

Supporting Information

Transition metal catalysed C7- and *ortho*-selective halogenation of 2-arylbenzo[d]oxazoles

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1. General Information

Chemicals and solvents were purchased from commercial suppliers and used as received. ^1H NMR, ^{13}C NMR, and ^{19}F spectra were recorded on a Bruker AVANCE III HD (400 MHz) spectrometer. Chemical shifts were calibrated using residual undeuterated solvent as an internal reference (CDCl_3 : 7.26 ppm ^1H NMR, 77.0 ppm ^{13}C NMR). Multiplicity was indicated as follows: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), dd (doublet of doublet), brs (broad singlet). All high-resolution mass spectra (HRMS) were obtained on a Bruker McriOTOF11 spectrometer. All GC analyses was performed on PE680-ST8 GC-MS.

Single crystal X-ray diffraction data for compounds were collected on a Bruker D8 VENTURE-MetalJet diffractometer equipped with a PHOTON II area detector and HELIOS multilayer optics monochromated Ga-K alpha radiation ($\lambda = 1.34138 \text{ \AA}$). The data reduction was performed using the APEX III software. Structure were solved by direct methods and refined by full-matrix least-squares methods based on F2 using the SHELXL-2014 software. If not noted hydrogen atoms were positioned geometrically in idealized positions and refined with isotropic displacement parameters as riding atoms. If not noted otherwise all non-hydrogen atoms were refined anisotropically. Geometrical calculations were performed using the SHELXL-2014 programs.

2. Experiment Procedure

2-1 General Halogenation Reactions

A 25 mL Schlenk tube was charged with 2-arylbenzoxazole **1** (0.5 mmol), N-halosuccinimide (chloro-, bromo-, or iodo-) (0.6 mmol), $[\text{RhCp}^*(\text{MeCN})_3](\text{SbF}_6)_2$ (16.7 mg, 4 mol%), and 1,2-dichloroethane (DCE). Then the reaction mixture was degassed and charged with N_2 at the temperature of liquid nitrogen. Then the reaction mixture was warmed gradually to room temperature and was stirred at 60 °C for 18 hours. The solvent was removed on a rotary evaporator under reduced pressure and the residue was subjected to column chromatography isolation on silica gel with petroleum ether / ethyl acetate (50:1-10:1) to afford the pure product.

2-2 KIE Study for *ortho*-Bromination

a) Preparation Procedure of Isotope Labeled Substrates

A 25 mL Schlenk tube was charged with 5-methyl-2-(*o*-tolyl)benzo[*d*]oxazole **1a** (223.3 mg, 1 mmol), CD₃COOD (0.5 mL), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%), and 1,2-dichloroethane (DCE). The reaction mixture was degassed and charged with N₂ in the temperature of liquid nitrogen. Then the reaction mixture was warmed gradually to room temperature and was stirred at 60 °C for 18 hours. The solvent was removed on a rotary evaporator under reduced pressure and the residue was subjected to column chromatography isolation on silica gel with petroleum ether / ethyl acetate (50:1) to afford the deuterized substrate **1a+1a-*d***. The H/D ratio were calculated by the peak area of corresponding ¹HNMR signal.

b) Parallel experiments for the *o*-bromination of **1a**

As per general procedure, **1a+1a-*d*** (44.6 mg, 0.2 mmol), N-bromosuccinimide (0.24 mmol), [RhCp*(MeCN)₃](SbF₆)₂ (6.7 mg, 4 mol%), and 1,2-dichloroethane (2.0 mL) were added under N₂ atmosphere into two 25 mL Schlenk tubes. The mixtures were stirred at 60 °C and were stopped at 30 and 60 minutes. The mixture of substrate **1a+1a-D** and product **2a** were roughly isolated by column chromatography isolation on silica gel with petroleum ether / ethyl acetate (50:1), and characterized by ¹HNMR (**Table S1**). Rates were determined as the slopes of the linear regression of the data obtained from a concentration of product (mol/L) versus reaction time (min) plot (**Figure S1**). The KIE value was determined as the ratio of the rates (k_H/k_D).

Table S1. Results from competition experiments of *o*-bromination

| Time (h) | Relative Peak Area | | | Conversion | Concentration (mol/L) | | |
|-------------|--------------------|---------------|---------------|------------|-----------------------|--------------------|-----------|
| | $\delta=2.52$ | $\delta=2.54$ | $\delta=8.17$ | | 1a | 1a-<i>d</i> | 2a |
| 0 | 3.00 | 0.00 | 0.60 | 0 | 0.0600 | 0.0400 | - |
| 0.50 | 2.61 | 0.39 | 0.59 | 13% | 0.0513 | 0.0357 | 0.0130 |
| 1.00 | 2.19 | 0.81 | 0.58 | 27% | 0.0423 | 0.0307 | 0.0270 |

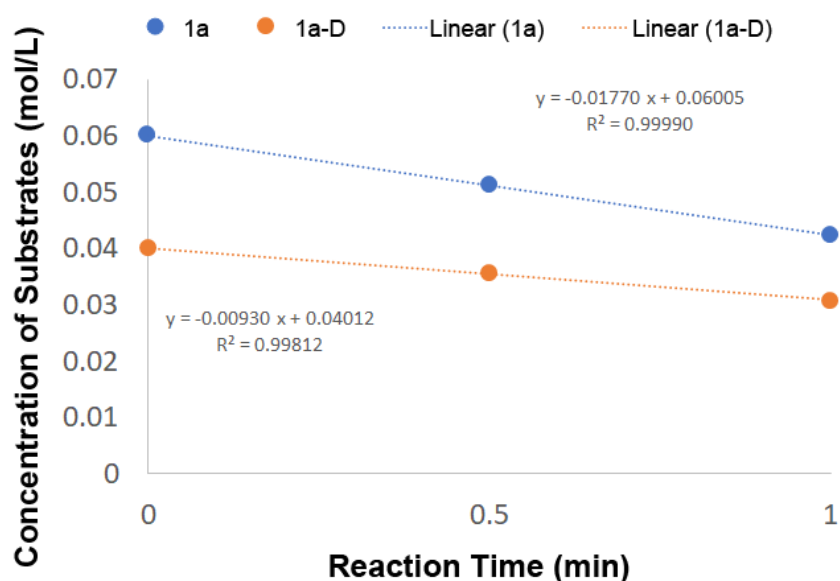


Figure S1. KIE experiment result: $k_H/k_D = 1.27$

c) Experiments for the 7-bromination of **1i**

As per general procedure, **1i**+**1i**- d_2 (44.6 mg, 0.2 mmol), N-bromosuccinimide (0.24 mmol), [RhCp*(MeCN)₃](SbF₆)₂ (6.7 mg, 4 mol%), and 1,2-dichloroethane (2.0 mL) were added under N₂ atmosphere into two 25 mL Schlenk tubes. The mixtures were stirred at 60 °C for 18 hours. The product **5i**+**5i**- d_2 was isolated in 61% yield by column chromatography isolation on silica gel with petroleum ether / ethyl acetate (50:1). Rates were determined as the slopes of the linear regression of the data obtained from a concentration of product (mol/L) versus reaction time (min) plot (**Table S2**). The KIE value was determined as the ratio of the rates (k_H/k_D).

Table S2. Results from competition experiments of *o*-bromination. $k_H/k_D = 1.23$

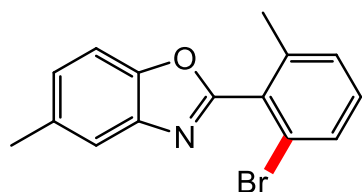
| Time (h) | Relative Peak Area | | H/D ratio | Concentration (mol/L) | | | |
|----------|-------------------------------------|-------------------------------------|------------|-----------------------|-------------------|-----------|-------------------|
| | $\delta=2.48$ or $\delta=2.56$ (3H) | $\delta=8.13$ or $\delta=8.11$ (2H) | | 1i | 1i - d_2 | 6i | 6i - d_2 |
| 0 | 3.00 | 0.48 | 0.24: 0.76 | 0.0240 | 0.0760 | - | - |
| 18 | 3.00 | 0.56 | 0.28: 0.72 | - | - | 0.0171 | 0.0439 |

2-4 General Procedure for Radical Scavenging Experiments

A 25 mL Schlenk tube was charged with 2-arylbenzoxazole **1** (0.5 mmol), N-bromo succinimide (0.6 mmol), catalyst (4 mol%), TEMPO (78.1 mg, 0.5 mmol) or BHT (110.2 mg, 0.5 mmol), and 5 mL of 1,2-dichloroethane (DCE). The reaction mixture was degassed and charged with N₂ in the temperature of liquid nitrogen. Then the reaction mixture was warmed gradually to room temperature and was stirred at 60 °C for 18 hours. The solvent was removed on a rotary evaporator under reduced pressure and the residue was subjected to column chromatography isolation on silica gel with petroleum ether / ethyl acetate (50:1-10:1) to afford the pure product.

3. Analytical Data of the Products.

3-1 ortho-brominated products



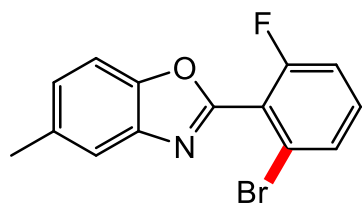
2-(2-bromo-6-methylphenyl)-5-methylbenzo[d]oxazole (**2a**)

Following the typical procedure, 5-methyl-2-(o-tolyl)benzo[d]oxazole (111.6 mg, 0.5 mmol, 1.0 equiv), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%) and N-bromosuccinimide (106.8 mg, 0.6 mmol) in DCE (5.0 mL) were employed to give the product **2a** (145.1 mg) in 96% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 7.87 – 7.84 (m, 1H), 7.64 – 7.61 (m, 1H), 7.54 (dt, J = 6.9, 3.0 Hz, 1H), 7.44 – 7.39 (m, 2H), 7.31 – 7.26 (m, 2H), 2.29 (s, 3H), 2.16 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 161.34, 150.64, 141.20, 141.07, 131.62, 130.25, 129.94, 129.04, 125.44, 124.51, 123.80, 120.51, 110.86, 30.89, 20.40.

HRMS (ESI): m/z calcd. for C₁₅H₁₃BrNO [M+H]⁺: 305.0181 found: 305.0184.



2-(2-bromo-6-fluorophenyl)-5-methylbenzo[d]oxazole (**2b**)

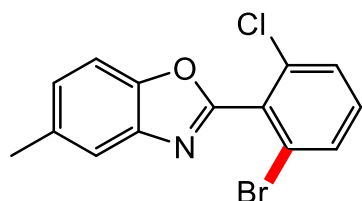
Following the typical procedure, 2-(2-fluorophenyl)-5-methylbenzo[d]oxazole (113.6 mg, 0.5 mmol, 1.0 equiv), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%) and N-bromosuccinimide (106.8 mg, 0.6 mmol) in DCE (5.0 mL) were employed to give the product **2b** (114.8 mg) in 75% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 7.66 (s, 1H), 7.53 (dd, J = 15.7, 8.2 Hz, 2H), 7.39 (td, J = 8.2, 5.9 Hz, 1H), 7.25 – 7.18 (m, 2H), 2.52 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 162.91, 160.36, 149.16, 141.46, 134.61, 132.98, 132.89, 129.09, 129.06, 126.98, 124.22, 120.54, 115.29, 115.07, 114.61, 110.31, 21.48.

¹⁹F NMR (376 MHz, CDCl₃): δ -107.87, -107.89.

HRMS (ESI): m/z calcd. for C₁₄H₉BrFNO [M+H]⁺: 305.9930, found: 305.9937.



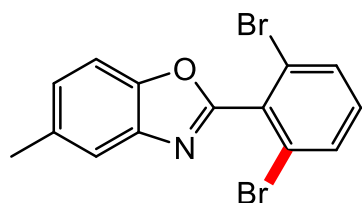
2-(2-bromo-6-chlorophenyl)-5-methylbenzo[d]oxazole (**2c**)¹

Following the typical procedure, 2-(2-chlorophenyl)-5-methylbenzo[d]oxazole (121.8 mg, 0.5 mmol, 1.0 equiv), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%) and N-bromosuccinimide (106.8 mg, 0.6 mmol) in DCE (5.0 mL) were employed to give the product **2c** (159.4 mg) in 99% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.12 (dd, J = 7.5, 1.3 Hz, 1H), 7.83 (s, 1H), 7.70 (s, 1H), 7.56 (d, J = 7.8 Hz, 1H), 7.43 (ddd, J = 16.2, 11.2, 6.9 Hz, 2H), 2.53 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 161.42, 149.31, 141.33, 134.32, 133.56, 132.06, 131.80, 131.47, 126.96, 125.97, 121.34, 114.38, 109.18, 29.70, 23.38.

GC/MS: M/Z = 321.97



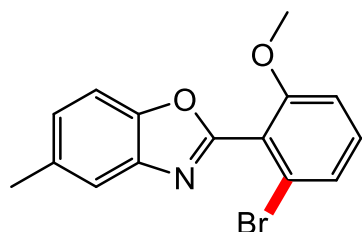
2-(2,6-dibromophenyl)-5-methylbenzo[d]oxazole (**2m**)

Following the typical procedure, 2-(2-bromophenyl)-5-methylbenzo[*d*]oxazole (144.07 mg, 0.5 mmol, 1.0 equiv), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%) and N-bromosuccinimide (106.8 mg, 0.6 mmol) in DCE (5.0 mL) were employed to give the product **2m** (168.6 mg) in 92% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.06 (dd, J = 7.8, 1.2 Hz, 1H), 7.83 (s, 1H), 7.77 (d, J = 8.0 Hz, 1H), 7.71 (s, 1H), 7.46 (t, J = 7.6 Hz, 1H), 7.40 – 7.35 (m, 1H), 2.54 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 161.94, 149.33, 141.24, 134.77, 134.31, 132.57, 132.12, 128.04, 127.47, 121.92, 121.36, 121.30, 114.40, 23.39.

HRMS (ESI): m/z calcd. for C₁₄H₁₀Br₂NO [M+H]⁺: 367.9109 found: 367.9104.



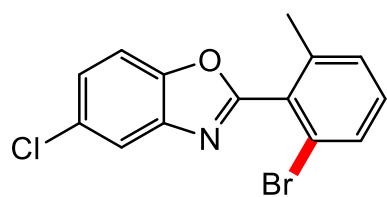
2-(2-bromo-6-methoxyphenyl)-5-methylbenzo[*d*]oxazole (**2n**)

Following the typical procedure, 2-(2-methoxyphenyl)-5-methylbenzo[*d*]oxazole (119.6 mg, 0.5 mmol, 1.0 equiv), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%), N-bromosuccinimide (106.8 mg, 0.6 mmol), and AcOH (30.0 mg, 0.5 mmol, 1.0 equiv) in DCE (5.0 mL) were employed to give the product **2n** (121.2 mg) in 89% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 7.66 (s, 1H), 7.61 (d, J = 8.9 Hz, 1H), 7.51 (d, J = 8.3 Hz, 1H), 7.25 (d, J = 8.8 Hz, 1H), 6.96 (d, J = 8.9 Hz, 1H), 3.95 (s, 3H), 2.52 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 160.38, 155.61, 148.83, 141.13, 134.55, 132.99, 132.05, 126.88, 120.61, 115.00, 114.76, 114.58, 110.38, 56.77, 21.49.

HRMS (ESI): m/z calcd. for C₁₅H₁₃BrNO [M+H]⁺: 318.0130 found: 318.0128.



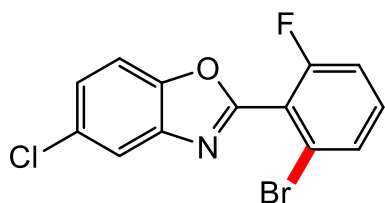
2-(2-bromo-6-methylphenyl)-5-chlorobenzo[*d*]oxazole (**2o**)¹

Following the typical procedure, 5-chloro-2-(*o*-tolyl)benzo[*d*]oxazole (121.8 mg, 0.5 mmol, 1.0 equiv), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%) and N-bromosuccinimide (106.8 mg, 0.6 mmol) in DCE (5.0 mL) were employed to give the product **2o** (130.5 mg) in 81% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 7.86 (s, 1H), 7.82 (s, 1H), 7.57 (s, 1H), 7.42 (s, 1H), 7.32 (s, 1H), 7.15 (d, J = 6.7 Hz, 1H), 2.29 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 164.35, 149.16, 142.32, 140.63, 136.76, 133.69, 132.03, 130.17, 129.85, 125.92, 120.61, 111.71, 97.54, 20.72.

GC/MS: M/Z = 321.95



2-(2-bromo-6-fluorophenyl)-5-chlorobenzo[*d*]oxazole (**2p**)

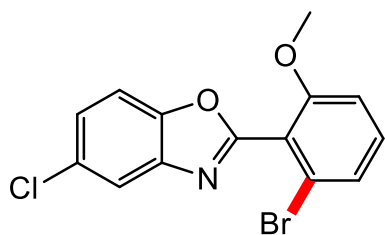
Following the typical procedure, 5-chloro-2-(2-fluorophenyl)benzo[*d*]oxazole (123.8 mg, 0.5 mmol, 1.0 equiv), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%) and N-bromosuccinimide (106.8 mg, 0.6 mmol) in DCE (5.0 mL) under 80 °C were employed to give the product **2p** (67.0 mg) in 41% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.20 (t, J = 7.5 Hz, 1H), 7.91 (s, 2H), 7.57 (dd, J = 13.3, 7.1 Hz, 1H), 7.35 – 7.29 (m, 1H), 7.26 (d, J = 8.9 Hz, 1H).

¹³C NMR (101 MHz, CDCl₃): δ 162.25, 159.66, 149.33, 142.18, 133.92, 133.84, 130.76, 130.66, 124.68, 124.64, 121.23, 118.73, 117.35, 117.14, 115.56, 114.80, 114.69.

¹⁹F NMR (376 MHz, CDCl₃): δ -109.32, -109.34, -109.35, -109.37, -109.38.

HRMS (ESI): m/z calcd. for C₁₃H₇BrClFNO [M+H]⁺: 325.9363 found: 325.9357.



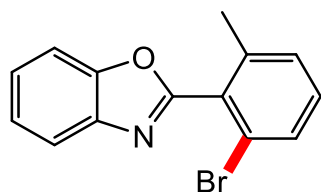
2-(2-bromo-6-methoxyphenyl)-5-chlorobenzo[*d*]oxazole (**2q**)²

Following the typical procedure, 5-chloro-2-(2-methoxyphenyl)benzo[d]oxazole (129.8 mg, 0.5 mmol, 1.0 equiv), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%), N-bromosuccinimide (106.8 mg, 0.6 mmol) and AcOH (30.0 mg, 0.5 mmol, 1.0 equiv) in DCE (5.0 mL) were employed to give the product **2q** (147.2 mg) in 87% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.23 (s, 1H), 7.77 (s, 1H), 7.58 (d, J = 8.9 Hz, 1H), 7.49 (d, J = 8.6 Hz, 1H), 7.32 (d, J = 8.6 Hz, 1H), 6.96 (d, J = 8.9 Hz, 1H), 3.99 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 161.47, 157.64, 148.96, 143.05, 135.65, 133.71, 131.40, 130.01, 125.63, 120.25, 117.47, 113.97, 112.89, 111.30, 56.51.

GC/MS: M/Z = 337.95



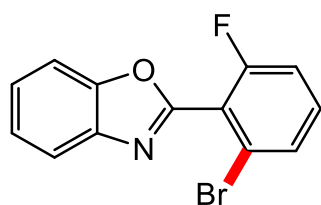
2-(2-bromo-6-methylphenyl)benzo[d]oxazole (**2r**)

Following the typical procedure, 2-(o-tolyl)benzo[d]oxazole (104.6 mg, 0.5 mmol, 1.0 equiv), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%) and N-bromosuccinimide (106.8 mg, 0.6 mmol) in DCE (5.0 mL) were employed to give the product **2r** (128.1 mg) in 89% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.17 (d, J = 7.4 Hz, 1H), 7.78 (s, 1H), 7.68 (d, J = 8.4 Hz, 1H), 7.50 (d, J = 8.5 Hz, 1H), 7.44 (d, J = 7.1 Hz, 1H), 7.38 (d, J = 7.2 Hz, 2H), 2.82 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 163.88, 150.78, 141.39, 139.06, 131.90, 131.22, 129.94, 127.82, 126.15, 125.72, 121.09, 117.92, 114.01, 22.22.

HRMS (ESI): m/z calcd. for C₁₄H₁₁BrNO [M+H]⁺: 288.0024, found: 288.0023.



2-(2-bromo-6-fluorophenyl)benzo[d]oxazole (**2s**)

Following the typical procedure, 2-(2-fluorophenyl)benzo[d]oxazole (106.6 mg, 0.5 mmol, 1.0 equiv), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%) and N-bromosuccinimide (106.8 mg,

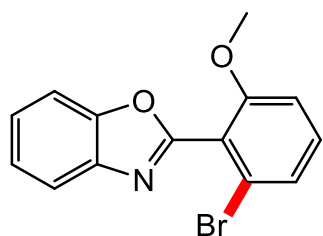
0.6 mmol) in DCE (5.0 mL) were employed to give the product **2s** (51.4 mg) in 35% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 7.91 (s, 1H), 7.66 (s, 1H), 7.58 (s, 1H), 7.45 (s, 3H), 7.24 (d, J = 6.6 Hz, 1H).

¹³C NMR (101 MHz, CDCl₃): δ 162.93, 160.37, 156.89, 150.90, 141.27, 133.25, 133.09, 133.00, 129.14, 128.25, 125.84, 124.71, 124.21, 121.72, 120.76, 115.33, 115.11, 114.52, 110.96.

¹⁹F NMR (376 MHz, CDCl₃): δ -107.79, -107.81.

HRMS (ESI): m/z calcd. for C₁₃H₈BrFNO [M+H]⁺: 291.9773, found: 291.9768.



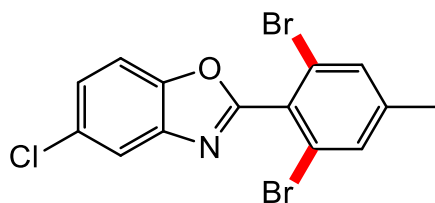
2-(2-bromo-6-methoxyphenyl)benzo[d]oxazole (**2t**)²

Following the typical procedure, 2-(2-methoxyphenyl)benzo[d]oxazole (112.6 mg, 0.5 mmol, 1.0 equiv), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%), N-bromosuccinimide (106.8 mg, 0.6 mmol), and AcOH (30.0 mg, 0.5 mmol, 1.0 equiv) in DCE (5.0 mL) were employed to give the product **2t** (138.6 mg) in 91% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 7.87 – 7.81 (m, 1H), 7.61 – 7.55 (m, 1H), 7.40 – 7.34 (m, 2H), 7.33 – 7.24 (m, 2H), 6.91 (d, J = 8.0 Hz, 1H), 3.72 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 160.00, 150.94, 141.45, 132.77, 131.31, 125.32, 124.85, 124.37, 120.55, 112.12, 110.88, 110.48, 110.08, 56.29, 56.22.

GC/MS: M/Z = 303.99



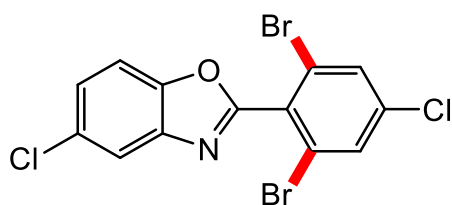
5-chloro-2-(2,6-dibromo-4-methylphenyl)benzo[d]oxazole (**2u**)

Following the typical procedure, 5-chloro-2-(p-tolyl)benzo[d]oxazole (121.8 mg, 0.5 mmol, 1.0 equiv), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%) and N-bromosuccinimide (195.8 mg, 1.1 mmol) in DCE (5.0 mL) were employed to give the product **2u** (142.7 mg) in 71% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 7.88 (d, J = 1.7 Hz, 1H), 7.78 (s, 2H), 7.59 (d, J = 8.7 Hz, 1H), 7.44 (dd, J = 8.7, 1.8 Hz, 1H), 2.37 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 165.16, 149.02, 144.23, 142.02, 139.45, 136.06, 130.27, 126.25, 120.86, 111.86, 96.58, 20.43.

HRMS (ESI): m/z calcd. for C₁₄H₉Br₂ClNO [M+H]⁺: 401.8719 found: 401.8716.



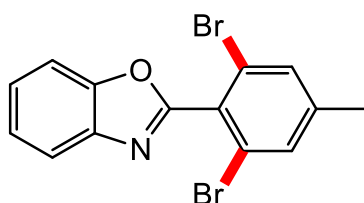
5-chloro-2-(2,6-dibromo-4-chlorophenyl)benzo[d]oxazole (**2v**)

Following the typical procedure, 5-chloro-2-(4-chlorophenyl)benzo[d]oxazole (132.1 mg, 0.5 mmol, 1.0 equiv), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%) and N-bromosuccinimide (195.8 mg, 1.1 mmol) in DCE (5.0 mL) were employed to give the product **2v** (137.1 mg) in 65% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 7.97 (s, 2H), 7.89 (s, 1H), 7.60 (d, J = 8.7 Hz, 1H), 7.46 (d, J = 8.7 Hz, 1H). ¹³C NMR (400 MHz, CDCl₃).

¹³C NMR (101 MHz, CDCl₃): δ 164.29, 149.01, 141.87, 138.46, 137.77, 130.50, 129.02, 126.55, 120.98, 111.93, 96.62.

HRMS (ESI): m/z calcd. for C₁₃H₆Br₂Cl₂NO [M+H]⁺: 421.8173 found: 421.8175.



2-(2,6-dibromo-4-methylphenyl)benzo[d]oxazole (**2w**)

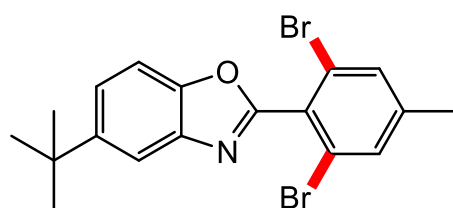
Following the typical procedure, 2-(p-tolyl)benzo[d]oxazole (104.6 mg, 0.5 mmol, 1.0 equiv), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%) and N-bromosuccinimide (195.8 mg, 1.1

mmol) in DCE (5.0 mL) were employed to give the product **2w** (112.1 mg) in 61% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 7.91 – 7.84 (m, 1H), 7.67 – 7.61 (m, 1H), 7.49 (s, 2H), 7.47 – 7.38 (m, 2H), 2.41 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 160.46, 150.63, 143.90, 141.02, 132.37, 128.79, 125.70, 124.61, 124.30, 120.75, 110.97, 20.95.

HRMS (ESI): m/z calcd. for C₁₄H₁₀Br₂NO [M+H]⁺: 367.9109 found: 367.9110.



5-(tert-butyl)-2-(2,6-dibromo-4-methylphenyl)benzo[d]oxazole (**2x**)

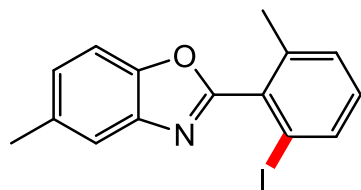
Following the typical procedure, 5-(tert-butyl)-2-(p-tolyl)benzo[d]oxazole (132.7 mg, 0.5 mmol, 1.0 equiv), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%) and N-bromosuccinimide (195.8 mg, 1.1 mmol) in DCE (5.0 mL) were employed to give the product **2x** (128.8 mg) in 63% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 7.90 (d, J = 1.4 Hz, 1H), 7.58 – 7.53 (m, 1H), 7.53 – 7.51 (m, 1H), 7.50 (d, J = 3.5 Hz, 2H), 2.42 (s, 3H), 1.43 (s, 9H).

¹³C NMR (101 MHz, CDCl₃): δ 160.51, 148.63, 148.09, 143.75, 140.94, 132.34, 128.97, 124.33, 123.52, 117.13, 110.06, 34.96, 31.74, 20.91.

HRMS (ESI): m/z calcd. for C₁₈H₁₈Br₂NO [M+H]⁺: 423.9735 found: 423.9736.

3-2 *ortho*-iodinated products



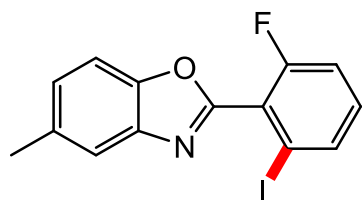
2-(2-iodo-6-methylphenyl)-5-methylbenzo[d]oxazole (**3a**)

Following the typical procedure, 5-methyl-2-(*o*-tolyl)benzo[*d*]oxazole (111.6 mg, 0.5 mmol, 1.0 equiv), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%) and N-iodosuccinimide (135.0 mg, 0.6 mmol) in DCE (5.0 mL) were employed to give the product **3a** (165.9 mg) in 95% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 7.66 (s, 1H), 7.58 – 7.48 (m, 2H), 7.29 (s, 2H), 2.53 (s, 3H), 2.30 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 161.47, 148.94, 141.47, 141.09, 134.42, 131.77, 131.56, 130.26, 130.17, 129.03, 126.58, 123.89, 121.44, 120.41, 110.26.

HRMS (ESI): *m/z* calcd. for C₁₅H₁₃INO [M+H]⁺: 350.0042 found: 350.0038.



2-(2-fluoro-6-iodophenyl)-5-methylbenzo[*d*]oxazole (**3b**)

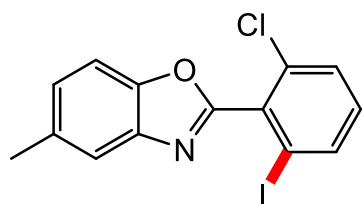
Following the typical procedure, 2-(2-fluorophenyl)-5-methylbenzo[*d*]oxazole (113.6 mg, 0.5 mmol, 1.0 equiv), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%) and N-iodosuccinimide (135.0 mg, 0.6 mmol) in DCE (5.0 mL) were employed to give the product **3b** (139.5 mg) in 89% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 7.81 (s, 1H), 7.69 (s, 1H), 7.53 (s, 1H), 7.25 (s, 3H), 2.54 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 162.26, 159.70, 149.13, 141.41, 135.47, 134.63, 133.41, 133.33, 127.28, 127.00, 120.82, 120.58, 116.05, 115.84, 110.49, 110.34, 97.55, 21.48.

¹⁹F NMR (376 MHz, CDCl₃): δ -106.97, -106.98.

HRMS (ESI): *m/z* calcd. for C₁₄H₉FINO [M+H]⁺: 354.9791 found: 354.9786.



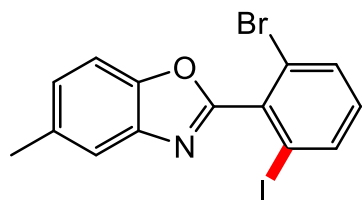
2-(2-chloro-6-iodophenyl)-5-methylbenzo[*d*]oxazole (**3c**)¹

Following the typical procedure, 2-(2-chlorophenyl)-5-methylbenzo[*d*]oxazole (121.8 mg, 0.5 mmol, 1.0 equiv), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%) and N-iodosuccinimide (135.0 mg, 0.6 mmol) in DCE (5.0 mL) were employed to give the product **3c** (183.0 mg) in 89% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 7.88 (d, J = 7.9 Hz, 1H), 7.68 (s, 1H), 7.53 (dd, J = 8.1, 4.5 Hz, 2H), 7.27 (d, J = 7.8 Hz, 1H), 7.18 (t, J = 8.1 Hz, 1H), 2.54 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 161.03, 148.89, 141.20, 137.51, 135.33, 134.63, 133.97, 132.69, 129.34, 127.01, 120.67, 110.42, 98.34, 21.53.

GC/MS: M/Z = 369.95



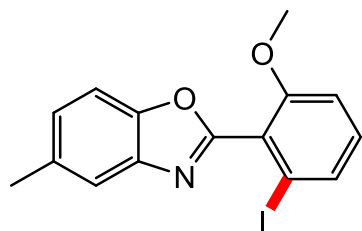
2-(2-bromo-6-iodophenyl)-5-methylbenzo[*d*]oxazole (**3m**)

Following the typical procedure, 2-(2-bromophenyl)-5-methylbenzo[*d*]oxazole (144.07 mg, 0.5 mmol, 1.0 equiv), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%) and N-iodosuccinimide (135.0 mg, 0.6 mmol) in DCE (5.0 mL) were employed to give the product **3m** (202.7 mg) in 98% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 7.90 (d, J = 8.0 Hz, 1H), 7.68 (d, J = 9.0 Hz, 2H), 7.52 (d, J = 8.3 Hz, 1H), 7.25 (d, J = 6.8 Hz, 1H), 7.08 (t, J = 8.0 Hz, 1H), 2.52 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 162.09, 148.73, 141.06, 137.95, 135.79, 134.61, 132.88, 132.38, 126.99, 123.89, 120.65, 110.39, 98.16, 21.48.

HRMS (ESI): m/z calcd. for C₁₄H₁₀BrINO [M+H]⁺: 413.8990 found: 413.8983.



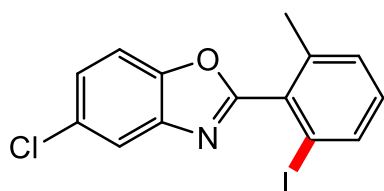
2-(2-iodo-6-methoxyphenyl)-5-methylbenzo[*d*]oxazole (**3n**)

Following the typical procedure, 2-(2-methoxyphenyl)-5-methylbenzo[*d*]oxazole (104.6 mg, 0.5 mmol, 1.0 equiv), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%), N-iodosuccinimide (135.0 mg, 0.6 mmol), and AcOH (30.0 mg, 0.5 mmol, 1.0 equiv) in DCE (5.0 mL) were employed to give the product **3n** (181.1 mg) in 99% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 7.66 (s, 1H), 7.55 (d, J = 7.9 Hz, 1H), 7.51 (d, J = 8.3 Hz, 1H), 7.21 (dd, J = 16.1, 7.8 Hz, 2H), 7.00 (d, J = 8.4 Hz, 1H), 3.78 (s, 3H), 2.53 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 161.28, 159.46, 149.04, 141.52, 134.17, 132.91, 131.05, 126.39, 120.37, 112.03, 110.76, 110.21, 98.67, 56.10, 29.65, 21.45.

HRMS (ESI): m/z calcd. for C₁₅H₁₃BrNO [M+H]⁺: 365.9991 found: 365.9999.



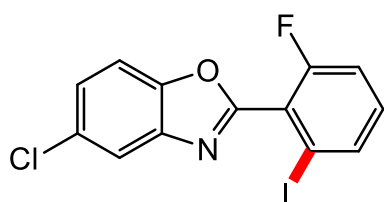
5-chloro-2-(2-iodo-6-methylphenyl)benzo[*d*]oxazole (**3o**)¹

Following the typical procedure, 5-chloro-2-(*o*-tolyl)benzo[*d*]oxazole (121.8 mg, 0.5 mmol, 1.0 equiv), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%) and N-iodosuccinimide (135.0 mg, 0.6 mmol) in DCE (5.0 mL) were employed to give the product **3o** (162.6 mg) in 88% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 7.86 (s, 1H), 7.82 (s, 1H), 7.57 (s, 1H), 7.42 (s, 1H), 7.32 (s, 1H), 7.15 (d, J = 6.7 Hz, 1H), 2.29 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 164.35, 149.16, 142.32, 140.63, 136.76, 133.69, 132.03, 130.17, 129.85, 125.92, 120.61, 111.71, 97.54, 20.72.

GC/MS: M/Z = 369.95



5-chloro-2-(2-fluoro-6-iodophenyl)benzo[*d*]oxazole (**3p**)

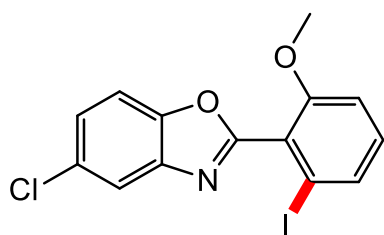
Following the typical procedure, 5-chloro-2-(2-(2-fluorophenyl)benzo[*d*]oxazole (123.8 mg, 0.5 mmol, 1.0 equiv), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%) and N-iodosuccinimide (135.0 mg, 0.6 mmol) in DCE (5.0 mL) under 80 °C were employed to give the product **3p** (91.6 mg) in 49% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 7.86 (d, J = 2.0 Hz, 1H), 7.82 – 7.78 (m, 1H), 7.56 (d, J = 8.7 Hz, 1H), 7.41 (dd, J = 8.7, 2.1 Hz, 1H), 7.27 – 7.21 (m, 2H).

¹³C NMR (101 MHz, CDCl₃): δ 162.25, 159.68, 149.43, 142.26, 135.61, 135.58, 133.78, 133.69, 130.34, 126.27, 125.82, 120.73, 120.29, 116.14, 115.92, 111.77, 111.46, 97.33.

¹⁹F NMR (376 MHz, CDCl₃): δ -106.84, -106.86.

HRMS (ESI): m/z calcd. for C₁₃H₇BrClFNO [M+H]⁺: 373.9245 found: 373.9239.



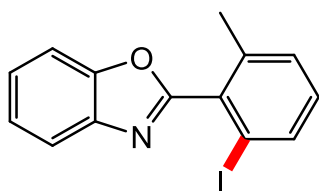
5-chloro-2-(2-iodo-6-methoxyphenyl)benzo[*d*]oxazole (3q) ²

Following the typical procedure, 5-chloro-2-(2-(2-methoxyphenyl)benzo[*d*]oxazole (129.8 mg, 0.5 mmol, 1.0 equiv), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%), N-iodosuccinimide (135.0 mg, 0.6 mmol), and AcOH (30.0 mg, 0.5 mmol, 1.0 equiv) in DCE (5.0 mL) were employed to give the product **3q** (179.4 mg) in 93% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 7.81 (d, J = 18.0 Hz, 1H), 7.58 – 7.42 (m, 2H), 7.38 (dd, J = 8.6, 1.9 Hz, 1H), 7.23 – 7.15 (m, 1H), 6.99 (d, J = 8.4 Hz, 1H), 3.77 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 159.47, 142.45, 133.23, 131.35, 131.16, 129.89, 125.66, 120.75, 120.51, 112.13, 111.63, 110.83, 98.41, 77.32, 77.00, 76.68, 56.15.

GC/MS: M/Z = 385.94



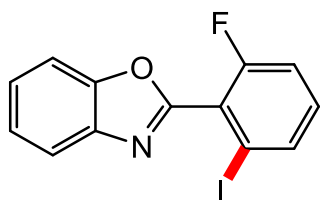
2-(2-iodo-6-methylphenyl)-5-methylbenzo[*d*]oxazole (3r)

Following the typical procedure, 2-(*o*-tolyl)benzo[*d*]oxazole (104.6 mg, 0.5 mmol, 1.0 equiv), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%) and N-iodosuccinimide (135.0 mg, 0.6 mmol) in DCE (5.0 mL) were employed to give the product **3r** (142.3 mg) in 85% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 7.89 – 7.83 (m, 1H), 7.79 (d, J = 7.9 Hz, 1H), 7.66 – 7.60 (m, 1H), 7.46 – 7.38 (m, 2H), 7.29 (d, J = 7.7 Hz, 1H), 7.12 (t, J = 7.8 Hz, 1H), 2.27 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 162.93, 150.53, 141.16, 140.62, 136.65, 134.10, 131.78, 129.75, 125.47, 124.54, 120.57, 110.88, 97.70, 77.32, 77.01, 76.69, 20.72.

HRMS (ESI): m/z calcd. for C₁₄H₁₁INO [M+H]⁺: 335.9885, found: 335.9880.



2-(2-fluoro-6-iodophenyl)benzo[*d*]oxazole (**3s**)

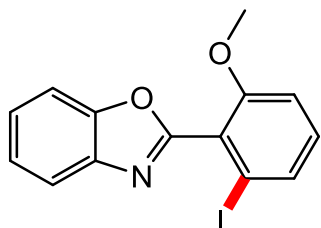
Following the typical procedure, 2-(2-fluorophenyl)benzo[*d*]oxazole (106.6 mg, 0.5 mmol, 1.0 equiv), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%) and N-iodosuccinimide (135.0 mg, 0.6 mmol) in DCE (5.0 mL) were employed to give the product **3s** (71.2 mg) in 42% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 7.91 (s, 1H), 7.81 (s, 1H), 7.66 (s, 1H), 7.45 (s, 2H), 7.24 (s, 2H).

¹³C NMR (101 MHz, CDCl₃): δ 133.09, 133.00, 129.14, 125.84, 124.71, 120.76, 115.33, 115.11, 110.96.

¹⁹F NMR (376 MHz, CDCl₃): δ 106.90, 106.92.

HRMS (ESI): m/z calcd. for C₁₄H₁₁BrNO [M+H]⁺: 339.9629, found: 339.9621.



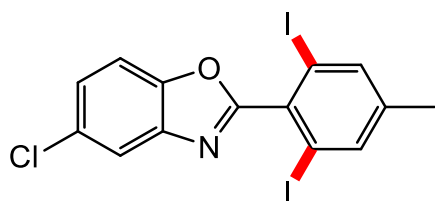
2-(2-iodo-6-methoxyphenyl)benzo[*d*]oxazole (**3t**)²

Following the typical procedure, 2-(2-methoxyphenyl)benzo[*d*]oxazole (112.6 mg, 0.5 mmol, 1.0 equiv), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%), N-iodosuccinimide (135.0 mg, 0.6 mmol), and AcOH (30.0 mg, 0.5 mmol, 1.0 equiv) in DCE (5.0 mL) were employed to give the product **3t** (166.6 mg) in 95% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 7.90 – 7.85 (m, 1H), 7.64 (dt, J = 4.9, 2.8 Hz, 1H), 7.57 (d, J = 7.9 Hz, 1H), 7.46 – 7.39 (m, 2H), 7.22 (t, J = 8.2 Hz, 1H), 7.01 (d, J = 8.4 Hz, 1H), 3.78 (d, J = 8.6 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 199.06, 161.24, 159.55, 150.87, 141.42, 133.02, 131.17, 125.30, 124.36, 123.92, 120.60, 110.88, 98.66, 56.18.

GC/MS: M/Z = 351.99



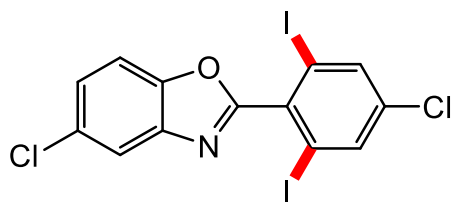
5-chloro-2-(2,6-diiodo-4-methylphenyl)benzo[*d*]oxazole (3u)

Following the typical procedure, 5-chloro-2-(*p*-tolyl)benzo[*d*]oxazole (121.6 mg, 0.5 mmol, 1.0 equiv), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%) and N-iodosuccinimide (247.5 mg, 1.1 mmol) in DCE (5.0 mL) were employed to give the product **3u** (180.6 mg) in 73% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 7.88 (d, J = 1.7 Hz, 1H), 7.78 (s, 2H), 7.59 (d, J = 8.7 Hz, 1H), 7.44 (dd, J = 8.7, 1.8 Hz, 1H), 2.37 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 165.16, 149.02, 144.23, 142.02, 139.45, 136.06, 130.27, 126.25, 120.86, 111.86, 96.58, 20.43.

HRMS (ESI): m/z calcd. for C₁₄H₉ClI₂NO [M+H]⁺: 495.8462 found: 495.8456.



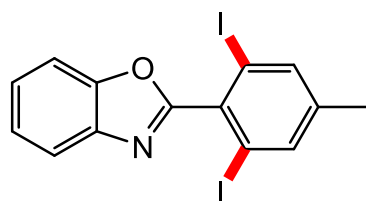
5-chloro-2-(4-chloro-2,6-diiodophenyl)benzo[*d*]oxazole (3v)

Following the typical procedure, 5-chloro-2-(4-chlorophenyl)benzo[*d*]oxazole (132.1 mg, 0.5 mmol, 1.0 equiv), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%) and N-iodosuccinimide (247.5 mg, 1.1 mmol) in DCE (5.0 mL) were employed to give the product **3v** (170.2 mg) in 66% yield as white solid.).

¹H NMR (400 MHz, CDCl₃): δ 7.97 (s, 2H), 7.89 (s, 1H), 7.60 (d, J = 8.7 Hz, 1H), 7.46 (d, J = 8.7 Hz, 1H).

¹³C NMR (101 MHz, CDCl₃): δ 164.29, 149.01, 141.87, 138.46, 137.77, 130.50, 129.02, 126.55, 120.98, 111.93, 96.62.

HRMS (ESI): m/z calcd. for C₁₃H₆Cl₂I₂NO [M+H]⁺: 515.7916 found: 515.7920.



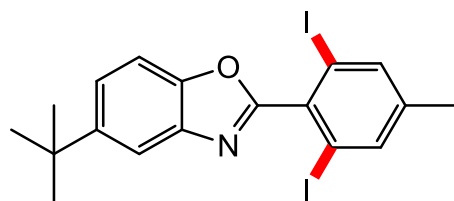
2-(2,6-diiodo-4-methylphenyl)benzo[*d*]oxazole (**3w**)

Following the typical procedure, 2-(*p*-tolyl)benzo[*d*]oxazole (104.6 mg, 0.5 mmol, 1.0 equiv), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%) and N-iodosuccinimide (247.5 mg, 1.1 mmol) in DCE (5.0 mL) were employed to give the product **3w** (159.0 mg) in 69% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 7.90 – 7.83 (m, 1H), 7.66 – 7.60 (m, 1H), 7.49 (s, 2H), 7.46 – 7.37 (m, 2H), 2.40 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 160.46, 150.63, 143.90, 141.02, 132.37, 128.79, 125.70, 124.61, 124.30, 120.75, 110.97, 20.95.

HRMS (ESI): m/z calcd. for C₁₃H₈I₂NO [M+H]⁺: 447.8695 found: 447.8689.



5-(*tert*-butyl)-2-(2,6-diiodo-4-methylphenyl)benzo[*d*]oxazole (**3x**)

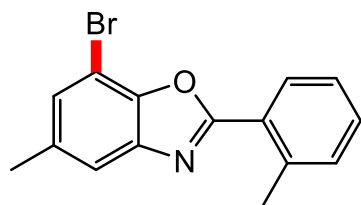
Following the typical procedure, 5-(tert-butyl)-2-(p-tolyl)benzo[*d*]oxazole (132.7 mg, 0.5 mmol, 1.0 equiv), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%) and N-iodosuccinimide (247.5 mg, 1.1 mmol) in DCE (5.0 mL) were employed to give the product **3x** (152.9 mg) in 59% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 7.89 (d, J = 1.4 Hz, 1H), 7.78 (s, 2H), 7.57 (d, J = 8.6 Hz, 1H), 7.52 (dd, J = 8.6, 1.8 Hz, 1H), 2.37 (s, 3H), 1.44 (s, 9H).

¹³C NMR (101 MHz, CDCl₃): δ 163.88, 148.38, 148.08, 143.82, 140.80, 139.36, 136.63, 123.63, 117.20, 110.06, 96.80, 34.97, 31.75, 20.34.

HRMS (ESI): m/z calcd. for C₁₈H₁₈I₂NO [M+H]⁺: 517.9478 found: 517.9481.

3-3 C7-brominated products



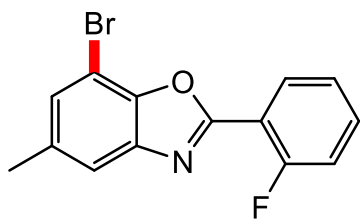
7-bromo-5-methyl-2-(o-tolyl)benzo[*d*]oxazole (**5a**)

Following the typical procedure, 5-methyl-2-(o-tolyl)benzo[*d*]oxazole (111.6 mg, 0.5 mmol, 1.0 equiv), [(p-cymene)Ru(MeCN)₃]₂ SbF₆ (14.6 mg, 5 mol%) and N-bromosuccinimide (106.8 mg, 0.6 mmol) in MeCN (5.0 mL) were employed to give the product **5a** (109.8 mg) in 73% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.14 (d, J = 7.5 Hz, 1H), 7.79 (s, 1H), 7.65 (s, 1H), 7.41 (d, J = 7.1 Hz, 1H), 7.34 (d, J = 6.9 Hz, 2H), 2.79 (s, 3H), 2.51 (d, J = 7.5 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃): ¹³C NMR (101 MHz, CDCl₃) δ 149.04, 141.80, 138.97, 133.90, 131.86, 131.75, 131.09, 130.77, 129.92, 126.11, 121.05, 114.11, 109.83, 23.35, 22.23.

HRMS (ESI): m/z calcd. for C₁₅H₁₃BrNO [M+H]⁺: 302.0181 found: 302.0186.



7-bromo-2-(2-fluorophenyl)-5-methylbenzo[d]oxazole (**5b**)

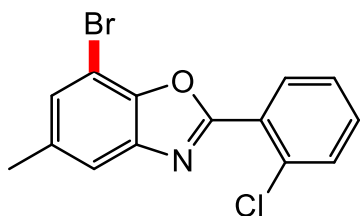
Following the typical procedure, 2-(2-fluorophenyl)-5-methylbenzo[d]oxazole (113.6 mg, 0.5 mmol, 1.0 equiv), [(p-cymene)Ru(MeCN)₃]₂ SbF₆ (14.6 mg, 5 mol%) and N-bromosuccinimide (106.8 mg, 0.6 mmol) in MeCN (5.0 mL) were employed to give the product **5b** (130.5 mg) in 73% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.18 (t, J = 7.5 Hz, 1H), 7.79 (s, 1H), 7.66 (s, 1H), 7.51 (dd, J = 12.9, 7.0 Hz, 1H), 7.28 (dd, J = 16.0, 8.3 Hz, 2H), 2.51 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 162.10, 159.90, 159.52, 149.16, 141.40, 134.33, 133.30 (d, J = 8.64), 130.50, 124.53 (d, J = 3.39), 121.18, 117.13 (d, J = 21.44), 115.23 (d, J = 10.83), 114.31, 23.41.

¹⁹F NMR (376 MHz, CDCl₃): δ -109.74, -109.75.

HRMS (ESI): m/z calcd. for C₁₄H₁₀BrFNO [M+H]⁺: 305.9930 found: 305.9927.



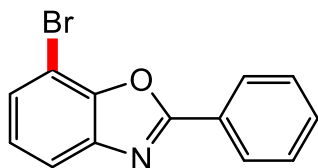
7-bromo-2-(2-chlorophenyl)-5-methylbenzo[d]oxazole (**5c**)

Following the typical procedure, 2-(2-chlorophenyl)-5-methylbenzo[d]oxazole (121.8 mg, 0.5 mmol, 1.0 equiv), [(p-cymene)Ru(MeCN)₃]₂ SbF₆ (14.6 mg, 5 mol%) and N-bromosuccinimide (106.8 mg, 0.6 mmol) in MeCN (5.0 mL) were employed to give the product **5c** (127.4 mg) in 79% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.11 (d, J = 7.5 Hz, 1H), 7.81 (s, 1H), 7.69 (s, 1H), 7.55 (d, J = 7.8 Hz, 1H), 7.48 – 7.37 (m, 2H), 2.52 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 161.40, 149.29, 141.32, 134.31, 133.54, 132.06, 131.79, 131.47, 126.96, 125.94, 121.34, 114.37, 23.40.

HRMS (ESI): m/z calcd. for C₁₄H₁₀BrCINO [M+H]⁺: 321.9635 found: 321.9639.



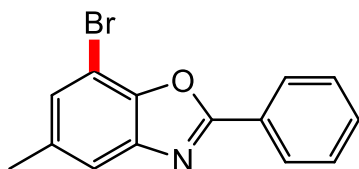
7-bromo-2-phenylbenzo[d]oxazole (**5d**)

Following the typical procedure, 2-phenylbenzo[d]oxazole (97.6 mg, 0.5 mmol, 1.0 equiv), [(p-cymene)Ru(MeCN)₃]₂ SbF₆ (14.6 mg, 5 mol%) and N-bromosuccinimide (106.8 mg, 0.6 mmol) in MeCN (5.0 mL) were employed to give the product **5d** (125.0 mg) in 91% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.22 (d, J = 6.9 Hz, 2H), 7.74 (s, 1H), 7.62 (d, J = 8.4 Hz, 1H), 7.54 (t, J = 10.2 Hz, 3H), 7.47 (d, J = 8.4 Hz, 1H).

¹³C NMR (101 MHz, CDCl₃): δ 163.56, 151.24, 141.35, 131.85, 128.99, 128.04, 127.72, 126.69, 120.96, 117.98, 114.13.

HRMS (ESI): m/z calcd. for C₁₃H₉BrNO [M+H]⁺: 273.9868 found: 273.9864.



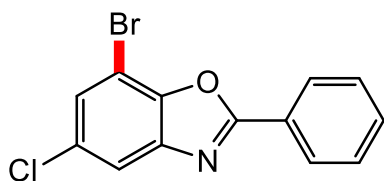
7-bromo-5-methyl-2-phenylbenzo[d]oxazole (**5e**)

Following the typical procedure, 5-methyl-2-phenylbenzo[d]oxazole (121.6 mg, 0.5 mmol, 1.0 equiv), [(p-cymene)Ru(MeCN)₃]₂ SbF₆ (14.6 mg, 5 mol%) and N-bromosuccinimide (106.8 mg, 0.6 mmol) in MeCN (5.0 mL) were employed to give the product **5e** (142.4 mg) in 99% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.21 (d, J = 6.7 Hz, 2H), 7.77 (s, 1H), 7.61 (s, 1H), 7.53 (t, J = 9.5 Hz, 3H), 2.51 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 163.52, 149.49, 141.77, 134.14, 131.69, 128.94, 127.67, 126.89, 120.91, 120.66, 114.22, 23.38.

HRMS (ESI): m/z calcd. for C₁₄H₁₁BrNO [M+H]⁺: 288.0025 found: 288.0027.



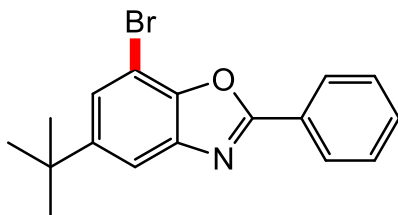
7-bromo-5-chloro-2-phenylbenzo[d]oxazole (**5f**)

Following the typical procedure, 5-chloro-2-phenylbenzo[d]oxazole (114.8 mg, 0.5 mmol, 1.0 equiv), [(p-cymene)Ru(MeCN)₃]₂ SbF₆ (14.6 mg, 5 mol%) and N-bromosuccinimide (106.8 mg, 0.6 mmol) in MeCN (5.0 mL) were employed to give the product **5f** (95.7 mg) in 62% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.21 (d, J = 7.2 Hz, 2H), 7.86 (s, 2H), 7.61 – 7.50 (m, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 164.72, 149.61, 142.58, 132.24, 130.56, 129.07, 127.89, 126.31, 120.93, 118.19, 115.40.

HRMS (ESI): m/z calcd. for C₁₃H₈BrClNO [M+H]⁺: 307.9478 found: 307.9478.



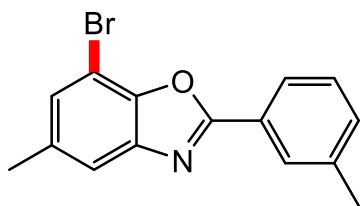
7-bromo-5-(*tert*-butyl)-2-phenylbenzo[d]oxazole (**5g**)

Following the typical procedure, 5-(*tert*-butyl)-2-phenylbenzo[d]oxazole (125.7 mg, 0.5 mmol, 1.0 equiv), [(p-cymene)Ru(MeCN)₃]₂ SbF₆ (14.6 mg, 5 mol%) and N-bromosuccinimide (106.8 mg, 0.6 mmol) in MeCN (5.0 mL) were employed to give the product **5g** (123.1 mg) in 75% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.29 (d, J = 7.0 Hz, 1H), 8.22 (d, J = 7.0 Hz, 2H), 7.89 (s, 1H), 7.83 (s, 1H), 7.51 (s, 2H), 7.43 (dt, J = 14.8, 7.5 Hz, 1H), 1.59 (s, 9H).

¹³C NMR (101 MHz, CDCl₃): δ 149.13, 144.61, 141.53, 131.73, 128.98, 127.67, 126.88, 124.49, 118.80, 117.28, 108.59, 36.99, 30.14.

HRMS (ESI): m/z calcd. for C₁₇H₁₇BrNO [M+H]⁺: 330.0494 found: 330.0498.



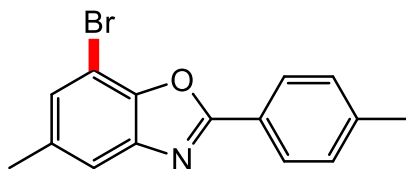
7-bromo-5-methyl-2-(*m*-tolyl)benzo[*d*]oxazole (**5h**)

Following the typical procedure, 5-methyl-2-(*m*-tolyl)benzo[*d*]oxazole (111.6 mg, 0.5 mmol, 1.0 equiv), [(*p*-cymene)Ru(MeCN)₃]₂ SbF₆ (14.6 mg, 5 mol%) and N-bromosuccinimide (106.8 mg, 0.6 mmol) in MeCN (5.0 mL) were employed to give the product **5h** (111.6 mg) in 74% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.05 (s, 1H), 8.00 (d, J = 7.6 Hz, 1H), 7.77 (s, 1H), 7.60 (s, 1H), 7.43 – 7.37 (m, 1H), 7.35 (d, J = 7.5 Hz, 1H), 2.51 (s, 3H), 2.45 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 163.75, 149.48, 141.77, 138.80, 134.11, 132.56, 128.86, 128.22, 126.74, 124.82, 120.84, 120.57, 114.18, 23.38, 21.34.

HRMS (ESI): *m/z* calcd. for C₁₅H₁₃BrNO [M+H]⁺: 302.0181, found: 302.0179.



7-bromo-5-methyl-2-(*p*-tolyl)benzo[*d*]oxazole (**5i**)

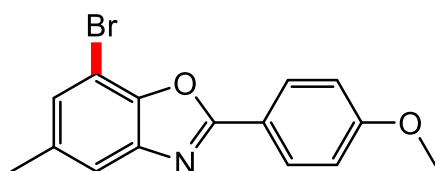
Ru method: Following the typical procedure, 5-methyl-2-(*p*-tolyl)benzo[*d*]oxazole (111.6 mg, 0.5 mmol, 1.0 equiv), [(*p*-cymene)Ru(MeCN)₃]₂ SbF₆ (14.6 mg, 5 mol%) and N-bromosuccinimide (106.8 mg, 0.6 mmol) in MeCN (5.0 mL) were employed to give the product **5i** (119.3 mg) in 79% yield as white solid.

Rh method: Following the typical procedure, 5-methyl-2-(*p*-tolyl)benzo[*d*]oxazole (111.6 mg, 0.5 mmol, 1.0 equiv), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%) (14.6 mg, 5 mol%) and N-bromosuccinimide (106.8 mg, 0.6 mmol) in MeCN (5.0 mL) were employed to give the product **5i** (78.5 mg) in 52% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.12 (d, J = 7.8 Hz, 2H), 7.78 (s, 1H), 7.62 (s, 1H), 7.34 (d, J = 7.7 Hz, 2H), 2.53 (s, 3H), 2.46 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 163.68, 149.28, 142.21, 133.90, 129.57, 127.51, 125.85, 123.95, 120.60, 120.24, 119.63, 113.99, 109.71, 23.26, 21.56.

HRMS (ESI): m/z calcd. for C₁₅H₁₃BrNO [M+H]⁺: 302.0181, found: 302.0183.



7-bromo-2-(4-methoxyphenyl)-5-methylbenzo[d]oxazole (5j)

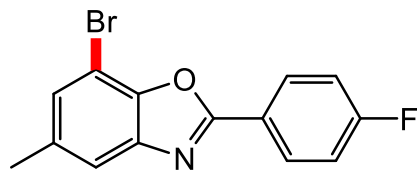
Ru method: Following the typical procedure, 2-(4-methoxyphenyl)-5-methylbenzo[d]oxazole (119.6 mg, 0.5 mmol, 1.0 equiv), [(p-cymene)Ru(MeCN)₃]₂ SbF₆ (14.6 mg, 5 mol%) and N-bromosuccinimide (106.8 mg, 0.6 mmol) in MeCN (5.0 mL) were employed to give the product **5j** (152.5 mg) in 96% yield as white solid.

Rh method: Following the typical procedure, 2-(4-methoxyphenyl)-5-methylbenzo[d]oxazole (119.6 mg, 0.5 mmol, 1.0 equiv), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%) and N-bromosuccinimide (106.8 mg, 0.6 mmol) in MeCN (5.0 mL) were employed to give the product **5j** (76.2 mg) in 48% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.14 (d, J = 7.6 Hz, 2H), 7.73 (s, 1H), 7.57 (s, 1H), 7.01 (d, J = 7.6 Hz, 2H), 3.89 (s, 3H), 2.50 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 164.03, 162.85, 149.77, 142.31, 134.26, 130.09, 129.80, 129.65, 120.88, 120.35, 119.74, 114.76, 114.34, 55.81, 23.68.

HRMS (ESI): m/z calcd. for C₁₅H₁₃BrNO₂ [M+H]⁺: 318.0130, found: 318.0125.



7-bromo-2-(4-fluorophenyl)-5-methylbenzo[d]oxazole (**5k**)

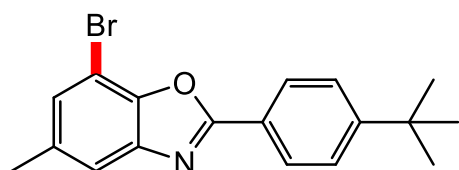
Following the typical procedure, 2-(4-fluorophenyl)-5-methylbenzo[d]oxazole (113.6 mg, 0.5 mmol, 1.0 equiv), [(p-cymene)Ru(MeCN)₃] SbF₆ (14.6 mg, 5 mol%) and N-bromosuccinimide (106.8 mg, 0.6 mmol) in MeCN (5.0 mL) were employed to give the product **5k** (140.8 mg) in 92% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.21 (dd, J = 7.9, 5.7 Hz, 2H), 7.76 (s, 1H), 7.60 (s, 1H), 7.21 (t, J = 8.4 Hz, 2H), 2.52 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 164.91 (d, J = 253.1 Hz), 149.45, 141.67, 134.25, 129.88 (d, J = 8.9 Hz), 123.18, 120.85, 120.68, 116.24 (d, J = 22.2 Hz), 114.18, 23.38.

¹⁹F NMR (376 MHz, CDCl₃): δ -106.96, -106.97, -106.98, -107.00, -107.01.

HRMS (ESI): m/z calcd. for C₁₄H₁₀BrFNO [M+H]⁺: 305.9930, found: 305.9934.



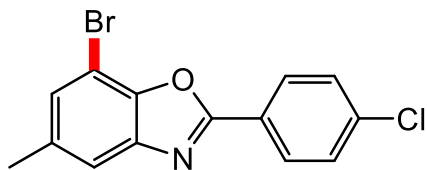
7-bromo-2-(4-(tert-butyl)phenyl)-5-methylbenzo[d]oxazole (**5y**)

Following the typical procedure, 2-(4-(tert-butyl)phenyl)-5-methylbenzo[d]oxazole (131.7 mg, 0.5 mmol, 1.0 equiv), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%) and N-bromosuccinimide (106.8 mg, 0.6 mmol) in DCE (5.0 mL) were employed to give the product **5y** (84.5 mg) in 49% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.20 (d, J = 8.3 Hz, 2H), 7.53 (d, J = 8.3 Hz, 2H), 7.40 (d, J = 8.2 Hz, 1H), 7.23 (d, J = 8.2 Hz, 1H), 2.58 (s, 3H), 1.37 (s, 9H).

¹³C NMR (101 MHz, CDCl₃): δ 212.89, 155.38, 147.09, 137.75, 127.77, 126.05, 125.80, 124.04, 110.00, 109.55, 77.33, 77.02, 76.70, 35.10, 31.16, 27.27.

HRMS (ESI): m/z calcd. for C₁₅H₁₂BrNOH [M+H]⁺: 344.0650, found: 344.0649



2-(4-chlorophenyl)-7-bromo-5-methylbenzo[d]oxazole (**5z**)

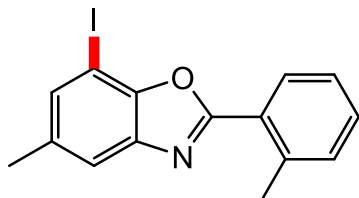
Following the typical procedure, 2-(4-chlorophenyl)-5-methylbenzo[d]oxazole (121.6 mg, 0.5 mmol, 1.0 equiv), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%) and N-bromosuccinimide (106.8 mg, 0.6 mmol) in DCE (5.0 mL) were employed to give the product **5z** (75.5 mg) in 47% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.16 (d, J = 8.4 Hz, 2H), 7.79 (s, 1H), 7.62 (s, 1H), 7.51 (d, J = 8.4 Hz, 2H), 2.53 (d, J = 4.5 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 164.03, 162.85, 149.77, 142.31, 134.26, 130.09, 129.80, 129.65, 120.88, 120.35, 119.74, 114.76, 114.34, 55.81, 23.68.

HRMS (ESI): m/z calcd. for C₁₄H₁₀BrClNO [M+H]⁺: 321.9634, found: 321.9633.

3-4 C7-iodinated products



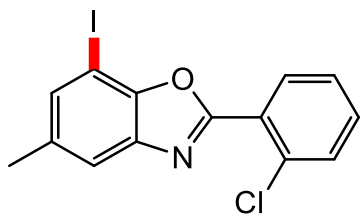
7-Iodo-5-methyl-2-(*o*-tolyl)benzo[d]oxazole (**6a**)

Following the typical procedure, 5-methyl-2-(*o*-tolyl)benzo[d]oxazole (111.6 mg, 0.5 mmol, 1.0 equiv), [(*p*-cymene)Ru(MeCN)₃]₂ SbF₆ (14.6 mg, 5 mol%) and N-iodosuccinimide (135.0 mg, 0.6 mmol) in MeCN (5.0 mL) were employed to give the product **6a** (130.4 mg) in 75% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.14 (d, J = 7.5 Hz, 1H), 7.79 (s, 1H), 7.65 (s, 1H), 7.41 (d, J = 7.1 Hz, 1H), 7.34 (d, J = 6.9 Hz, 2H), 2.79 (s, 3H), 2.51 (d, J = 7.5 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃): ¹³C NMR (101 MHz, CDCl₃) δ 149.04, 141.80, 138.97, 133.90, 131.86, 131.75, 131.09, 130.77, 129.92, 126.11, 121.05, 114.11, 109.83, 23.35, 22.23.

HRMS (ESI): m/z calcd. for C₁₅H₁₃INO [M+H]⁺: 350.0042, found: 350.0041.



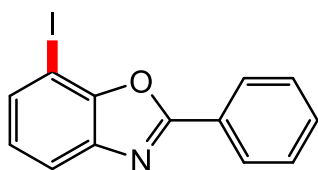
2-(2-chlorophenyl)-7-iodo-5-methylbenzo[d]oxazole (**6c**)

Following the typical procedure, 2-(2-chlorophenyl)-5-methylbenzo[d]oxazole (121.8 mg, 0.5 mmol, 1.0 equiv), [(p-cymene)Ru(MeCN)₃]₂ SbF₆ (14.6 mg, 5 mol%) and N-iodosuccinimide (135.0 mg, 0.6 mmol) in MeCN (5.0 mL) were employed to give the product **6c** (130.0 mg) in 70% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.17 – 8.13 (m, 1H), 8.13 (s, 1H), 7.75 (s, 1H), 7.59 (d, J = 7.8 Hz, 1H), 7.48 (dd, J = 12.0, 4.2 Hz, 1H), 7.44 (t, J = 7.6 Hz, 1H), 2.60 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): ¹³C NMR (101 MHz, CDCl₃) δ 161.29, 149.39, 142.36, 137.40, 133.58, 132.10, 131.84, 131.48, 131.24, 126.98, 125.94, 120.62, 120.38, 28.52.

HRMS (ESI): m/z calcd. for C₁₄H₁₀ClINO [M+H]⁺: 353.9792, found: 353.9788.



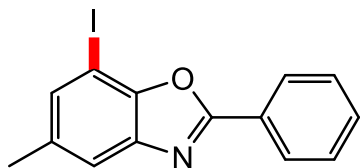
7-iodo-2-phenylbenzo[d]oxazole (**6d**)

Following the typical procedure, 2-phenylbenzo[d]oxazole (97.6 mg, 0.5 mmol, 1.0 equiv), [(p-cymene)Ru(MeCN)₃]₂ SbF₆ (14.6 mg, 5 mol%) and N-iodosuccinimide (135.0 mg, 0.6 mmol) in MeCN (5.0 mL) were employed to give the product **6d** (136.5 mg) in 85% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.25 (d, J = 6.9 Hz, 2H), 7.76 (s, 1H), 7.64 (d, J = 8.4 Hz, 1H), 7.57 (t, J = 10.2 Hz, 3H), 7.49 (d, J = 8.4 Hz, 1H).

¹³C NMR (101 MHz, CDCl₃): δ 163.56, 151.24, 141.35, 131.85, 128.99, 128.04, 127.72, 126.69, 120.96, 117.98, 114.13.

HRMS (ESI): m/z calcd. for C₁₃H₉INO [M+H]⁺: 321.9729, found: 321.9726.



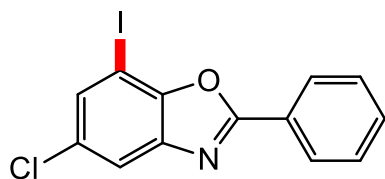
7-iodo-5-methyl-2-phenylbenzo[d]oxazole (**6e**)

Following the typical procedure, 5-methyl-2-phenylbenzo[d]oxazole (104.6 mg, 0.5 mmol, 1.0 equiv), [(p-cymene)Ru(MeCN)₃]₂ SbF₆ (14.6 mg, 5 mol%) and N-iodosuccinimide (135.0 mg, 0.6 mmol) in MeCN (5.0 mL) were employed to give the product **6e** (134.5 mg) in 80% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.21 (d, J = 6.7 Hz, 2H), 7.77 (s, 1H), 7.61 (s, 1H), 7.53 (t, J = 9.5 Hz, 3H), 2.51 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 163.52, 149.49, 141.77, 134.14, 131.69, 128.94, 127.67, 126.89, 120.91, 120.66, 114.22, 23.38.

HRMS (ESI): m/z calcd. for C₁₄H₁₁INO [M+H]⁺: 335.9886, found: 335.9886.



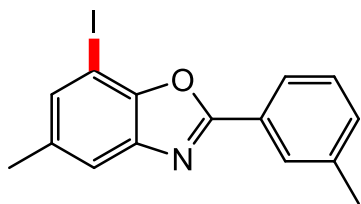
5-chloro-7-iodo-2-phenylbenzo[d]oxazole (**6f**)

Following the typical procedure, 5-chloro-2-phenylbenzo[d]oxazole (114.8 mg, 0.5 mmol, 1.0 equiv), [(p-cymene)Ru(MeCN)₃]₂ SbF₆ (14.6 mg, 5 mol%) and N-iodosuccinimide (135.0 mg, 0.6 mmol) in MeCN (5.0 mL) were employed to give the product **6f** (115.7 mg) in 65% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.21 (d, J = 7.2 Hz, 2H), 7.86 (s, 2H), 7.61 – 7.50 (m, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 164.72, 149.61, 142.58, 132.24, 130.56, 129.07, 127.89, 126.31, 120.93, 118.19, 115.40.

HRMS (ESI): m/z calcd. for C₁₃H₈ClINO [M+H]⁺: 355.9339, found: 355.9337.



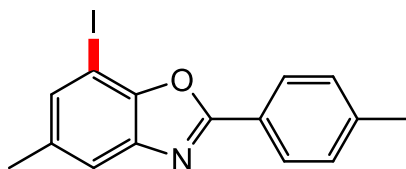
7-iodo-5-methyl-2-(*m*-tolyl)benzo[*d*]oxazole (**6h**)

Following the typical procedure, 5-methyl-2-(*m*-tolyl)benzo[*d*]oxazole (111.6 mg, 0.5 mmol, 1.0 equiv), [(*p*-cymene)Ru(MeCN)₃]₂ SbF₆ (14.6 mg, 5 mol%) and N-iodosuccinimide (135.0 mg, 0.6 mmol) in MeCN (5.0 mL) were employed to give the product **6h** (124.8 mg) in 71% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.05 (s, 1H), 8.01 (d, J = 7.6 Hz, 1H), 7.58 (s, 2H), 7.40 (t, J = 7.5 Hz, 1H), 7.35 (d, J = 7.5 Hz, 1H), 2.48 (s, 3H), 2.45 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 163.82, 149.29, 141.30, 141.13, 138.80, 132.51, 130.92, 128.85, 128.19, 126.78, 124.79, 120.92, 111.09, 21.33, 20.56.

HRMS (ESI): m/z calcd. for C₁₅H₁₃INO [M+H]⁺: 350.0042, found: 350.0044.



