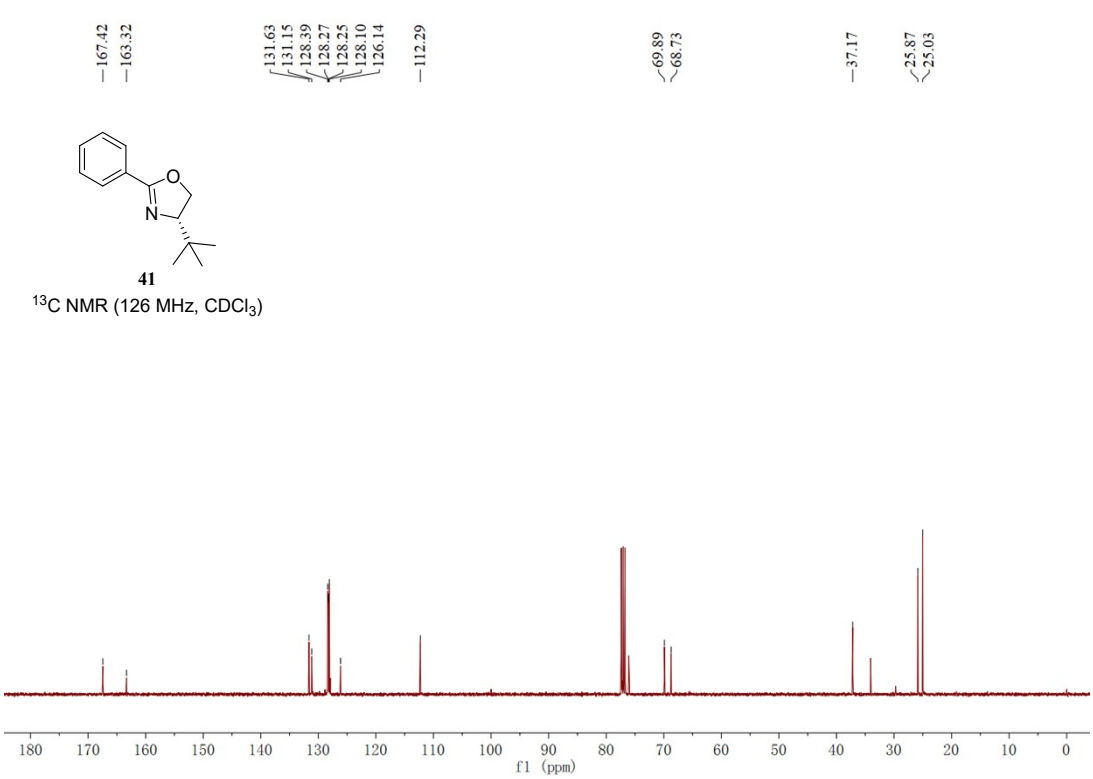

Temperature (°C)
Pressure (bar)
Power (W)
300
250
200
150
100
50
0
30
25
20
15
10
5
0
450
375
300
225
150
75
0
0 10 20 30 40 50 60
Time (min)

NMR spectra and microwave data of compound 41



41

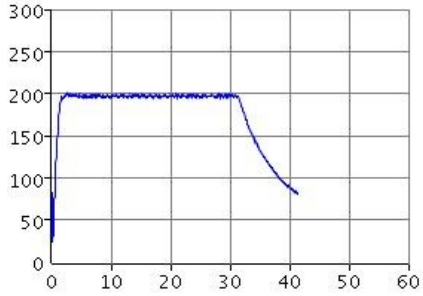
^{1}H NMR (500 MHz, $CDCl_3$)



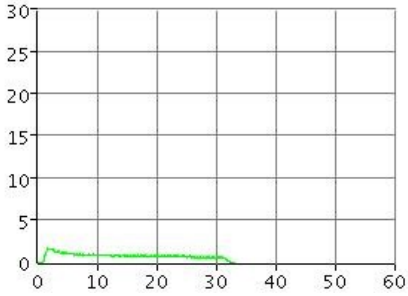
41

^{13}C NMR (126 MHz, $CDCl_3$)

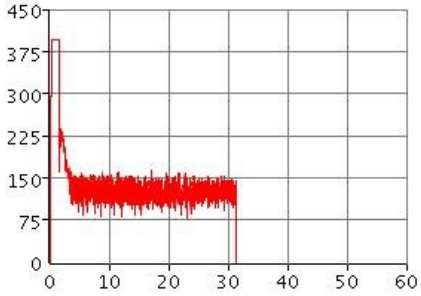
Temperature (°C)



Pressure (bar)

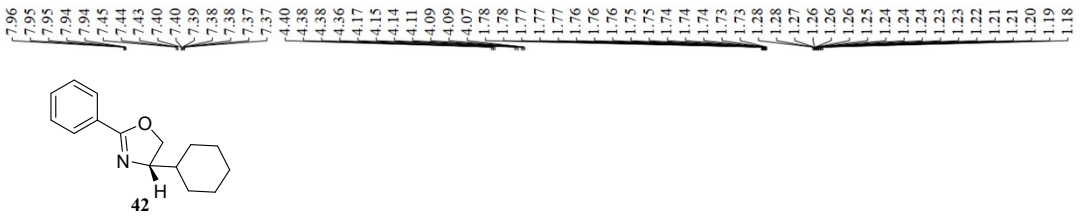


Power (W)



