

Supporting Information

One-pot Synthesis of 1,3,4-Oxadiazol-2(3*H*)-ones with CO₂ as C1

Synthon Promoted by Hypoiodite

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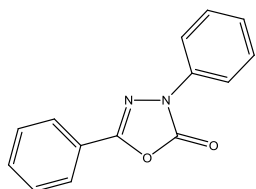
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1. General methods

^1H and ^{13}C NMR spectra were recorded by using a Bruker DRX-400 spectrometer and CDCl_3 as the solvent. The chemical shifts were referenced to signals at 7.26 and 77.23 ppm, respectively. Mass spectra were recorded on a Thermo Scientific ISQ gas chromatograph-mass spectrometer. The data of HRMS were obtained on a high resolution mass spectrometer (LCMS-IT-TOF). Melting points were determined with a Büchi Melting Point B-545 instrument.

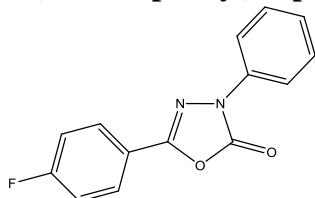
2. Characterization data

3,5-diphenyl-1,3,4-oxadiazol-2(3H)-one (3a)¹



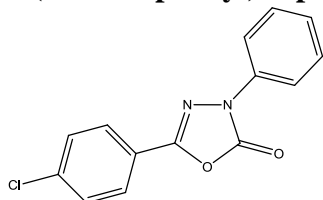
White solid, mp 108–110 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3): δ (ppm) 7.95 – 7.92 (m, 4H), 7.53 – 7.44 (m, 5H), 7.27 (t, $J = 7.4$ Hz, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ (ppm) 153.7, 150.8, 136.2, 132.1, 129.4, 129.2, 126.3, 126.1, 123.6, 118.5.

5-(4-fluorophenyl)-3-phenyl-1,3,4-oxadiazol-2(3H)-one (3b)¹



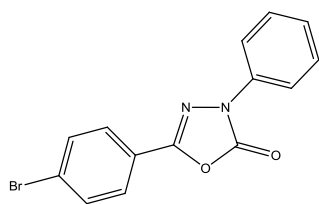
White solid, mp 142–144 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3): δ (ppm) 7.94 (t, $J = 9.5$ Hz, 4H), 7.47 (t, $J = 7.8$ Hz, 2H), 7.28 (t, $J = 8.5$ Hz, 1H), 7.20 (t, $J = 8.4$ Hz, 2H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ (ppm) 165.1 (d, $J = 252.2$ Hz), 153.0, 150.8, 136.2, 129.4, 128.5 (d, $J = 8.9$ Hz), 126.4, 120.0 (d, $J = 3.3$ Hz), 118.5, 116.7 (d, $J = 22.3$ Hz).

5-(4-chlorophenyl)-3-phenyl-1,3,4-oxadiazol-2(3H)-one (3c)¹



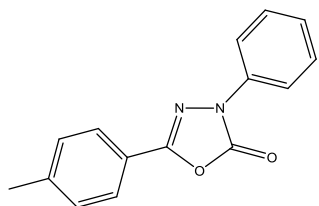
White solid, mp 133–135 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3): δ (ppm) 7.92 (d, $J = 8.1$ Hz, 2H), 7.88 (d, $J = 8.2$ Hz, 2H), 7.47 (dd, $J = 11.0, 8.3$ Hz, 4H), 7.28 (t, $J = 7.5$ Hz, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ (ppm) 153.0, 150.7, 138.5, 136.2, 129.7, 129.5, 127.4, 126.5, 122.1, 118.5.

5-(4-bromophenyl)-3-phenyl-1,3,4-oxadiazol-2(3H)-one (3d)¹



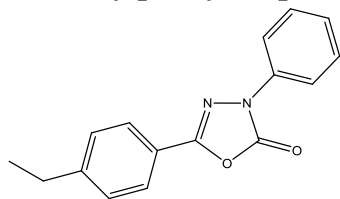
White solid, mp 121–123 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3): δ (ppm) 7.91 (d, $J = 8.0$ Hz, 2H), 7.78 (d, $J = 8.5$ Hz, 2H), 7.63 (d, $J = 8.5$ Hz, 2H), 7.45 (t, $J = 8.0$ Hz, 2H), 7.27 (t, $J = 7.5$ Hz, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ (ppm) 153.0, 150.6, 136.1, 132.6, 129.4, 127.5, 126.9, 126.5, 122.6, 118.5.

3-phenyl-5-(*p*-tolyl)-1,3,4-oxadiazol-2(3*H*)-one (3e)¹



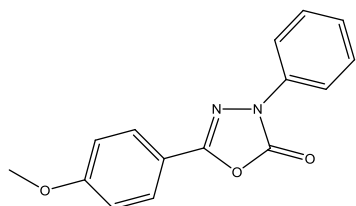
White solid, mp 148–150 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3): δ (ppm) 7.94 (d, $J = 8.2$ Hz, 2H), 7.82 (d, $J = 8.1$ Hz, 2H), 7.46 (t, $J = 7.9$ Hz, 2H), 7.29 (t, $J = 8.0$ Hz, 3H), 2.42 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ (ppm) 154.0, 151.0, 142.8, 136.3, 130.0, 129.4, 126.2, 126.1, 120.9, 118.5, 21.9.

5-(4-ethylphenyl)-3-phenyl-1,3,4-oxadiazol-2(3*H*)-one (3f)¹



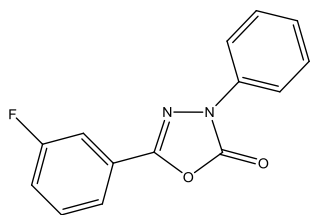
White solid, mp 72–74 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3): δ (ppm) 7.94 – 7.92 (m, 2H), 7.84 – 7.81 (m, 2H), 7.46 – 7.42 (m, 2H), 7.31 – 7.22 (m, 3H), 2.69 (q, $J = 7.6$ Hz, 2H), 1.25 (t, $J = 7.6$ Hz, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ (ppm) 153.9, 150.9, 149.0, 136.3, 129.3, 128.7, 126.2, 126.2, 121.0, 118.4, 29.1, 15.3.

5-(4-methoxyphenyl)-3-phenyl-1,3,4-oxadiazol-2(3*H*)-one (3g)¹



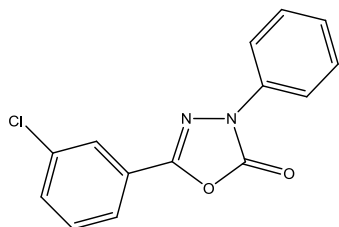
White solid, mp 144–146 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3): δ (ppm) 7.93 (d, $J = 8.1$ Hz, 2H), 7.86 (d, $J = 8.5$ Hz, 2H), 7.45 (t, $J = 7.8$ Hz, 2H), 7.26 (t, $J = 7.4$ Hz, 1H), 6.99 (d, $J = 8.5$ Hz, 2H), 3.86 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ (ppm) 162.7, 153.8, 151.0, 136.4, 129.3, 128.0, 126.1, 118.4, 116.0, 114.7, 55.7.

5-(3-fluorophenyl)-3-phenyl-1,3,4-oxadiazol-2(3*H*)-one (3h)



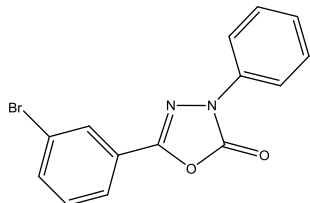
Brown solid, mp 80–82 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3): δ (ppm) 7.89 (d, $J = 8.2$ Hz, 2H), 7.68 (d, $J = 7.7$ Hz, 1H), 7.58 (d, $J = 9.0$ Hz, 1H), 7.44 (dd, $J = 16.3, 8.2$ Hz, 3H), 7.22 (dt, $J = 16.8, 7.8$ Hz, 2H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ (ppm) 162.9 (d, $J = 246.6$ Hz), 152.6, 150.4, 136.0, 131.0 (d, $J = 8.2$ Hz), 129.3, 126.4, 125.5 (d, $J = 8.6$ Hz), 121.8 (d, $J = 3.1$ Hz), 119.1 (d, $J = 21.1$ Hz), 118.3, 113.1 (d, $J = 24.4$ Hz); **HRMS** (ESI) m/z : calcd for $\text{C}_{14}\text{H}_9\text{FN}_2\text{NaO}_2$ $[\text{M}+\text{Na}]^+$, 279.0540, found 279.0544.

5-(3-chlorophenyl)-3-phenyl-1,3,4-oxadiazol-2(3H)-one (3i)⁴



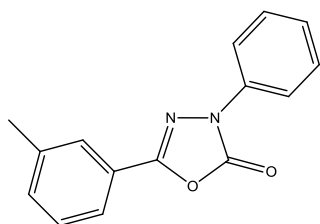
White solid, mp 115–117 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3): δ (ppm) 7.92 – 7.91 (m, 3H), 7.79 (d, $J = 7.6$ Hz, 1H), 7.46 (dq, $J = 11.7, 8.1$ Hz, 4H), 7.28 (d, $J = 7.4$ Hz, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ (ppm) 152.5, 150.5, 136.1, 135.5, 132.2, 130.6, 129.4, 126.5, 126.1, 125.3, 124.2, 118.5.

5-(3-bromophenyl)-3-phenyl-1,3,4-oxadiazol-2(3H)-one (3j)



White solid, mp 88–90 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3): δ (ppm) 8.02 (s, 1H), 7.89 (d, $J = 8.1$ Hz, 2H), 7.79 (d, $J = 7.8$ Hz, 1H), 7.61 (d, $J = 8.0$ Hz, 1H), 7.43 (t, $J = 7.9$ Hz, 2H), 7.32 (t, $J = 7.9$ Hz, 1H), 7.25 (t, $J = 7.4$ Hz, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ (ppm) 152.2, 150.4, 136.0, 135.0, 130.7, 129.3, 128.9, 126.4, 125.4, 124.5, 123.2, 118.3; **HRMS** (ESI) m/z : calcd for $\text{C}_{14}\text{H}_9\text{BrN}_2\text{NaO}_2$ $[\text{M}+\text{Na}]^+$, 338.9740, found 338.9742.

