# Supporting Information

## Unconventional oxazole formation from isocyanides

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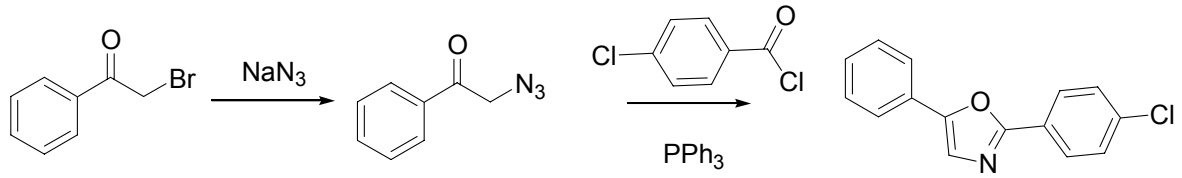
## General procedures

$^{1}H$ NMR spectra were recorded on a Bruker Avance 400 spectrometer, using $CDCl_3$ solvent as reference and/or internal deuterium lock. $^{13}C$ NMR spectra were recorded on a Bruker Avance 400 (100.6 MHz) spectrometer. Two-dimensional NMR spectroscopy [$^{1}H$-$^{1}H$ COSY spectra, $^{1}H$-$^{13}C$ COSY spectra (HSQC) and long-range $^{1}H$-$^{13}C$ COSY spectra (HMBC)], were carried out to determine the correlation between $^{1}H$ and $^{13}C$. The chemical shifts for all NMR spectra are expressed in parts per million to high frequency of TMS reference. Coupling constants (J) are quoted in Hz and are recorded to the nearest 0.1 Hz.

The IR spectra were obtained on a Brucker IFS 66 or a Perkin-Elmer FT 1600 spectrometer. Low resolution mass spectral analysis (EI and CI) were recorded using a Hewlett-Packard HP5989 mass spectrometer via either direct injection or GC/MS coupling with a Hewlett-Packard HP5890 chromatograph. High-resolution (HR) mass spectra were performed on a JEOL JMS-Gcmate II, GC/MS system spectrometer. TLC was carried out using precoated plates of silica gel 60F254.

**Preparation of 2-(4-Chloro phenyl)-5-phenyl oxazole by Staudinger-Aza-Wittig Reaction[1] to confirm the structure:**



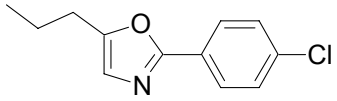

Procedure for Synthesis of 2-azido-1-phenyl ethanone: To a stirred solution of sodium azide (0.98 g, 3.0 equiv.) in dimethylsulfoxide (25 mL, 0.2 M) was added 2-bromo-1-phenyl-ethanone (1.0 g, 1.0 equiv.) at room temperature. After 10 minutes of vigorous stirring, the mixture was poured onto ice-water and extracted with ether (3x50 mL). The combined organic phases were dried ($MgSO_4$), filtered and evaporated in vacuo. The product was obtained quantitatively (809 mg).

Procedure for Synthesis of 2-(4-Chloro phenyl)-5-phenyl oxazole: To a stirred solution of 2-azido-1-phenyl ethanone (400 mg, 1.0 equiv.) with 4-chloro benzoyl chloride (450 µL, 1.4 equiv.) in distilled toluene (5.0 mL, 0.5 M) was added triphenyl phosphine (650 mg, 1.0 equiv.). The mixture was warmed to 100°C under argon for 2 hours with stirring. The solution was evaporated in vacuo and purified on a silica gel column, eluting with a diethyl ether-petroleum ether system to provide 230 mg (yield of 36%) of pure product.

[1]E. Zbiral, E. Bauer, J. Stroh, *Monatsh. Chem.* **1971**, 102, 168-179.
H. Takeuchi, S-I. Yanagida, T.Ozaki, S. Hagiwara, S. Eguchi, *J. Org. Chem*. **1989**, 54, 431-434.

**General Procedure for preparation of oxazoles:**
A solution of 1.0 mmol (1.0 equiv.) of isocyanide, 1.0 mmol (1.0 equiv.) of acyl chloride and 1.0 mmol (1.0 equiv., 115 µL) of 2,6-lutidine in 2 mL of toluene was warmed at 80°C with stirring under an atmosphere of argon overnight. The solution was then washed with water and citric acid. The layers were separated and the aqueous layer was extracted twice with $CH_2Cl_2$. The combined organic phases were concentrated in vacuo and purified on flash column chromatography silica gel using a mixture of petroleum ether/diethyl ether as eluent.

***3c : 2-(4-Chloro phenyl)-5-propyl oxazole***

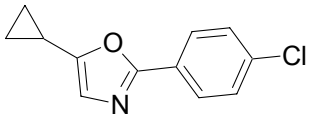



$C_{12}H_{12}ClNO$
M.W.=221.68 g.mol$^{-1}$

The general procedure was followed starting from butyryl chloride (105 µL, 1.0 mmol) and 1-chloro-4-isocyanomethyl benzene (152 mg, 1.0 mmol).

Yellow oil
**Yield** : 59% ($m_{product}$= 131 mg)
**$R_f$ :** 0.5 (50:50 $Et_2O$/E.P.)
**$^1$H NMR** ($CDCl_3$, 400 MHz) δ 7.96 (d, 2H, *J* = 8.6 Hz), 7.44 (d, 2H, *J* = 8.6 Hz), 6.87 (s, 1H), 2.72 (t, 2H, *J* = 7.6 Hz), 1.75 (sext, 2H, *J* = 7.6 Hz), 1.04 (t, 3H, *J* = 7.6 Hz).
**$^{13}$C NMR** ($CDCl_3$, 100.6 MHz) δ 160.1, 153.5, 136.2, 129.4, 127.7, 126.7, 124.4, 28.0, 21.0, 13.6.
**IR** (thin film) υ 1014, 1092, 1123, 1406, 1483, 1545, 1609 cm$^{-1}$.
**HRMS** Calculated for $C_{12}H_{12}ClNO$ 221.0607, found 221.0616.

***3d : 2-(4-Chloro phenyl)-5-cyclopropyl oxazole***

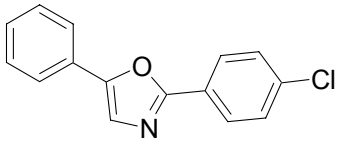



$C_{12}H_{10}ClNO$
M.W.=219.67 g.mol$^{-1}$

The general procedure was followed starting from cyclopropanecarbonyl chloride (90 µL, 1.0 mmol) and 1-chloro-4-isocyanomethyl benzene (152 mg, 1.0 mmol).

Yellow oil
**Yield** : 81% ($m_{product}$= 178 mg)
**$R_f$ :** 0.6 (50:50 $Et_2O$/E.P.)
**$^1$H NMR** ($CDCl_3$, 400 MHz) δ 7.92 (d, 2H, *J* = 8.6 Hz), 7.42 (d, 2H, *J* = 8.6 Hz), 6.83 (s, 1H), 2.01-1.93 (m, 1H), 1.05-0.85 (m, 4H).
**$^{13}$C NMR** ($CDCl_3$, 100.6 MHz) δ 159.6, 155.3, 136.2, 129.4, 127.6, 126.6, 123.3, 7.3, 7.0.
**IR** (thin film) υ1065, 1090, 1122, 1406, 1482, 1608, 3009 cm$^{-1}$.
**HRMS** Calculated for $C_{12}H_{10}ClNO$ 219.0451, found 219.0446.

***3a : 2-(4-Chloro phenyl)-5-phenyl oxazole***

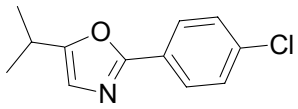



$C_{15}H_{10}ClNO$
M.W.=255.70 g.mol$^{-1}$

The general procedure was followed starting from benzoyl chloride (120 µL, 1.0 mmol) and 1-chloro-4-isocyanomethyl benzene (152 mg, 1.0 mmol).

Yellow solid, **mp** = 117-118°C
**Yield** : 60% ($m_{product}$= 152 mg)
**$R_f$ :** 0.5 (50:50 $Et_2O$/E.P.)
**$^1$H NMR** ($CDCl_3$, 400 MHz) δ 8.06 (d, 2H, *J* = 8.6 Hz), 7.74 (d, 2H, *J* = 7.3 Hz), 7.48 (d, 2H, *J* = 8.6 Hz,), 7.47 (s, 1H), 7.49-7.45 (m, 2H), 7.38 (t, 1H, *J* = 7.3 Hz).
**$^{13}$C NMR** ($CDCl_3$, 100.6 MHz) δ 160.6, 151.3, 136.8, 129.6, 129.4, 129.0, 128.2, 127.9, 126.3, 124.7, 124.0.
**IR** (thin film) υ 1089, 1133, 1403, 1478, 1604 cm$^{-1}$.
**HRMS** Calculated for $C_{15}H_{10}ClNO$ 255.0451, found 255.0448.

***3e : 2-(4-Chloro phenyl)-5-isopropyl oxazole***

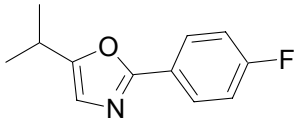



$C_{12}H_{12}ClNO$
M.W.=221.68 g.mol$^{-1}$

The general procedure was followed starting from isobutyryl chloride (105 µL, 1.0 mmol) and 1-chloro-4-isocyanomethyl benzene (152 mg, 1.0 mmol).

Yellow solid, **mp** = 142-143°C
**Yield** : 73% ($m_{product}$= 162 mg)
**$R_f$ :** 0.6 (50:50 $Et_2O$/E.P.)
**$^1$H NMR** ($CDCl_3$, 400 MHz) δ 7.96 (d, 2H, *J* = 8.6 Hz), 7.43 (d, 2H, *J* = 8.6 Hz), 6.84 (d, 1H, *J* = 1.3 Hz), 3.07 (sept , 1H, *J* = 6.8 Hz), 1.34 (d, 6H, *J* = 6.8 Hz).
**$^{13}$C NMR** ($CDCl_3$, 100.6 MHz) δ 160.0, 159.1, 136.3, 129.4, 127.7, 126.8, 122.4, 26.5, 21.1.
**IR (**thin film) υ 1014, 1092, 1265, 1405, 1483, 2961 cm$^{-1}$.
**HRMS** Calculated for $C_{12}H_{12}ClNO$ 221.0607, found 221.0601.

***3h : 2-(4-Fluoro phenyl)-5-isopropyl oxazole***



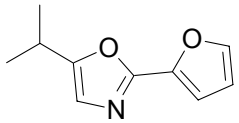

$C_{12}H_{12}FNO$

M.W.=205.23 g.mol$^{-1}$

The general procedure was followed starting from isobutyryl chloride (105 µL, 1.0 mmol) and 1-fluoro-4-isocyanomethyl benzene (135 mg, 1.0 mmol).

Yellow oil
**Yield** : 58% ($m_{product}$= 119 mg)
**$R_f$ :** 0.6 (50:50 $Et_2O$/E.P.)
**$^1$H NMR** ($CDCl_3$, 400 MHz) δ 8.02 (dd, 2H, $J_{H-F}$ = 4.8 Hz, $J$ = 8.8 Hz), 7.15 (dd, 2H, $J_{H-F}$ = 9.3 Hz, $J$ = 8.8 Hz), 6.82 (s, 1H), 3.06 (sept, 1H, $J$ = 6.8 Hz,), 1.34 (d, 6H, $J$ = 7.1 Hz).
**$^{13}$C NMR** ($CDCl_3$, 100.6 MHz) δ 164.2 (d, $J_{C-F}$ = 251.8 Hz), 160.1, 158.8, 128.4 (d, $J_{C-F}$ = 8.1 Hz,), 124.6 (d, $J_{C-F}$ = 3.7 Hz,), 122.2, 116.2 (d, $J_{C-F}$ = 22.0 Hz), 26.5, 21.2.
**IR (**thin film) υ 1093, 1121, 1156, 1233, 1369, 1415, 1497, 1557, 1610, 2971 (cm$^{-1}$).
**HRMS** Calculated for $C_{12}H_{12}FNO$ 205.0903, found 205.0898.

***3l : 2-Furan-2-yl-5-isopropyl oxazole***

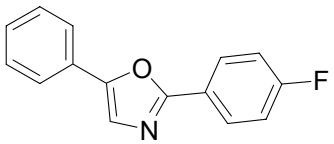



$C_{10}H_{11}NO_2$
M.W.=177.20 g.mol$^{-1}$

The general procedure was followed starting from isobutyryl chloride (105 µL, 1.0 mmol) and 2-isocyanomethyl furan (107 mg, 1.0 mmol).

Yellow oil
**Yield** : 51% ($m_{product}$= 91 mg)
**$R_f$ :** 0.5 (50:50 $Et_2O$/E.P.)
**$^1$H NMR** ($CDCl_3$, 400 MHz) δ 7.50 (d, 1H, $J$ = 1.5 Hz), 6.92 (d, 1H, $J$ = 3.3 Hz), 6.77 (s, 1H), 6.49 (dd, 1H, $J$ = 3.3, 1.5 Hz), 3.00 (sept, 1H, $J$ = 6.8 Hz), 1.28 (d, 6H, $J$ = 6.8 Hz).
**$^{13}$C NMR** ($CDCl_3$, 100.6 MHz) δ 158.4, 153.8, 144.3, 143.7, 122.0, 112.1, 110.9, 26.4, 21.1.
**IR (**thin film) υ 1010, 1120, 1451, 1537, 1591, 2970 cm$^{-1}$.
**HRMS** Calculated for $C_{10}H_{11}NO_2$ 177.0790, found 177.0789.