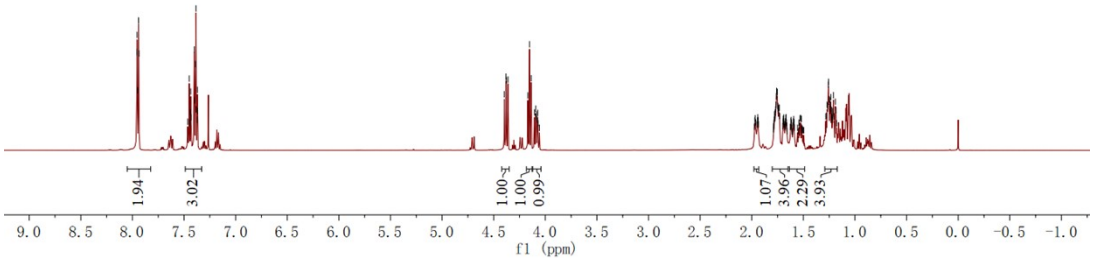
Time (min)

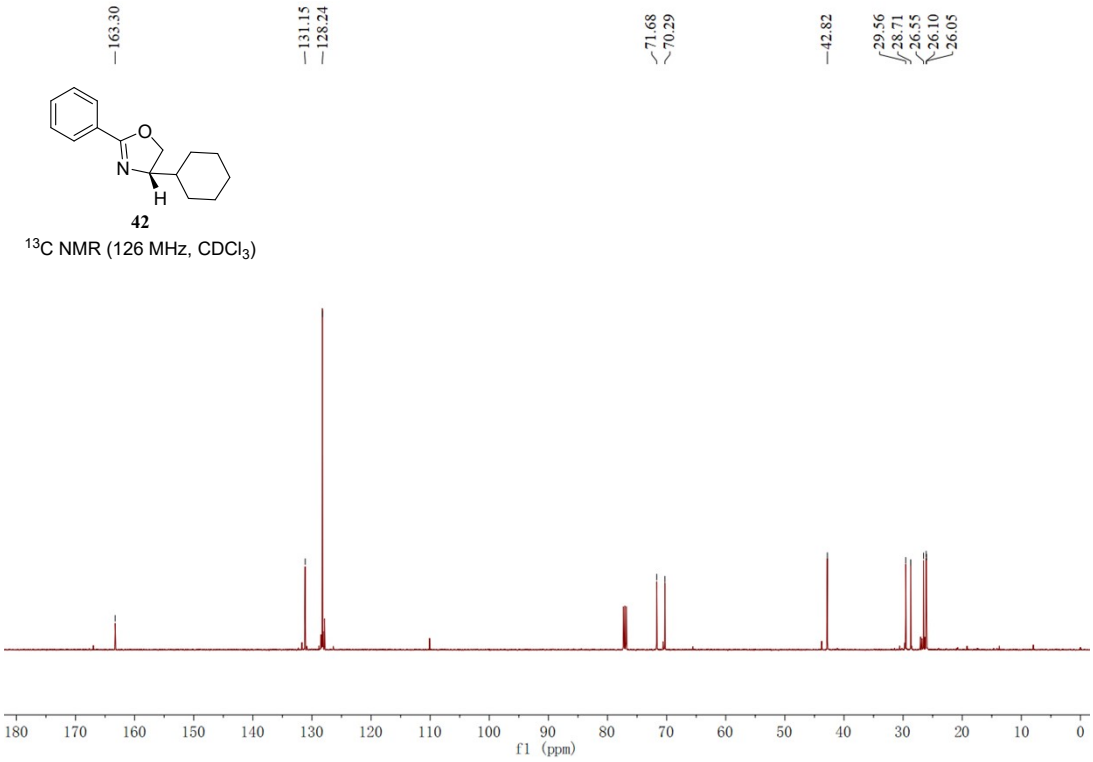
NMR spectra and microwave data of compound 42



42

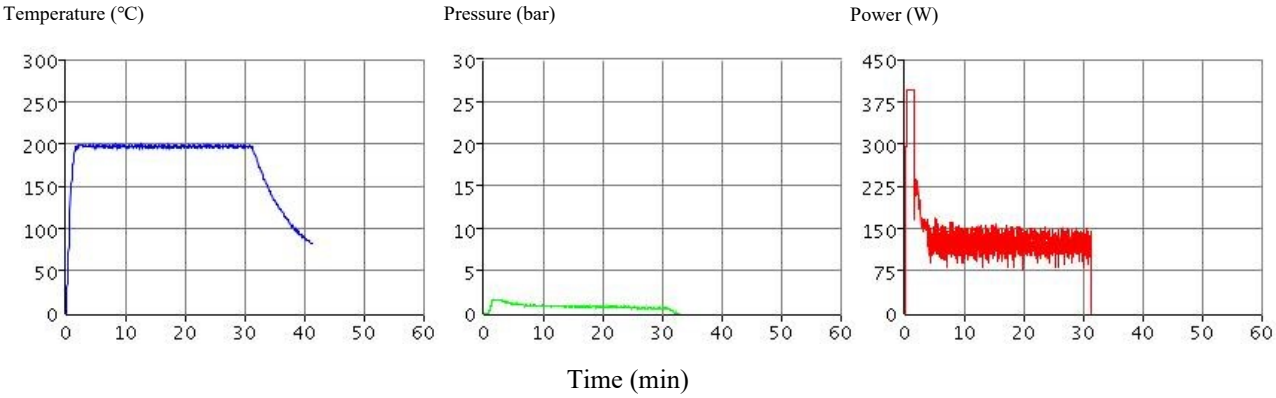
^{1}H NMR (500 MHz, $CDCl_3$)