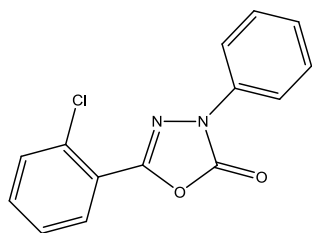
3-phenyl-5-(*m*-tolyl)-1,3,4-oxadiazol-2(3H)-one(3k)¹



White solid, mp 123–125 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3): δ (ppm) 7.94 (d, $J = 8.2$ Hz, 2H), 7.75 – 7.72 (m, 2H), 7.46 (t, $J = 7.8$ Hz, 2H), 7.38 – 7.33 (m, 2H), 7.29 –

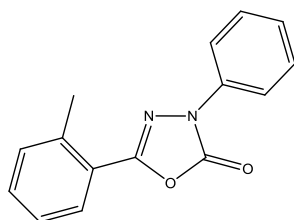
7.25 (m, 1H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 153.9, 150.9, 139.2, 136.3, 133.0, 129.4, 129.1, 126.6, 126.3, 123.5, 123.4, 118.5, 21.5

5-(2-chlorophenyl)-3-phenyl-1,3,4-oxadiazol-2(3H)-one (3l)²



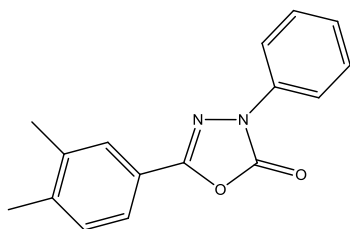
White solid, mp 116–118 °C; ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.95 (d, $J = 8.1$ Hz, 2H), 7.88 (d, $J = 7.7$ Hz, 1H), 7.54 (d, $J = 7.9$ Hz, 1H), 7.46 (t, $J = 5.8$ Hz, 3H), 7.41 – 7.38 (m, 1H), 7.28 (t, $J = 7.7$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 151.8, 150.4, 136.1, 133.1, 132.6, 131.7, 130.2, 129.4, 127.2, 126.4, 122.4, 118.5.

3-phenyl-5-(*o*-tolyl)-1,3,4-oxadiazol-2(3H)-one (3m)²



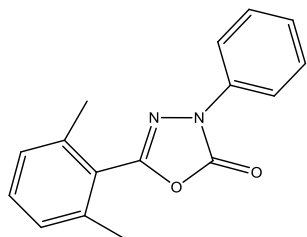
White solid, mp 96–98 °C; ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.95 (d, $J = 8.3$ Hz, 2H), 7.87 (d, $J = 7.9$ Hz, 1H), 7.49 – 7.40 (m, 3H), 7.34 – 7.28 (m, 3H), 2.70 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 154.1, 150.6, 138.3, 136.4, 132.1, 131.6, 129.4, 128.4, 126.5, 126.3, 122.4, 118.4, 22.4.

5-(3,4-dimethylphenyl)-3-phenyl-1,3,4-oxadiazol-2(3H)-one (3n)



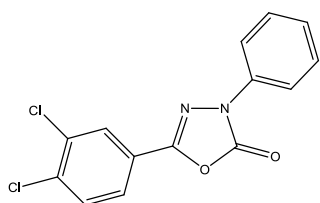
White solid, mp 119–121 °C; ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.90 (d, $J = 8.2$ Hz, 2H), 7.63 (s, 1H), 7.58 (d, $J = 7.8$ Hz, 1H), 7.41 (t, $J = 7.9$ Hz, 2H), 7.22 (t, $J = 7.4$ Hz, 1H), 7.17 (d, $J = 7.8$ Hz, 1H), 2.25 (d, $J = 6.7$ Hz, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 153.8, 150.7, 141.4, 137.6, 136.3, 130.3, 129.2, 126.9, 126.0, 123.6, 121.0, 118.2, 20.0, 19.8; HRMS (ESI) m/z : calcd for $\text{C}_{16}\text{H}_{14}\text{N}_2\text{NaO}_2$ [$\text{M}+\text{Na}$] $^+$, 289.0947, found 289.0951.

5-(2,6-dimethylphenyl)-3-phenyl-1,3,4-oxadiazol-2(3H)-one (3o)



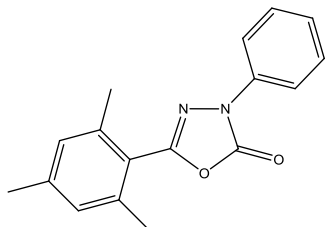
White solid, mp 79–81 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3): δ (ppm) 7.96 – 7.93 (m, 2H), 7.47 – 7.43 (m, 2H), 7.32 – 7.24 (m, 2H), 7.13 (d, $J = 7.6$ Hz, 2H), 2.41 (s, 6H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ (ppm) 153.6, 151.2, 139.1, 136.3, 131.3, 129.4, 128.4, 126.2, 123.5, 118.4, 20.6; **HRMS** (ESI) m/z : calcd for $\text{C}_{16}\text{H}_{14}\text{N}_2\text{NaO}_2$ $[\text{M}+\text{Na}]^+$, 289.0947, found 289.0950.

5-(3,4-dichlorophenyl)-3-phenyl-1,3,4-oxadiazol-2(3H)-one (3p)



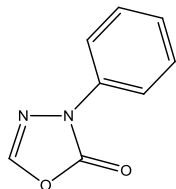
Brown solid, mp 145–147 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3): δ (ppm) 8.00 (d, $J = 1.7$ Hz, 1H), 7.90 (d, $J = 8.0$ Hz, 2H), 7.73 (dd, $J = 8.4, 1.6$ Hz, 1H), 7.57 (d, $J = 8.4$ Hz, 1H), 7.45 (t, $J = 7.9$ Hz, 2H), 7.28 (t, $J = 7.5$ Hz, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ (ppm) 151.9, 150.4, 136.7, 136.0, 134.0, 131.5, 129.5, 127.9, 126.6, 125.1, 123.4, 118.5; **HRMS** (ESI) m/z : calcd for $\text{C}_{14}\text{H}_8\text{Cl}_2\text{N}_2\text{NaO}_2$ $[\text{M}+\text{Na}]^+$, 328.9855, found 328.9853.

5-mesityl-3-phenyl-1,3,4-oxadiazol-2(3H)-one (3q)²



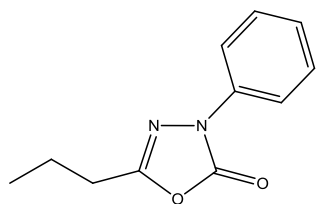
White solid, mp 62–64 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3): δ (ppm) 7.94 (d, $J = 8.4$ Hz, 2H), 7.45 (t, $J = 7.9$ Hz, 2H), 7.26 (t, $J = 7.4$ Hz, 1H), 6.96 (s, 2H), 2.39 (s, 6H), 2.33 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ (ppm) 153.9, 151.3, 141.6, 139.0, 136.4, 129.4, 129.3, 126.2, 120.7, 118.4, 21.4, 20.6.

3-phenyl-1,3,4-oxadiazol-2(3H)-one (3r)



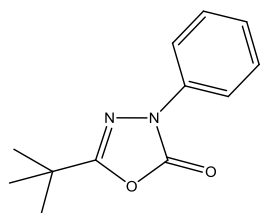
Brown solid, mp 69–71 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3): δ (ppm) 7.85 (d, $J = 7.9$ Hz, 2H), 7.71 (s, 1H), 7.45 (t, $J = 7.7$ Hz, 2H), 7.28 (t, $J = 7.5$ Hz, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ (ppm) 150.5, 144.1, 135.9, 129.4, 126.6, 118.5; **HRMS** (ESI) m/z : calcd for $\text{C}_8\text{H}_6\text{N}_2\text{NaO}_2$ $[\text{M}+\text{Na}]^+$, 185.0321, found 185.0316.

3-phenyl-5-propyl-1,3,4-oxadiazol-2(3H)-one (3s)



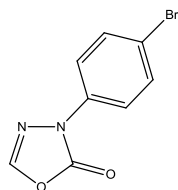
Brown solid, mp 59–61 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3): δ (ppm) 7.84 (d, $J = 8.4$ Hz, 2H), 7.43 (t, $J = 8.0$ Hz, 2H), 7.26 – 7.22 (m, 1H), 2.62 (t, $J = 7.4$ Hz, 2H), 1.80 (dd, $J = 14.8, 7.4$ Hz, 2H), 1.05 (t, $J = 7.4$ Hz, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ (ppm) 157.0, 151.4, 136.3, 129.4, 126.1, 118.3, 28.4, 19.2, 13.6; **HRMS** (ESI) m/z : calcd for $\text{C}_{11}\text{H}_{12}\text{N}_2\text{NaO}_2$ $[\text{M}+\text{Na}]^+$, 227.0791, found 227.0793.

5-(*tert*-butyl)-3-phenyl-1,3,4-oxadiazol-2(3H)-one (3t)³



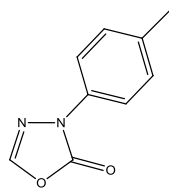
Light yellow oil; $^1\text{H NMR}$ (400 MHz, CDCl_3): δ (ppm) 7.86 (d, $J = 8.3$ Hz, 2H), 7.42 (t, $J = 7.9$ Hz, 2H), 7.23 (t, $J = 7.4$ Hz, 1H), 1.37 (s, 9H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ (ppm) 162.9, 151.5, 136.3, 129.3, 126.0, 118.3, 33.0, 27.2.