7-iodo-5-methyl-2-(*p*-tolyl)benzo[*d*]oxazole (**6i**)

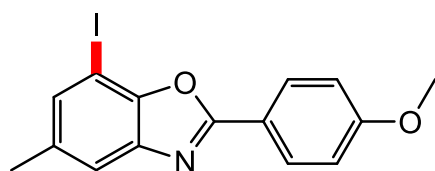
Ru method: Following the typical procedure, 5-methyl-2-(*p*-tolyl)benzo[*d*]oxazole (111.6 mg, 0.5 mmol, 1.0 equiv), [(*p*-cymene)Ru(MeCN)₃]₂ SbF₆ (14.6 mg, 5 mol%) and N-iodosuccinimide (135.0 mg, 0.6 mmol) in MeCN (5.0 mL) were employed to give the product **6i** (142.2 mg) in 81% yield as white solid.

Rh method: Following the typical procedure, 5-methyl-2-(*p*-tolyl)benzo[*d*]oxazole (111.6 mg, 0.5 mmol, 1.0 equiv), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%) and N-iodosuccinimide (135.0 mg, 0.6 mmol) in MeCN (5.0 mL) were employed to give the product **6i** (107.1 mg) in 61% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.11 (d, J = 7.9 Hz, 1H), 8.04 (s, 1H), 7.63 (s, 1H), 7.32 (s, 2H), 2.56 (s, 3H), 2.44 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 163.51, 149.37, 142.23, 136.98, 129.56, 127.55, 125.84, 123.90, 120.18, 119.66, 109.71, 94.67, 28.37, 21.57.

HRMS (ESI): m/z calcd. for C₁₅H₁₂INONa [M+Na]⁺: 371.9861, found: 371.9869.



7-iodo-2-(4-methoxyphenyl)-5-methylbenzo[d]oxazole (**6j**)

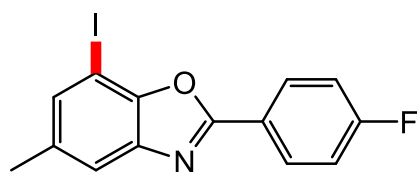
Ru method: Following the typical procedure, 2-(4-methoxyphenyl)-5-methylbenzo[d]oxazole (119.6 mg, 0.5 mmol, 1.0 equiv), [(p-cymene)Ru(MeCN)₃]₂ SbF₆ (14.6 mg, 5 mol%) and N-iodosuccinimide (135.0 mg, 0.6 mmol) in MeCN (5.0 mL) were employed to give the product **6j** (173.0 mg) in 95% yield as white solid.

Rh method: Following the typical procedure, 2-(4-methoxyphenyl)-5-methylbenzo[d]oxazole (119.6 mg, 0.5 mmol, 1.0 equiv), [(p-cymene)Ru(MeCN)₃]₂ SbF₆ (14.6 mg, 5 mol%) and N-iodosuccinimide (135.0 mg, 0.6 mmol) in MeCN (5.0 mL) were employed to give the product **6j** (92.9 mg) in 51% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.15 (d, J = 8.7 Hz, 2H), 8.00 (s, 1H), 7.60 (s, 1H), 7.01 (d, J = 8.7 Hz, 2H), 3.88 (d, J = 8.7 Hz, 3H), 2.54 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 162.51, 136.95, 129.46, 125.58, 120.13, 119.58, 119.35, 115.77, 114.37, 109.95, 94.21, 55.39, 28.33.

HRMS (ESI): m/z calcd. for C₁₅H₁₂INO₂Na [M+Na]⁺: 387.9810, found: 387.9815.



2-(4-fluorophenyl)-7-iodo-5-methylbenzo[d]oxazole (**6k**)

Following the typical procedure, 2-(4-fluorophenyl)-5-methylbenzo[d]oxazole (113.6 mg, 0.5 mmol, 1.0 equiv), [(p-cymene)Ru(MeCN)₃]₂ SbF₆ (14.6 mg, 5 mol%) and N-

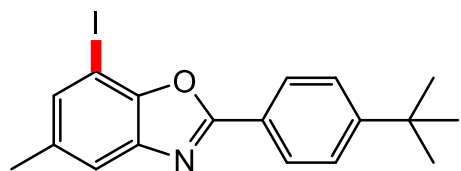
iodosuccinimide (135.0 mg, 0.6 mmol) in MeCN (5.0 mL) were employed to give the product **6k** (167.2 mg) in 95% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.22 (dd, J = 8.6, 5.1 Hz, 2H), 8.03 (d, J = 4.4 Hz, 1H), 7.62 (d, J = 3.6 Hz, 1H), 7.20 (td, J = 8.7, 2.7 Hz, 2H), 2.55 (d, J = 2.8 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 164.96 (d, J = 253.4 Hz), 149.58, 142.74, 137.38, 129.96 (d, J = 8.8 Hz), 123.18, 120.41, 119.93, 116.26 (d, J = 22.2 Hz), 105.27, 95.13, 28.50.

¹⁹F NMR (376 MHz, CDCl₃): δ -106.91, -106.92, -106.92, -106.93, -106.94, -106.95, -106.95.

HRMS (ESI): m/z calcd. for C₁₄H₁₀FINO [M+H]⁺: 353.9792, found: 353.9789.



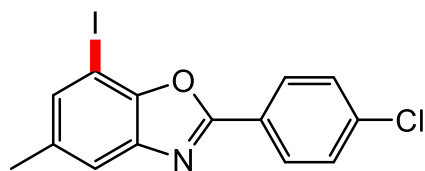
7-iodo-2-(4-(tert-butyl)phenyl)-5-methylbenzo[d]oxazole (6y)

Following the typical procedure, 2-(4-(tert-butyl)phenyl)-5-methylbenzo[d]oxazole (131.6 mg, 0.5 mmol, 1.0 equiv), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%) and N-iodosuccinimide (70.8 mg, 0.6 mmol) in DCE (5.0 mL) were employed to give the product **6y** (111.1 mg) in 57% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.20 (d, J = 8.3 Hz, 2H), 7.53 (d, J = 8.3 Hz, 2H), 7.40 (d, J = 8.2 Hz, 1H), 7.23 (d, J = 8.2 Hz, 1H), 2.58 (s, 3H), 1.37 (s, 9H).

¹³C NMR (101 MHz, CDCl₃): δ 212.89, 155.38, 147.09, 137.75, 127.77, 126.05, 125.80, 124.04, 110.00, 109.55, 77.33, 77.02, 76.70, 35.10, 31.16, 27.27.

HRMS (ESI): m/z calcd. for C₁₅H₁₂INOH [M+H]⁺: 392.2605, found: 392.2610.



2-(4-chlorophenyl)-7-iodo-5-methylbenzo[d]oxazole (6z)

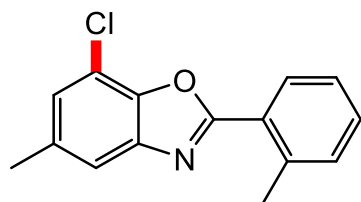
Following the typical procedure, 2-(4-chlorophenyl)-5-methylbenzo[*d*]oxazole (121.8 mg, 0.5 mmol, 1.0 equiv), [RhCp*(MeCN)₃](SbF₆)₂ (16.7 mg, 4 mol%) and N-iodosuccinimide (70.8 mg, 0.6 mmol) in DCE (5.0 mL) were employed to give the product **6z** (90.6 mg) in 49% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.15 (d, J = 8.6 Hz, 2H), 8.05 (s, 1H), 7.64 (s, 1H), 7.50 (d, J = 8.6 Hz, 2H), 2.54 (d, J = 14.5 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 164.03, 162.85, 149.77, 142.31, 134.26, 130.09, 129.80, 129.65, 120.88, 120.35, 119.74, 114.76, 114.34, 55.81, 23.68.

HRMS (ESI): m/z calcd. for C₁₄H₉INONa [M+Na]⁺: 391.9315, found: 391.9312.

3-5 C7-Chlorinated products



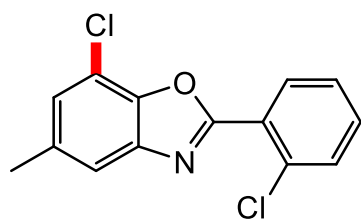
7-chloro-5-methyl-2-(*o*-tolyl)benzo[*d*]oxazole (**7a**)

Following the typical procedure, 5-methyl-2-(*o*-tolyl)benzo[*d*]oxazole (111.6 mg, 0.5 mmol, 1.0 equiv), [(*p*-cymene)Ru(MeCN)₃]₂ SbF₆ (14.6 mg, 5 mol%) and N-chlorosuccinimide (135.0 mg, 0.6 mmol) in MeCN (5.0 mL) were employed to give the product **7a** (107.0 mg) in 83% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.13 (d, J = 7.9 Hz, 1H), 7.62 (s, 1H), 7.58 (s, 1H), 7.44 – 7.37 (m, 1H), 7.37 – 7.30 (m, 2H), 2.79 (s, 3H), 2.48 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 163.89, 148.81, 141.14, 138.93, 132.34, 131.84, 131.04, 130.91, 129.88, 126.09, 125.92, 121.11, 111.00, 22.26, 20.56.

HRMS (ESI): m/z calcd. for C₁₅H₁₃ClNO [M+H]⁺: 258.0686, found: 258.0691.



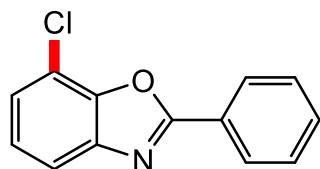
7-chloro-2-(2-chlorophenyl)-5-methylbenzo[*d*]oxazole (**7c**)

Following the typical procedure, 2-(2-chlorophenyl)-5-methylbenzo[*d*]oxazole (121.8 mg, 0.5 mmol, 1.0 equiv), [(*p*-cymene)Ru(MeCN)₃]₂ SbF₆ (14.6 mg, 5 mol%) and N-chlorosuccinimide (135.0 mg, 0.6 mmol) in MeCN (5.0 mL) were employed to give the product **7c** (130.9 mg) in 75% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.12 (d, *J* = 7.6 Hz, 1H), 7.68 (s, 1H), 7.64 (s, 1H), 7.57 (d, *J* = 7.7 Hz, 1H), 7.49 – 7.38 (m, 2H), 2.50 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 161.47, 149.12, 140.68, 133.53, 132.80, 132.05, 131.79, 131.61, 131.46, 126.96, 125.99, 121.43, 111.28, 20.60.

HRMS (ESI): *m/z* calcd. for C₁₅H₁₃ClNO [M+H]⁺: 278.0140, found: 278.0141.



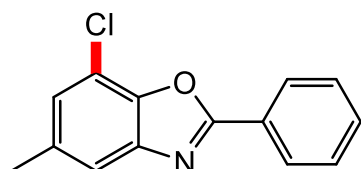
7-chloro-2-phenylbenzo[*d*]oxazole (**7d**)

Following the typical procedure, 2-phenylbenzo[*d*]oxazole 97.6 mg, 0.5 mmol, 1.0 equiv), [(*p*-cymene)Ru(MeCN)₃]₂ SbF₆ (14.6 mg, 5 mol%) and N-chlorosuccinimide (135.0 mg, 0.6 mmol) in MeCN (5.0 mL) were employed to give the product **7d** (91.2 mg) in 79% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.25 (d, *J* = 6.9 Hz, 2H), 7.76 (s, 1H), 7.64 (d, *J* = 8.4 Hz, 1H), 7.57 (t, *J* = 10.2 Hz, 3H), 7.49 (d, *J* = 8.4 Hz, 1H).

¹³C NMR (101 MHz, CDCl₃): δ 163.56, 151.24, 141.35, 131.85, 128.99, 128.04, 127.72, 126.69, 120.96, 117.98, 114.13.

HRMS (ESI): *m/z* calcd. for C₁₃H₉ClNO [M+H]⁺: 230.0373, found: 237.0370.



7-chloro-5-methyl-2-(*o*-tolyl)benzo[*d*]oxazole (**7e**)

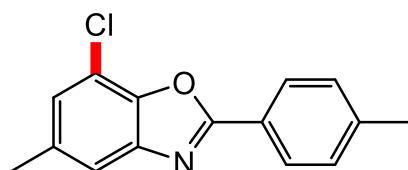
Following the typical procedure, 7-chloro-5-methyl-2-phenylbenzo[*d*]oxazole (104.6 mg, 0.5 mmol, 1.0 equiv), [(*p*-cymene)Ru(MeCN)₃]₂ SbF₆ (14.6 mg, 5 mol%) and N-

chlorosuccinimide (135.0 mg, 0.6 mmol) in MeCN (5.0 mL) were employed to give the product **7e** (118.4 mg) in 97% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.22 – 8.16 (m, 2H), 7.58 (s, 1H), 7.56 (s, 1H), 7.53 – 7.47 (m, 3H), 2.46 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 163.57, 149.28, 141.09, 132.61, 131.65, 130.99, 128.93, 127.62, 126.90, 120.96, 111.12, 20.57.

HRMS (ESI): m/z calcd. for C₁₄H₁₁ClNO [M+H]⁺: 244.0530, found: 244.0526.



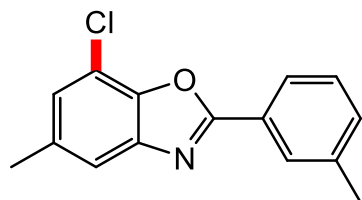
7-chloro-5-methyl-2-(p-tolyl)benzo[d]oxazole (**7i**)

Following the typical procedure, 5-methyl-2-(p-tolyl)benzo[d]oxazole (111.6 mg, 0.5 mmol, 1.0 equiv), [(p-cymene)Ru(MeCN)₃]₂ SbF₆ (14.6 mg, 5 mol%) and N-chlorosuccinimide (135.0 mg, 0.6 mmol) in MeCN (5.0 mL) were employed to give the product **7i** (97.0 mg) in 75% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.12 (d, J = 7.8 Hz, 2H), 7.78 (s, 1H), 7.62 (s, 1H), 7.34 (d, J = 7.7 Hz, 2H), 2.53 (s, 3H), 2.46 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 163.68, 149.28, 142.21, 133.90, 129.57, 127.51, 125.85, 123.95, 120.60, 120.24, 119.63, 113.99, 109.71, 23.26, 21.56.

HRMS (ESI): m/z calcd. for C₁₅H₁₃ClNO [M+H]⁺: 258.0686, found: 258.0689.



7-chloro-5-methyl-2-(m-tolyl)benzo[d]oxazole (**7h**)

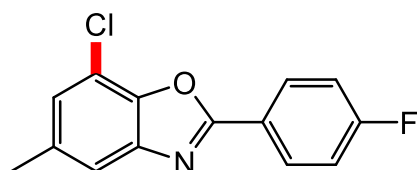
Following the typical procedure, 5-methyl-2-(m-tolyl)benzo[d]oxazole (111.6 mg, 0.5 mmol, 1.0 equiv), [(p-cymene)Ru(MeCN)₃]₂ SbF₆ (14.6 mg, 5 mol%) and N-chlorosuccinimide

(135.0 mg, 0.6 mmol) in MeCN (5.0 mL) were employed to give the product **7h** (117.7 mg) in 91% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.05 (s, 1H), 8.01 (d, J = 7.6 Hz, 1H), 7.58 (s, 2H), 7.40 (t, J = 7.5 Hz, 1H), 7.35 (d, J = 7.5 Hz, 1H), 2.48 (s, 3H), 2.45 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 163.82, 149.29, 141.30, 141.13, 138.80, 132.51, 130.92, 128.85, 128.19, 126.78, 124.79, 120.92, 111.09, 21.33, 20.56.

HRMS (ESI): m/z calcd. for C₁₅H₁₃ClNO [M+H]⁺: 258.0686, found: 258.0687.



7-chloro-2-(4-fluorophenyl)-5-methylbenzo[d]oxazole (**7k**)

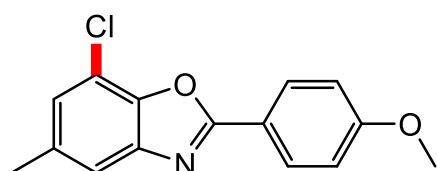
Following the typical procedure, 2-(4-fluorophenyl)-5-methylbenzo[d]oxazole (113.6 mg, 0.5 mmol, 1.0 equiv), [(p-cymene)Ru(MeCN)₃]₂ SbF₆ (14.6 mg, 5 mol%) and N-chlorosuccinimide (135.0 mg, 0.6 mmol) in MeCN (5.0 mL) were employed to give the product **7k** (85.4 mg) in 65% yield as white solid.

¹H NMR (400 MHz, CDCl₃): δ 8.26 (dd, J = 7.7, 5.6 Hz, 2H), 7.37 (d, J = 8.2 Hz, 1H), 7.19 (dd, J = 18.4, 8.7 Hz, 3H), 2.56 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 164.95 (d, J = 253.1 Hz), 162.06, 147.10, 145.36, 138.00, 130.16 (d, J = 8.9 Hz), 126.34, 123.16, 116.12 (d, J = 22.2 Hz), 109.61, 91.13, 27.26.

¹⁹F NMR (376 MHz, CDCl₃): δ -106.99, -107.01, -107.01, -107.03, -107.04, -107.05, -107.06.

HRMS (ESI): m/z calcd. for C₁₄H₁₀ClFNO [M+H]⁺: 262.0435, found: 262.0439.



7-chloro-2-(4-methoxyphenyl)-5-methylbenzo[d]oxazole (**7j**)

Following the typical procedure, 2-(4-methoxyphenyl)-5-methylbenzo[d]oxazole (119.6 mg, 0.5 mmol, 1.0 equiv), [(p-cymene)Ru(MeCN)₃]₂ SbF₆ (14.6 mg, 5 mol%) and N-

chlorosuccinimide (135.0 mg, 0.6 mmol) in MeCN (5.0 mL) were employed to give the product **7j** (132.0 mg) in 96% yield as white solid.

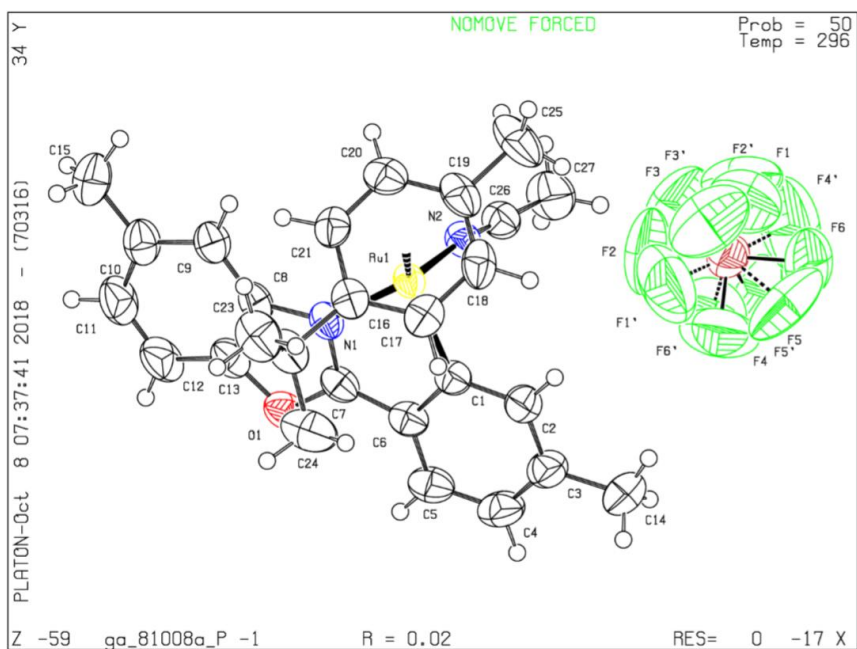
¹H NMR (400 MHz, CDCl₃): δ 8.15 (d, J = 7.7 Hz, 2H), 7.55 (s, 2H), 7.02 (d, J = 7.8 Hz, 2H), 3.89 (s, 3H), 2.47 (s, 3H).

¹³C NMR (101 MHz, CDCl₃): δ 163.75 162.47, 149.24, 141.32, 132.37, 130.39, 129.42, 120.79, 120.61, 119.45, 114.41, 110.93, 55.47, 20.54.

HRMS (ESI): m/z calcd. for C₁₅H₁₃CINO₂ [M+H]⁺: 274.0635, found: 274.0634.

4. Crystallographic Data

| Identification code | Ru-1i |
|---|--|
| CCDC Number | 1904128 |
| Empirical formula | C ₂₇ H ₂₉ F ₆ N ₂ OPRu |
| <i>M_r</i> | 643.56 |
| Crystal system | Triclinic |
| Space group | P-1 |
| <i>a</i> [Å] | 10.7138(3) |
| <i>b</i> [Å] | 10.8978(3) |
| <i>c</i> [Å] | 12.0990(3) |
| <i>α</i> [°] | 92.7480(10) |
| <i>β</i> [°] | 96.7020(10) |
| <i>γ</i> [°] | 90.4760(10) |
| <i>V</i> [Å ³] | 1401.24(7) |
| <i>Z</i> | 2 |
| <i>ρ</i> _{calc} [mg·mm ⁻³] | 1.525 |
| <i>μ</i> [mm ⁻¹] | 3.783 |
| <i>F</i> [000] | 652 |
| <i>T</i> [K] | 296(2) |
| <i>θ</i> range [°] | 3.204 to 58.144 |
| reflns collected/indep reflns | 40468/5953 |
| <i>R</i> _(int) | 0.0258 |
| data / restraints / params | 5953 / 72 / 404 |
| GOF | 1.053 |
| <i>R</i> ₁ (I > 2σ(I)) | 0.0242 |
| <i>wR</i> ₂ | 0.0659 |



5. Theoretical Calculations

B3LYP³ level of density functional theory (DFT) calculations were carried out using Gaussian 09 software package⁴. The LanI2DZ pseudopotential⁵ basis set is used for Rh and Br, and the standard 6-31G(d) basis set for other atoms. The NBO program in Gaussian 09, Version 5.9, was used to obtain more information about some special bonds.⁶ Truhlar and coworkers' SMD solvation model was employed to consider the solvent effect of dichloroethane⁷. In addition, introduced in the DFT by Parr and Yang, the condensed Fukui function is the most important local reactivity index⁸. It has become a valuable tool to deal with the site selectivity in a wide range of organic reactions⁹. For the free radical attack of the atom site k of the molecule, the condensed Fukui function is defined as the following equation in terms of the atomic charges:

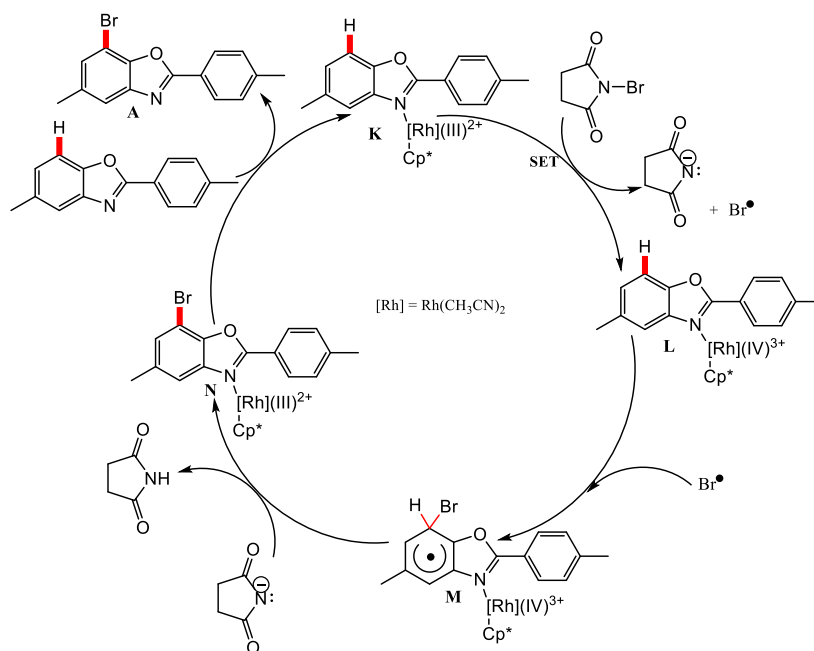
$$f_k^0 = [q_k(N+1) - q_k(N-1)]/2$$

Electrophilic-aromatic-substitution-like (S_EAr -like) reaction mechanism¹⁰ was examined theoretically as well, and four pathways (Path1-4) were located. The reaction of an electrophilic Br with an electron-rich, nucleophilic aromatic ring is involved in the C-H bond cleavage. And the rate-determining steps are activation of Br atom except Path4. Br adds to α -carbon of aromatic ring attached to benzo[*a*]oxazole via different intermediates (**E** and **E'**)

in Path1 and Path2. However, in Path3 and Path4, β -carbon of the aromatic ring is the attacked site of Br atom, the sequence of 1,2-Br shift and proton elimination differentiate the two pathways. The most preferred pathway out of four is Path1 shown in **Figure S3**. The total barrier height is 39.6 kcal/mol which makes this way far less favorable than the substitution mechanism.

On the basis of the experimental observations, a plausible free radical mechanism to rationalize the remote-halogenation is presented in **Scheme S1**. First, an intermolecular SET from Rh(III) complex **K** to NBS leads to the formation of Rh(IV) complex **L** and a Br radical. Then, a nucleophilic addition of Br radical to intermediate **L** generates the intermediate **M**. Finally, abstraction a proton of **M** with pyrrolidine-2,5-dione anion and ligand exchange provides product **L** along with the regeneration of intermediate **K**.

Scheme S1 The plausible mechanism of Rh catalyzed remote bromination .



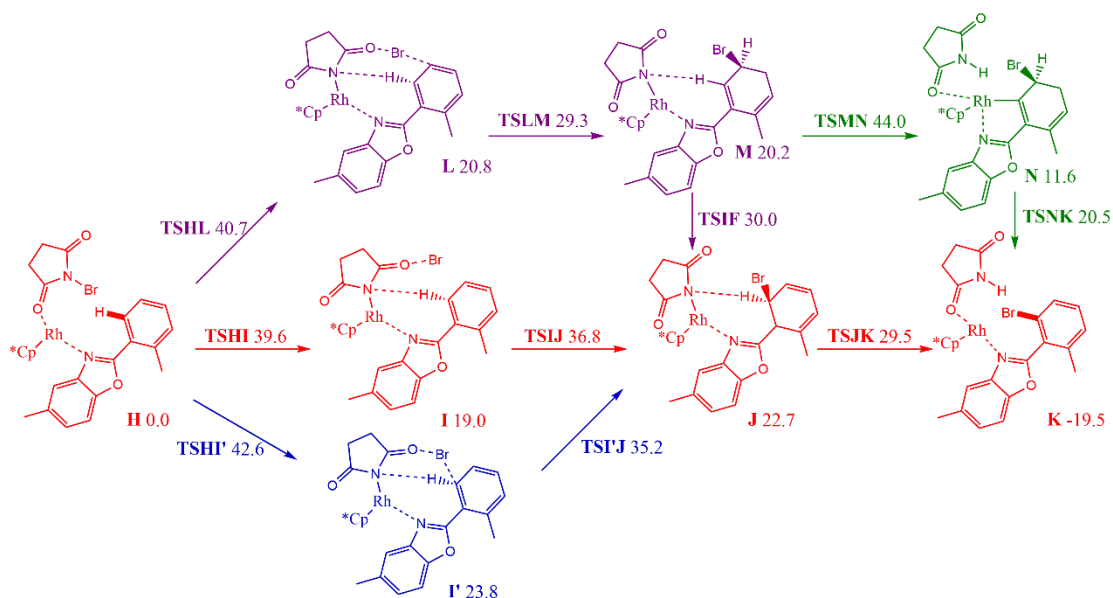


Figure S2. Free-energy reaction profiles (kcal mol⁻¹) of four pathways for the ortho-bromination reaction, calculated at the SMD (dichloroethane) B3LYP/6-31G(d)/LanI2DZ level. Path1 in red, Path2 in blue, Path3 in purple and Path4 in green.

Electrophilic-aromatic-substitution-like (SEAr-like) reaction mechanism was examined theoretically as well, and four pathways (Path1-4) were located (**Figure S2**). The reaction of an electrophilic Br with an electron-rich, nucleophilic aromatic ring is involved in the C-H bond cleavage. And the rate-determining steps are activation of Br atom except Path4. Br adds to α -carbon of aromatic ring attached to benzo[*d*]oxazole via different intermediates (**I** and **I'**) in Path1 and Path2. However, in Path3 and Path4, β -carbon of the aromatic ring is the attacked site of Br atom, the sequence of 1,2-Br shift and proton elimination differentiate the two pathways. The most preferred pathway out of the four paths is Path1 shown in **Figure S3**. The total barrier height is 39.6 kcal/mol, which makes this way far less favorable than the substitution mechanism.

In Path1, firstly NBS and benzo[*d*]oxazole coordinate with Rh(III) cation to form complex **H** with one O atom of NBS and N atom of benzo[*d*]oxazole. Transformation from **H** to **I** makes the Br atom more positive charged (from 0.283 e in **H** to 0.309 e in **I** out of NBO analysis). Then partially positive charged Br' s electrophilic attack to α -carbon of aromatic

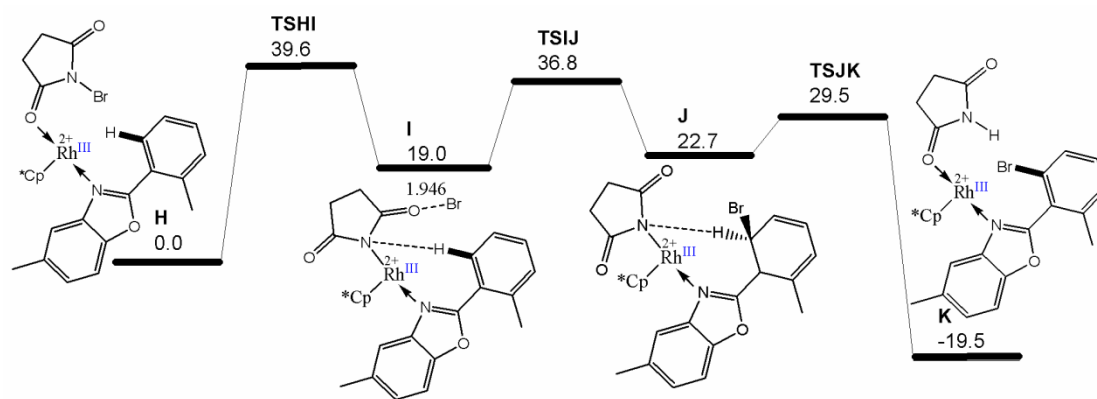


Figure S3. Free-energy reaction profile (kcal mol⁻¹) for the ortho-halogenation reaction (Path1), calculated at the SMD (dichloroethane) B3LYP/6-31G(d)/Lanl2DZ level.

ring attached to benzo[*d*]oxazole gives intermediate **J**. Finally, elimination of α -proton of the aromatic ring assisted by 2,5-dioxo-pyrrolidine anion results in the Rh(III) cation complex **K** coordinated with 2,5-dioxo-pyrrolidine and the product via **TSJK**. The optimized structures of **TSHI**, **TSIJ** and **TSJK** are shown in **Figure S4**. The electrophilic attack and the elimination of proton of the last two steps of this pathway is similar with S_EAr reaction. In this pathway, the activation of Br atom in the first step is the rate-determining step with the barrier of 39.6 kcal/mol. Path2 is very similar with Path1 with a shared intermediate **F**, the difference is that **H** via a higher barrier **TSHI'** (the relative free energy is 42.6 kcal/mol) transformed to a less stable intermediate **I'** (23.8 kcal/mol), which is converted to **J** via **TSI' J** (35.2 kcal/mol). The total barrier is higher than that of the preferred Path1 by 3 kcal/mol. Path3 also has the same intermediate **J**, while it is formed from electrophilic 1,2-Br shift of another intermediate **M** in which Br is added to β -carbon of the aromatic ring attached to benzo[*d*]oxazole. In this pathway, **M** is obtained through a two-step process via **TSHL** (40.7 kcal/mol) and **TSLM** (29.3 kcal/mol). Thus, the total barrier of Path3 is 40.7, higher than that of Path1, so Path3 is disfavored as well. The sequence of 1,2-Br shift and proton elimination differentiate Path3 and Path4. In Path3, proton elimination follows 1,2-Br shift, while conversely in Path4, 1,2-Br shift follows proton elimination. The rate-determining step in Path4 is the proton-elimination step, and the total barrier is 45.2 kcal/mol.

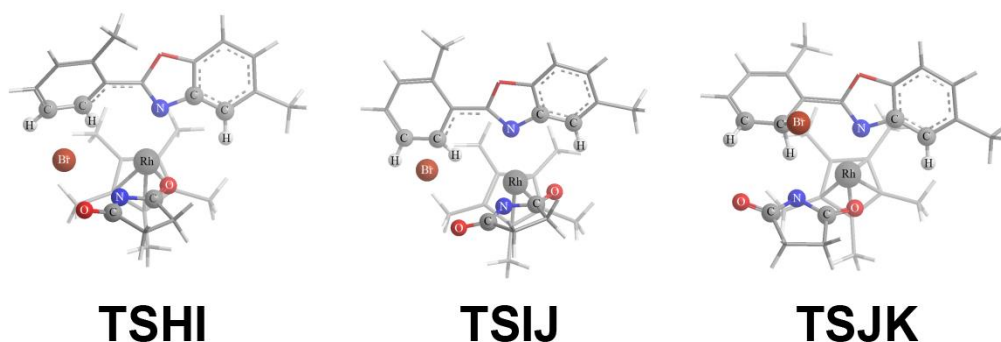


Figure S4. The optimized structures of **TSHI**, **TSIJ** and **TSJK** at the SMD (dichloroethane) B3LYP/6-31G(d)/Lan12DZ level

Table S3. Coordinate data sets and free energies for DFT optimized complexes at the SMD (Dimethylsulfoxide) B3LYP/6-31G(d) /Lan12DZ level.

| | | | | | | |
|----------|---------------------|--|----|-------------|-------------|-------------|
| | | | C | -1.93988600 | 2.04997600 | -4.01529600 |
| A | -1581.071852 | | C | -2.53975300 | 2.62600100 | -2.89464900 |
| | | | C | -2.42196400 | 1.90668300 | -1.71706700 |
| | | | H | 1.72396200 | -2.33375400 | 2.53861900 |
| | | | H | 1.39905100 | -4.02547600 | 2.94047700 |
| | | | H | 0.56776300 | -2.73382000 | 3.82495400 |
| | | | H | 2.02100900 | -2.29163700 | 0.11355800 |
| | | | H | 1.98338700 | -4.05521500 | 0.00538000 |
| | | | H | 1.38009700 | -3.07795900 | -1.34353700 |
| | | | H | -1.75077900 | -4.48477300 | -1.91503300 |
| | | | H | -2.28588200 | -2.80994600 | -2.04793100 |
| | | | H | -0.58518200 | -3.22357600 | -2.34317900 |
| | | | H | -3.89710100 | -4.45029300 | 0.48094900 |
| | | | H | -4.26486400 | -2.94882000 | 1.34818500 |
| | | | H | -3.98261400 | -2.92003600 | -0.40535900 |
| | | | H | -2.41413500 | -4.58542600 | 3.45573100 |
| | | | H | -1.60073000 | -3.22369300 | 4.23214900 |
| | | | H | -3.18699800 | -2.99621700 | 3.46584800 |
| | | | H | -1.78508100 | -1.00862600 | 4.22874200 |
| | | | H | -2.92164400 | 0.69531600 | 5.59439400 |
| | | | H | -3.96753500 | 2.67169200 | 4.54069800 |
| | | | H | -3.28675000 | 4.00875500 | 1.44374000 |
| | | | H | -4.78637600 | 3.12335900 | 1.18407300 |
| | | | H | -4.51560700 | 3.96713400 | 2.71918000 |
| | | | H | -0.62267600 | -0.82372400 | -2.69041600 |
| | | | H | -2.00022500 | 2.57218900 | -4.96634100 |
| | | | H | -3.05995100 | 3.57666300 | -2.94076700 |
| | | | Rh | -1.22623900 | -1.29817300 | 1.02817300 |
| | | | C | -2.51290400 | 1.22208100 | 0.34399000 |
| | | | C | 0.93810200 | -3.03267800 | 2.84081300 |
| | | | C | 1.43317800 | -3.14026200 | -0.25368900 |
| | | | C | -1.45616700 | -3.44408600 | -1.72135500 |
| | | | C | -3.66840600 | -3.37609900 | 0.53775500 |
| | | | C | -2.22389600 | -3.50577400 | 3.37989400 |
| | | | Br | 2.03742200 | 2.43059400 | 3.20744800 |
| | | | C | -2.16451000 | -0.01515500 | 2.34760800 |
| | | | C | -2.22988200 | -0.15181400 | 3.73452700 |
| | | | C | -2.87395300 | 0.81801400 | 4.51492600 |
| | | | C | -3.46146400 | 1.93487600 | 3.92264000 |
| | | | C | -3.40432600 | 2.13830700 | 2.53739400 |
| | | | C | -2.74077300 | 1.15215300 | 1.77123400 |
| | | | C | -4.03140500 | 3.37394000 | 1.93792900 |
| | | | O | -2.89831300 | 2.23469400 | -0.45944600 |
| | | | N | -1.84537600 | 0.27526600 | -0.28959900 |
| | | | C | -1.75634200 | 0.68108100 | -1.62138400 |
| | | | C | -1.15417800 | 0.11990400 | -2.75041800 |
| | | | C | -1.25109900 | 0.81514600 | -3.96123000 |

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|---|-------------|-------------|-------------|
| N | 3.57900200 | 1.62809400 | 2.39539800 |
| C | 4.88010700 | 2.11196800 | 2.63539100 |
| C | 5.81038500 | 1.22864600 | 1.81994100 |
| C | 4.90909200 | 0.19874300 | 1.11628700 |
| C | 3.48653800 | 0.53065800 | 1.53624400 |
| O | 5.15282400 | 3.04464500 | 3.35236400 |
| O | 2.45750200 | -0.02576400 | 1.21210000 |
| H | 6.36137200 | 1.86490100 | 1.12077100 |
| H | 6.53752200 | 0.77318700 | 2.49866100 |
| H | 4.96730100 | 0.24945200 | 0.02496000 |
| H | 5.12233500 | -0.83282900 | 1.41302900 |
| C | -0.63013800 | 0.25509400 | -5.21991500 |
| H | -1.39671300 | 0.02915600 | -5.97194600 |
| H | 0.06316900 | 0.97265200 | -5.67527800 |
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B -1581.063686

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| C | -1.94303900 | 1.78215600 | 0.34292500 |
| C | -2.45014700 | 3.09553500 | 0.48788100 |
| C | -3.83865800 | 3.24501800 | 0.47120300 |
| C | -4.68017000 | 2.14437900 | 0.31169700 |
| Rh | -1.81748500 | -1.16672100 | 0.09584000 |
| C | -0.55710900 | 1.41826000 | 0.31790400 |
| C | -2.03635100 | -1.28103400 | 2.37313900 |
| C | -0.74202700 | -1.97294500 | 2.28228400 |
| C | -0.91252600 | -3.23958300 | 1.64108300 |
| C | -2.28423300 | -3.38538100 | 1.37040700 |
| C | -3.00223600 | -2.16171000 | 1.84238600 |
| C | -2.26951900 | -0.09327200 | 3.25526200 |
| C | 0.48815500 | -1.50647700 | 2.95418200 |
| C | 0.15100800 | -4.27126400 | 1.44241200 |
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| C | -4.47342100 | -2.10221100 | 2.07258700 |
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| C | -0.25182800 | -0.96868800 | -4.02436700 |
| C | -0.84526900 | -0.36090800 | -2.75335600 |

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| O | -0.44772800 | -3.59627900 | -1.55709200 |
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| C | 1.16986900 | 0.09960300 | 0.07577200 |
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| H | -0.86097700 | 4.18478000 | 1.48915000 |
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| H | 1.08760000 | -2.69341700 | -3.69368500 |
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| H | 0.64387400 | -0.40704500 | -4.30683800 |
| H | -0.98000700 | -0.85559300 | -4.83442000 |
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| H | 4.88146500 | 0.98401600 | -0.39340100 |
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| C | -3.91665800 | 3.38259100 | 0.50666600 |
| Rh | -0.00145100 | -1.05411800 | 0.32636400 |
| C | 0.16239500 | 2.13001900 | 0.00654400 |
| C | -0.32259500 | -0.79112200 | 2.52066900 |
| C | 0.75327800 | -1.72301500 | 2.25303800 |
| C | 0.18639500 | -2.90617000 | 1.61816400 |
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| C | -0.49944300 | 4.34689500 | 1.85733000 |
| O | 1.02858900 | 3.16033600 | -0.18078100 |
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| Br | -2.02514100 | 0.36258400 | -1.67460600 |
| N | 0.69022800 | -1.69018500 | -1.59233600 |
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| C | 1.54028500 | -1.77289000 | -3.84085300 |
| C | 1.20726100 | -0.90494400 | -2.62626100 |
| O | 0.04073500 | -3.91433300 | -1.38113800 |
| O | 1.37316300 | 0.30482500 | -2.60058100 |
| C | 3.26035800 | 0.39835900 | -0.01297800 |
| C | 4.51746300 | 0.99251800 | -0.14514800 |
| C | 4.62344500 | 2.39721600 | -0.30218200 |
| C | 3.51126300 | 3.23511200 | -0.33393500 |
| C | 2.28374900 | 2.60266000 | -0.19331200 |
| C | 2.13623300 | 1.22851500 | -0.03675900 |
| H | -4.43584200 | 1.79898900 | -0.86606500 |
| H | -3.10775200 | 4.83921800 | 1.86037200 |
| H | -4.94190900 | 3.71904900 | 0.62813100 |
| H | -0.40516100 | 0.26533600 | 4.36261900 |
| H | 0.80186800 | 0.89690000 | 3.23836400 |
| H | -0.92515100 | 1.22911500 | 2.97472900 |
| H | 2.85217000 | -2.17846600 | 2.14003300 |
| H | 2.19285100 | -2.01908900 | 3.77393000 |
| H | 2.48530300 | -0.56854900 | 2.80429400 |
| H | 1.91975900 | -3.99318800 | 0.95349900 |
| H | 1.11812400 | -4.63204700 | 2.39208100 |

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| H | 0.39478800 | -4.87756400 | 0.78284900 |
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| H | -1.74166700 | -4.31245300 | 0.14754300 |
| H | -2.68793400 | -4.13473300 | 1.64706700 |
| H | -3.40635200 | -1.22369100 | 2.88110800 |
| H | -2.85348500 | 0.32091800 | 2.21910300 |
| H | -3.46391600 | -0.95721700 | 1.13852400 |
| H | 0.24993200 | 3.67489400 | 2.28655000 |
| H | 0.03308900 | 5.08225200 | 1.24452600 |
| H | -0.97999400 | 4.88488800 | 2.67959100 |
| H | 1.83152000 | -3.93193900 | -3.46797000 |
| H | 0.23018200 | -3.52831200 | -4.08510400 |
| H | 2.62023100 | -1.72406900 | -4.01801600 |
| H | 1.04744000 | -1.35479700 | -4.72412100 |
| H | 3.15975300 | -0.67670800 | 0.08683700 |
| H | 5.61254300 | 2.83564600 | -0.40449900 |
| H | 3.59709300 | 4.30904700 | -0.45869000 |
| C | 5.77140500 | 0.14915100 | -0.13330200 |
| H | 6.32085900 | 0.24437200 | -1.07815400 |
| H | 6.45398000 | 0.46012600 | 0.66731500 |
| H | 5.53805500 | -0.90987400 | 0.01480000 |

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| C | -4.00576200 | 0.97596800 | 0.65298800 |
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| C | -1.75112900 | 1.80996000 | 0.36060400 |
| C | -2.19627300 | 3.15499700 | 0.36204800 |
| C | -3.56915100 | 3.36692600 | 0.51086900 |
| C | -4.46062000 | 2.29899000 | 0.64585900 |
| Rh | -1.80163600 | -1.15567700 | 0.52075200 |
| C | -0.39558600 | 1.37053700 | 0.16308800 |
| C | -2.38713800 | -1.43864200 | 2.64956200 |
| C | -0.99449800 | -1.82619000 | 2.48412400 |
| C | -0.94266900 | -3.08597300 | 1.76305100 |
| C | -2.26557200 | -3.41082500 | 1.40070600 |
| C | -3.17165800 | -2.39044700 | 1.92955700 |
| C | -2.88228800 | -0.38396500 | 3.58887400 |
| C | 0.15934800 | -1.17736100 | 3.17379000 |
| C | 0.26371000 | -3.94934400 | 1.56774000 |
| C | -2.69616700 | -4.65614200 | 0.70107700 |
| C | -4.66054900 | -2.48349100 | 1.89812800 |
| C | -1.25833400 | 4.32718200 | 0.20705800 |
| O | 0.67708100 | 2.15968400 | -0.04808200 |
| N | -0.10751200 | 0.08164900 | 0.13931400 |

| | | | |
|----|-------------|-------------|-------------|
| Br | -3.70758600 | -1.88171500 | -1.61053200 |
| N | -1.50782600 | -1.46456000 | -1.91307600 |
| C | -0.66080300 | -2.53634600 | -2.22574600 |
| C | 0.24364000 | -2.11325400 | -3.37680900 |
| C | -0.10673100 | -0.64425700 | -3.64330700 |
| C | -1.32887500 | -0.36069700 | -2.77487300 |
| O | -0.64980000 | -3.60946300 | -1.65518100 |
| O | -2.01999600 | 0.63294900 | -2.80256600 |
| C | 2.12533200 | -1.10264200 | -0.28086800 |
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| C | 1.74087400 | 1.29108800 | -0.22815500 |
| C | 1.26051400 | -0.01744500 | -0.11657300 |
| H | -4.72046700 | 0.16653500 | 0.75870700 |
| H | -3.94619400 | 4.38575700 | 0.51577800 |
| H | -5.52432500 | 2.49938900 | 0.74852800 |
| H | -2.98212700 | -0.82157200 | 4.59183100 |
| H | -2.18642300 | 0.45536700 | 3.66293000 |
| H | -3.85883600 | 0.00412700 | 3.29403400 |
| H | 1.09836400 | -1.34142400 | 2.64026300 |
| H | 0.26260800 | -1.62043300 | 4.17479900 |
| H | 0.00609400 | -0.10325800 | 3.30315900 |
| H | 1.19250400 | -3.37991600 | 1.65120100 |
| H | 0.28815000 | -4.72612200 | 2.34535500 |
| H | 0.24520300 | -4.45034100 | 0.59723500 |
| H | -3.72122200 | -4.58562800 | 0.33234200 |
| H | -2.03271500 | -4.88749700 | -0.13455000 |
| H | -2.65416900 | -5.49412900 | 1.41179600 |
| H | -4.99100800 | -3.35873500 | 2.47374900 |
| H | -5.13145800 | -1.59879700 | 2.33151100 |
| H | -5.04014300 | -2.61553400 | 0.87704800 |
| H | -0.48183500 | 4.33247100 | 0.98066800 |
| H | -0.74489800 | 4.30876500 | -0.76139200 |
| H | -1.81374900 | 5.26696800 | 0.27724000 |
| H | 1.28734300 | -2.28083300 | -3.09870300 |
| H | 0.01868700 | -2.76267800 | -4.23027300 |
| H | 0.69338300 | 0.04142700 | -3.34641400 |
| H | -0.35982000 | -0.42743400 | -4.68492100 |
| H | 1.76396800 | -2.12312200 | -0.21770700 |
| H | 4.97278800 | 0.69015000 | -0.84467900 |
| H | 3.41438200 | 2.62224600 | -0.57228800 |
| C | 4.46061700 | -1.96341200 | -0.71869700 |
| H | 4.97631800 | -1.89432700 | -1.68406700 |

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|---|------------|-------------|-------------|
| H | 5.23373200 | -1.93809600 | 0.05955600 |
| H | 3.96486600 | -2.93761500 | -0.66767200 |

TSBC -1581.03122

| | | | |
|----|-------------|-------------|-------------|
| C | -4.26172600 | 1.05776400 | 0.76042900 |
| C | -2.97079800 | 0.85593300 | 0.30097800 |
| C | -2.00025800 | 1.87466200 | 0.29779200 |
| C | -2.37460200 | 3.17899000 | 0.74222300 |
| C | -3.67891400 | 3.37146700 | 1.20016300 |
| C | -4.59936300 | 2.32564500 | 1.23950200 |
| Rh | -1.62933700 | -1.30342000 | 0.20578200 |
| C | -0.63274600 | 1.49505000 | 0.03774700 |
| C | -2.25239100 | -1.38871500 | 2.42027000 |
| C | -0.92110400 | -1.90790700 | 2.25254000 |
| C | -0.99562000 | -3.12216500 | 1.46977000 |
| C | -2.37477000 | -3.32397100 | 1.10209900 |
| C | -3.14316700 | -2.27119800 | 1.71170600 |
| C | -2.61890700 | -0.29200700 | 3.36557000 |
| C | 0.29148900 | -1.40181400 | 2.95841700 |
| C | 0.14321600 | -4.07137200 | 1.30556300 |
| C | -2.99990600 | -4.52726600 | 0.47181000 |
| C | -4.63290500 | -2.24905800 | 1.73653400 |
| C | -1.40844700 | 4.33958600 | 0.77336000 |
| O | 0.34639000 | 2.38166600 | -0.22000800 |
| N | -0.20284200 | 0.25558700 | 0.11500400 |
| Br | -3.49757000 | -0.58183500 | -1.62182200 |
| N | -0.67605700 | -1.87347700 | -1.64976800 |
| C | -0.55326500 | -3.17547300 | -2.10059000 |
| C | 0.04204500 | -3.20200600 | -3.50614200 |
| C | 0.22022800 | -1.73163000 | -3.86870900 |
| C | -0.31776200 | -0.97276300 | -2.65673200 |
| O | -0.87367500 | -4.18504500 | -1.48689600 |
| O | -0.41229700 | 0.24425800 | -2.61512400 |
| C | 2.16190300 | -0.69117300 | -0.18356400 |
| C | 3.47492400 | -0.28467100 | -0.44187300 |
| C | 3.76807200 | 1.08734700 | -0.63424400 |
| C | 2.78973400 | 2.07888100 | -0.57905600 |
| C | 1.50256200 | 1.63400900 | -0.32371300 |
| C | 1.17151300 | 0.29346600 | -0.12280000 |
| H | -5.01895200 | 0.28931800 | 0.70262800 |
| H | -3.97384400 | 4.35971400 | 1.53947700 |
| H | -5.61071100 | 2.49744000 | 1.59732600 |
| H | -2.54909800 | -0.67496100 | 4.39298900 |
| H | -1.93266900 | 0.55597900 | 3.28516400 |

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|---|-------------|-------------|-------------|
| H | -3.63676700 | 0.06575900 | 3.21009100 |
| H | 1.21187000 | -1.65551000 | 2.42958200 |
| H | 0.33375500 | -1.87487900 | 3.95014100 |
| H | 0.25199900 | -0.32054600 | 3.10992200 |
| H | 1.06465100 | -3.55324700 | 1.02297200 |
| H | 0.32919600 | -4.55146800 | 2.27723500 |
| H | -0.06883700 | -4.83463200 | 0.56109400 |
| H | -3.63542300 | -4.25203900 | -0.37555100 |
| H | -2.25327300 | -5.23402100 | 0.11866000 |
| H | -3.64099200 | -5.02048600 | 1.21519400 |
| H | -4.97223300 | -3.07861000 | 2.37338400 |
| H | -5.03032600 | -1.32528000 | 2.15519600 |
| H | -5.06173500 | -2.41588500 | 0.74414000 |
| H | -0.55901600 | 4.14912100 | 1.43908800 |
| H | -0.99898700 | 4.55632500 | -0.21806000 |
| H | -1.92492500 | 5.23373300 | 1.13266000 |
| H | 0.97792900 | -3.76980800 | -3.48273400 |
| H | -0.64754300 | -3.73676400 | -4.16727900 |
| H | 1.26459600 | -1.44198800 | -4.02675600 |
| H | -0.34250000 | -1.42265100 | -4.75512700 |
| H | 1.92255900 | -1.73967300 | -0.04643300 |
| H | 4.79582400 | 1.37764600 | -0.83500300 |
| H | 3.01764400 | 3.12816200 | -0.73218600 |
| C | 4.59025800 | -1.30116700 | -0.51635200 |
| H | 5.13160900 | -1.22652600 | -1.46710900 |
| H | 5.32472500 | -1.14409100 | 0.28371000 |
| H | 4.20642000 | -2.32187600 | -0.42443300 |

TSAC -1581.039301

| | | | |
|----|-------------|-------------|-------------|
| C | -1.33674000 | -2.97107700 | 2.49002200 |
| C | -0.03429900 | -3.07419300 | 1.91997700 |
| C | -0.17338900 | -3.11079700 | 0.46645700 |
| C | -1.57768900 | -3.04370500 | 0.15537000 |
| C | -2.30167500 | -2.92132100 | 1.39869100 |
| Rh | -0.98080000 | -1.19689900 | 1.19773000 |
| C | -2.11215000 | 1.33899900 | 0.26918200 |
| C | 1.26393300 | -3.17970400 | 2.64550200 |
| C | 0.95885000 | -3.28499500 | -0.48504900 |
| C | -2.18954200 | -3.13453800 | -1.20317100 |
| C | -3.78377400 | -2.88927000 | 1.55270400 |
| C | -1.67746800 | -2.99810800 | 3.94384000 |
| Br | 0.61332200 | 0.74645500 | 2.16097500 |
| C | -1.52916900 | 0.73840600 | 2.56112000 |
| C | -1.83698800 | 0.60118600 | 3.91722300 |

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|---|-------------|-------------|-------------|
| C | -3.04137700 | 1.10928800 | 4.40571700 |
| C | -3.92006300 | 1.77447900 | 3.55034900 |
| C | -3.65429000 | 1.92759900 | 2.18023100 |
| C | -2.44374100 | 1.39445500 | 1.68905700 |
| C | -4.66168600 | 2.61949300 | 1.29395300 |
| O | -2.43936800 | 2.29305700 | -0.62350600 |
| N | -1.43453000 | 0.34127800 | -0.24921300 |
| C | -1.25648700 | 0.64442400 | -1.59914800 |
| C | -0.59344700 | -0.01003600 | -2.64048400 |
| C | -0.60861500 | 0.59139800 | -3.90222500 |
| C | -1.27938000 | 1.82546800 | -4.09053900 |
| C | -1.93708100 | 2.49352500 | -3.05875100 |
| C | -1.89881800 | 1.86594500 | -1.82346900 |
| H | 2.05360500 | -2.62534300 | 2.12818900 |
| H | 1.56036200 | -4.23772100 | 2.68301500 |
| H | 1.18516100 | -2.81578900 | 3.67261800 |
| H | 1.79532600 | -2.62755400 | -0.22345300 |
| H | 1.31954300 | -4.32195600 | -0.42507200 |
| H | 0.65616800 | -3.09417200 | -1.51719300 |
| H | -2.42070500 | -4.18710800 | -1.41702600 |
| H | -3.12325900 | -2.57001200 | -1.26504500 |
| H | -1.51052800 | -2.77618100 | -1.97913800 |
| H | -4.15132600 | -3.91792400 | 1.67790900 |
| H | -4.08777400 | -2.32085700 | 2.43549100 |
| H | -4.27409000 | -2.46625700 | 0.67239600 |
| H | -1.89472800 | -4.03532900 | 4.23458700 |
| H | -0.84911200 | -2.64634400 | 4.56299400 |
| H | -2.56397700 | -2.40062700 | 4.16795600 |
| H | -1.13111400 | 0.13133300 | 4.59426500 |
| H | -3.28573300 | 1.00641500 | 5.45902600 |
| H | -4.84580000 | 2.18144600 | 3.94677600 |
| H | -4.27045300 | 3.56821500 | 0.90991400 |
| H | -4.93323200 | 2.00605400 | 0.42746800 |
| H | -5.57431800 | 2.83425400 | 1.85653700 |
| H | -0.07461600 | -0.94805700 | -2.47217800 |
| H | -1.27500600 | 2.27259600 | -5.08091800 |
| H | -2.43958600 | 3.44255000 | -3.21022600 |
| N | 2.99358700 | 0.80854900 | 1.71005000 |
| C | 3.75059800 | -0.15863200 | 1.11916500 |
| C | 5.19763000 | 0.33234000 | 0.94902500 |
| C | 5.18220000 | 1.74249000 | 1.54661200 |
| C | 3.72183400 | 1.94252200 | 1.98564700 |
| O | 3.36583100 | -1.27679600 | 0.76197100 |
| O | 3.28406700 | 2.96359200 | 2.50504500 |

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|---|-------------|-------------|-------------|
| H | 5.87379100 | -0.35865600 | 1.46386300 |
| H | 5.45883400 | 0.30942200 | -0.11465500 |
| H | 5.83631000 | 1.85604600 | 2.41786100 |
| H | 5.45408100 | 2.52759500 | 0.83309400 |
| C | 0.08248000 | -0.06510500 | -5.07421700 |
| H | -0.63531500 | -0.31916100 | -5.86426600 |
| H | 0.82722100 | 0.60440400 | -5.52111400 |
| H | 0.59312500 | -0.98467400 | -4.77291800 |

D-*o*Me -1473.830875

| | | | |
|----|-------------|-------------|-------------|
| Rh | 0.74104900 | -0.83036000 | 0.00688800 |
| N | 1.43158200 | 0.20890300 | 1.78719600 |
| N | -0.80918400 | -1.55090600 | 1.32564200 |
| C | 1.77240500 | 0.71930900 | 2.76763000 |
| C | 0.69262400 | 4.99185800 | -0.66787300 |
| C | 1.75939600 | 4.06696500 | -0.56032600 |
| C | 1.49120000 | 2.69898000 | -0.44758600 |
| C | 0.15535200 | 2.28612200 | -0.44978800 |
| C | 0.79141900 | -2.20861700 | -1.73591400 |
| C | 1.61543600 | -1.06707400 | -2.05745800 |
| C | 2.66979500 | -0.98831600 | -1.08834600 |
| C | 2.53124100 | -2.12245000 | -0.18105800 |
| C | 1.39236300 | -2.87825600 | -0.59476500 |
| C | -0.30808400 | -2.77383800 | -2.57419100 |
| C | 1.41658200 | -0.15181000 | -3.21768200 |
| C | 3.83085000 | -0.04969400 | -1.09906700 |
| C | 3.48851300 | -2.48416500 | 0.90574300 |
| C | 0.92382000 | -4.16185300 | 0.00294700 |
| C | -1.49987800 | -2.01590700 | 2.12856000 |
| C | -2.37791300 | -2.59461700 | 3.13119000 |
| C | 2.19915300 | 1.37172300 | 3.99411700 |
| C | -0.86270800 | 3.23221500 | -0.54664800 |
| C | -0.64315500 | 4.59729100 | -0.65984800 |
| N | -0.45360200 | 1.02150500 | -0.35178600 |
| C | -1.75161100 | 1.24528900 | -0.38985600 |
| O | -2.06072200 | 2.56137500 | -0.50622800 |
| C | -2.89113700 | 0.31763000 | -0.36256400 |
| C | -2.93346800 | -0.71891900 | -1.30618800 |
| C | -4.01405200 | -1.59719600 | -1.34772700 |
| C | -5.05810600 | -1.44024400 | -0.43465100 |
| C | -5.01925700 | -0.40439700 | 0.50130500 |
| C | -3.95062400 | 0.49958500 | 0.55827400 |
| C | 3.18364400 | 4.57131100 | -0.56966700 |
| H | 0.92644400 | 6.04945300 | -0.75532100 |

| | | | |
|---|-------------|-------------|-------------|
| H | 2.29872700 | 1.98462000 | -0.35197300 |
| H | -0.72463300 | -2.03211200 | -3.25848900 |
| H | -1.11344900 | -3.19043100 | -1.96396800 |
| H | 0.10165500 | -3.59257600 | -3.18170100 |
| H | 1.91849700 | -0.58382100 | -4.09461200 |
| H | 1.84920200 | 0.83458000 | -3.03815200 |
| H | 0.35894800 | -0.03514000 | -3.46621600 |
| H | 4.08505300 | 0.29324900 | -0.09221500 |
| H | 3.65200100 | 0.81577800 | -1.73911900 |
| H | 4.70775300 | -0.58199800 | -1.49232700 |
| H | 2.99326400 | -3.01162300 | 1.72476200 |
| H | 3.99778500 | -1.60447700 | 1.30618900 |
| H | 4.25569900 | -3.15379100 | 0.49309500 |
| H | 1.45246000 | -4.98874400 | -0.49137700 |
| H | -0.14681800 | -4.31570300 | -0.14960500 |
| H | 1.14626700 | -4.21836300 | 1.07132900 |
| H | -2.13473800 | -3.65327800 | 3.26678600 |
| H | -3.41852700 | -2.50069100 | 2.80592600 |
| H | -2.24618100 | -2.06894600 | 4.08233000 |
| H | 2.21325800 | 0.64541400 | 4.81300700 |
| H | 1.50374900 | 2.18083300 | 4.23881100 |
| H | 3.20341100 | 1.78654800 | 3.86110900 |
| H | -1.45943600 | 5.30752400 | -0.73575300 |
| H | -2.12653800 | -0.81296000 | -2.02278300 |
| H | -4.04446500 | -2.38834600 | -2.09116000 |
| H | -5.83669400 | -0.28887800 | 1.20813200 |
| H | 3.89647400 | 3.76228900 | -0.38231100 |
| H | 3.33639000 | 5.34220400 | 0.19507400 |
| H | 3.43684500 | 5.02522400 | -1.53614400 |
| H | -5.90666100 | -2.11865000 | -0.45233500 |
| C | -3.96101400 | 1.60708400 | 1.58507600 |
| H | -2.98736100 | 1.72680200 | 2.07408700 |
| H | -4.21622600 | 2.57152100 | 1.13069100 |
| H | -4.70473700 | 1.39905400 | 2.35995700 |

D-*p*Me -1473.836562

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|----|-------------|-------------|-------------|
| Rh | 0.49590400 | -1.02871900 | 0.02002000 |
| N | 1.84412700 | -0.43429500 | 1.63352500 |
| N | -0.92246800 | -1.12709300 | 1.65196300 |
| C | 2.50863000 | -0.22657800 | 2.55719900 |
| C | 2.69024000 | 4.34877800 | -0.45274700 |
| C | 3.29113300 | 3.06753700 | -0.44943800 |
| C | 2.49471300 | 1.92069100 | -0.36832600 |
| C | 1.10621700 | 2.07868700 | -0.29428100 |

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|---|-------------|-------------|-------------|
| C | -2.20552800 | 2.19344300 | -0.16103000 |
| C | -3.00435400 | 1.20385900 | -0.74941100 |
| C | -4.38694600 | 1.35749500 | -0.80560800 |
| C | -5.01267400 | 2.49411200 | -0.27265000 |
| C | -4.20301600 | 3.48074300 | 0.31708300 |
| C | -2.82140600 | 3.34414500 | 0.36949300 |
| C | -6.50905600 | 2.66590500 | -0.32969300 |
| H | 4.48565400 | 3.74882500 | -0.01714900 |
| H | 2.67621300 | -0.16540000 | -0.29502800 |
| H | -3.35213500 | -1.34464000 | -2.35980700 |
| H | -3.70448200 | -2.06579900 | -0.76936100 |
| H | -3.47772800 | -3.09907400 | -2.18290500 |
| H | -0.63265300 | -1.34955400 | -4.23648100 |
| H | 0.12663900 | -0.05847200 | -3.29783800 |
| H | -1.64231200 | -0.24036300 | -3.29434700 |
| H | 2.80426700 | -2.22914300 | -1.49928200 |
| H | 2.11787000 | -1.03487500 | -2.62373500 |
| H | 2.14708400 | -2.74929400 | -3.05553400 |
| H | 0.93945800 | -4.36306300 | 1.11694000 |
| H | 2.27736200 | -3.63564900 | 0.19286700 |
| H | 1.41055700 | -5.03698800 | -0.44923100 |
| H | -2.12937300 | -5.05848500 | -0.07460500 |
| H | -2.83952800 | -3.66190000 | 0.74649200 |
| H | -1.33766800 | -4.38950800 | 1.36101600 |
| H | -4.42533000 | -0.92262700 | 3.35108300 |
| H | -3.75510200 | 0.71750800 | 3.57000400 |
| H | -3.04757900 | -0.66213300 | 4.45682100 |
| H | 1.79432100 | -1.62843200 | 4.71511300 |
| H | 2.61165700 | -0.11983300 | 4.21896600 |
| H | 3.30523900 | -1.70173500 | 3.76666000 |
| H | 2.25767400 | 4.82958400 | 0.06040900 |
| H | -2.53124200 | 0.32619700 | -1.16957500 |
| H | -4.99149700 | 0.58667400 | -1.27632800 |
| H | -4.66600600 | 4.36995500 | 0.73739400 |
| H | -2.21905100 | 4.12230200 | 0.82606100 |
| H | -6.78045700 | 3.57061900 | -0.88803300 |
| H | -6.93233500 | 2.77550300 | 0.67669200 |
| H | -6.99402200 | 1.81177500 | -0.81202800 |
| C | 5.17533000 | 1.12435800 | -0.19543500 |
| C | 5.92099300 | 1.50895300 | 1.10447700 |
| H | 6.93951900 | 1.10269600 | 1.08797800 |
| H | 5.99894600 | 2.59428600 | 1.22816800 |
| H | 5.41044000 | 1.10598700 | 1.98765700 |
| C | 5.94464700 | 1.69364000 | -1.41075000 |

| | | | |
|---|------------|-------------|-------------|
| H | 6.95962300 | 1.27924400 | -1.44121600 |
| H | 5.44491500 | 1.43518200 | -2.35205300 |
| H | 6.03422200 | 2.78423600 | -1.36552800 |
| C | 5.17153400 | -0.41143200 | -0.30734100 |
| H | 4.66664600 | -0.88402900 | 0.54407400 |
| H | 4.68726800 | -0.75423400 | -1.22880600 |
| H | 6.20374000 | -0.77864600 | -0.32183800 |

D-Cl -1483.667369

| | | | |
|----|-------------|-------------|-------------|
| Rh | 0.14074500 | -1.15227000 | -0.01464200 |
| N | 1.58845500 | -0.95383200 | 1.58354100 |
| N | -1.27941100 | -1.00589600 | 1.65759000 |
| C | 2.29064200 | -0.92831700 | 2.50241400 |
| C | 3.39375000 | 3.74727000 | -0.19720100 |
| C | 3.69226200 | 2.37580800 | -0.26872700 |
| C | 2.71962300 | 1.37856700 | -0.26228900 |
| C | 1.39309700 | 1.80919800 | -0.17998600 |
| C | -1.07318700 | -2.51362600 | -1.31693400 |
| C | -0.32382300 | -1.63514100 | -2.16038000 |
| C | 1.08768600 | -1.83993000 | -1.88233300 |
| C | 1.19576900 | -2.90705100 | -0.91561100 |
| C | -0.13103700 | -3.28184900 | -0.51256300 |
| C | -2.55040900 | -2.72252300 | -1.30856000 |
| C | -0.85935700 | -0.71184200 | -3.20207600 |
| C | 2.21084500 | -1.23682300 | -2.65985000 |
| C | 2.46651300 | -3.52181200 | -0.43807300 |
| C | -0.49923700 | -4.37591000 | 0.43548700 |
| C | -1.94498700 | -1.00835800 | 2.60347300 |
| C | -2.79278300 | -1.00081100 | 3.78347200 |
| C | 3.18201400 | -0.88156100 | 3.64854000 |
| C | 1.10840000 | 3.17408800 | -0.11412600 |
| C | 2.06780000 | 4.17353500 | -0.11803600 |
| N | 0.17380600 | 1.11596400 | -0.14595000 |
| C | -0.76234300 | 2.04706300 | -0.08027700 |
| O | -0.25310900 | 3.30866900 | -0.05284200 |
| C | -2.21454100 | 1.95758000 | -0.05610700 |
| C | -2.87826100 | 0.76657200 | -0.38537500 |
| C | -4.26840700 | 0.71228200 | -0.38336000 |
| C | -5.03864900 | 1.83759000 | -0.05298500 |
| C | -4.36561700 | 3.02641000 | 0.27834200 |
| C | -2.97855600 | 3.09550400 | 0.27457700 |
| C | -6.54420600 | 1.78620000 | -0.06994700 |
| H | 4.19700000 | 4.47575500 | -0.20521200 |
| H | 2.98229700 | 0.33154400 | -0.31891400 |

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | -3.08645400 | -1.92205300 | -1.82125300 | C | 0.18377600 | -3.13163200 | -0.69010200 |
| H | -2.93865000 | -2.82107900 | -0.29079800 | C | -1.52274500 | -2.19279000 | -2.44257400 |
| H | -2.76944600 | -3.66238500 | -1.83402200 | C | 1.01780000 | -0.47120900 | -3.24345700 |
| H | -0.78177300 | -1.20622700 | -4.18032600 | C | 3.50039700 | -1.52855000 | -1.48806100 |
| H | -0.27742900 | 0.21249000 | -3.25625000 | C | 2.41928700 | -3.73186400 | 0.52335800 |
| H | -1.90838800 | -0.46328500 | -3.03331500 | C | -0.70863400 | -4.13638500 | -0.04422200 |
| H | 3.14893500 | -1.24433100 | -2.10072500 | C | -1.44408400 | -1.34422700 | 2.68112700 |
| H | 1.98766500 | -0.21020400 | -2.95976800 | C | -2.23025500 | -1.50930300 | 3.89171700 |
| H | 2.36226000 | -1.82543800 | -3.57548100 | C | 3.47857900 | 0.11971200 | 3.62936400 |
| H | 2.35392500 | -3.98806500 | 0.54278900 | C | 0.42754700 | 3.33561900 | -0.31314100 |
| H | 3.28572000 | -2.79971200 | -0.40296500 | C | 1.12162400 | 4.52762600 | -0.45167900 |
| H | 2.75123500 | -4.30822600 | -1.15140500 | N | 0.00208900 | 1.12156400 | -0.18036300 |
| H | -0.55618000 | -5.32675100 | -0.11162100 | C | -1.11974000 | 1.81262400 | -0.05082900 |
| H | -1.47556800 | -4.19599200 | 0.89191400 | O | -0.91870900 | 3.15641700 | -0.11914000 |
| H | 0.24274700 | -4.49089800 | 1.22982300 | C | -2.50265200 | 1.40542200 | 0.13592000 |
| H | -3.72437500 | -1.53516000 | 3.57120800 | C | -2.95111700 | 0.10948200 | -0.18338300 |
| H | -3.02414600 | 0.03232900 | 4.06138300 | C | -4.28068000 | -0.23912600 | -0.02558000 |
| H | -2.27546700 | -1.49236000 | 4.61333900 | C | -5.20912400 | 0.69967400 | 0.46373900 |
| H | 2.69619100 | -1.34606500 | 4.51246100 | C | -4.77708300 | 1.99816000 | 0.78351300 |
| H | 3.42053200 | 0.16067200 | 3.88372800 | C | -3.44070600 | 2.34145000 | 0.61276900 |
| H | 4.10613800 | -1.42198400 | 3.41963200 | C | 4.63891000 | 3.09070200 | -0.90965500 |
| H | 1.80709500 | 5.22462500 | -0.06431200 | H | 3.09232500 | 5.30581000 | -0.76448200 |
| H | -2.29444200 | -0.10737700 | -0.64045300 | H | 2.89543700 | 1.00747400 | -0.59570900 |
| H | -4.76784700 | -0.21717500 | -0.64350700 | H | -1.77946500 | -1.20405100 | -2.82983900 |
| H | -4.94074800 | 3.91042700 | 0.54135700 | H | -2.33952700 | -2.55147700 | -1.81245100 |
| H | -2.48588700 | 4.02610300 | 0.53361600 | H | -1.44689300 | -2.87440500 | -3.30154400 |
| H | -6.94253100 | 2.34471700 | -0.92740300 | H | 1.16435800 | -1.00929100 | -4.19025500 |
| H | -6.96788600 | 2.24233400 | 0.83223700 | H | 1.84388500 | 0.23329500 | -3.12674300 |
| H | -6.90991400 | 0.75746400 | -0.14255400 | H | 0.08452000 | 0.09163400 | -3.32397000 |
| Cl | 5.38454700 | 1.89092400 | -0.37040400 | H | 3.99960800 | -1.40853600 | -0.52323400 |