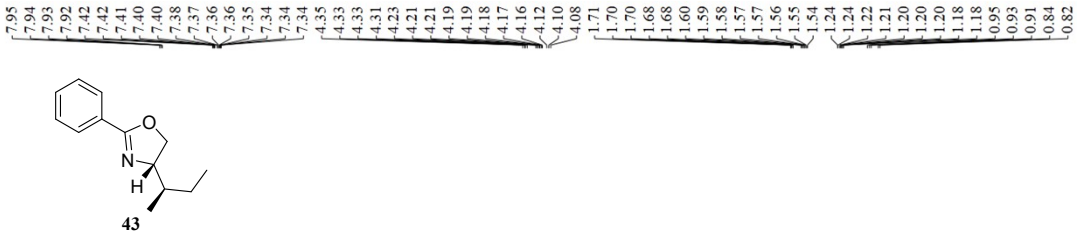


42

^{13}C NMR (126 MHz, $CDCl_3$)

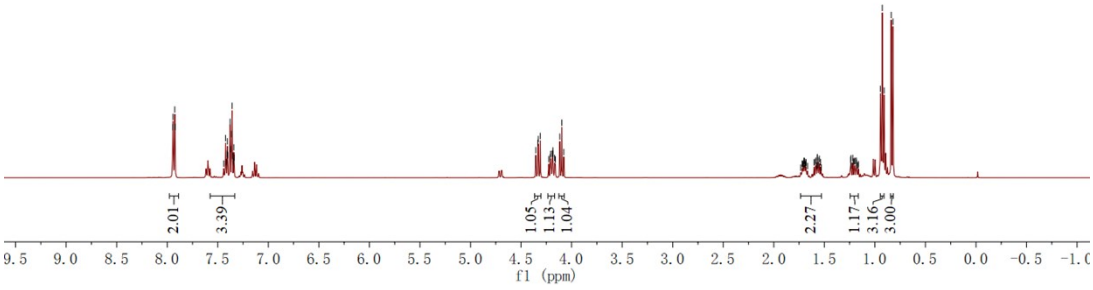

Temperature (°C)
Pressure (bar)
Power (W)
300
250
200
150
100
50
0
30
25
20
15
10
5
0
450
375
300
225
150
75
0
0 10 20 30 40 50 60
Time (min)

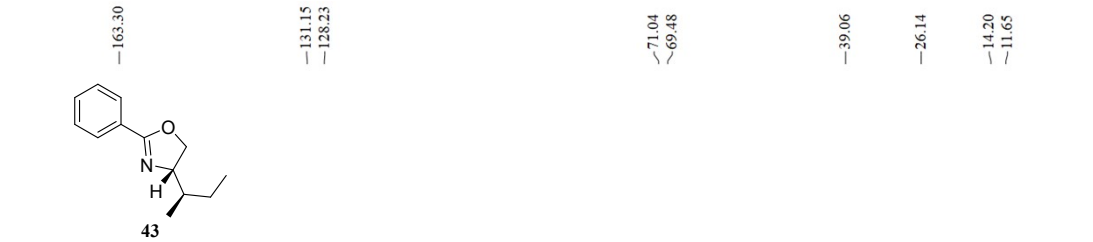
NMR spectra and microwave data of compound 43



43

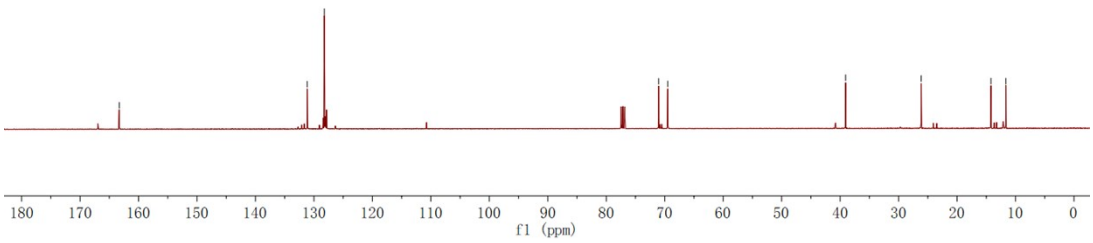
^{1}H NMR (500 MHz, $CDCl_3$)



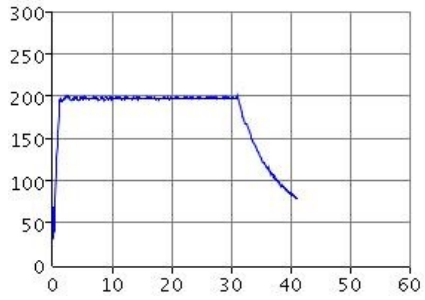


43

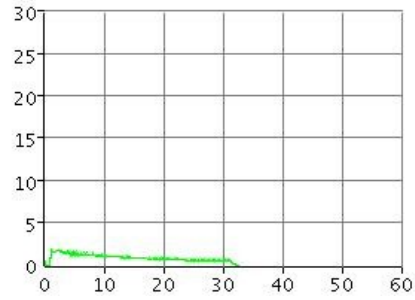
^{13}C NMR (126 MHz, $CDCl_3$)



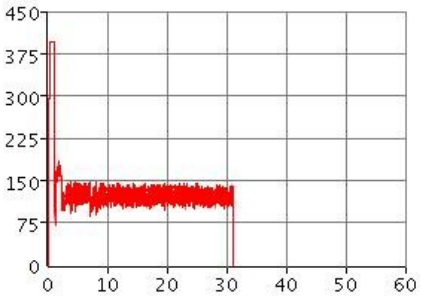
Temperature (°C)



Pressure (bar)

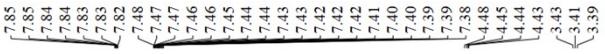


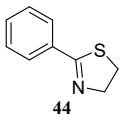
Power (W)



Time (min)