3-(4-bromophenyl)-1,3,4-oxadiazol-2(3H)-one (3v)⁴



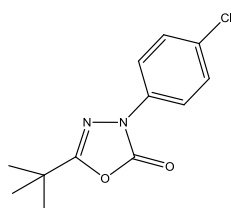
Brown solid, mp 114–116 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3): δ (ppm) 7.78 – 7.71 (m, 3H), 7.56 (d, $J = 8.3$ Hz, 2H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ (ppm) 150.1, 144.2, 135.0, 132.5, 119.9, 119.8.

3-(*p*-tolyl)-1,3,4-oxadiazol-2(3H)-one (3w)⁴



Brown solid, mp 83–85 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3): δ (ppm) 7.70 (d, $J = 7.5$ Hz, 3H), 7.23 (d, $J = 8.1$ Hz, 2H), 2.36 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ (ppm) 150.5, 143.9, 136.5, 133.4, 129.9, 118.5, 21.1.

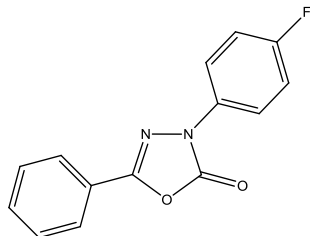
5-(*tert*-butyl)-3-(4-chlorophenyl)-1,3,4-oxadiazol-2(3H)-one (3x)



Light Yellow oil; $^1\text{H NMR}$ (400 MHz, CDCl_3): δ (ppm) 7.83 (d, $J = 8.5$ Hz,

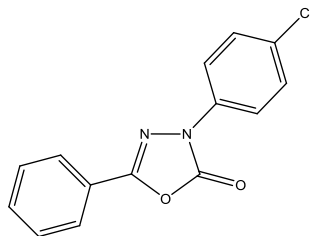
2H), 7.39 (d, $J = 8.6$ Hz, 2H), 1.38 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 163.2, 151.3, 134.9, 131.4, 129.4, 119.5, 33.1, 27.2; HRMS (ESI) m/z : calcd for $\text{C}_{12}\text{H}_{14}\text{ClN}_2\text{O}_2$ $[\text{M}+\text{H}]^+$, 253.0738, found 253.0733.

3-(4-fluorophenyl)-5-phenyl-1,3,4-oxadiazol-2(3H)-one (4a)¹



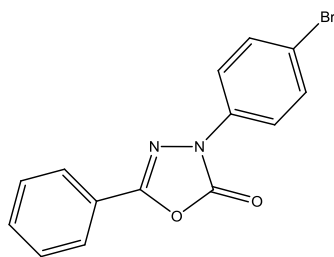
White solid, mp 145–147 °C; ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.92 (t, $J = 7.1$ Hz, 4H), 7.53 (dq, $J = 14.9, 7.5$ Hz, 3H), 7.16 (t, $J = 7.9$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 160.8 (d, $J = 244.7$ Hz), 153.9, 150.9, 132.4 (d, $J = 2.9$ Hz), 132.3, 129.3, 126.2, 123.6, 120.4 (d, $J = 8.1$ Hz), 116.3 (d, $J = 22.8$ Hz).

3-(4-chlorophenyl)-5-phenyl-1,3,4-oxadiazol-2(3H)-one (4b)¹



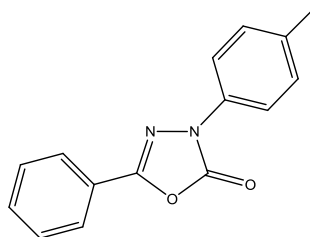
White solid, mp 141–143 °C; ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.92 (t, $J = 8.4$ Hz, 4H), 7.56 – 7.49 (m, 3H), 7.43 (d, $J = 7.9$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 153.9, 150.7, 134.8, 132.4, 131.7, 129.5, 129.3, 126.2, 123.4, 119.6.

3-(4-bromophenyl)-5-phenyl-1,3,4-oxadiazol-2(3H)-one (4c)²



White solid, mp 132–135 °C; ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.92 (d, $J = 7.2$ Hz, 2H), 7.84 (d, $J = 7.5$ Hz, 2H), 7.57 – 7.48 (m, 5H); ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 153.9, 150.6, 135.3, 132.4, 132.3, 129.3, 126.2, 123.4, 119.9, 119.5.

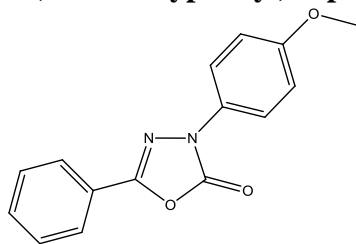
5-phenyl-3-(*p*-tolyl)-1,3,4-oxadiazol-2(3H)-one (4d)³



White solid, mp 155–157 °C; ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.92 (d, $J = 7.0$ Hz, 2H), 7.80 (d, $J = 8.1$ Hz, 2H), 7.53 – 7.47 (m, 3H), 7.25 (d, $J = 7.9$ Hz, 2H),

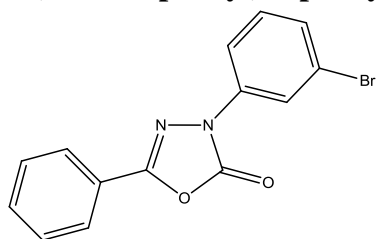
2.37 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 153.6, 150.9, 136.2, 133.8, 132.0, 129.9, 129.2, 126.1, 123.7, 118.6, 21.1.

3-(4-methoxyphenyl)-5-phenyl-1,3,4-oxadiazol-2(3H)-one (4e)³



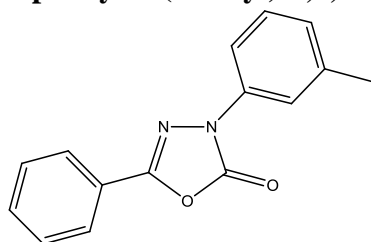
White solid, mp 135–137 °C; ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.92 (d, $J = 7.3$ Hz, 2H), 7.81 (d, $J = 8.4$ Hz, 2H), 7.53 – 7.47 (m, 3H), 6.98 (d, $J = 8.4$ Hz, 2H), 3.83 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 158.1, 153.6, 151.1, 132.0, 129.5, 129.2, 126.1, 123.7, 120.5, 114.5, 55.7.

3-(3-bromophenyl)-5-phenyl-1,3,4-oxadiazol-2(3H)-one (4f)⁵



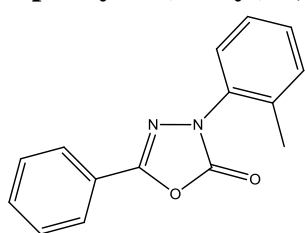
White solid, mp 128–130 °C; ^1H NMR (400 MHz, CDCl_3): δ (ppm) 8.13 (s, 1H), 7.94 (d, $J = 7.7$ Hz, 3H), 7.58 – 7.49 (m, 3H), 7.40 (d, $J = 7.8$ Hz, 1H), 7.32 (t, $J = 7.9$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 154.0, 150.5, 137.3, 132.4, 130.7, 129.3, 129.3, 126.3, 123.4, 123.1, 121.3, 116.7.

5-phenyl-3-(*m*-tolyl)-1,3,4-oxadiazol-2(3H)-one (4g)⁵



Brown solid, mp 99–101 °C; ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.95 (d, $J = 7.4$ Hz, 2H), 7.75 (d, $J = 12.5$ Hz, 2H), 7.55 – 7.49 (m, 3H), 7.35 (t, $J = 7.8$ Hz, 1H), 7.09 (d, $J = 7.5$ Hz, 1H), 2.43 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 153.7, 151.0, 139.5, 136.2, 132.1, 129.2, 127.2, 126.2, 123.7, 119.2, 115.8, 21.8.

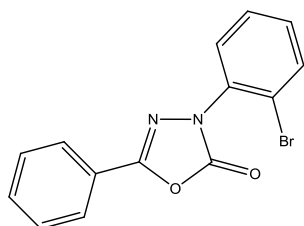
5-phenyl-3-(*o*-tolyl)-1,3,4-oxadiazol-2(3H)-one (4h)⁵



Brown solid, mp 104–106 °C; ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.92 (d, $J = 7.3$ Hz, 2H), 7.54 – 7.48 (m, 3H), 7.44 (d, $J = 7.3$ Hz, 1H), 7.33 (d, $J = 11.5$ Hz, 3H),

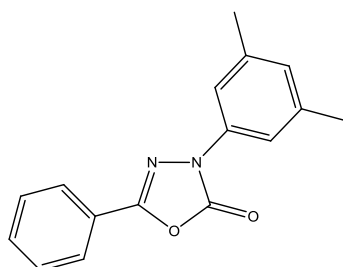
2.39 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 154.2, 152.3, 135.3, 134.0, 132.0, 131.7, 129.7, 129.2, 127.1, 126.7, 126.0, 123.9, 18.3.

3-(2-bromophenyl)-5-phenyl-1,3,4-oxadiazol-2(3H)-one (4i)⁵



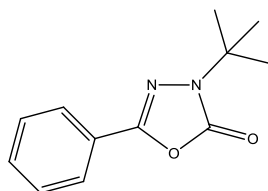
Brown solid, mp 123–125 °C; ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.92 (d, $J = 7.4$ Hz, 2H), 7.74 (d, $J = 8.1$ Hz, 1H), 7.54 – 7.45 (m, 5H), 7.36 (t, $J = 8.0$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 154.4, 151.8, 134.3, 134.2, 132.2, 131.5, 129.5, 129.3, 128.7, 126.1, 123.8, 121.9.