***3g : 2-(4-Fluoro phenyl)-5-phenyl oxazole***



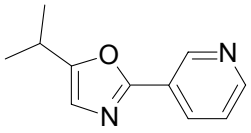

$C_{15}H_{10}FNO$
M.W.=239.24 g.mol$^{-1}$

The general procedure was followed starting from benzoyl chloride (120 µL, 1.0 mmol) and 1-fluoro-4-isocyanomethyl benzene (135 mg, 1.0 mmol).

White powder, **mp** = 81-82°C
**Yield** : 57% ($m_{product}$= 136 mg)

**$R_f$ :** 0.5 (50:50 $Et_2O$/E.P.)
**$^1$H NMR** ($CDCl_3$, 400 MHz) δ 8.13 (dd, 2H, $J_{H-F}$ = 3.0 Hz, $J$ = 5.3Hz), 7.74 (d, 2H, $J$ = 7.8 Hz), 7.47 (dd, 2H, $J$ = 8.0, 7.3 Hz) , 7.45 (s, 1H), 7.48 (t, 1H, $J$ = 7.6 Hz), 7.20 (dd, 1H, $J_{H-F}$ = 9.3 Hz, $J$ = 8.0 Hz).
**$^{13}$C NMR** ($CDCl_3$, 100.6 MHz) δ 164.5 (d, $J_{C-F}$ = 250.3 Hz), 160.8, 151.8, 129.4, 128.9, 128.8 (d, $J_{C-F}$ = 8.8 Hz), 128.3, 124.6, 124.2 (d, $J_{C-F}$ = 2.2 Hz), 123.8, 116.4 (d, $J_{C-F}$ = 22.0 Hz,).
**IR** (thin film) υ 1094, 1133, 1155, 1221, 1414, 1494, 1607, 1668 $cm^{-1}$.
**HRMS** Calculated for $C_{15}H_{10}FNO$ 239.0746, found 239.0743.

***3i : 3-(5-Isopropyl oxazol-2-yl)-pyridine***

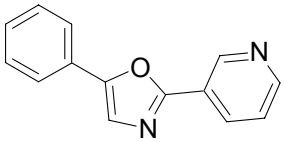



$C_{11}H_{12}N_2O$
M.W.=188.23 $g.mol^{-1}$

The general procedure was followed starting from isobutyryl chloride (105 µL, 1.0 mmol) and 3-isocyanomethyl pyridine (118 mg, 1.0 mmol).

Yellow oil
**Yield**: 62% ($m_{product}$= 117 mg)
**$R_f$ :** 0.2 (50:50 $Et_2O$/E.P.)
**$^1$H NMR** ($CDCl_3$, 400 MHz) δ 9.25 (d, 1H, $J$ = 2.3 Hz), 8.67 (dd, 1H, $J$ = 4.8, 1.7 Hz), 8.28 (ddd, 1H, $J$ = 8.1, 2.3, 1.7 Hz), 7.40 (dd, 1H, $J$ = 8.1, 4.8 Hz), 6.87 (s, 1H), 3.10 (sept, 1H, $J$ = 6.8 Hz), 1.35 (d, 6H, $J$ = 6.8 Hz).
**$^{13}$C NMR** ($CDCl_3$, 100.6 MHz) δ 159.6, 158.7, 151.0, 147.7, 133.5, 124.5, 123.9, 122.6, 26.6, 21.1.
**IR** (thin film) υ 1021, 1115, 1411, 1466, 1577, 2360, 2970 $cm^{-1}$.
**HRMS** Calculated for $C_{11}H_{12}N_2O$ 188.0950, found 188.0955

***3j : 3-(5-Phenyl oxazol-2-yl)-pyridine***



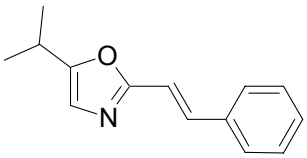

$C_{14}H_{10}N_2O$
M.W.=222.24 $g.mol^{-1}$

The general procedure was followed starting from benzoyl chloride (120 µL, 1.0 mmol) and 3-isocyanomethyl pyridine (118 mg, 1.0 mmol).

Yellow powder, **mp** = 83-84°C
**Yield** : 50% ($m_{product}$= 111 mg)
**$R_f$ :** 0.2 (50:50 $Et_2O$/E.P.)

**$^1$H NMR** ($CDCl_3$, 400 MHz) δ 9.36 (d, 1H, *J* = 2.3 Hz), 8.72 (dd, 1H, *J* = 4.8, 1.8 Hz), 8.38 (ddd, 1H, *J* = 8.0, 2.3, 1.8 Hz), 7.76 (d, 2H, *J* = 7.1 Hz), 7.51 (s, 1H), 7.50-7.47 (m, 2H), 7.45 (dd, 1H, *J* = 8.0, 4.8 Hz), 7.41-7.39 (m, 1H).
**$^{13}$C NMR** ($CDCl_3$, 100.6 MHz) δ 159.2, 152.4, 151.4, 148.0, 133.8, 129.5, 129.3, 128.0, 124.8, 124.1, 124.1, 124.0.
**IR** (thin film) υ 1023, 1134, 1410, 1487 $cm^{-1}$.
**HRMS** Calculated for $C_{14}H_{10}N_2O$ 222.0793, found 222.0802.

***3n : 5-Isopropyl-2-styryl oxazole***

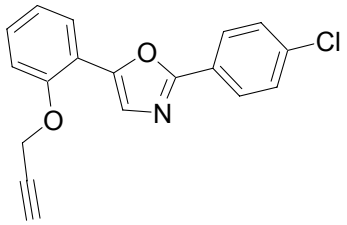



$C_{14}H_{15}NO$
M.W.=213.28 $g.mol^{-1}$

The general procedure was followed starting from isobutyryl chloride (40 µL, 0.4 mmol) and (3-isocyano propenyl)-benzene (59 mg, 0.4 mmol).

Yellow oil
**Yield** : 48% ($m_{product}$= 41 mg)
**$R_f$ :** 0.3 (50:50 $Et_2O$/E.P.)
**$^1$H NMR** ($CDCl_3$, 400 MHz) δ 7.54 (d, 2H, *J* = 8.1 Hz), 7.44 (d, 1H, *J* = 16.2 Hz), 7.41-7.38 (m, 2H), 7.35-7.32 (m, 1H), 6.93 (d, 1H, *J* = 16.2 Hz), 6.79 (s, 1H), 3.03 (sept, 1H, *J* = 7.1 Hz), 1.33 (d, 6H, *J* = 7.1 Hz).
**$^{13}$C NMR** ($CDCl_3$, 100.6 MHz) δ 160.8, 158.6, 136.2, 135.1, 129.3, 129.2, 127.4, 122.5, 114.8, 26.6, 21.2.
**IR** (thin film) υ 1206, 1450, 1523, 1629, 1668, 2972 $cm^{-1}$.
**HRMS** Calculated for $C_{14}H_{15}NO$ 213.1154, found 213.1150.

***3o : 2-(4-Chloro phenyl)-5-(2-prop-2-ynyloxy phenyl)-oxazole***



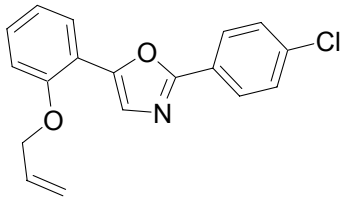

$C_{18}H_{12}ClNO_2$
M.W.=309.75 $g.mol^{-1}$

The general procedure was followed starting from 2-prop-2-ynyloxy benzoyl chloride (162 mg, 1.0 mmol) and 1-chloro-4-isocyanomethyl benzene (152 mg, 1.0 mmol).

White solid, **mp** = 143-144°C
**Yield** : 49% ($m_{product}$= 151 mg)
**$R_f$ :** 0.5 (50:50 $Et_2O$/E.P.)

**$^1$H NMR** ($CDCl_3$, 400 MHz) δ 8.08 (d, 2H, *J* = 8.6 Hz), 7.90 (dd, 1H, *J* = 7.6, 1.6 Hz), 7.74 (s, 1H), 7.48 (d, 2H, *J* = 8.6 Hz), 7.36 (ddd, 1H, *J* = 8.3, 7.6, 1.6 Hz), 7.15 (dd, 1H, *J* = 8.3, 7.6 Hz), 7.13 (d, 1H, *J* = 8.3 Hz), 4.9 (d, 2H, *J* = 2.5 Hz), 2.6 (t, 1H, *J* = 2.5 Hz).
**$^{13}$C NMR** ($CDCl_3$, 100.6 MHz) δ 159.6, 154.1, 148.1, 136.7, 129.5, 129.4, 128.5, 128.4, 128.0, 126.4, 122.2, 118.0, 112.7, 78.4, 76.5, 55.6.
**IR** (thin film) υ 1022, 1057, 1093, 1136, 1231, 1480, 3302 $cm^{-1}$.
**HRMS** Calculated for $C_{18}H_{12}ClNO_2$ 309.0557, found 309.0557.

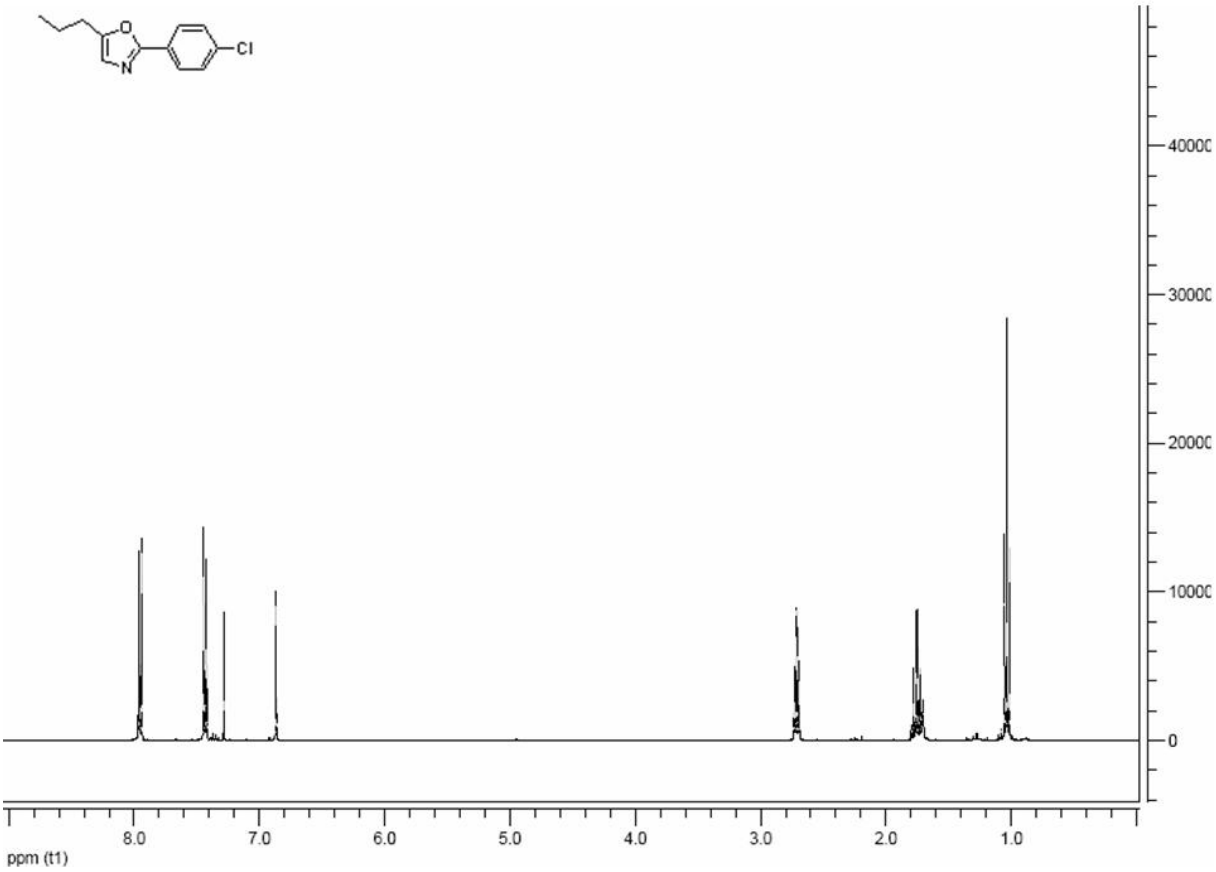
***3f : 5-(2-Allyloxy phenyl)-2-(4-chloro phenyl)-oxazole***




$C_{18}H_{14}ClNO_2$
M.W.=311.76 $g.mol^{-1}$

The general procedure was followed starting from 2-allyloxy benzoyl chloride (393 mg, 2.0 mmol) and 1-chloro-4-isocyanomethyl benzene (303 mg, 2.0 mmol).