D-*p*OMe -1549.5371102

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|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| Rh | 0.53347700 | -1.04107200 | 0.03287600 | H | 3.62257600 | -0.61526800 | -2.07266400 |
| N | 1.91665000 | -0.41629300 | 1.60858300 | H | 4.01607400 | -2.33872200 | -2.02219900 |
| N | -0.82931200 | -1.20317200 | 1.71176700 | H | 1.85185300 | -4.05485200 | 1.39997500 |
| C | 2.60660500 | -0.18067400 | 2.50661900 | H | 3.29100000 | -3.16446700 | 0.85827800 |
| C | 2.49584800 | 4.40493700 | -0.64852000 | H | 2.78356400 | -4.63173800 | 0.00938400 |
| C | 3.14310600 | 3.14822400 | -0.70243100 | H | -0.75020600 | -5.02925000 | -0.68338300 |
| C | 2.40142500 | 1.97021800 | -0.55905200 | H | -1.72926300 | -3.76172300 | 0.06615300 |
| C | 1.02047000 | 2.07566900 | -0.36027900 | H | -0.33358000 | -4.44309700 | 0.93453900 |
| C | -0.21340500 | -2.19677700 | -1.72358900 | H | -2.94269400 | -2.32977100 | 3.75980800 |
| C | 0.96668400 | -1.46497800 | -2.13244800 | H | -2.77820600 | -0.58500400 | 4.10131500 |
| C | 2.06650800 | -1.90945000 | -1.33182500 | H | -1.56878400 | -1.73693700 | 4.73360100 |
| C | 1.57565800 | -2.93837000 | -0.41971700 | H | 3.14934200 | -0.43833900 | 4.51165700 |
| | | | | H | 3.44257400 | 1.19218100 | 3.84574800 |
| | | | | H | 4.50676100 | -0.16471100 | 3.38420000 |

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|---|-------------|-------------|-------------|
| H | 0.62428900 | 5.49064000 | -0.41081400 |
| H | -2.24847000 | -0.61578300 | -0.56816000 |
| H | -4.63240700 | -1.23362300 | -0.28260200 |
| H | -5.47184400 | 2.73935700 | 1.16042100 |
| H | -3.12293700 | 3.34805800 | 0.86135300 |
| H | 4.99651400 | 2.05769600 | -0.96006600 |
| H | 5.17180000 | 3.59143800 | -0.09156500 |
| H | 4.93201500 | 3.59638000 | -1.83781900 |
| C | -7.47758000 | 1.16091700 | 1.07926900 |
| H | -8.40762800 | 0.59040300 | 1.08900600 |
| H | -7.24187700 | 1.49347400 | 2.09662300 |
| H | -7.58839300 | 2.02950000 | 0.42069800 |
| O | -6.47906800 | 0.26083300 | 0.58614400 |

E -1473.60006

| | | | |
|----|-------------|-------------|-------------|
| Rh | 0.47898400 | -1.07062300 | 0.01843700 |
| N | 1.84446500 | -0.45395600 | 1.60170100 |
| N | -0.93430000 | -1.13994000 | 1.67659000 |
| C | 2.52518500 | -0.25001500 | 2.51484300 |
| C | 2.70512300 | 4.39644300 | -0.24780800 |
| C | 3.29846300 | 3.08330200 | -0.36860400 |
| C | 2.49953900 | 1.95312200 | -0.35695300 |
| C | 1.10858800 | 2.13454400 | -0.23562700 |
| C | -0.40031900 | -2.40416400 | -1.53099900 |
| C | 0.60108200 | -1.59009800 | -2.17135100 |
| C | 1.86668800 | -1.83918500 | -1.53161700 |
| C | 1.65571400 | -2.85834200 | -0.51615500 |
| C | 0.26120800 | -3.20022800 | -0.51187000 |
| C | -1.81305600 | -2.58583600 | -1.97907100 |
| C | 0.36252000 | -0.65501300 | -3.30629300 |
| C | 3.19837300 | -1.31401300 | -1.95588700 |
| C | 2.71766000 | -3.49212200 | 0.31438500 |
| C | -0.38205700 | -4.25241400 | 0.32553800 |
| C | -1.55372000 | -1.26181900 | 2.64621300 |
| C | -2.33459900 | -1.40964500 | 3.86205300 |
| C | 3.38604400 | 0.01769800 | 3.65360100 |
| C | 0.57319100 | 3.45520900 | -0.13168800 |
| C | 1.33647000 | 4.60755100 | -0.12897600 |
| N | 0.06524800 | 1.25127300 | -0.20534900 |
| C | -1.04694700 | 2.00253800 | -0.12068100 |
| O | -0.77015600 | 3.34220100 | -0.05120300 |
| C | -2.42488100 | 1.65289200 | -0.13366300 |
| C | -2.84535400 | 0.32560600 | -0.41310500 |
| C | -4.18935700 | 0.02255900 | -0.46065300 |

| | | | |
|---|-------------|-------------|-------------|
| C | -5.16933100 | 1.01541300 | -0.22713300 |
| C | -4.74476100 | 2.33970600 | 0.05123000 |
| C | -3.40792600 | 2.66261300 | 0.09221500 |
| C | 4.78883200 | 2.99157500 | -0.50876400 |
| C | -6.62626900 | 0.68940500 | -0.28043400 |
| H | 3.37062100 | 5.25463800 | -0.25579100 |
| H | 2.92569200 | 0.96323400 | -0.44625600 |
| H | -2.17962600 | -1.72691500 | -2.54495500 |
| H | -2.48762500 | -2.77862900 | -1.14109200 |
| H | -1.85566500 | -3.46125100 | -2.64177700 |
| H | 0.43662400 | -1.22092300 | -4.24562000 |
| H | 1.10536600 | 0.14476600 | -3.34273800 |
| H | -0.63638300 | -0.21389800 | -3.26561500 |
| H | 3.86149800 | -1.15366300 | -1.10182300 |
| H | 3.11019800 | -0.38477100 | -2.52172600 |
| H | 3.67717400 | -2.05726400 | -2.60800200 |
| H | 2.34139600 | -3.79877100 | 1.29324600 |
| H | 3.57680600 | -2.83172900 | 0.44941200 |
| H | 3.06767000 | -4.39504600 | -0.20565600 |
| H | -0.27068800 | -5.21877200 | -0.18589600 |
| H | -1.44995300 | -4.06865600 | 0.46108400 |
| H | 0.09290000 | -4.33958900 | 1.30571800 |
| H | -3.04731100 | -2.23230800 | 3.74568900 |
| H | -2.88089900 | -0.48265900 | 4.06414800 |
| H | -1.66726400 | -1.62633700 | 4.70239100 |
| H | 3.04453100 | -0.56112800 | 4.51775000 |
| H | 3.35159600 | 1.08453300 | 3.89692600 |
| H | 4.41555000 | -0.26548700 | 3.41235000 |
| H | 0.90054800 | 5.59613700 | -0.04629300 |
| H | -2.10066100 | -0.43286200 | -0.60705600 |
| H | -4.50762700 | -0.98995900 | -0.68883500 |
| H | -5.49037600 | 3.10800300 | 0.23052000 |
| H | -3.10104700 | 3.67996400 | 0.30365100 |
| H | 5.12535000 | 1.95401400 | -0.57381800 |
| H | 5.28710200 | 3.47135300 | 0.34342800 |
| H | 5.12334200 | 3.52565700 | -1.40771700 |
| H | -7.11440500 | 1.26493800 | -1.07906300 |
| H | -7.12085600 | 0.98280500 | 0.65496000 |
| H | -6.80113300 | -0.37432000 | -0.45865300 |

H -1581.496673

| | | | |
|----|-------------|------------|-------------|
| Rh | -0.42829900 | 1.17993900 | -0.45386800 |
| C | -0.44788300 | 2.93560900 | -1.80627100 |
| C | -1.75831900 | 2.36791500 | -1.78891400 |

| | | | |
|----|-------------|-------------|-------------|
| H | -0.26485700 | -3.84538100 | -3.10061300 |
| H | -1.19850700 | -2.34912000 | -2.97829200 |
| H | -1.00140900 | -3.40160800 | -1.55568800 |
| H | 1.03123500 | 0.54558700 | -4.09225200 |
| H | -0.32436500 | -0.60596500 | -4.07081300 |
| H | 1.18021500 | -1.02255400 | -4.89830500 |
| H | 4.17957100 | 0.56053400 | -1.81084200 |
| H | 2.99719600 | 1.10433300 | -3.02207800 |
| H | 4.15224000 | -0.17475200 | -3.41971800 |
| H | 4.63632600 | -2.66777100 | -0.61326200 |
| H | 3.73694500 | -2.13070900 | 0.81002100 |
| H | 4.58004100 | -0.94303000 | -0.21611900 |
| H | 0.56798700 | -2.63948800 | 3.71261300 |
| H | 0.09109000 | -1.00825400 | 4.19386800 |
| H | -2.09864600 | -1.87519700 | 4.75221900 |
| H | -1.68656200 | -3.44596400 | 4.05153400 |
| C | 3.63056500 | 4.24279900 | 1.14244200 |
| C | 4.03927700 | 2.88489800 | 1.15057700 |
| C | 3.17929200 | 1.89259800 | 0.67255800 |
| C | 1.92341700 | 2.28648600 | 0.19616600 |
| C | 1.55778200 | 3.63146300 | 0.22513700 |
| C | 2.38087100 | 4.64936100 | 0.68332400 |
| N | 0.83426600 | 1.56391600 | -0.30902200 |
| C | -0.11488400 | 2.45598700 | -0.53036400 |
| O | 0.27016400 | 3.72107800 | -0.24339700 |
| C | -1.49591900 | 2.24416700 | -0.97345300 |
| C | -1.76997900 | 1.11314800 | -1.72532000 |
| C | -4.16328400 | 1.61135100 | -1.66599000 |
| C | -3.87948300 | 2.77131400 | -0.95474800 |
| C | -2.57450200 | 3.11908600 | -0.58220600 |
| H | 4.31831300 | 4.99435000 | 1.52026500 |
| H | 3.47436500 | 0.84942900 | 0.68413400 |
| H | -0.95958300 | 0.46360300 | -2.03653400 |
| H | -4.69385600 | 3.42418300 | -0.65844600 |
| C | -3.10276700 | 0.74994000 | -2.04966900 |
| H | -3.28600400 | -0.06662500 | -2.74070800 |
| Br | -3.36224600 | -0.69695700 | 0.07009900 |
| H | 2.06689800 | 5.68721000 | 0.69240700 |
| H | -5.18337200 | 1.36768100 | -1.94415300 |
| C | 5.40194600 | 2.52822900 | 1.69560500 |
| H | 6.19405200 | 3.07924700 | 1.17452000 |
| H | 5.47957700 | 2.78544500 | 2.75938100 |
| H | 5.60817900 | 1.45851600 | 1.59362100 |
| C | -2.38436300 | 4.36817000 | 0.23043200 |

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|---|-------------|------------|-------------|
| H | -1.82112400 | 4.17166700 | 1.14931000 |
| H | -1.82452800 | 5.12562400 | -0.32955600 |
| H | -3.35476800 | 4.78973700 | 0.50229600 |

I -1581.466461

| | | | |
|----|-----------|-----------|-----------|
| 45 | 0.871978 | -0.838924 | -0.508785 |
| 6 | 1.813661 | -2.670073 | -1.331066 |
| 6 | 0.652748 | -2.391599 | -2.105779 |
| 6 | 0.807106 | -1.070948 | -2.715659 |
| 6 | 2.079424 | -0.549842 | -2.324401 |
| 6 | 2.694726 | -1.512899 | -1.422205 |
| 6 | 2.106420 | -3.915159 | -0.561800 |
| 6 | -0.526120 | -3.279631 | -2.305573 |
| 6 | -0.132381 | -0.463558 | -3.700773 |
| 6 | 2.696751 | 0.725637 | -2.786531 |
| 6 | 4.059874 | -1.412310 | -0.835713 |
| 6 | 0.701949 | -1.754743 | 3.976712 |
| 6 | -0.632128 | -1.625347 | 4.727591 |
| 6 | -1.547728 | -1.217840 | 3.591555 |
| 7 | -1.020037 | -1.110846 | 2.405921 |
| 6 | 0.322544 | -1.418527 | 2.545844 |
| 8 | 1.131383 | -1.417063 | 1.608022 |
| 8 | -2.796003 | -1.008494 | 3.920303 |
| 1 | 1.195620 | -4.472631 | -0.331280 |
| 1 | 2.630548 | -3.695852 | 0.372354 |
| 1 | 2.757215 | -4.564600 | -1.162407 |
| 1 | -0.432957 | -3.779318 | -3.279988 |
| 1 | -1.459384 | -2.708991 | -2.321831 |
| 1 | -0.591429 | -4.052597 | -1.536766 |
| 1 | -0.031552 | 0.622879 | -3.743229 |
| 1 | -1.173136 | -0.715587 | -3.486664 |
| 1 | 0.105580 | -0.860160 | -4.698060 |
| 1 | 3.330483 | 1.175538 | -2.018743 |
| 1 | 1.943110 | 1.452411 | -3.097709 |
| 1 | 3.332437 | 0.508930 | -3.656312 |
| 1 | 4.780411 | -1.824098 | -1.557391 |
| 1 | 4.148212 | -1.992221 | 0.086304 |
| 1 | 4.345030 | -0.376235 | -0.638519 |
| 1 | 1.129507 | -2.760798 | 4.023271 |
| 1 | 1.462133 | -1.050420 | 4.328840 |
| 1 | -0.633484 | -0.854361 | 5.504003 |
| 1 | -0.984483 | -2.559099 | 5.175398 |
| 6 | 3.247609 | 3.702228 | 2.388075 |
| 6 | 3.662715 | 2.348725 | 2.332389 |

| | | | | | | | |
|----|-----------|-----------|-----------|---|-------------|-------------|-------------|
| 6 | 2.909379 | 1.415615 | 1.612735 | C | -1.07218900 | -2.20138500 | 2.59325400 |
| 6 | 1.753899 | 1.868436 | 0.968171 | N | -0.15590200 | -1.75406000 | 1.64267600 |
| 6 | 1.376518 | 3.207761 | 1.052863 | C | 1.02016500 | -1.53925700 | 2.23838400 |
| 6 | 2.096795 | 4.164622 | 1.751924 | O | 1.99580800 | -1.16871800 | 1.52168500 |
| 7 | 0.795900 | 1.221487 | 0.177874 | O | -2.24142500 | -2.50161900 | 2.39813900 |
| 6 | -0.095884 | 2.136518 | -0.150092 | H | -0.11389200 | -4.56706300 | -0.21607200 |
| 8 | 0.205371 | 3.360839 | 0.343799 | H | 1.57610100 | -4.60398100 | 0.33227400 |
| 6 | -1.335583 | 1.951031 | -0.901809 | H | 1.13203200 | -5.32085700 | -1.22396700 |
| 6 | -2.003813 | 0.720142 | -0.745706 | H | -1.05992000 | -3.87288800 | -3.09739000 |
| 6 | -3.715555 | 1.434645 | -2.276914 | H | -1.75844100 | -2.25988500 | -2.91883200 |
| 6 | -3.057586 | 2.655463 | -2.431806 | H | -1.65961400 | -3.36050900 | -1.51915500 |
| 6 | -1.867341 | 2.952328 | -1.754430 | H | 0.65993700 | 0.62515400 | -3.44777500 |
| 6 | 4.918344 | 1.925995 | 3.058356 | H | -0.77171300 | -0.40580100 | -3.67062400 |
| 1 | 3.850161 | 4.408244 | 2.953066 | H | 0.67494900 | -0.66242600 | -4.65697900 |
| 1 | 3.204866 | 0.372927 | 1.567788 | H | 4.11044200 | -0.30712700 | -1.85293200 |
| 1 | 1.783209 | 5.201540 | 1.802383 | H | 2.88155500 | 0.65689400 | -2.70087900 |
| 1 | -1.605798 | -0.014502 | -0.047761 | H | 3.70833200 | -0.66297000 | -3.53733600 |
| 1 | -3.472144 | 3.404532 | -3.100629 | H | 4.28789600 | -3.50613300 | -1.37044400 |
| 1 | 5.792863 | 2.478308 | 2.692997 | H | 3.53209100 | -3.48567400 | 0.23107300 |
| 1 | 5.115012 | 0.857422 | 2.927289 | H | 4.31900100 | -2.02318800 | -0.40472500 |
| 1 | 4.840803 | 2.126641 | 4.134083 | H | 1.81182300 | -2.52383000 | 3.97242100 |
| 6 | -3.187922 | 0.458827 | -1.428593 | H | 1.28937800 | -0.86007000 | 4.25422800 |
| 1 | -3.699537 | -0.489501 | -1.292664 | H | -0.95118300 | -1.64291800 | 4.67141200 |
| 35 | -4.020736 | -0.442346 | 2.519943 | H | -0.44228400 | -3.30111700 | 4.34115600 |
| 1 | -4.639795 | 1.248298 | -2.816597 | C | 2.97171700 | 3.81655400 | 1.74454300 |
| 6 | -1.211175 | 4.293950 | -1.978850 | C | 3.56048100 | 2.55422200 | 1.43837500 |
| 1 | -1.316617 | 4.944799 | -1.103722 | C | 2.80264000 | 1.55254900 | 0.84275000 |
| 1 | -0.139169 | 4.202066 | -2.184349 | C | 1.45141800 | 1.82747100 | 0.55747200 |
| 1 | -1.677577 | 4.800623 | -2.828478 | C | 0.93085600 | 3.09951800 | 0.84942200 |
| | | | | C | 1.64855800 | 4.12109400 | 1.45496100 |
| | | | | N | 0.44338600 | 1.07943300 | -0.03456300 |
| | | | | C | -0.60054500 | 1.90511100 | -0.13097900 |
| | | | | O | -0.35395000 | 3.12803400 | 0.41144300 |
| | | | | C | -1.86658100 | 1.74855900 | -0.81059500 |
| | | | | C | -2.26329100 | 0.37886100 | -1.19966800 |
| | | | | C | -4.11611100 | 1.28805300 | -2.53039500 |
| | | | | C | -3.78738300 | 2.55689100 | -2.02151900 |
| | | | | C | -2.68512500 | 2.83236200 | -1.17681200 |
| | | | | H | 3.59230200 | 4.57400700 | 2.21498300 |
| | | | | H | 1.20767200 | 5.08715900 | 1.67296700 |
| | | | | H | -1.42131400 | -0.29787300 | -1.33507100 |
| | | | | H | -4.40719900 | 3.39952000 | -2.31419400 |
| | | | | C | -3.36615000 | 0.20980800 | -2.14729500 |
| | | | | H | -3.58585100 | -0.79456100 | -2.49279700 |

TSIJ -1581.438065

| | | | | | | | |
|----|-------------|-------------|-------------|--|--|--|--|
| Rh | 0.91680300 | -1.21408800 | -0.40323000 | | | | |
| C | 1.17979100 | -3.19627000 | -1.24671500 | | | | |
| C | 0.22727200 | -2.51165200 | -2.11284000 | | | | |
| C | 0.87932100 | -1.36725300 | -2.66668700 | | | | |
| C | 2.23632300 | -1.32487200 | -2.15575000 | | | | |
| C | 2.43387800 | -2.49374700 | -1.32784600 | | | | |
| C | 0.92709400 | -4.48666500 | -0.53896700 | | | | |
| C | -1.14479400 | -3.01241300 | -2.41934500 | | | | |
| C | 0.32030000 | -0.39429500 | -3.65244800 | | | | |
| C | 3.28878600 | -0.34952400 | -2.57121500 | | | | |
| C | 3.70877900 | -2.89095900 | -0.66740300 | | | | |
| C | 1.04141900 | -1.78643600 | 3.72512400 | | | | |
| C | -0.39221800 | -2.27210000 | 3.97241900 | | | | |

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|----------|---------------------|-------------|-------------|-------------|---------------------|-------------|-------------|
| Br | -3.16122000 | -0.53860500 | 0.49275500 | 1 | 3.293273 | -3.588418 | 0.299513 |
| C | -2.46162600 | 4.27701800 | -0.80306100 | 1 | 4.310827 | -2.145417 | 0.090605 |
| H | -2.49955200 | 4.42339200 | 0.28051400 | 1 | 0.900857 | -2.992781 | 4.264048 |
| H | -1.48811200 | 4.63842800 | -1.14838800 | 1 | 0.201754 | -1.427968 | 4.680543 |
| H | -3.23626000 | 4.89592400 | -1.26097400 | 1 | -1.881939 | -2.132183 | 3.695678 |
| H | 3.23837100 | 0.58907500 | 0.62077700 | 1 | -1.141586 | -3.640181 | 3.161137 |
| C | 5.01560800 | 2.33194800 | 1.76645600 | 6 | 3.272324 | 4.374067 | 0.922401 |
| H | 5.65482800 | 3.01717200 | 1.19541300 | 6 | 3.653842 | 3.066952 | 1.353134 |
| H | 5.21208100 | 2.52168200 | 2.82855700 | 6 | 2.798166 | 1.989881 | 1.146546 |
| H | 5.32563100 | 1.30784800 | 1.53908800 | 6 | 1.577279 | 2.250297 | 0.505953 |
| H | -4.95707800 | 1.17610300 | -3.20528400 | 6 | 1.233957 | 3.553093 | 0.110180 |
| | | | | 6 | 2.059479 | 4.652081 | 0.301704 |
| J | -1581.438065 | | | 7 | 0.541374 | 1.411172 | 0.139922 |
| 45 | 1.161450 | -0.711807 | -0.206175 | 6 | -0.378438 | 2.190813 | -0.413451 |
| 6 | 1.195786 | -2.627377 | -1.273435 | 8 | -0.000363 | 3.497185 | -0.470168 |
| 6 | 0.474346 | -1.621362 | -2.037726 | 6 | -1.710803 | 1.846355 | -0.849161 |
| 6 | 1.422524 | -0.588859 | -2.445095 | 6 | -2.355049 | 0.691353 | -0.165635 |
| 6 | 2.676195 | -0.901640 | -1.870111 | 6 | -4.339048 | 0.974820 | -1.592590 |
| 6 | 2.536406 | -2.159687 | -1.121606 | 6 | -3.711895 | 2.105164 | -2.155603 |
| 6 | 0.633046 | -3.919997 | -0.782568 | 6 | -2.419014 | 2.573050 | -1.810252 |
| 6 | -0.944848 | -1.713135 | -2.477096 | 6 | 4.983162 | 2.881953 | 2.039424 |
| 6 | 1.098919 | 0.575074 | -3.322207 | 1 | 3.965346 | 5.192392 | 1.096815 |
| 6 | 3.950835 | -0.142982 | -2.017014 | 1 | 3.034606 | 0.990939 | 1.501666 |
| 6 | 3.655633 | -2.854397 | -0.423263 | 1 | 1.780877 | 5.651790 | -0.011427 |
| 6 | 0.327808 | -2.149527 | 3.866308 | 1 | -1.711824 | -0.168205 | 0.058918 |
| 6 | -0.998085 | -2.555146 | 3.208703 | 1 | -4.248118 | 2.656507 | -2.923138 |
| 6 | -0.888969 | -2.010161 | 1.786349 | 1 | 5.028205 | 3.460610 | 2.970319 |
| 7 | 0.339522 | -1.435245 | 1.597917 | 1 | 5.804003 | 3.234756 | 1.403040 |
| 6 | 1.113834 | -1.490233 | 2.736325 | 1 | 5.164010 | 1.830941 | 2.282205 |
| 8 | 2.266234 | -1.068977 | 2.806827 | 6 | -3.684941 | 0.269953 | -0.621838 |
| 8 | -1.773161 | -2.070185 | 0.926229 | 1 | -4.111861 | -0.612390 | -0.156865 |
| 1 | -0.411285 | -3.812619 | -0.482680 | 35 | -2.786791 | 1.359898 | 1.786944 |
| 1 | 1.203312 | -4.311398 | 0.062916 | 6 | -1.891802 | 3.790439 | -2.525002 |
| 1 | 0.680127 | -4.659627 | -1.593421 | 1 | -1.940473 | 4.671458 | -1.875233 |
| 1 | -0.992141 | -2.297944 | -3.407347 | 1 | -0.850295 | 3.667707 | -2.832681 |
| 1 | -1.362427 | -0.725188 | -2.688851 | 1 | -2.495735 | 3.993257 | -3.412627 |
| 1 | -1.561895 | -2.215493 | -1.729440 | 1 | -5.324657 | 0.679718 | -1.934309 |
| 1 | 1.784386 | 1.410407 | -3.158793 | | | | |
| 1 | 0.074762 | 0.924235 | -3.163415 | | | | |
| 1 | 1.182618 | 0.271450 | -4.374310 | | | | |
| 1 | 4.530870 | -0.140209 | -1.089415 | | | | |
| 1 | 3.779593 | 0.888009 | -2.334059 | | | | |
| 1 | 4.568222 | -0.632654 | -2.783208 | | | | |
| 1 | 4.265929 | -3.383812 | -1.168647 | | | | |
| | | | | TSJK | -1581.449722 | | |
| | | | | Rh | 1.20275300 | -0.71031700 | -0.50252000 |
| | | | | C | 1.00460700 | -2.46364400 | -1.81534800 |
| | | | | C | 0.97778100 | -1.25717200 | -2.64675600 |
| | | | | C | 2.21727500 | -0.57867900 | -2.47473300 |
| | | | | C | 3.00899500 | -1.33236900 | -1.50775400 |

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|---|-------------|-------------|-------------|-----------------------|-------------|-------------|-------------|
| C | 2.26225800 | -2.52231600 | -1.14087400 | C | -3.69429500 | 1.23584900 | -1.88523700 |
| C | -0.10178700 | -3.45585500 | -1.72445800 | C | -2.39539100 | 1.81020000 | -1.73784000 |
| C | -0.12047400 | -0.89276300 | -3.58754400 | C | 5.20565700 | 3.44372700 | 1.23218600 |
| C | 2.66662500 | 0.65850700 | -3.17574300 | H | 3.63447800 | 5.62123400 | 0.95321400 |
| C | 4.39973200 | -1.01999300 | -1.07890800 | H | 3.56048200 | 1.31970500 | 0.63625300 |
| C | 2.74624300 | -3.60652800 | -0.23590300 | H | 1.22471700 | 5.78044900 | 0.32884300 |
| C | 0.39908500 | -2.18828300 | 3.53131800 | H | -1.61628700 | -0.22851700 | 0.74560600 |
| C | -1.05206500 | -2.65539800 | 3.70088600 | H | -4.23867100 | 1.45751100 | -2.80002000 |
| C | -1.74574900 | -2.15929000 | 2.42867100 | H | 5.35107900 | 3.91768400 | 2.21035900 |
| N | -0.82257500 | -1.55553200 | 1.57383000 | H | 5.82447300 | 3.99489700 | 0.51339800 |
| C | 0.38436300 | -1.55716300 | 2.15012100 | H | 5.58526900 | 2.41939600 | 1.29252400 |
| O | 1.42940900 | -1.09916000 | 1.60145700 | C | -3.64400600 | 0.16741100 | 0.25583000 |
| O | -2.93960900 | -2.25948300 | 2.17995100 | H | -4.07584200 | -0.45201100 | 1.03435700 |
| H | -1.07965400 | -2.98137600 | -1.84204500 | Br | -2.27964000 | 1.64119600 | 2.29217400 |
| H | -0.08164300 | -4.00481200 | -0.78071600 | C | -1.86744300 | 2.67502800 | -2.85171700 |
| H | 0.00781100 | -4.18495000 | -2.54020200 | H | -2.34999100 | 3.65979000 | -2.81486700 |
| H | 0.03883800 | -1.41798300 | -4.53948200 | H | -0.78889700 | 2.83135500 | -2.79490200 |
| H | -0.13779100 | 0.17900800 | -3.79853900 | H | -2.10851600 | 2.23206900 | -3.82296200 |
| H | -1.09794100 | -1.19937100 | -3.20633100 | H | -5.28801300 | 0.00376500 | -1.11350400 |
| H | 3.30436200 | 1.27677100 | -2.53943900 | | | | |
| H | 1.82359000 | 1.25923500 | -3.52416000 | K -1581.527772 | | | |
| H | 3.25840200 | 0.37080200 | -4.05565400 | Rh | -0.06018500 | -1.27731600 | 0.60572100 |
| H | 4.57587500 | -1.31192900 | -0.04001300 | C | -0.90253000 | -2.64006900 | 2.10127600 |
| H | 4.63641700 | 0.03881200 | -1.20181100 | C | -1.40500200 | -3.00231500 | 0.80111700 |
| H | 5.09593700 | -1.59563300 | -1.70632700 | C | -0.28529100 | -3.40112700 | -0.03641400 |
| H | 3.33615400 | -4.32448900 | -0.82128400 | C | 0.90679400 | -3.27321800 | 0.74311600 |
| H | 1.91832500 | -4.15126800 | 0.22368600 | C | 0.53009100 | -2.77881900 | 2.06542200 |
| H | 3.39061100 | -3.21429000 | 0.55464900 | C | -1.72788500 | -2.23861600 | 3.27797000 |
| H | 1.13685600 | -2.99618500 | 3.56196900 | C | -2.83101000 | -2.99446100 | 0.38413600 |
| H | 0.70385200 | -1.43873500 | 4.26967500 | C | -0.38299300 | -3.98880900 | -1.40312300 |
| H | -1.55306500 | -2.22853400 | 4.57488300 | C | 2.27831700 | -3.66550700 | 0.31590500 |
| H | -1.14993600 | -3.74401400 | 3.76573000 | C | 1.46352600 | -2.56086200 | 3.20449900 |
| C | 3.07673100 | 4.71430500 | 0.73671400 | C | -0.27872100 | 2.32545400 | 3.37896300 |
| C | 3.75102700 | 3.46878900 | 0.82957400 | C | 0.98427100 | 2.89317400 | 4.04994300 |
| C | 3.06631300 | 2.28233000 | 0.55905300 | C | 2.14163900 | 2.11756800 | 3.44582800 |
| C | 1.71478300 | 2.37883000 | 0.20988700 | N | 1.58275000 | 1.18687000 | 2.53747500 |
| C | 1.08771800 | 3.62355700 | 0.13364300 | C | 0.23250400 | 1.24913700 | 2.44978100 |
| C | 1.73319900 | 4.82486300 | 0.38924700 | O | -0.48258400 | 0.53206800 | 1.72971100 |
| N | 0.75109400 | 1.40767900 | -0.09238400 | O | 3.32720800 | 2.21562900 | 3.65384500 |
| C | -0.35860500 | 2.06916500 | -0.31187500 | H | -2.62876500 | -1.69985700 | 2.97387900 |
| O | -0.23023500 | 3.41005000 | -0.20959800 | H | -1.16555800 | -1.61561800 | 3.97723300 |
| C | -1.70684000 | 1.53208200 | -0.57227000 | H | -2.04476400 | -3.14284400 | 3.81494200 |
| C | -2.29976600 | 0.67550500 | 0.46756700 | H | -3.24114200 | -4.00442900 | 0.53239900 |
| C | -4.29993700 | 0.41154200 | -0.93068400 | H | -2.94327800 | -2.75019200 | -0.67554100 |

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|----|-------------|-------------|-------------|
| H | -3.42658800 | -2.30179200 | 0.98298500 |
| H | 0.51944500 | -3.80682200 | -1.99025100 |
| H | -1.24790400 | -3.61239700 | -1.95236900 |
| H | -0.50178300 | -5.07708900 | -1.30471700 |
| H | 3.05505300 | -3.16073300 | 0.89405600 |
| H | 2.44371600 | -3.48045200 | -0.74844200 |
| H | 2.39164600 | -4.74626200 | 0.48523900 |
| H | 1.59891400 | -3.51629800 | 3.73172000 |
| H | 1.07113500 | -1.83874200 | 3.92341900 |
| H | 2.45015100 | -2.23354500 | 2.86714400 |
| H | -0.83183500 | 3.06820200 | 2.79641100 |
| H | -0.98409300 | 1.87623600 | 4.08508200 |
| H | 0.99201200 | 2.75181600 | 5.13486000 |
| H | 1.13180700 | 3.95947800 | 3.85547700 |
| C | 4.72134600 | 1.23898700 | -1.93559800 |
| C | 4.64630900 | 0.36258700 | -0.82490000 |
| C | 3.40684200 | -0.13567000 | -0.41259600 |
| C | 2.27032900 | 0.25733100 | -1.12701500 |
| C | 2.39021900 | 1.12176600 | -2.21431200 |
| C | 3.59908100 | 1.63920600 | -2.65656100 |
| N | 0.90440700 | -0.03255100 | -0.97547200 |
| C | 0.29169100 | 0.62972900 | -1.92927300 |
| O | 1.12762000 | 1.34152200 | -2.71626800 |
| C | -1.14627200 | 0.64266300 | -2.26815800 |
| C | -2.00750800 | 1.63405100 | -1.77642900 |
| C | -3.87358800 | 0.64112500 | -2.89455300 |
| C | -3.02701100 | -0.32019400 | -3.44448000 |
| C | -1.65625400 | -0.33173700 | -3.15986800 |
| C | 5.91050300 | -0.01496500 | -0.08999400 |
| H | 5.69576500 | 1.61429700 | -2.23544200 |
| H | 3.33779500 | -0.80869300 | 0.43664500 |
| H | 3.66274200 | 2.31335000 | -3.50361000 |
| H | 2.15760100 | 0.55579700 | 1.98374600 |
| H | -3.42747800 | -1.06790600 | -4.12276300 |
| H | 6.36979600 | 0.86360000 | 0.38013700 |
| H | 6.65498300 | -0.43823800 | -0.77457800 |
| H | 5.71352500 | -0.75193900 | 0.69467100 |
| C | -3.36636600 | 1.64303800 | -2.06491200 |
| H | -4.01486200 | 2.41566000 | -1.66776000 |
| Br | -1.28591700 | 3.13031500 | -0.71280000 |
| C | -0.74092300 | -1.30675800 | -3.86103600 |
| H | -0.21286500 | -0.80384700 | -4.68177800 |
| H | 0.01987000 | -1.72766100 | -3.19718700 |
| H | -1.31312600 | -2.13092700 | -4.29562300 |

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|---|-------------|------------|-------------|
| H | -4.93372400 | 0.63151700 | -3.12992600 |
|---|-------------|------------|-------------|

TSHI' -1581.428777

| | | | |
|----|-------------|-------------|-------------|
| Rh | 1.42662100 | 0.89752600 | 0.28517800 |
| C | 2.15631600 | 2.27119000 | -1.26545800 |
| C | 0.98699400 | 2.90567100 | -0.65236200 |
| C | 1.25623600 | 3.09772600 | 0.72985600 |
| C | 2.59181300 | 2.58244100 | 1.00011700 |
| C | 3.15805200 | 2.11797700 | -0.25485900 |
| C | 2.30368800 | 1.96851700 | -2.71814300 |
| C | -0.21265400 | 3.36410500 | -1.40925500 |
| C | 0.38009300 | 3.75686000 | 1.74288500 |
| C | 3.31556200 | 2.71099400 | 2.29438900 |
| C | 4.54178900 | 1.59601800 | -0.43915300 |
| C | 2.77206000 | -3.03543600 | -1.02062100 |
| C | 1.91182200 | -3.48800900 | -2.21225100 |
| C | 0.84816100 | -2.38200700 | -2.33430600 |
| N | 1.15632600 | -1.33698600 | -1.47996900 |
| C | 2.16878100 | -1.68042200 | -0.69639400 |
| O | 2.57585300 | -0.93181500 | 0.24907500 |
| O | -0.14154200 | -2.41363500 | -3.05189900 |
| H | 1.36088000 | 1.63705700 | -3.16044800 |
| H | 3.06451600 | 1.20619900 | -2.89761000 |
| H | 2.61320200 | 2.88520000 | -3.24005600 |
| H | 0.03415800 | 4.32226900 | -1.88889000 |
| H | -1.07537100 | 3.53734200 | -0.76229300 |
| H | -0.48643200 | 2.66909300 | -2.20710800 |
| H | 0.41636400 | 3.23618900 | 2.70433800 |
| H | -0.65805700 | 3.81664000 | 1.40982400 |
| H | 0.73705500 | 4.78172400 | 1.91213500 |
| H | 4.13689200 | 1.99654200 | 2.37870400 |
| H | 2.64608000 | 2.59689300 | 3.15018500 |
| H | 3.74562800 | 3.72223600 | 2.34549600 |
| H | 5.21703300 | 2.44603800 | -0.60894300 |
| H | 4.61372200 | 0.93055700 | -1.30190100 |
| H | 4.89284500 | 1.06384100 | 0.44853600 |
| H | 3.83639100 | -2.92826800 | -1.25389900 |
| H | 2.69229700 | -3.69603700 | -0.15063800 |
| H | 1.42062100 | -4.45342800 | -2.06168600 |
| H | 2.47686500 | -3.54588500 | -3.14854900 |
| Br | -1.46416400 | -0.28067300 | -0.94148100 |
| C | 1.97619200 | -1.70286600 | 5.41816400 |
| C | 2.88286000 | -1.18294300 | 4.44867500 |
| C | 2.40196100 | -0.59519900 | 3.28302700 |

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|----|--------------|-------------|-------------|----|-------------|-------------|-------------|
| C | 1.00917500 | -0.53245300 | 3.10323000 | C | 3.00543100 | -1.79330800 | -0.05859200 |
| C | 0.15931000 | -1.06201200 | 4.08539800 | O | 3.72928300 | -1.35643600 | 0.81244500 |
| C | 0.59757300 | -1.65577300 | 5.26147800 | O | 0.19233500 | -1.59222100 | -2.10162100 |
| N | 0.21559500 | -0.01138000 | 2.08741300 | H | 0.24960300 | 2.21724400 | -2.97716100 |
| C | -1.04145300 | -0.23758200 | 2.46687600 | H | 1.78625800 | 1.38025800 | -3.28835400 |
| O | -1.12011300 | -0.87349500 | 3.66661600 | H | 1.72009000 | 3.14807800 | -3.27579900 |
| C | -2.30083700 | 0.07781700 | 1.82456800 | H | -0.06586000 | 4.74627100 | -1.01901800 |
| C | -2.25562400 | 0.95016800 | 0.63531700 | H | -0.91756400 | 3.99299900 | 0.33271900 |
| C | -3.50378200 | 1.37626800 | 0.01486500 | H | -1.01635500 | 3.29377900 | -1.30512900 |
| C | -4.70093500 | 0.88926200 | 0.47187200 | H | 1.51834500 | 2.93372500 | 3.05978200 |
| C | -4.69934800 | 0.01431300 | 1.56891900 | H | 0.15000700 | 3.75013400 | 2.27146700 |
| C | -3.54159800 | -0.40406600 | 2.27316000 | H | 1.74902700 | 4.50798300 | 2.29455100 |
| C | 4.36521200 | -1.28613700 | 4.70618700 | H | 4.51175900 | 1.08486700 | 1.44149700 |
| H | 2.38607200 | -2.15752100 | 6.31566400 | H | 3.58224200 | 1.96869500 | 2.67380000 |
| H | 3.08211200 | -0.21890100 | 2.53155700 | H | 4.61164500 | 2.85117900 | 1.53727300 |
| H | -0.08943400 | -2.05405400 | 5.99945700 | H | 4.68523000 | 2.00497400 | -1.79910500 |
| H | -1.48013400 | 1.71311800 | 0.66652400 | H | 3.69210000 | 0.64580700 | -2.33929600 |
| H | -3.44697300 | 2.07108700 | -0.81613300 | H | 4.59696500 | 0.54244600 | -0.80925500 |
| H | -5.65276400 | -0.37696400 | 1.91104900 | H | 4.24398200 | -2.98106500 | -1.35051000 |
| H | 4.67347000 | -2.33386300 | 4.80882500 | H | 3.22748100 | -3.91599700 | -0.24789600 |
| H | 4.63847900 | -0.77933300 | 5.63989900 | H | 1.48837100 | -3.93332300 | -1.90988300 |
| H | 4.94467800 | -0.83954200 | 3.89294300 | H | 2.44238400 | -2.86980800 | -2.95150600 |
| H | -5.63698600 | 1.17038700 | 0.00252100 | Br | -1.13584900 | -0.27526200 | -1.06661000 |
| C | -3.75866200 | -1.34521900 | 3.43193100 | C | 1.58462700 | -1.21660800 | 5.75580200 |
| H | -3.15617400 | -2.25291600 | 3.33238800 | C | 2.55839300 | -0.98273200 | 4.75119200 |
| H | -3.49260900 | -0.87886200 | 4.38555800 | C | 2.16766700 | -0.56505700 | 3.47670600 |
| H | -4.81120000 | -1.63321100 | 3.47617300 | C | 0.79960200 | -0.39060600 | 3.23402400 |
| I' | -1581.458775 | | | C | -0.12363400 | -0.66333600 | 4.24466300 |
| Rh | 1.14246000 | 0.80591900 | 0.20463700 | C | 0.22019900 | -1.06959400 | 5.52567700 |
| C | 1.65841300 | 2.29231100 | -1.34259500 | N | 0.08053000 | 0.00272800 | 2.09397500 |
| C | 0.88567700 | 2.99945700 | -0.31936600 | C | -1.19382300 | -0.08516100 | 2.43993400 |
| C | 1.59715400 | 2.91515400 | 0.90898600 | O | -1.37640400 | -0.47053700 | 3.72521100 |
| C | 2.81898900 | 2.16029500 | 0.67034700 | C | -2.41237000 | 0.11808600 | 1.65273200 |
| C | 2.86985100 | 1.82925900 | -0.74091100 | C | -2.39698000 | 1.11432100 | 0.62552900 |
| C | 1.32650300 | 2.24066200 | -2.79625600 | C | -3.54280800 | 1.35512000 | -0.17133800 |
| C | -0.35793100 | 3.78127400 | -0.58046100 | C | -4.68251200 | 0.58743200 | 0.02716200 |
| C | 1.22117300 | 3.54823500 | 2.20640800 | C | -4.68284400 | -0.38928300 | 1.02351600 |
| C | 3.93539100 | 1.98980800 | 1.64087400 | C | -3.56838200 | -0.66045200 | 1.84924900 |
| C | 4.01760500 | 1.20169900 | -1.45699600 | C | 4.01797500 | -1.19288900 | 5.07671400 |
| C | 3.24939200 | -3.03662600 | -0.89971600 | H | 1.91817900 | -1.53837900 | 6.73864300 |
| C | 2.10887500 | -3.03303900 | -1.92182500 | H | 2.89499000 | -0.42682700 | 2.68685900 |
| C | 1.27726700 | -1.84622600 | -1.47364200 | H | -0.52498100 | -1.26733700 | 6.28810700 |
| N | 1.78575300 | -1.17781200 | -0.44752300 | H | -1.60460500 | 1.85122800 | 0.63763800 |
| | | | | H | -3.51943200 | 2.14861900 | -0.91102300 |

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|---|-------------|-------------|-------------|
| H | -5.57606300 | -0.99037300 | 1.16824800 |
| H | 4.19237500 | -2.19881800 | 5.47682500 |
| H | 4.35871500 | -0.48124400 | 5.83958200 |
| H | 4.64766200 | -1.06554800 | 4.19139800 |
| C | -3.68638900 | -1.78706100 | 2.84620400 |
| H | -2.80340800 | -2.43343600 | 2.84067400 |
| H | -3.80998400 | -1.40955500 | 3.86684100 |
| H | -4.55915100 | -2.39999400 | 2.60695800 |
| H | -5.56929300 | 0.74846800 | -0.57666000 |

TSI' J -1581.440615

| | | | |
|----|-------------|-------------|-------------|
| Rh | 1.53085800 | 0.79750000 | 0.35576700 |
| C | 1.38806700 | 2.33172600 | -1.18669800 |
| C | 0.94782600 | 3.00213000 | 0.03552600 |
| C | 2.00194900 | 2.92788000 | 0.97555300 |
| C | 3.13579100 | 2.24843600 | 0.33970200 |
| C | 2.76342600 | 1.92103200 | -1.01049300 |
| C | 0.63377100 | 2.20214600 | -2.46367600 |
| C | -0.35556400 | 3.70479400 | 0.22825000 |
| C | 2.00766300 | 3.48273800 | 2.36029600 |
| C | 4.48436400 | 2.05529400 | 0.93927400 |
| C | 3.64825600 | 1.35452900 | -2.06996600 |
| C | 3.73584800 | -2.98254500 | -0.37527100 |
| C | 2.78432200 | -3.03567300 | -1.57188900 |
| C | 1.96530900 | -1.75060300 | -1.45786100 |
| N | 2.29434100 | -1.08022200 | -0.29670000 |
| C | 3.36577400 | -1.68437900 | 0.33619800 |
| O | 3.95061900 | -1.23061700 | 1.31805000 |
| O | 1.14747900 | -1.37693400 | -2.29722300 |
| H | -0.42134800 | 2.45713900 | -2.35293700 |
| H | 0.71853200 | 1.18493800 | -2.85874700 |
| H | 1.07186700 | 2.88752400 | -3.20293000 |
| H | -0.20660900 | 4.77764300 | 0.04334400 |
| H | -0.73417900 | 3.60006500 | 1.24863700 |
| H | -1.11701100 | 3.35906300 | -0.47396300 |
| H | 2.60183900 | 2.86619900 | 3.04043100 |
| H | 0.99815100 | 3.58446100 | 2.76537100 |
| H | 2.46533200 | 4.48171000 | 2.34224700 |
| H | 4.95057300 | 1.13350800 | 0.58585000 |
| H | 4.44858300 | 2.03739100 | 2.03052300 |
| H | 5.12223900 | 2.89931100 | 0.63879400 |
| H | 4.08862600 | 2.18408200 | -2.64011300 |
| H | 3.08720600 | 0.72752500 | -2.76646900 |
| H | 4.46658200 | 0.77073300 | -1.64310000 |

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|----|-------------|-------------|-------------|
| H | 4.79311900 | -2.94772600 | -0.65707200 |
| H | 3.61197100 | -3.81808500 | 0.32154100 |
| H | 2.09968300 | -3.89031400 | -1.54850300 |
| H | 3.29306100 | -3.05321800 | -2.54059500 |
| Br | -1.51326700 | -0.86677900 | -1.15477200 |
| C | 1.31455100 | -1.40689700 | 5.60168100 |
| C | 2.29552200 | -0.93119800 | 4.67758500 |
| C | 1.90731000 | -0.47295300 | 3.42413400 |
| C | 0.53773700 | -0.50825100 | 3.11329000 |
| C | -0.39131200 | -0.98925500 | 4.05364100 |
| C | -0.04454300 | -1.44884200 | 5.31660900 |
| N | -0.14923800 | -0.12342500 | 1.98044600 |
| C | -1.43110500 | -0.36638800 | 2.24853200 |
| O | -1.62282900 | -0.89860300 | 3.49179300 |
| C | -2.60076700 | -0.11924800 | 1.44987600 |
| C | -2.37917500 | 0.54181700 | 0.13784000 |
| C | -3.54835100 | 0.98273600 | -0.63368100 |
| C | -4.80786700 | 0.69151700 | -0.20091100 |
| C | -4.96570500 | -0.01711300 | 1.00930900 |
| C | -3.91190000 | -0.42662700 | 1.85615100 |
| C | 3.74671100 | -0.93870700 | 5.08614900 |
| H | 1.65369500 | -1.75873200 | 6.57204600 |
| H | 2.63480700 | -0.15669100 | 2.68419400 |
| H | -0.77905300 | -1.81574800 | 6.02426300 |
| H | -1.58373500 | 1.28259400 | 0.17453200 |
| H | -3.36936500 | 1.52428000 | -1.55675800 |
| H | -5.97607700 | -0.26096700 | 1.32457800 |
| H | 4.04332800 | -1.92702300 | 5.45688600 |
| H | 3.92927100 | -0.22468200 | 5.89957700 |
| H | 4.39794100 | -0.67862900 | 4.24761000 |
| C | -4.29352200 | -1.13731000 | 3.13041900 |
| H | -3.79420600 | -2.10674600 | 3.21707000 |
| H | -4.02496200 | -0.54937000 | 4.01375800 |
| H | -5.37341400 | -1.30061700 | 3.14735700 |
| H | -5.68216700 | 0.99085400 | -0.76798400 |

TSHL -1581.431835

| | | | |
|----|------------|------------|-------------|
| Rh | 0.83173900 | 1.18999900 | 0.17795400 |
| C | 1.04521200 | 3.08785200 | -0.95548700 |
| C | 0.48262600 | 3.35938400 | 0.36754600 |
| C | 1.44274700 | 2.94801100 | 1.34811400 |
| C | 2.57741600 | 2.37625000 | 0.64166500 |
| C | 2.33431100 | 2.51115000 | -0.78796200 |
| C | 0.36320700 | 3.38707100 | -2.24677200 |

| | | | | | | | |
|----|-------------|-------------|-------------|-----------------------|-------------|-------------|-------------|
| C | -0.80860800 | 4.05635400 | 0.62947800 | C | -4.69349100 | 1.43814500 | 0.94585200 |
| C | 1.33453100 | 3.12274000 | 2.82402600 | C | -3.70242900 | 0.95256400 | 1.80996700 |
| C | 3.84221000 | 1.88553500 | 1.25397200 | C | 3.64021300 | -1.99518200 | 4.54287800 |
| C | 3.29265200 | 2.11525400 | -1.85908100 | H | 1.43317200 | -2.68379000 | 5.94512100 |
| C | 2.75819300 | -2.67228200 | -1.57897100 | H | 2.67856600 | -0.59660200 | 2.38343800 |
| C | 2.21141500 | -4.11394900 | -1.51827600 | H | -0.96855100 | -2.20339400 | 5.46459400 |
| C | 0.81509100 | -3.92105900 | -0.95048800 | H | -1.42391300 | 0.10766100 | -0.61347100 |
| N | 0.58474100 | -2.63629200 | -0.65349100 | H | -3.20280800 | 0.99742000 | -2.08533100 |
| C | 1.64595200 | -1.82451900 | -0.96967300 | H | -5.61870700 | 1.80836000 | 1.37841800 |
| O | 1.73140800 | -0.60266300 | -0.81599300 | H | 3.80641900 | -3.07895000 | 4.57876100 |
| O | -0.04682200 | -4.78778600 | -0.75994100 | H | 3.91100400 | -1.59744100 | 5.52850400 |
| H | -0.71379900 | 3.20691900 | -2.18520900 | H | 4.33148700 | -1.57276500 | 3.80693500 |
| H | 0.77539100 | 2.79875200 | -3.06930300 | C | -3.95989300 | 0.96653400 | 3.29816700 |
| H | 0.50275500 | 4.45022500 | -2.48759500 | H | -4.14504300 | -0.04278200 | 3.68277000 |
| H | -0.63573200 | 5.14109200 | 0.58781500 | H | -3.11455300 | 1.37510100 | 3.86182200 |
| H | -1.20509400 | 3.82006400 | 1.61925800 | H | -4.84151700 | 1.57464400 | 3.51925200 |
| H | -1.56324300 | 3.81487500 | -0.12260300 | H | -5.32513300 | 1.84123600 | -1.07154700 |
| H | 1.87100000 | 2.34178200 | 3.36726200 | | | | |
| H | 0.29507200 | 3.13996800 | 3.15844200 | | | | |
| H | 1.78884500 | 4.08676900 | 3.09225200 | L -1581.463555 | | | |
| H | 4.27910400 | 1.06754000 | 0.67489100 | Rh | 1.08909000 | 1.08592400 | 0.29783100 |
| H | 3.69990000 | 1.56277900 | 2.28691000 | C | 1.74858800 | 2.45023000 | -1.30260900 |
| H | 4.56989400 | 2.71051500 | 1.25657300 | C | 0.77579700 | 3.16901600 | -0.48320700 |
| H | 4.06461200 | 2.89138600 | -1.94887100 | C | 1.26704300 | 3.23240100 | 0.85620500 |
| H | 2.80175500 | 2.01263900 | -2.82908600 | C | 2.56305300 | 2.57925500 | 0.87624200 |
| H | 3.79586000 | 1.17512300 | -1.61779700 | C | 2.86414300 | 2.12565300 | -0.47354000 |
| H | 2.94474100 | -2.32889900 | -2.60163400 | C | 1.61523400 | 2.20923500 | -2.76975400 |
| H | 3.68020300 | -2.53011600 | -1.00716900 | C | -0.47909900 | 3.77226600 | -1.00951400 |
| H | 2.77012600 | -4.76907400 | -0.84315000 | C | 0.63329200 | 3.91098200 | 2.02527900 |
| H | 2.13725800 | -4.60811200 | -2.49045100 | C | 3.50128400 | 2.56207700 | 2.03097200 |
| Br | -1.73148400 | -3.28194200 | 0.10602600 | C | 4.12542400 | 1.45023400 | -0.88828100 |
| C | 1.16697100 | -2.11721700 | 5.05696600 | C | 1.62149400 | -3.04614200 | -1.30609000 |
| C | 2.20447900 | -1.67320300 | 4.20057700 | C | 0.40681900 | -3.50877400 | -2.12980600 |
| C | 1.89523400 | -0.94239900 | 3.04918700 | C | -0.53087600 | -2.33441100 | -1.93576900 |
| C | 0.54788300 | -0.67363500 | 2.78725500 | N | -0.08175800 | -1.33737200 | -1.22343400 |
| C | -0.44275900 | -1.13108100 | 3.65495100 | C | 1.19355300 | -1.67655500 | -0.81852300 |
| C | -0.17915300 | -1.85834600 | 4.80586700 | O | 1.89330900 | -0.91503400 | -0.13129900 |
| N | -0.09674400 | 0.02770700 | 1.76122000 | O | -1.70797600 | -2.42535200 | -2.49079100 |
| C | -1.38931300 | -0.03969800 | 2.01966600 | H | 0.58197400 | 1.98032600 | -3.04594000 |
| O | -1.65979700 | -0.72539800 | 3.15462700 | H | 2.25868700 | 1.39318000 | -3.10739700 |
| C | -2.49766500 | 0.48700000 | 1.22351200 | H | 1.90893100 | 3.11740000 | -3.31373900 |
| C | -2.33551200 | 0.51317200 | -0.17679000 | H | -0.21462500 | 4.69443700 | -1.54705300 |
| C | -3.33923200 | 0.99875200 | -1.00823000 | H | -1.17971300 | 4.03627300 | -0.21554300 |
| C | -4.52672000 | 1.46352300 | -0.43926500 | H | -0.97386800 | 3.11394500 | -1.72935000 |
| | | | | H | 0.77379400 | 3.33330000 | 2.94324900 |

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|----|-------------|-------------|-------------|
| H | -0.43476800 | 4.07673200 | 1.87274100 |
| H | 1.10847700 | 4.88974500 | 2.17488100 |
| H | 4.23615800 | 1.75758600 | 1.95662300 |
| H | 2.97577100 | 2.48689600 | 2.98578700 |
| H | 4.05187800 | 3.51464600 | 2.03117500 |
| H | 4.90219400 | 2.21370800 | -1.03269400 |
| H | 4.00542100 | 0.90793300 | -1.82801400 |
| H | 4.48418700 | 0.75753500 | -0.12209800 |
| H | 2.54022300 | -2.96290800 | -1.89417100 |
| H | 1.83047700 | -3.69608300 | -0.45045700 |
| H | -0.06177000 | -4.42450100 | -1.75852200 |
| H | 0.62030800 | -3.64494400 | -3.19434900 |
| Br | -2.97509800 | -0.98232200 | -2.10950800 |
| C | 1.83946800 | -1.82720300 | 5.30532600 |
| C | 2.76420800 | -1.29820600 | 4.37157100 |
| C | 2.30453400 | -0.61011700 | 3.24453400 |
| C | 0.92267700 | -0.46488500 | 3.08017100 |
| C | 0.04951800 | -1.01853500 | 4.01446200 |
| C | 0.46076000 | -1.70464500 | 5.14723100 |
| N | 0.14250000 | 0.12885300 | 2.07594200 |
| C | -1.11547700 | -0.09742800 | 2.41458100 |
| O | -1.23167300 | -0.77573800 | 3.58132600 |
| C | -2.34232600 | 0.26607800 | 1.70639400 |
| C | -2.29100900 | 1.40211100 | 0.88272800 |
| C | -3.39233900 | 1.80556800 | 0.13662200 |
| C | -4.57633000 | 1.06475000 | 0.21751100 |
| C | -4.63777100 | -0.05674600 | 1.04807700 |
| C | -3.54342600 | -0.48721100 | 1.80927000 |
| C | 4.24459900 | -1.48772700 | 4.60577200 |
| H | 2.22181600 | -2.35821000 | 6.17287600 |
| H | 3.00105800 | -0.21953600 | 2.51201500 |
| H | -0.24520700 | -2.12336200 | 5.85612600 |
| H | -1.37283300 | 1.97562300 | 0.85532500 |
| H | -3.33489800 | 2.69270400 | -0.48606500 |
| H | -5.56165000 | -0.62494200 | 1.10442400 |
| H | 4.48973500 | -2.54668400 | 4.75059400 |
| H | 4.57393000 | -0.95677600 | 5.50787900 |
| H | 4.83479900 | -1.11592400 | 3.76251300 |
| C | -3.69995100 | -1.72870500 | 2.65596300 |
| H | -2.88877600 | -2.44552400 | 2.49021500 |
| H | -3.70737400 | -1.49283900 | 3.72557700 |
| H | -4.64451600 | -2.22521500 | 2.41577700 |
| H | -5.45318800 | 1.36641000 | -0.34881600 |

TSLM -1581.450042

| | | | |
|----|-------------|-------------|-------------|
| Rh | 1.16039300 | 0.79199400 | 0.17526500 |
| C | 1.86276700 | 2.16050700 | -1.37970900 |
| C | 0.83652400 | 2.84469800 | -0.61383200 |
| C | 1.30439400 | 2.96838900 | 0.74483700 |
| C | 2.60401800 | 2.37073200 | 0.83029600 |
| C | 2.95251500 | 1.87278700 | -0.49176400 |
| C | 1.81535100 | 1.91050800 | -2.85220600 |
| C | -0.35859400 | 3.51150900 | -1.20797800 |
| C | 0.59535900 | 3.66572100 | 1.85828100 |
| C | 3.51742000 | 2.41498700 | 2.01132200 |
| C | 4.24607300 | 1.22757700 | -0.85792600 |
| C | 1.31090900 | -3.04203400 | -1.39824800 |
| C | 0.33917200 | -2.75450300 | -2.55425200 |
| C | -0.10380300 | -1.29441900 | -2.34841600 |
| N | 0.46437200 | -0.81524200 | -1.17562400 |
| C | 1.33655500 | -1.71336500 | -0.68377400 |
| O | 2.08334400 | -1.35219100 | 0.26114700 |
| O | -0.82131900 | -0.67743600 | -3.12432000 |
| H | 0.81051200 | 1.63390000 | -3.18030900 |
| H | 2.50737700 | 1.11975400 | -3.15085800 |
| H | 2.10571400 | 2.82846200 | -3.38124200 |
| H | -0.04221700 | 4.48590400 | -1.60725300 |
| H | -1.14348400 | 3.70577700 | -0.47375100 |
| H | -0.77288800 | 2.93777400 | -2.03902300 |
| H | 0.85766000 | 3.24446800 | 2.83200700 |
| H | -0.49005100 | 3.63382300 | 1.73872000 |
| H | 0.89550400 | 4.72262600 | 1.86227200 |
| H | 4.23070000 | 1.58754600 | 2.01145700 |
| H | 2.96781800 | 2.40607500 | 2.95522300 |
| H | 4.09611000 | 3.34865800 | 1.97244700 |
| H | 4.98238400 | 2.01312900 | -1.07831000 |
| H | 4.15111600 | 0.59985600 | -1.74669000 |
| H | 4.64492100 | 0.62171300 | -0.04025100 |
| H | 2.31912100 | -3.31735400 | -1.72282000 |
| H | 0.95907300 | -3.82396900 | -0.71638700 |
| H | -0.54842300 | -3.39465600 | -2.54434800 |
| H | 0.80271400 | -2.85068300 | -3.54059200 |
| Br | -2.98640000 | 0.78449100 | -1.81973500 |
| C | 1.81945500 | -1.40275900 | 5.54034300 |
| C | 2.73177500 | -1.07407700 | 4.50569400 |
| C | 2.26092300 | -0.60420300 | 3.27793100 |
| C | 0.87651100 | -0.47306500 | 3.10924300 |
| C | 0.01836700 | -0.82862100 | 4.14947200 |

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|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | 0.44099200 | -1.29282500 | 5.38669200 | O | -2.08606000 | -2.37973600 | 1.12917300 |
| N | 0.08391000 | -0.04997300 | 2.02525100 | H | -0.52829900 | -3.79704200 | -0.73683700 |
| C | -1.15577300 | -0.18540600 | 2.43886700 | H | 0.99982800 | -4.42245400 | -0.09071900 |
| O | -1.26919000 | -0.64137000 | 3.70825900 | H | 0.57142500 | -4.70991400 | -1.78488000 |
| C | -2.41319000 | 0.09504600 | 1.73292500 | H | -0.74420600 | -2.30192600 | -3.69508500 |
| C | -2.46032200 | 1.16817800 | 0.88392100 | H | -1.11335600 | -0.69997700 | -3.04878000 |
| C | -3.64561900 | 1.46302500 | 0.07386700 | H | -1.47899000 | -2.15724800 | -2.09343700 |
| C | -4.83523700 | 0.65012600 | 0.33084700 | H | 2.13868500 | 1.32635500 | -3.08165000 |
| C | -4.78508400 | -0.39144700 | 1.21288600 | H | 0.44969300 | 0.85848500 | -3.39443200 |
| C | -3.59174000 | -0.72396200 | 1.90928200 | H | 1.74826100 | 0.21847700 | -4.40323600 |
| C | 4.21287300 | -1.24954400 | 4.74411500 | H | 4.73000000 | -0.53869900 | -0.95720400 |
| H | 2.21400500 | -1.76468200 | 6.48583900 | H | 4.07286600 | 0.66103200 | -2.09176900 |
| H | 2.94699300 | -0.37205300 | 2.47443400 | H | 4.76299500 | -0.85331900 | -2.69445200 |
| H | -0.25603200 | -1.55576500 | 6.17453400 | H | 4.20841400 | -3.69480200 | -1.08571800 |
| H | -1.58834700 | 1.80202700 | 0.77508500 | H | 3.11555000 | -3.85367100 | 0.29957200 |
| H | -3.83711100 | 2.52324100 | -0.09938900 | H | 4.24318700 | -2.48426300 | 0.20079500 |
| H | -5.66334100 | -1.00640600 | 1.37670200 | H | 1.14819100 | -2.63336300 | 4.09113200 |
| H | 4.45241300 | -2.29345300 | 4.98141800 | H | 0.38272100 | -1.07466100 | 4.40878700 |
| H | 4.55283900 | -0.64193300 | 5.59180400 | H | -1.75591500 | -2.05219000 | 3.87218500 |
| H | 4.79665800 | -0.96181400 | 3.86447500 | H | -0.97150500 | -3.56698100 | 3.42322300 |
| C | -3.61114500 | -1.92424600 | 2.78386500 | C | 3.27343600 | 4.40260800 | 1.16358300 |
| H | -2.70512700 | -2.52745900 | 2.66347800 | C | 3.84335600 | 3.10588300 | 1.23815300 |
| H | -3.63547800 | -1.60818800 | 3.83730400 | C | 3.08048800 | 1.98516800 | 0.90318800 |
| H | -4.49567000 | -2.53286300 | 2.58967300 | C | 1.75659500 | 2.19455700 | 0.50097100 |
| H | -5.74621100 | 0.88136700 | -0.21228800 | C | 1.23445000 | 3.48658600 | 0.44786200 |

M -1581.464525

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|------------|-------------|
| Rh | 1.22223400 | -0.83228700 | -0.28238600 | C | 1.95713800 | 4.62646600 | 0.76927300 |
| C | 1.21102500 | -2.72141300 | -1.39486600 | N | 0.74018200 | 1.31035200 | 0.10141800 |
| C | 0.61148400 | -1.66382500 | -2.19207200 | C | -0.30009300 | 2.06883400 | -0.14716000 |
| C | 1.64597900 | -0.68759400 | -2.49211100 | O | -0.07582600 | 3.39003900 | 0.03448200 |
| C | 2.83800700 | -1.08500800 | -1.82515600 | C | -1.67282400 | 1.67058400 | -0.50708100 |
| C | 2.56961300 | -2.35294000 | -1.14529900 | C | -2.26121500 | 0.66621600 | 0.21079100 |
| C | 0.52406400 | -3.97740600 | -0.96767700 | C | -4.35013300 | 0.90733900 | -1.14311300 |
| C | -0.76098800 | -1.69750500 | -2.77718600 | C | -3.75431200 | 1.92311200 | -1.83029400 |
| C | 1.48254700 | 0.50344700 | -3.37584700 | C | -2.42336700 | 2.34255900 | -1.54093100 |
| C | 4.16774400 | -0.40764600 | -1.88536100 | C | 5.27664700 | 2.95219300 | 1.68760200 |
| C | 3.58147000 | -3.13491900 | -0.37763400 | H | 3.89070600 | 5.25591300 | 1.43114900 |
| C | 0.44945600 | -1.89520800 | 3.68574800 | H | 3.49266400 | 0.98611600 | 0.97578400 |
| C | -0.92472600 | -2.47963000 | 3.30337100 | H | 1.52527800 | 5.61979700 | 0.71978900 |
| C | -1.09995400 | -2.13597100 | 1.81700300 | H | -1.71777500 | 0.18147900 | 1.01000500 |
| N | 0.03206900 | -1.47881400 | 1.38080300 | H | -4.28871700 | 2.43199400 | -2.62495300 |
| C | 0.95561600 | -1.36832500 | 2.36007500 | H | 5.42096100 | 3.36370800 | 2.69394300 |
| O | 2.07388800 | -0.88872000 | 2.07452400 | H | 5.96021600 | 3.49072500 | 1.01969900 |
| | | | | H | 5.57827500 | 1.90072600 | 1.70584200 |
| | | | | C | -3.63072300 | 0.21024100 | -0.06646700 |

| | | | |
|----|-------------|-------------|-------------|
| H | -3.68611800 | -0.88286400 | -0.12353500 |
| Br | -4.70266400 | 0.59518800 | 1.67853000 |
| C | -1.85655500 | 3.47581700 | -2.30817100 |
| H | -1.95485600 | 4.39037200 | -1.69938300 |
| H | -0.78822900 | 3.35425500 | -2.50933700 |
| H | -2.40586500 | 3.63897100 | -3.23763300 |
| H | -5.35899900 | 0.58677800 | -1.38419500 |

TSMJ -1581.448892

| | | | |
|----|-------------|-------------|-------------|
| Rh | 1.23805700 | -0.86374800 | -0.26898100 |
| C | 1.19428800 | -2.77634000 | -1.35029100 |
| C | 0.60960200 | -1.72127200 | -2.16231300 |
| C | 1.65898900 | -0.76798300 | -2.47915000 |
| C | 2.84483100 | -1.17185800 | -1.80221000 |
| C | 2.55818700 | -2.42446800 | -1.10316700 |
| C | 0.49232400 | -4.01776700 | -0.90727500 |
| C | -0.76730700 | -1.73486500 | -2.74005400 |
| C | 1.51577100 | 0.40983400 | -3.38364100 |
| C | 4.18216000 | -0.51024100 | -1.86995600 |
| C | 3.55776300 | -3.21159700 | -0.32454100 |
| C | 0.51038100 | -1.82851100 | 3.73046500 |
| C | -0.88347700 | -2.39730500 | 3.40092800 |
| C | -1.09479400 | -2.08229700 | 1.91383200 |
| N | 0.03912000 | -1.46352600 | 1.42534900 |
| C | 0.98489300 | -1.33905700 | 2.38022900 |
| O | 2.10120200 | -0.87945200 | 2.05507400 |
| O | -2.10688800 | -2.31307600 | 1.26014700 |
| H | -0.56211200 | -3.82880100 | -0.69354100 |
| H | 0.95438800 | -4.45155500 | -0.01756400 |
| H | 0.54439800 | -4.76432900 | -1.71156300 |
| H | -0.76114100 | -2.32314500 | -3.66855100 |
| H | -1.11155900 | -0.72950700 | -2.99304900 |
| H | -1.48594900 | -2.20097000 | -2.06150300 |
| H | 2.17125500 | 1.23444500 | -3.09298100 |
| H | 0.48489700 | 0.76798400 | -3.42466800 |
| H | 1.79715500 | 0.10585300 | -4.40142100 |
| H | 4.74755200 | -0.64762500 | -0.94459200 |
| H | 4.09803800 | 0.55950600 | -2.07595300 |
| H | 4.76797700 | -0.96208900 | -2.68246600 |
| H | 4.17555700 | -3.79185800 | -1.02405400 |
| H | 3.08063600 | -3.91245800 | 0.36354600 |
| H | 4.22943600 | -2.56279100 | 0.24438100 |
| H | 1.20915400 | -2.56992600 | 4.12990000 |
| H | 0.47872700 | -0.99241600 | 4.43768700 |

| | | | |
|----|-------------|-------------|-------------|
| H | -1.69052900 | -1.94362300 | 3.98363300 |
| H | -0.94484600 | -3.48104700 | 3.54518600 |
| C | 3.23760300 | 4.41140800 | 1.06751400 |
| C | 3.78075400 | 3.11282000 | 1.25582100 |
| C | 3.02528700 | 1.98442600 | 0.93502500 |
| C | 1.73292800 | 2.18615600 | 0.43338400 |
| C | 1.23642100 | 3.48161200 | 0.27067700 |
| C | 1.95457200 | 4.62891100 | 0.57412000 |
| N | 0.73376600 | 1.29619800 | 0.01815700 |
| C | -0.28027100 | 2.05210100 | -0.34777900 |
| O | -0.04142800 | 3.37950500 | -0.22318700 |
| C | -1.62488000 | 1.66305900 | -0.77856200 |
| C | -2.19266800 | 0.50877700 | -0.16134400 |
| C | -4.33373200 | 0.87449700 | -1.36979300 |
| C | -3.74134100 | 1.95085400 | -1.97314000 |
| C | -2.38387500 | 2.38132400 | -1.70229800 |
| C | 5.17319700 | 2.96953800 | 1.82076700 |
| H | 3.84991000 | 5.27106400 | 1.32572600 |
| H | 3.41358900 | 0.98576800 | 1.09378300 |
| H | 1.54351200 | 5.62302800 | 0.43858000 |
| H | -1.55252300 | -0.20924300 | 0.33674800 |
| H | -4.29768400 | 2.52122400 | -2.71076800 |
| H | 5.22301500 | 3.35902900 | 2.84529300 |
| H | 5.90213100 | 3.53437500 | 1.22730300 |
| H | 5.48857500 | 1.92226500 | 1.84279000 |
| C | -3.56577400 | 0.09583200 | -0.46414300 |
| H | -3.86688000 | -0.90601100 | -0.17354800 |
| Br | -3.51697800 | 1.03988500 | 1.69357200 |
| C | -1.89034700 | 3.57523700 | -2.45375800 |
| H | -2.14865300 | 4.48932600 | -1.89885500 |
| H | -0.80811200 | 3.57120500 | -2.59343700 |
| H | -2.38530900 | 3.63903100 | -3.42711500 |
| H | -5.35139000 | 0.58323000 | -1.60270400 |

TSMN -1581.426631

| | | | |
|----|-------------|-------------|-------------|
| Rh | 1.07192200 | -0.88682800 | -0.66025600 |
| C | 0.87797700 | -2.62332000 | -2.01609700 |
| C | 0.79461600 | -1.39399900 | -2.80798500 |
| C | 2.02198900 | -0.68796400 | -2.65880500 |
| C | 2.86125000 | -1.44652200 | -1.73761300 |
| C | 2.15438300 | -2.66600500 | -1.38257700 |
| C | -0.19060500 | -3.65863800 | -1.93853700 |
| C | -0.35101400 | -1.02376100 | -3.68910700 |
| C | 2.41397100 | 0.57824000 | -3.34236400 |