3-(3,5-dimethylphenyl)-5-phenyl-1,3,4-oxadiazol-2(3H)-one (4j)⁵



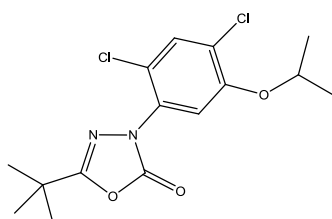
Brown oil; ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.95 (d, $J = 7.4$ Hz, 2H), 7.56 – 7.48 (m, 5H), 6.91 (s, 1H), 2.38 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 153.6, 151.0, 139.3, 136.1, 132.1, 129.2, 128.2, 126.2, 123.8, 116.4, 21.7.

3-(tert-butyl)-5-phenyl-1,3,4-oxadiazol-2(3H)-one (4k)



Light yellow oil; ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.84 (s, 2H), 7.46 (s, 3H), 1.61 (d, $J = 8.3$ Hz, 9H); ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 152.6, 152.1, 131.3, 129.0, 125.7, 124.5, 58.5, 28.1; HRMS (ESI) m/z : calcd for $\text{C}_{12}\text{H}_{14}\text{N}_2\text{NaO}_2$ $[\text{M}+\text{Na}]^+$, 241.0947, found 241.0949.

5-(tert-butyl)-3-(2,4-dichloro-5-isopropoxyphenyl)-1,3,4-oxadiazol-2(3H)-one (5a)³



White solid, mp 84–86 °C; ^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.38 (s, 1H), 7.14 (s, 1H), 4.51 (dd, $J = 11.4, 5.6$ Hz, 1H), 1.34 (d, $J = 5.4$ Hz, 6H), 1.25 (s, 9H);

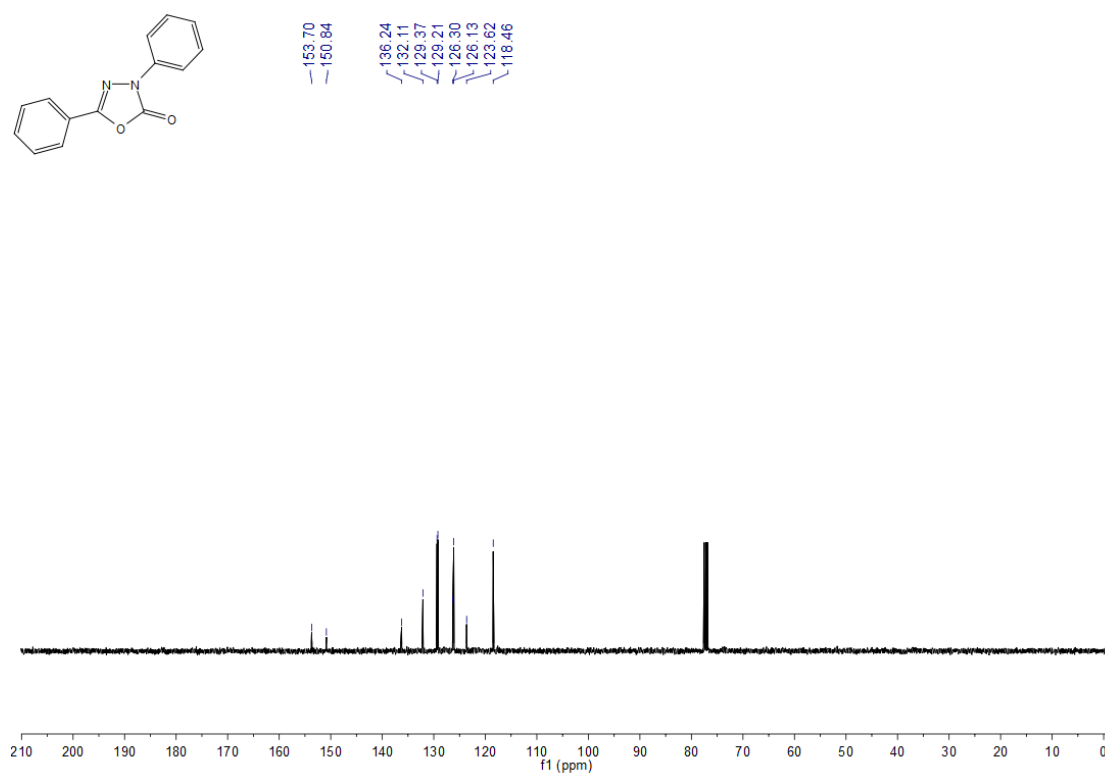
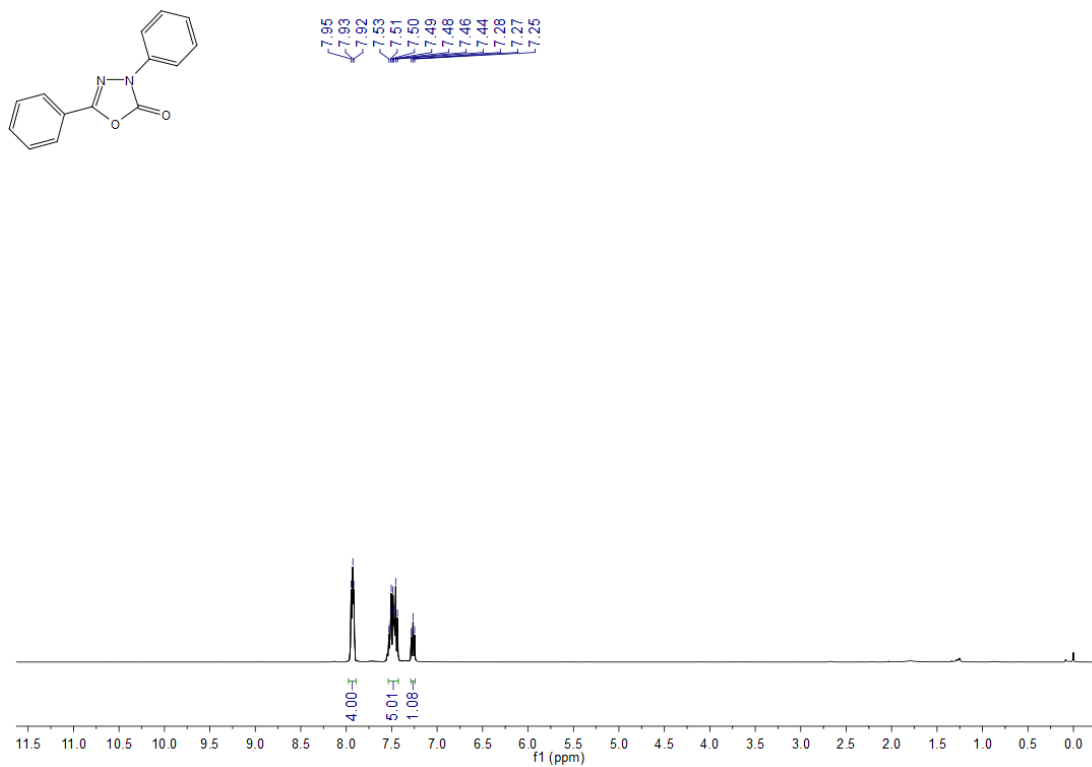
¹³C NMR (100 MHz, CDCl₃): δ (ppm) 178.5, 159.0, 153.1, 140.5, 130.9, 123.0, 121.7, 114.9, 72.4, 38.0, 27.5, 21.9.