White solid, **mp** = 96-97°C
**Yield** : 58% ($m_{product}$= 363 mg)
**$R_f$ :** 0.6 (50:50 $Et_2O$/E.P.)
**$^1$H NMR** ($CDCl_3$, 400 MHz) δ 8.08 (d, 2H, *J* = 8.5 Hz), 7.90 (dd, 1H, *J* = 8.0, 1.8 Hz), 7.72 (s, 1H), 7.48 (d, 2H, *J* = 8.5 Hz), 7.33 (ddd, 1H, *J* = 8.0, 7.3, 1.8 Hz), 7.10 (ddd, 1H, *J* = 8.0, 7.3, 1.8), 7.01 (d, 1H, *J* = 8.0 Hz), 6.18 (ddt, 1H, *J* = 16.9, 10.3, 5.6 Hz), 5.50 (dd, 1H, *J* = 16.9, 1.3 Hz), 5.38 (dd, 1H, *J* = 10.3, 1.3 Hz), 4.73 (dt, 2H, *J* = 5.6, 1.5 Hz).
**$^{13}$C NMR** ($CDCl_3$, 100.6 MHz) δ 159.5, 155.2, 148.5, 136.7, 133.1, 129.5, 129.5, 128.3, 127.9, 126.5, 126.4, 121.5, 119.0, 117.6, 112.5, 69.8.
**IR** (thin film) υ 1011, 1091, 1131, 1248, 1404, 1424, 1480, 1494, 1563 $cm^{-1}$.
**HRMS** Calculated for $C_{18}H_{14}ClNO_2$ 311.0713, found 311.0717.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30000
20000
10000
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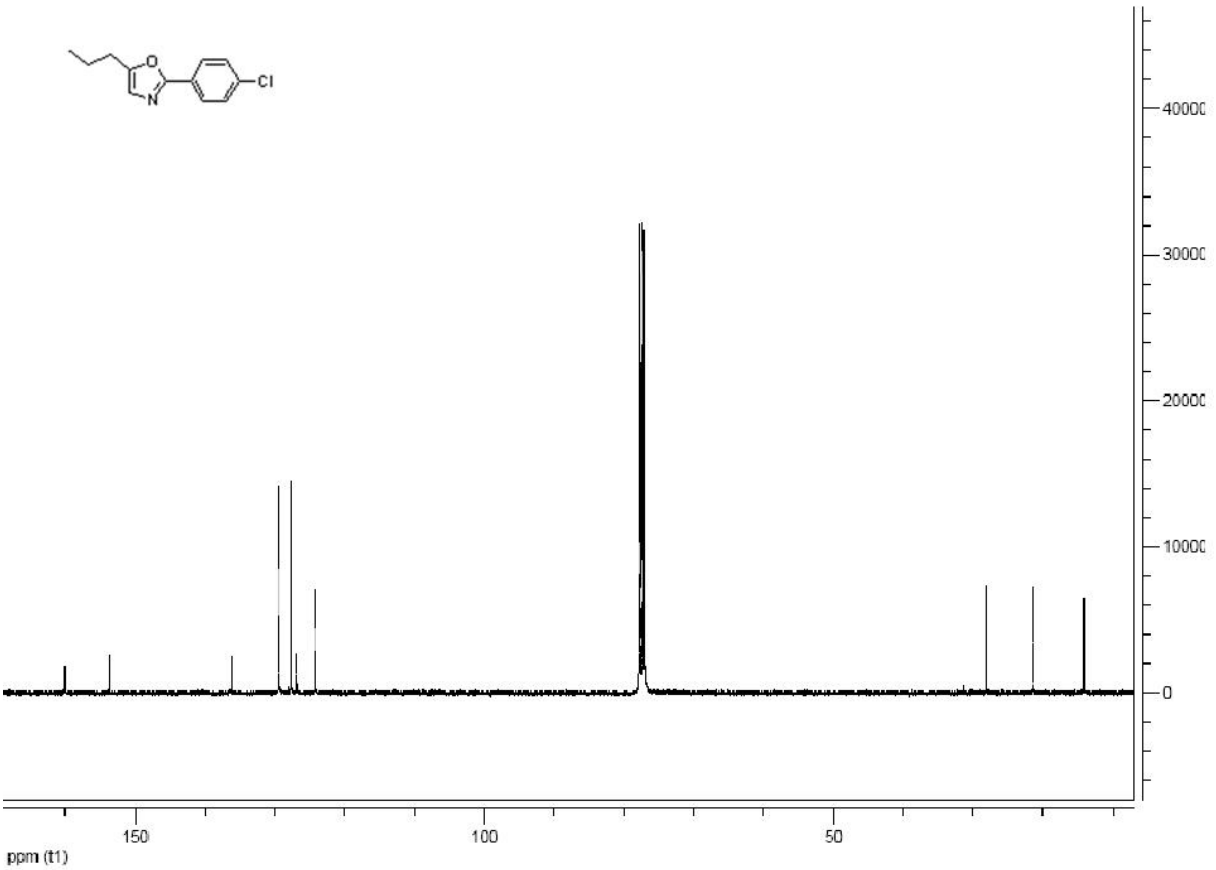
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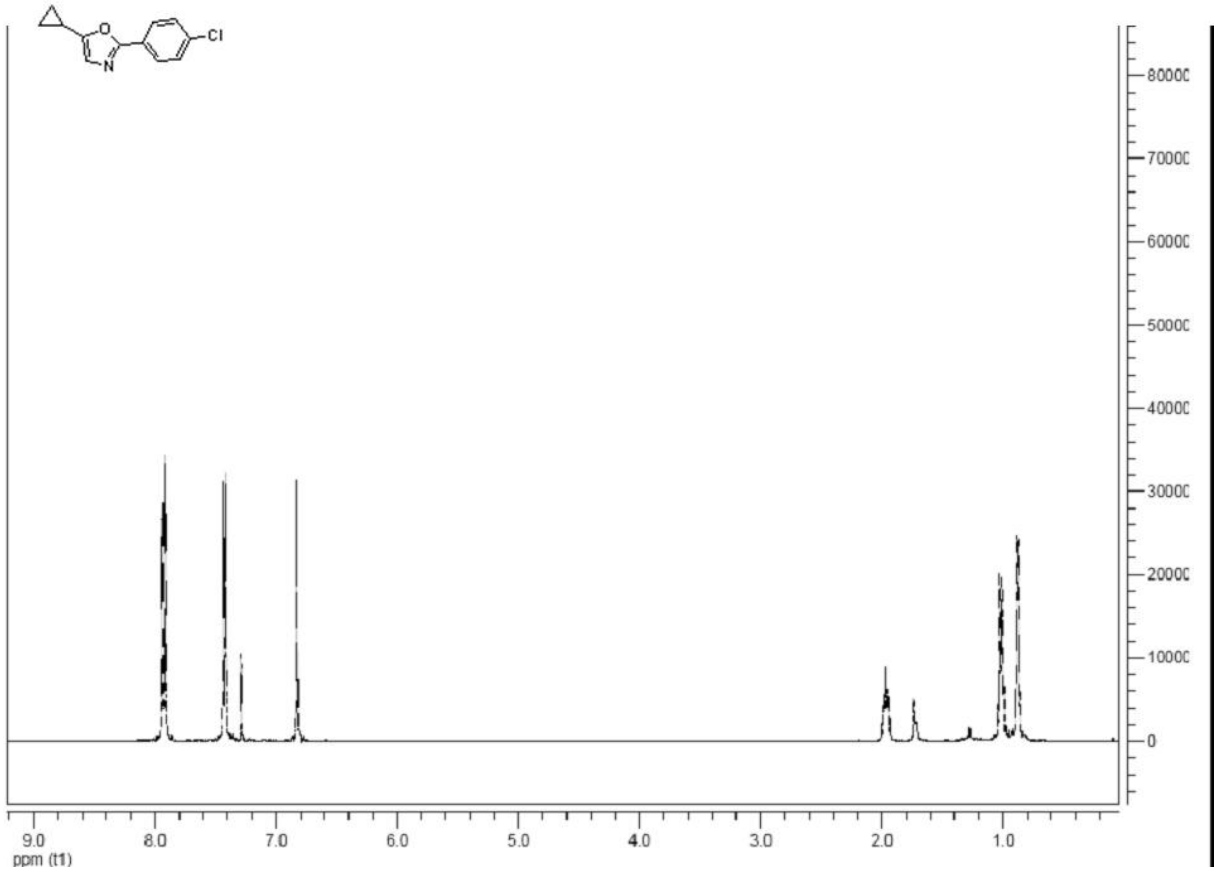