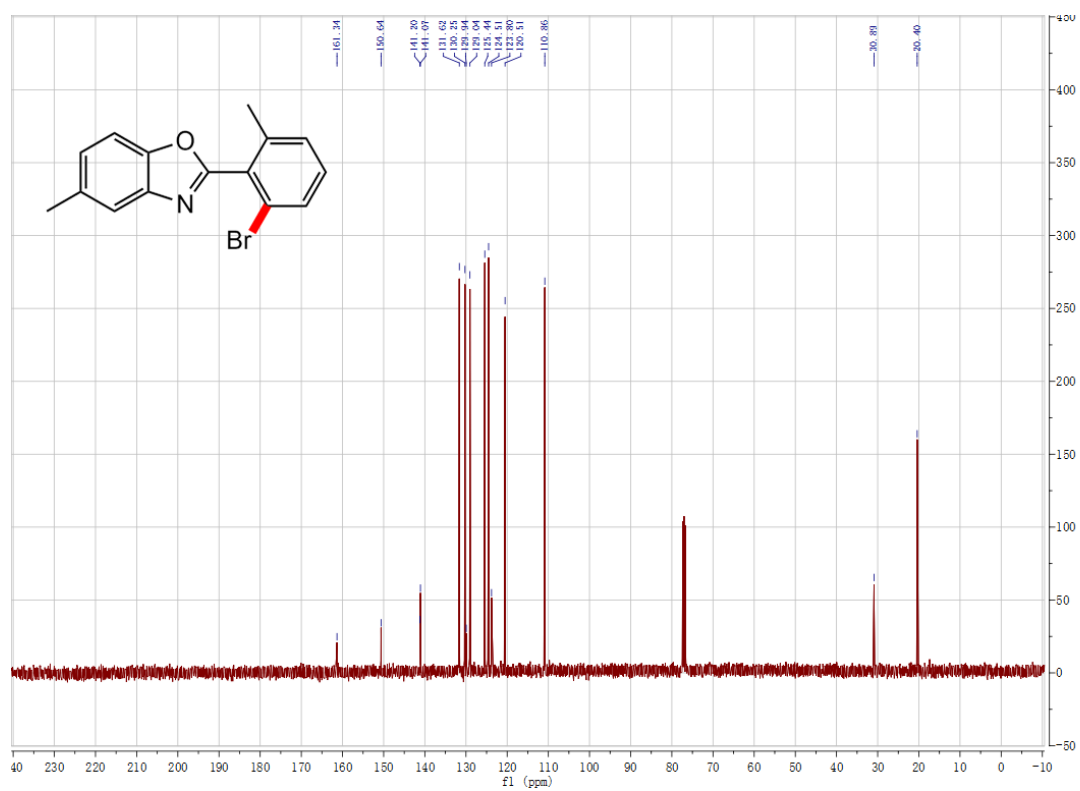
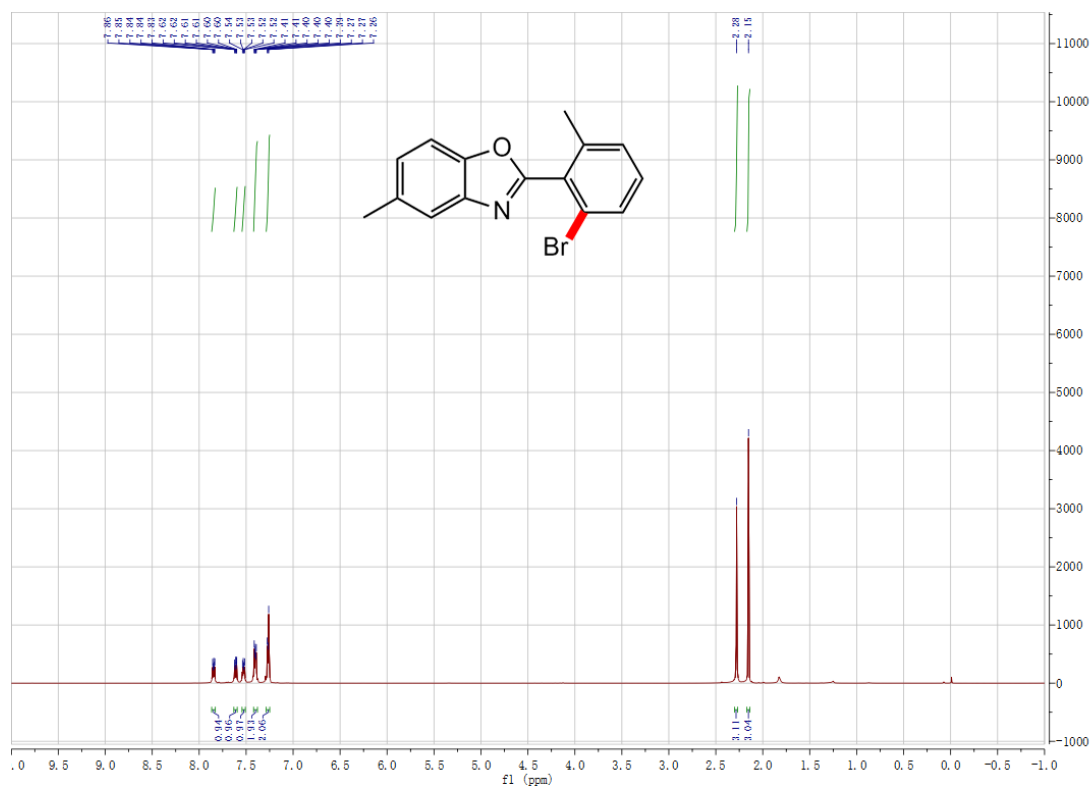
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|---|-------------|-------------|-------------|----------|---------------------|-------------|-------------|
| C | 4.26164200 | -1.11325900 | -1.35886600 | H | 3.55007600 | 1.06146000 | 0.62318700 |
| C | 2.68811400 | -3.75769900 | -0.51610300 | H | 1.10713500 | 5.45029400 | 1.06039000 |
| C | 0.93147000 | -1.28429100 | 3.79332300 | H | -1.16389700 | -0.41230600 | 1.00425100 |
| C | -0.33276900 | -0.78619500 | 4.50710500 | H | -4.67138100 | 1.94500500 | -2.17272700 |
| C | -1.25110200 | -0.32803800 | 3.37456800 | H | 5.30034600 | 3.41327300 | 2.59447600 |
| N | -0.61746200 | -0.57569100 | 2.14542000 | H | 5.74879400 | 3.76029400 | 0.92476700 |
| C | 0.61029400 | -1.07052000 | 2.32679400 | H | 5.54786800 | 2.08011600 | 1.45254200 |
| O | 1.43777800 | -1.33121600 | 1.40830100 | C | -3.07833000 | -0.71642900 | -0.67326000 |
| O | -2.34798100 | 0.18266300 | 3.47956700 | H | -2.71302400 | -1.47809700 | -1.38622500 |
| H | -1.18638900 | -3.22273000 | -2.05886800 | Br | -3.94545000 | -1.91532800 | 0.76752900 |
| H | -0.15390500 | -4.21365200 | -0.99809100 | C | -2.56981800 | 3.47372900 | -1.60354400 |
| H | -0.04906000 | -4.37847600 | -2.75711600 | H | -2.65573700 | 4.06045500 | -0.67731500 |
| H | -0.20998700 | -1.48795300 | -4.67500900 | H | -1.58904600 | 3.71063300 | -2.02858200 |
| H | -0.41957200 | 0.05660000 | -3.83802800 | H | -3.35832400 | 3.79894200 | -2.28463600 |
| H | -1.29989600 | -1.39197000 | -3.29000700 | H | -5.03031200 | -0.45155300 | -1.69120600 |
| H | 3.07589900 | 1.18745000 | -2.72211400 | | | | |
| H | 1.54283700 | 1.17392300 | -3.62478300 | N | -1581.478222 | | |
| H | 2.96116300 | 0.32842900 | -4.26189900 | Rh | -0.21382400 | -0.98722700 | 0.28466500 |
| H | 4.50933000 | -1.47781400 | -0.35878000 | C | -1.27743000 | -2.47428500 | 1.60099100 |
| H | 4.45367500 | -0.03923600 | -1.40907000 | C | -1.50497700 | -2.84550200 | 0.24378800 |
| H | 4.94184700 | -1.60710200 | -2.06831700 | C | -0.20951200 | -3.07718900 | -0.36197100 |
| H | 3.29200600 | -4.43891400 | -1.13043400 | C | 0.79438600 | -3.07086500 | 0.71103200 |
| H | 1.88489900 | -4.34002000 | -0.05875900 | C | 0.15369200 | -2.67317700 | 1.89302700 |
| H | 3.33133600 | -3.36519500 | 0.27531800 | C | -2.30803000 | -2.15696800 | 2.63561800 |
| H | 1.14653200 | -2.34400800 | 3.96579200 | C | -2.82115400 | -3.06554100 | -0.42631500 |
| H | 1.83395400 | -0.72054200 | 4.05073900 | C | 0.03376700 | -3.56212400 | -1.75497000 |
| H | -0.14564100 | 0.05268800 | 5.18391800 | C | 2.21989100 | -3.47879000 | 0.52870100 |
| H | -0.83942400 | -1.56657600 | 5.08345500 | C | 0.75587300 | -2.47157800 | 3.24409000 |
| C | 2.98582100 | 4.37739100 | 1.29046300 | C | 0.50063400 | 2.30983700 | 3.50982500 |
| C | 3.68857500 | 3.15106100 | 1.17551000 | C | 1.02462200 | 3.72667300 | 3.21991000 |
| C | 3.03013100 | 2.00949300 | 0.71142600 | C | 1.16847600 | 3.79764000 | 1.70892100 |
| C | 1.67769600 | 2.12935000 | 0.37553600 | N | 0.78815800 | 2.53802600 | 1.19969000 |
| C | 1.02147300 | 3.35352500 | 0.50946700 | C | 0.40338800 | 1.64793400 | 2.15102400 |
| C | 1.63839000 | 4.51006700 | 0.96251600 | O | 0.02354000 | 0.48552600 | 1.95829800 |
| N | 0.74053300 | 1.21069000 | -0.10842000 | O | 1.53156100 | 4.71820600 | 1.01427700 |
| C | -0.39023300 | 1.87015500 | -0.22379500 | H | -3.23283300 | -1.78465200 | 2.18867400 |
| O | -0.29091600 | 3.17136700 | 0.12493700 | H | -1.93997500 | -1.41217900 | 3.34691800 |
| C | -1.68246300 | 1.28261100 | -0.60638700 | H | -2.55104800 | -3.06512700 | 3.20438300 |
| C | -1.88396500 | -0.02571100 | -0.17462000 | H | -3.03808300 | -4.14256600 | -0.41033600 |
| C | -4.13159400 | 0.05781600 | -1.35689900 | H | -2.81226400 | -2.75552600 | -1.47474000 |
| C | -3.91942800 | 1.37031800 | -1.64225500 | H | -3.64198100 | -2.56592700 | 0.09428600 |
| C | -2.70195700 | 2.02628000 | -1.28021900 | H | 1.02022500 | -3.25904500 | -2.11687600 |
| C | 5.14880300 | 3.09350400 | 1.55645400 | H | -0.72353600 | -3.18943000 | -2.44922900 |
| H | 3.52174100 | 5.24968800 | 1.65456400 | H | -0.00331200 | -4.66022100 | -1.77444800 |

| | | | | | | | |
|--------------------------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | 2.84947100 | -3.16087000 | 1.36210500 | C | -1.26086100 | -2.40595300 | 1.61460800 |
| H | 2.64172100 | -3.08830300 | -0.40126100 | C | -1.60647000 | -2.71337000 | 0.26750600 |
| H | 2.27062600 | -4.57490600 | 0.47113600 | C | -0.36602800 | -2.93655400 | -0.45550200 |
| H | 0.40706500 | -3.25649200 | 3.92809200 | C | 0.72305800 | -2.97064600 | 0.52878400 |
| H | 0.44728400 | -1.50988900 | 3.66696700 | C | 0.18858600 | -2.61194400 | 1.77766000 |
| H | 1.84753300 | -2.50580800 | 3.21505500 | C | -2.19265900 | -2.10197800 | 2.74106600 |
| H | -0.49122000 | 2.30196400 | 3.97274900 | C | -2.98496600 | -2.88158100 | -0.28416000 |
| H | 1.16598600 | 1.71946200 | 4.14714600 | C | -0.23836900 | -3.39330000 | -1.87258300 |
| H | 1.99898800 | 3.92466800 | 3.67688000 | C | 2.13178000 | -3.34735600 | 0.20755300 |
| H | 0.34117100 | 4.51476300 | 3.54910700 | C | 0.90545000 | -2.48271400 | 3.08145500 |
| C | 5.23231200 | 0.73515500 | -1.87267000 | C | 0.31310500 | 2.26126100 | 3.73770100 |
| C | 5.03897200 | 0.03136000 | -0.65777000 | C | 1.12916700 | 3.56000000 | 3.62481300 |
| C | 3.74676300 | -0.29800200 | -0.23867900 | C | 1.68994400 | 3.55632700 | 2.21278600 |
| C | 2.67890100 | 0.08931800 | -1.05339200 | N | 1.20429600 | 2.39441300 | 1.57940100 |
| C | 2.91266800 | 0.79057900 | -2.24065000 | C | 0.42214900 | 1.61250900 | 2.37195300 |
| C | 4.17726800 | 1.13361000 | -2.69179000 | O | -0.11860900 | 0.54892100 | 2.04677800 |
| N | 1.29463300 | -0.05229700 | -0.93768600 | O | 2.41465700 | 4.36017700 | 1.67295600 |
| C | 0.77493200 | 0.53658100 | -1.99194000 | H | -3.17546200 | -1.78353300 | 2.38528700 |
| O | 1.68691900 | 1.06825600 | -2.82494900 | H | -1.78440400 | -1.32378100 | 3.39258300 |
| C | -0.66848000 | 0.62714600 | -2.13101100 | H | -2.33249700 | -3.00374900 | 3.35279400 |
| C | -1.33663300 | 0.07307300 | -1.01500900 | H | -3.27716300 | -3.93385800 | -0.16332000 |
| C | -3.49505300 | 0.78047600 | -2.16957600 | H | -3.03627300 | -2.65099700 | -1.35122000 |
| C | -2.78307200 | 1.20528600 | -3.24099700 | H | -3.72187200 | -2.27630600 | 0.24928800 |
| C | -1.34771600 | 1.17881300 | -3.24106300 | H | 0.71280000 | -3.07712800 | -2.31021800 |
| C | 6.23781300 | -0.35275000 | 0.17657100 | H | -1.05408300 | -3.02093200 | -2.49696700 |
| H | 6.24705200 | 0.97909700 | -2.17474800 | H | -0.26760800 | -4.49133000 | -1.90516700 |
| H | 3.58014000 | -0.83345000 | 0.68987900 | H | 2.81613900 | -3.10650800 | 1.02348100 |
| H | 4.33431500 | 1.67954800 | -3.61555900 | H | 2.48395800 | -2.85892800 | -0.70538300 |
| H | 0.79342800 | 2.33586300 | 0.20438100 | H | 2.18057300 | -4.43116200 | 0.03518900 |
| H | -3.28840300 | 1.59432400 | -4.11827000 | H | 0.66128100 | -3.33856300 | 3.72491800 |
| H | 6.82528100 | 0.53120300 | 0.45296900 | H | 0.59529600 | -1.57773600 | 3.61280100 |
| H | 6.90739500 | -1.02251500 | -0.37701000 | H | 1.98967000 | -2.45866300 | 2.94950900 |
| H | 5.93717900 | -0.86165200 | 1.09738400 | H | -0.74383600 | 2.42901100 | 3.96645300 |
| C | -2.81416100 | 0.25518200 | -0.96629600 | H | 0.70602200 | 1.56794400 | 4.48815600 |
| H | -3.34654700 | -0.57481600 | -0.50682300 | H | 1.95716300 | 3.61474400 | 4.33751000 |
| Br | -3.13397800 | 1.77137000 | 0.45641300 | H | 0.52079400 | 4.45993200 | 3.75817100 |
| C | -0.62881100 | 1.72915000 | -4.42613200 | C | 5.18157300 | 0.77388600 | -1.88957900 |
| H | -0.02881200 | 2.60249300 | -4.13631700 | C | 4.97571700 | 0.19146700 | -0.61070700 |
| H | 0.07595600 | 0.99494700 | -4.83484200 | C | 3.68048600 | -0.08539800 | -0.16986500 |
| H | -1.32779100 | 2.02863100 | -5.20874300 | C | 2.62086500 | 0.22442000 | -1.03018100 |
| H | -4.57985200 | 0.82096400 | -2.15834200 | C | 2.86794300 | 0.80165400 | -2.28352900 |
| | | | | C | 4.13772600 | 1.09601100 | -2.75369600 |
| TSNK -1581.463926 | | | | N | 1.23847200 | 0.10332300 | -0.90979100 |
| Rh | -0.28516000 | -0.88807800 | 0.27139000 | C | 0.73025700 | 0.57064000 | -2.03435700 |

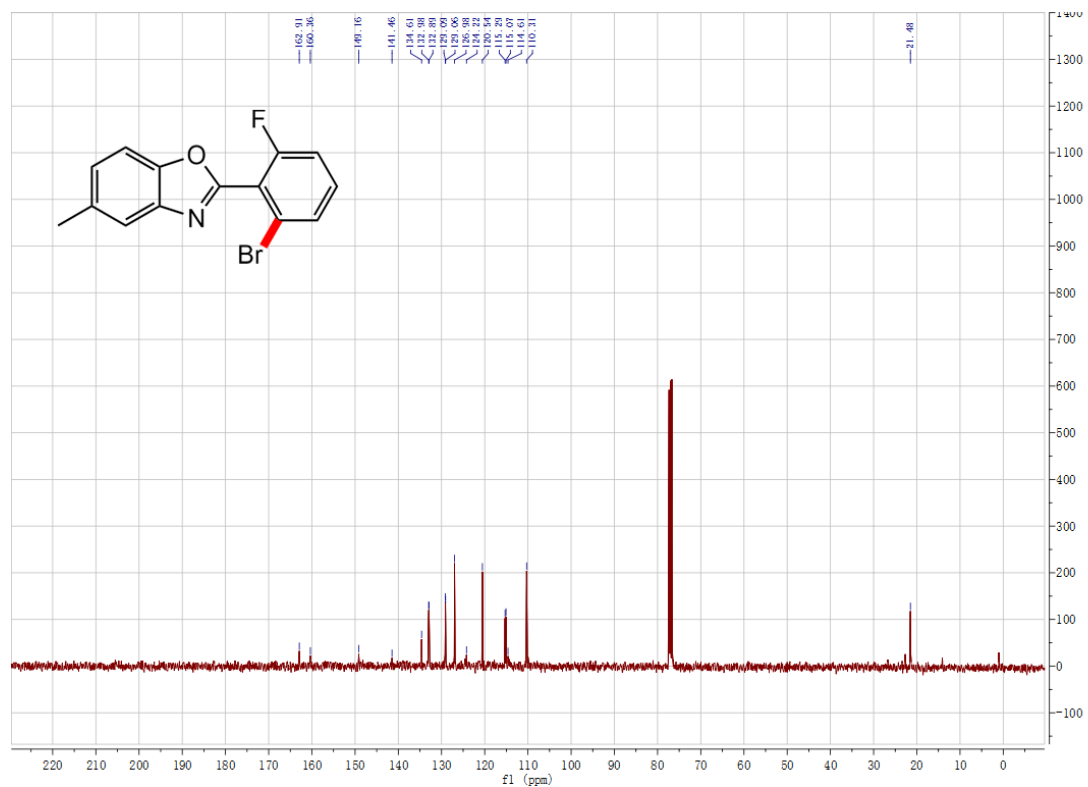
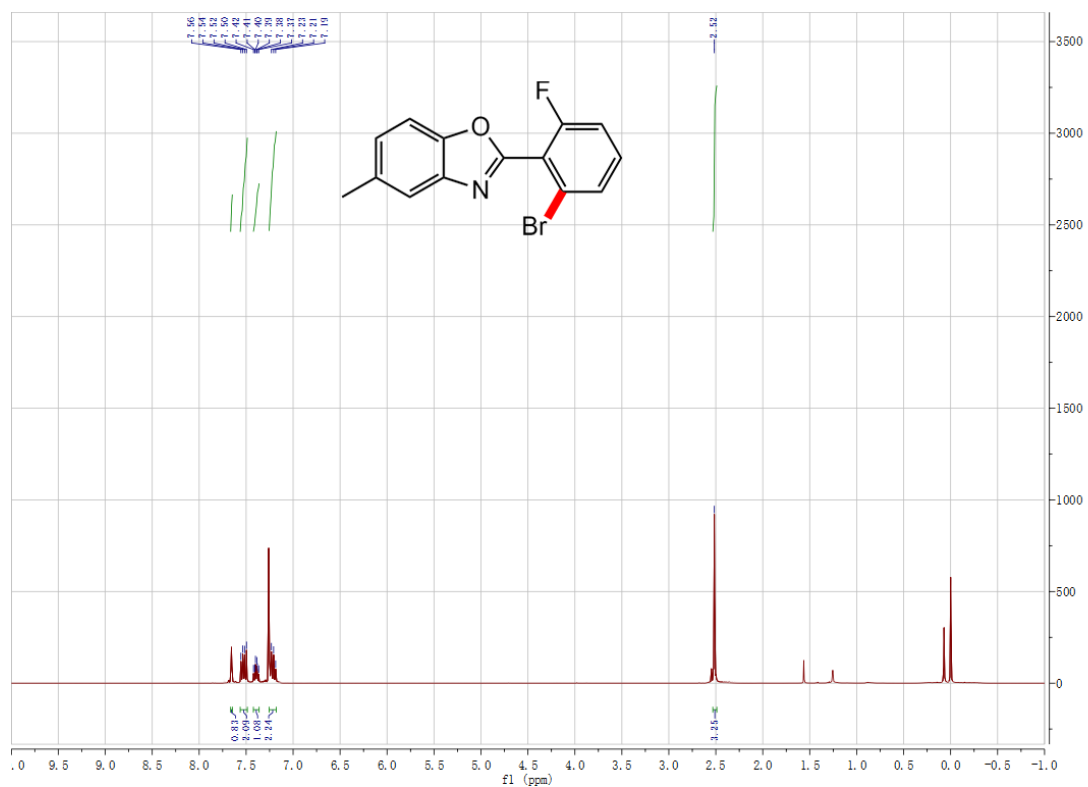
| | | | | | | | |
|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| O | 1.65267500 | 1.01261100 | -2.90684800 | H | 6.82809600 | -0.85226000 | -0.22913300 |
| C | -0.69743600 | 0.57753000 | -2.24714500 | H | 5.86380500 | -0.53293700 | 1.22454600 |
| C | -1.41521500 | 0.21290100 | -1.02122400 | C | -2.87946200 | 0.26702700 | -1.09980300 |
| C | -3.52966500 | 0.43285700 | -2.34644000 | H | -3.45403800 | -0.03079700 | -0.23123600 |
| C | -2.77818100 | 0.64952500 | -3.47587600 | Br | -2.13340100 | 2.35790400 | -0.13520500 |
| C | -1.34073100 | 0.74441200 | -3.46286800 | C | -0.62199700 | 0.99035900 | -4.75928900 |
| C | 6.16975400 | -0.12228800 | 0.25781800 | H | -0.14366200 | 1.97742400 | -4.75627700 |
| H | 6.20035400 | 0.98018700 | -2.20524700 | H | 0.16794300 | 0.25114100 | -4.92872200 |
| H | 3.50328400 | -0.52560500 | 0.80562400 | H | -1.32066000 | 0.95167900 | -5.59786600 |
| H | 4.30523000 | 1.54757800 | -3.72524400 | H | -4.61263400 | 0.39920500 | -2.39366000 |
| H | 1.44327700 | 2.17057500 | 0.61866200 | | | | |
| H | -3.27739500 | 0.76471000 | -4.43368100 | | | | |
| H | 6.76934500 | 0.77693300 | 0.44311600 | | | | |

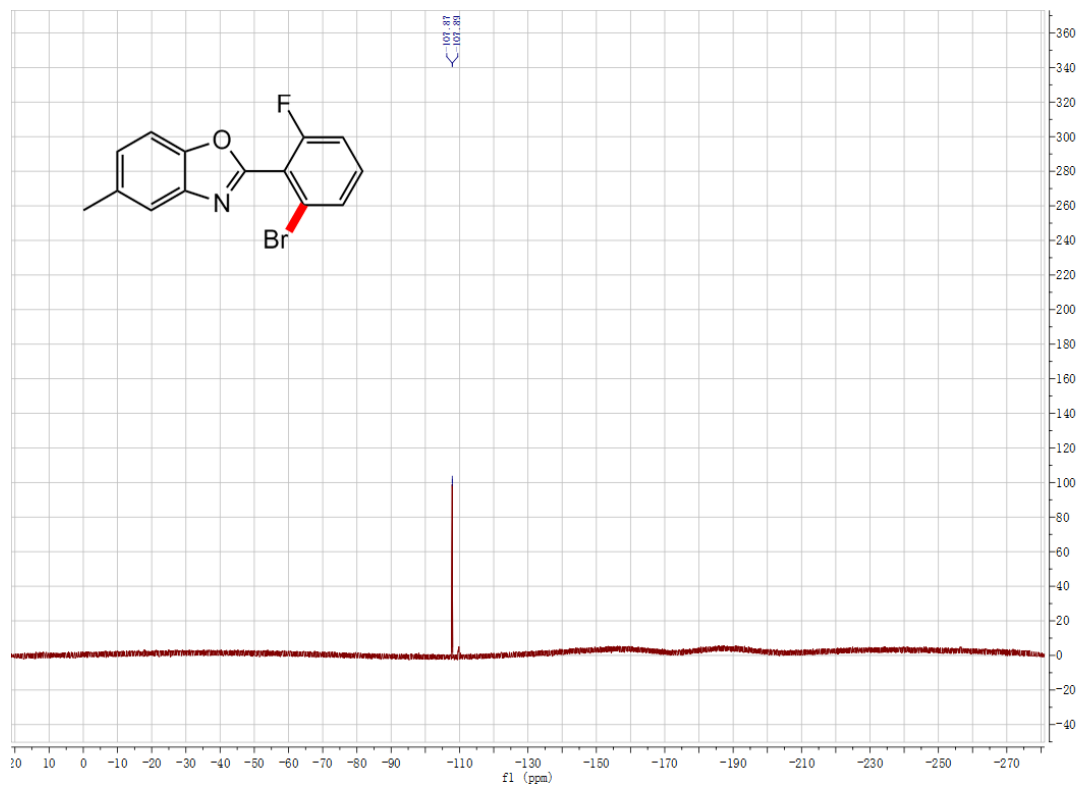
6. NMR Spectra of products

2-(2-bromo-6-methylphenyl)-5-methylbenzo[d]oxazole (2a)

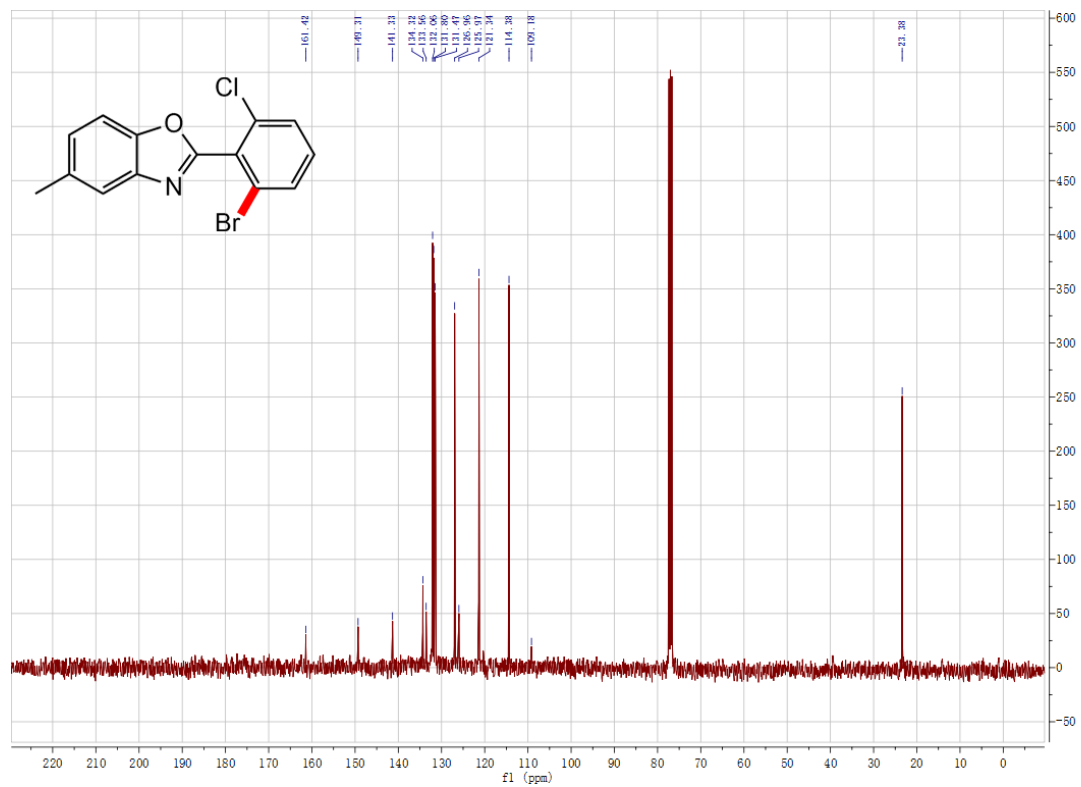
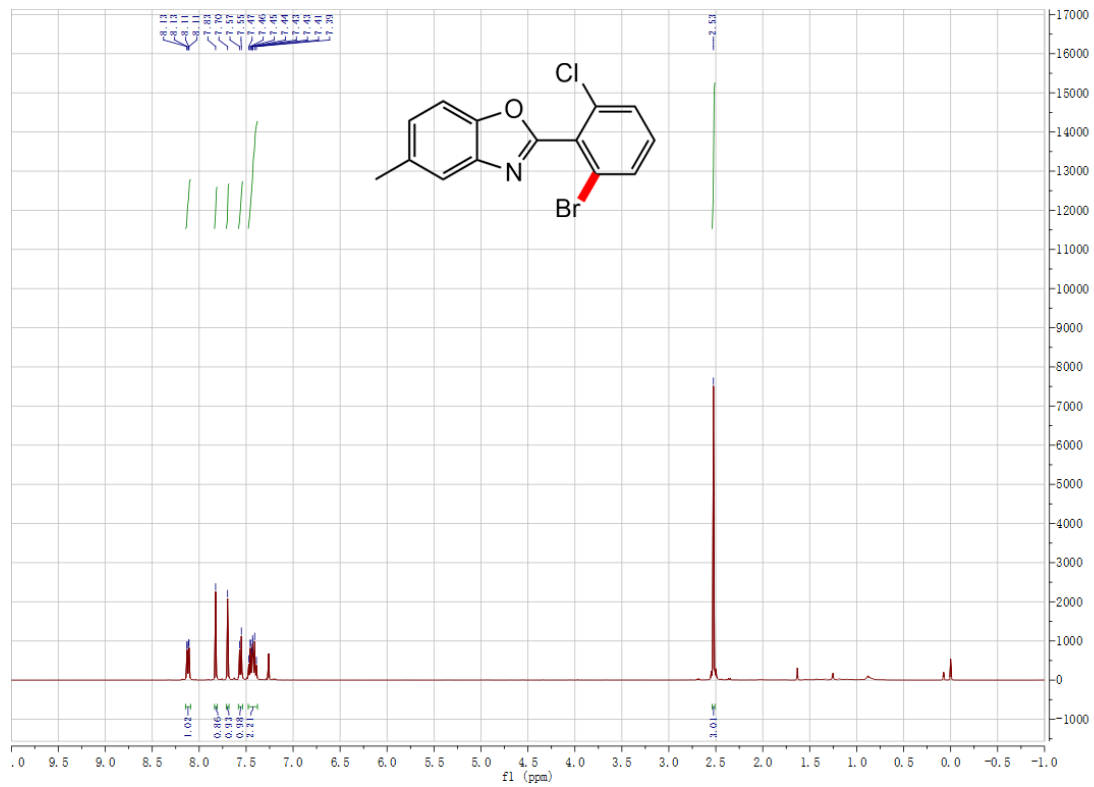


2-(2-bromo-6-fluorophenyl)-5-methylbenzo[d]oxazole (2b)

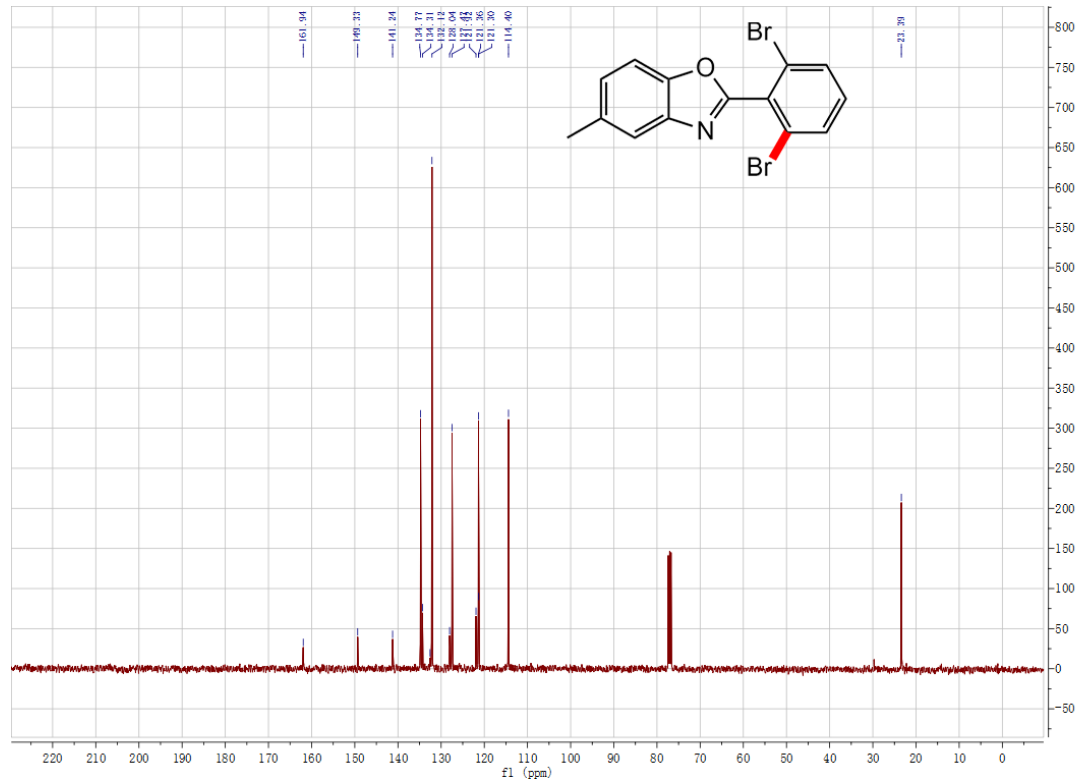
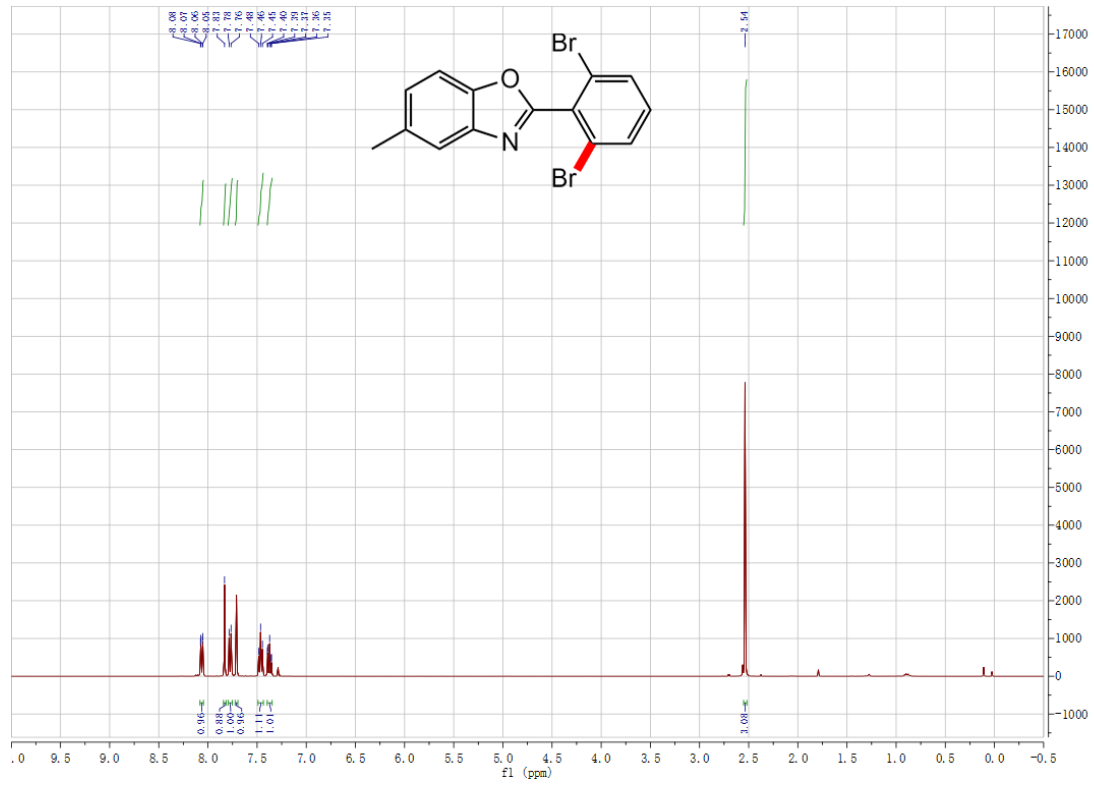




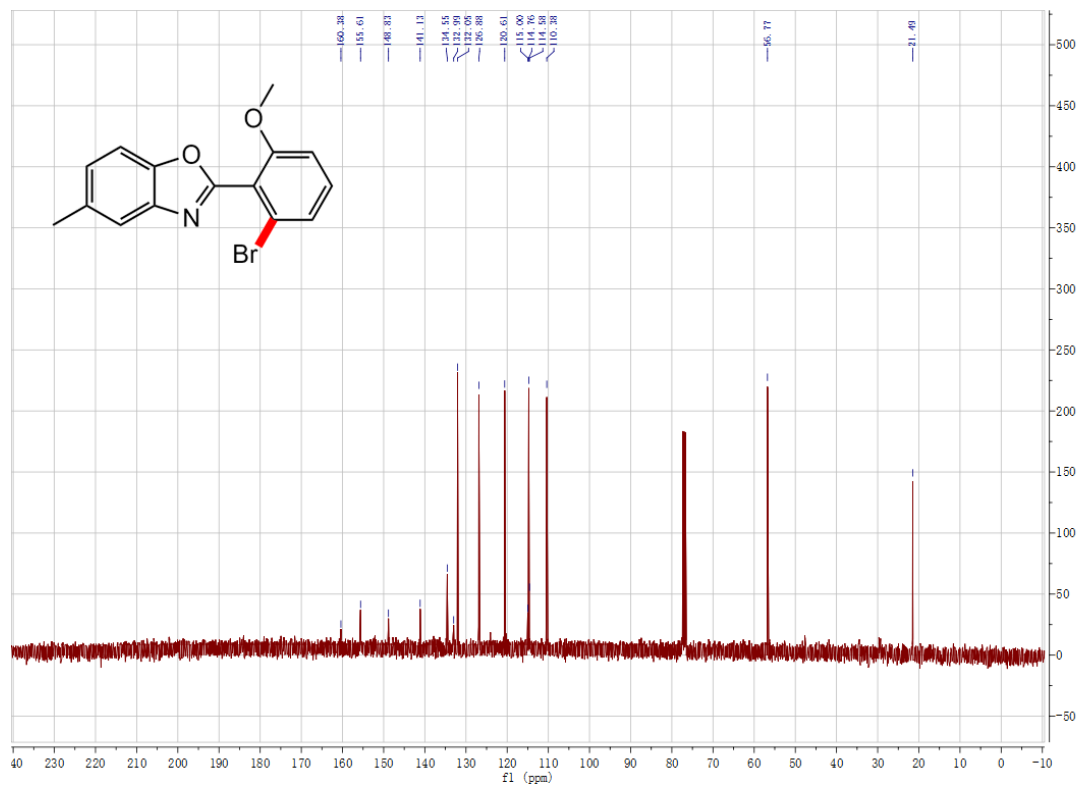
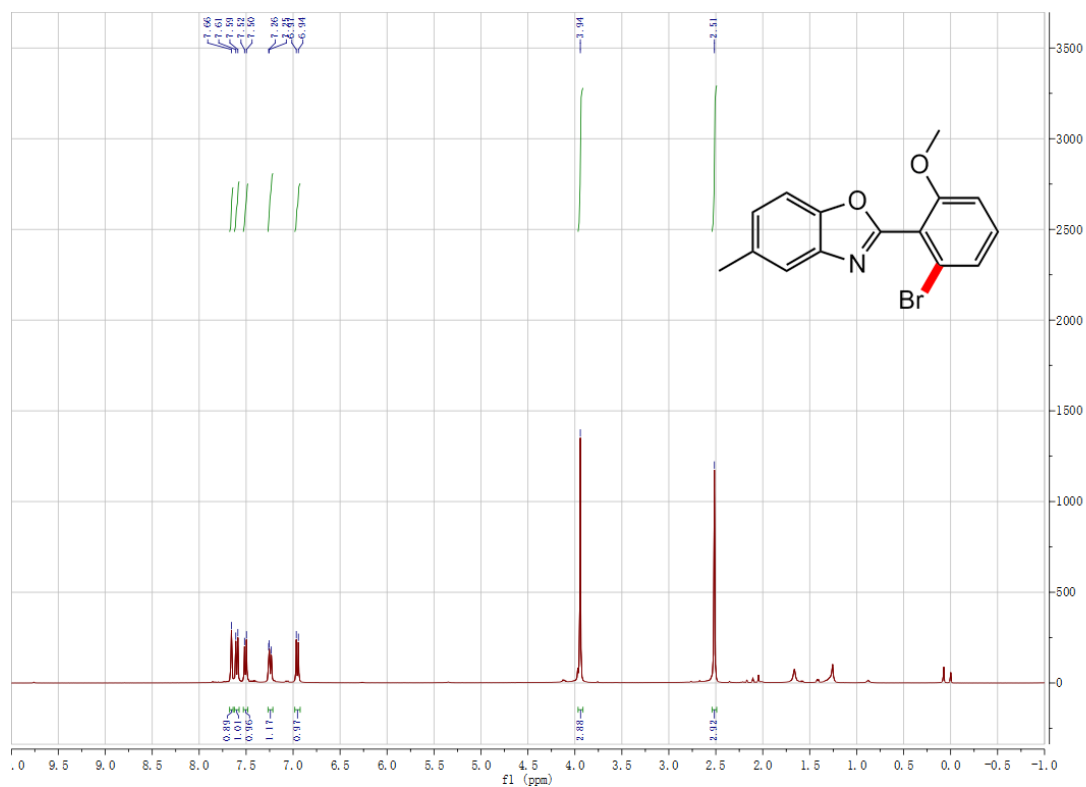
2-(2-bromo-6-chlorophenyl)-5-methylbenzo[d]oxazole (2c)



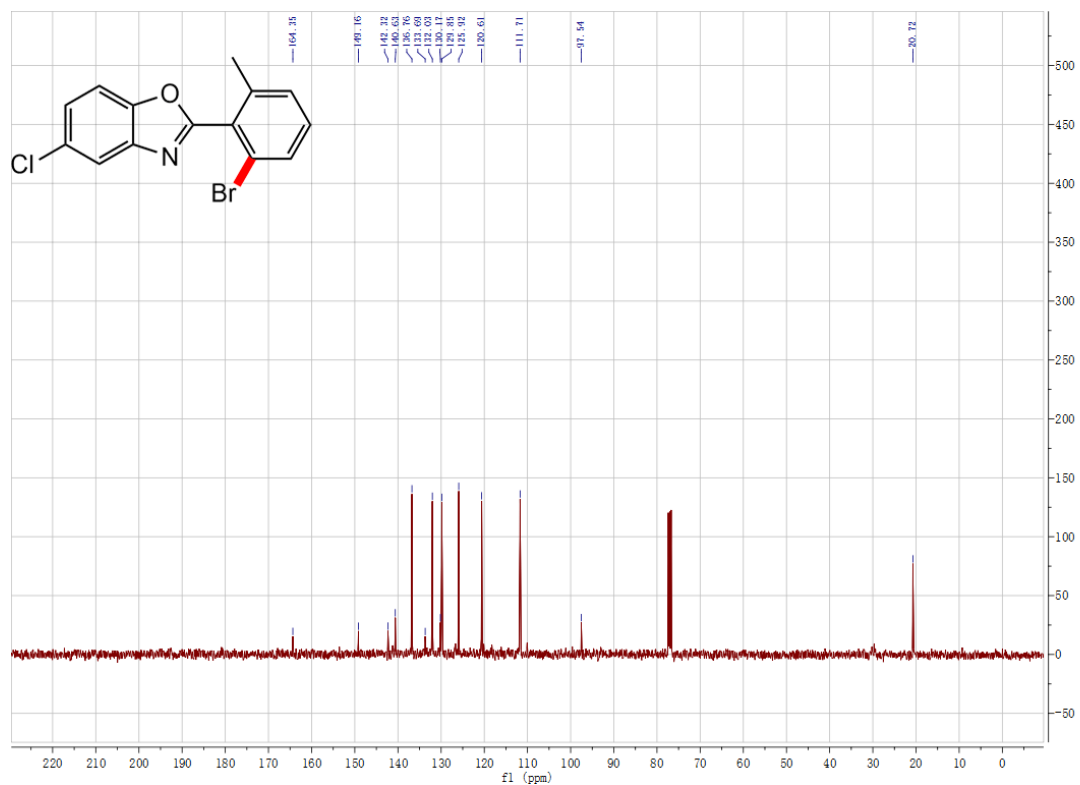
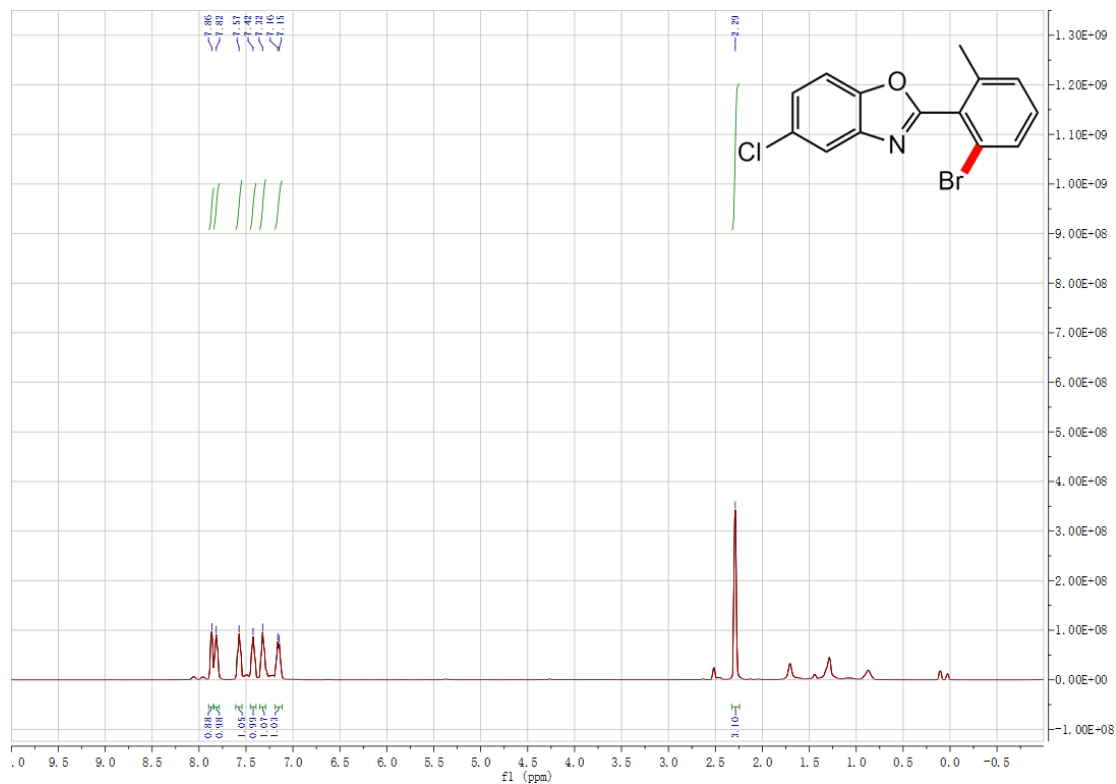
2-(2,6-dibromophenyl)-5-methylbenzo[d]oxazole (2m)



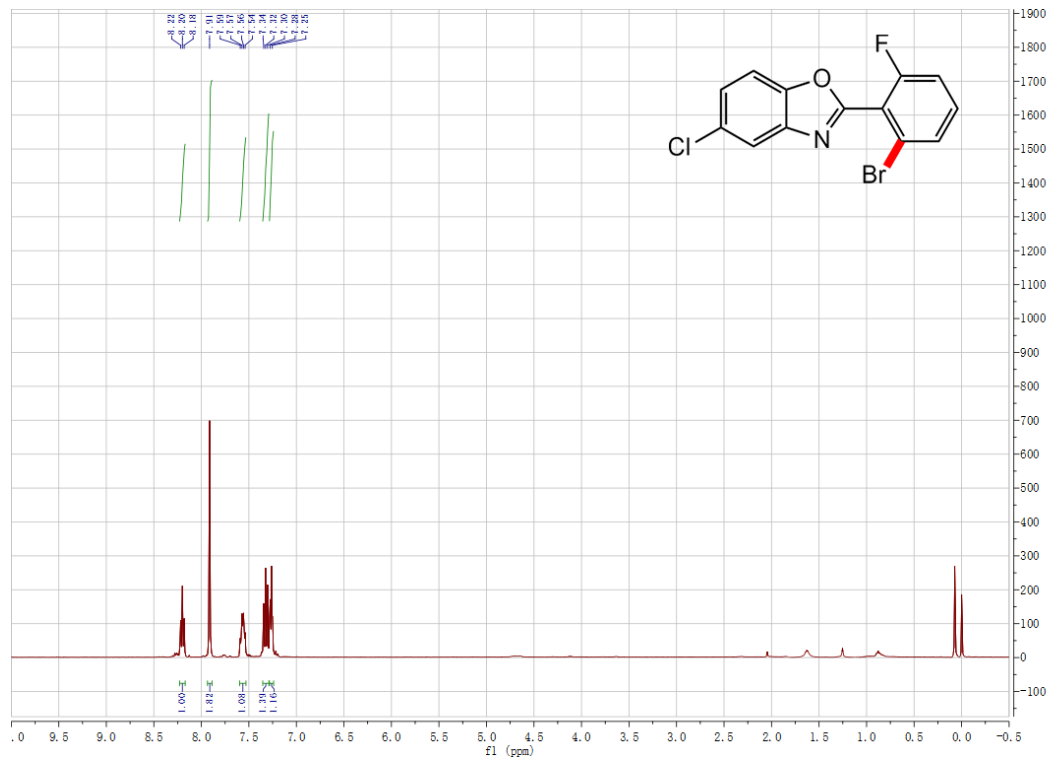
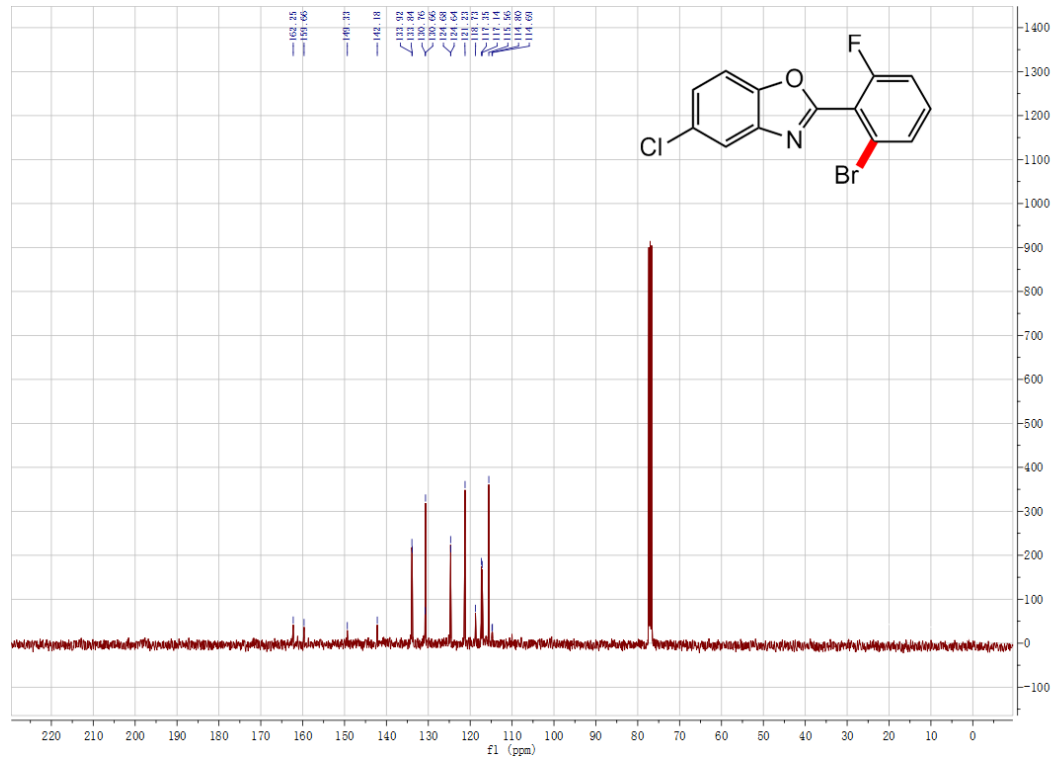
2-(2-bromo-6-methoxyphenyl)-5-methylbenzo[d]oxazole (2n)

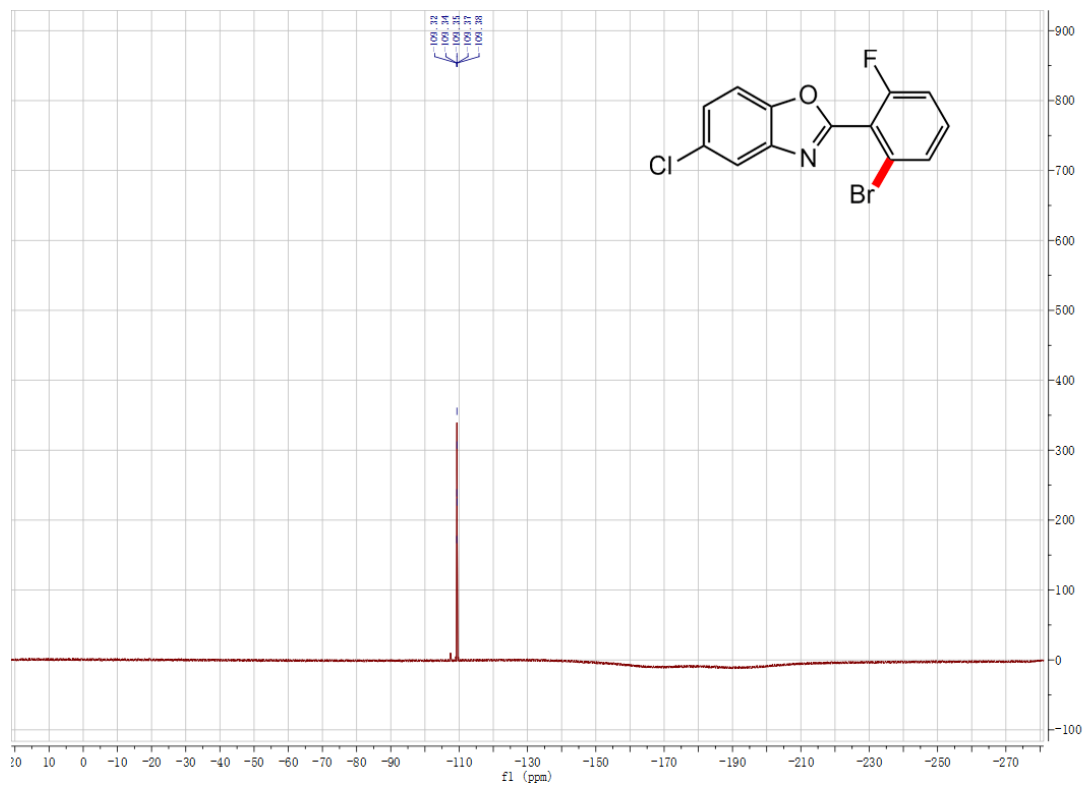


2-(2-bromo-6-methylphenyl)-5-chlorobenzo[d]oxazole (2o)

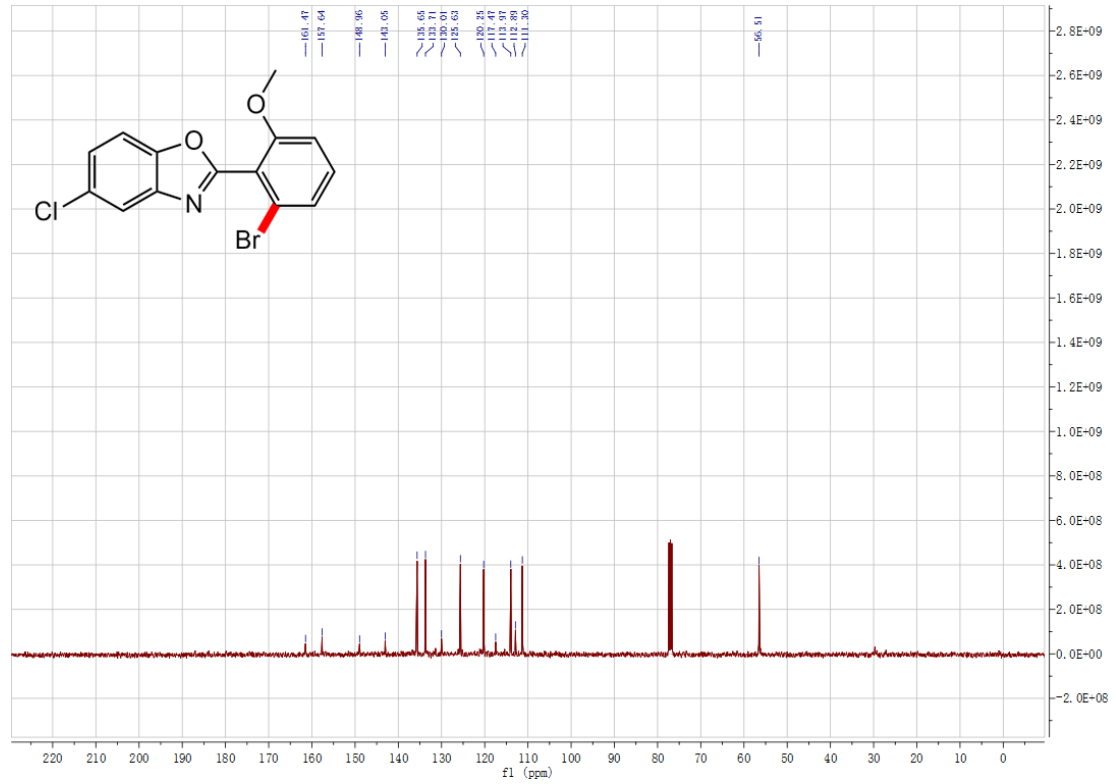
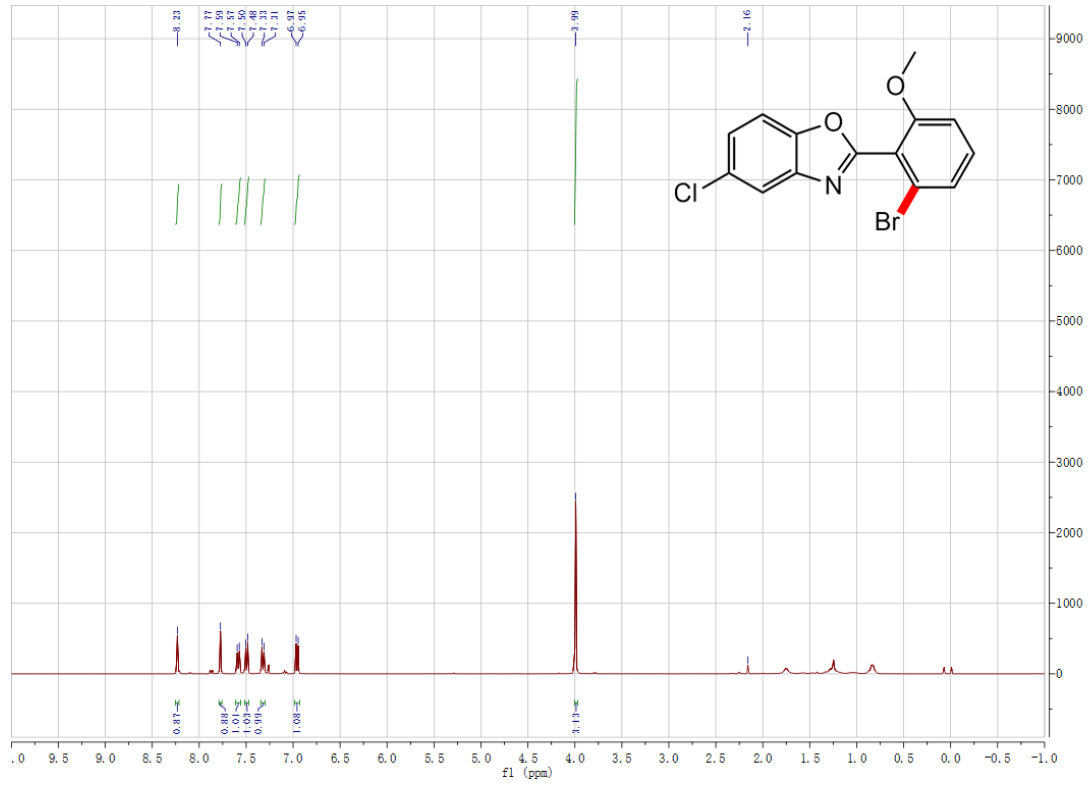


2-(2-bromo-6-fluorophenyl)-5-chlorobenzo[d]oxazole (2p)

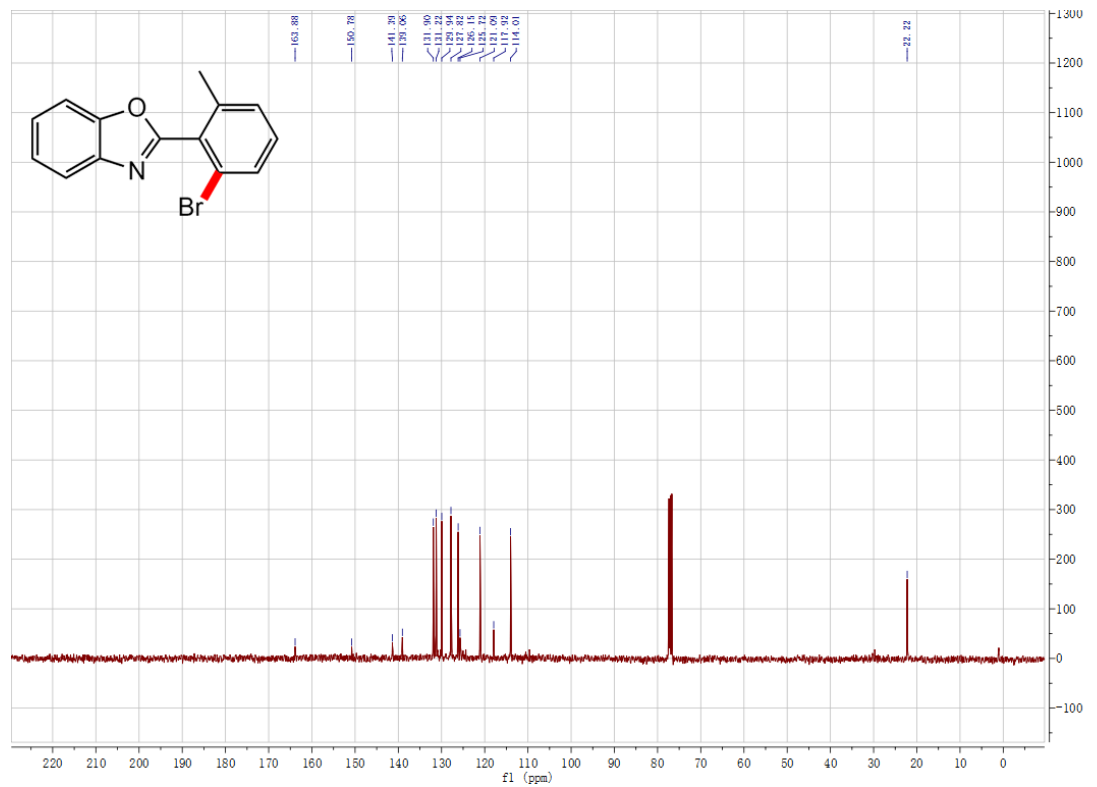
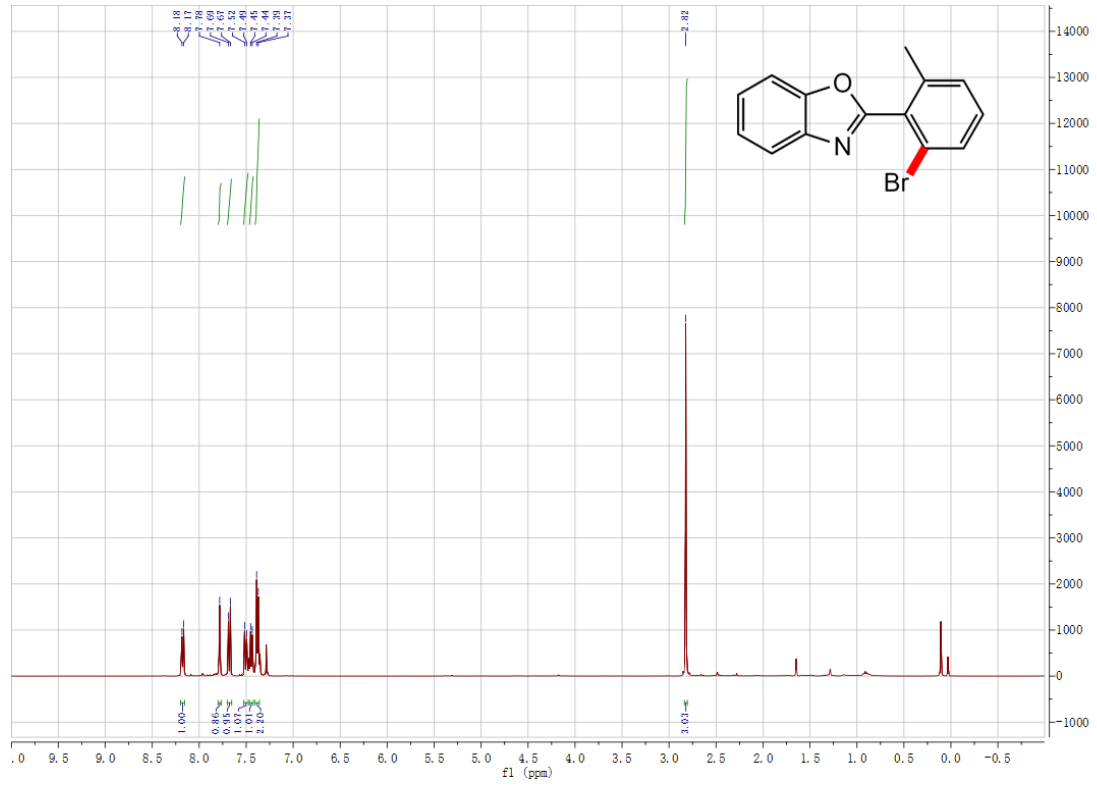




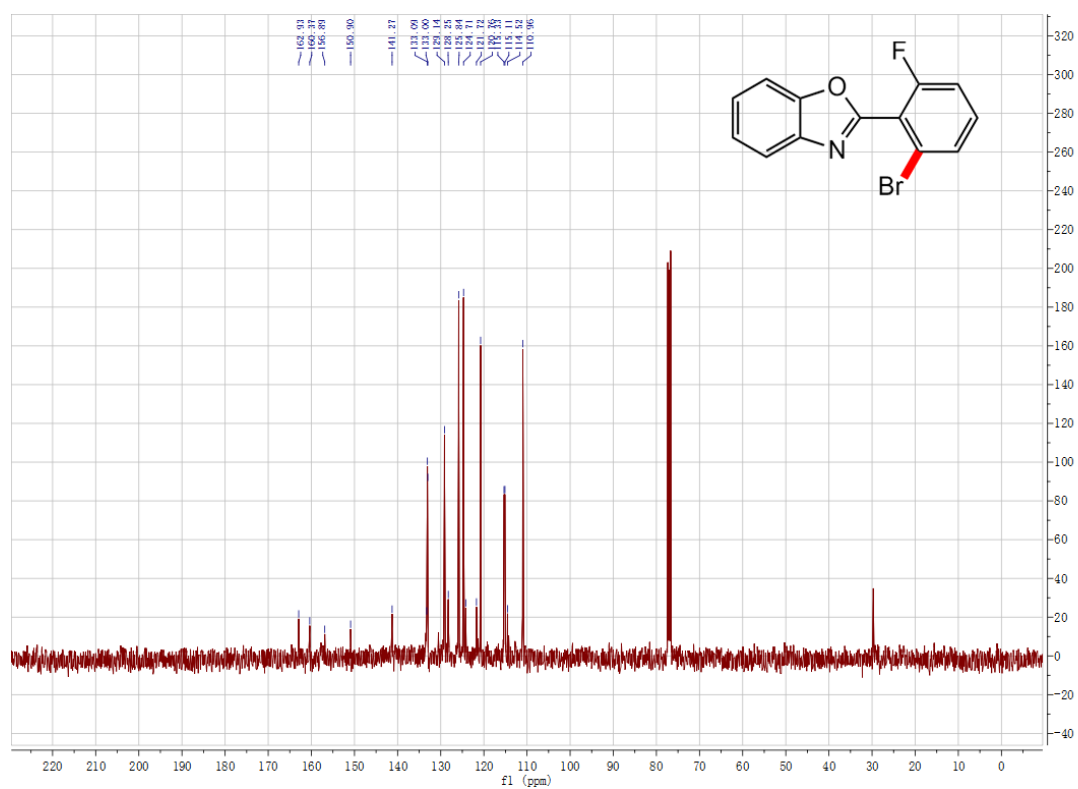
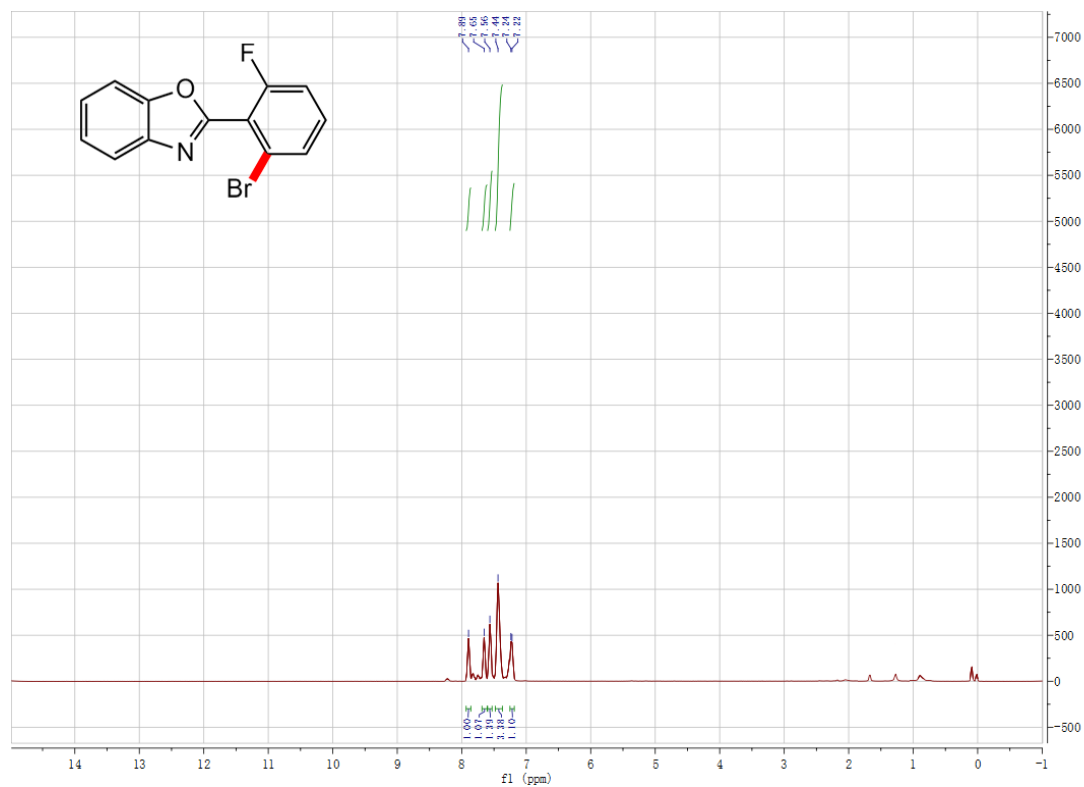
2-(2-bromo-6-methoxyphenyl)-5-chlorobenzo[d]oxazole (2q)