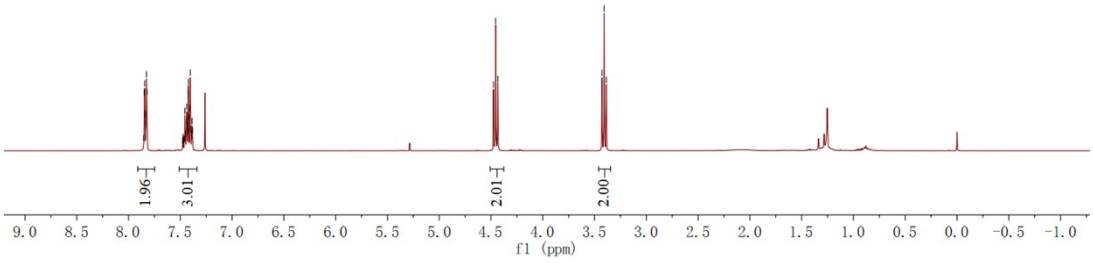
NMR spectra and microwave data of compound 44

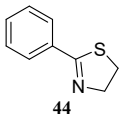




44

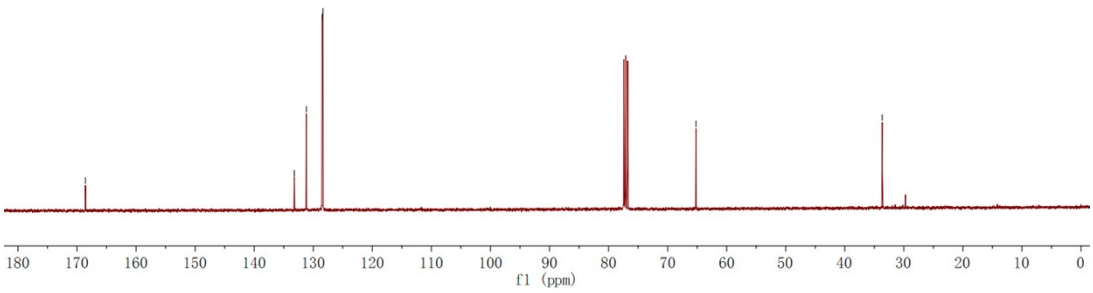
^{1}H NMR (500 MHz, $CDCl_3$)

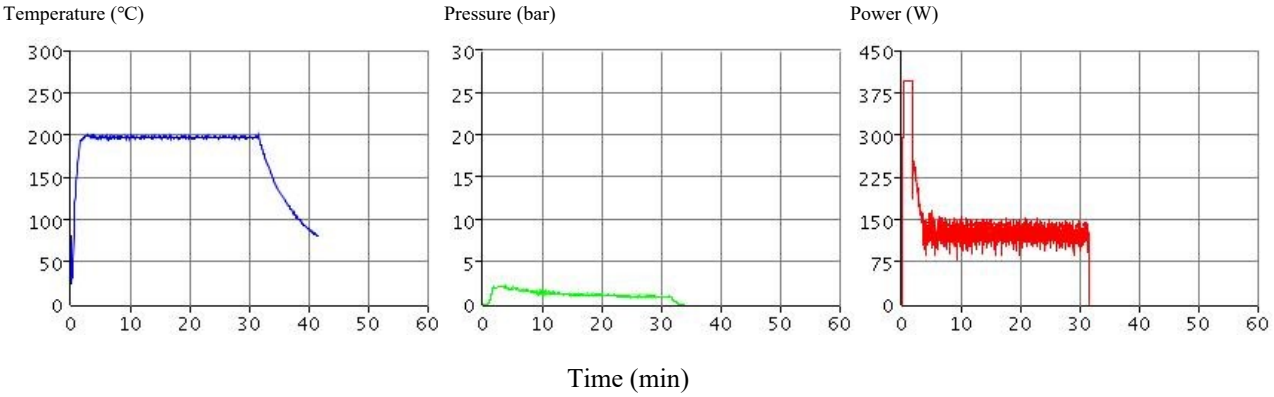


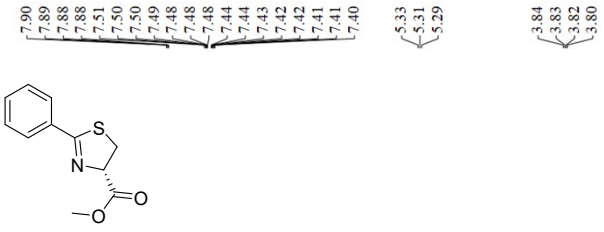


44

^{13}C NMR (126 MHz, $CDCl_3$)