3. Reference

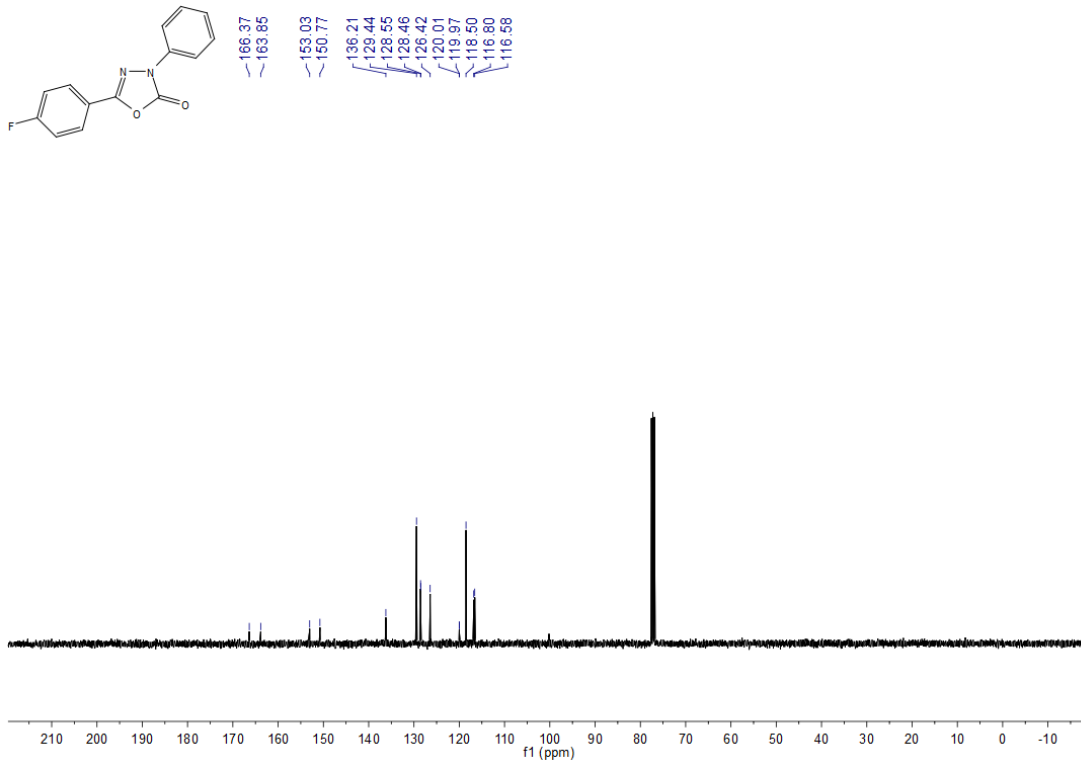
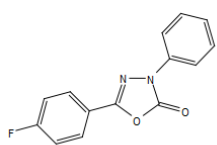
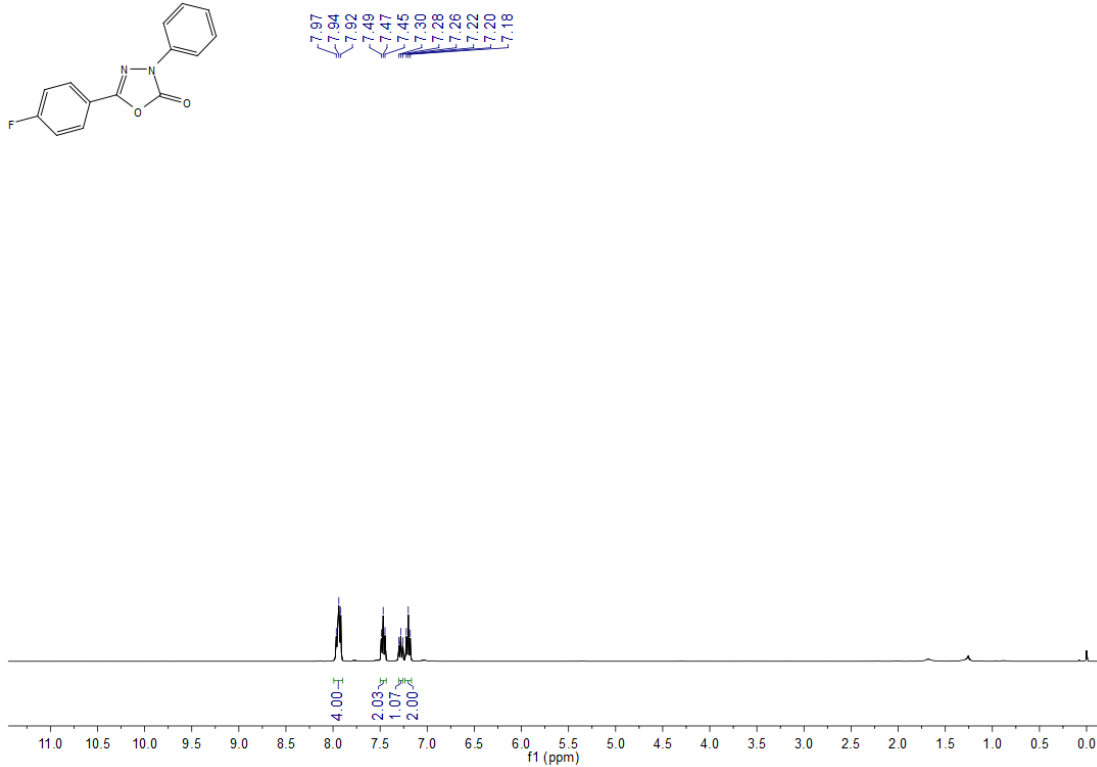
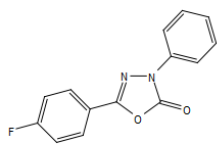
- (1) Y. Wang, X. Meng, Y. T. Yang, L. T. Zhang, S. B. Guo, D. Tang, Y.-X. Li and B. H. Chen, *Chem. Commun.*, 2015, **51**, 1905-1907.
- (2) F. H. Ji, X. W. Li, W. Guo, W. Q. Wu and H. F. Jiang, *J. Org. Chem.*, 2015, **80**, 5713-5718.
- (3) C. X. Guo, W. Z. Zhang, N. Zhang and X. B. Lu, *J. Org. Chem.* 2017, **82**, 7637-7642.
- (4) N. Yang, Q. Lai, H. F. Jiang and G. Q. Yuan, *Electrochem. Commun.* 2016, **72**, 109-112.
- (5) N. Yang, H. Zhang and G. Q. Yuan, *Org. Chem. Front.*, 2019, **6**, 532-536.