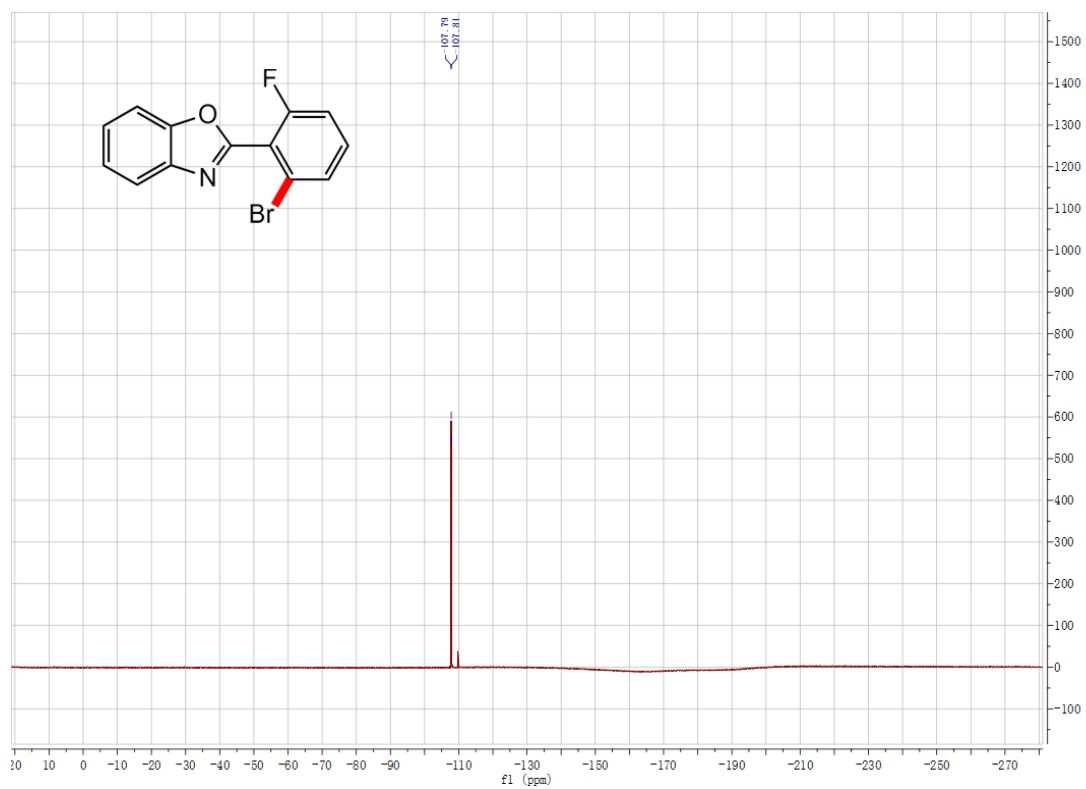


2-(2-bromo-6-methylphenyl)benzo[d]oxazole (2r)

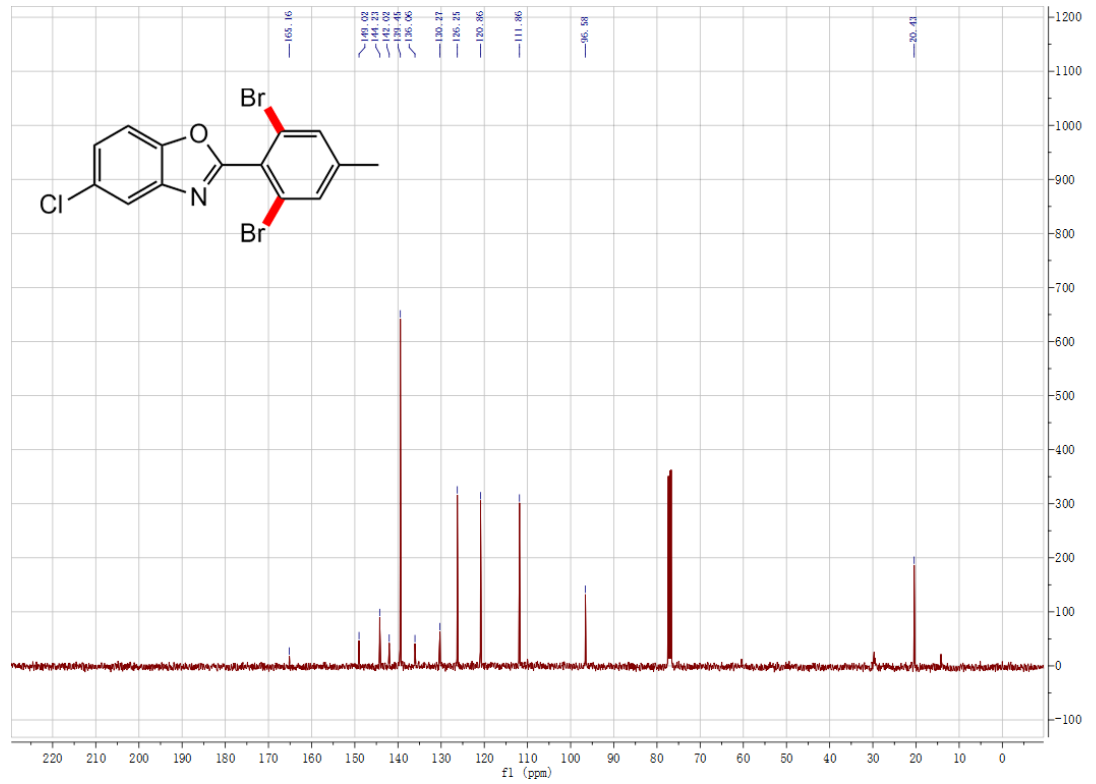
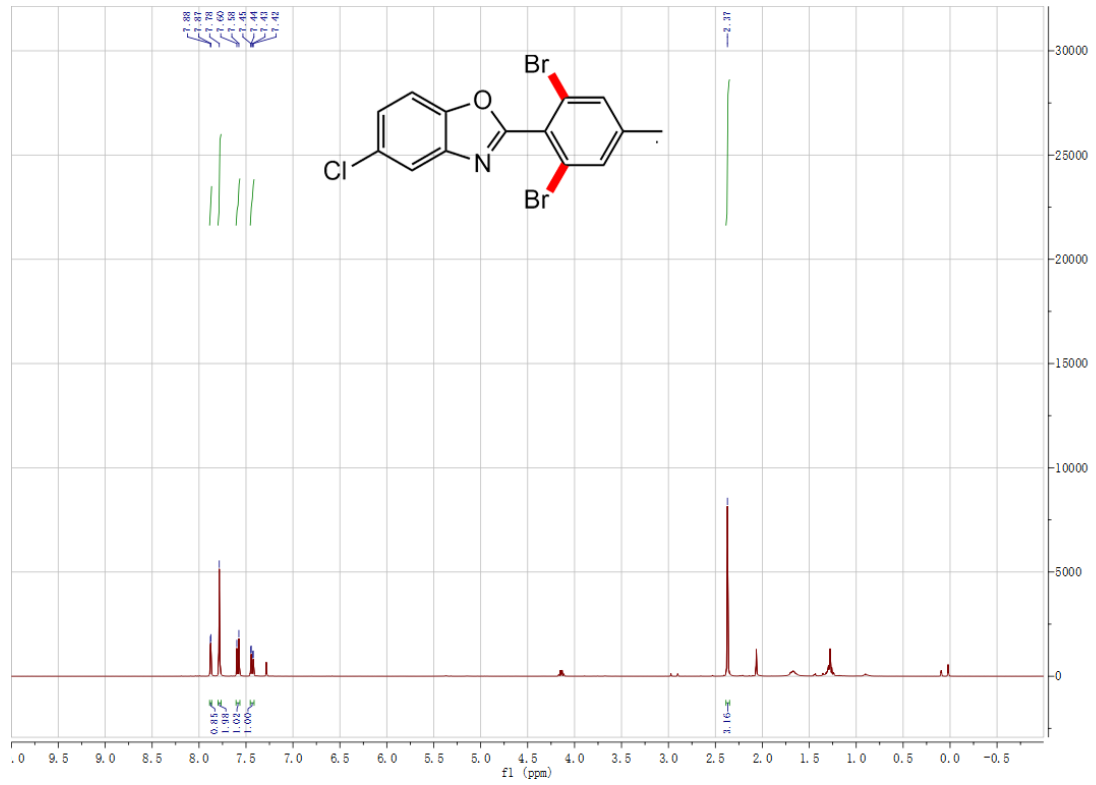


2-(2-bromo-6-fluorophenyl)benzo[d]oxazole (2s)

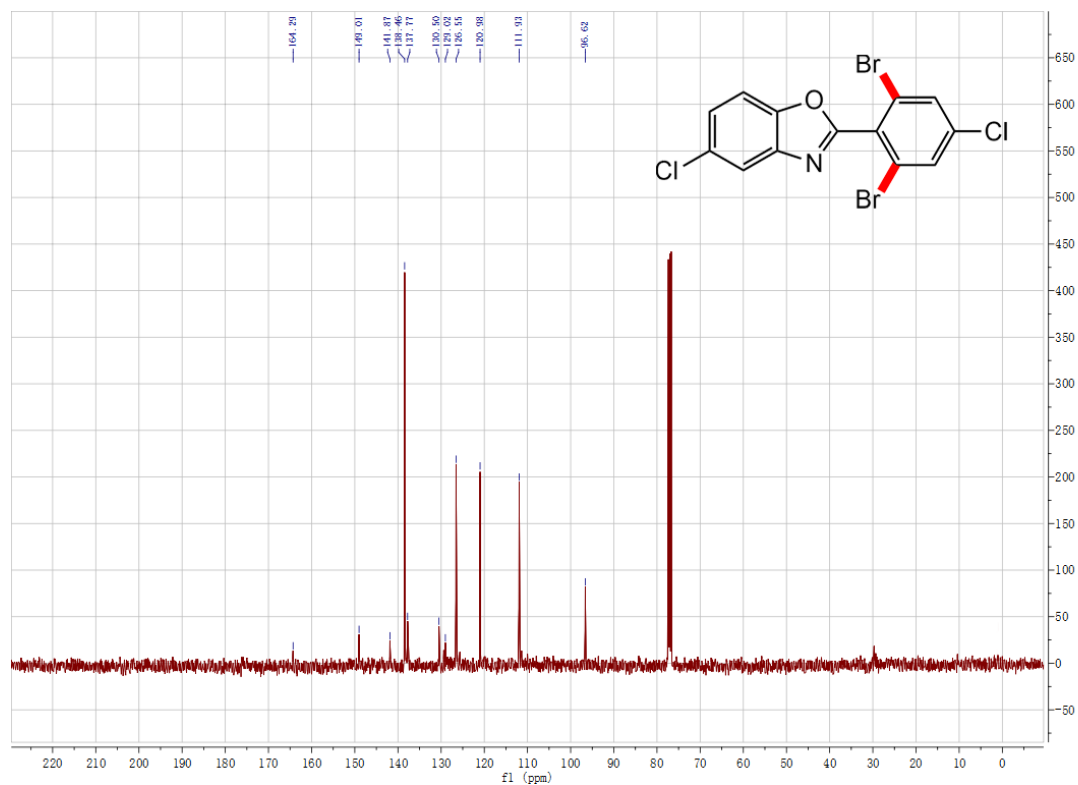
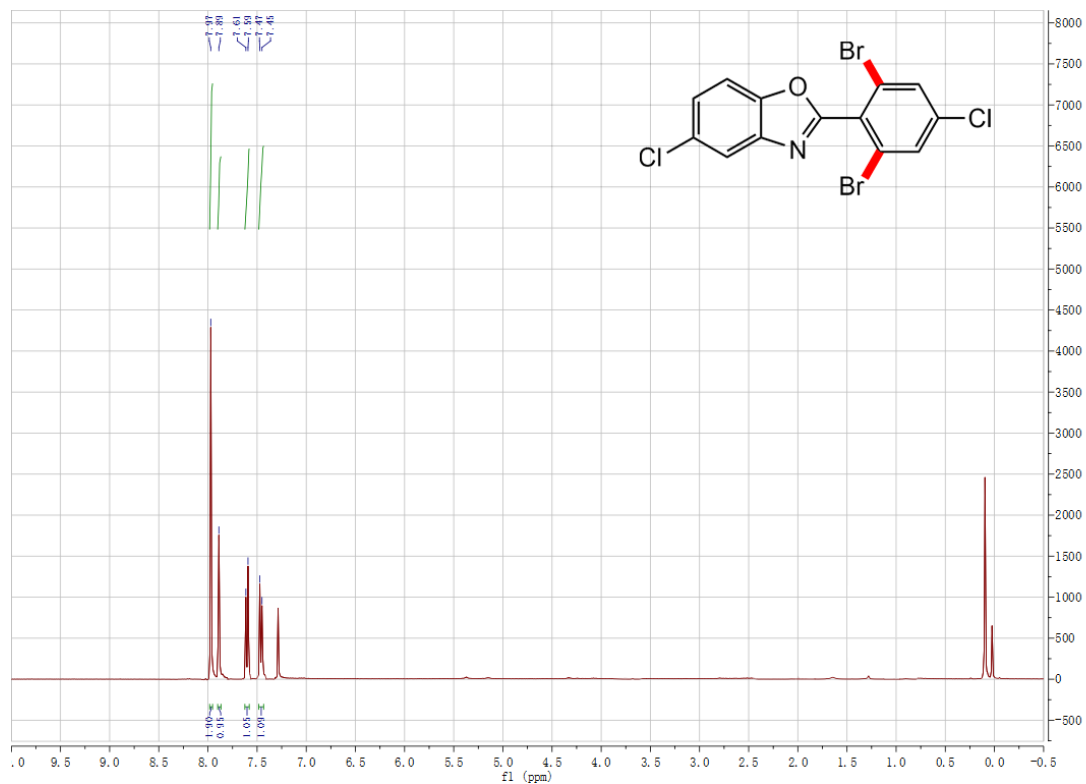




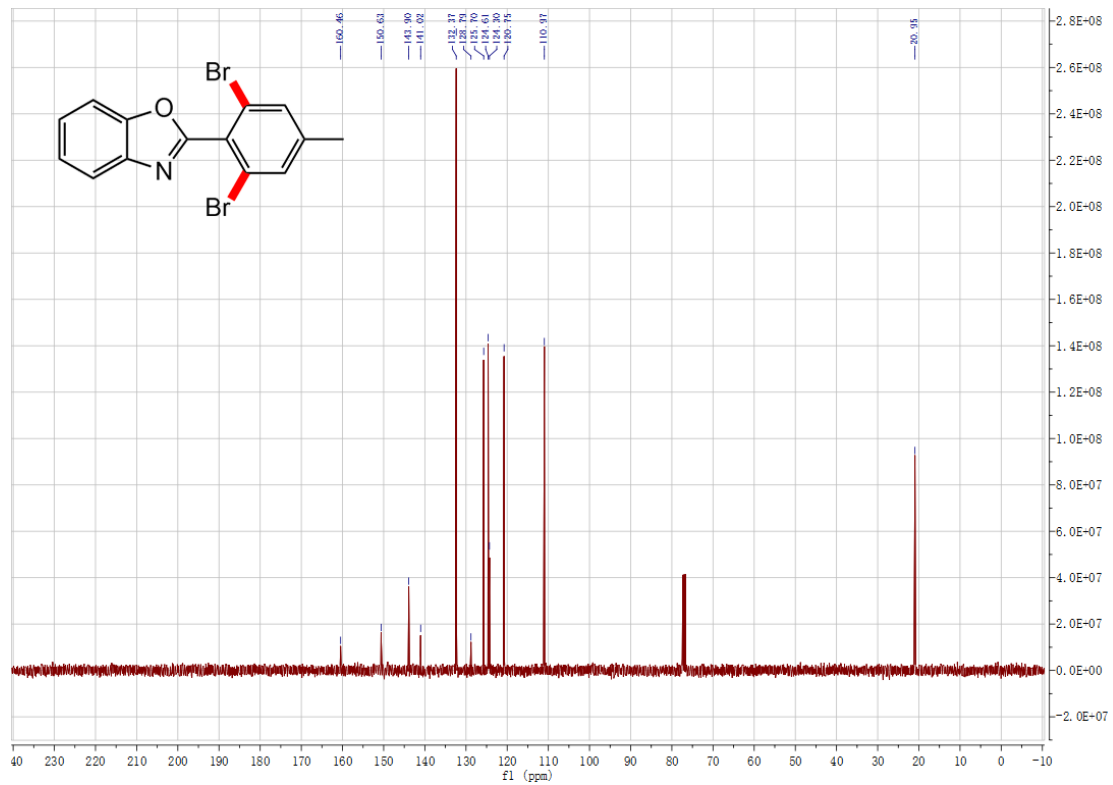
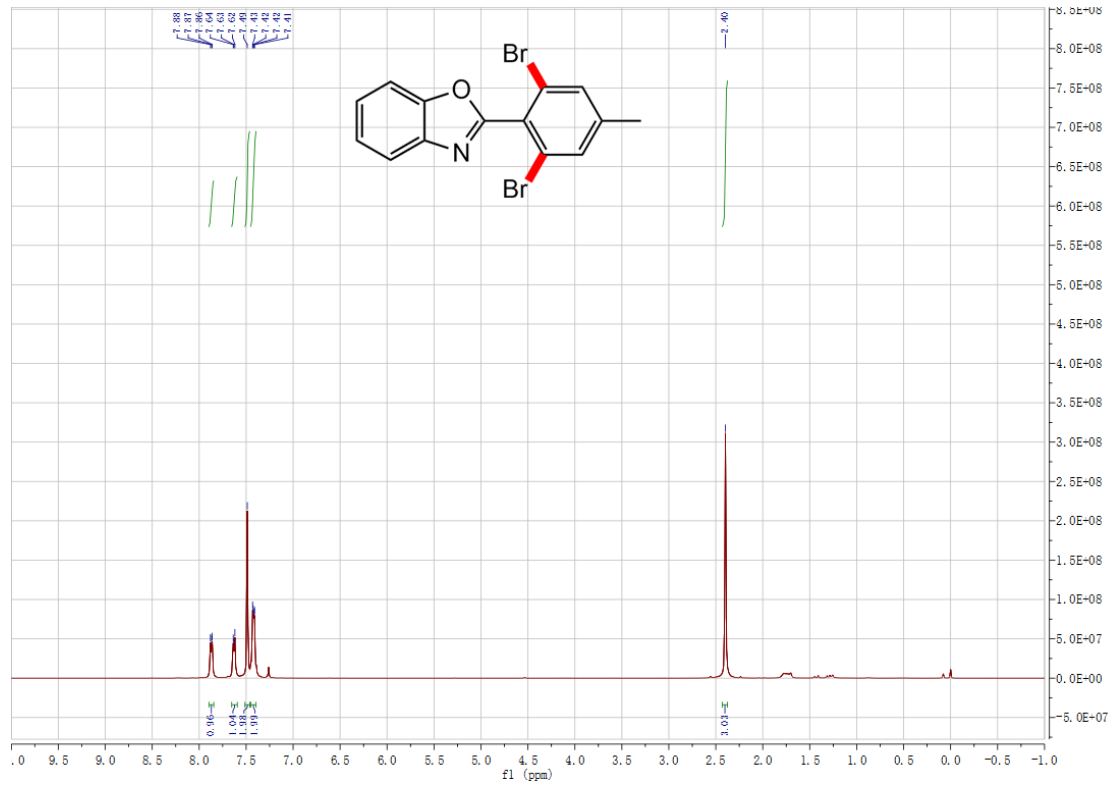
5-chloro-2-(2,6-dibromo-4-methylphenyl)benzo[d]oxazole (2u)



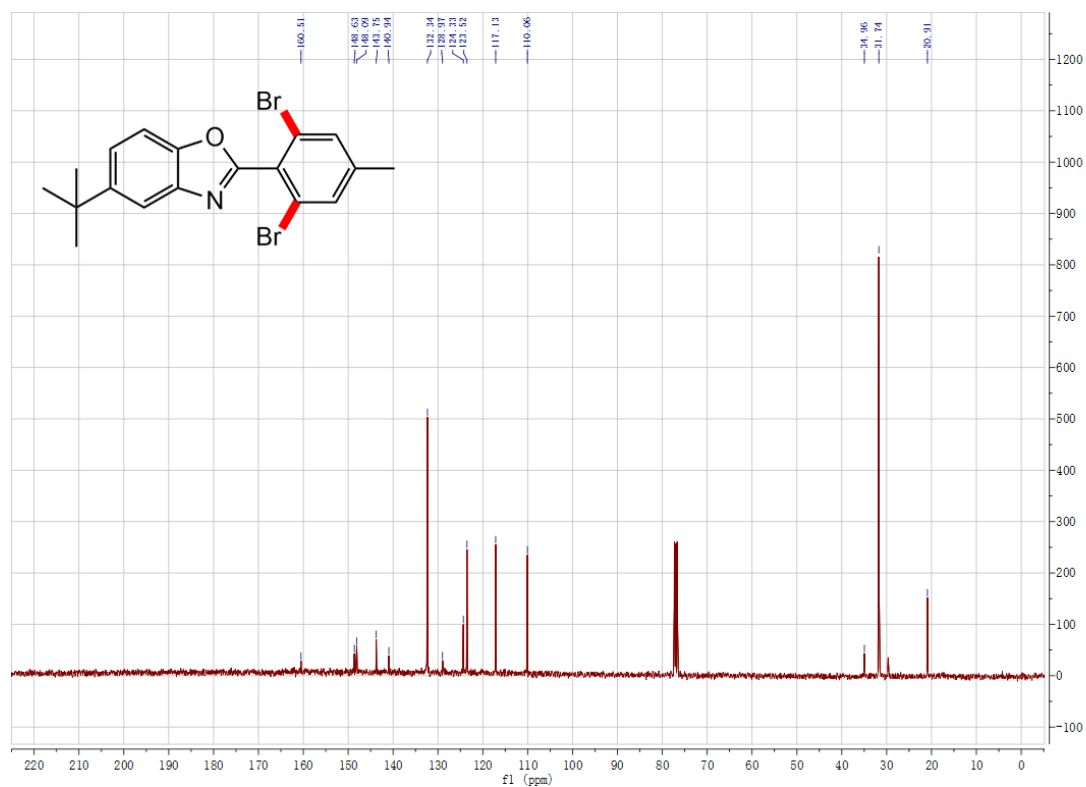
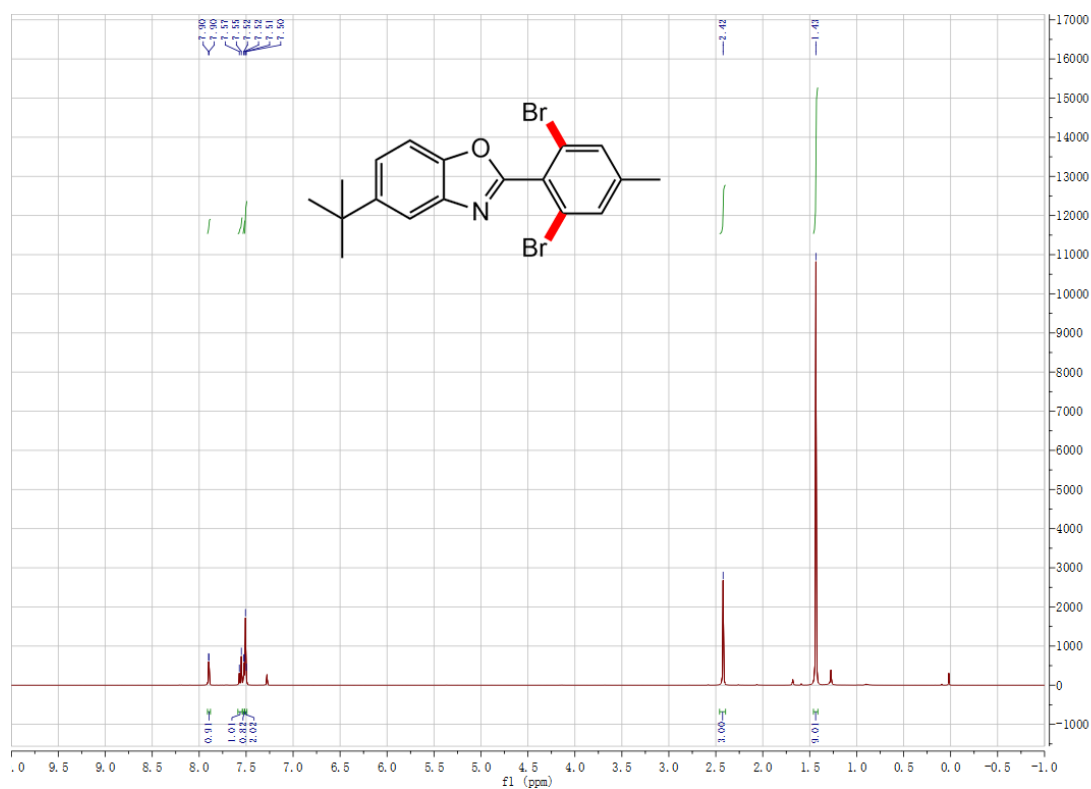
5-chloro-2-(2,6-dibromo-4-chlorophenyl)benzo[d]oxazole (2v)



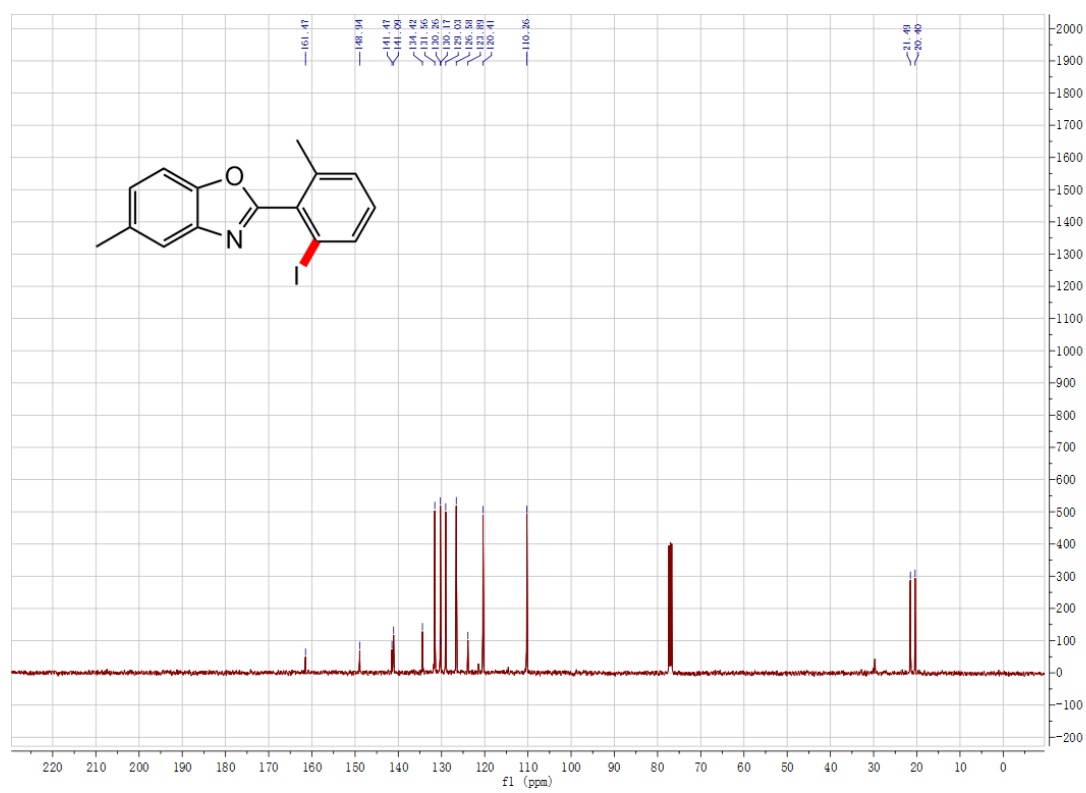
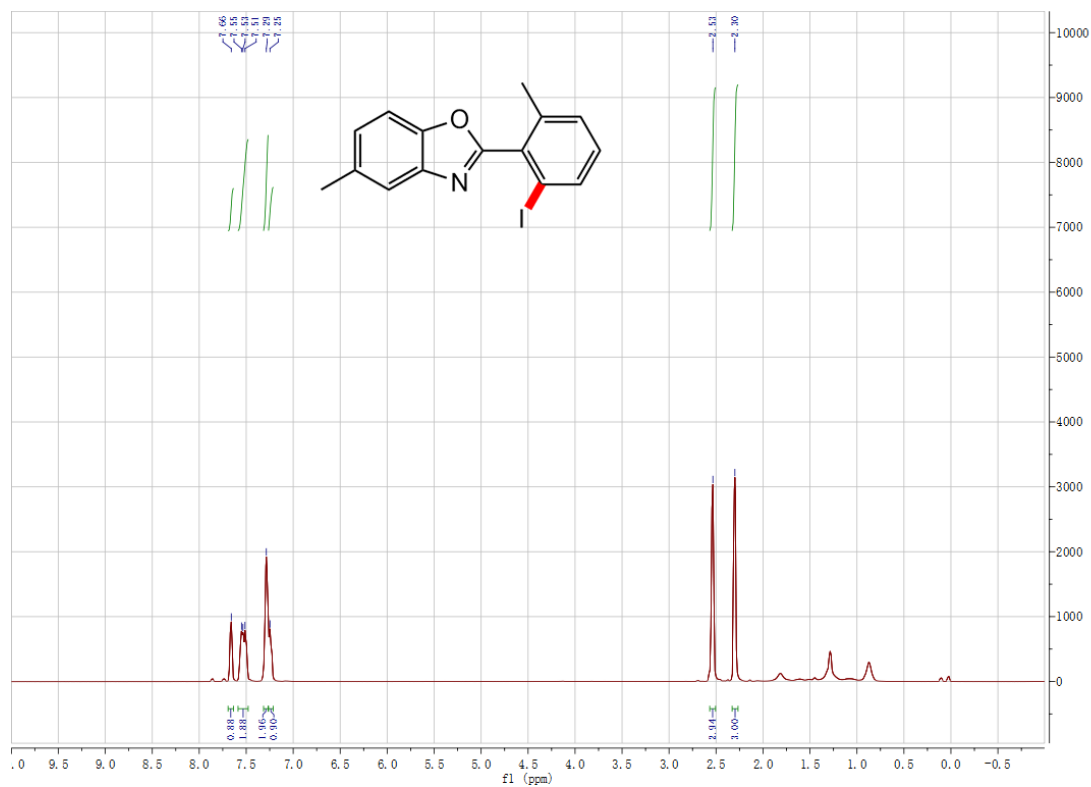
2-(2,6-dibromo-4-methylphenyl)benzo[d]oxazole (2w)



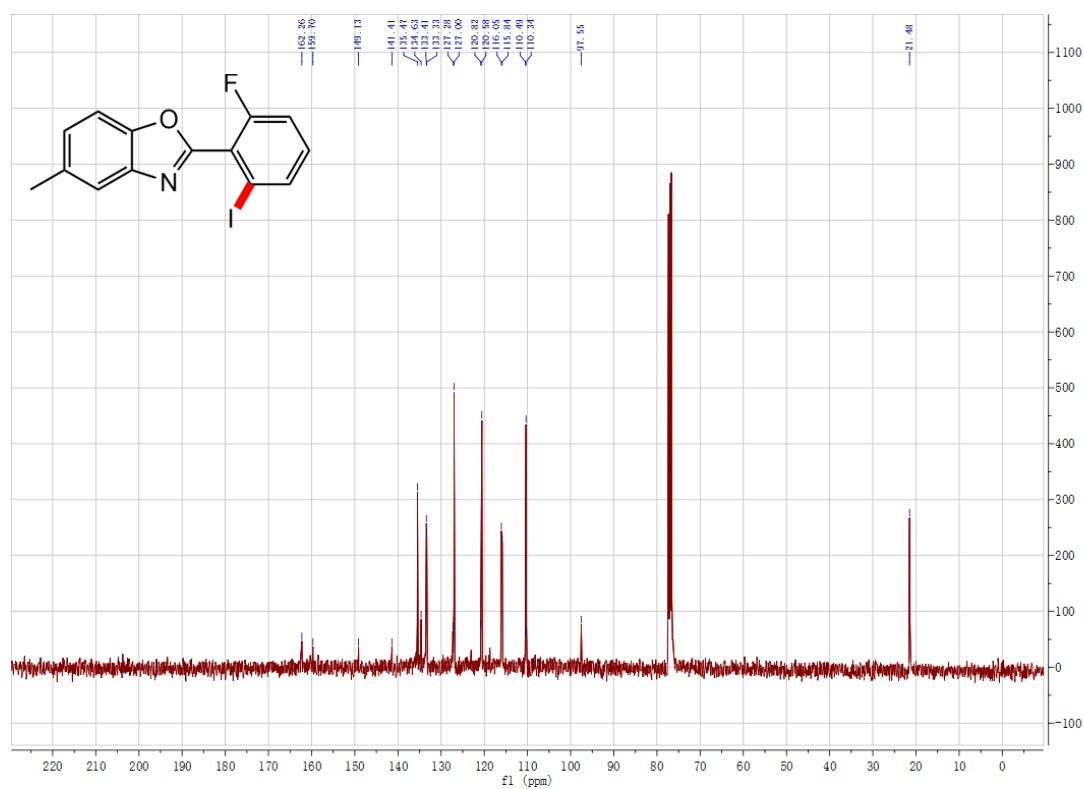
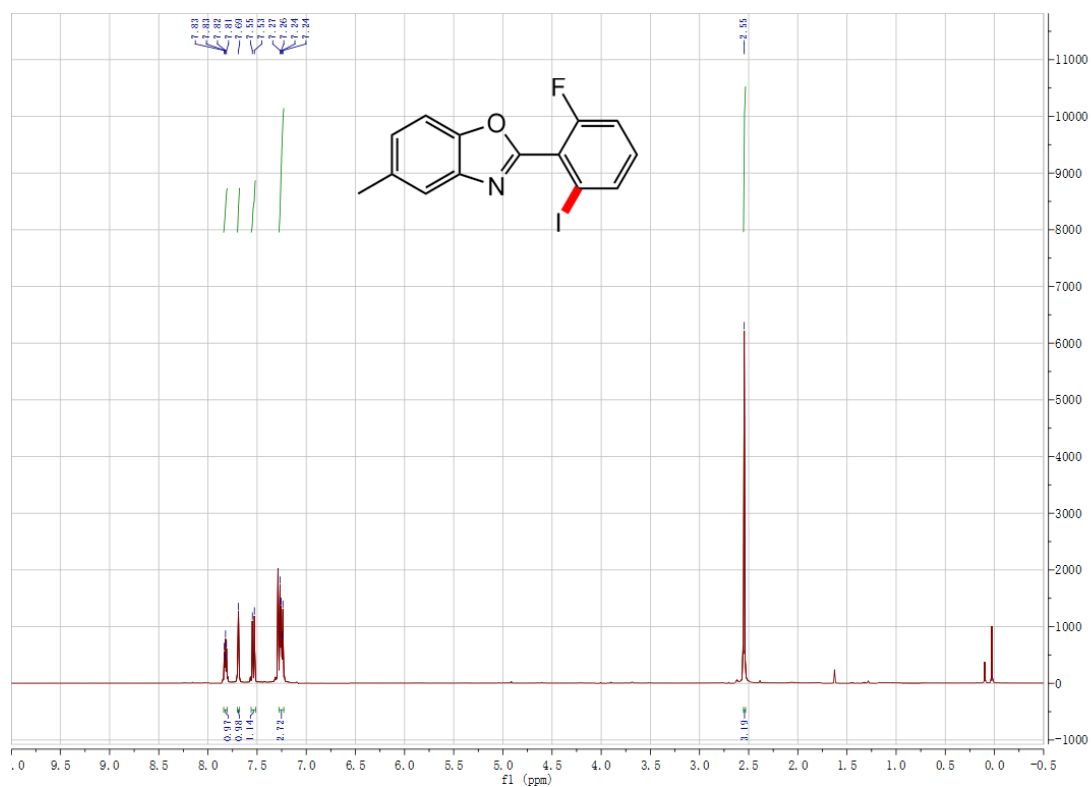
5-(tert-butyl)-2-(2,6-dibromo-4-methylphenyl)benzo[d]oxazole (2x)

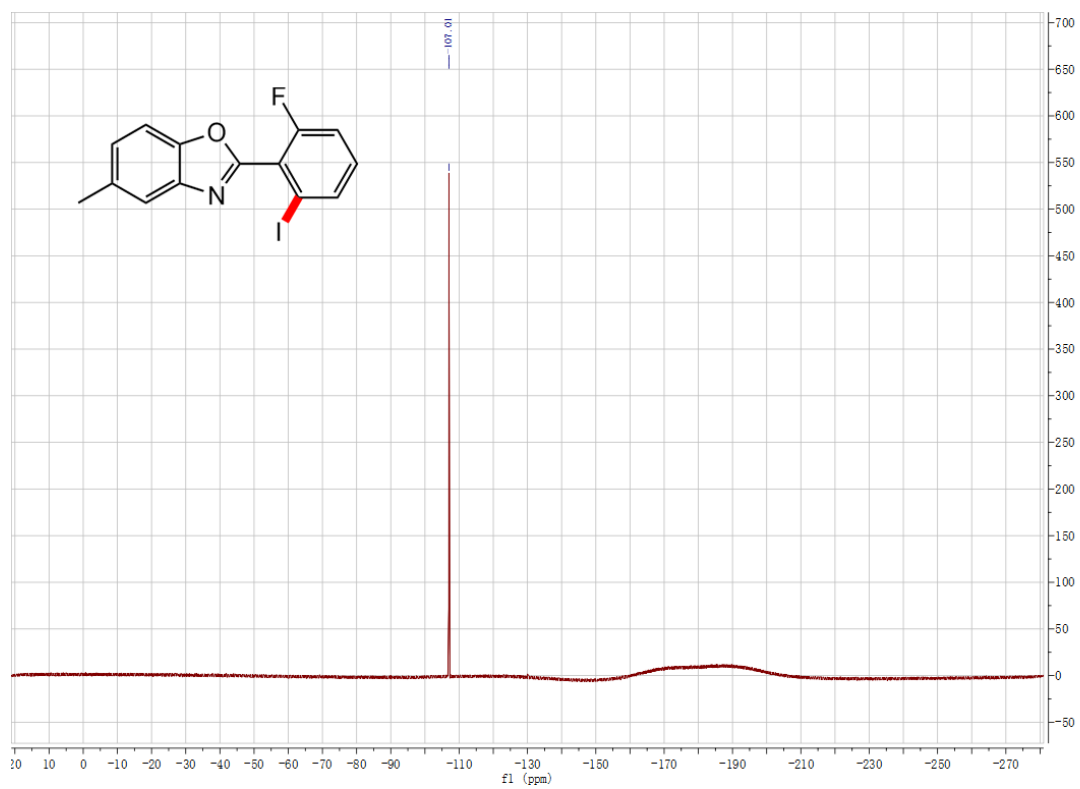


2-(2-iodo-6-methylphenyl)-5-methylbenzo[d]oxazole (3a)

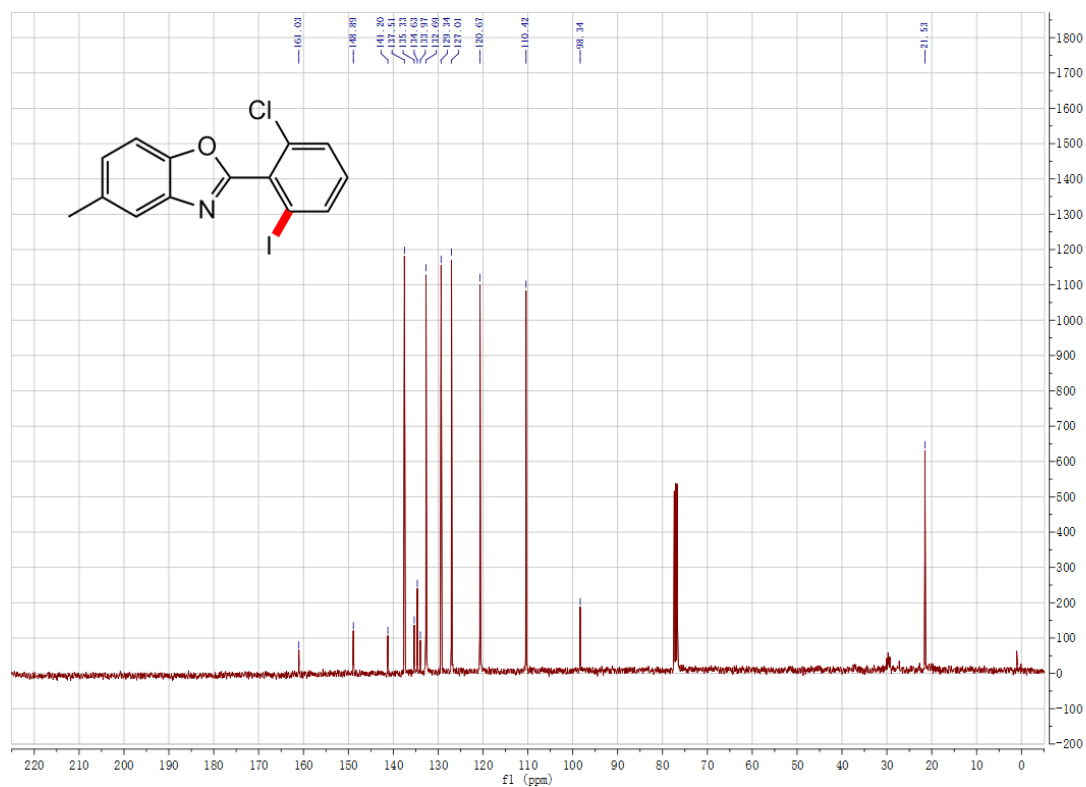
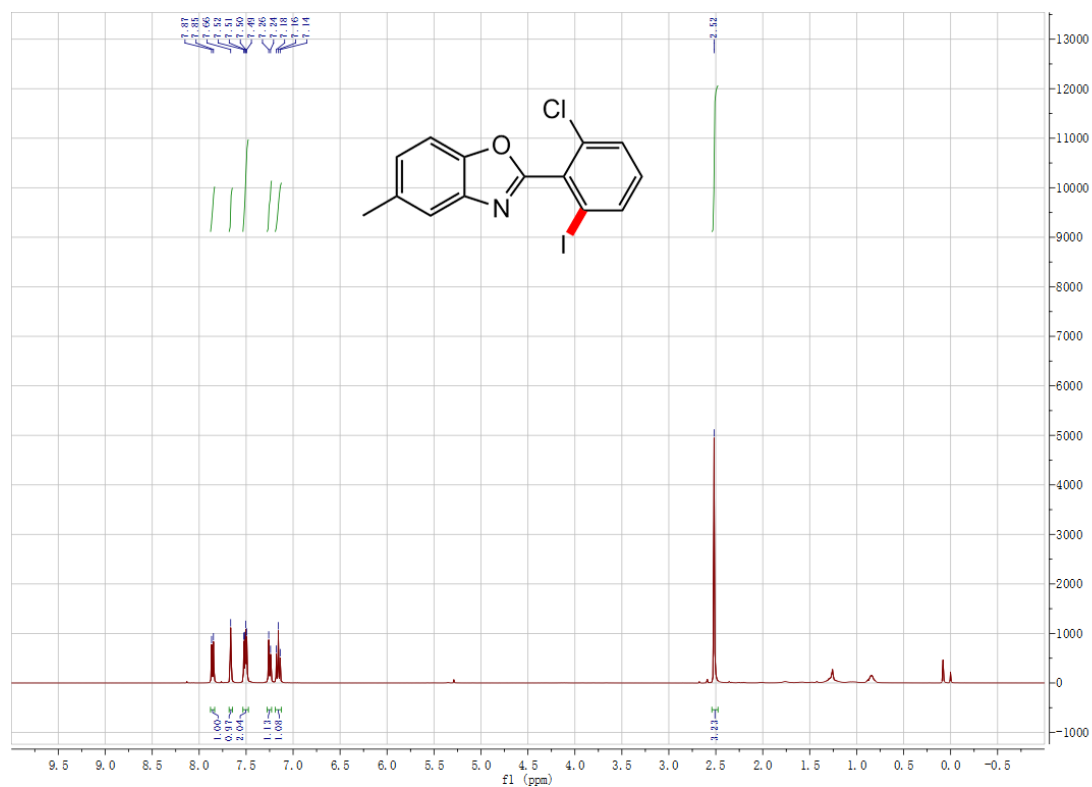


2-(2-fluoro-6-iodophenyl)-5-methylbenzo[d]oxazole (3b)

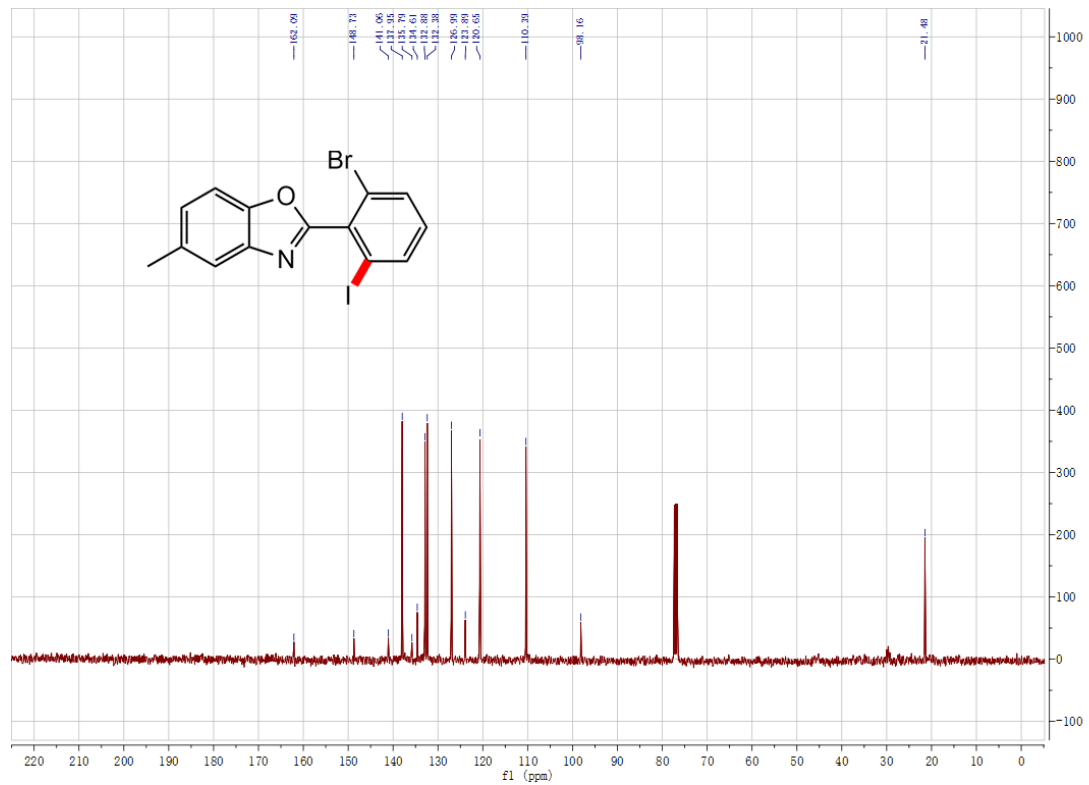
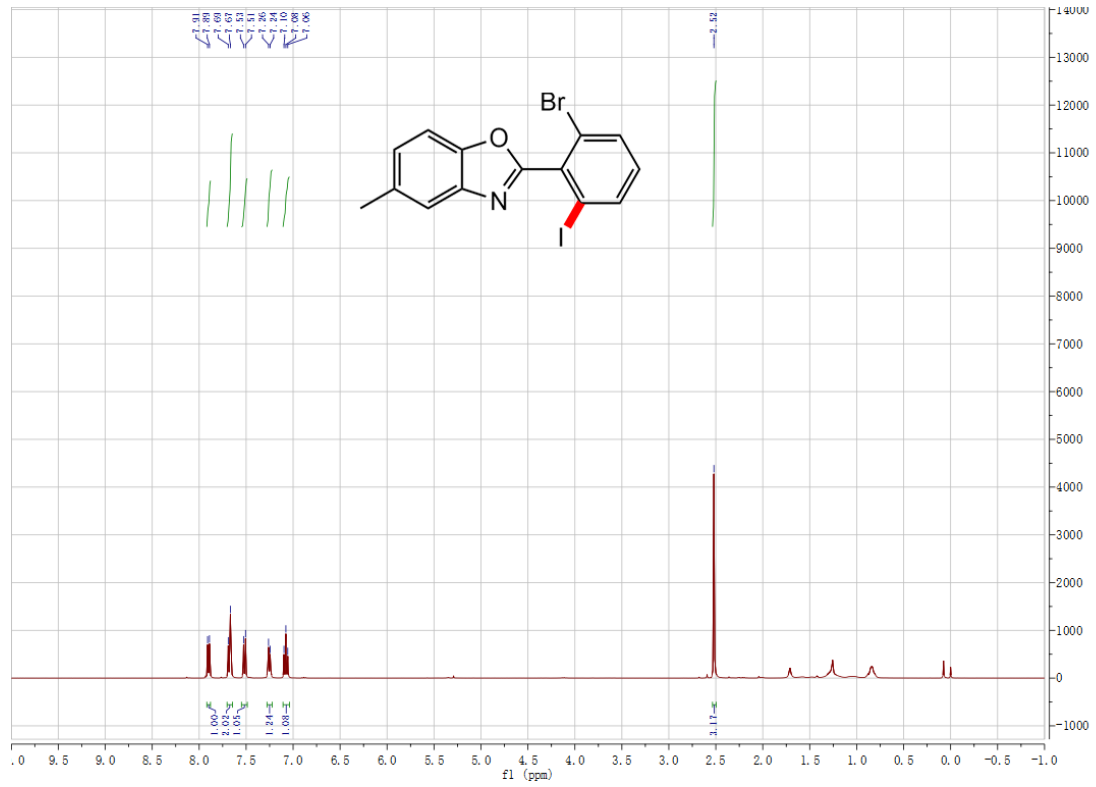




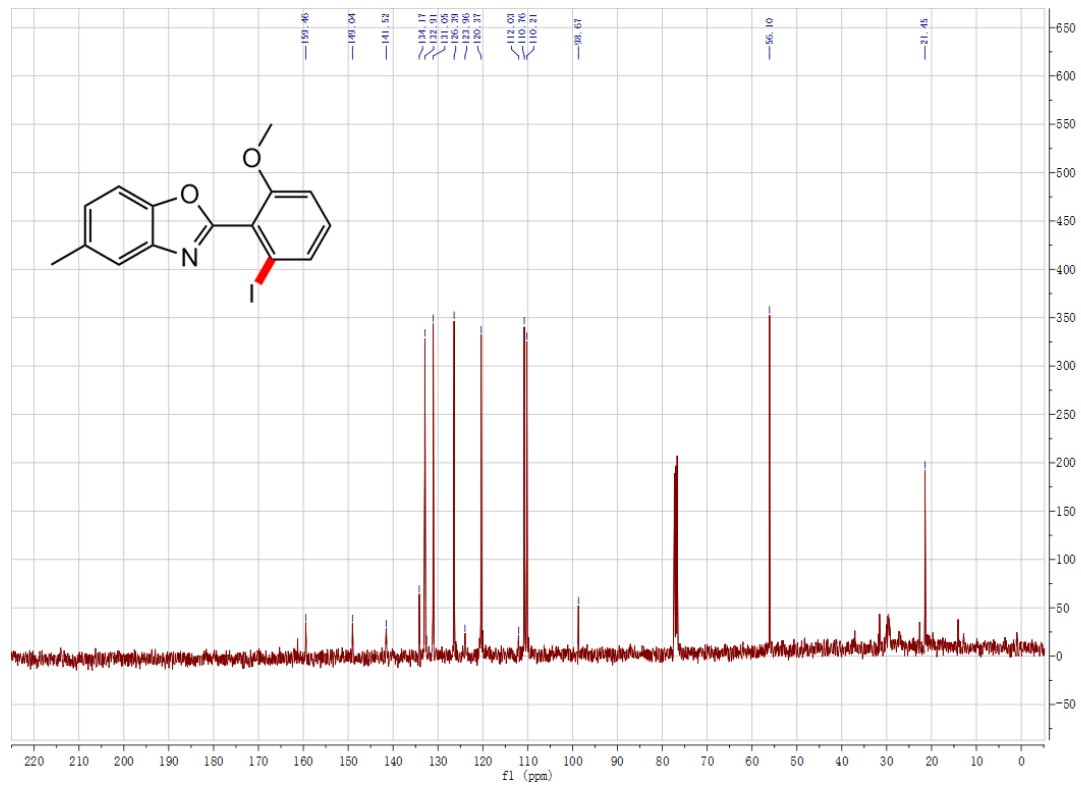
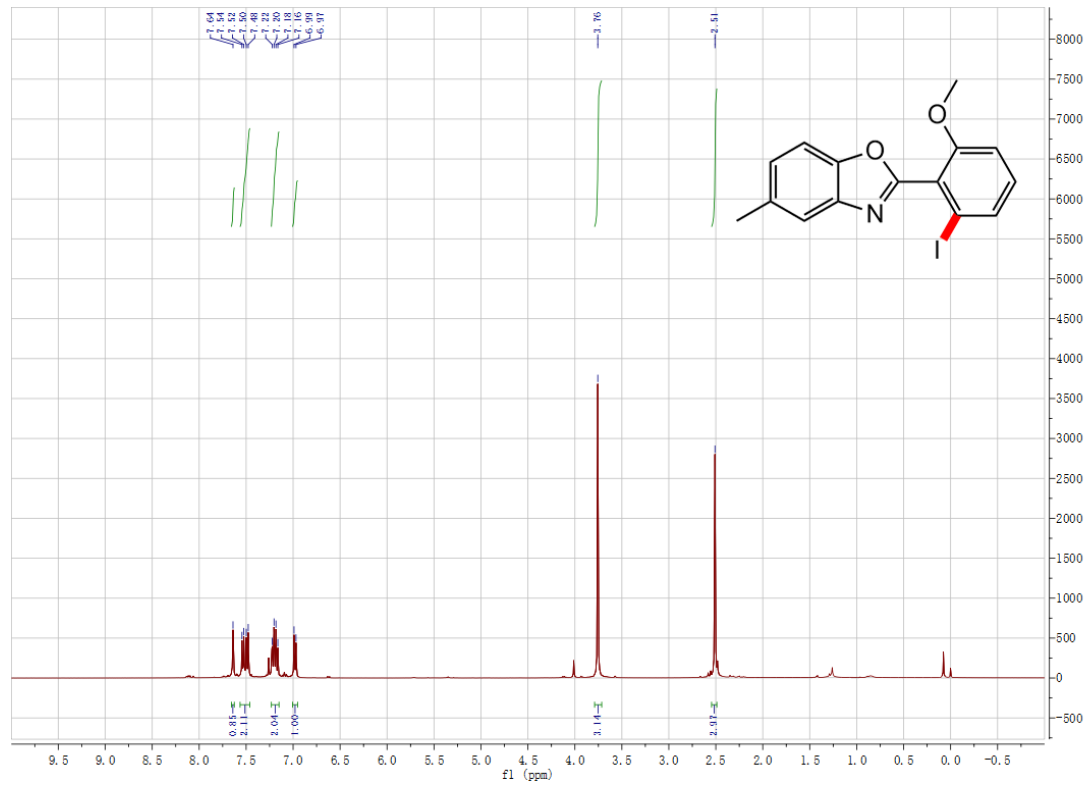
2-(2-chloro-6-iodophenyl)-5-methylbenzo[d]oxazole (3c)



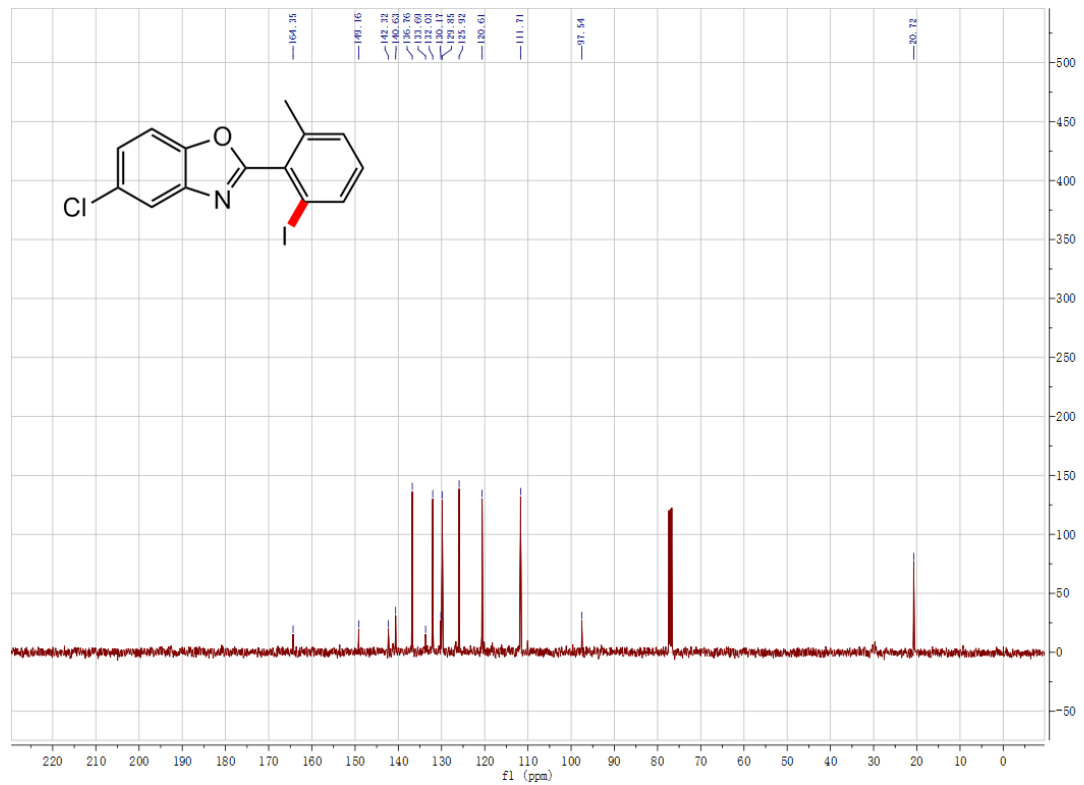
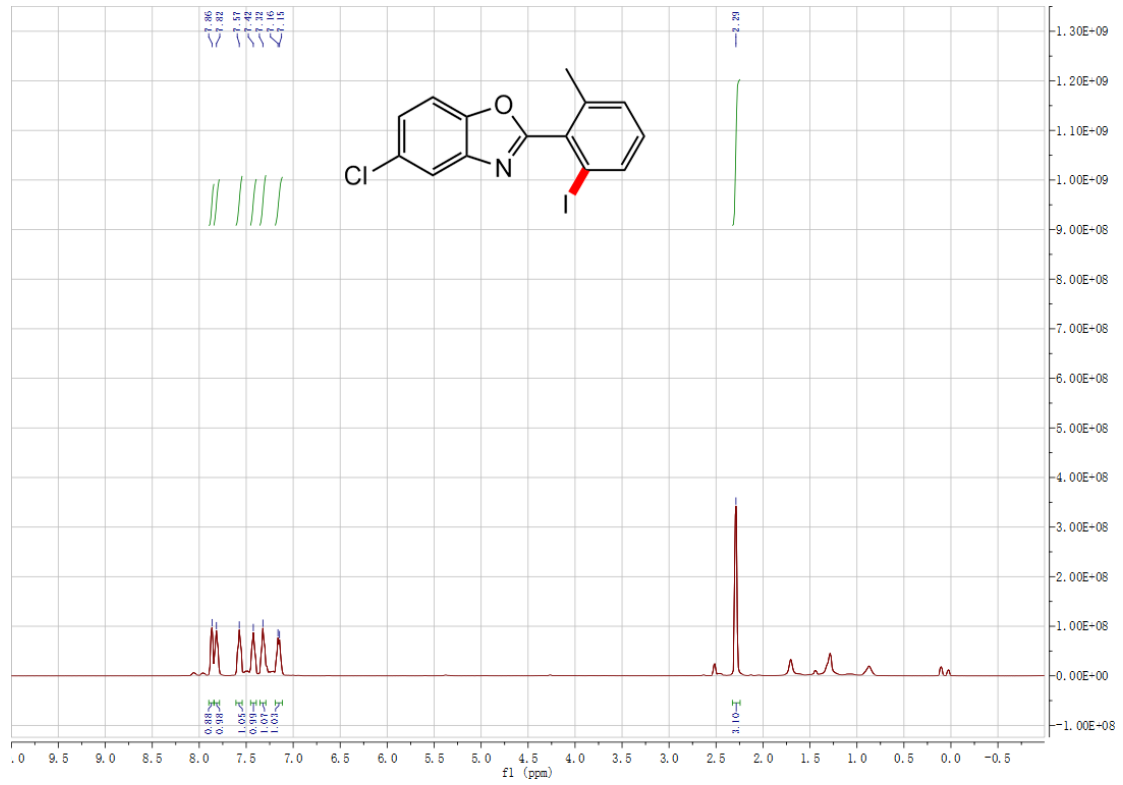
2-(2-bromo-6-iodophenyl)-5-methylbenzo[d]oxazole (3m)



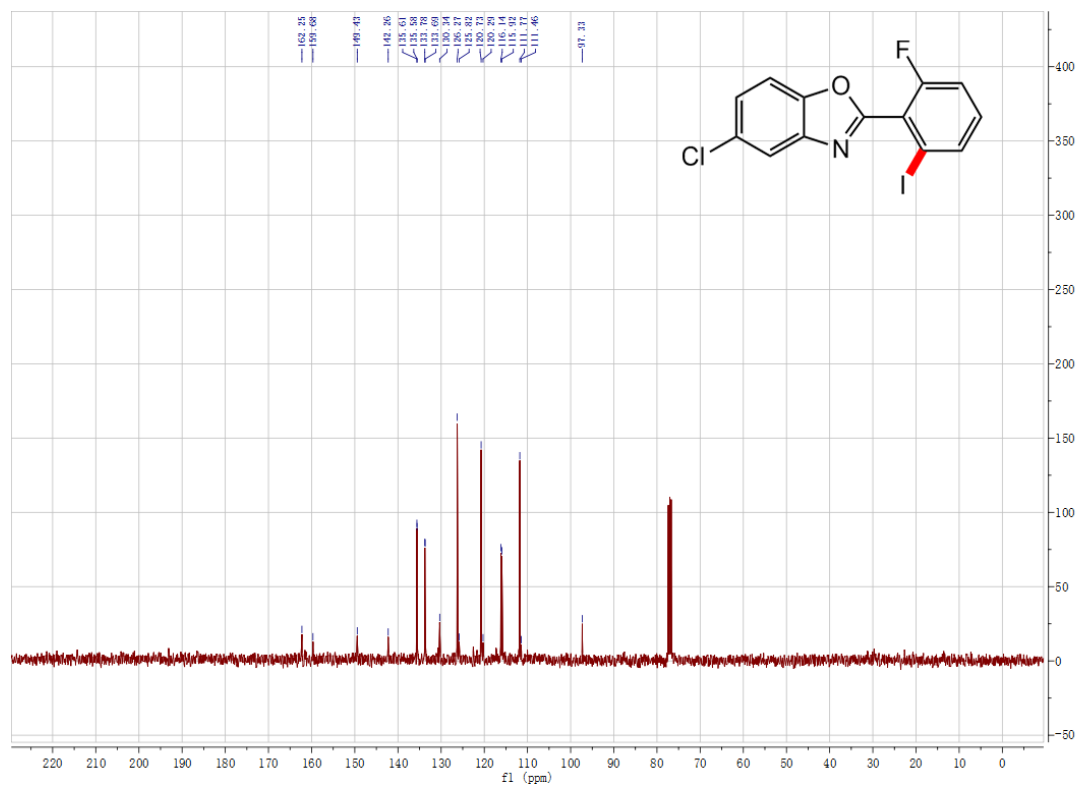
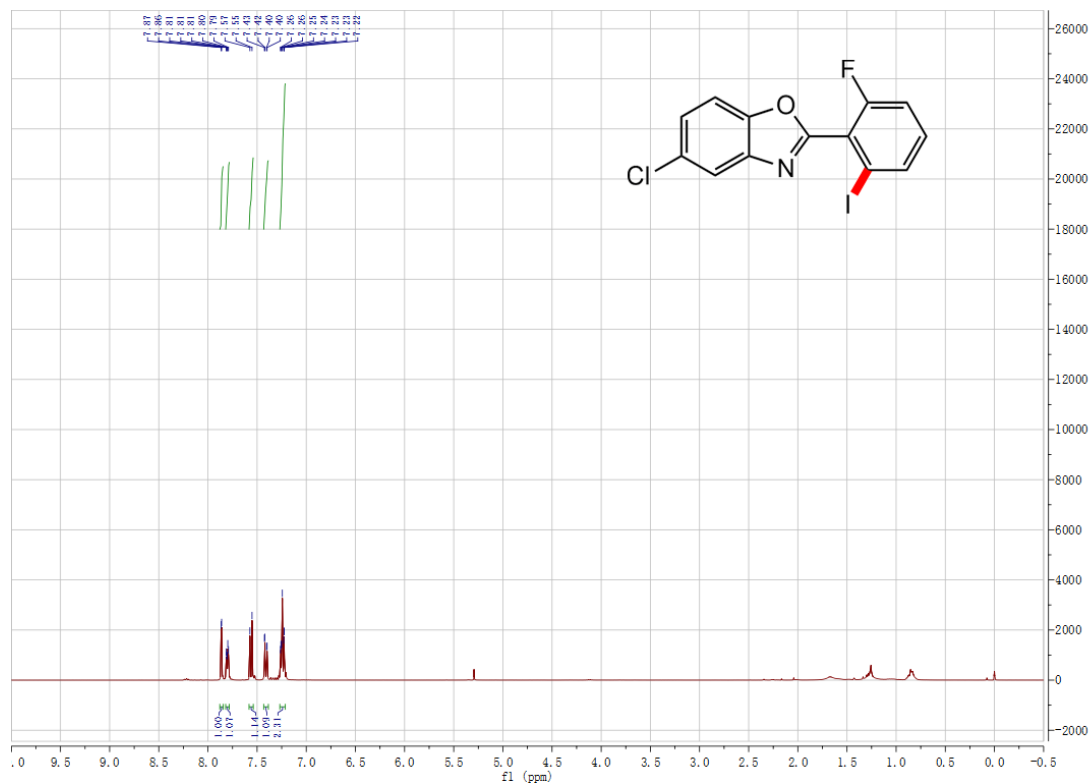
2-(2-iodo-6-methoxyphenyl)-5-methylbenzo[d]oxazole (3n)

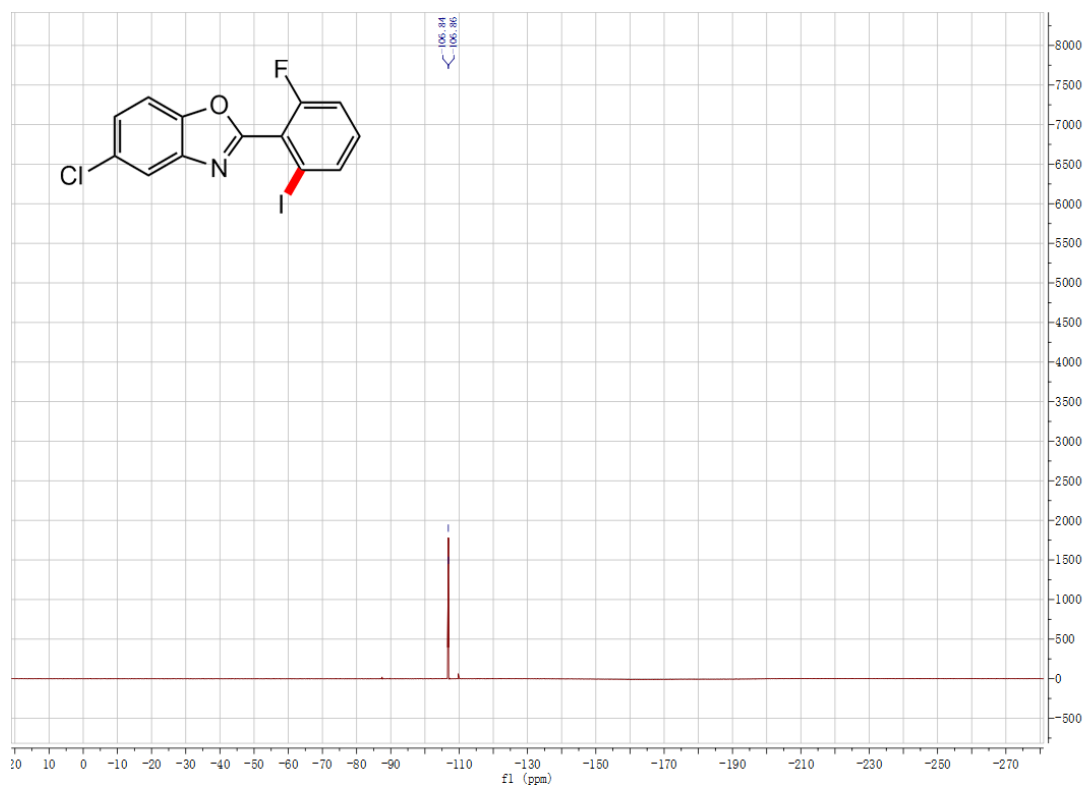


5-chloro-2-(2-iodo-6-methylphenyl)benzo[d]oxazole (3o)

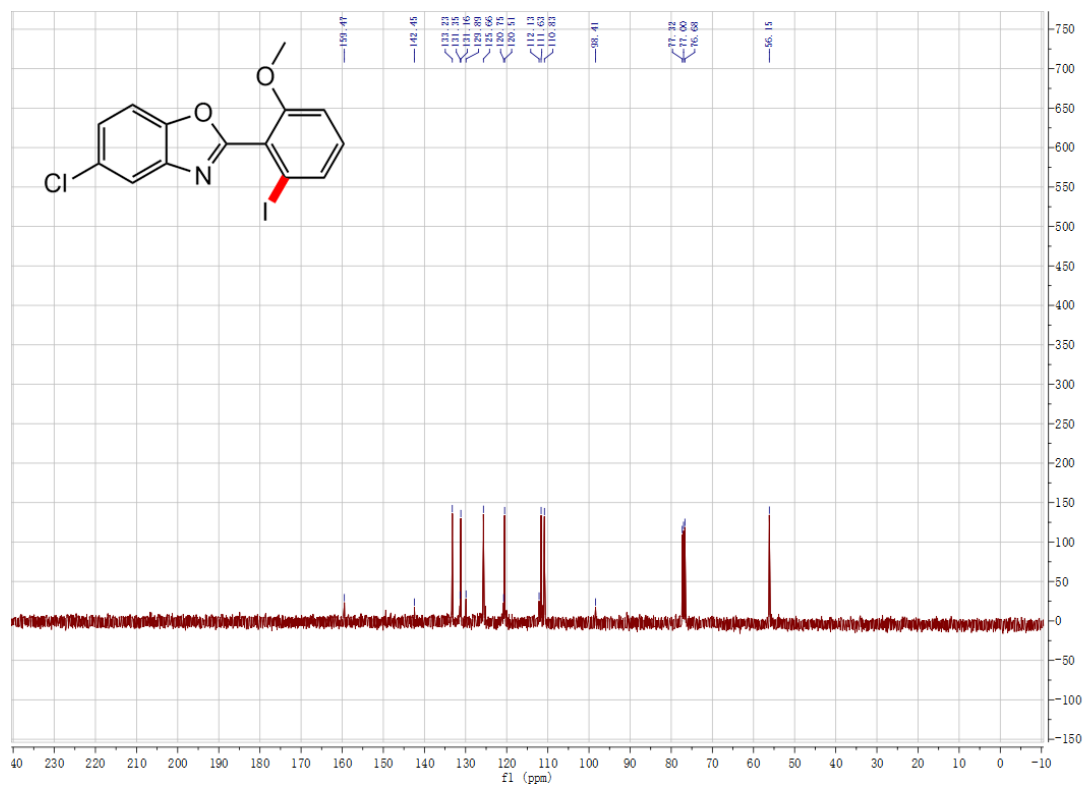
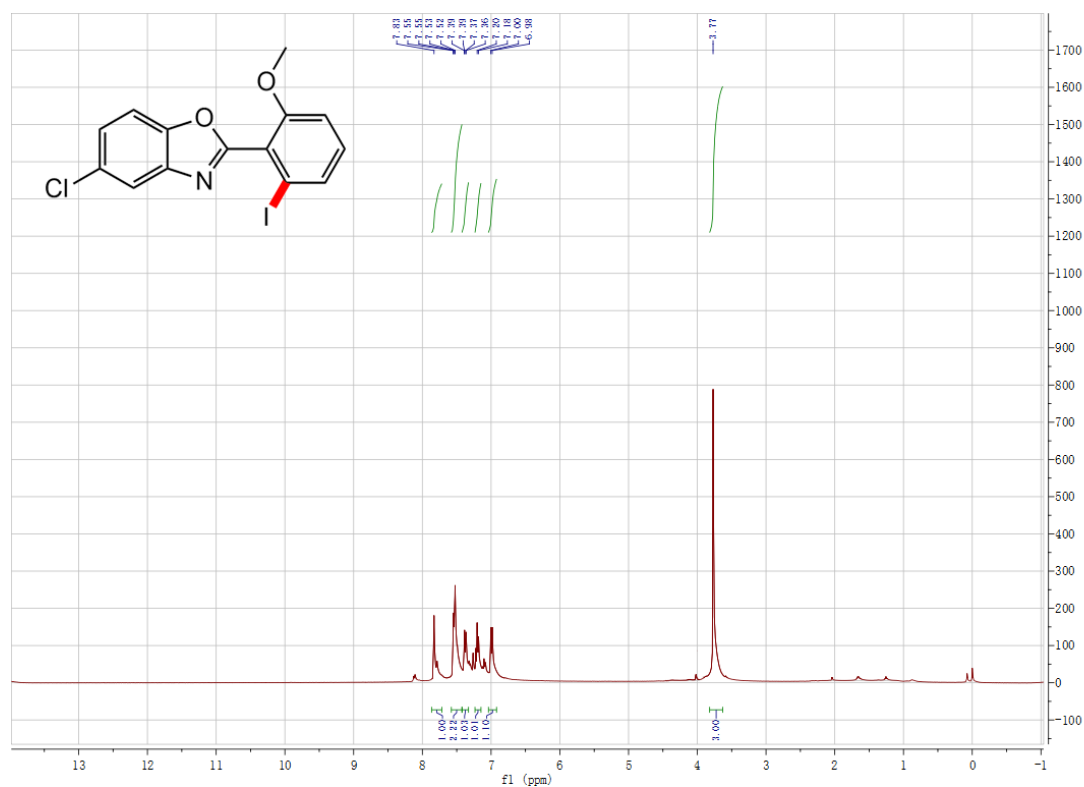