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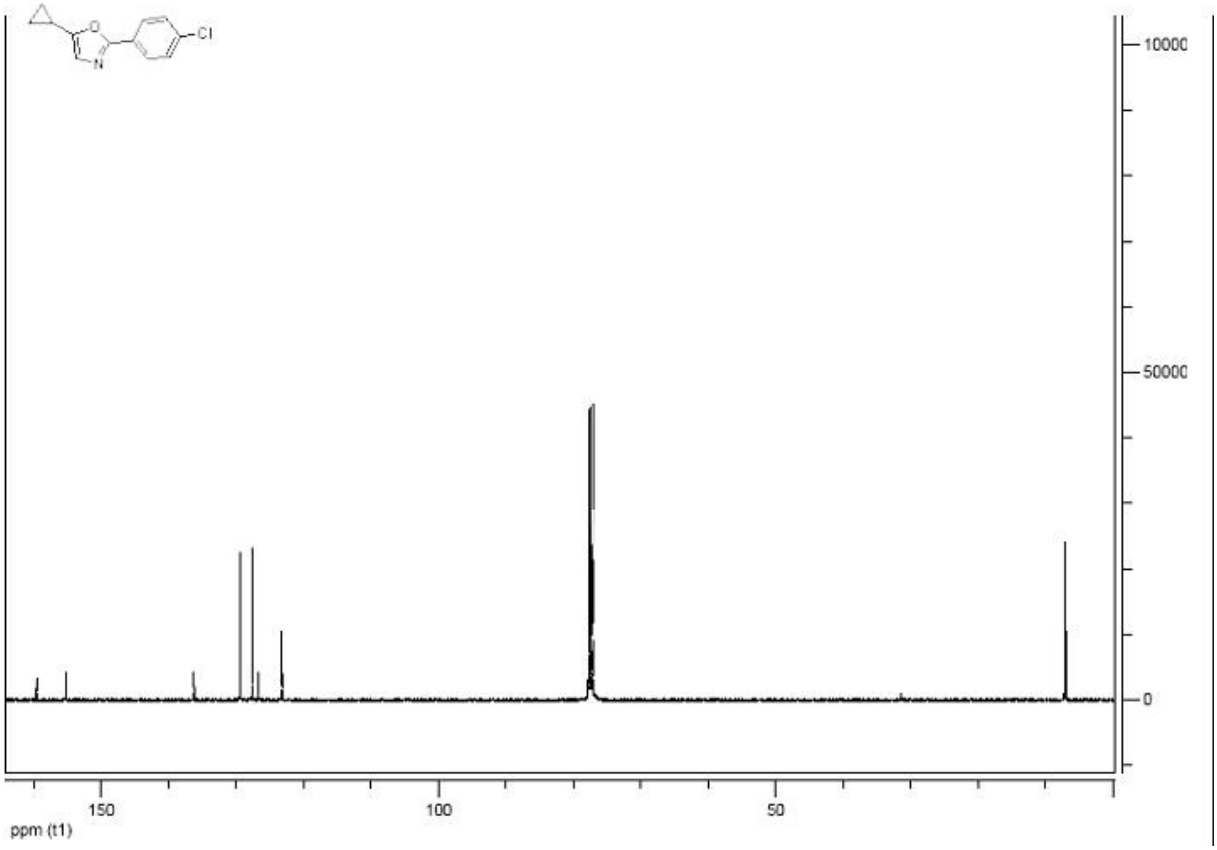
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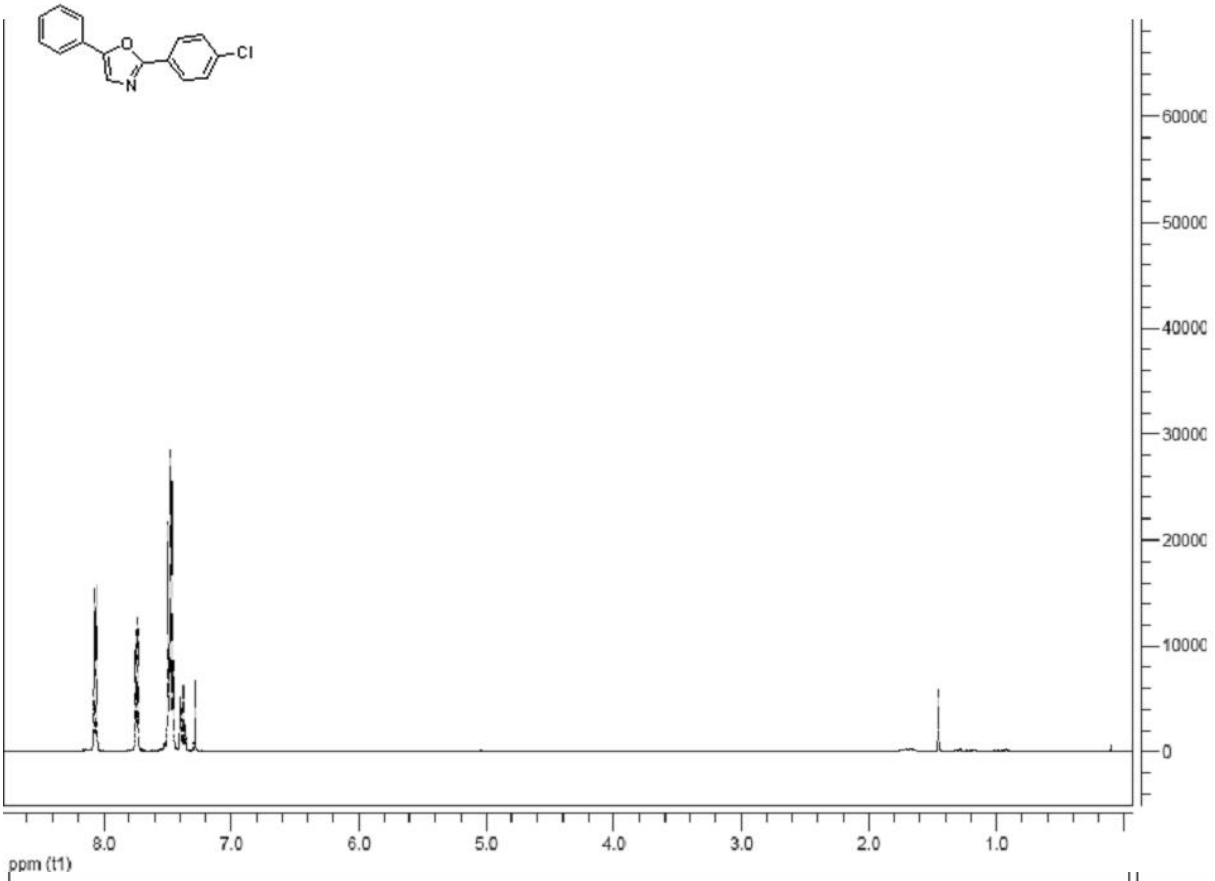
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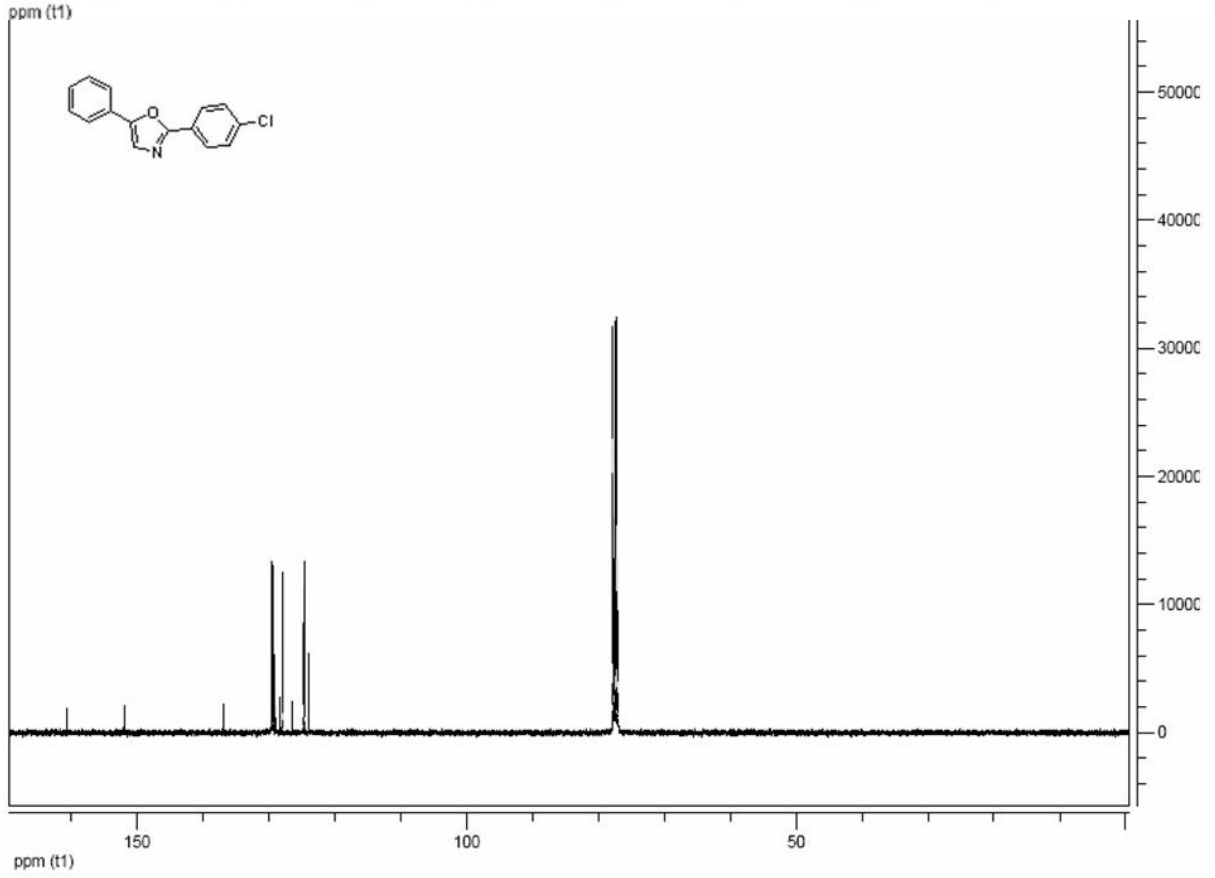
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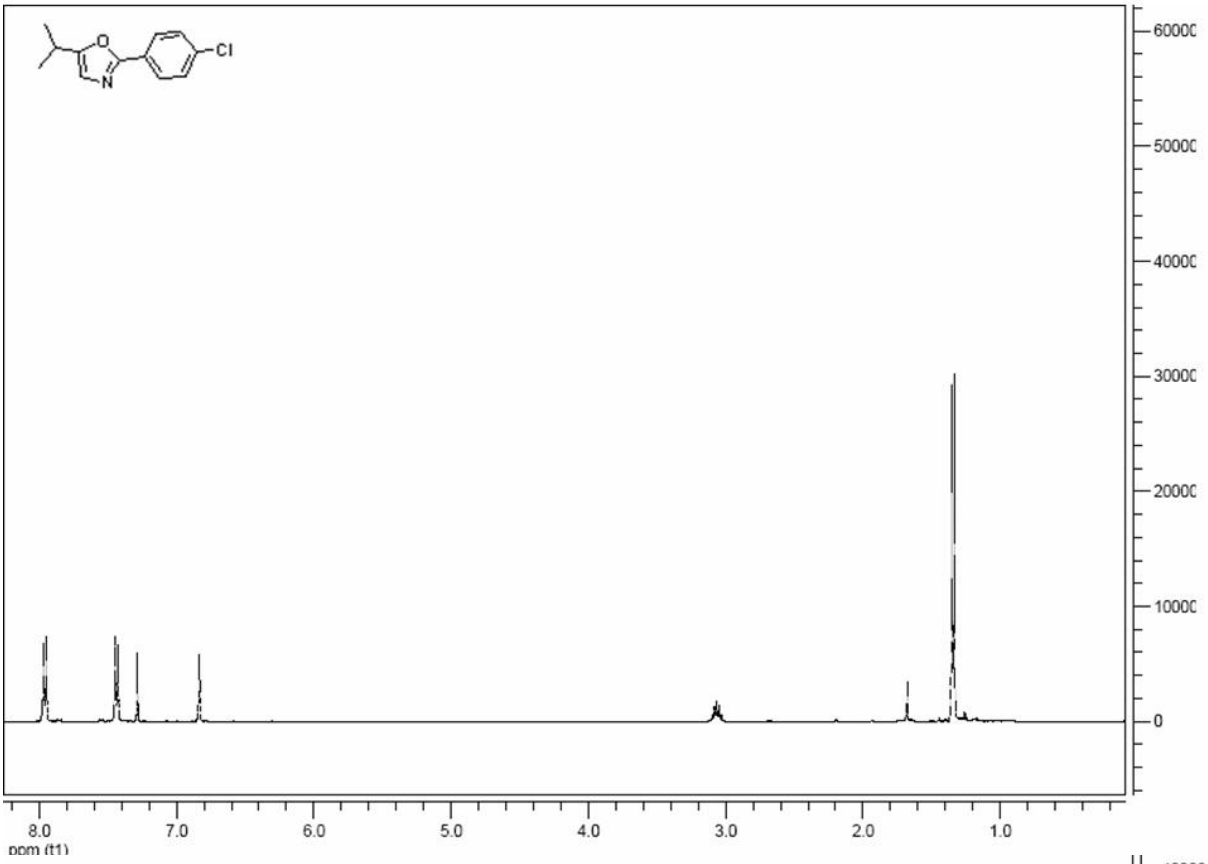
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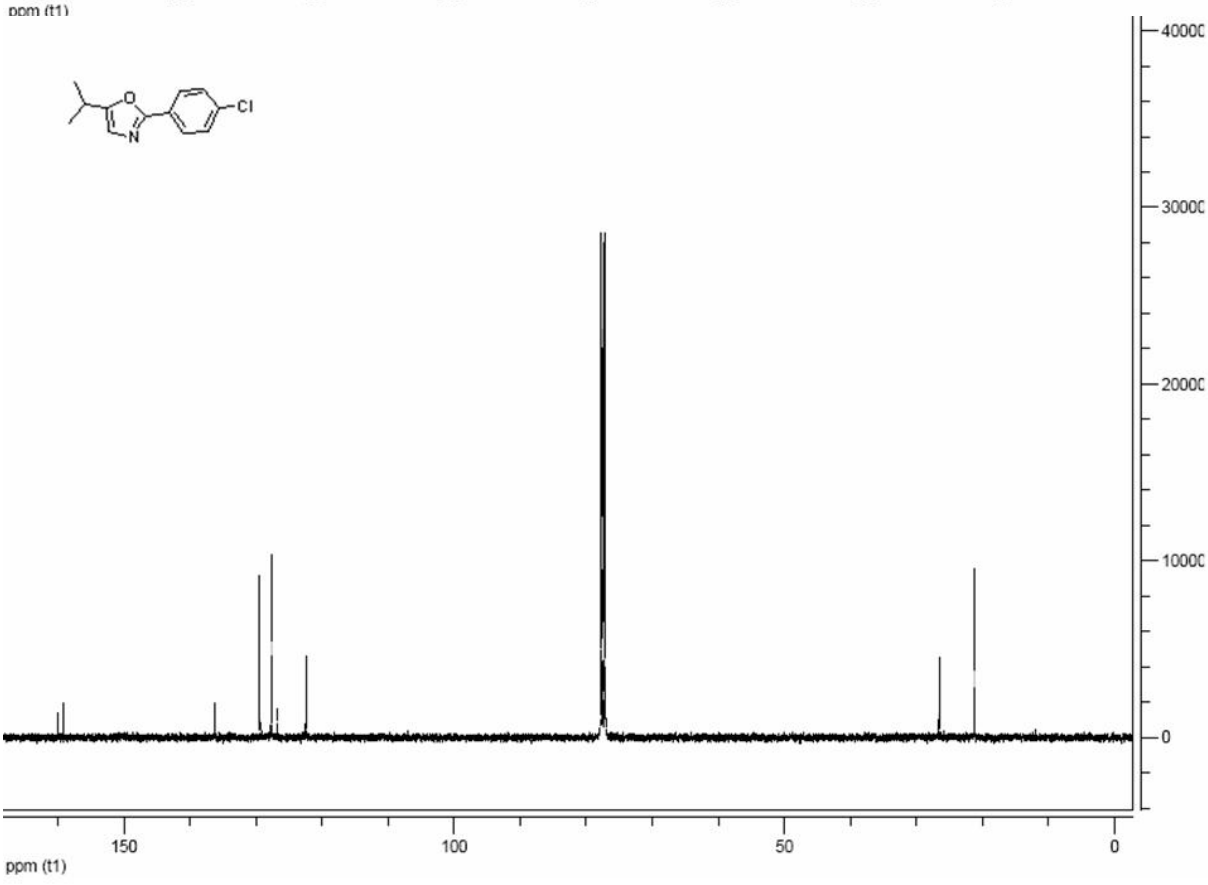