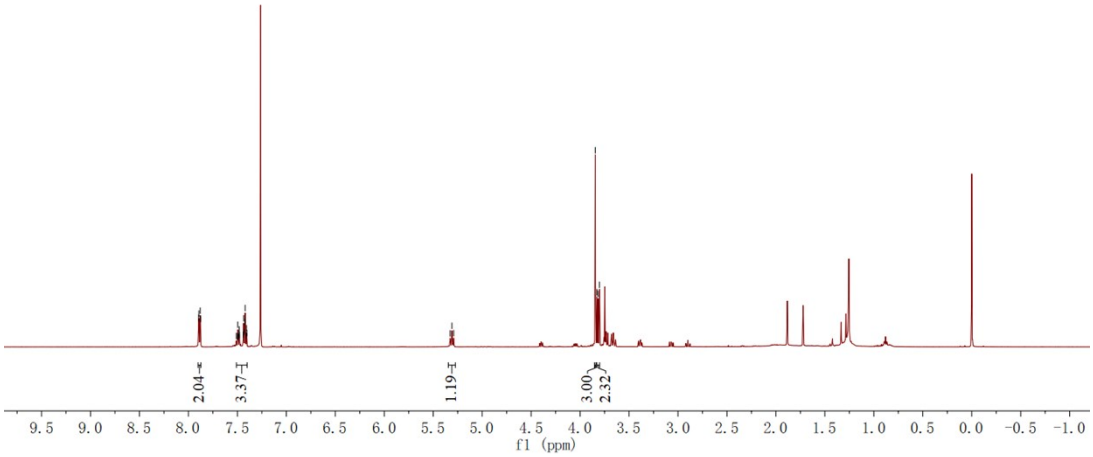


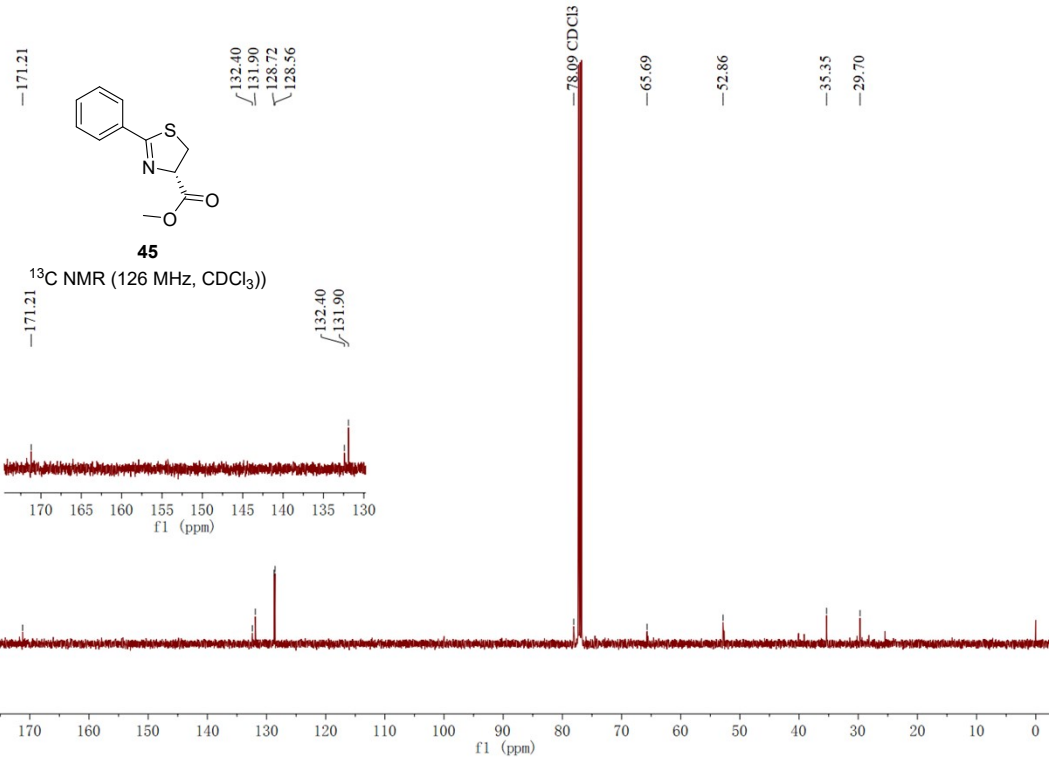

Temperature (°C)
Pressure (bar)
Power (W)
300
250
200
150
100
50
0
30
25
20
15
10
5
0
450
375
300
225
150
75
0
0 10 20 30 40 50 60
Time (min)



45

^{1}H NMR (500 MHz, $CDCl_3$)

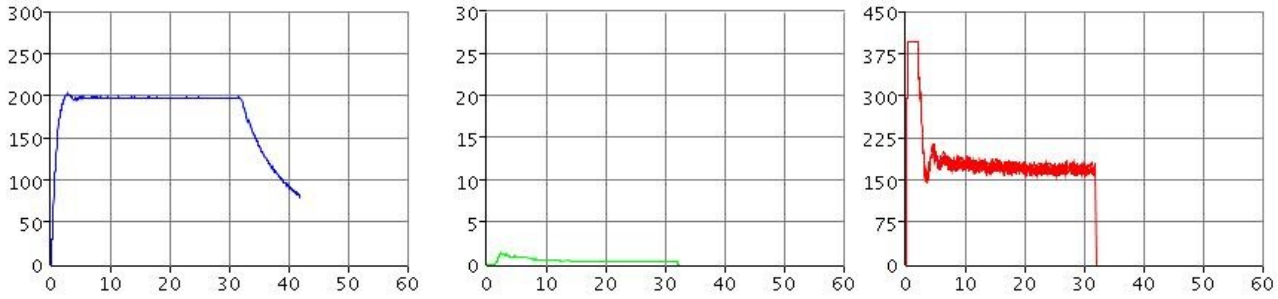




45

^{13}C NMR (126 MHz, $CDCl_3$))

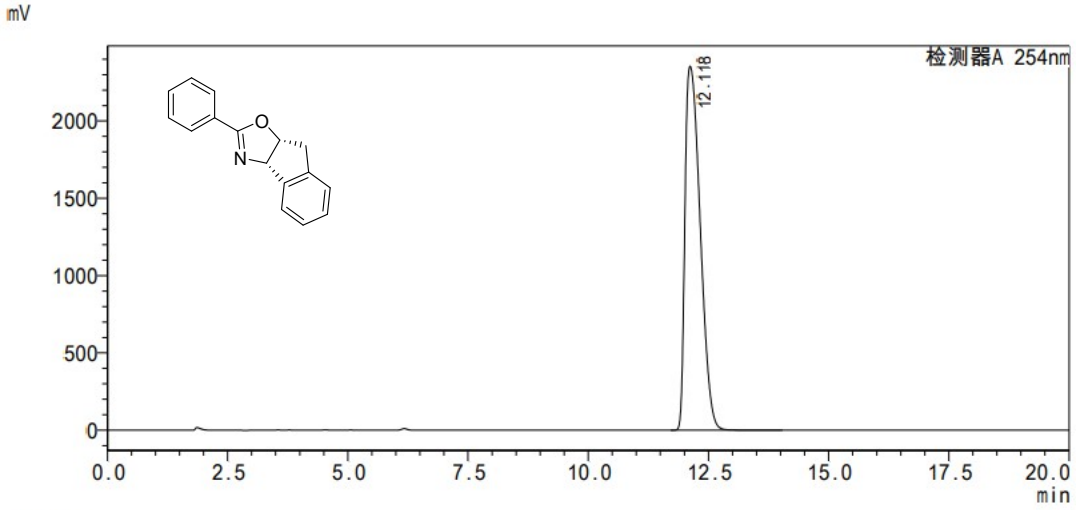
Temperature (℃)