5-chloro-2-(2-fluoro-6-iodophenyl)benzo[*a*]oxazole (3p)

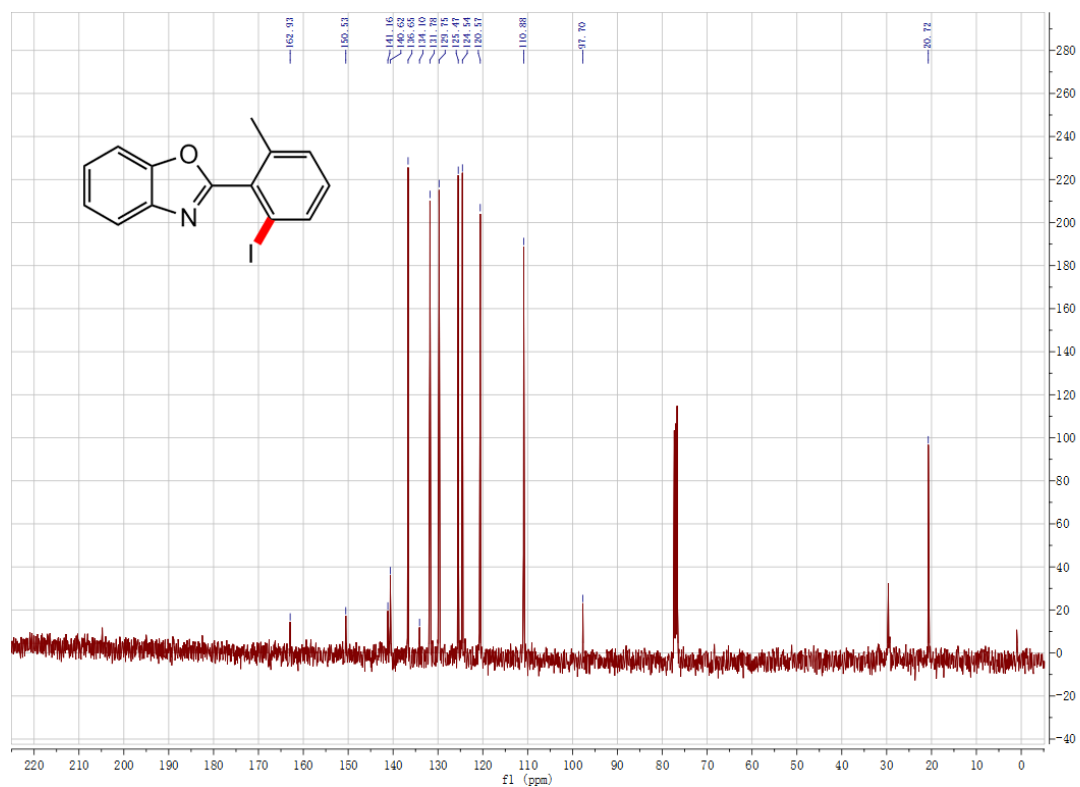
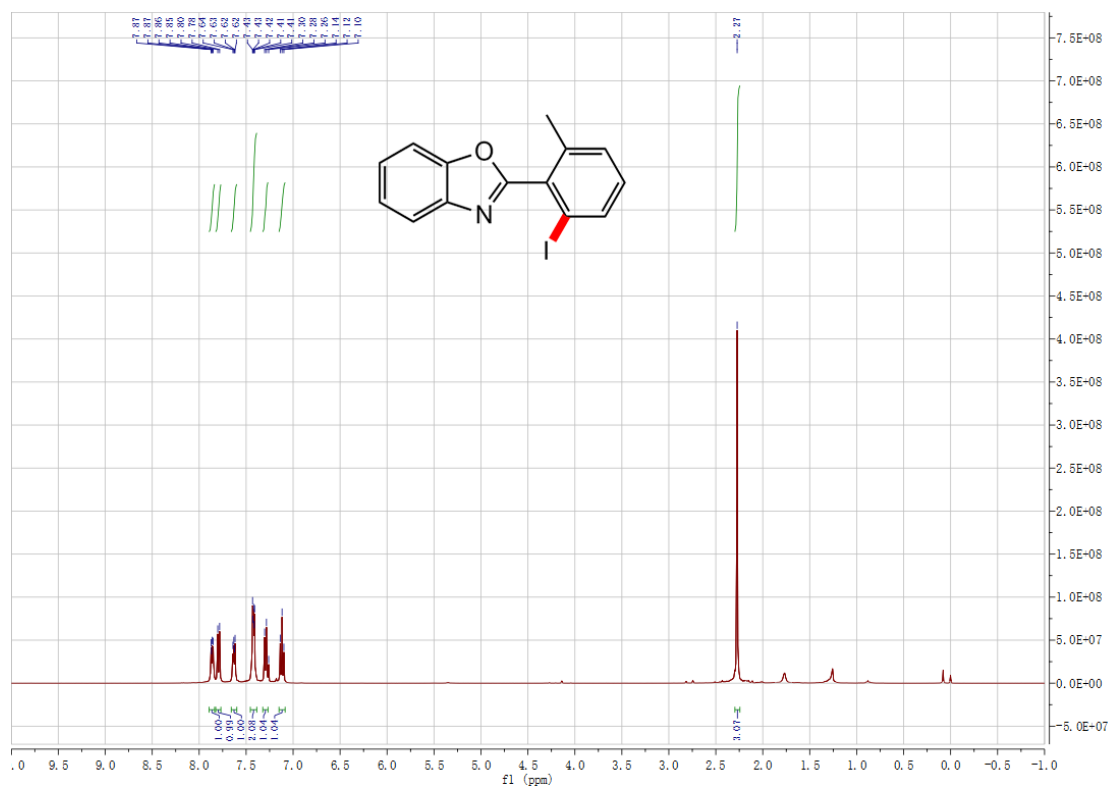




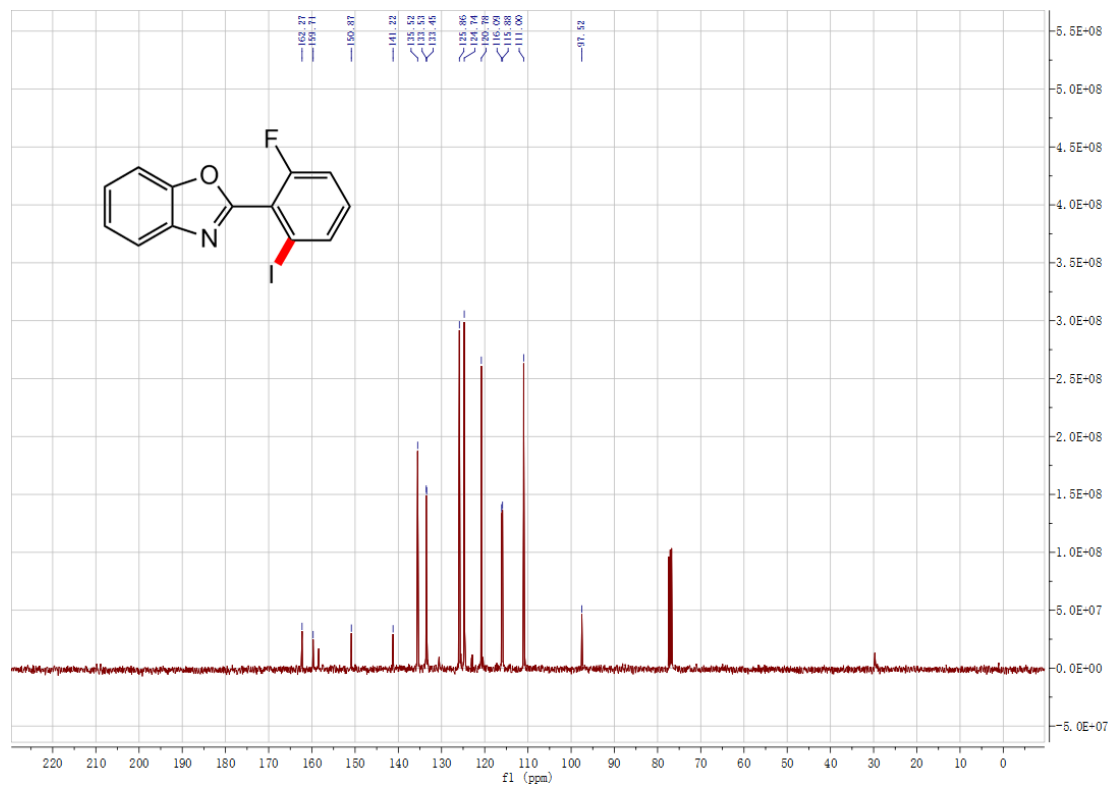
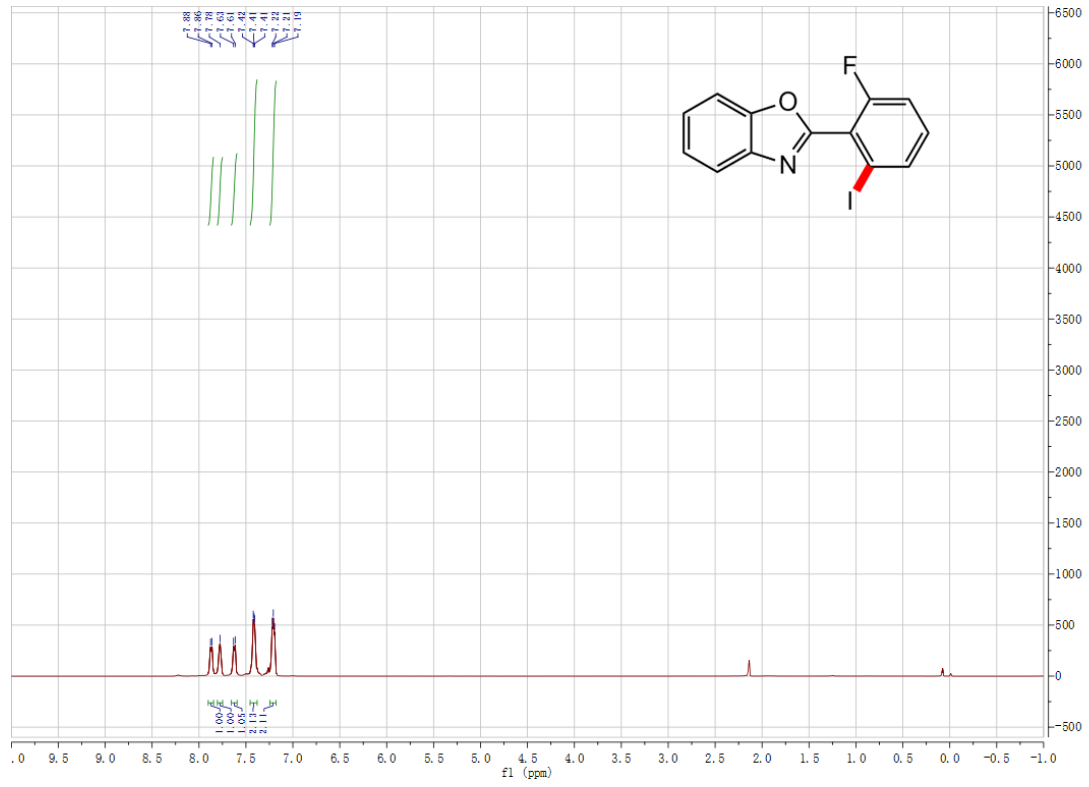
5-chloro-2-(2-iodo-6-methoxyphenyl)benzo[d]oxazole (3q)

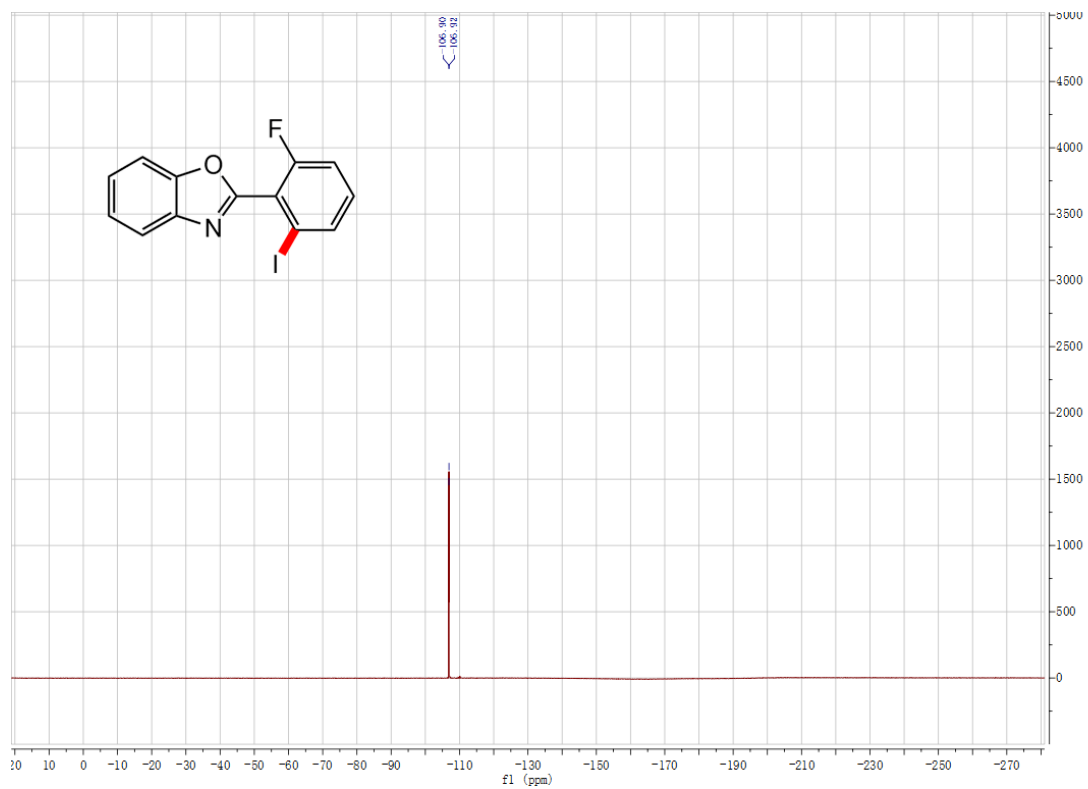


2-(2-iodo-6-methylphenyl)-5-methylbenzo[d]oxazole (3r)

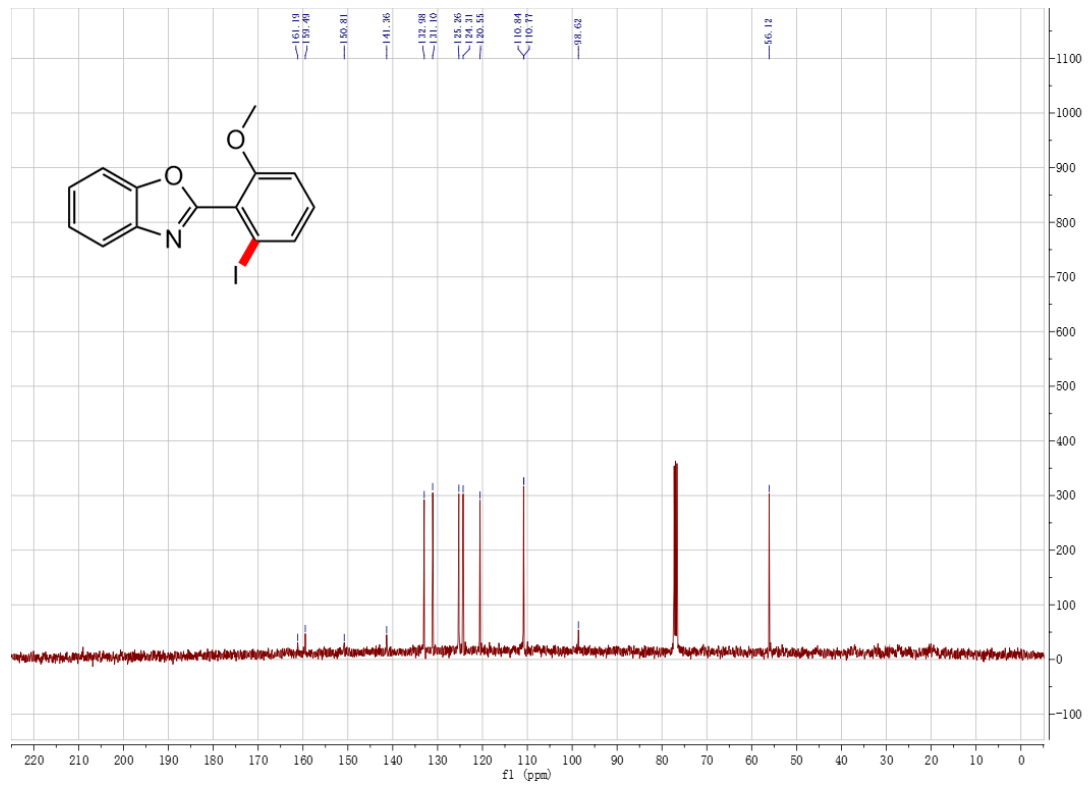
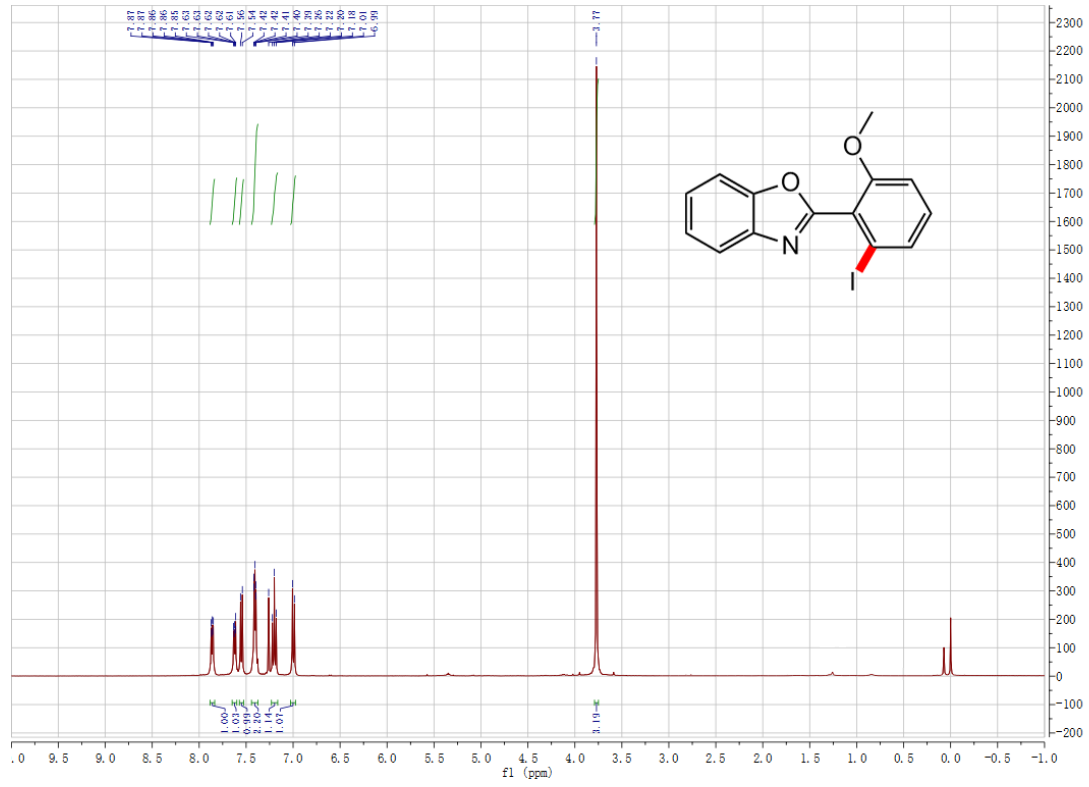


2-(2-fluoro-6-iodophenyl)benzo[d]oxazole (3s)

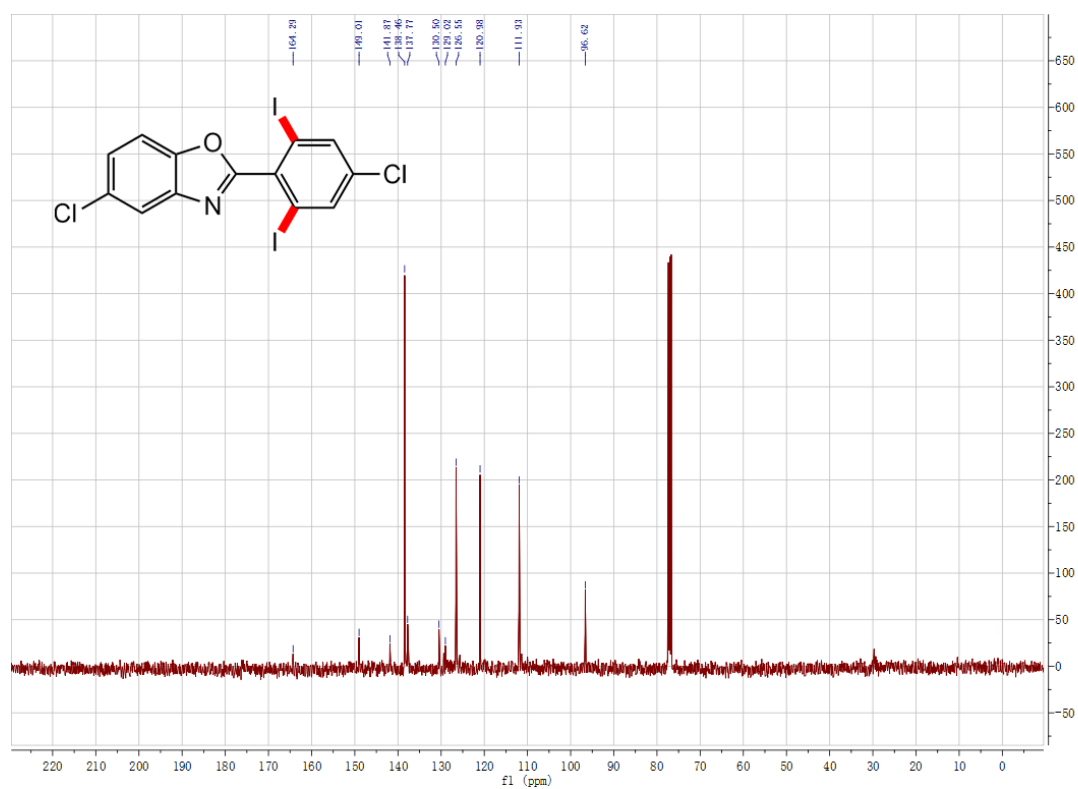
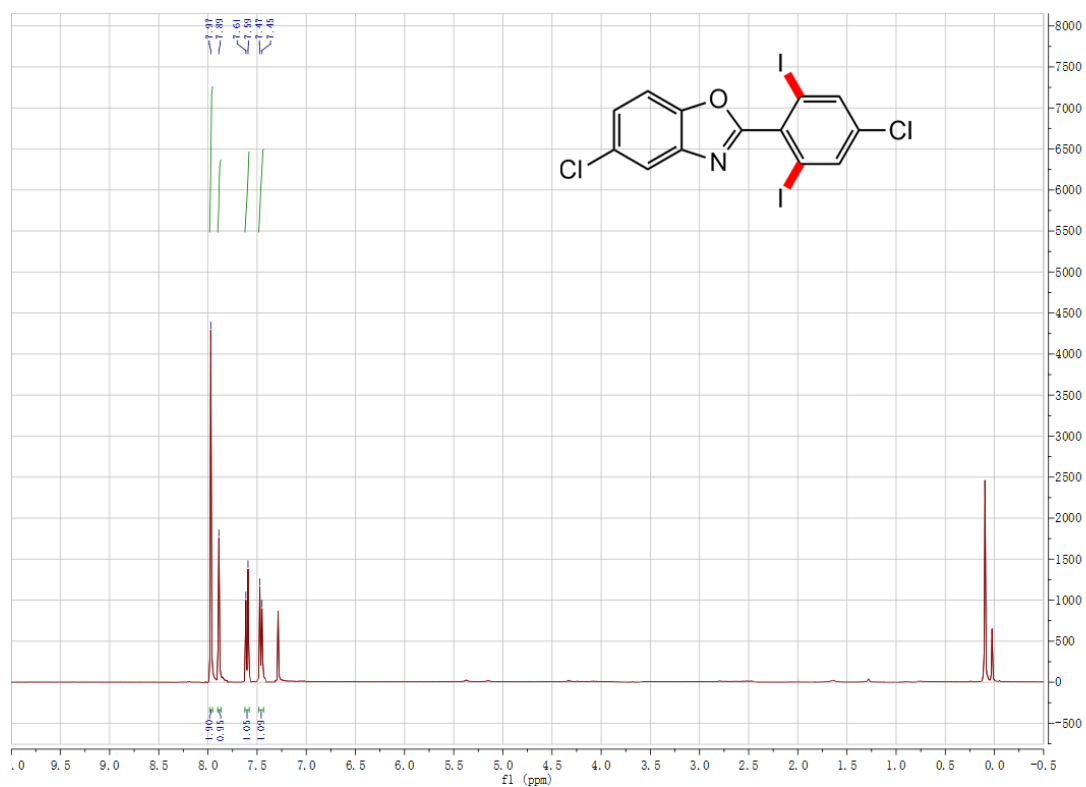




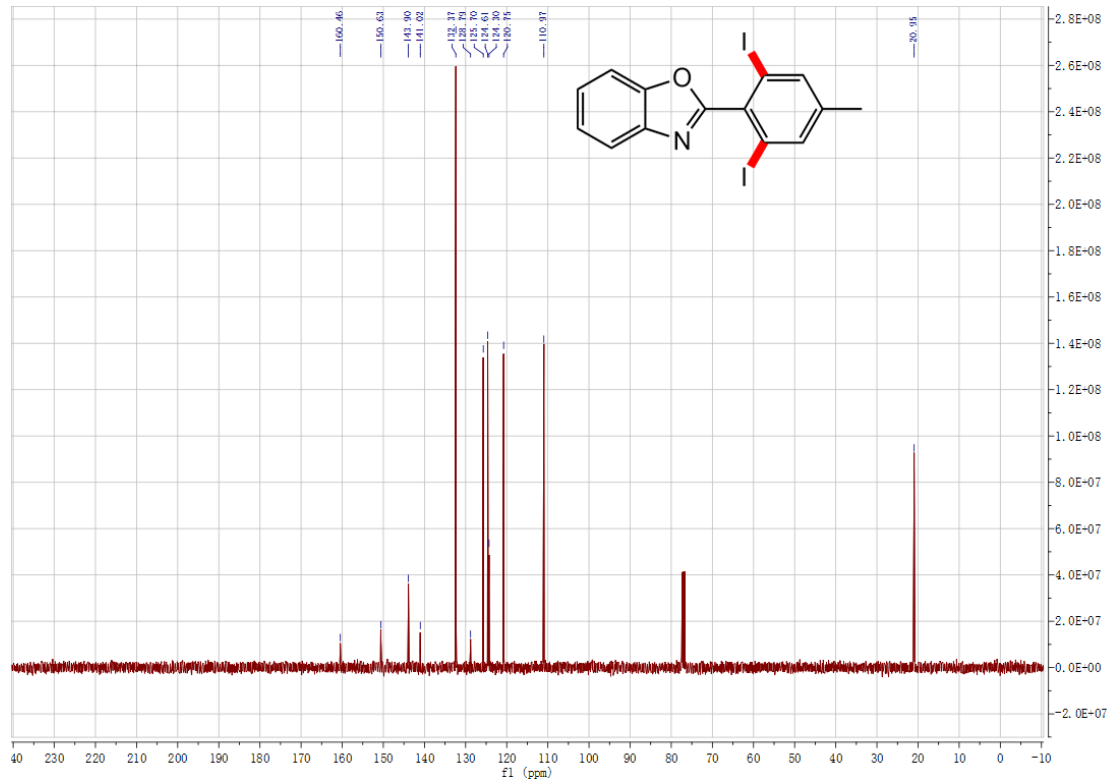
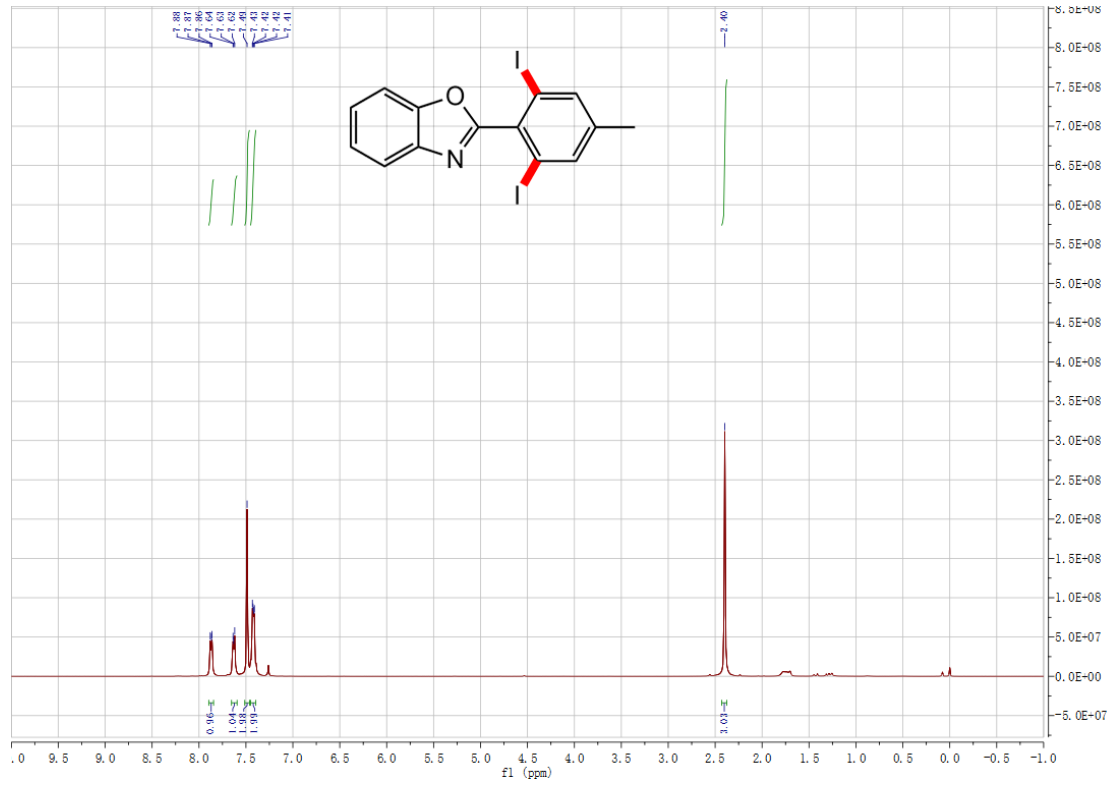
2-(2-iodo-6-methoxyphenyl)benzo[d]oxazole (3t)



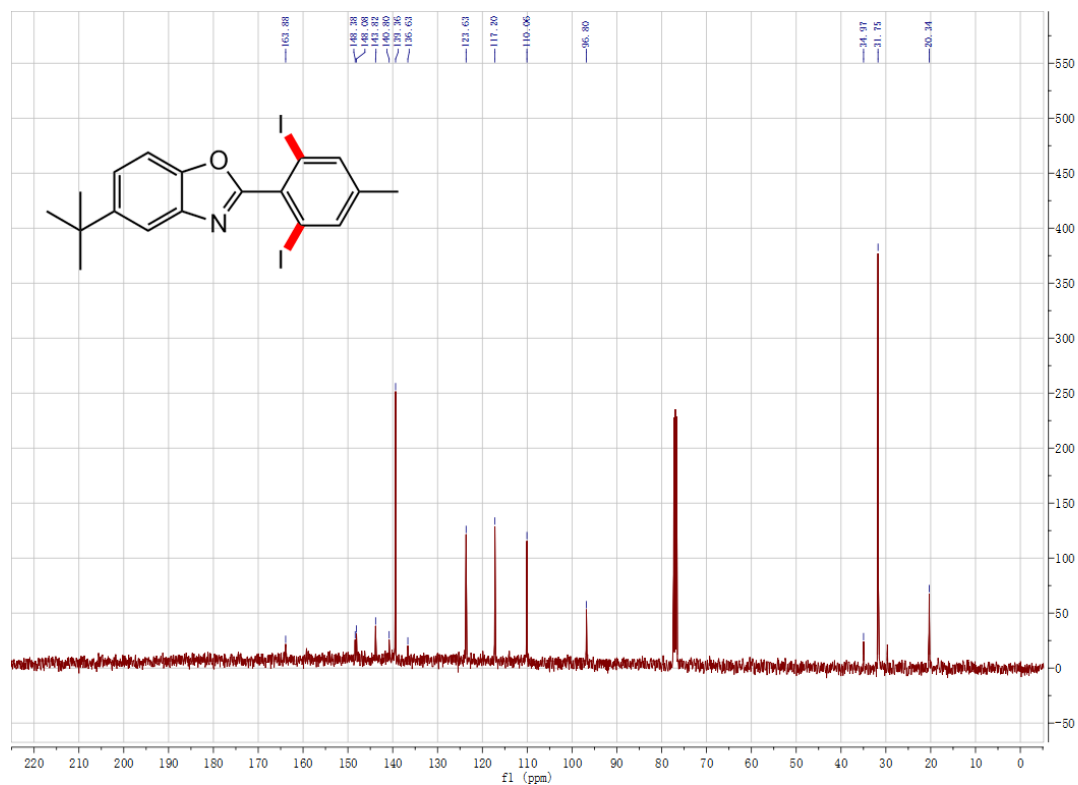
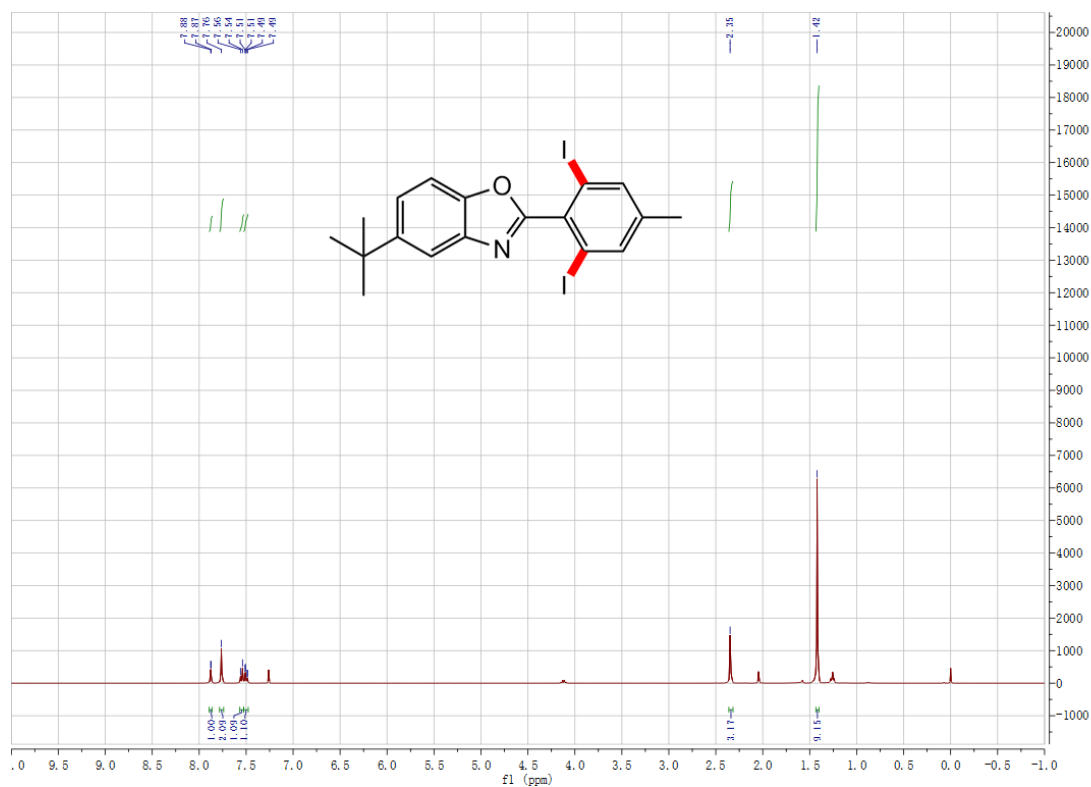
5-chloro-2-(4-chloro-2,6-diiodophenyl)benzo[d]oxazole (3v)



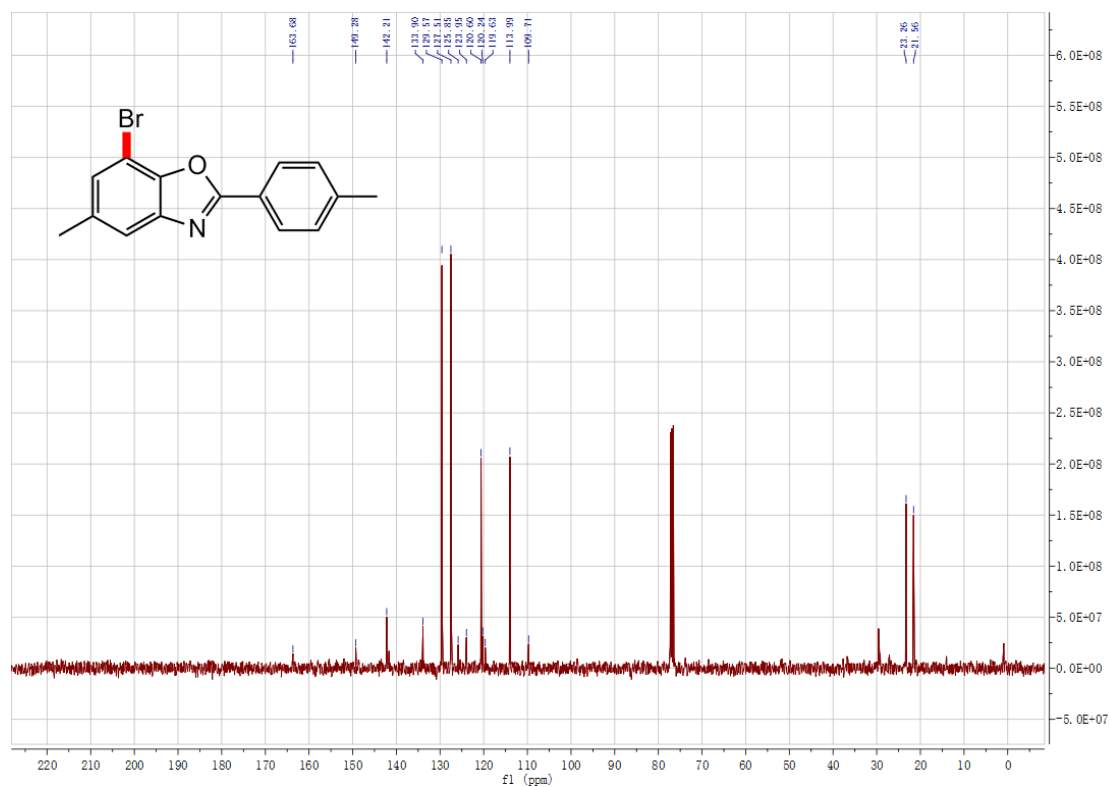
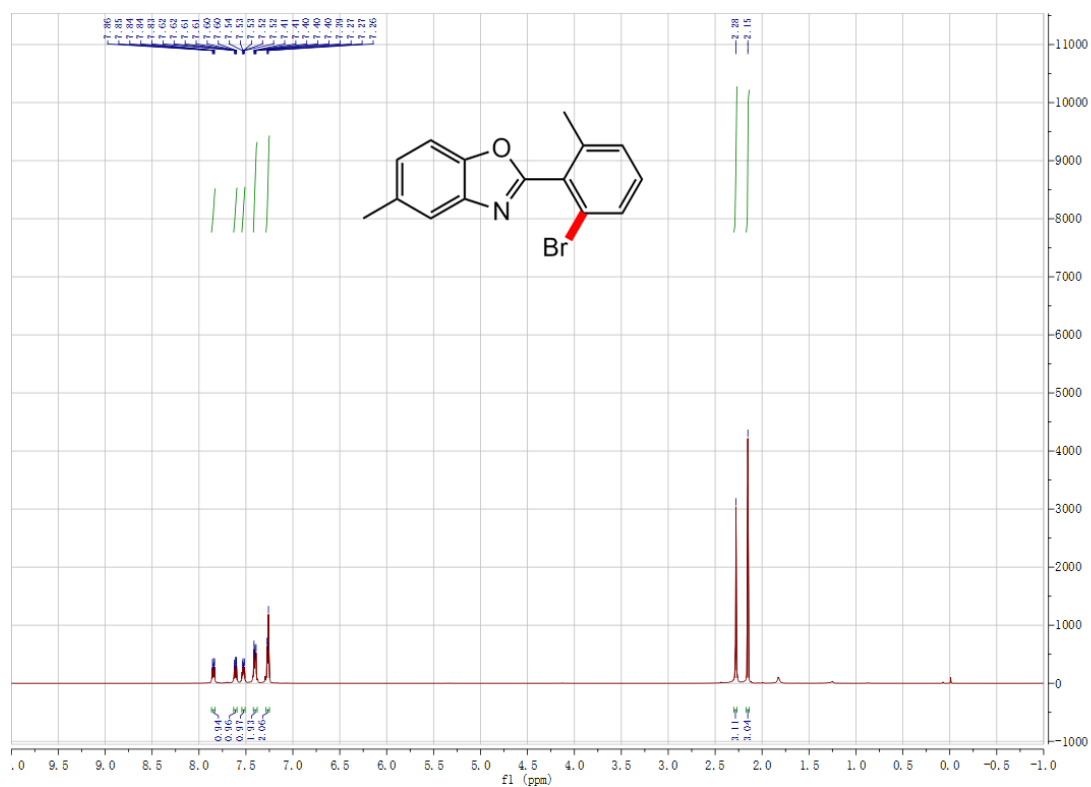
2-(2,6-diiodo-4-methylphenyl)benzo[d]oxazole (3w)



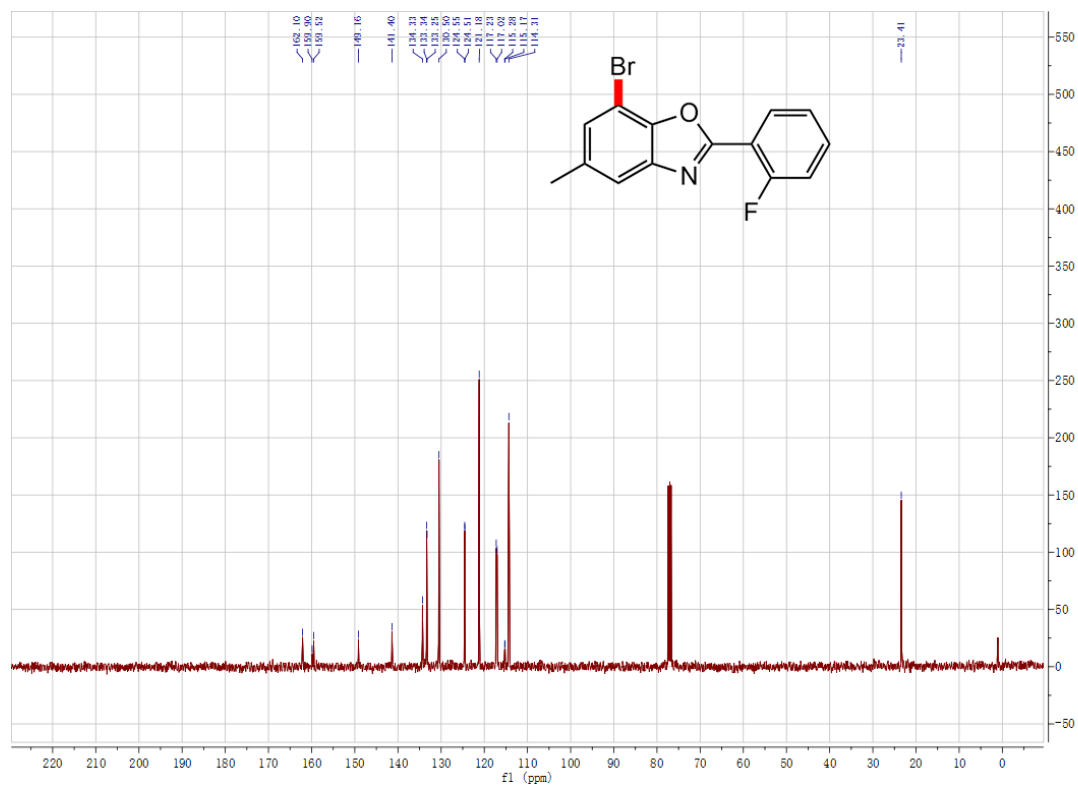
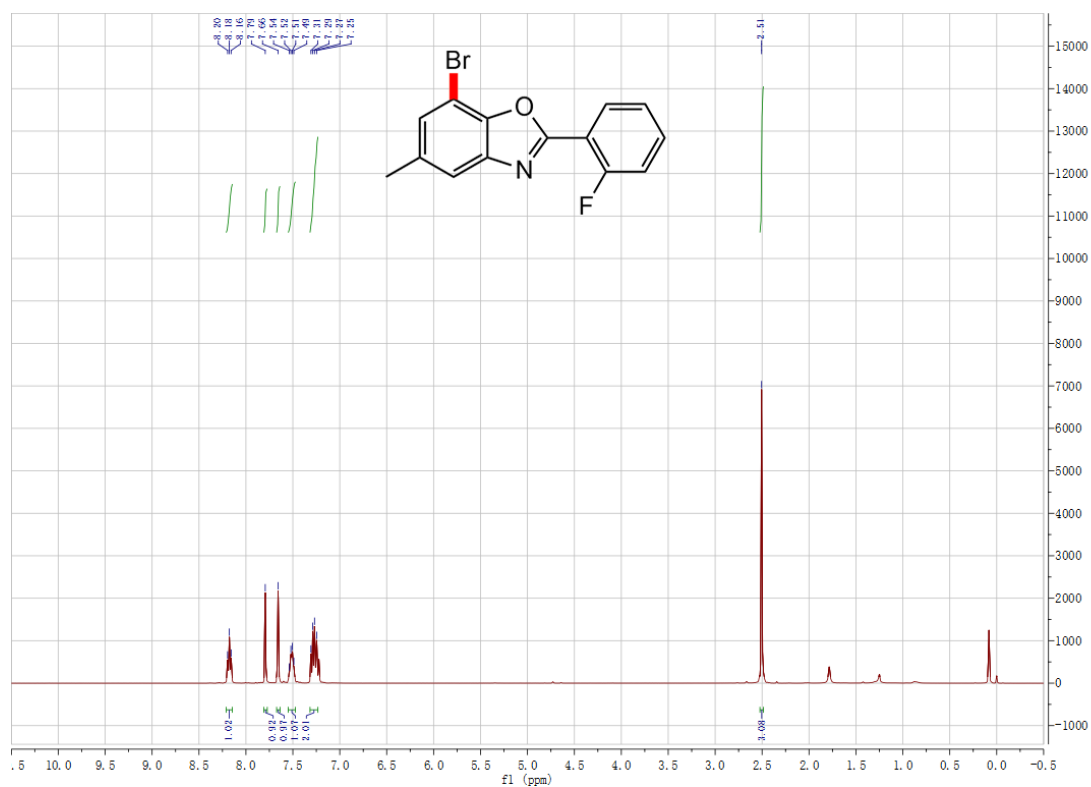
5-(*tert*-butyl)-2-(2,6-diiodo-4-methylphenyl)benzo[*d*]oxazole (3x)

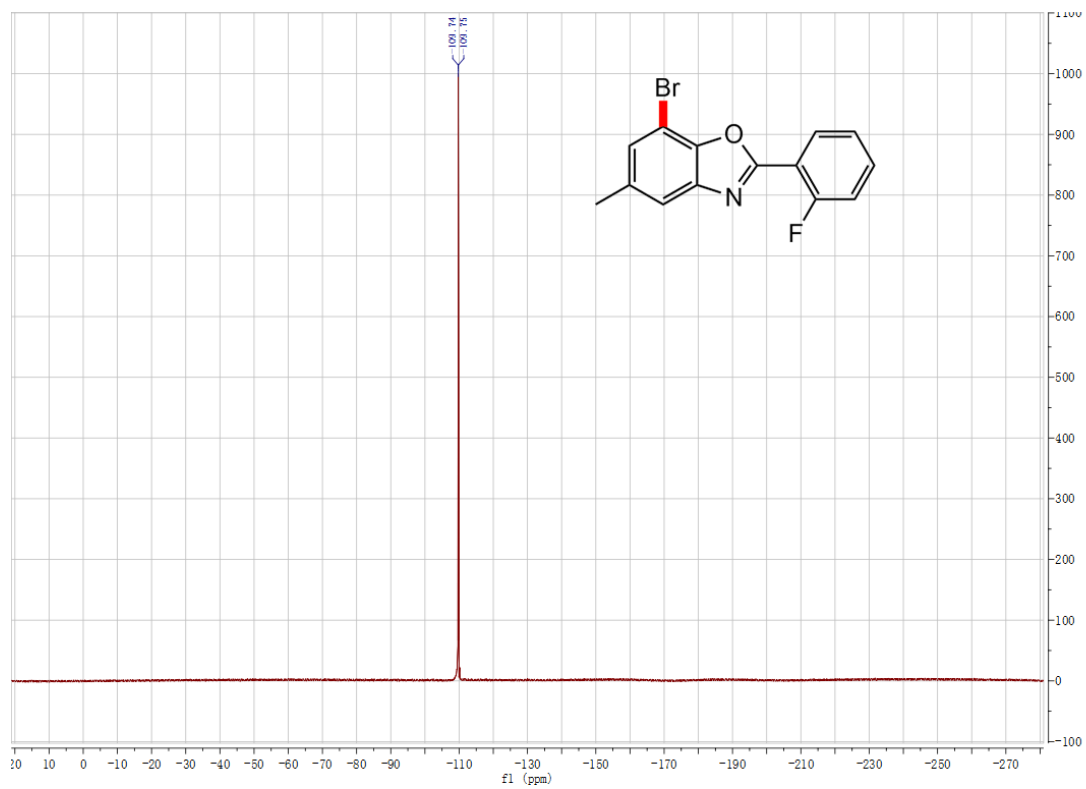


7-bromo-5-methyl-2-(o-tolyl)benzo[d]oxazole (5a)

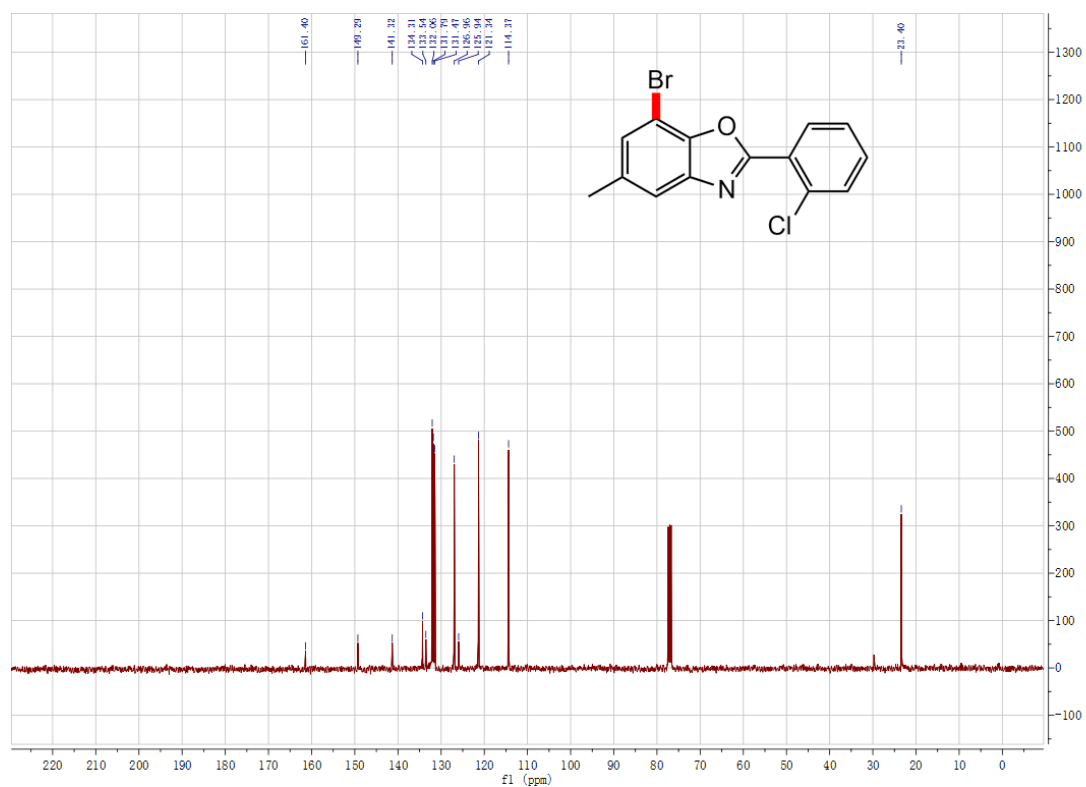
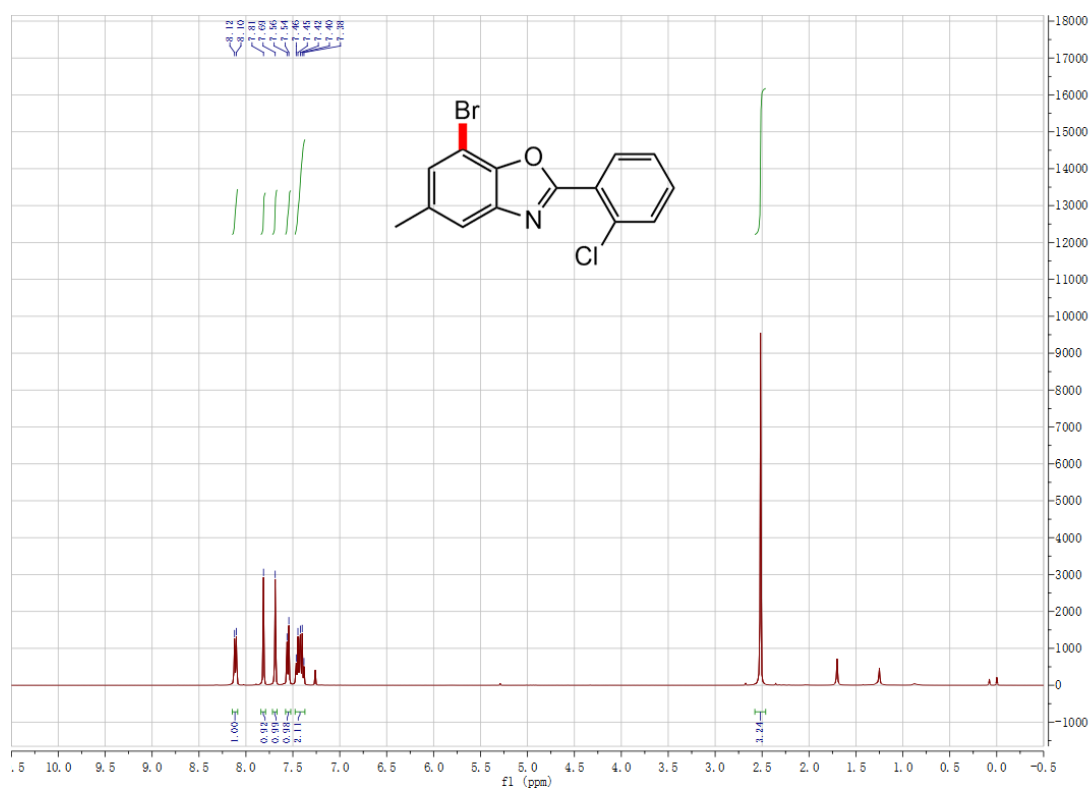


7-bromo-2-(2-fluorophenyl)-5-methylbenzo[d]oxazole (5b)

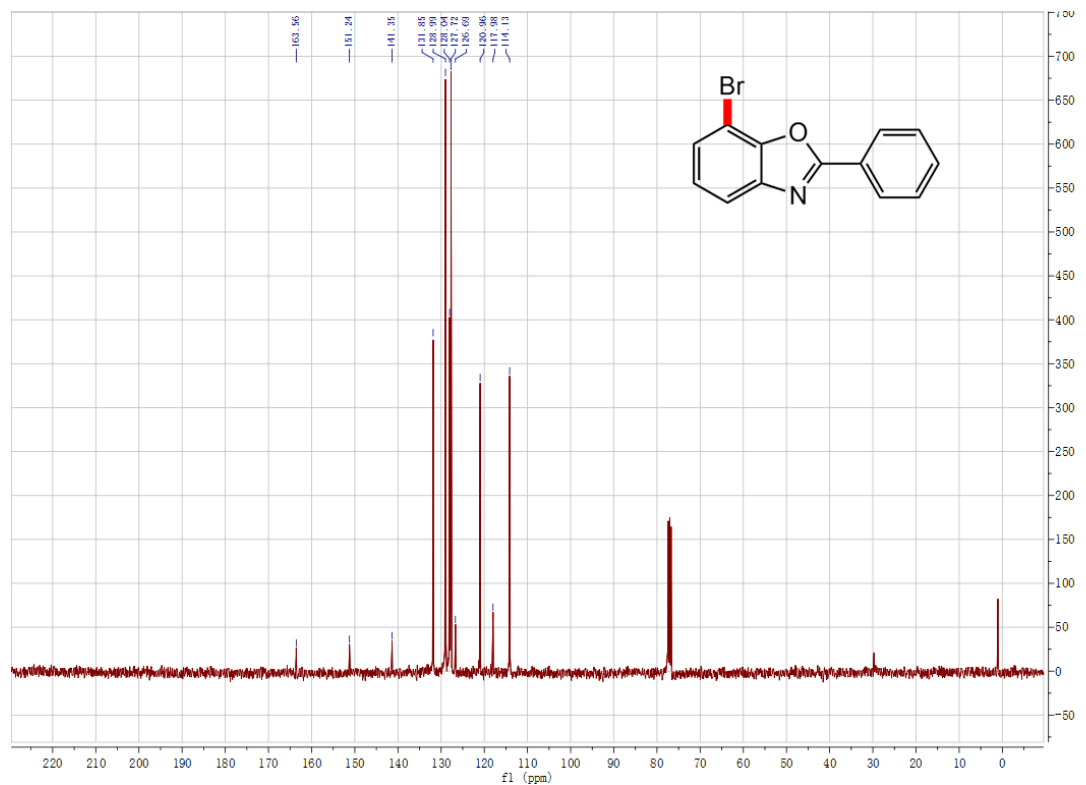
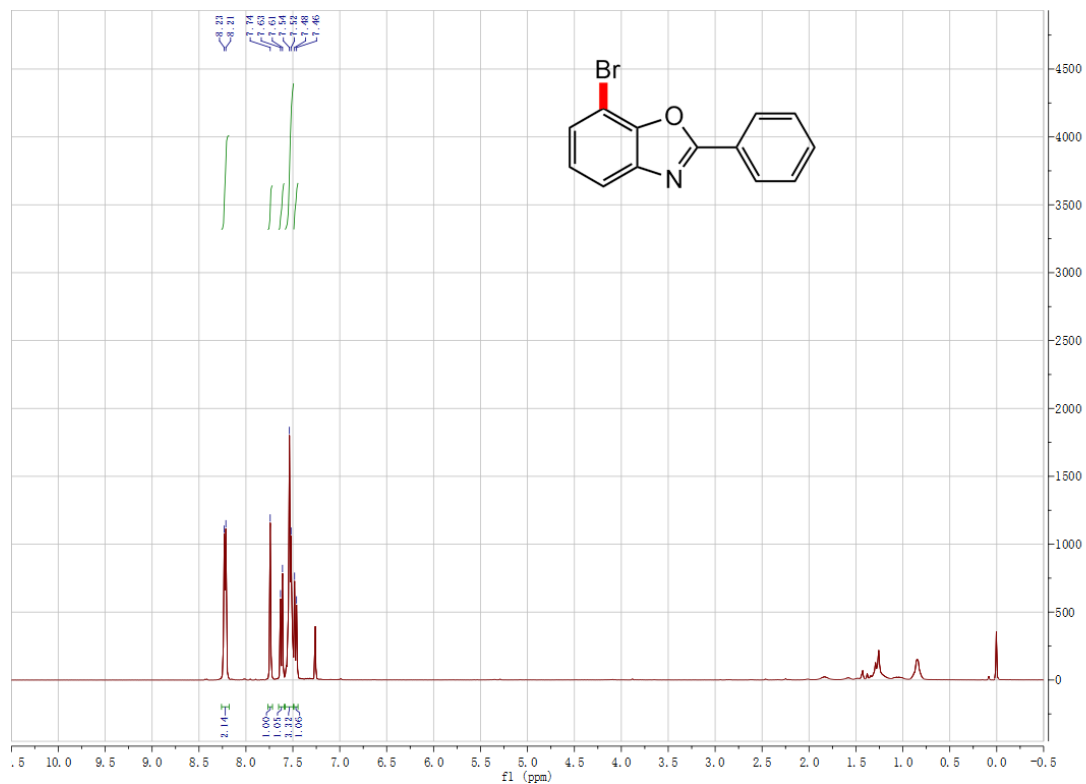




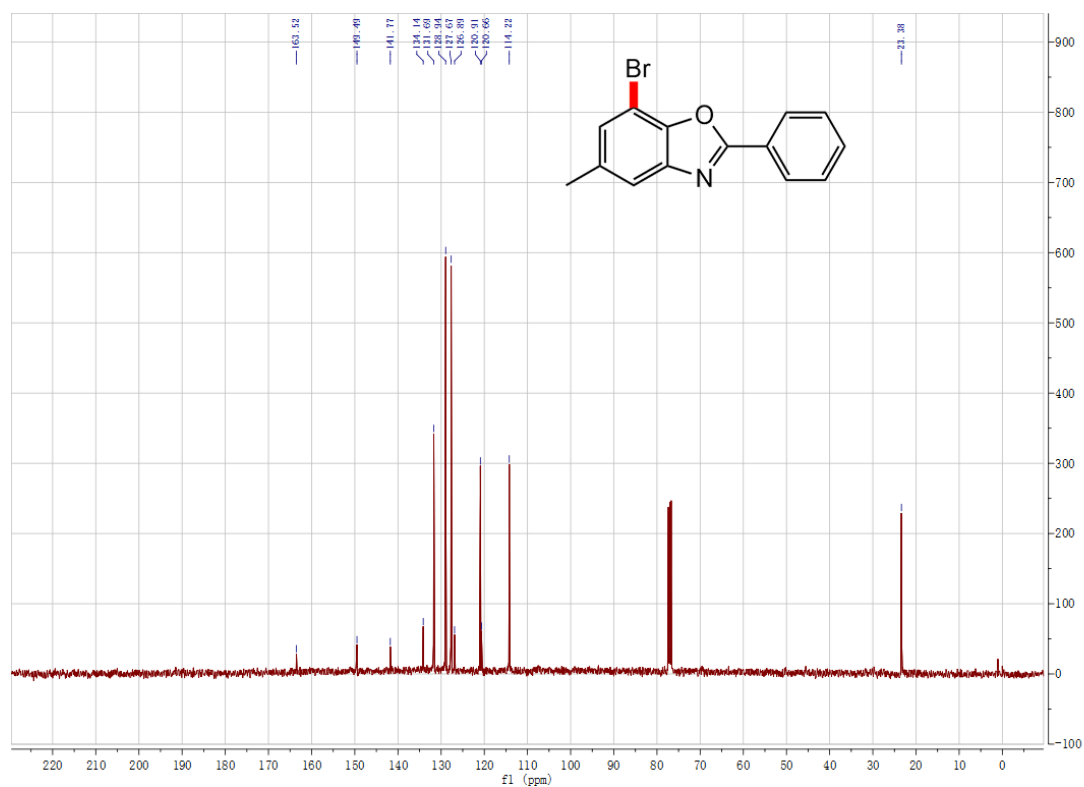
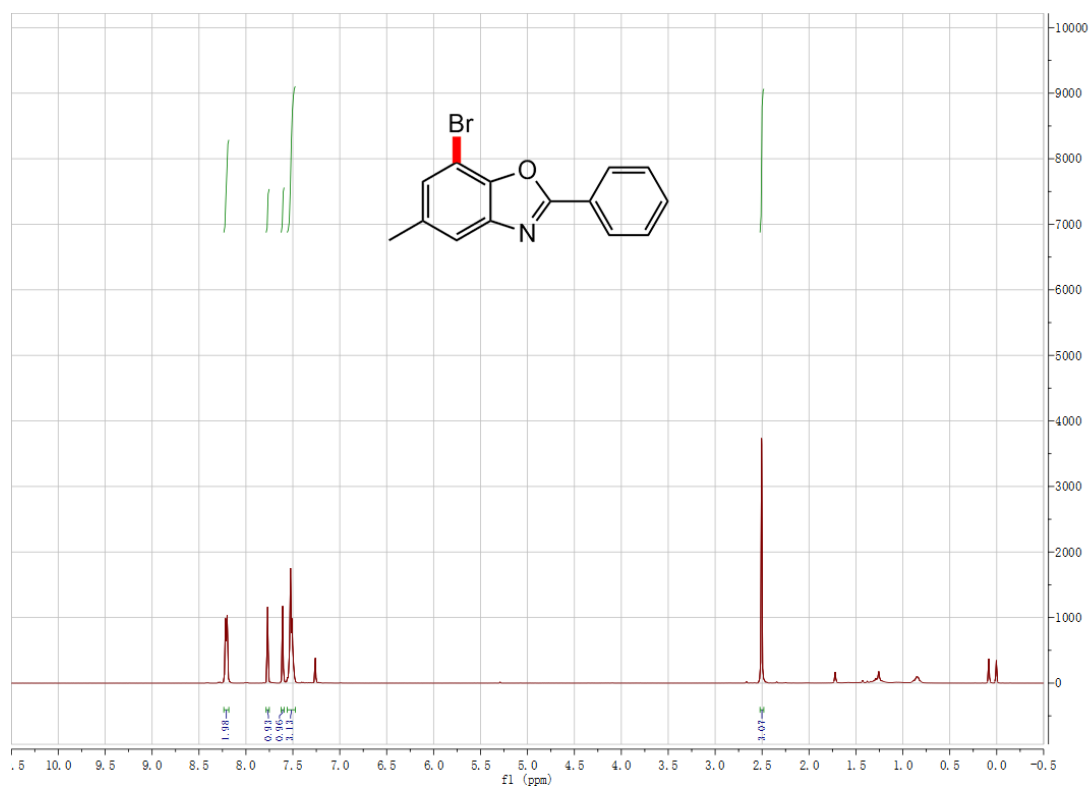
7-bromo-2-(2-chlorophenyl)-5-methylbenzo[d]oxazole (5c)



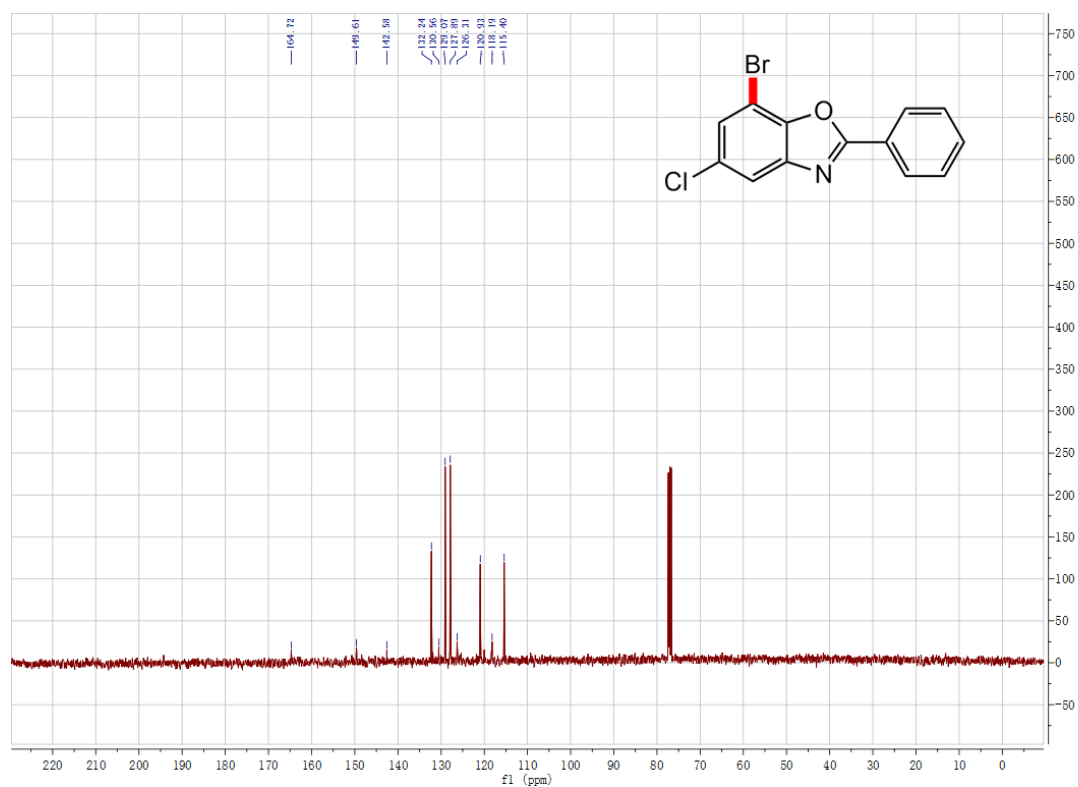
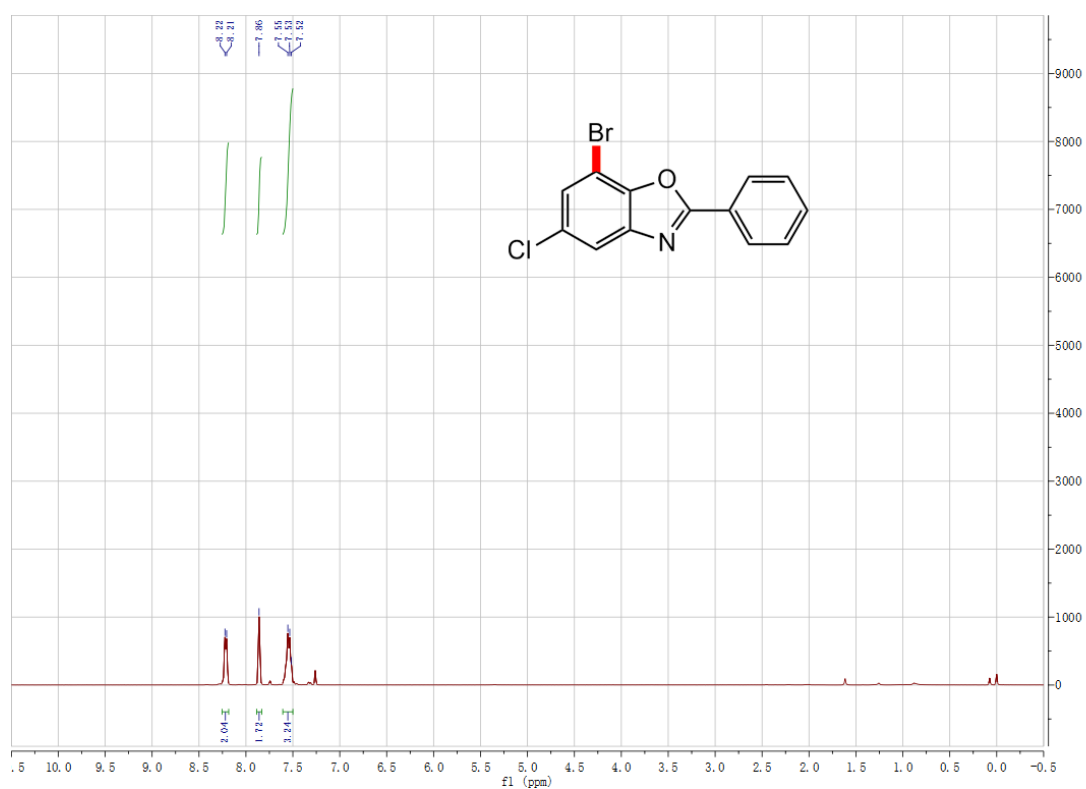
7-bromo-2-phenylbenzo[d]oxazole (5d)