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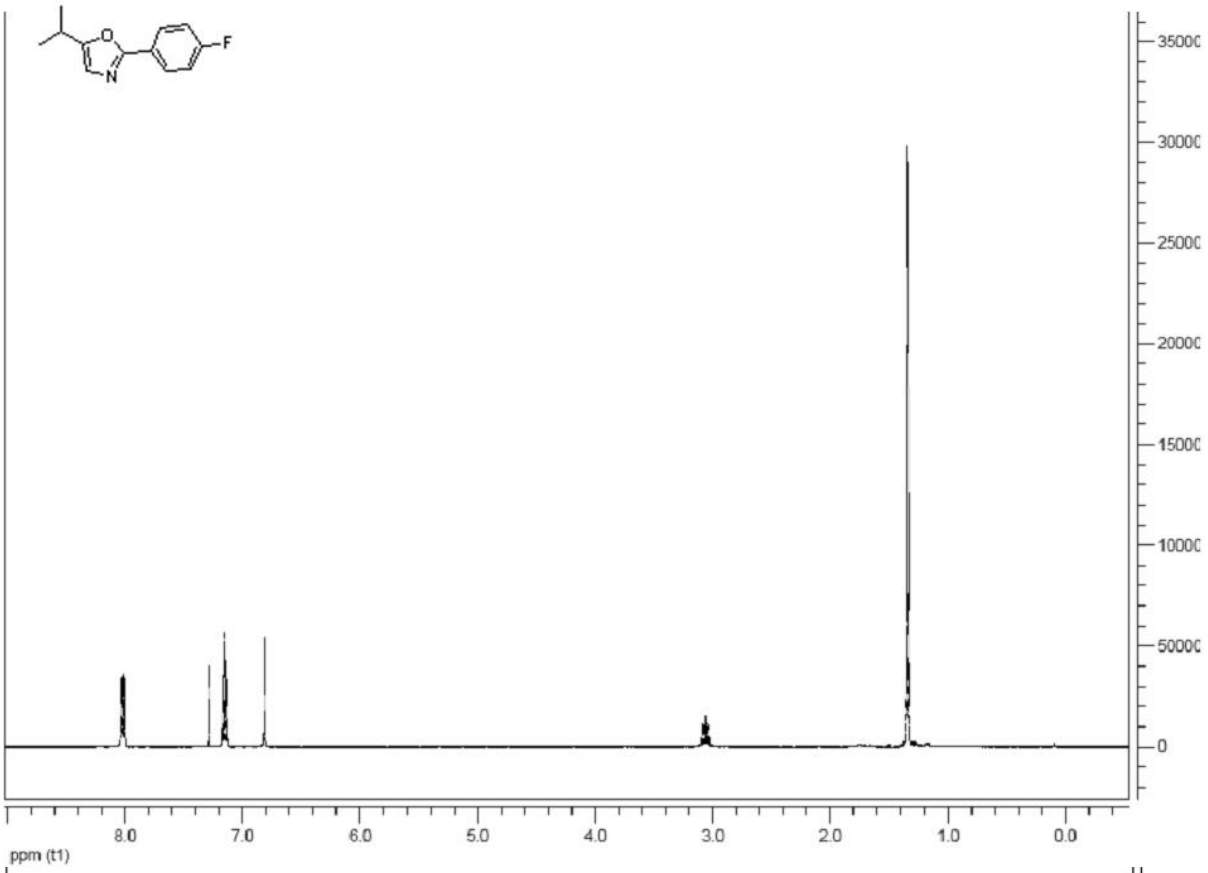
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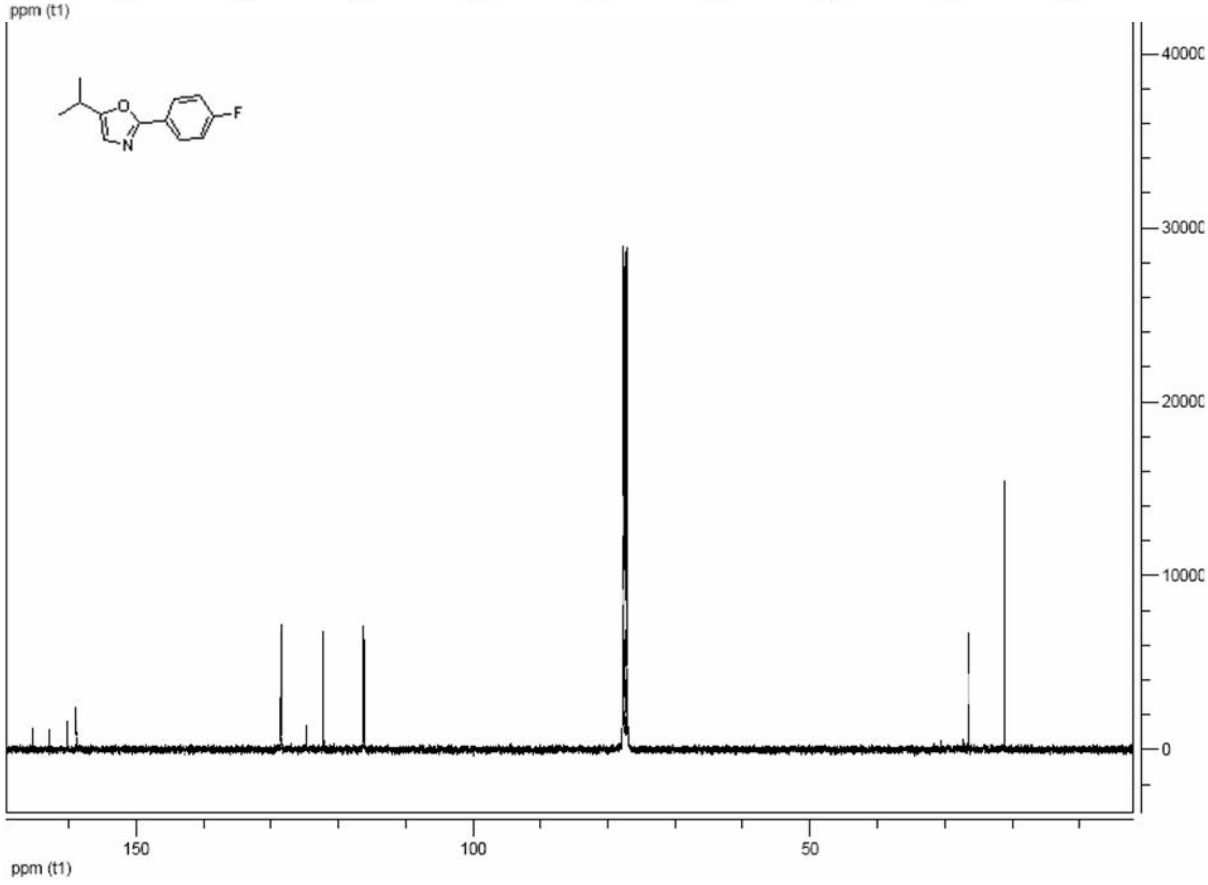
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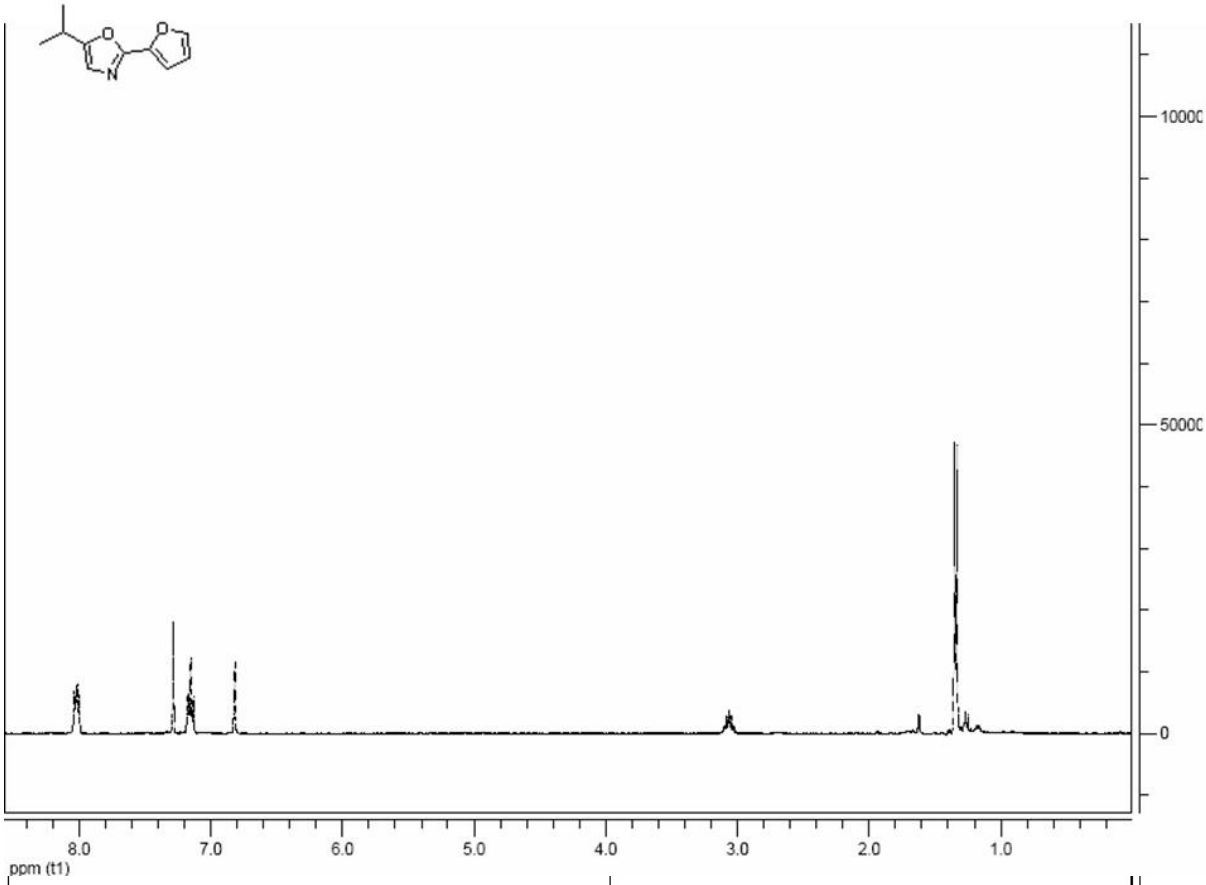
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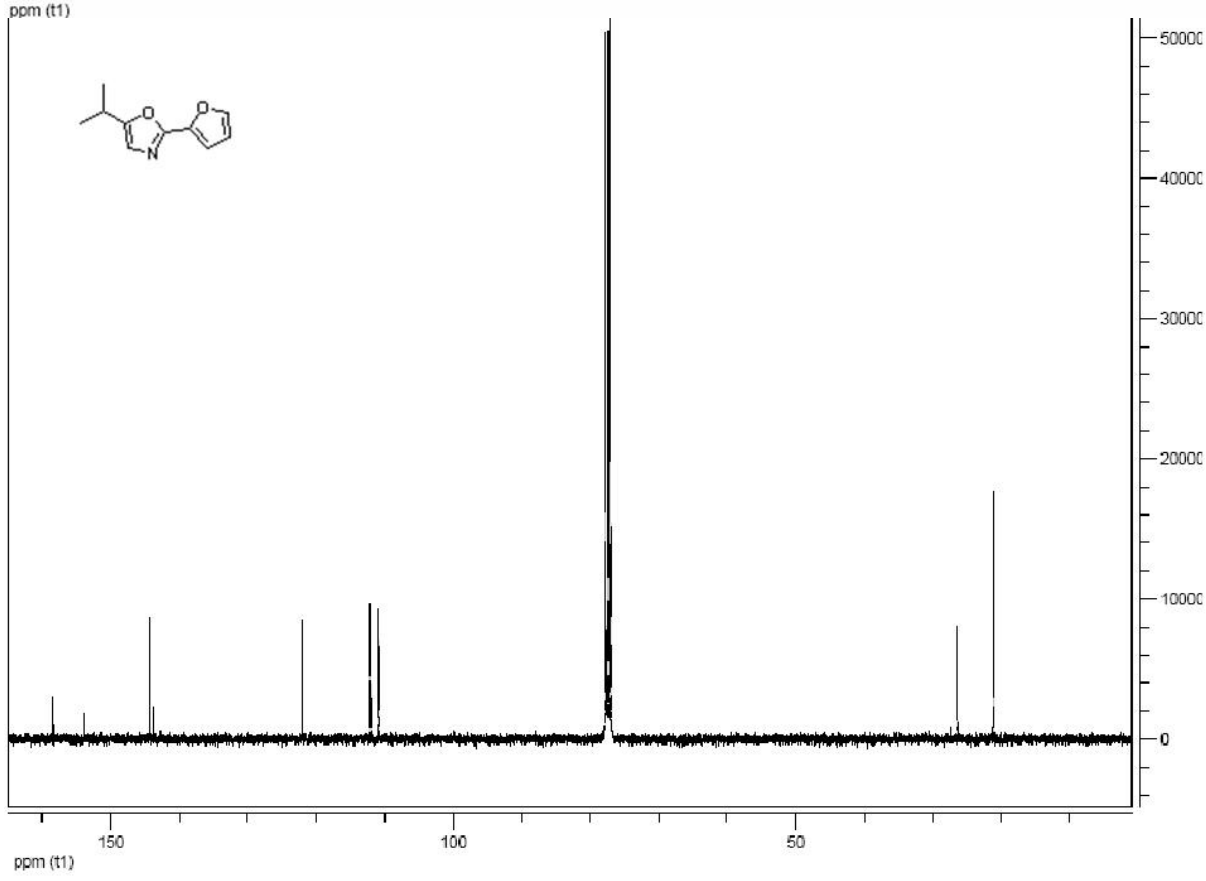
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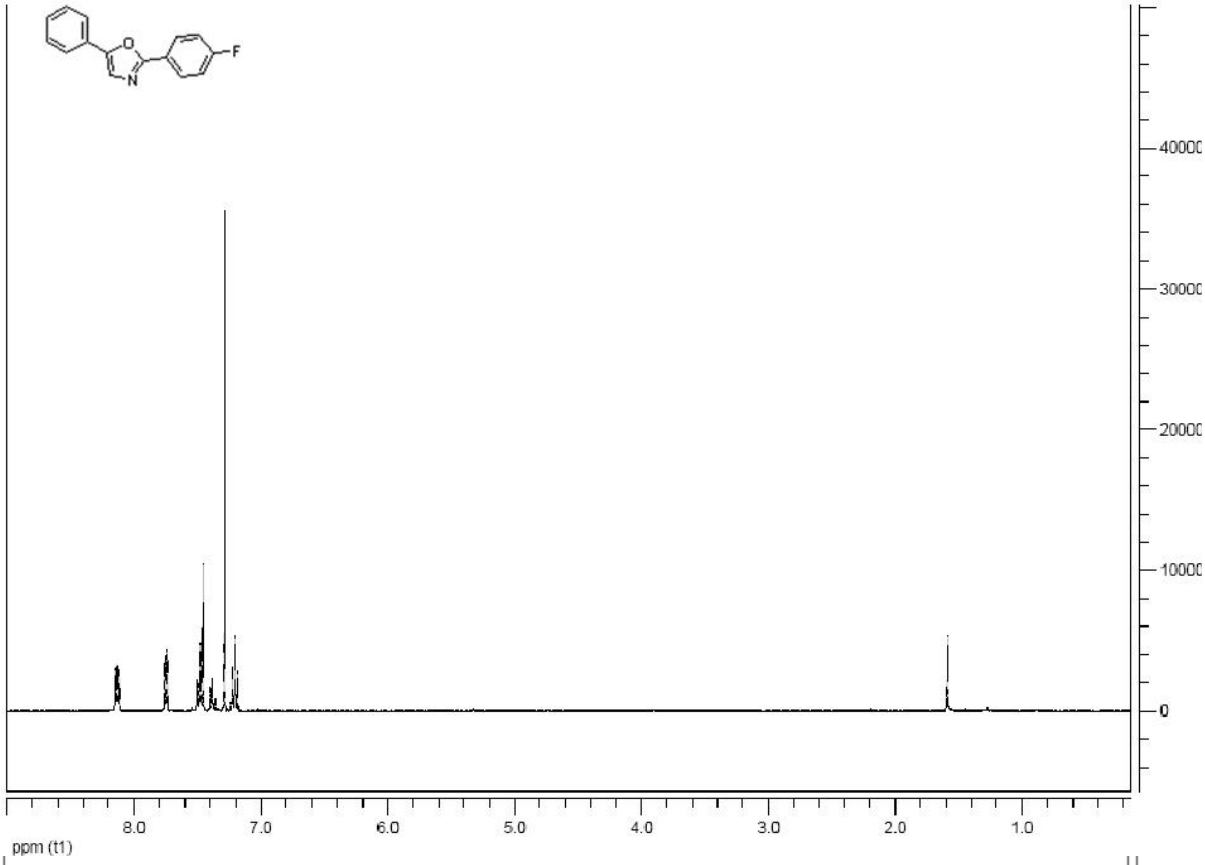
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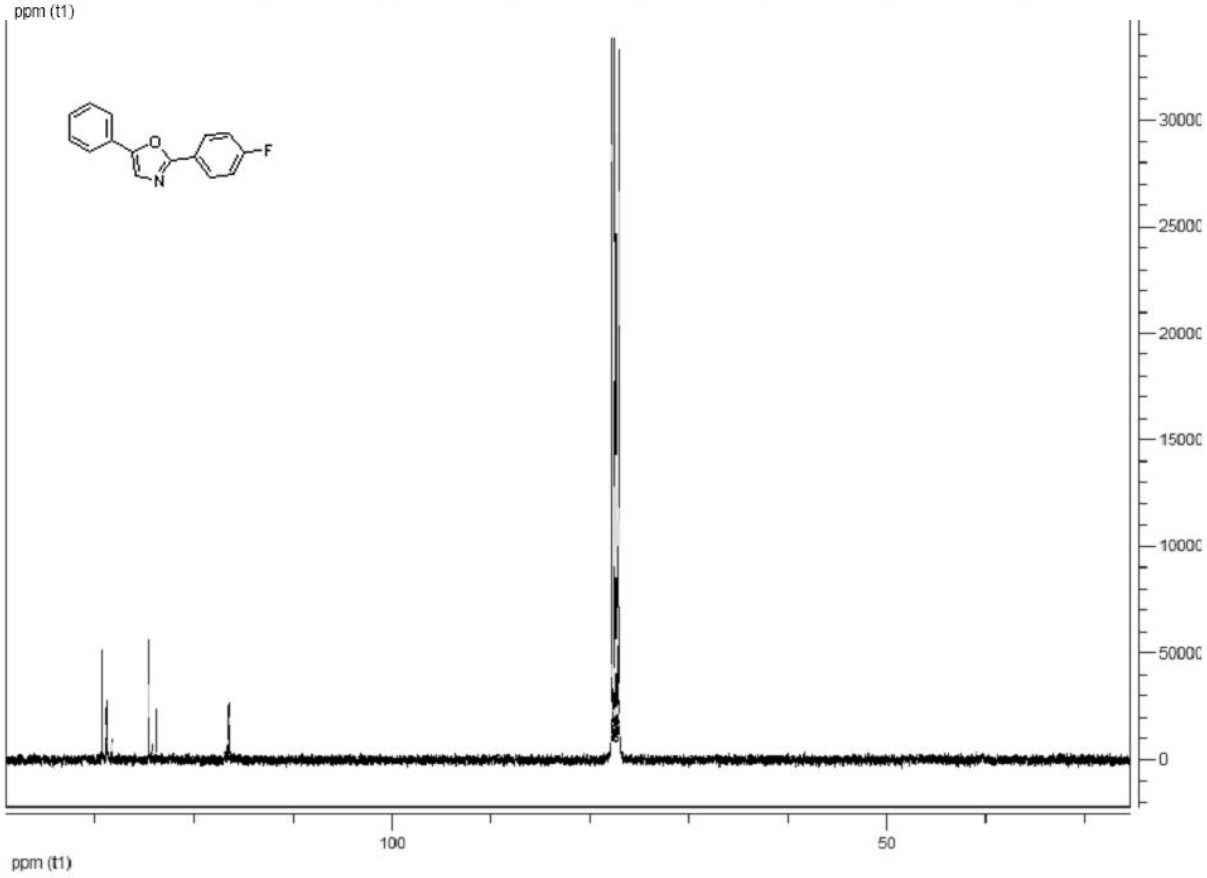