(min) Time (min)

Spectroscopic Data (HPLC Trace)

Fig S1. (3a*S*,8a*R*)-2-phenyl-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazole (3)

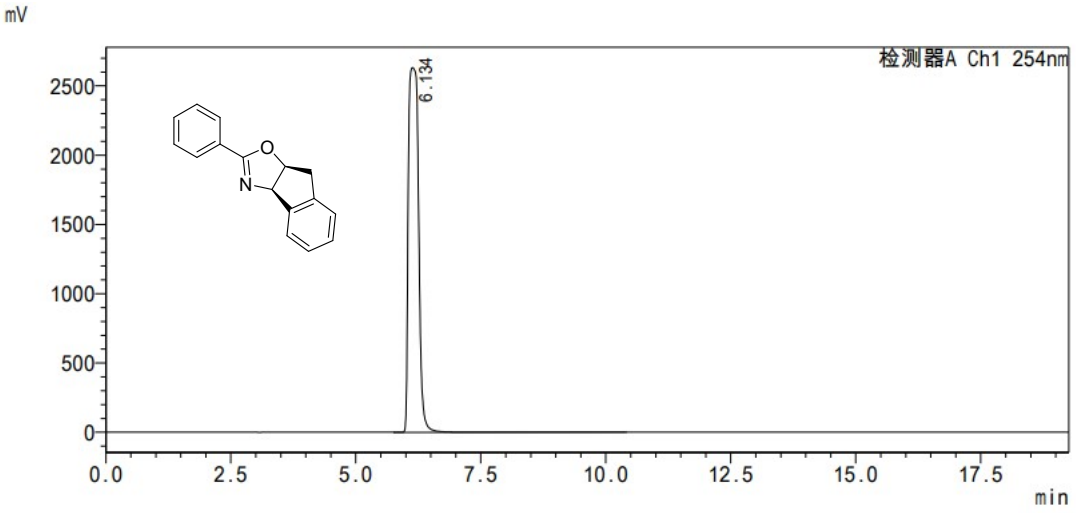


<峰表>

检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	12.118	51729947	2354037	100.000			
总计		51729947	2354037				

Fig S2. (3a*R*,8a*S*)-2-phenyl-3a,8a-dihydro-8*H*-indeno[1,2-*d*]oxazole

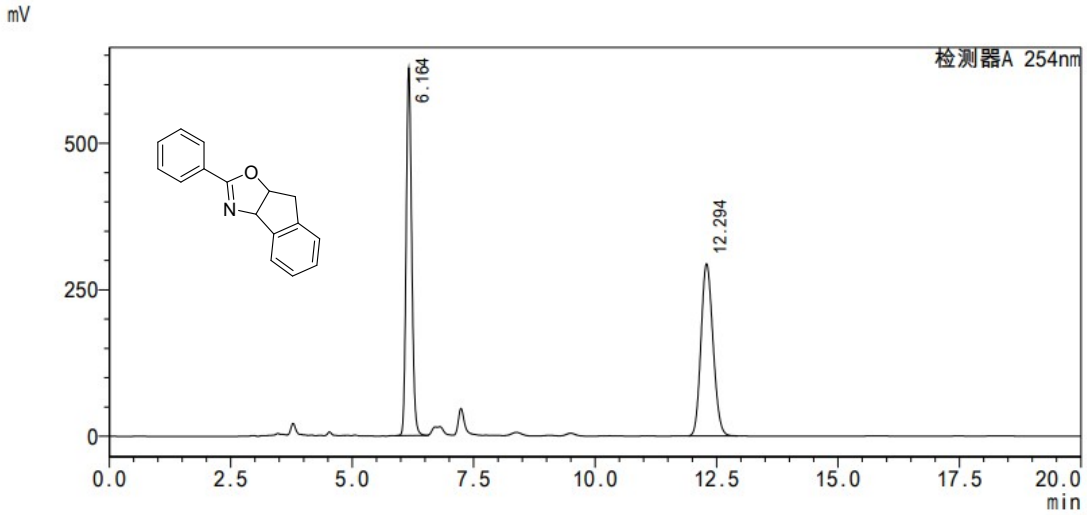


<峰表>

检测器A Ch1 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.134	37429911	2631916	100.000		S	
总计		37429911	2631916				

Fig S3. The racemate of compound 3



<峰表>

检测器A 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.164	4966992	627066	49.517		M	
2	12.294	5063884	293785	50.483		M	
总计		10030876	920851				

X-ray crystalline structure of compound 13:

Table S1. Crystalline data and structure refinement for compound 13

Identification code	mo220823a_pl
Empirical formula	$C_{16}H_{12}INO$
Formula weight	361.17
Temperature/K	296.15
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	4.896(5)
b/Å	10.615(12)
c/Å	26.62(3)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1383(3)
Z	4
ρ_{calc}g/cm^3	1.734
μ/mm^{-1}	2.305
F(000)	704.0
Crystal size/mm^3	0.25 × 0.25 × 0.1
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.06 to 57.014
Index ranges	$-6 \le h \le 6$, $-14 \le k \le 13$, $-32 \le l \le 35$
Reflections collected	9381
Independent reflections	3461 [R_{int} = 0.0370, R_{sigma} = 0.0505]
Data/restraints/parameters	3461/0/181
Goodness-of-fit on F^2	0.997
Final R indexes [I>=2σ (I)]	R_1 = 0.0346, wR_2 = 0.0581
Final R indexes [all data]	R_1 = 0.0765, wR_2 = 0.0695
Largest diff. peak/hole / e Å^{-3}	0.33/-0.55
Flack parameter	0.04(3)

Table S2. Fractional Atomic Coordinates (×104) and Equivalent Isotropic Displacement Parameters (Å2×103) for compound 13. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
I(1)	5287.1(10)	2805.9(4)	2440.9(2)	93.0(2)
O(1)	2112(7)	4271(3)	539.8(12)	51.2(9)
N(1)	3961(9)	6145(3)	337.9(14)	46.7(12)
C(3)	3803(10)	5406(4)	-538.7(17)	39.8(12)
C(2)	2182(11)	5812(5)	-87.6(17)	45.4(13)
C(1)	3781(10)	5254(4)	647.5(17)	41.2(12)
C(11)	5279(11)	5163(4)	1123.4(15)	41.7(12)
C(9)	1030(12)	3631(5)	-327(2)	50.1(15)
C(8)	3117(10)	4177(4)	-673.3(17)	40.6(11)
C(10)	688(10)	4614(4)	79.0(16)	47.6(12)
C(15)	6218(11)	4202(5)	1912.2(18)	51.7(14)
C(16)	4752(11)	4220(4)	1466.3(15)	46.3(11)
C(4)	5736(11)	6068(4)	-806.2(17)	52.2(14)
C(12)	7233(11)	6063(5)	1229.6(19)	54.4(14)
C(14)	8178(12)	5088(5)	2013(2)	58.8(16)
C(13)	8675(12)	6015(5)	1671(2)	66.1(17)
C(7)	4323(12)	3647(5)	-1090.9(18)	58.4(15)
C(6)	6188(13)	4330(6)	-1360(2)	69.6(18)
C(5)	6919(13)	5522(6)	-1220(2)	69.0(17)

Table S3. Anisotropic Displacement Parameters (Å2×103) for compound 13. The Anisotropic displacement factor exponent takes the form: -2π2[h2a*2U11+2hka*b*U12+…].

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
I(1)	129.6(4)	97.6(3)	51.8(2)	22.49(18)	-30.8(3)	-28.9(3)
O(1)	49(2)	58(2)	47(2)	13.5(16)	-7.8(18)	-11.0(19)
N(1)	65(3)	33(2)	42(2)	-2.3(16)	2(2)	7(2)
C(3)	40(3)	38(3)	42(2)	7(2)	-7(2)	7(3)
C(2)	53(4)	40(3)	42(3)	1(2)	-7(3)	15(3)
C(1)	39(3)	42(3)	43(3)	-10(2)	6(2)	2(2)
C(11)	47(3)	39(2)	39(2)	-8.9(17)	5(3)	1(3)
C(9)	46(4)	53(4)	51(3)	8(3)	-13(3)	-1(3)
C(8)	39(3)	43(3)	40(3)	1(2)	-10(2)	2(2)
C(10)	30(3)	63(3)	50(3)	7(2)	4(2)	3(3)
C(15)	62(4)	54(3)	39(3)	1(2)	-1(2)	-2(3)
C(16)	50(3)	48(3)	41(2)	-1.7(18)	-3(3)	-6(3)
C(4)	65(4)	46(3)	45(3)	12(2)	-10(3)	-1(3)
C(12)	61(4)	51(3)	51(3)	-4(2)	3(3)	-13(3)
C(14)	57(4)	73(4)	47(3)	-17(3)	-6(3)	-1(3)
C(13)	67(4)	70(4)	62(4)	-24(3)	4(3)	-20(3)
C(7)	66(4)	57(3)	52(3)	-12(2)	-12(3)	6(3)
C(6)	68(4)	99(5)	42(3)	-6(3)	3(3)	19(4)
C(5)	66(4)	89(5)	51(3)	22(3)	6(3)	-1(4)

Table S4 Bond Lengths for compound 13.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
I(1)	C(15)	2.094(5)	C(11)	C(12)	1.382(7)
O(1)	C(1)	1.356(5)	C(9)	C(8)	1.494(7)
O(1)	C(10)	1.457(6)	C(9)	C(10)	1.511(7)
N(1)	C(2)	1.472(6)	C(8)	C(7)	1.379(6)
N(1)	C(1)	1.257(6)	C(15)	C(16)	1.387(6)
C(3)	C(2)	1.502(7)	C(15)	C(14)	1.370(7)
C(3)	C(8)	1.394(6)	C(4)	C(5)	1.373(7)
C(3)	C(4)	1.378(7)	C(12)	C(13)	1.371(7)
C(2)	C(10)	1.532(7)	C(14)	C(13)	1.363(8)
C(1)	C(11)	1.467(6)	C(7)	C(6)	1.369(8)
C(11)	C(16)	1.379(6)	C(6)	C(5)	1.367(8)