4. NMR spectra

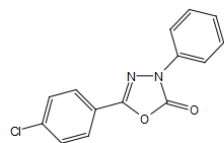
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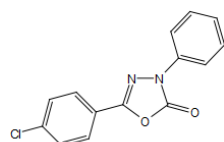
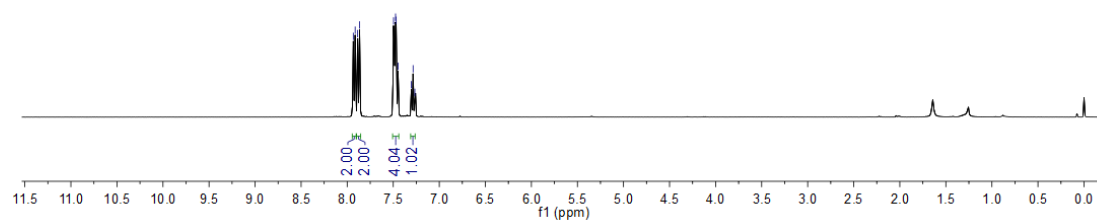
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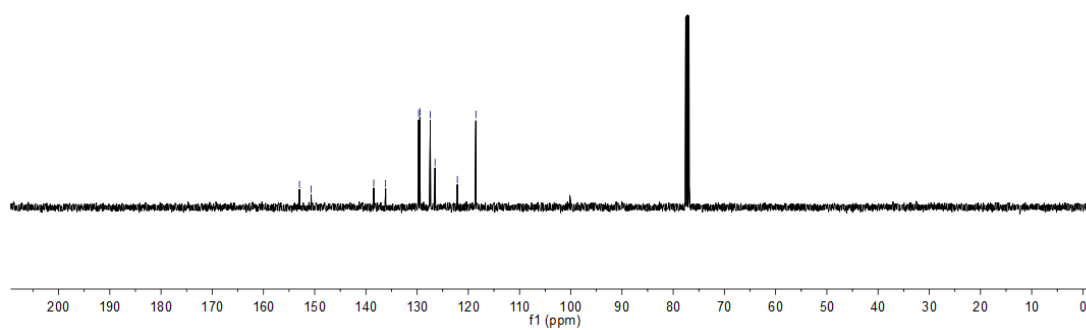
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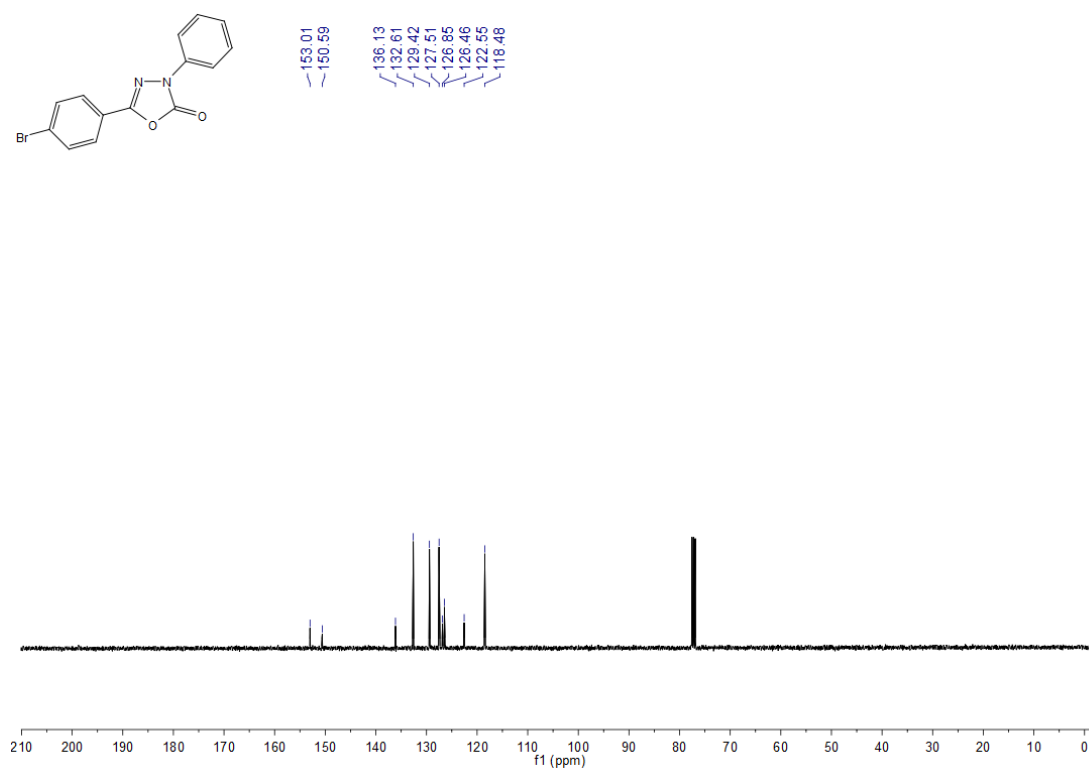
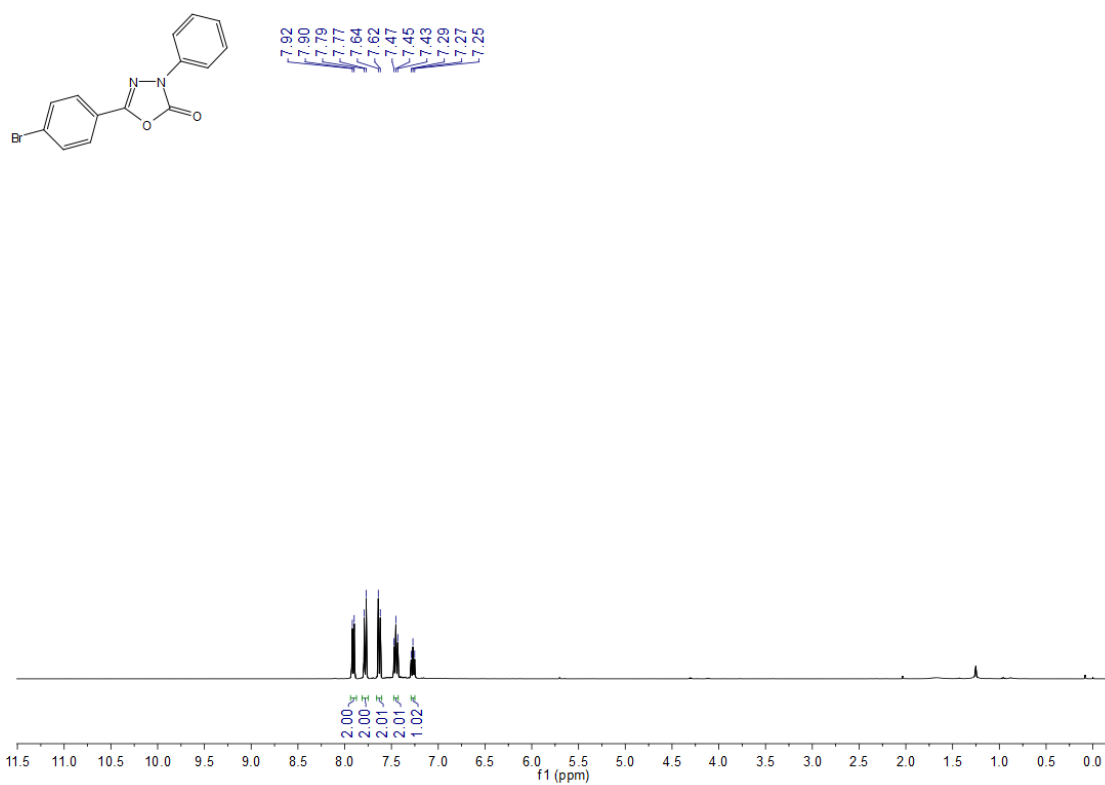