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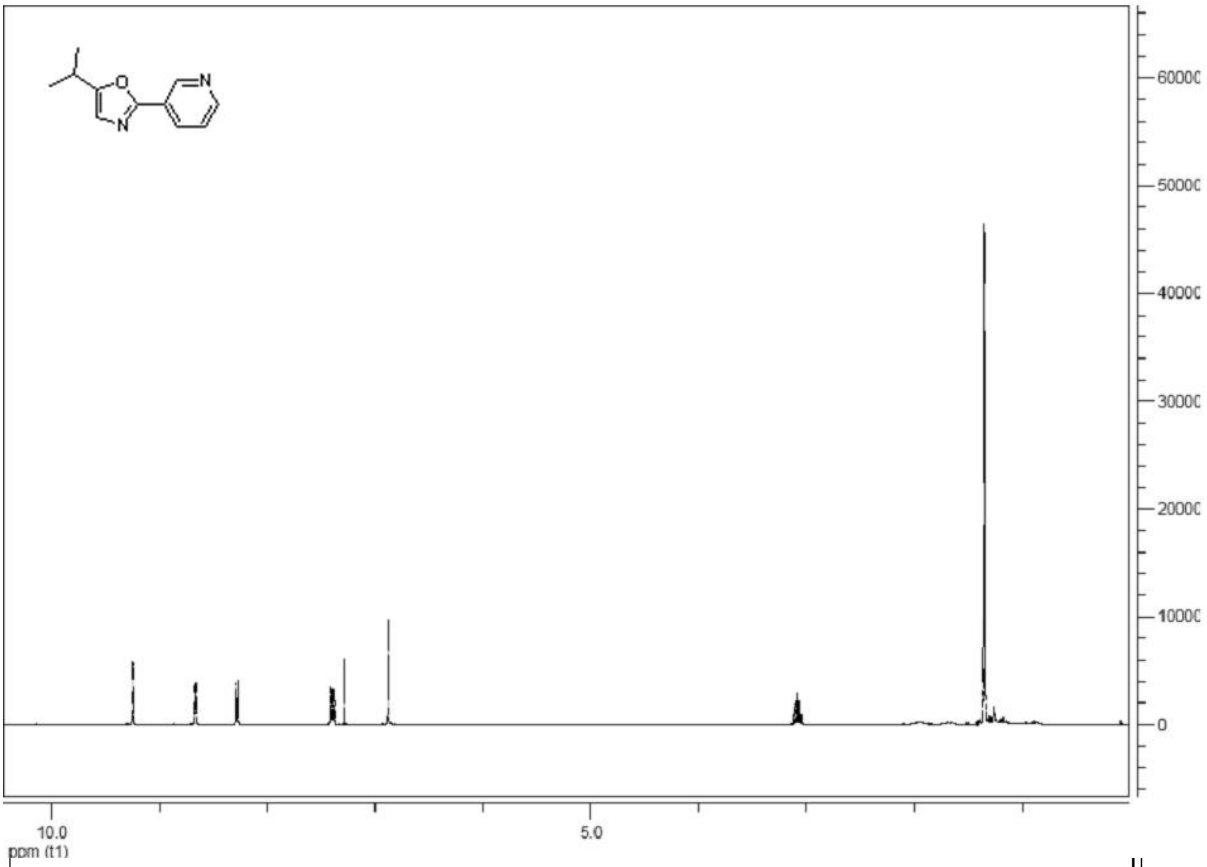
ppm (t1)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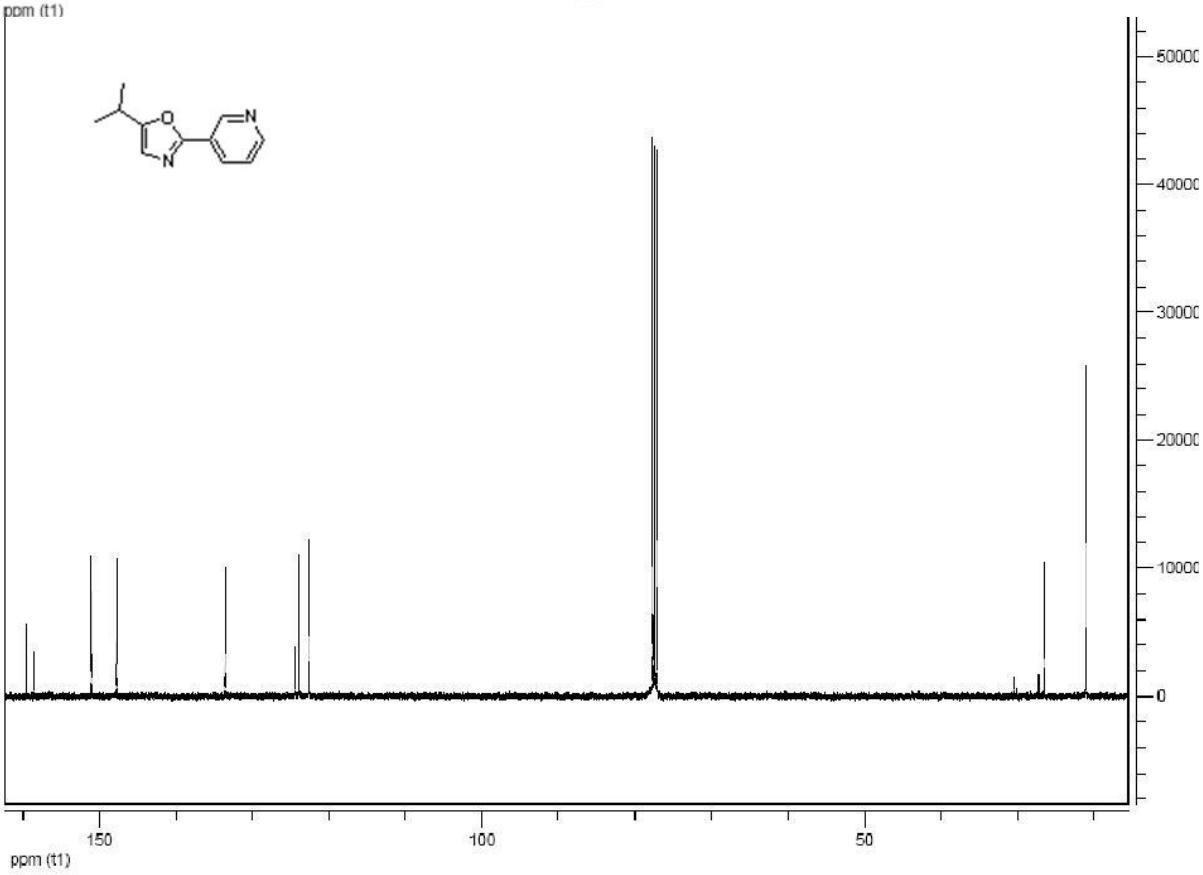
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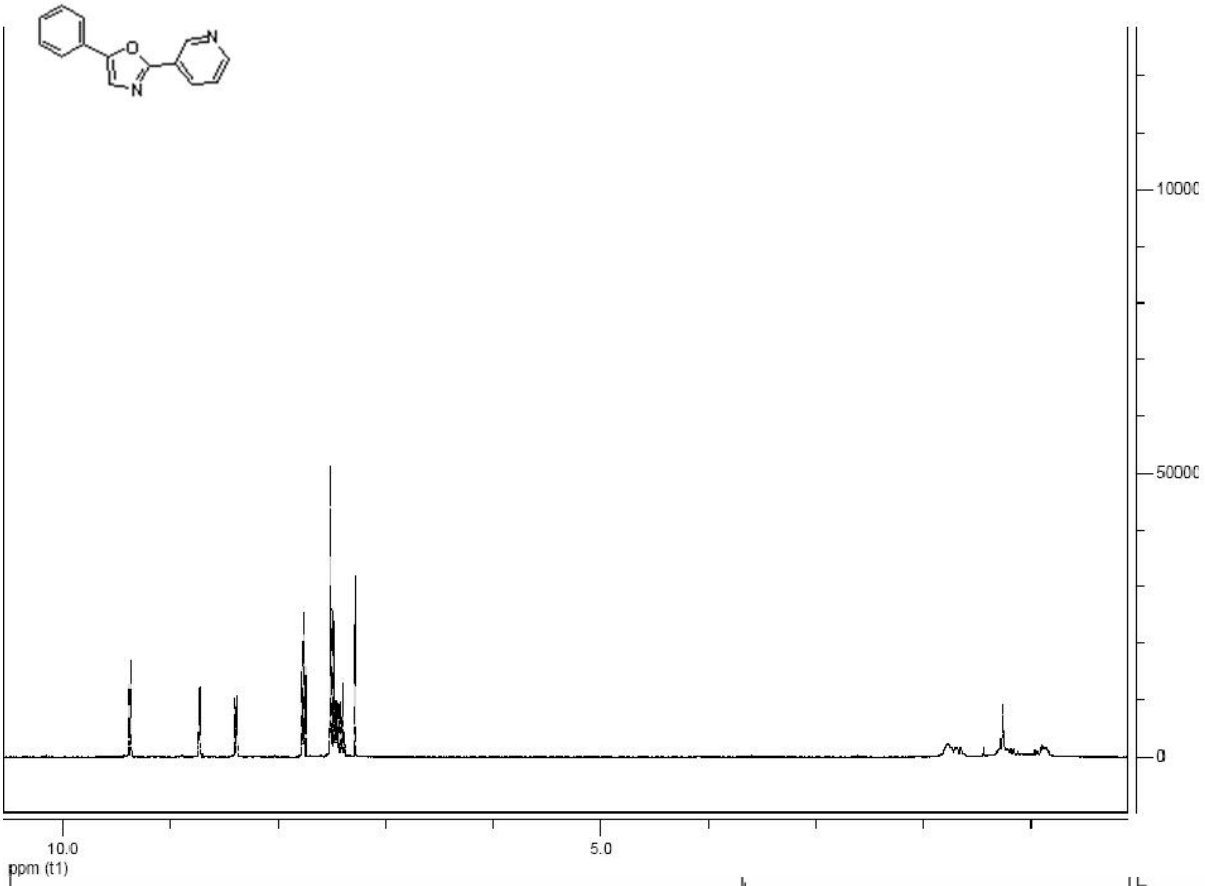
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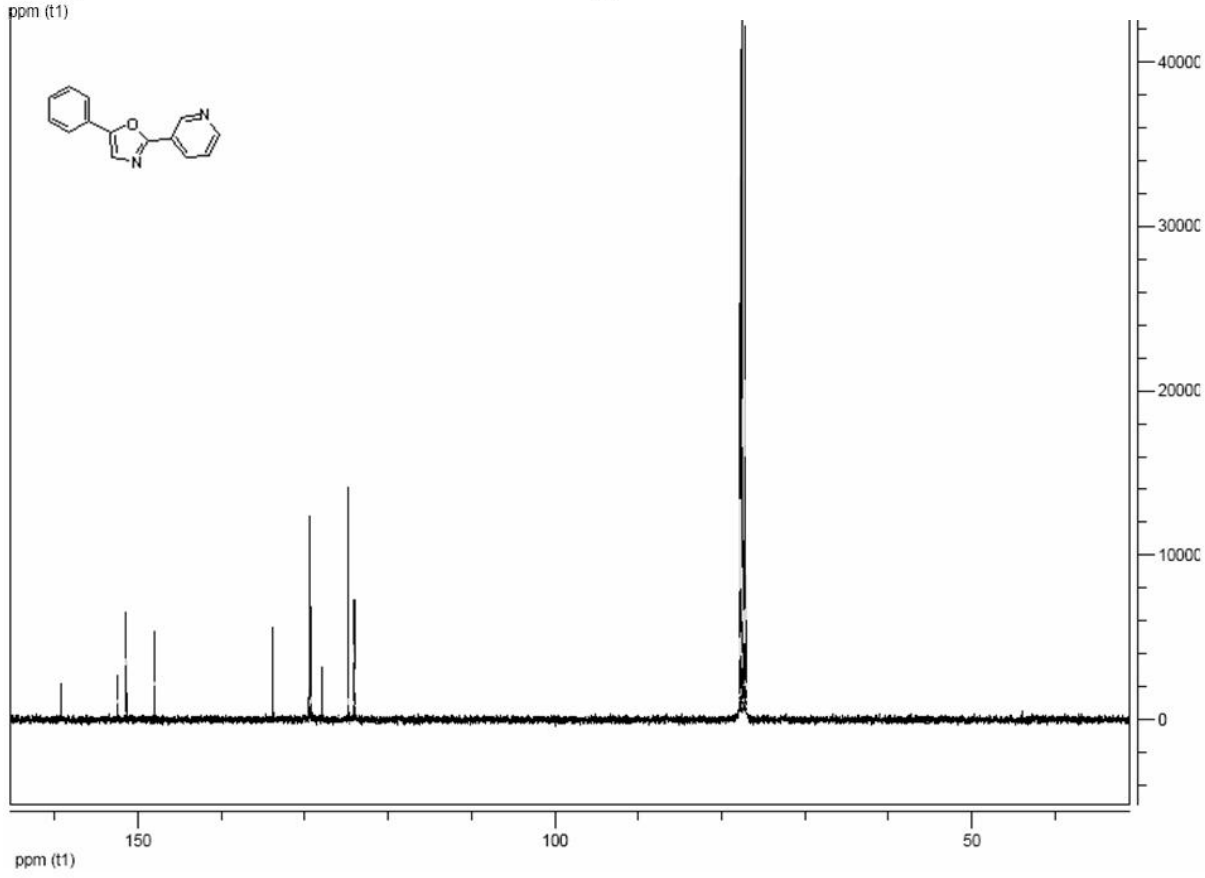
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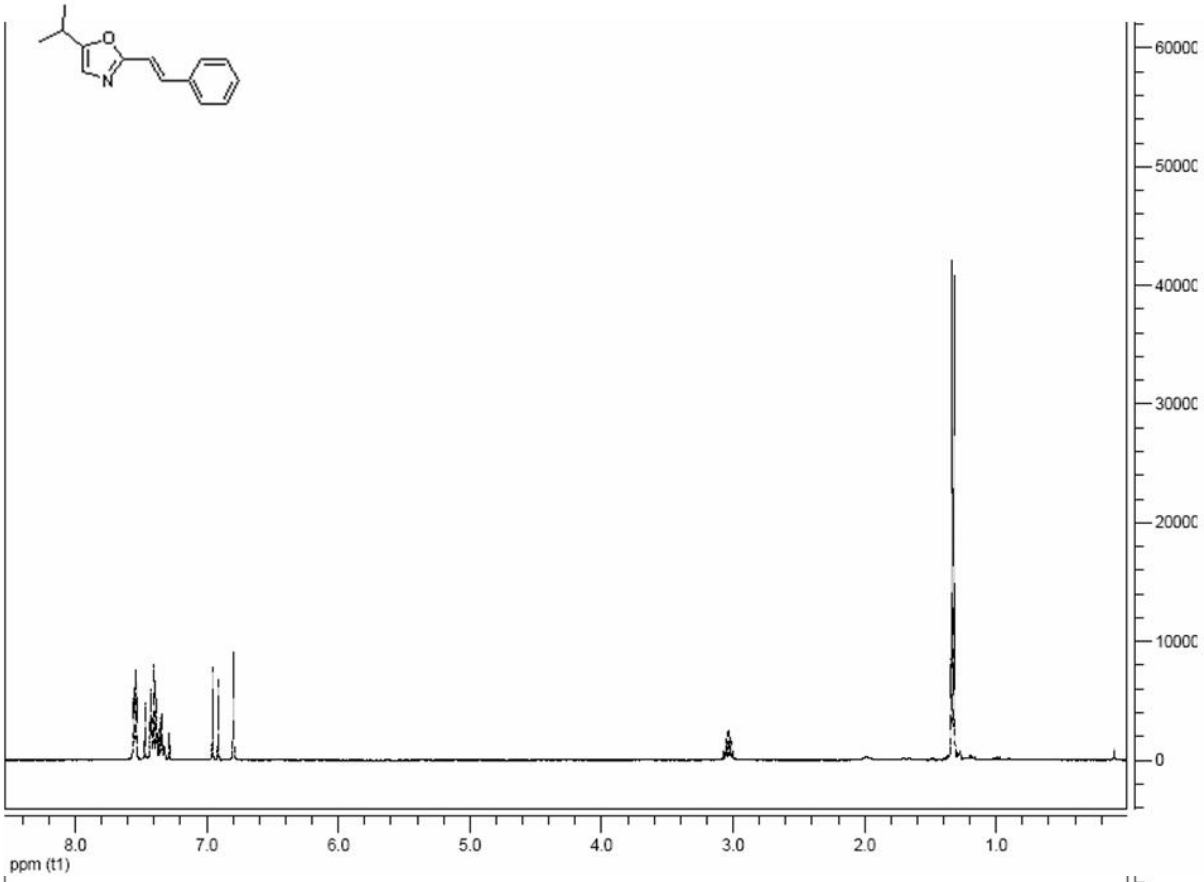