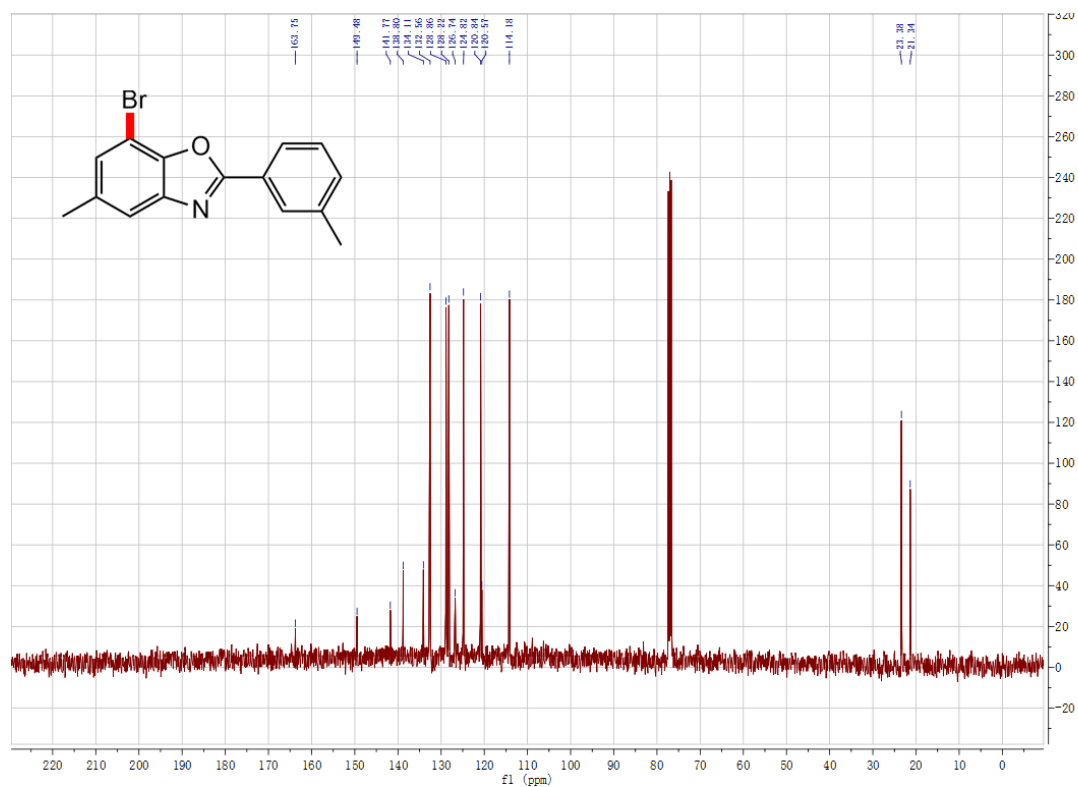
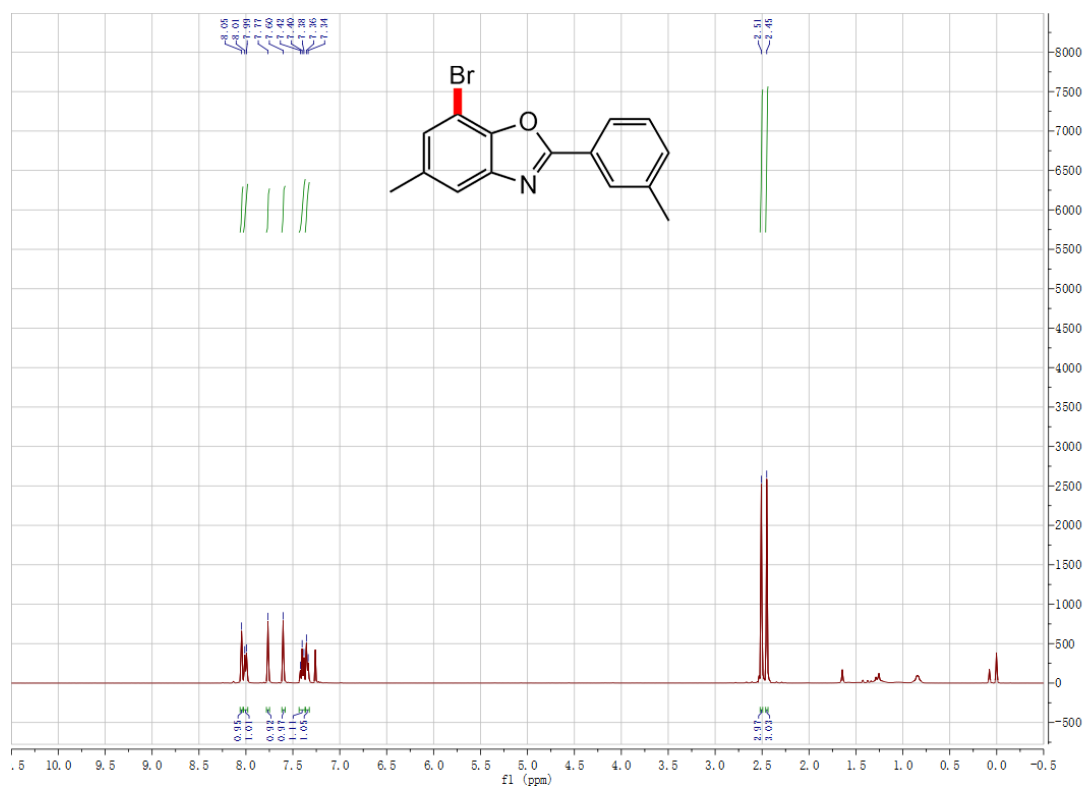
7-bromo-5-methyl-2-phenylbenzo[d]oxazole (5e)



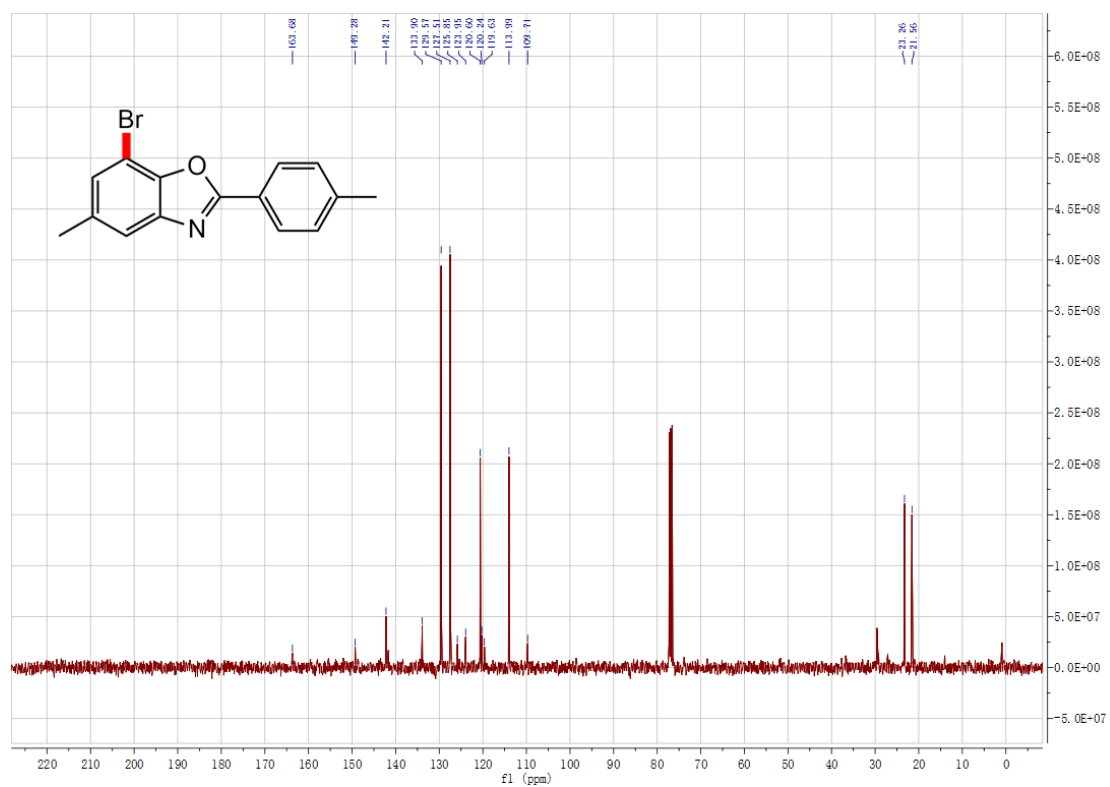
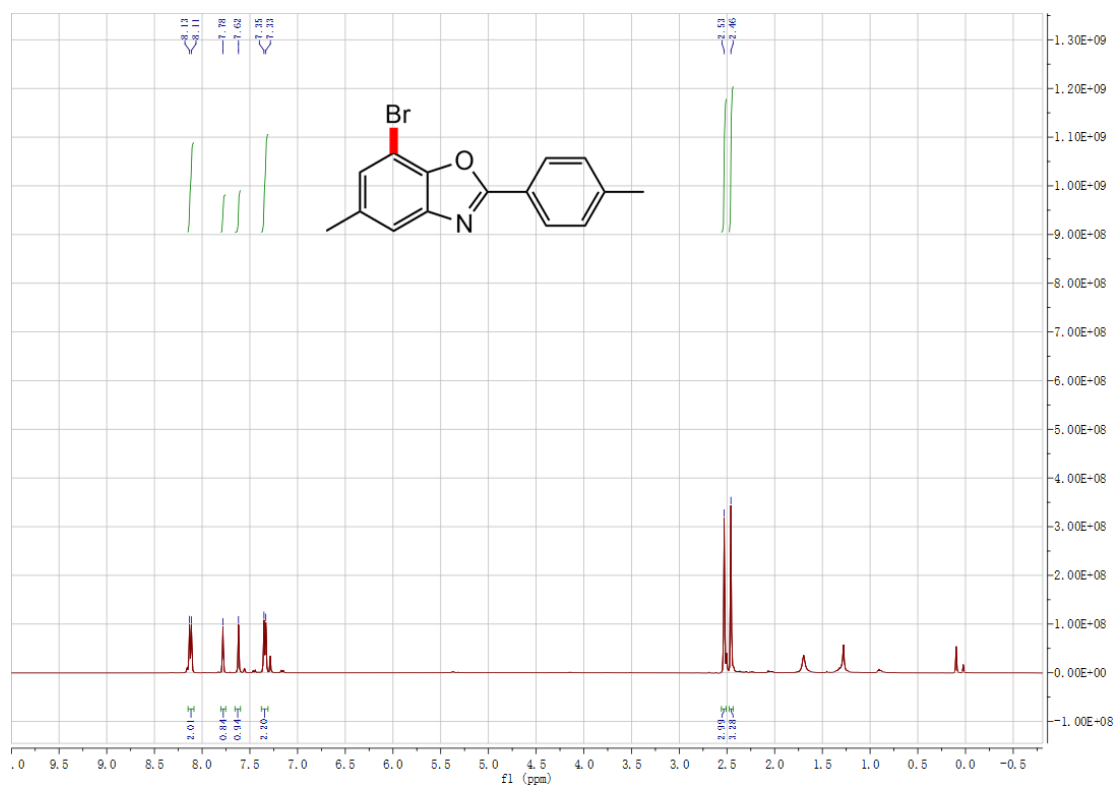
7-bromo-5-chloro-2-phenylbenzo[d]oxazole (5f)



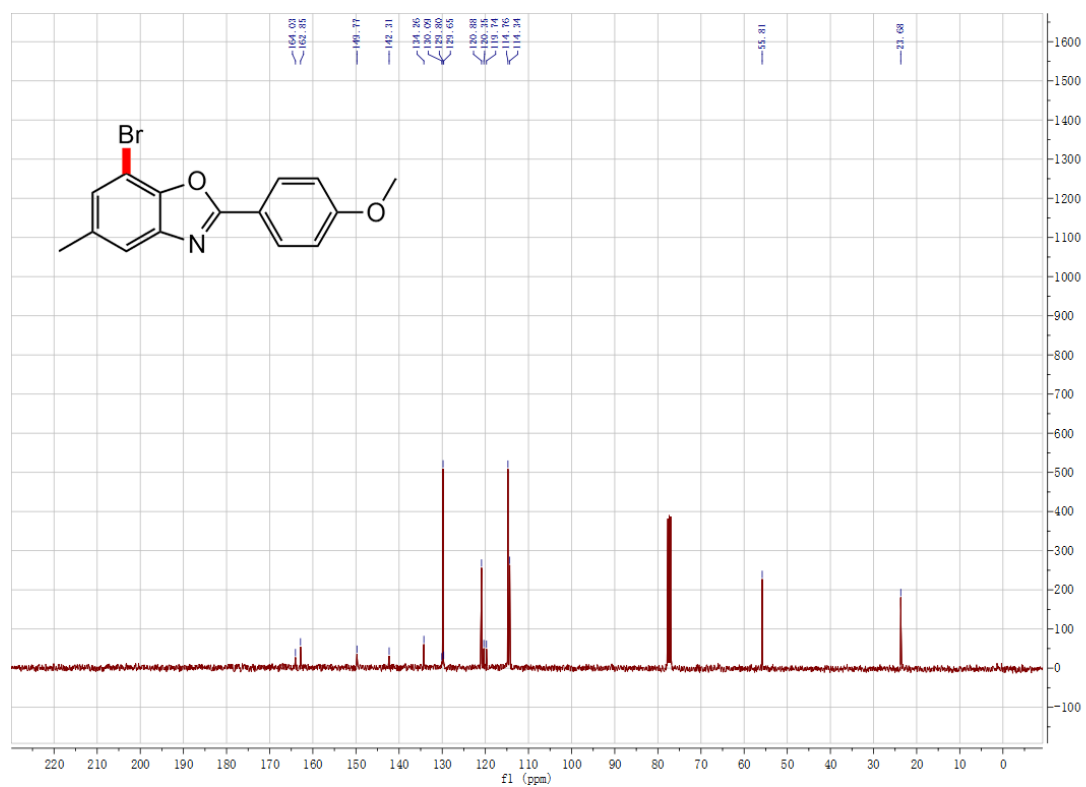
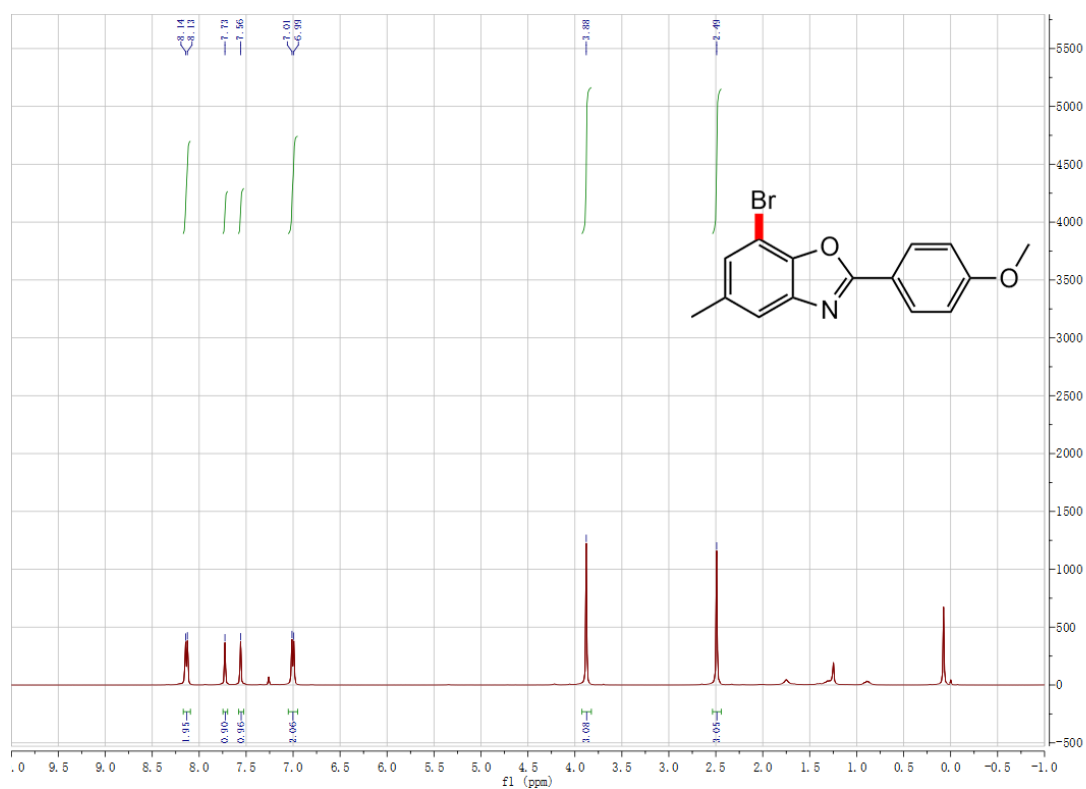
7-bromo-5-methyl-2-(*m*-tolyl)benzo[*d*]oxazole (5h)



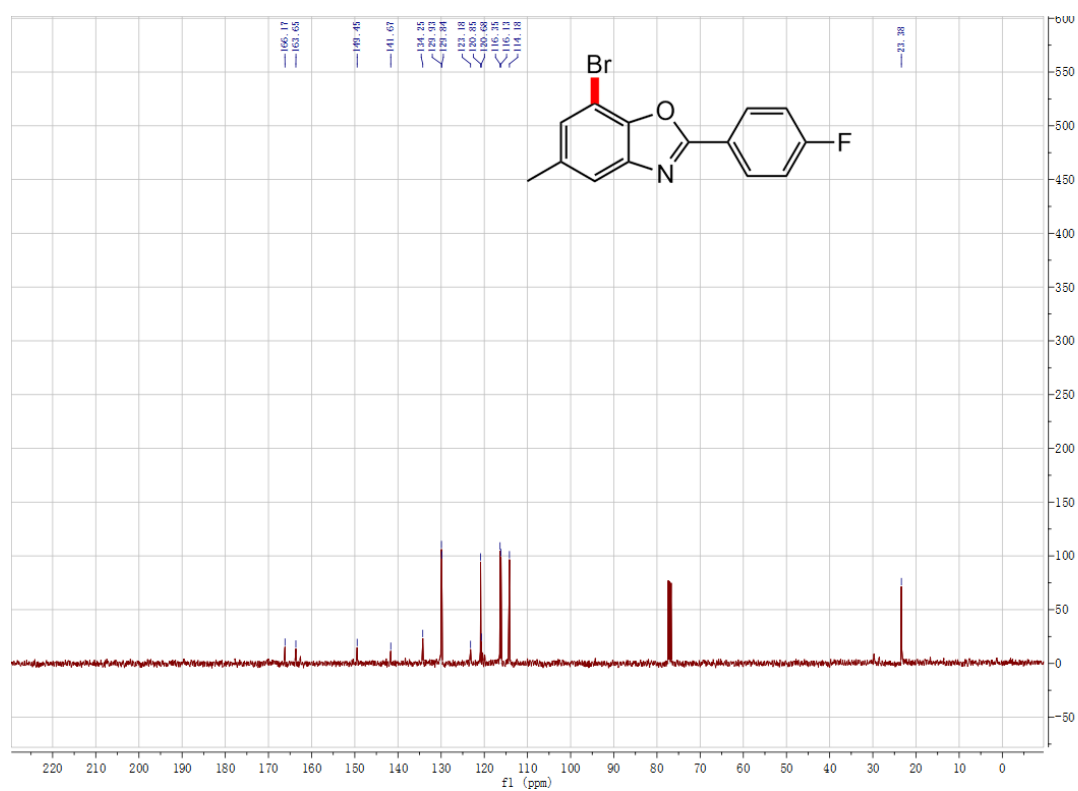
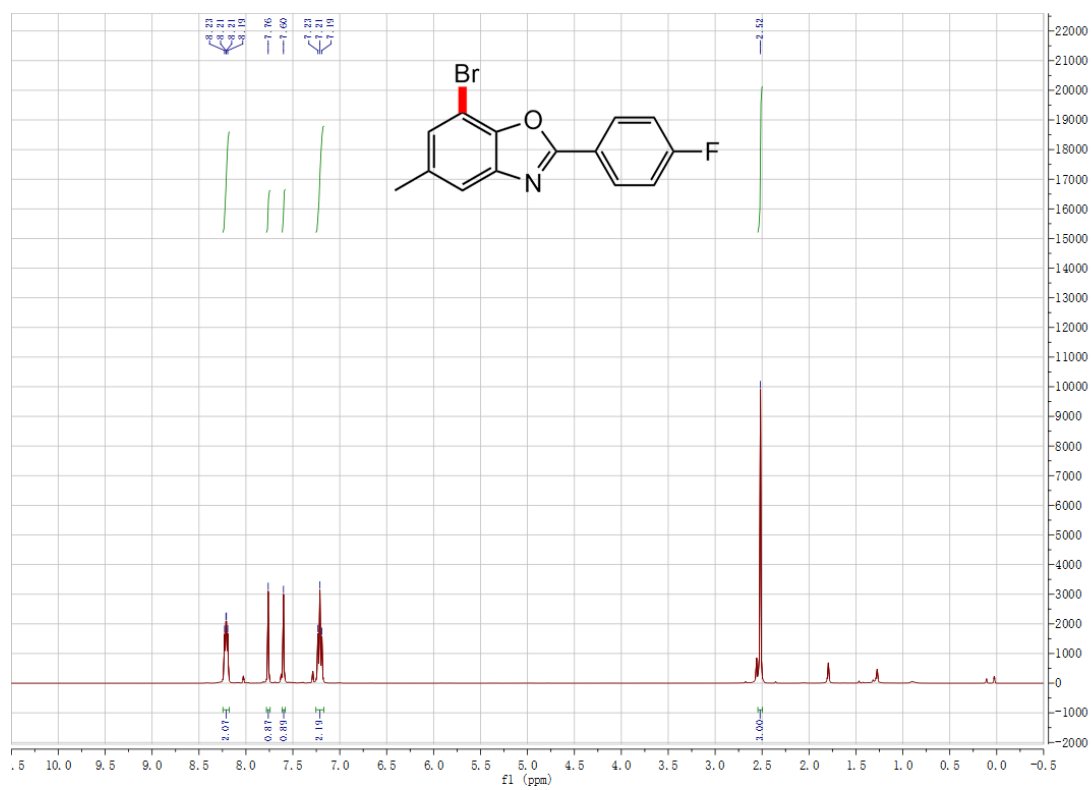
7-bromo-5-methyl-2-(p-tolyl)benzo[d]oxazole (5i)

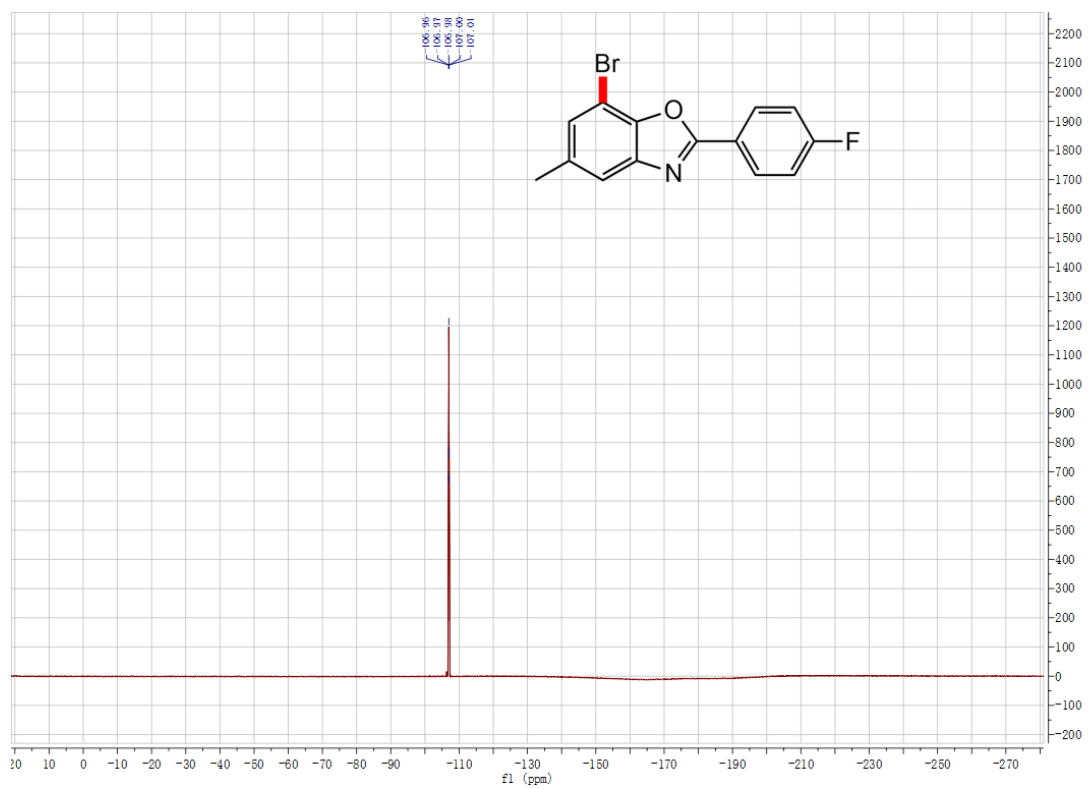


7-bromo-2-(4-methoxyphenyl)-5-methylbenzo[d]oxazole (5j)

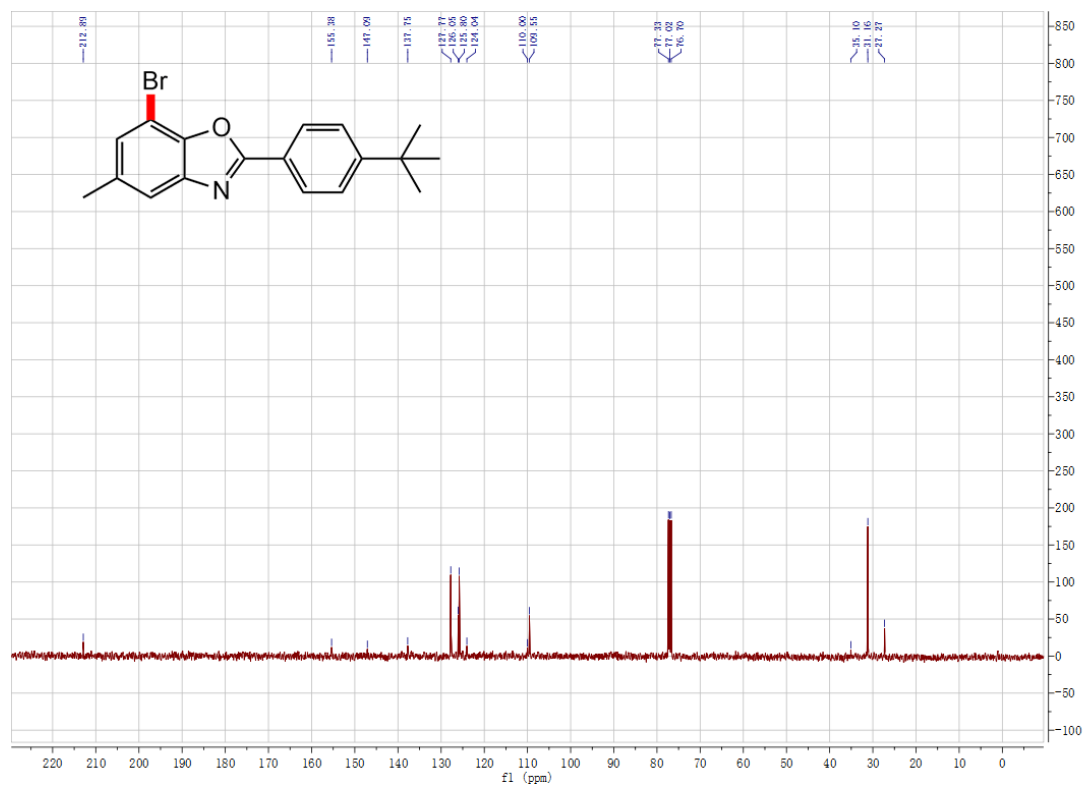
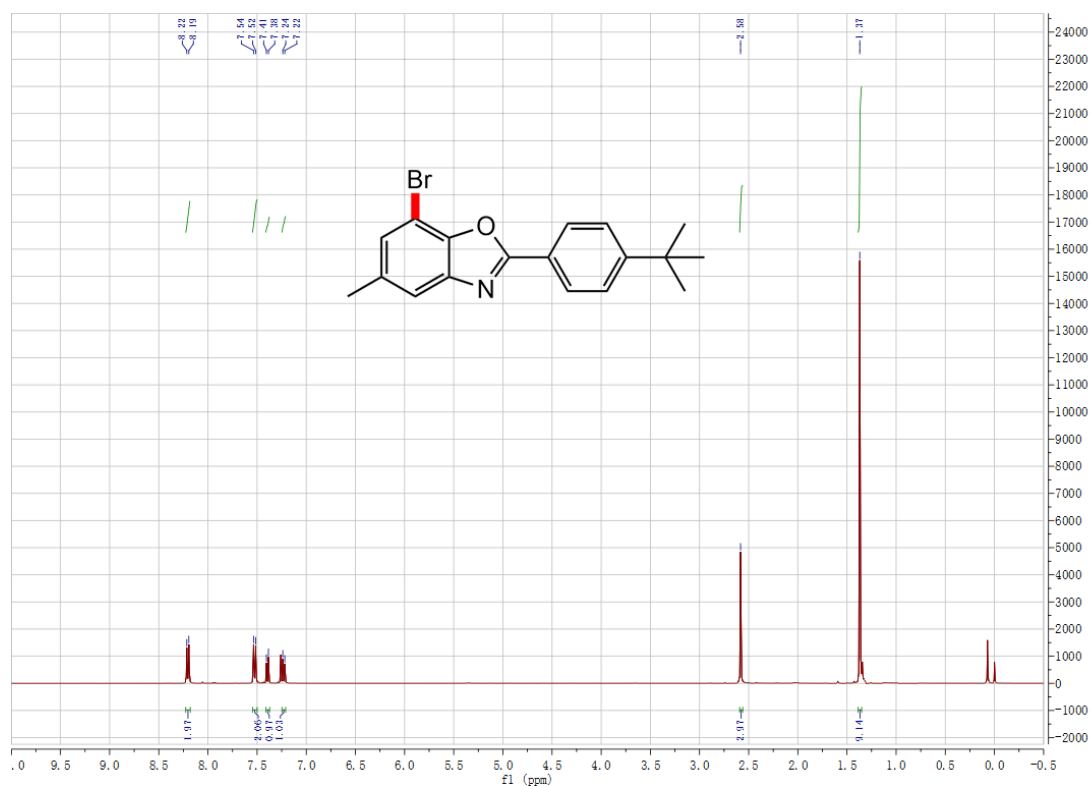


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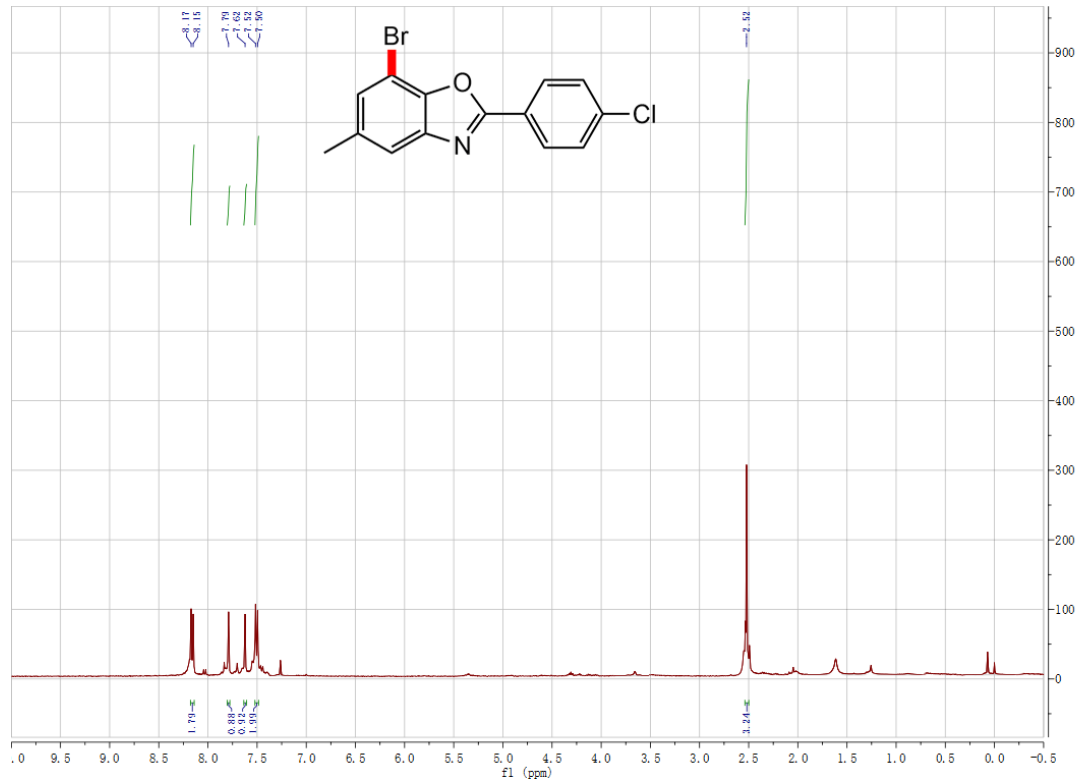
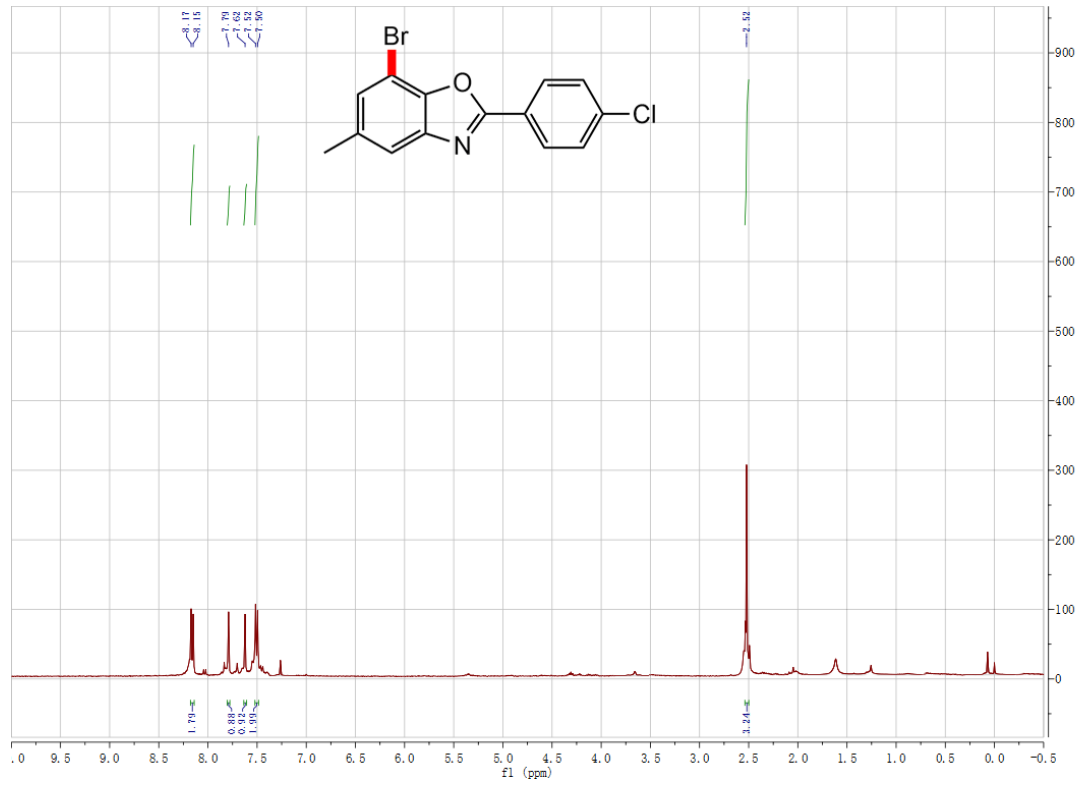




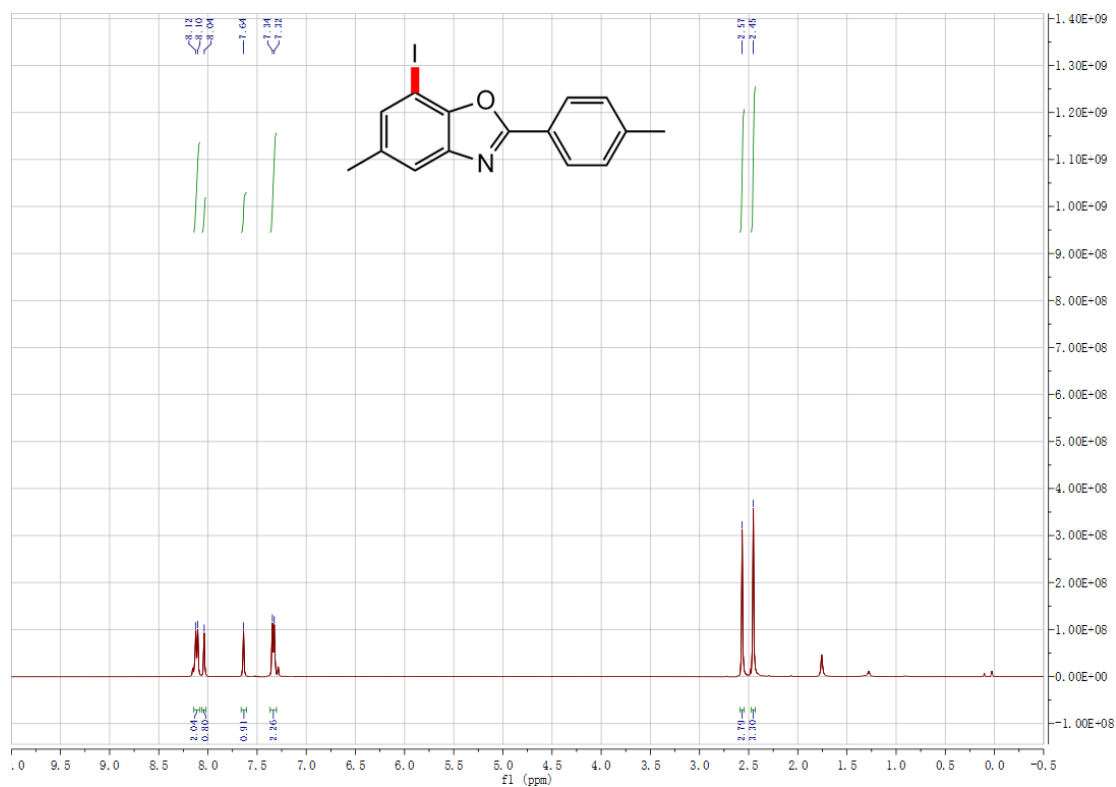
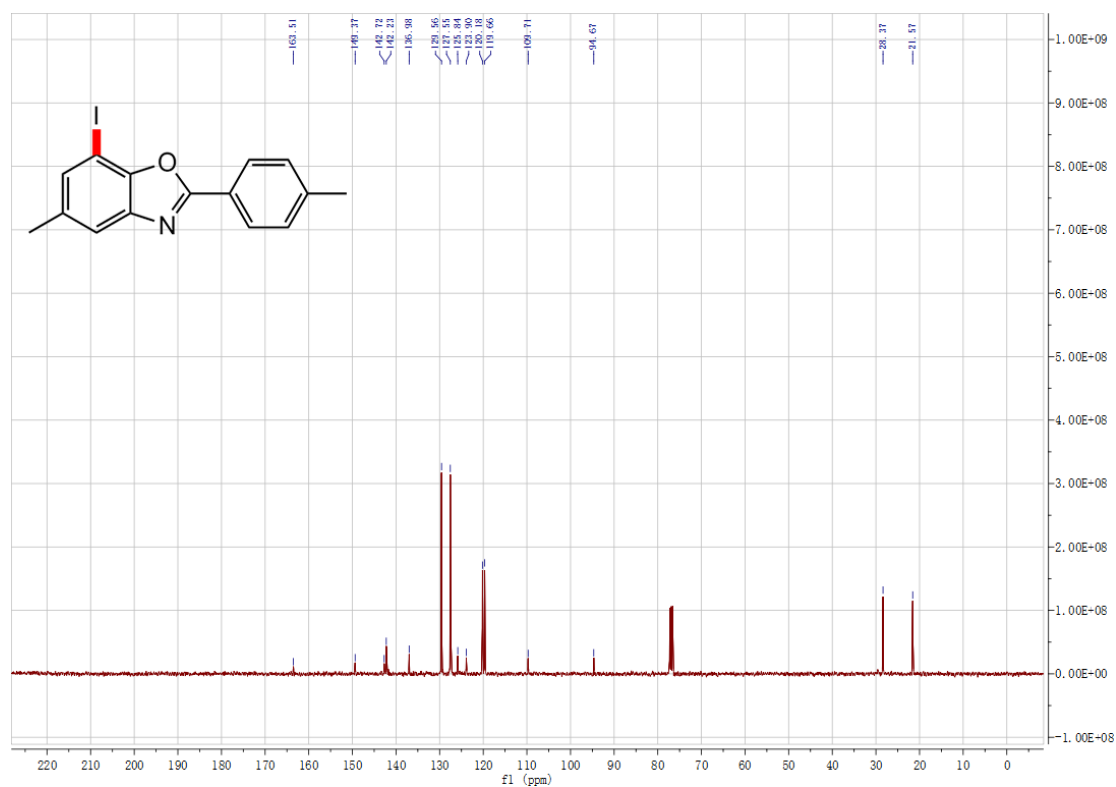
7-bromo-2-(4-(tert-butyl)phenyl)-5-methylbenzo[d]oxazole (5y)



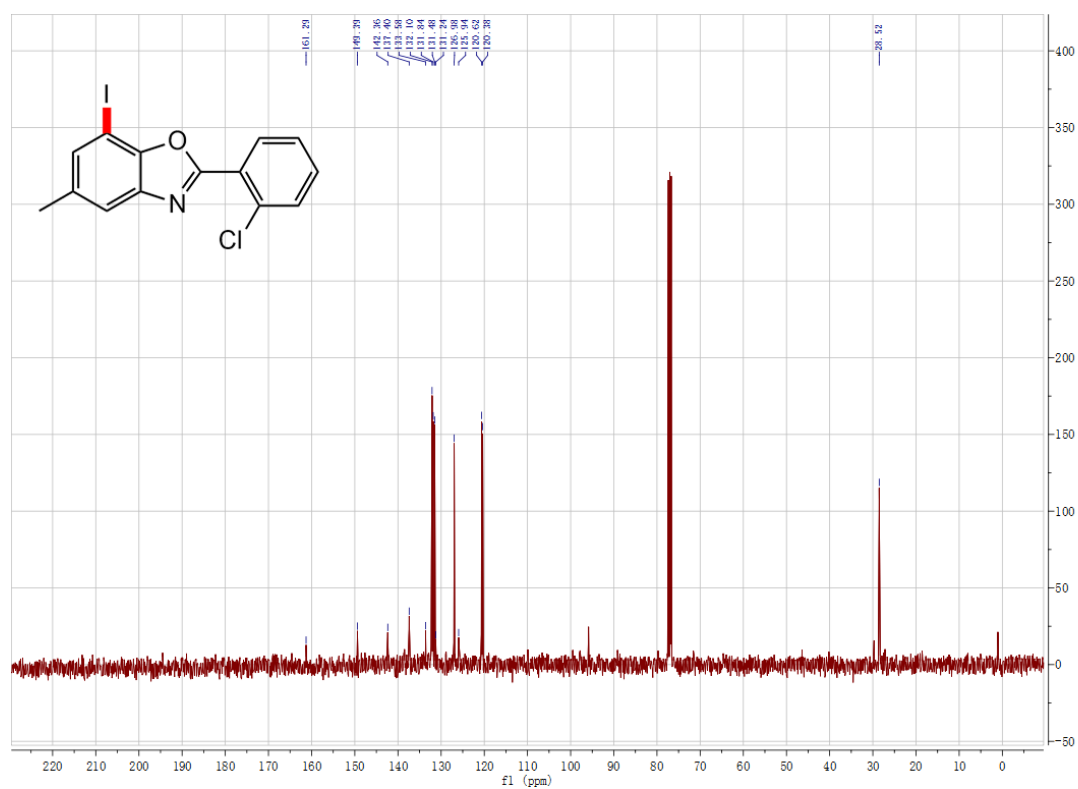
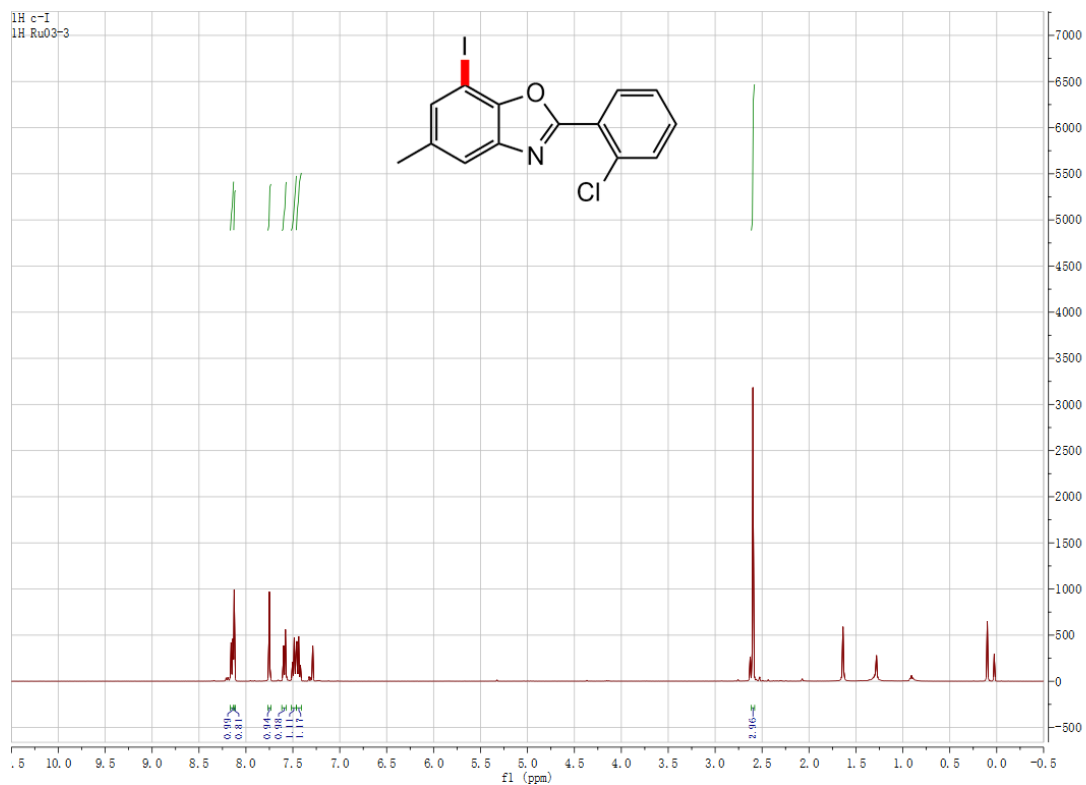
2-(4-chlorophenyl)-7-bromo-5-methylbenzo[d]oxazole (5z)



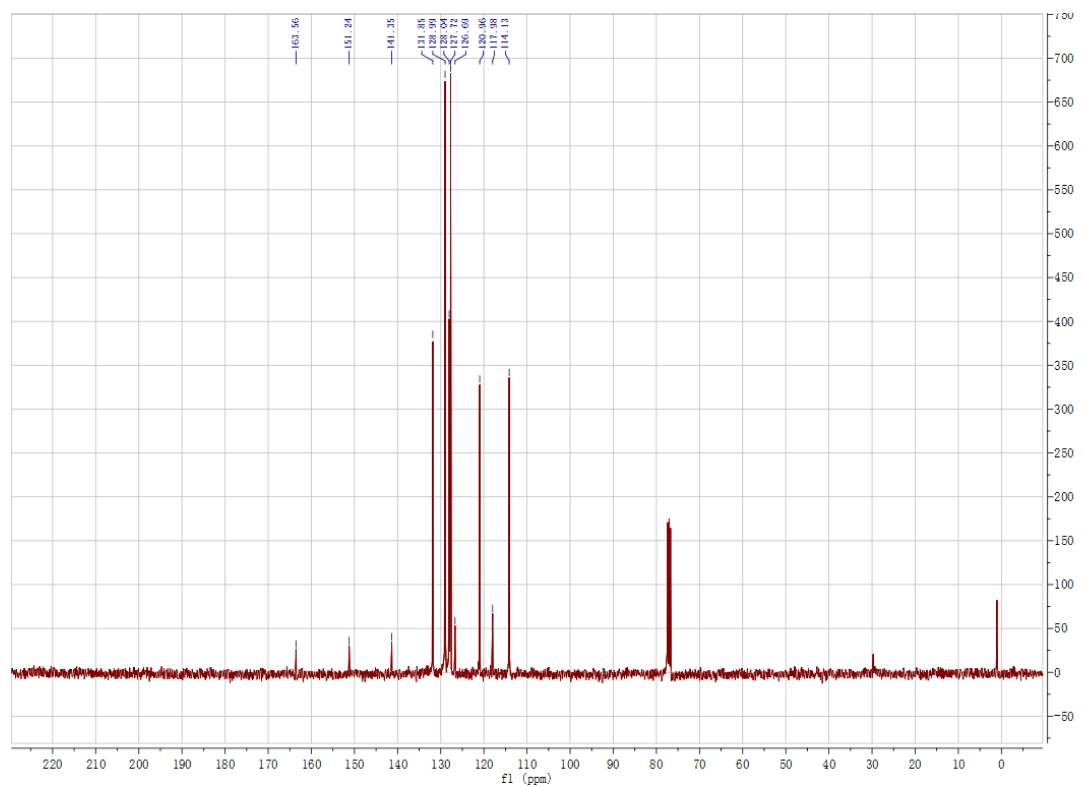
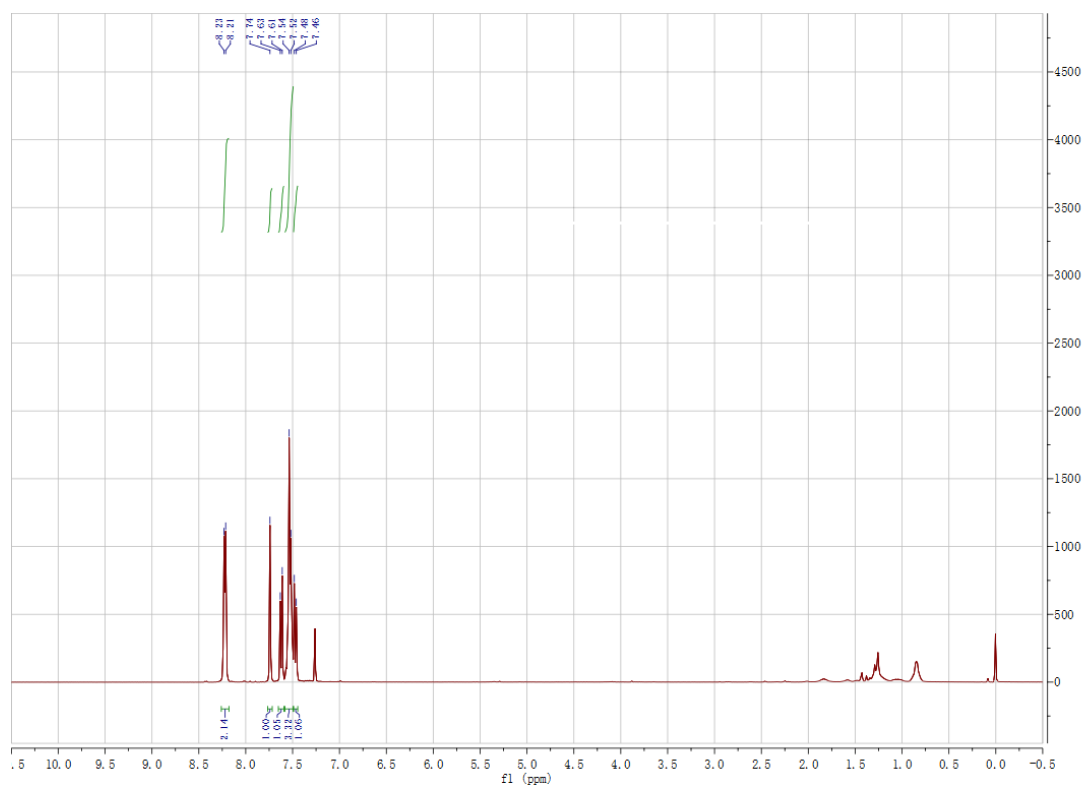
7-Iodo-5-methyl-2-(*o*-tolyl)benzo[*d*]oxazole (6a)



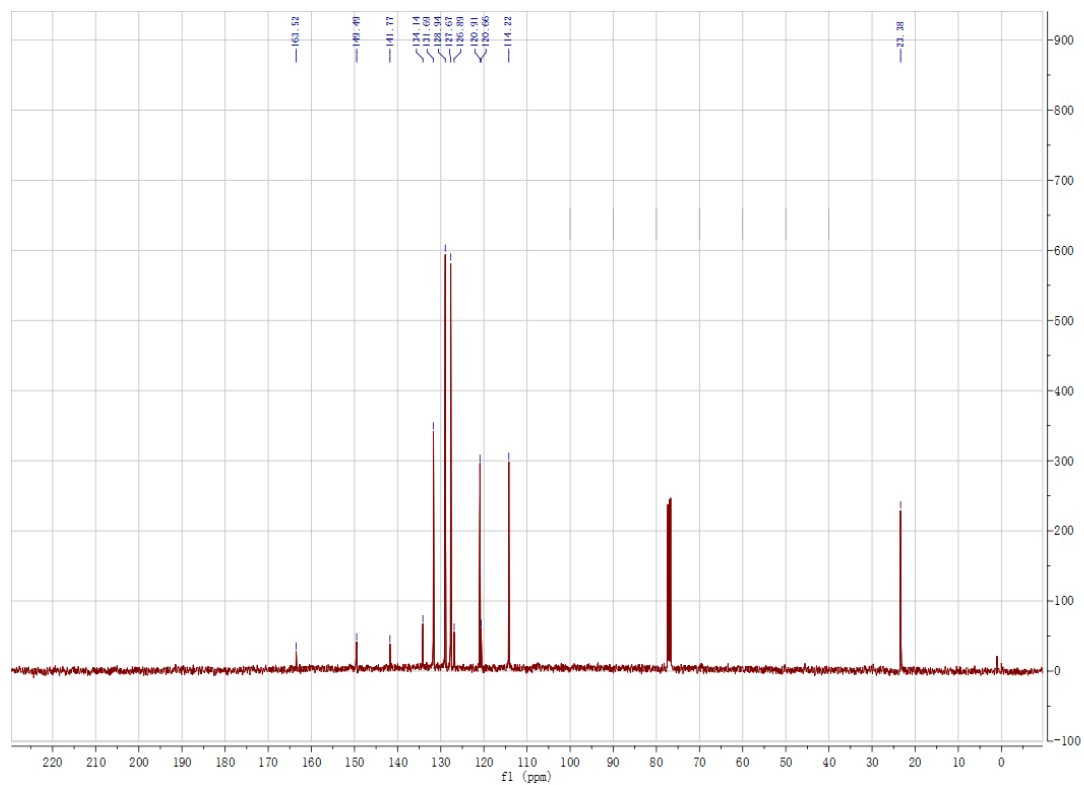
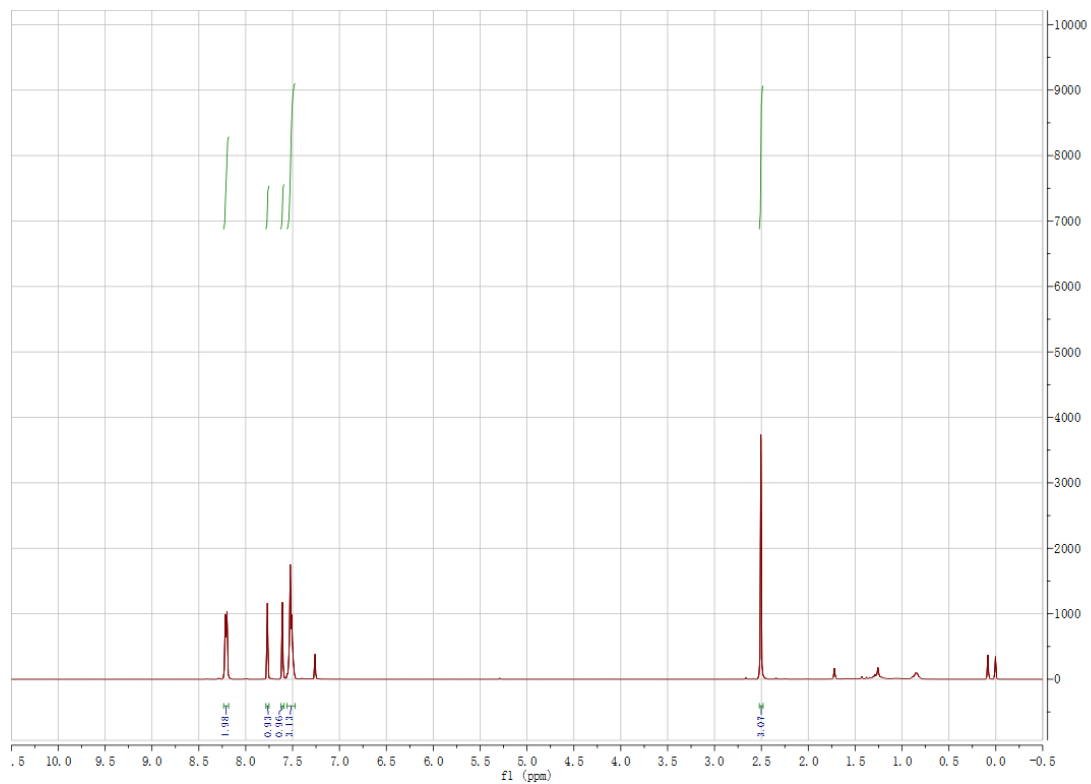
2-(2-chlorophenyl)-7-iodo-5-methylbenzo[d]oxazole (6c)



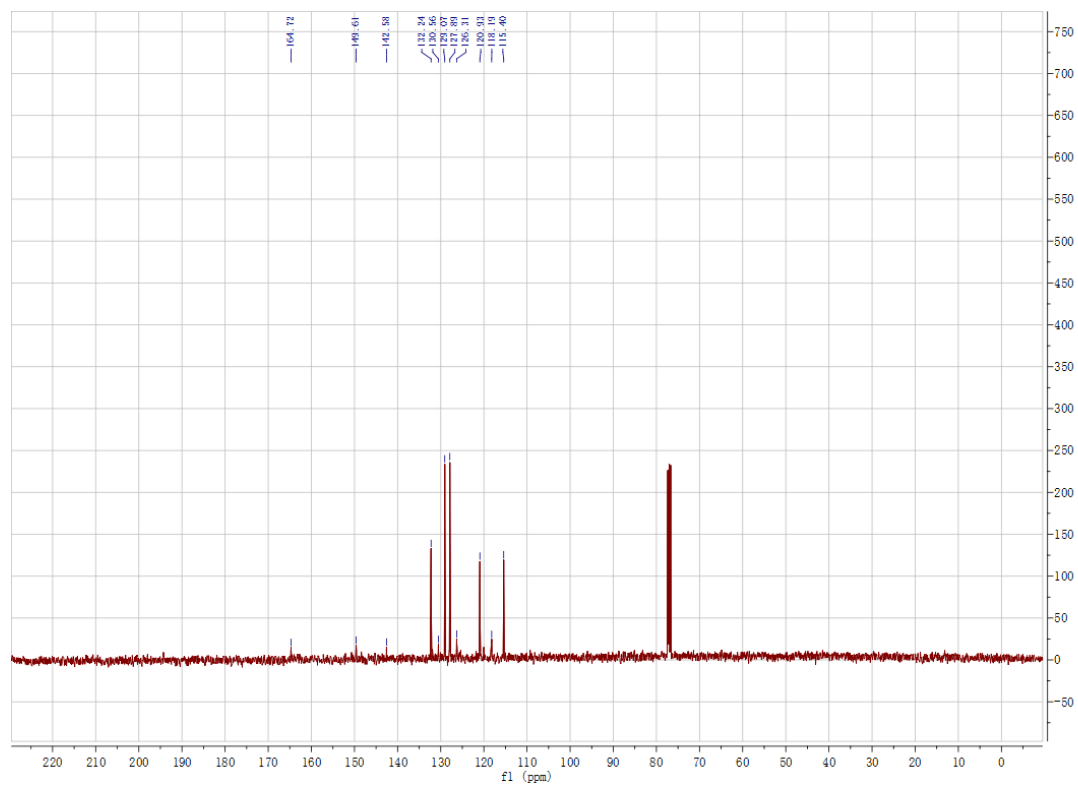
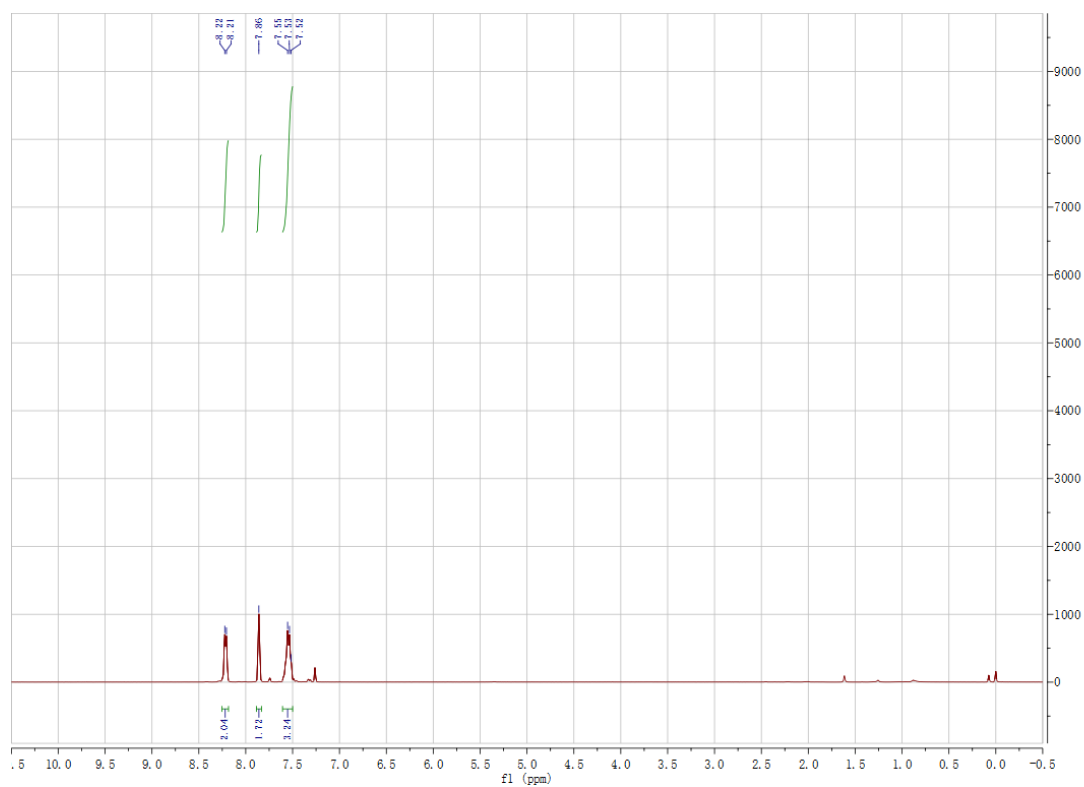
7-iodo-2-phenylbenzo[d]oxazole (6d)



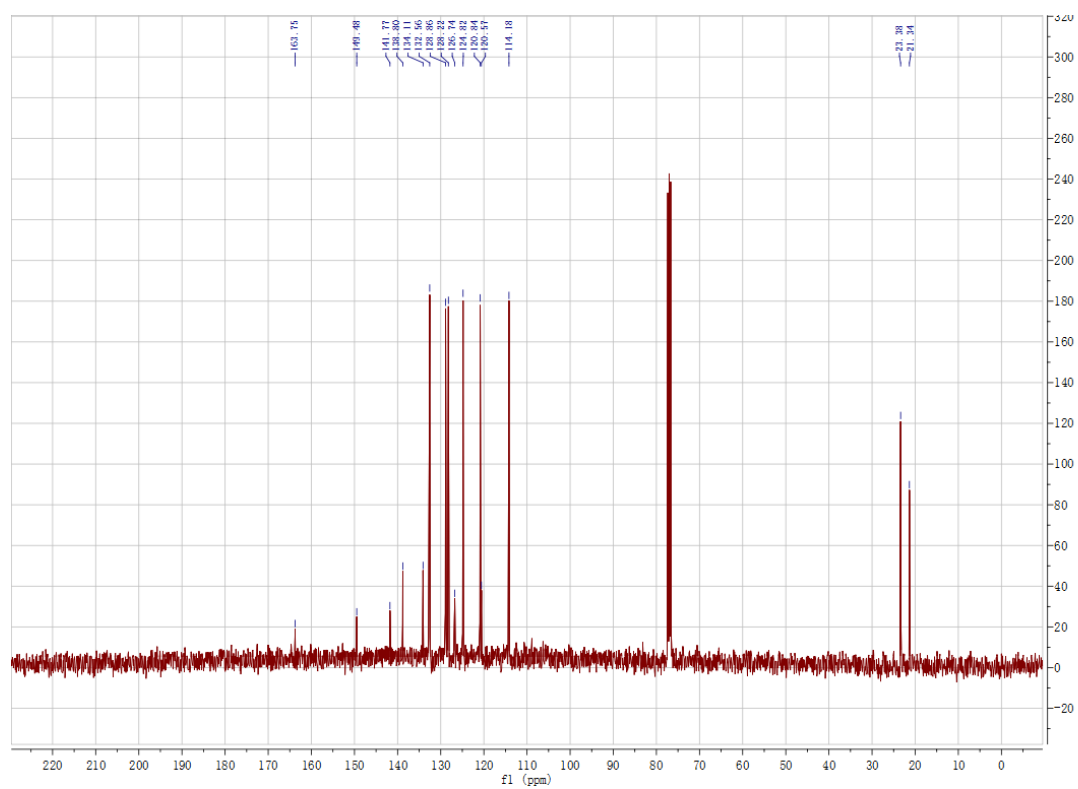
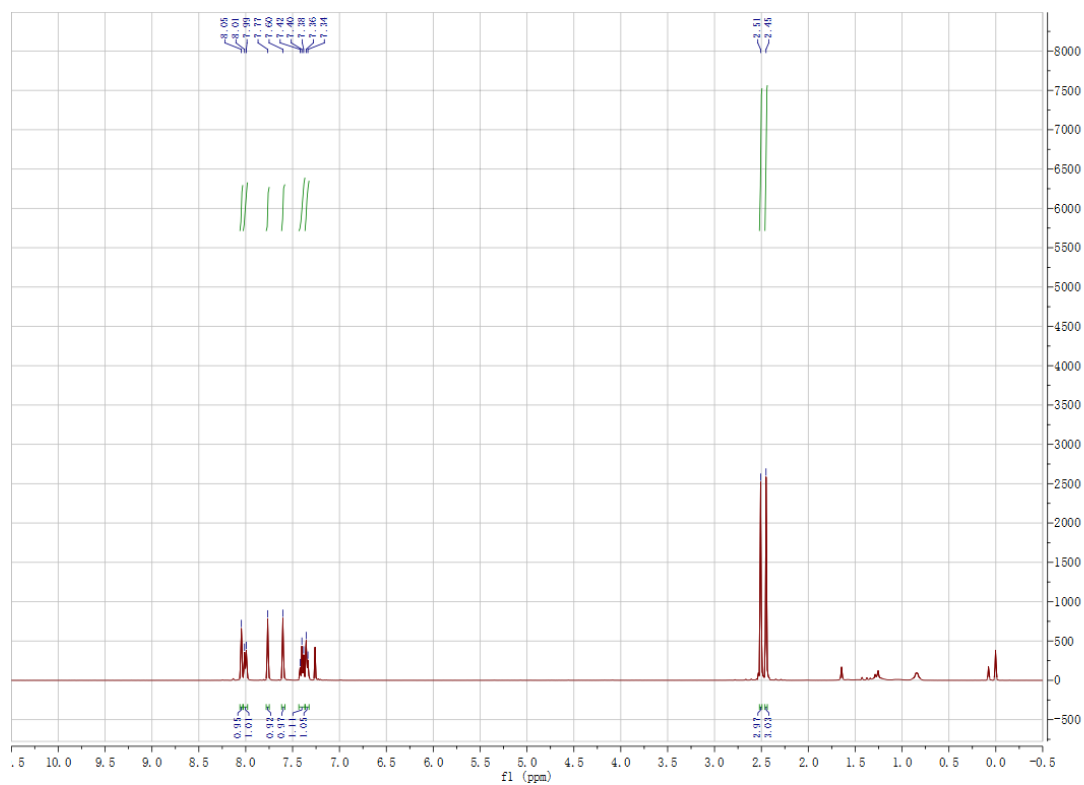
7-iodo-5-methyl-2-phenylbenzo[d]oxazole (6e)



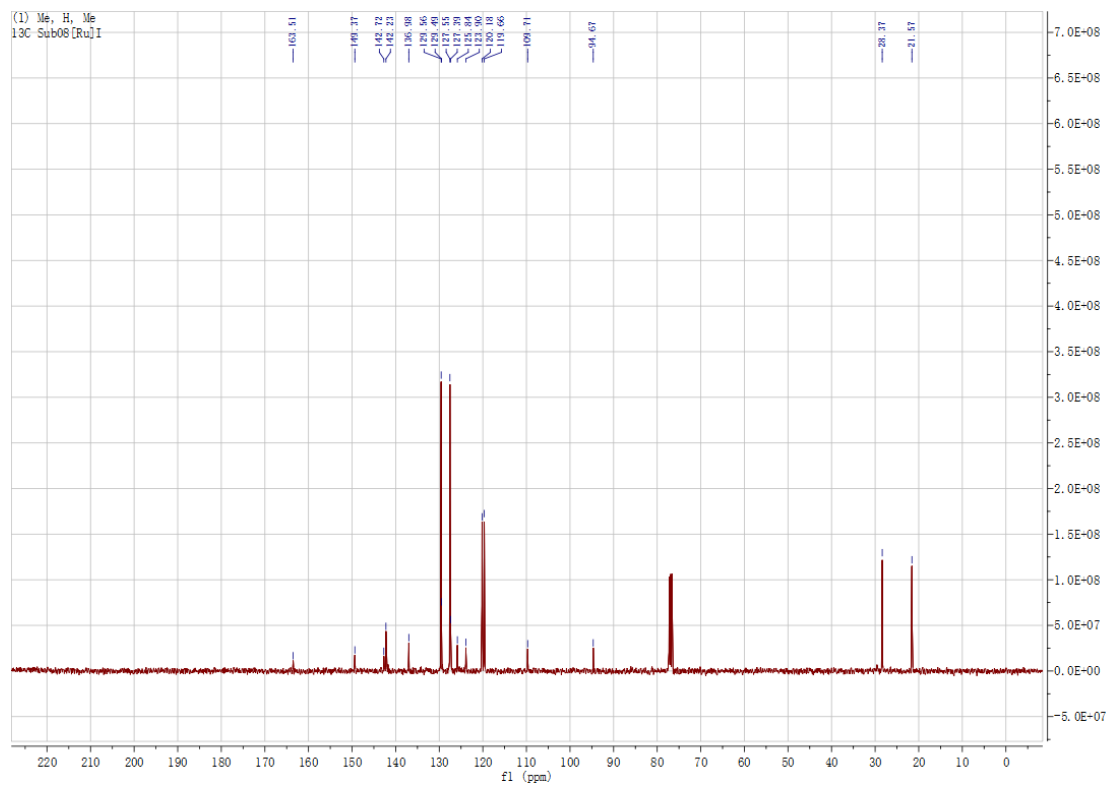
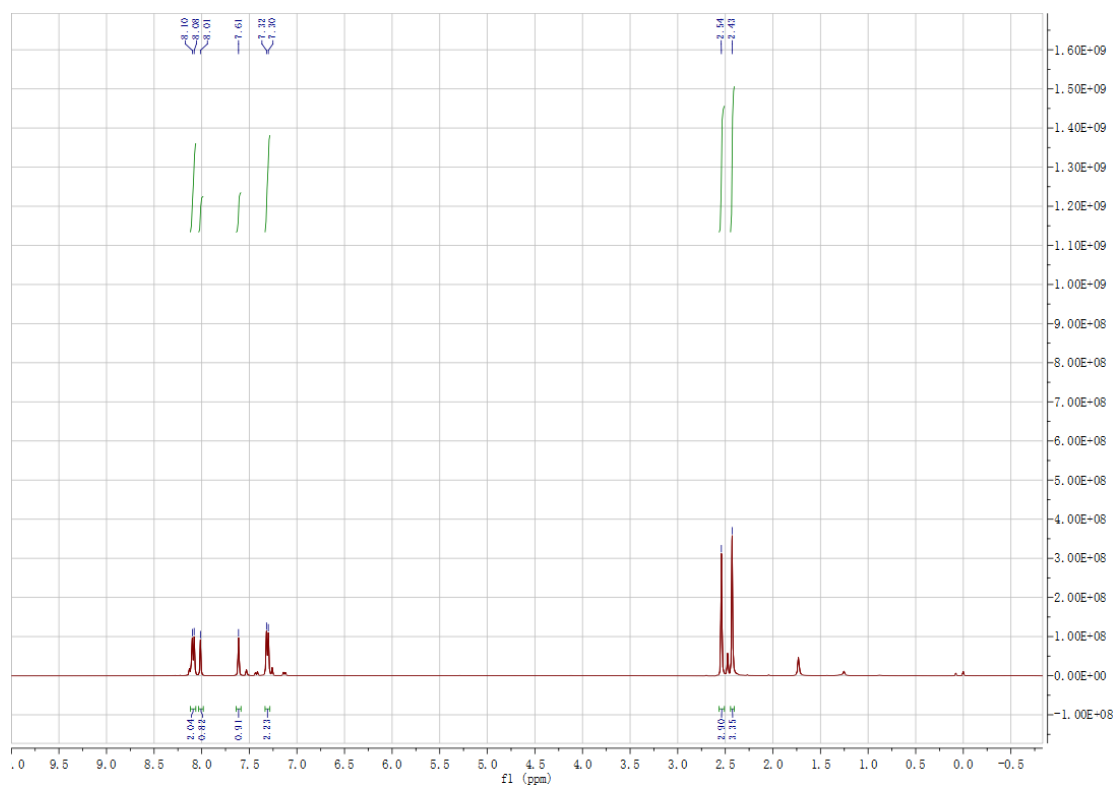
5-chloro-7-iodo-2-phenylbenzo[d]oxazole (6f)