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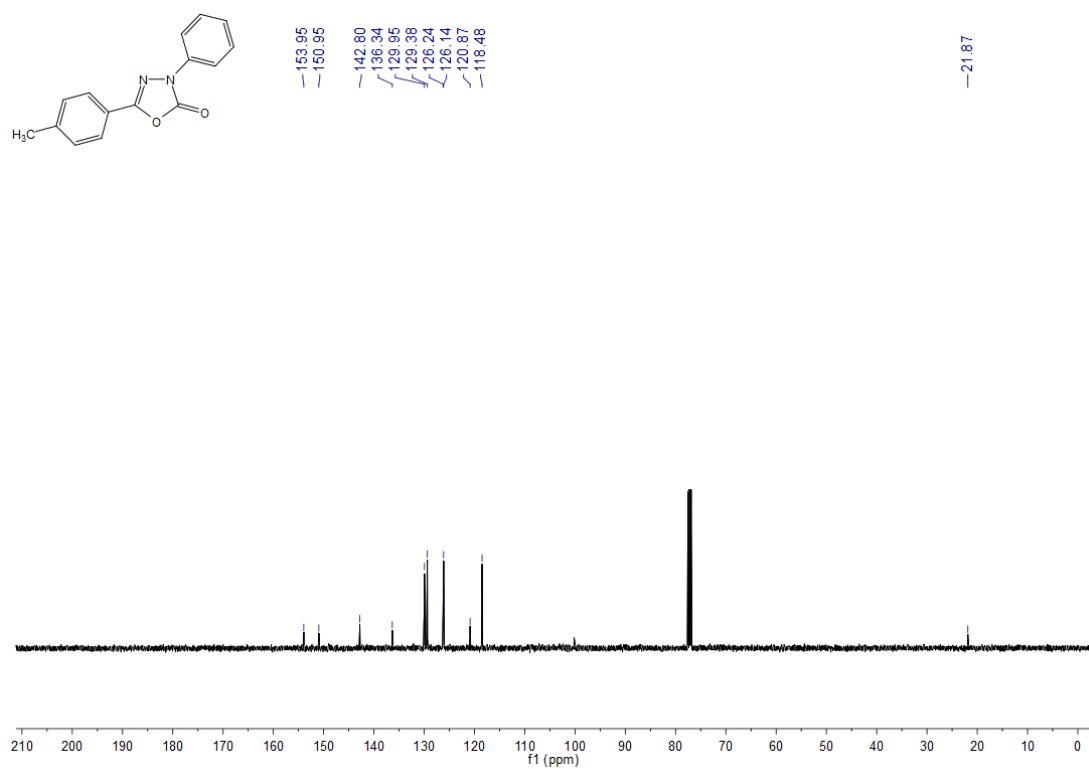
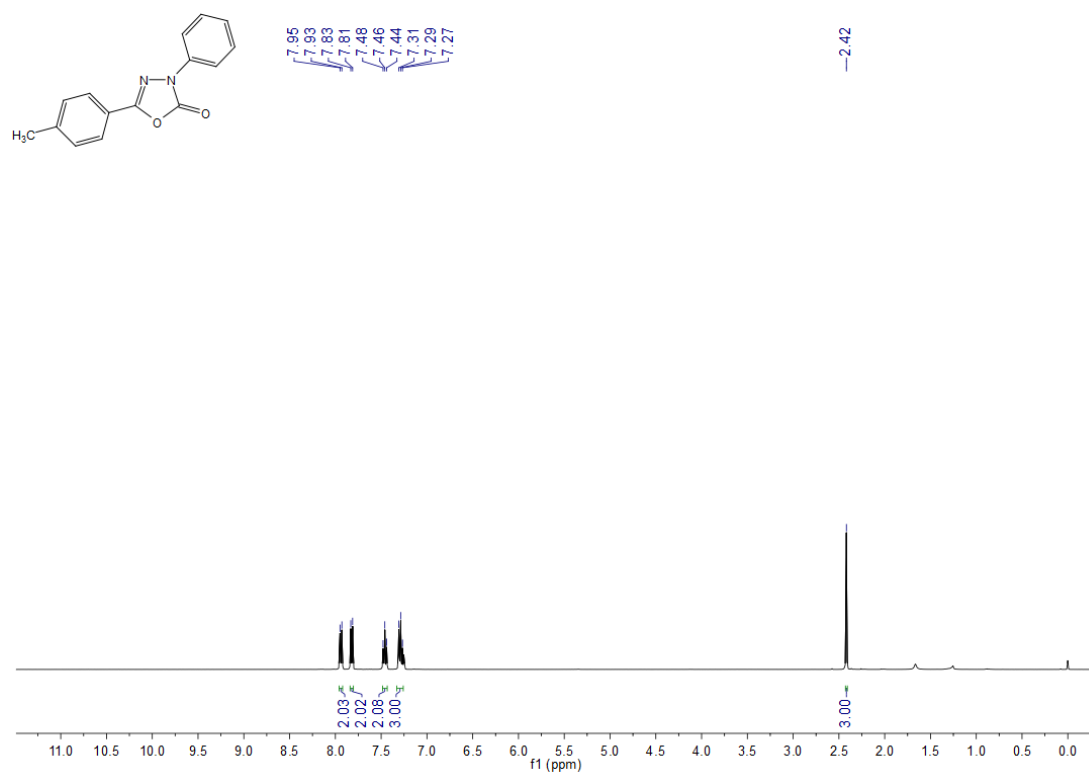
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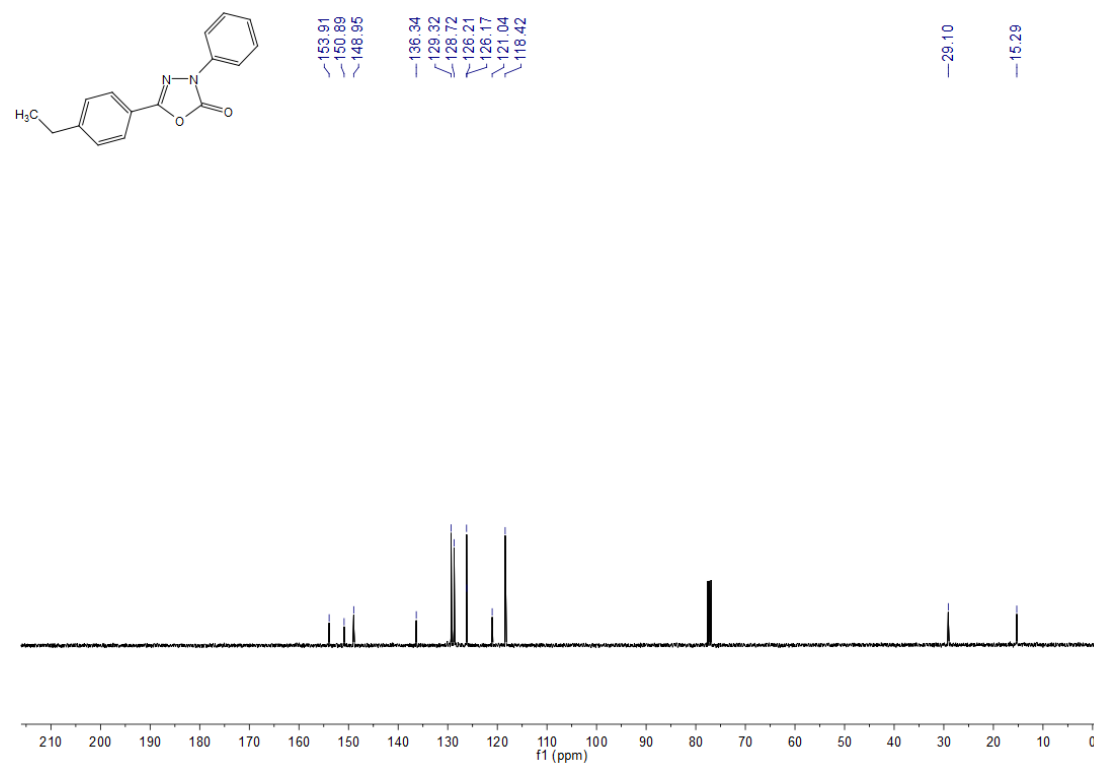
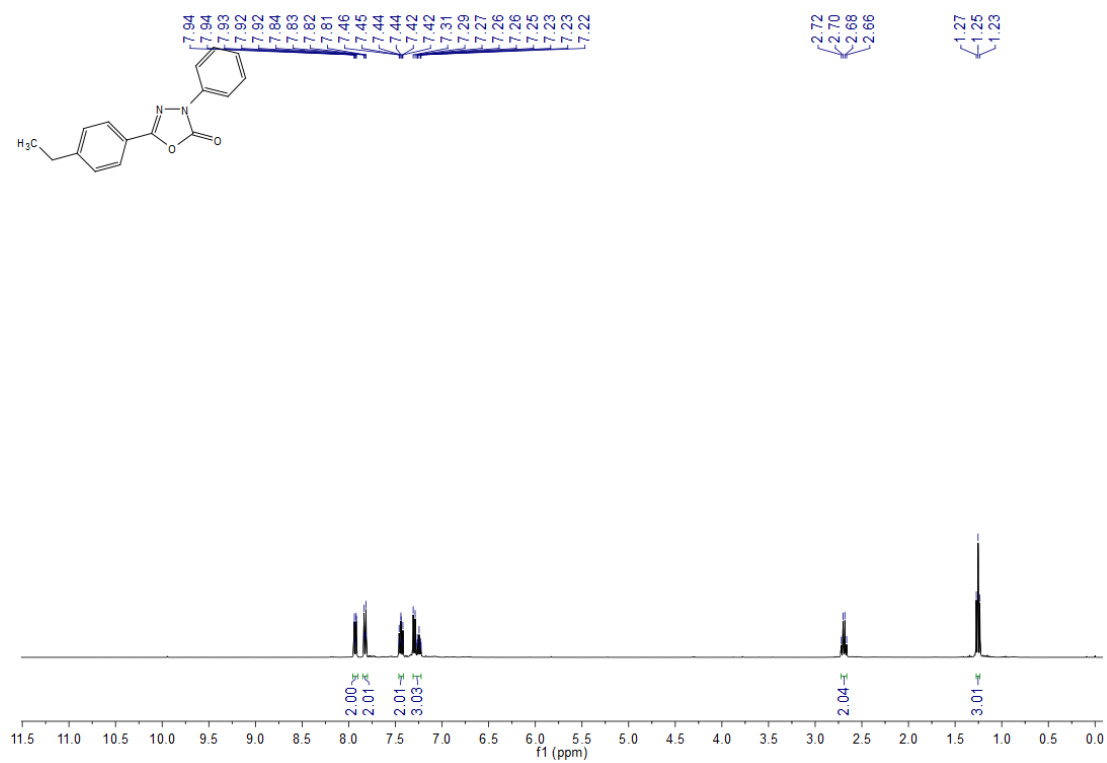
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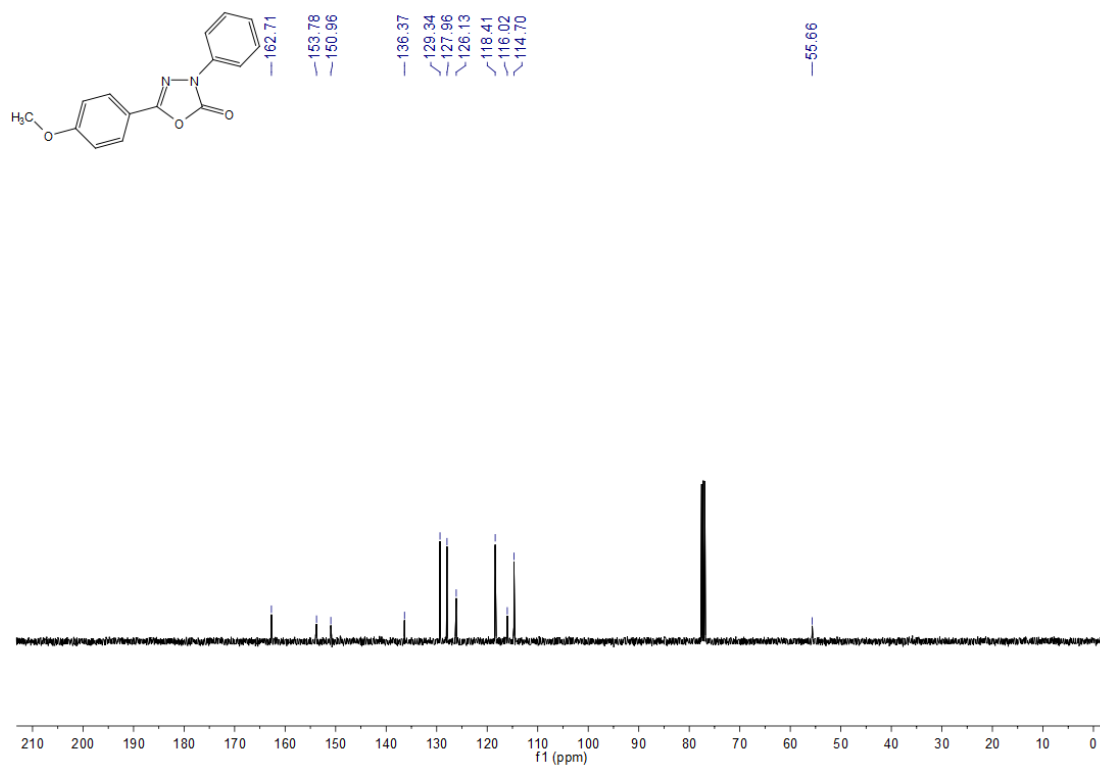
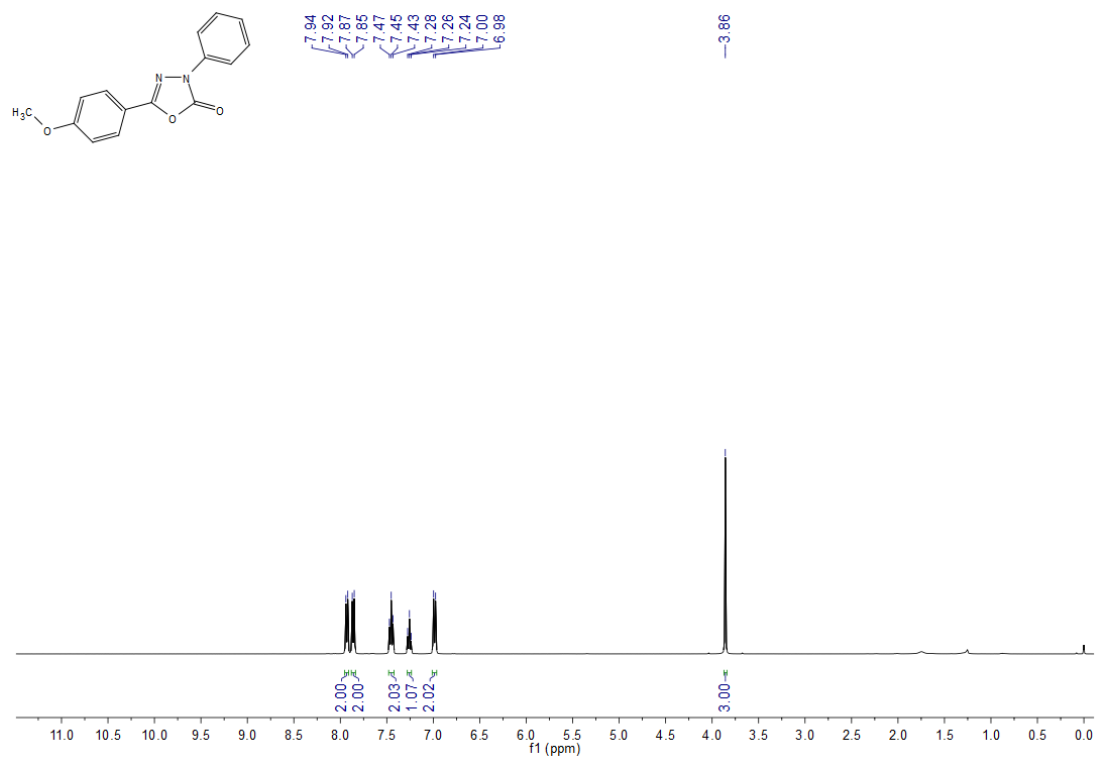