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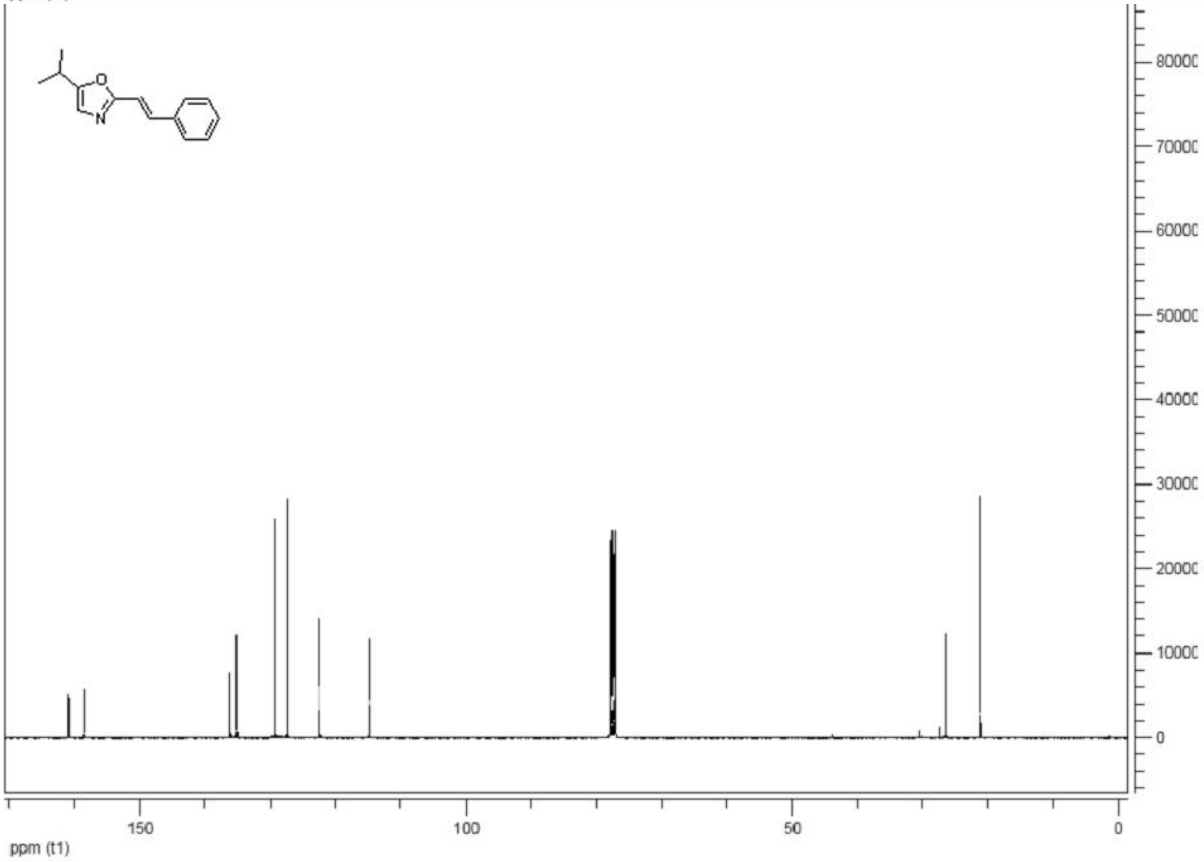
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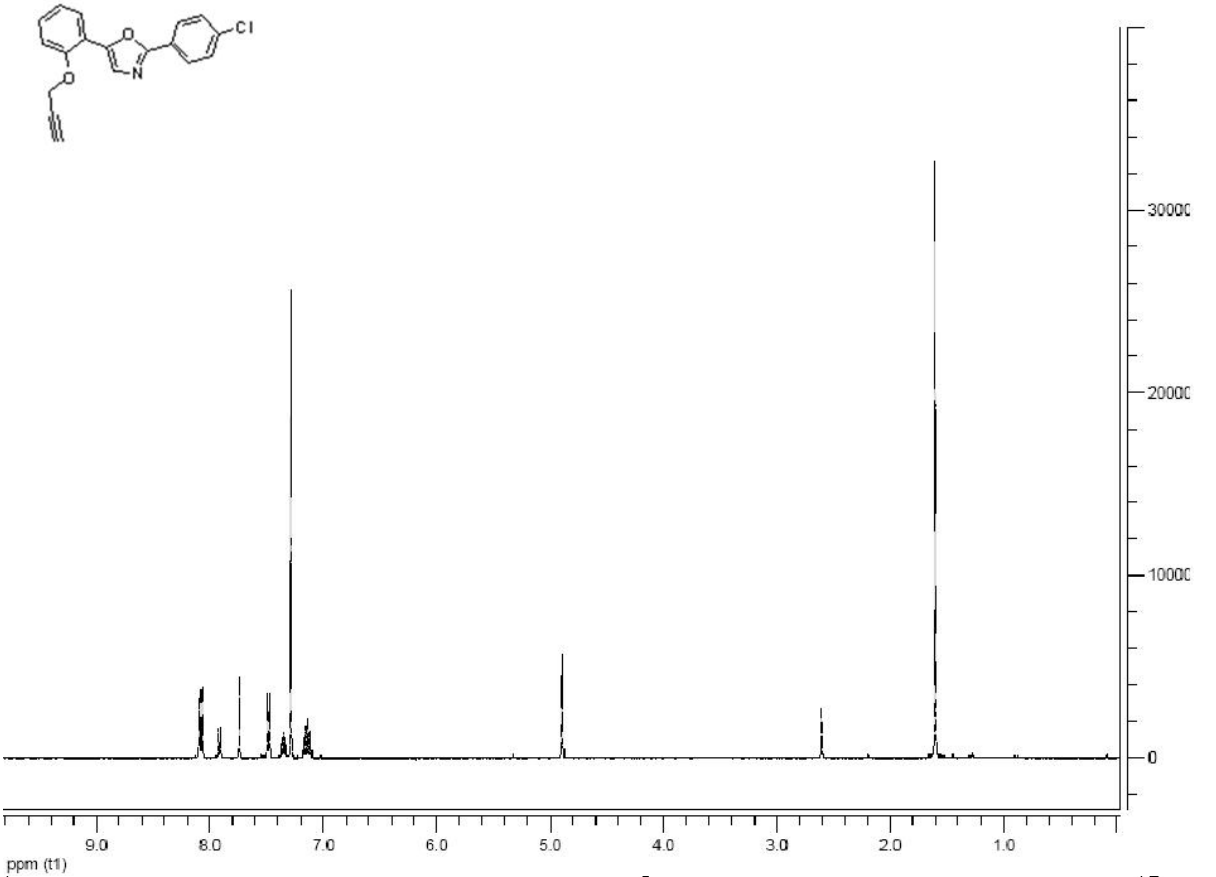
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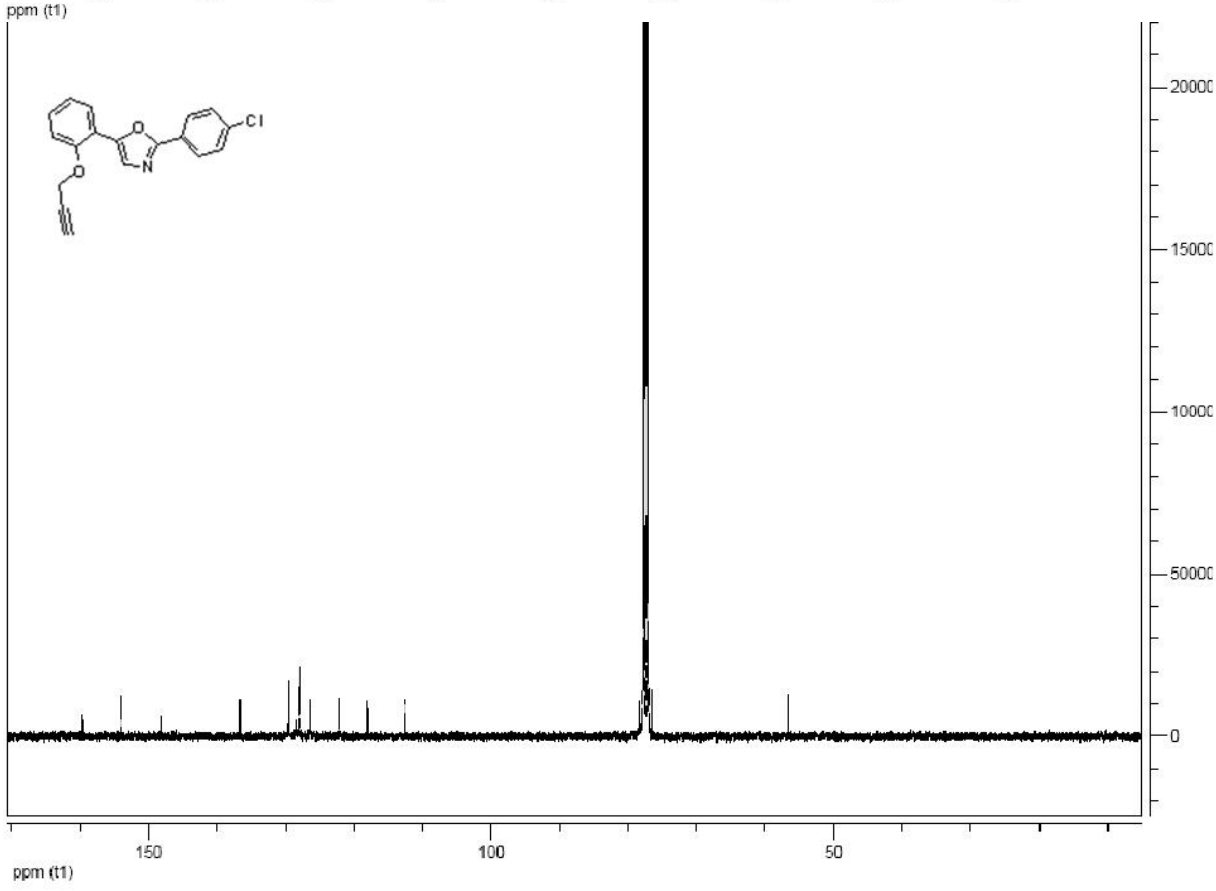
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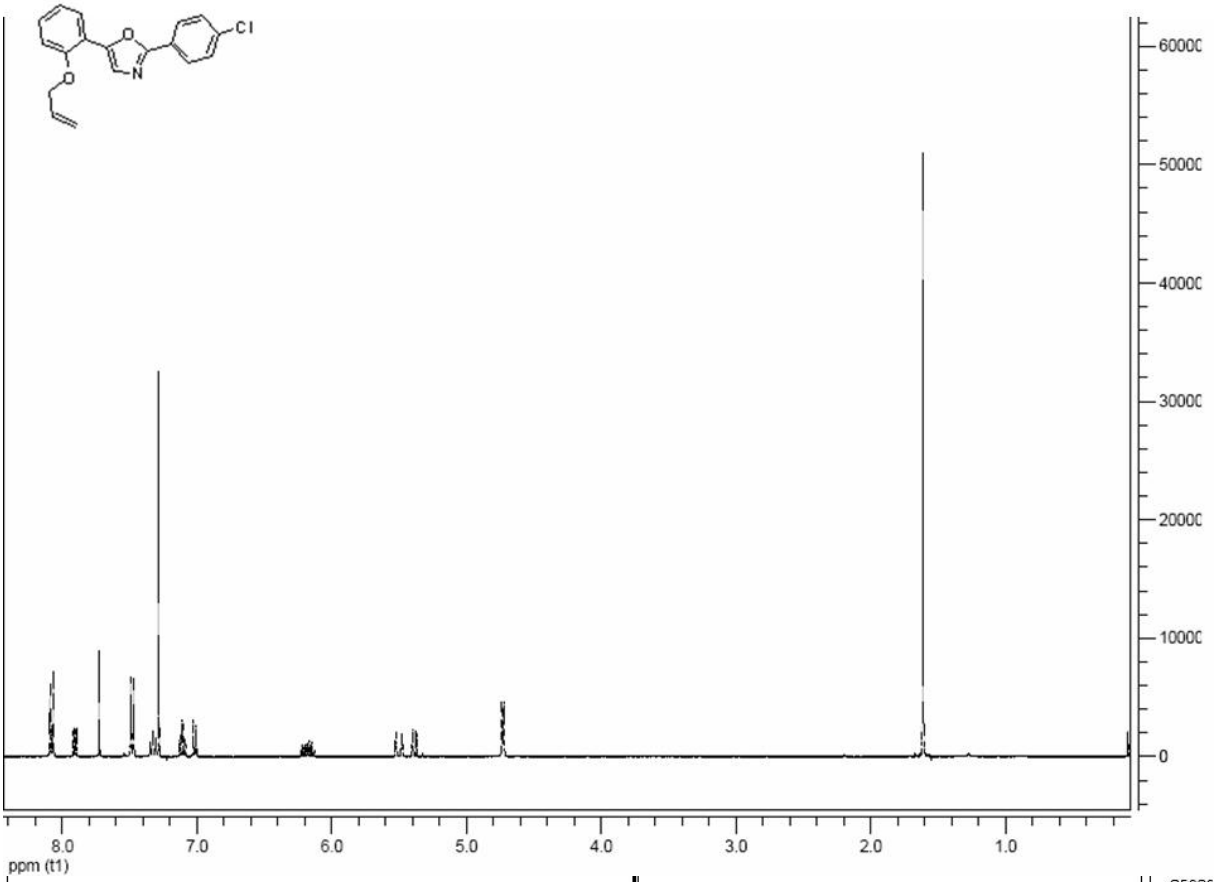
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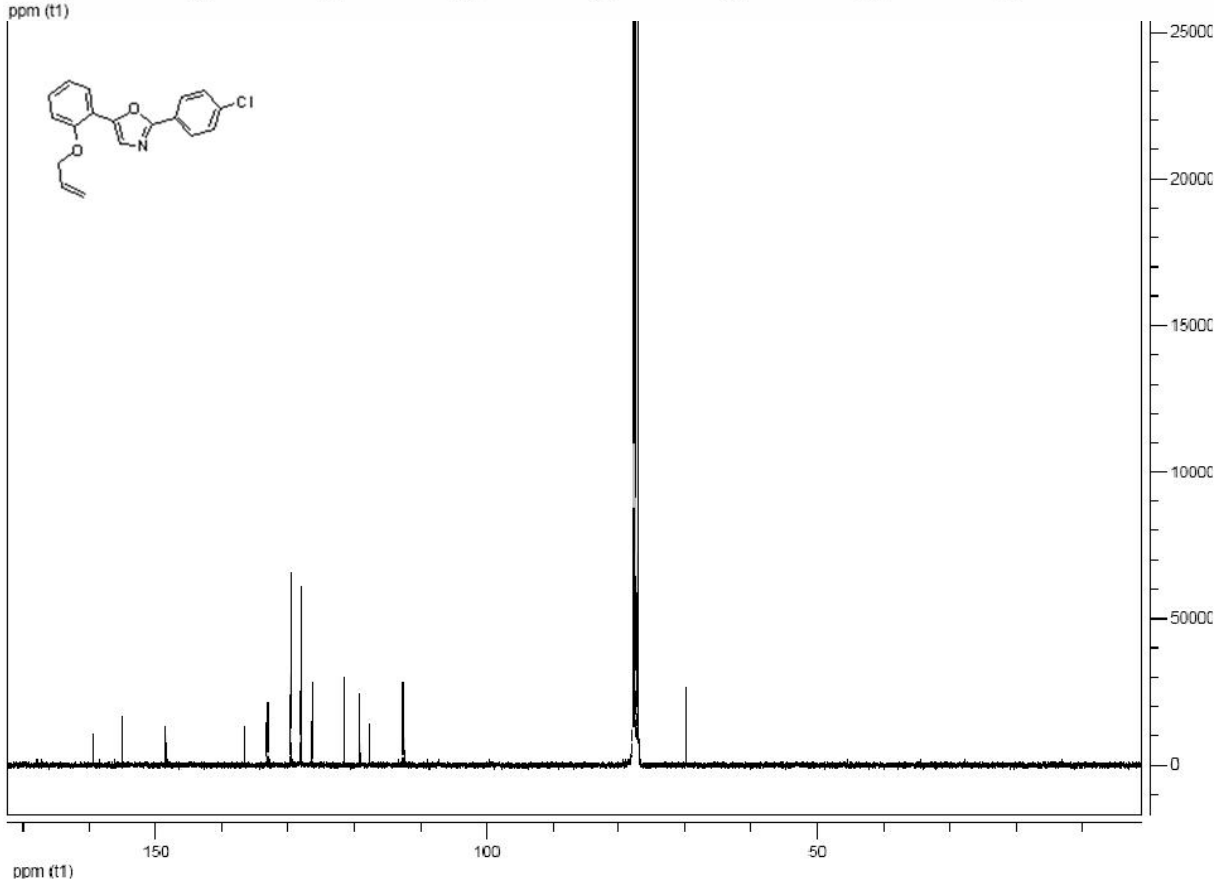
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ppm (t1)