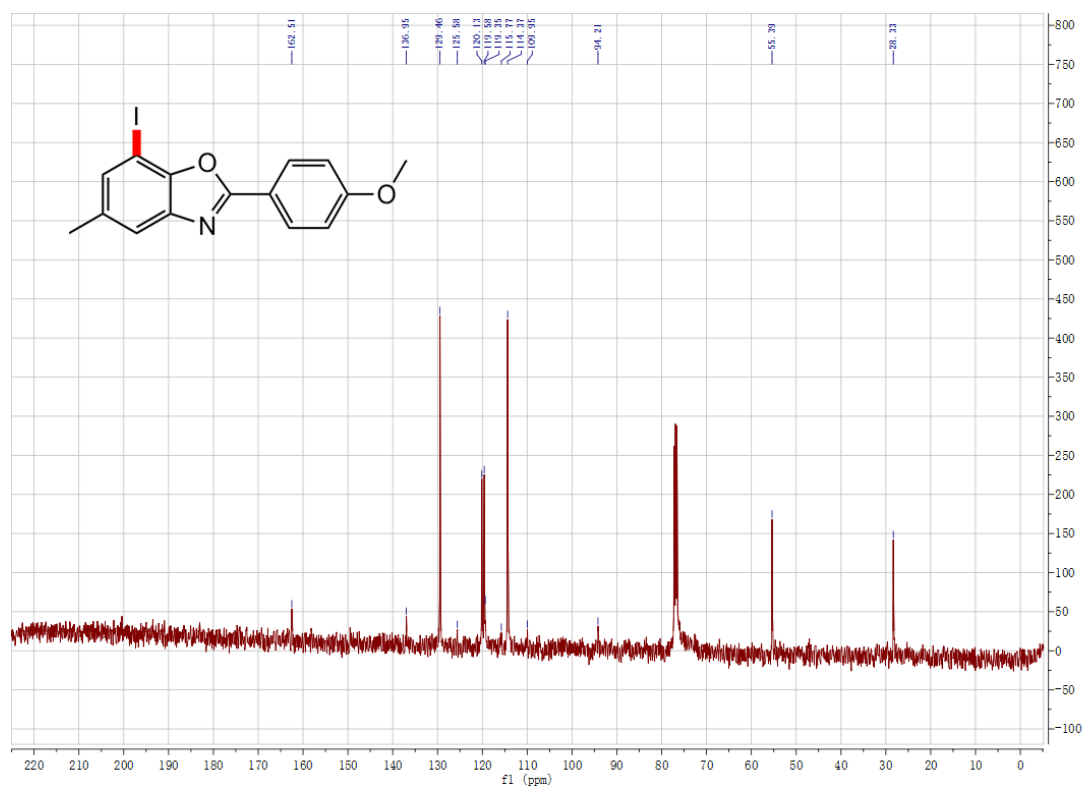
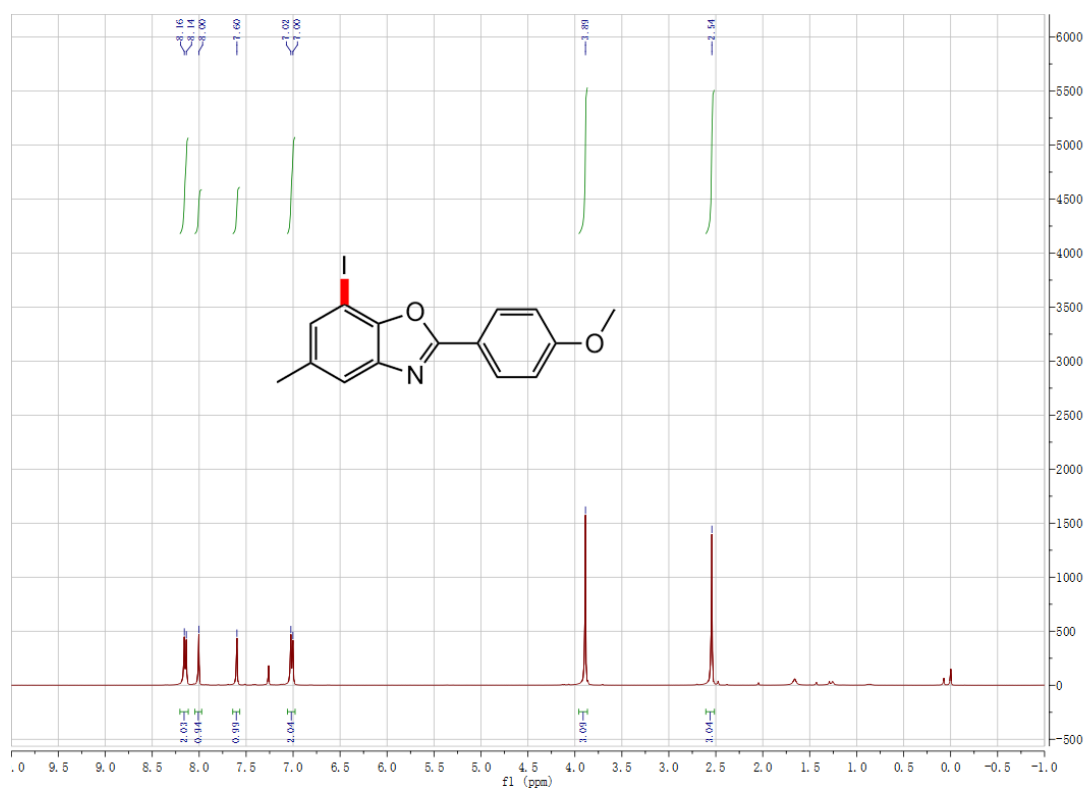
7-iodo-5-methyl-2-(m-tolyl)benzo[d]oxazole (6h)



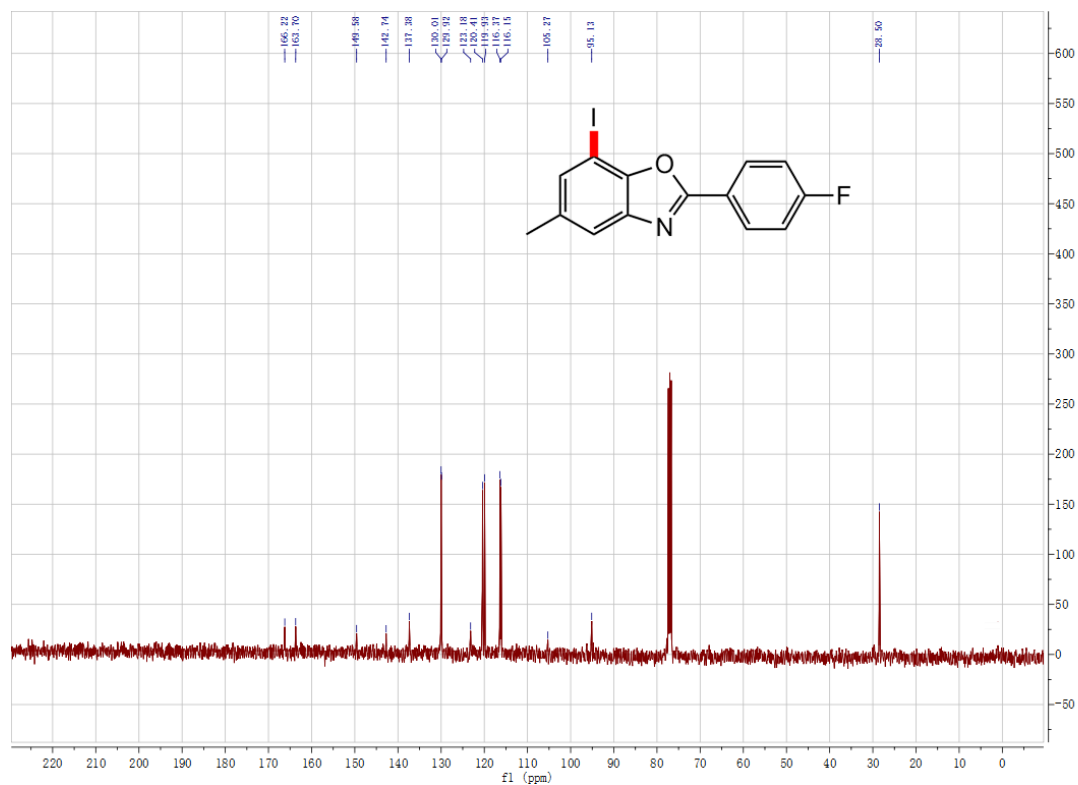
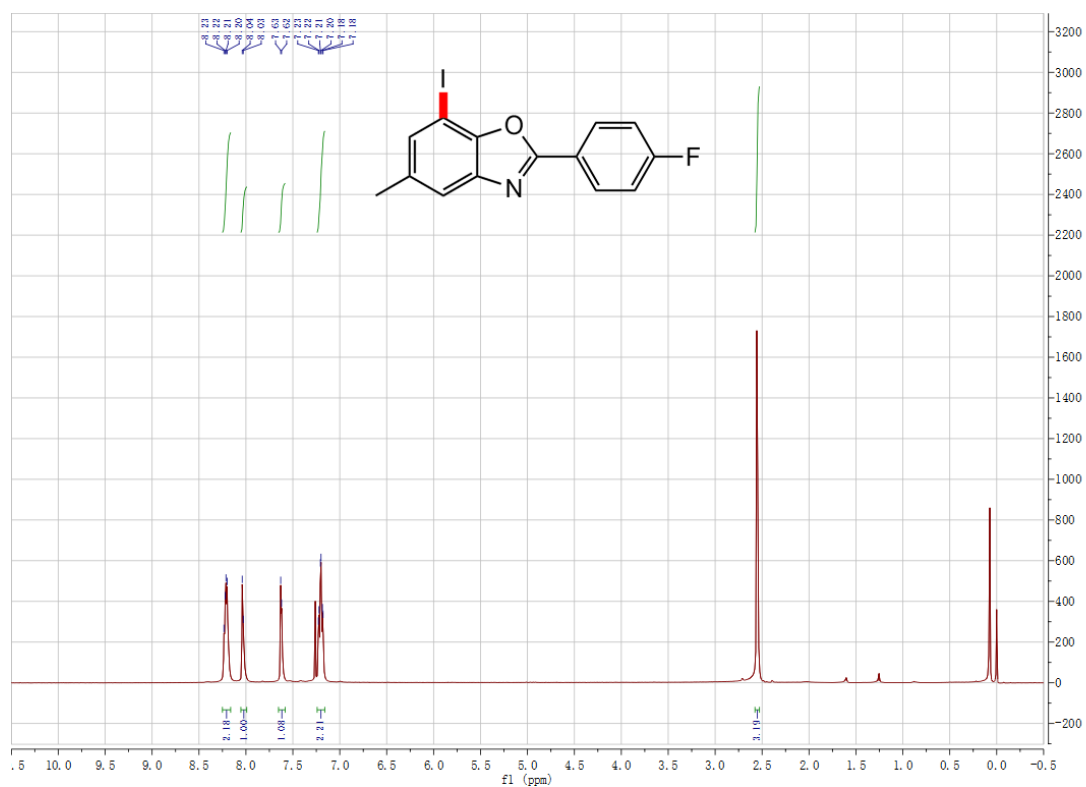
7-iodo-5-methyl-2-(p-tolyl)benzo[d]oxazole (6i)

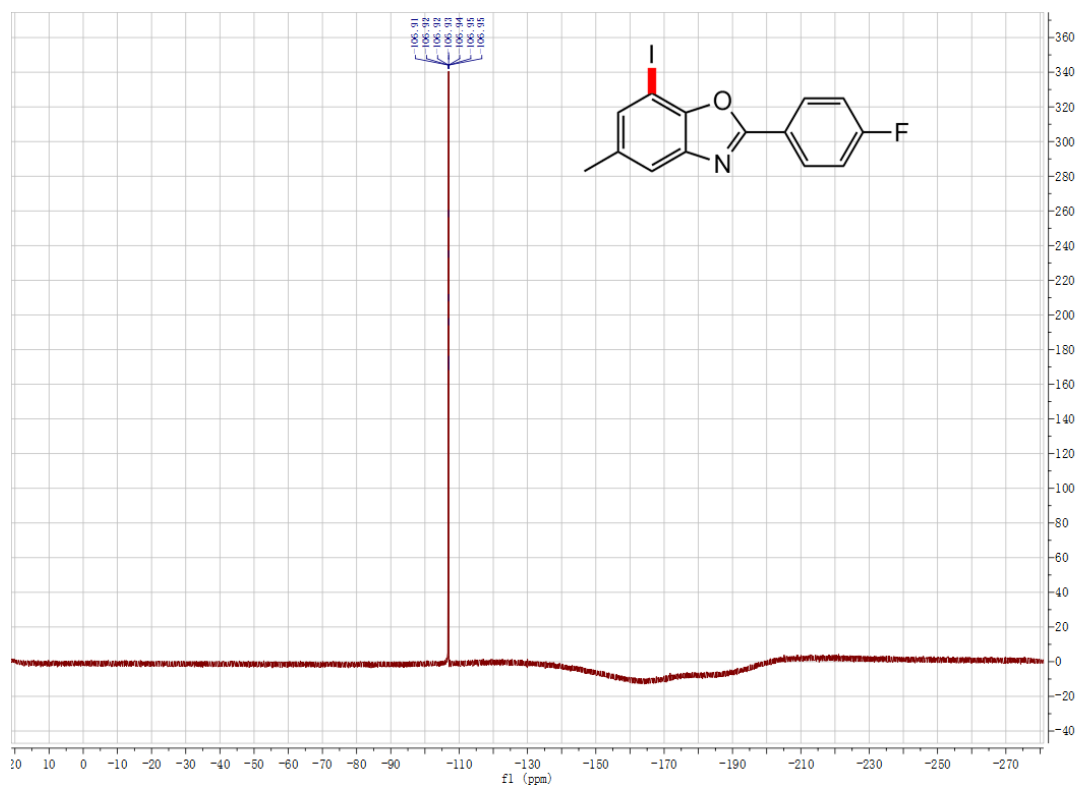


7-iodo-2-(4-methoxyphenyl)-5-methylbenzo[d]oxazole (6j)

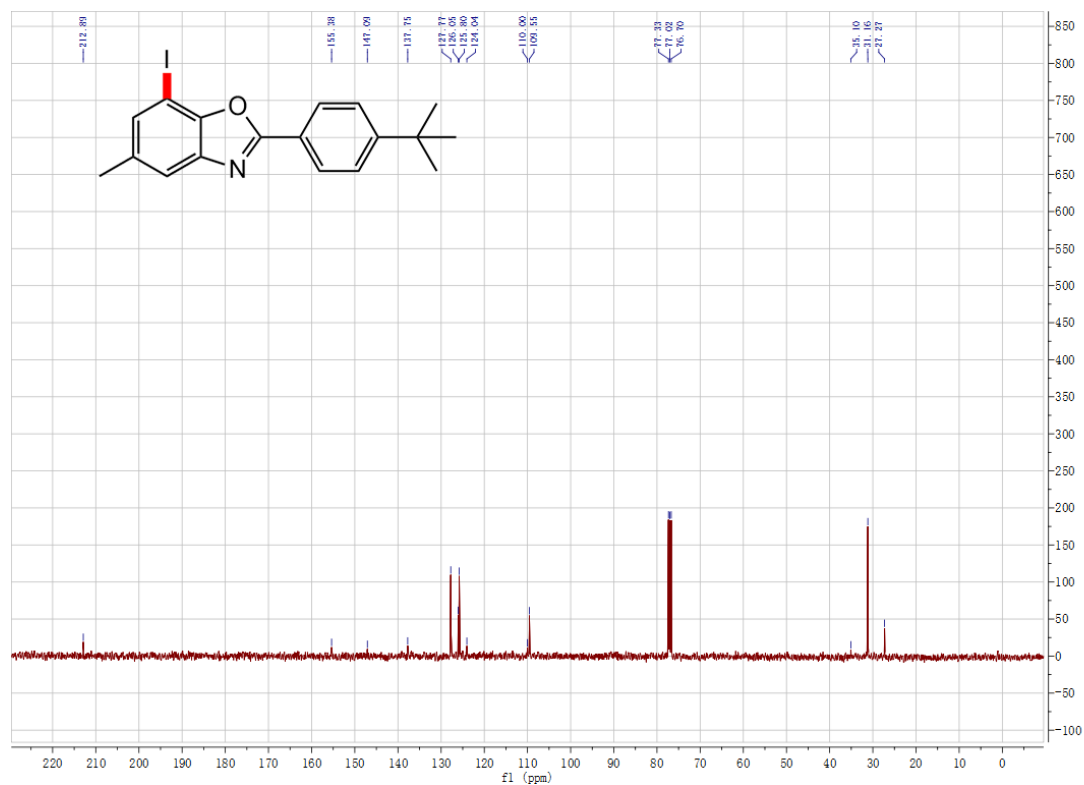
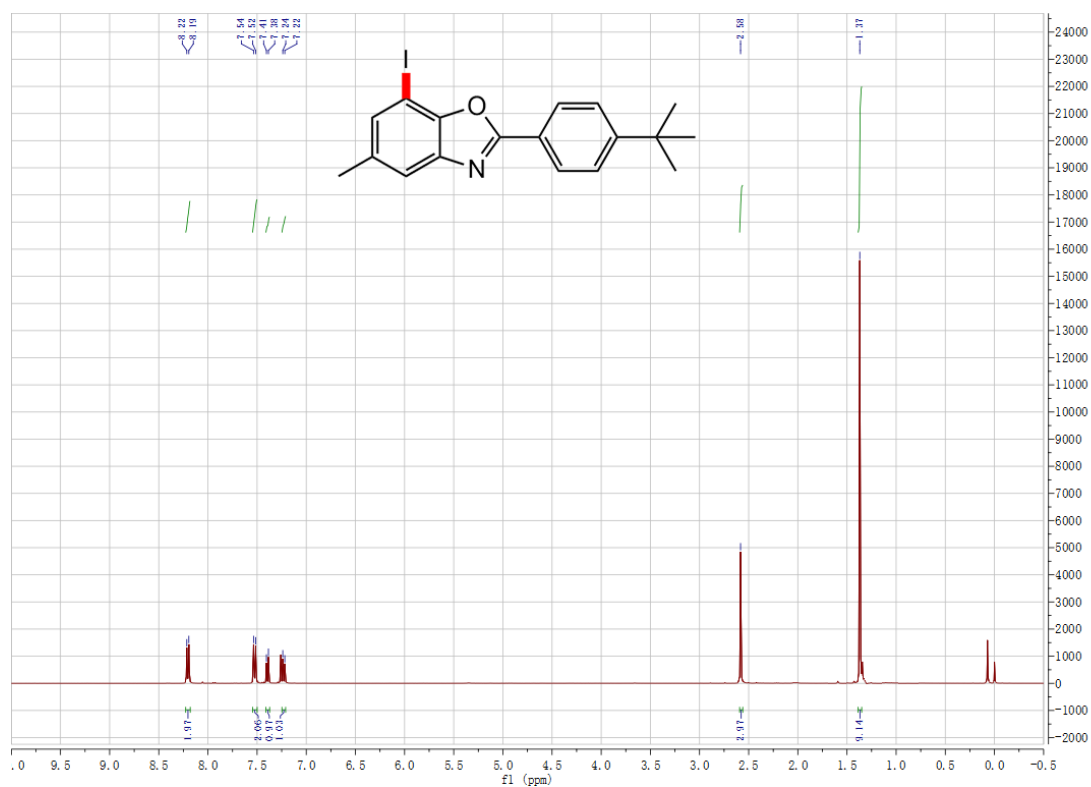


2-(4-fluorophenyl)-7-iodo-5-methylbenzo[d]oxazole (6k)

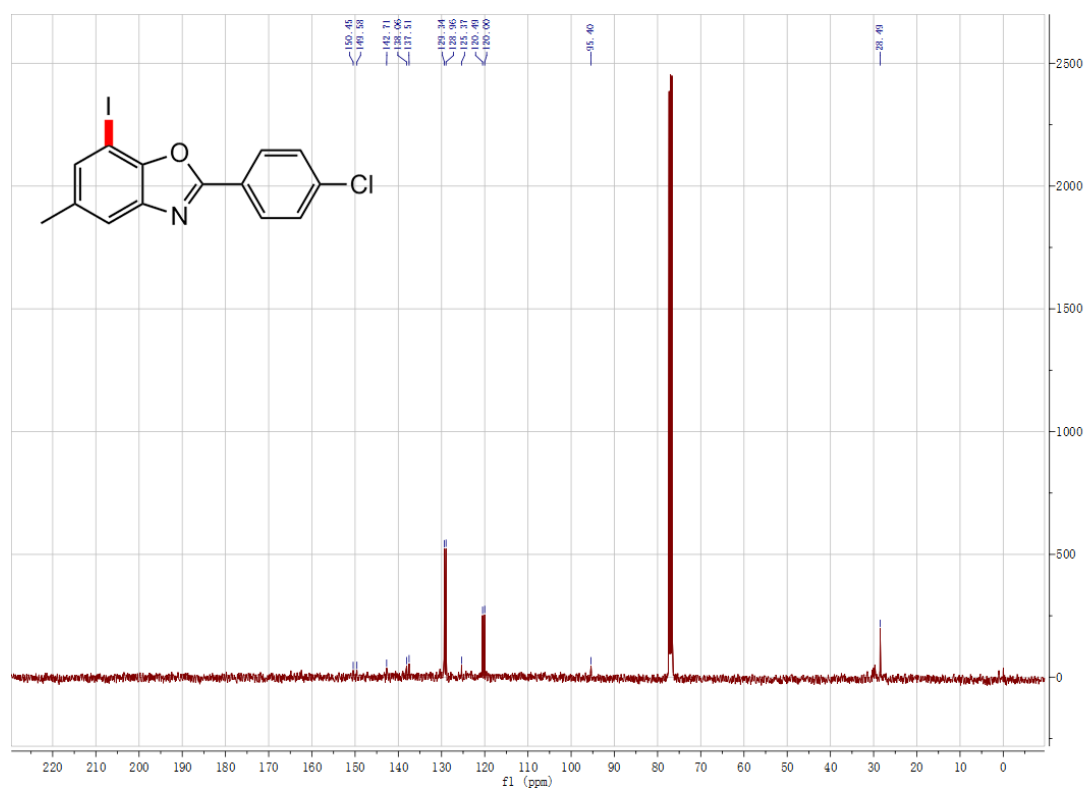
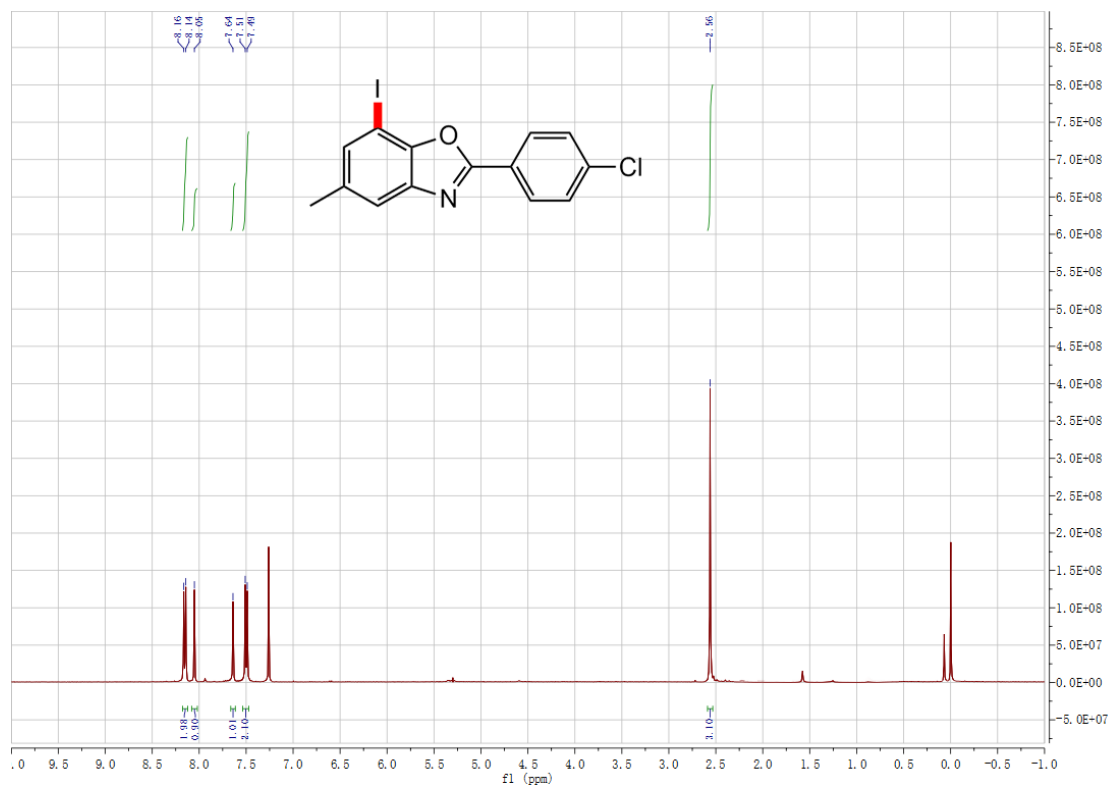




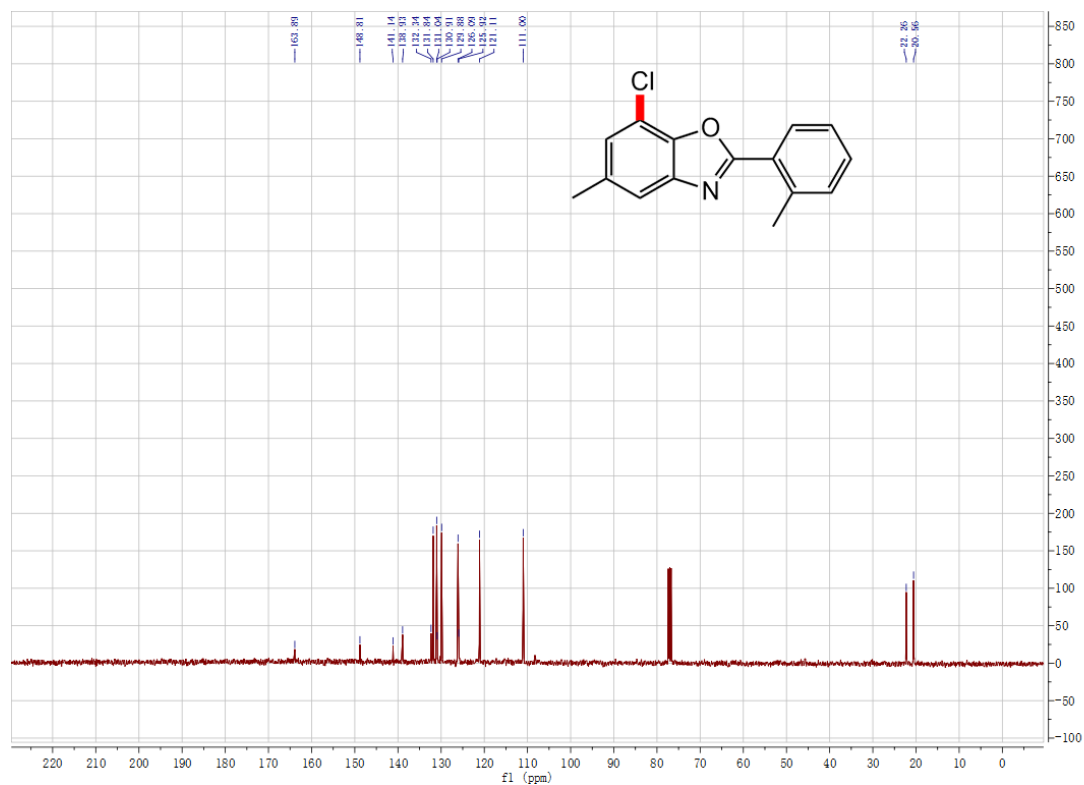
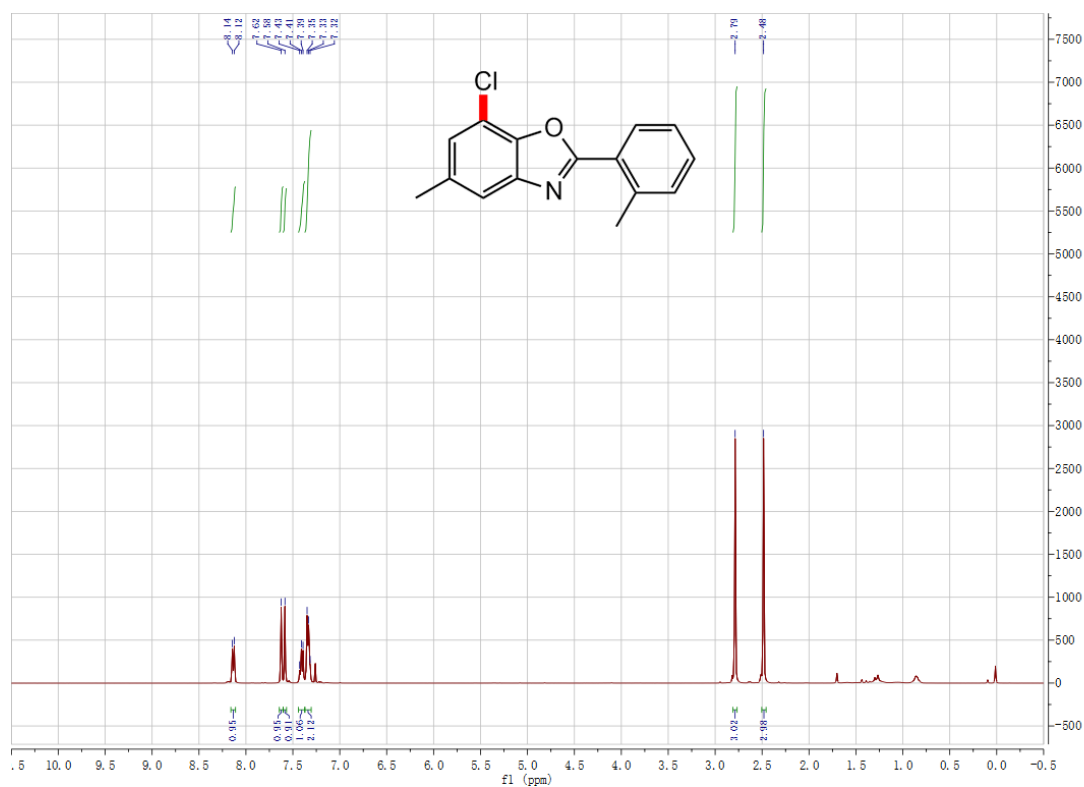
7-iodo-2-(4-(tert-butyl)phenyl)-5-methylbenzo[d]oxazole (6y)



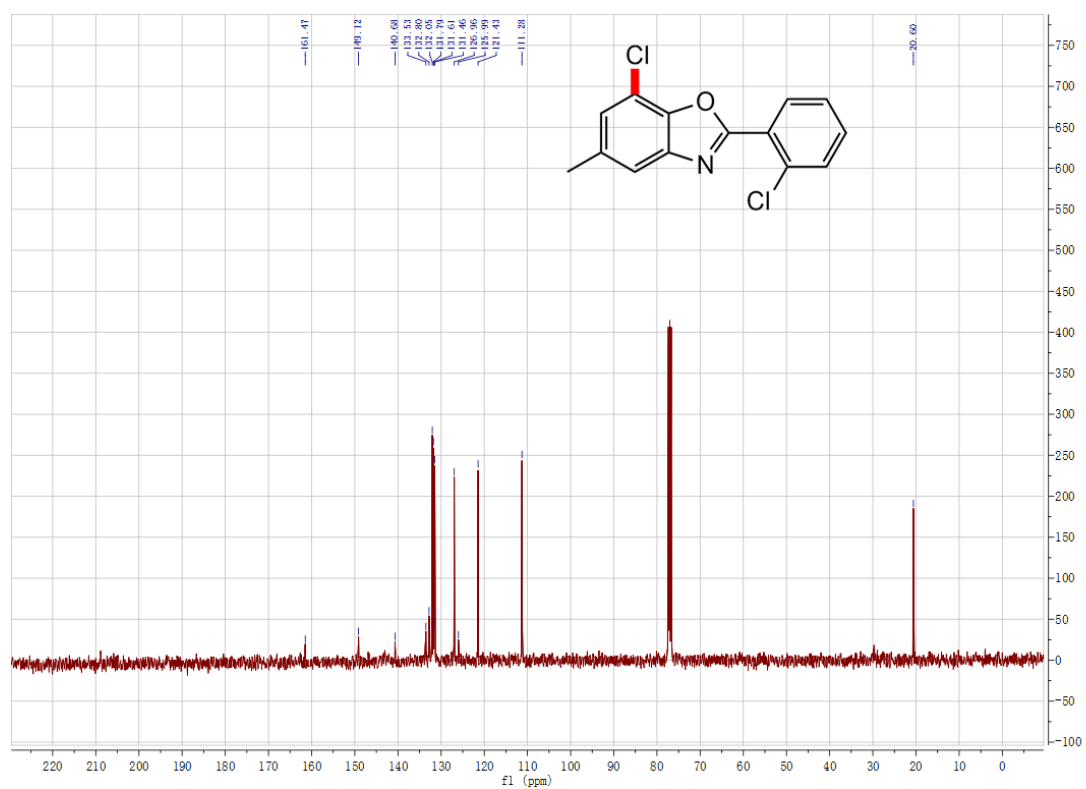
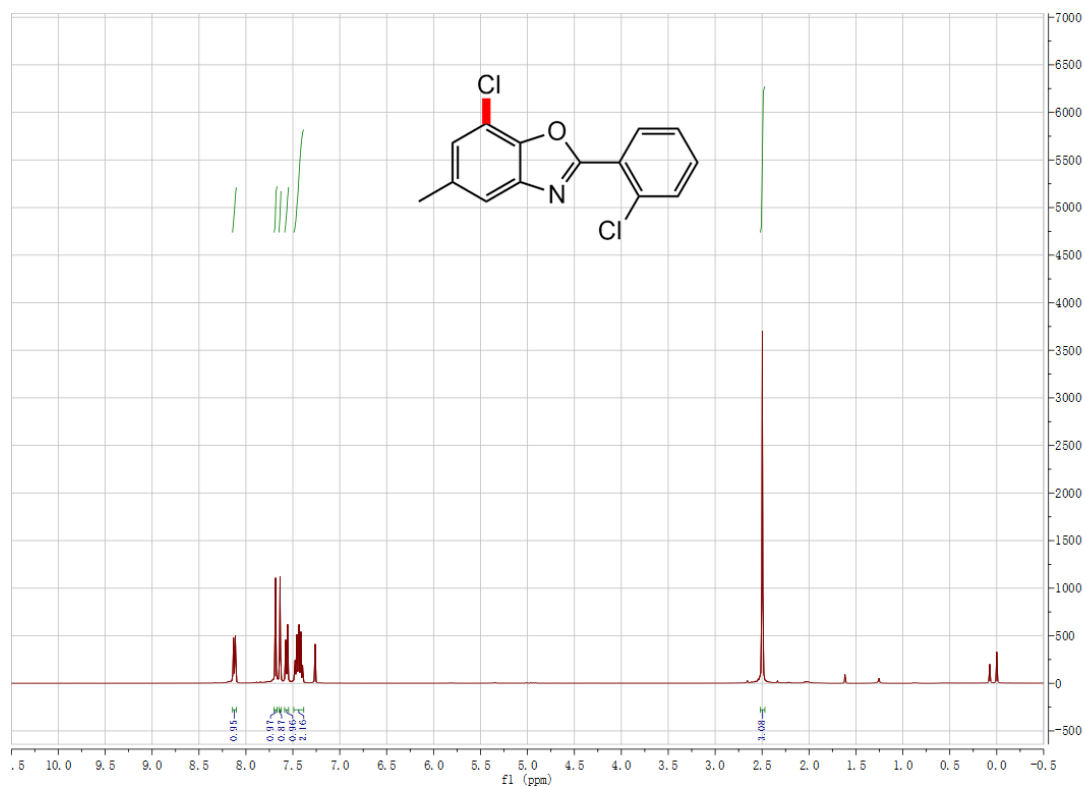
2-(4-chlorophenyl)-7-iodo-5-methylbenzo[d]oxazole (6z)



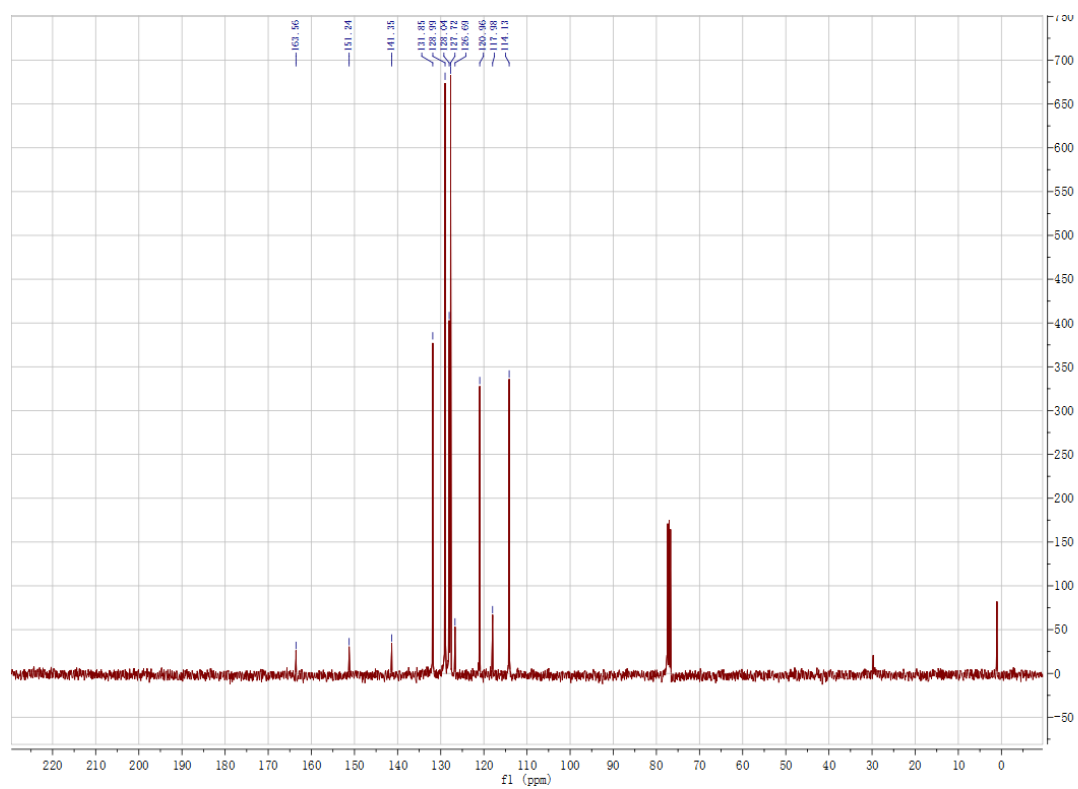
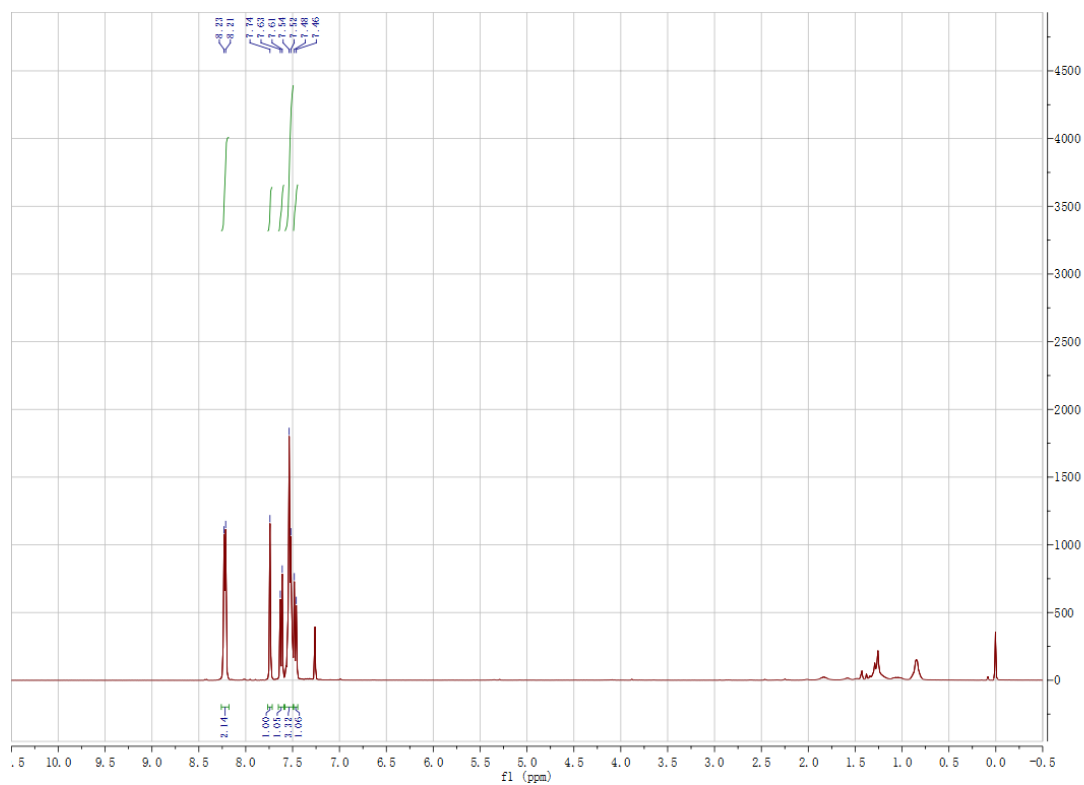
7-chloro-5-methyl-2-(o-tolyl)benzo[d]oxazole (7a)



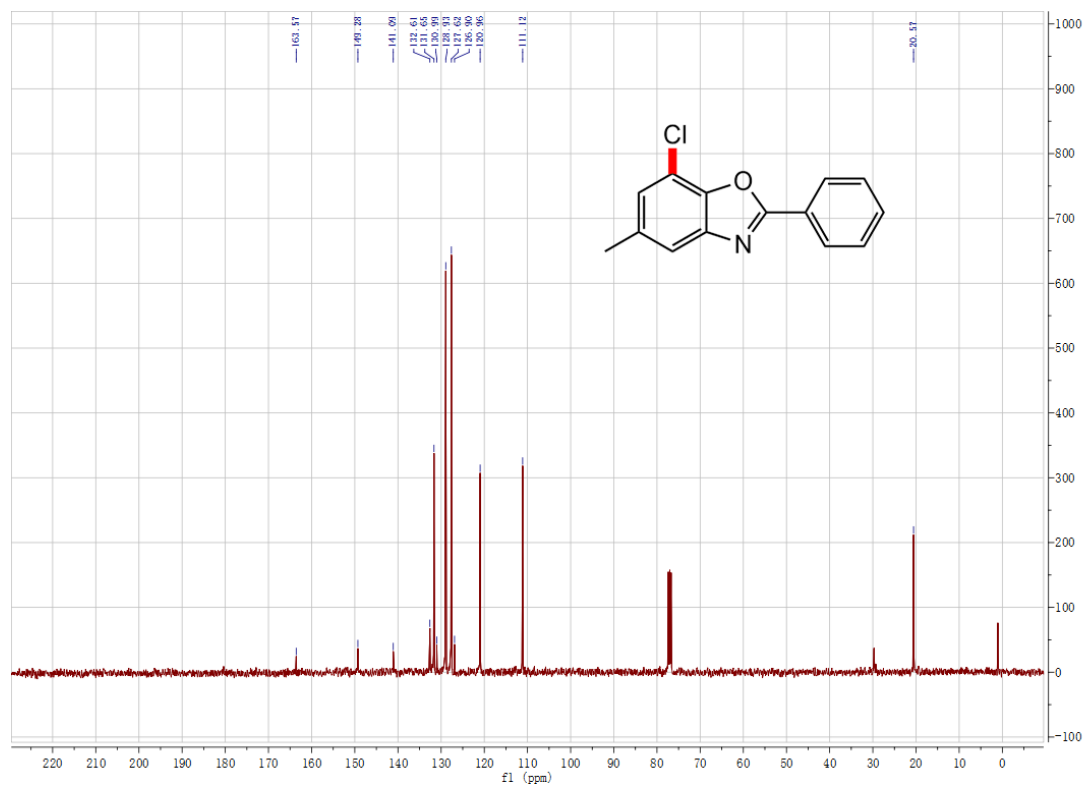
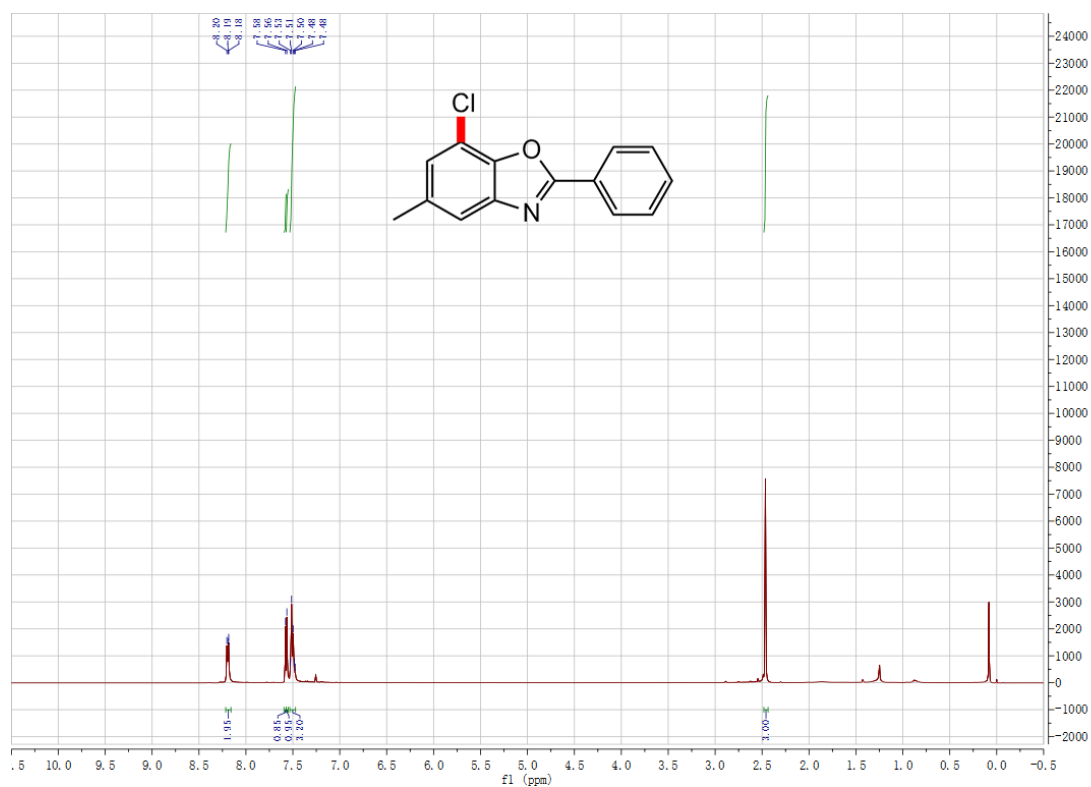
7-chloro-2-(2-chlorophenyl)-5-methylbenzo[d]oxazole (7c)



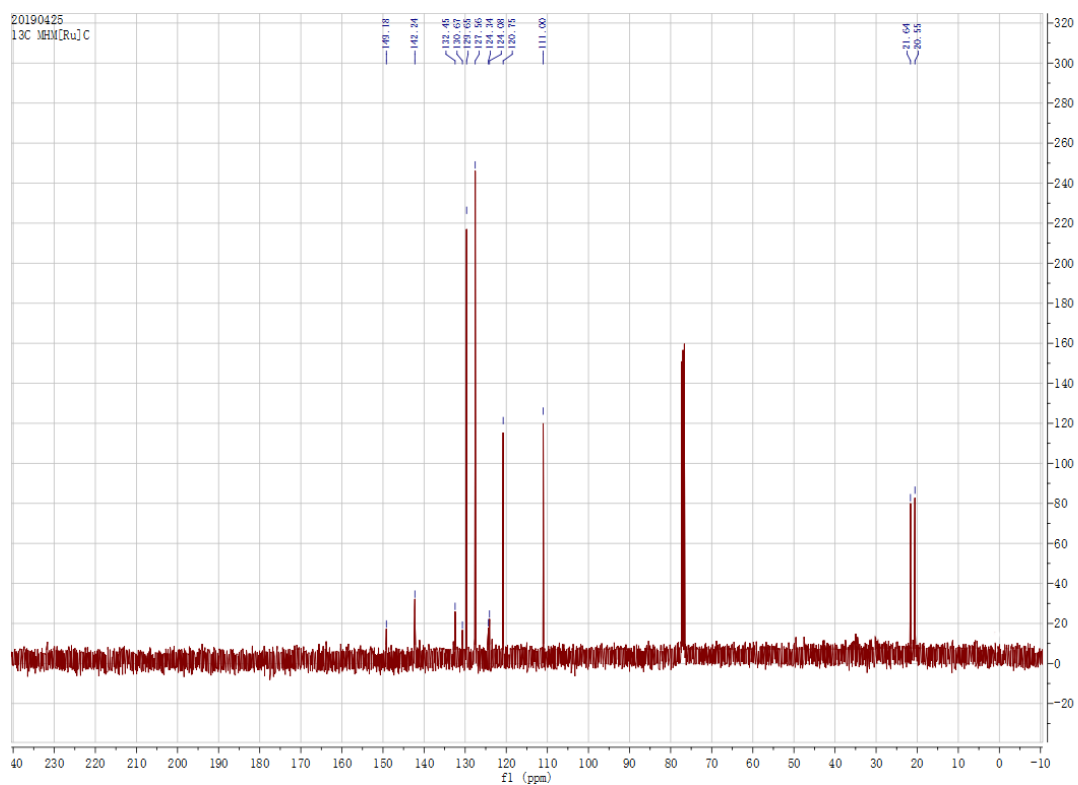
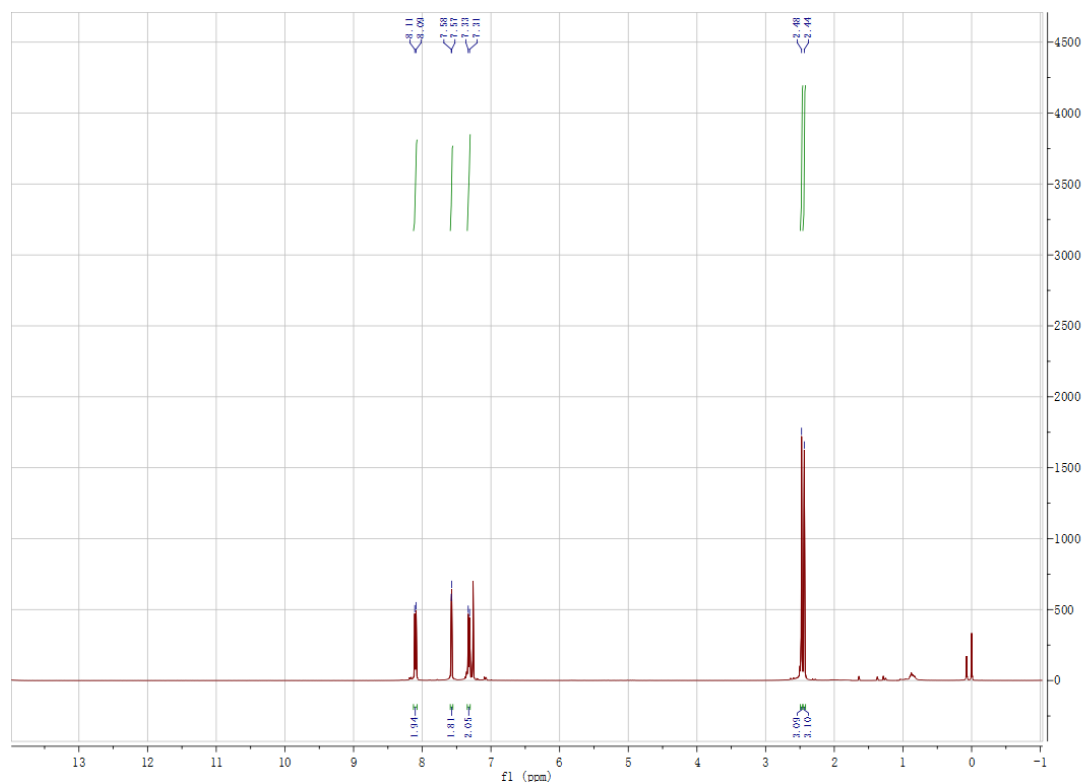
7-chloro-2-phenylbenzo[d]oxazole (7d)



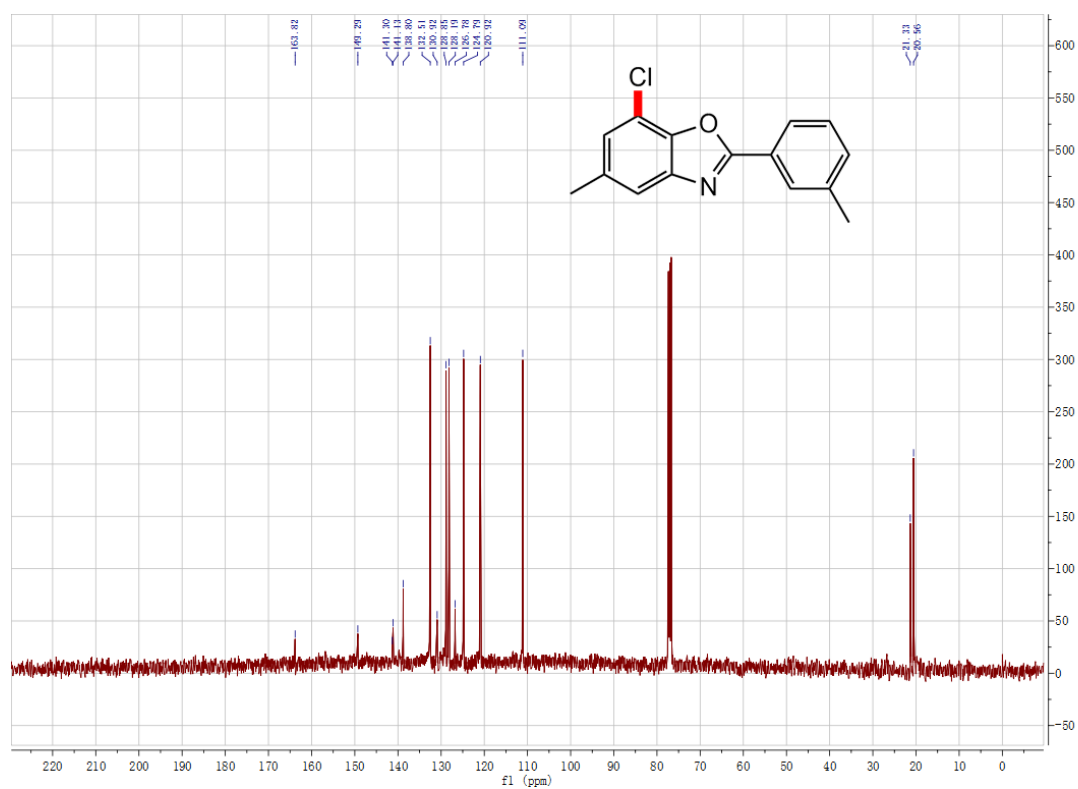
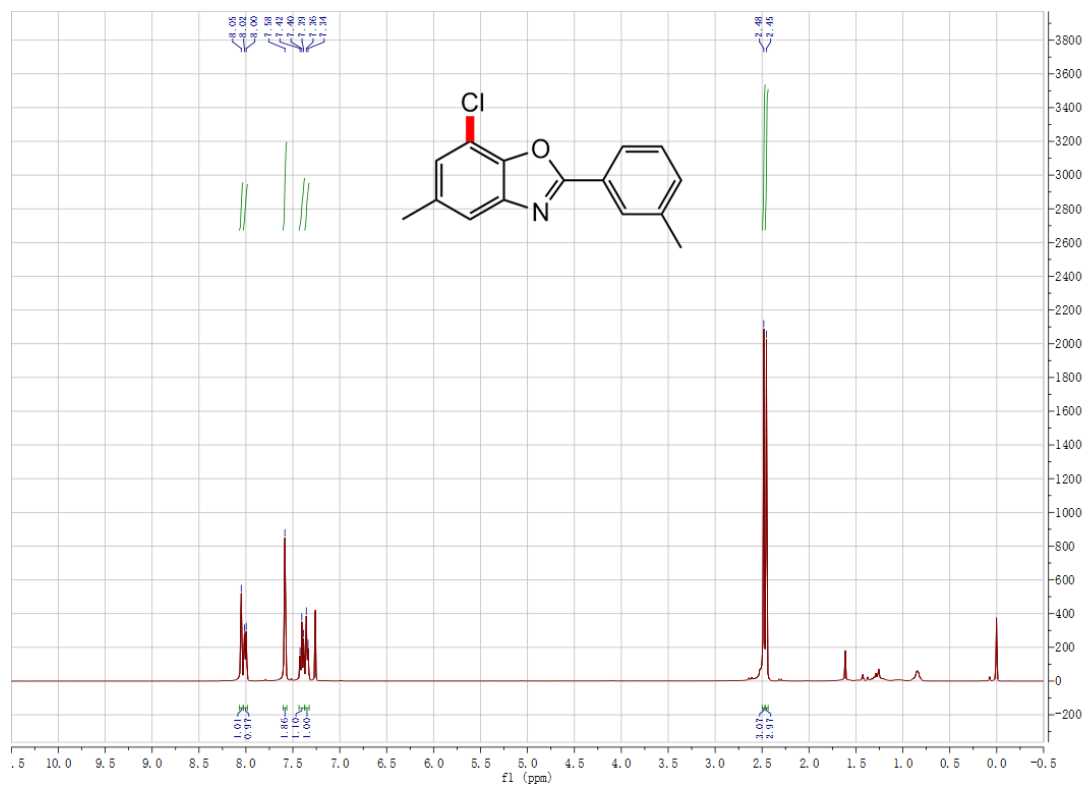
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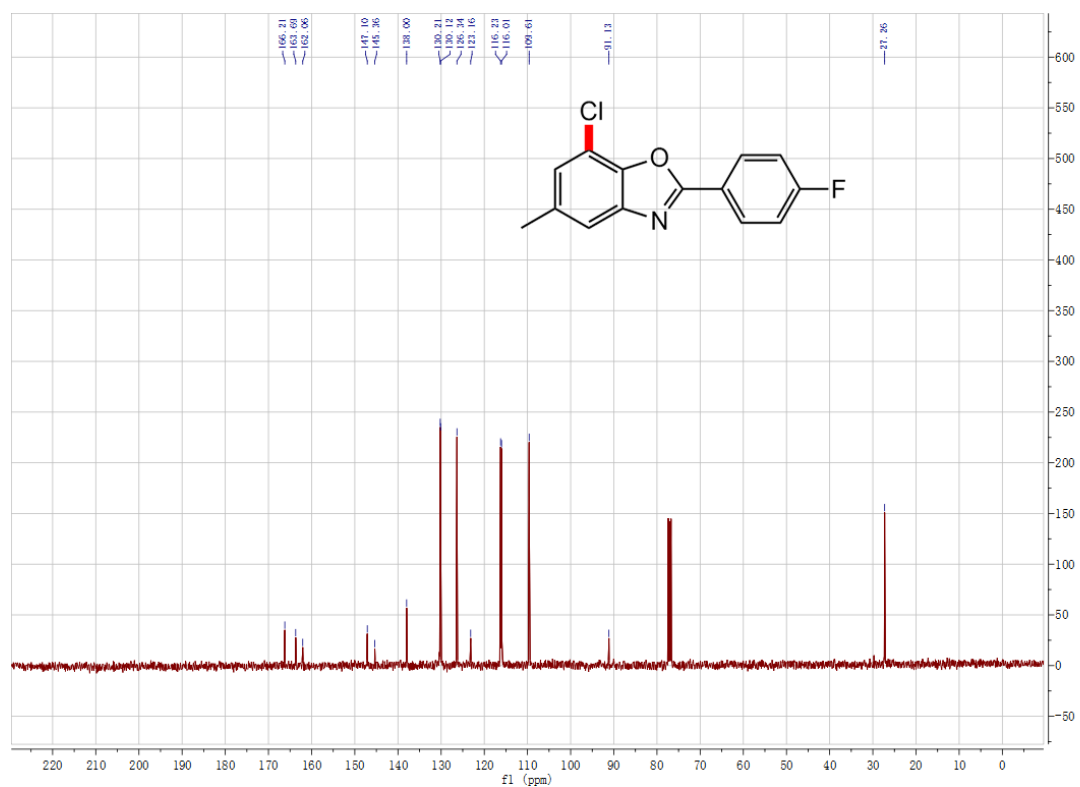
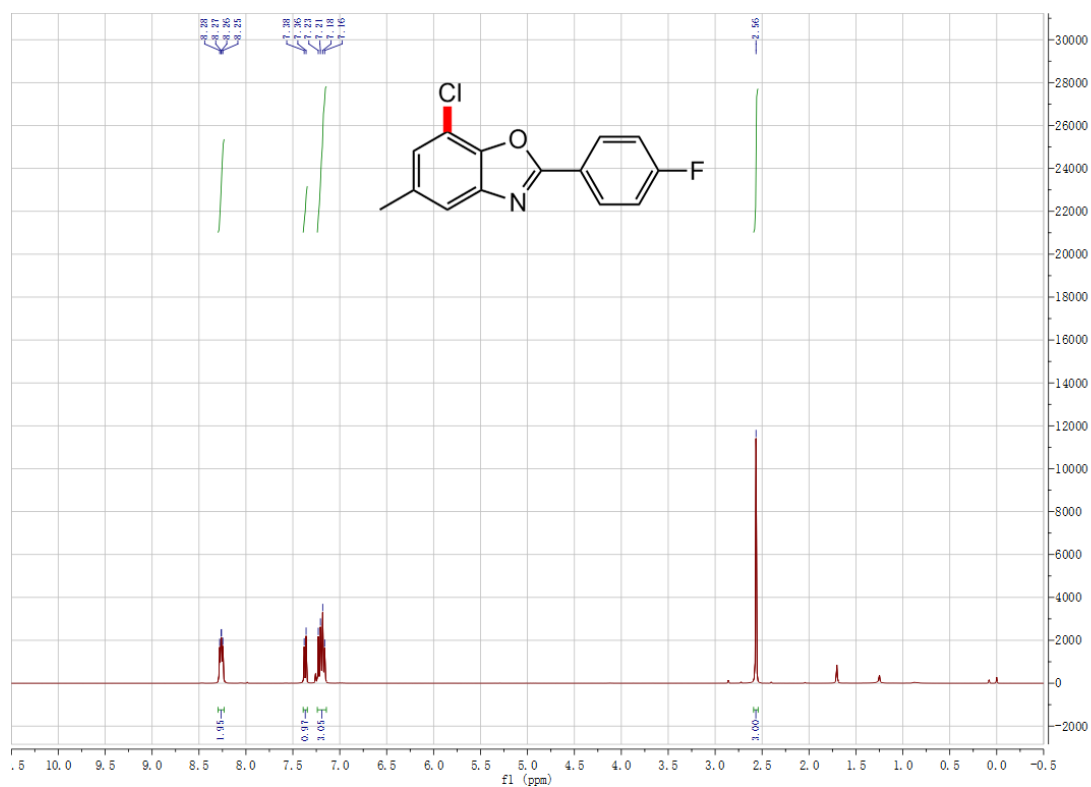
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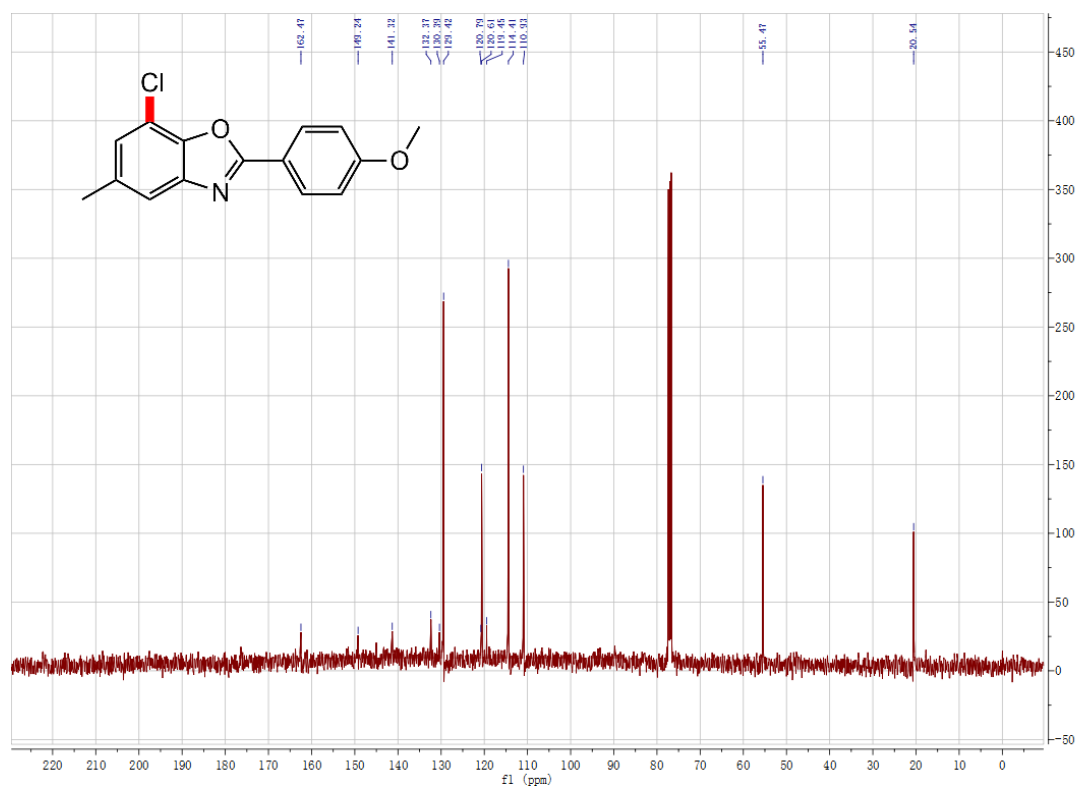
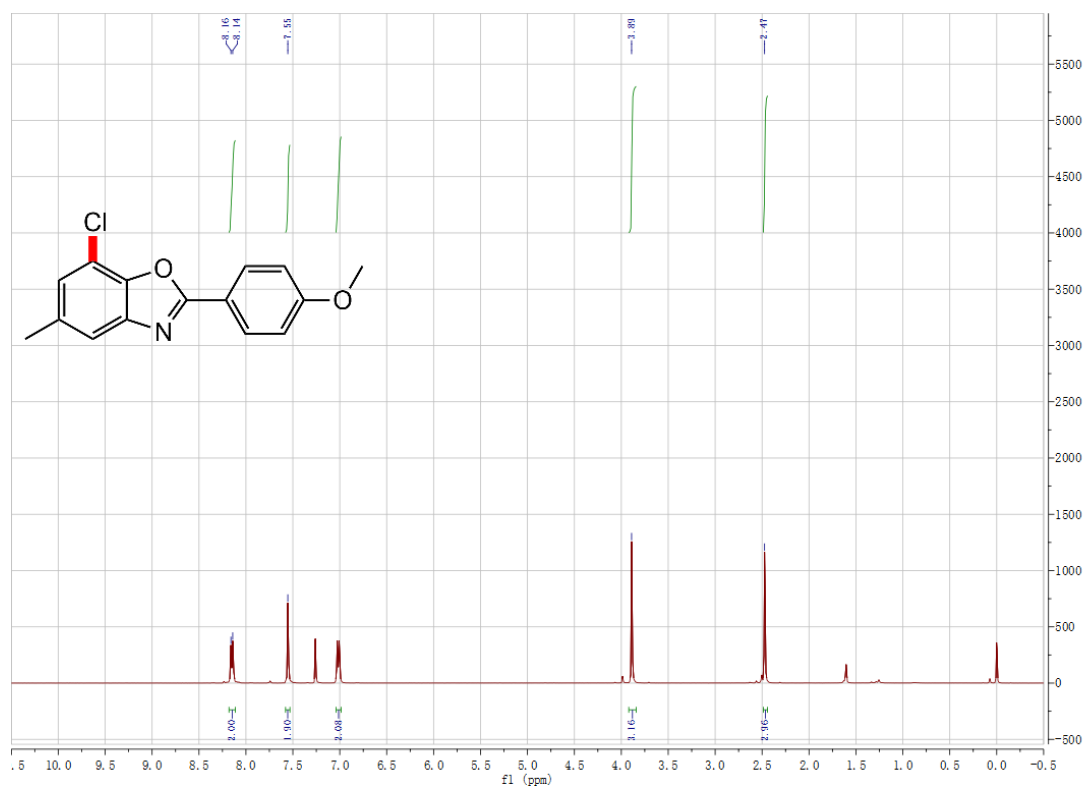
7-chloro-5-methyl-2-(m-tolyl)benzo[d]oxazole (7h)



7-chloro-2-(4-fluorophenyl)-5-methylbenzo[d]oxazole (7k)



7-chloro-2-(4-methoxyphenyl)-5-methylbenzo[d]oxazole (7j)



7. Reference

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- 2 For examples, see: (a) Lane, B. S.; Brown, M. A.; Sames, D. J. Am. Chem. Soc. 2005, 127, 8050-8057. (b) Park, C. H.; Ryabova, V.; Seregin, I. V.; Sromek, A. W.; Gevorgyan, V. Org. Lett. 2004, 6, 1159-1162. (c) Lafrance, M.; Rowley, C. N.; Woo, T. K.; Fagnou, K. J. Am. Chem. Soc. 2006, 128, 8754-8756.
- 3 (a) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648-5652. (b) Stephens, P. J.; Devlin, F. J.; Chabalowski, C. F.; Frisch, M. J. *J. Phys. Chem.* **1994**, *98*, 11623-11627. (c) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B*, **1988**, *37*, 785-789.
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- 5 Hay, P. J.; Wadt, W. R. *J. Chem. Phys.*, **1985**, *82*, 270-283.
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- 8 (a) Parr, R. G.; Yang, W. Density Functional Theory of Atoms and Molecules; Oxford University Press: New York, 1999. (b) Yang, W.; Mortier, W. J. J. Am. Chem. Soc. 1986, 108, 5708.
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