Table S5 Bond Angles for compound 13.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C(1)	O(1)	C(10)	105.9(3)	C(7)	C(8)	C(3)	119.1(5)
C(1)	N(1)	C(2)	106.4(4)	C(7)	C(8)	C(9)	129.2(5)
C(8)	C(3)	C(2)	110.3(4)	O(1)	C(10)	C(2)	102.9(4)
C(4)	C(3)	C(2)	129.0(5)	O(1)	C(10)	C(9)	112.1(4)
C(4)	C(3)	C(8)	120.7(5)	C(9)	C(10)	C(2)	108.3(4)
N(1)	C(2)	C(3)	111.8(5)	C(16)	C(15)	I(1)	118.2(4)
N(1)	C(2)	C(10)	105.0(4)	C(14)	C(15)	I(1)	120.4(4)
C(3)	C(2)	C(10)	104.2(4)	C(14)	C(15)	C(16)	121.4(5)
O(1)	C(1)	C(11)	115.6(4)	C(11)	C(16)	C(15)	118.7(5)
N(1)	C(1)	O(1)	118.8(4)	C(5)	C(4)	C(3)	119.3(5)
N(1)	C(1)	C(11)	125.5(5)	C(13)	C(12)	C(11)	120.4(5)
C(16)	C(11)	C(1)	121.8(5)	C(13)	C(14)	C(15)	119.3(5)
C(16)	C(11)	C(12)	119.8(4)	C(14)	C(13)	C(12)	120.5(5)
C(12)	C(11)	C(1)	118.5(4)	C(6)	C(7)	C(8)	119.5(5)
C(8)	C(9)	C(10)	104.4(4)	C(5)	C(6)	C(7)	121.4(6)
C(3)	C(8)	C(9)	111.7(4)	C(6)	C(5)	C(4)	120.0(6)

Table S6 Torsion Angles for compound 13.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
I(1)	C(15)	C(16)	C(11)	177.7(4)	C(11)	C(12)	C(13)	C(14)	-0.8(9)
I(1)	C(15)	C(14)	C(13)	-177.6(4)	C(9)	C(8)	C(7)	C(6)	179.3(5)
O(1)	C(1)	C(11)	C(16)	-8.0(7)	C(8)	C(3)	C(2)	N(1)	120.1(4)
O(1)	C(1)	C(11)	C(12)	173.0(4)	C(8)	C(3)	C(2)	C(10)	7.2(5)
N(1)	C(2)	C(10)	O(1)	-9.6(5)	C(8)	C(3)	C(4)	C(5)	2.3(7)
N(1)	C(2)	C(10)	C(9)	-128.3(5)	C(8)	C(9)	C(10)	O(1)	-102.7(4)
N(1)	C(1)	C(11)	C(16)	173.0(5)	C(8)	C(9)	C(10)	C(2)	10.1(5)
N(1)	C(1)	C(11)	C(12)	-5.9(7)	C(8)	C(7)	C(6)	C(5)	1.1(8)
C(3)	C(2)	C(10)	O(1)	108.1(4)	C(10)	O(1)	C(1)	N(1)	-5.7(6)
C(3)	C(2)	C(10)	C(9)	-10.7(5)	C(10)	O(1)	C(1)	C(11)	175.3(4)
C(3)	C(8)	C(7)	C(6)	0.8(7)	C(10)	C(9)	C(8)	C(3)	-5.8(6)
C(3)	C(4)	C(5)	C(6)	-0.4(8)	C(10)	C(9)	C(8)	C(7)	175.6(5)
C(2)	N(1)	C(1)	O(1)	-0.9(6)	C(15)	C(14)	C(13)	C(12)	0.0(9)
C(2)	N(1)	C(1)	C(11)	178.0(5)	C(16)	C(11)	C(12)	C(13)	0.9(8)
C(2)	C(3)	C(8)	C(9)	-1.0(6)	C(16)	C(15)	C(14)	C(13)	0.8(8)
C(2)	C(3)	C(8)	C(7)	177.8(4)	C(4)	C(3)	C(2)	N(1)	-59.6(6)
C(2)	C(3)	C(4)	C(5)	-178.0(5)	C(4)	C(3)	C(2)	C(10)	-172.5(5)
C(1)	O(1)	C(10)	C(2)	9.1(5)	C(4)	C(3)	C(8)	C(9)	178.7(4)
C(1)	O(1)	C(10)	C(9)	125.2(4)	C(4)	C(3)	C(8)	C(7)	-2.5(7)
C(1)	N(1)	C(2)	C(3)	-105.6(5)	C(12)	C(11)	C(16)	C(15)	-0.1(7)
C(1)	N(1)	C(2)	C(10)	6.7(5)	C(14)	C(15)	C(16)	C(11)	-0.7(8)
C(1)	C(11)	C(16)	C(15)	-179.0(5)	C(7)	C(6)	C(5)	C(4)	-1.3(9)
C(1)	C(11)	C(12)	C(13)	179.8(5)					

Table S7 Hydrogen Atom Coordinates (Å×104) and Isotropic Displacement Parameters (Å2×103) for compound 13.

Atom	*x*	*y*	*z*	U(eq)
H(2)	904.88	6492.84	-169.33	54
H(10)	-1247.25	4784.06	143.9	57
H(16)	3439.99	3608.61	1400	56
H(4)	6234.56	6876.77	-707.56	63
H(12)	7571.93	6706.15	1000.55	65
H(14)	9159.22	5057.3	2311.94	71
H(13)	10003.19	6618.86	1736.9	79
H(7)	3872.35	2832.2	-1188.75	70
H(6)	6975.29	3975.39	-1645.2	83
H(5)	8217.52	5962.93	-1404.71	83
H(9A)	-750(110)	3570(50)	-514(18)	63(16)
H(9B)	1580(110)	2850(50)	-199(18)	69(16)

III. References

1. S. Roshandel, S. C. Suri, J. C. Marcischak, G. Rasul and G. K. Surya Prakash, *Green Chem.*, 2018, **20**, 3700-3704.