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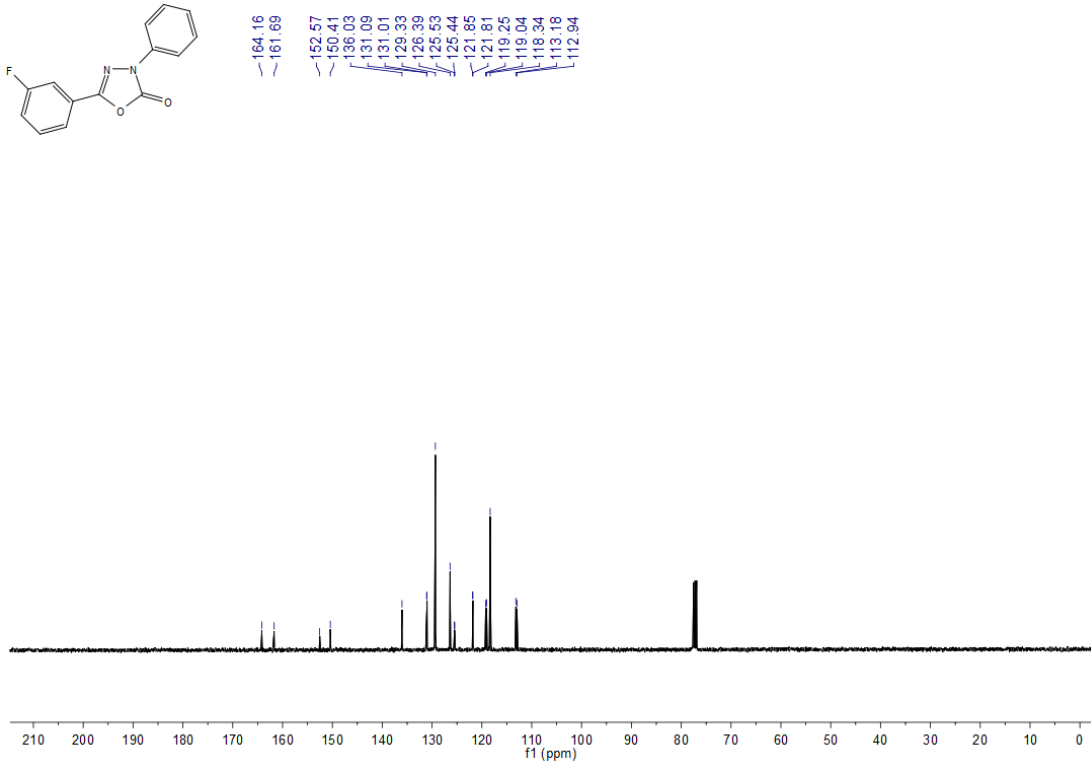
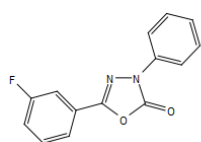
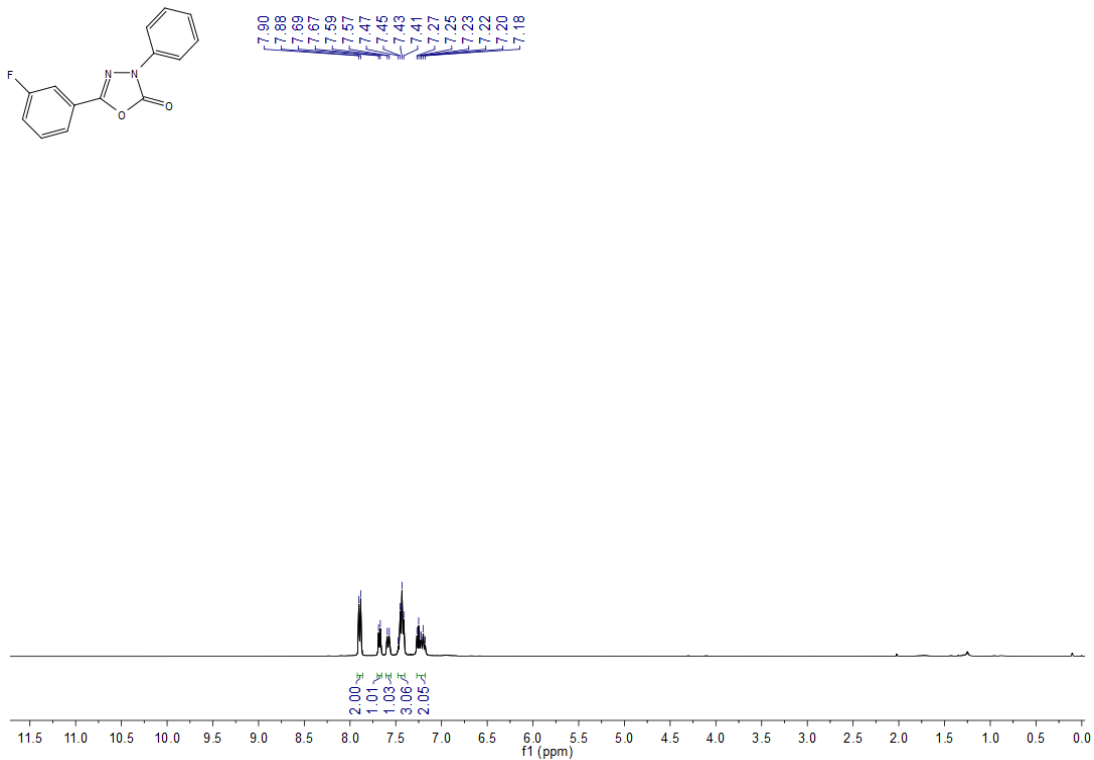
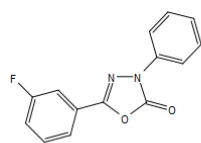
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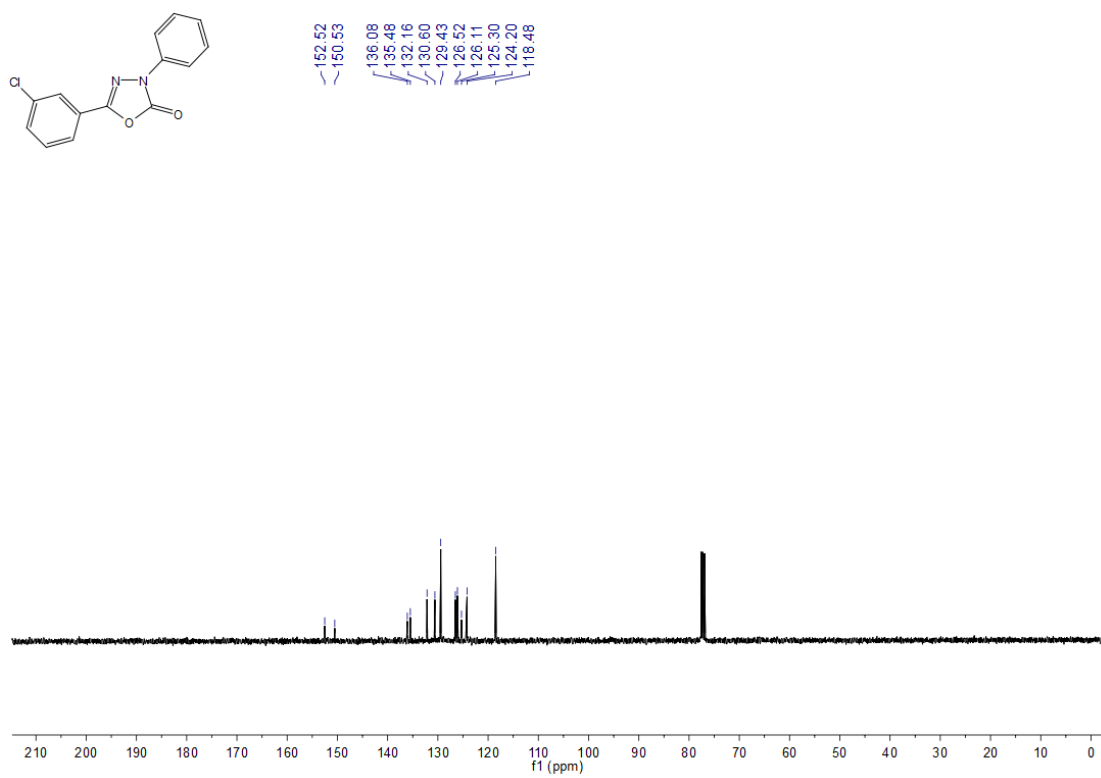
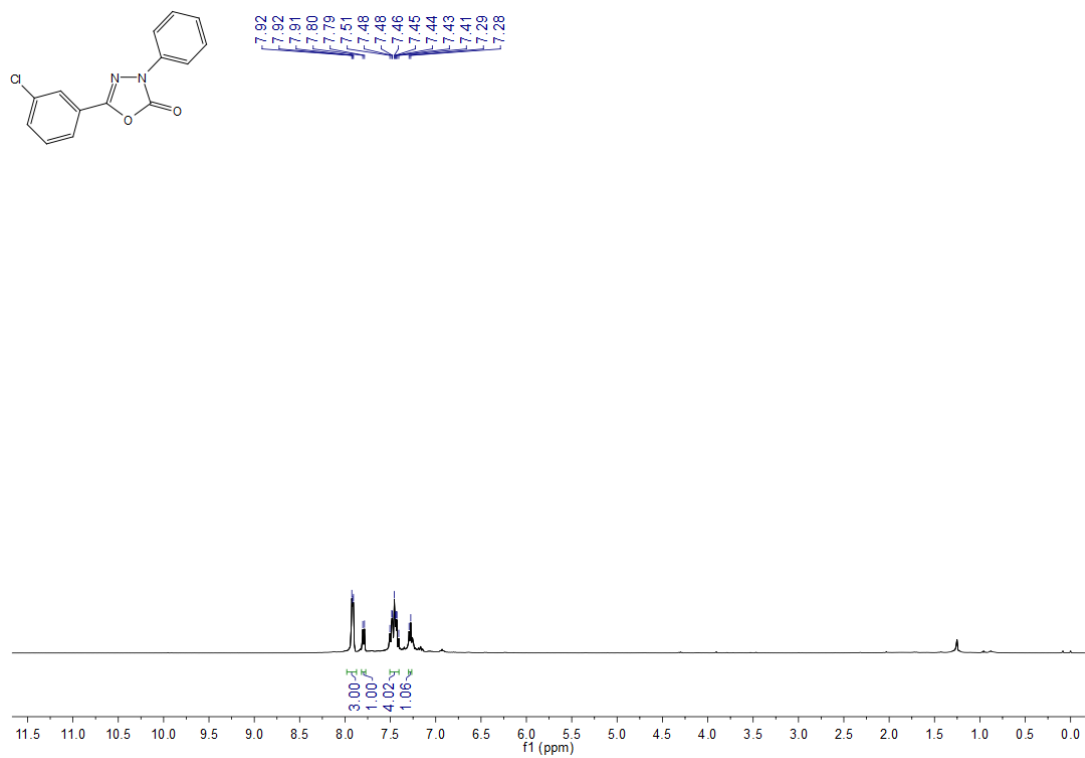
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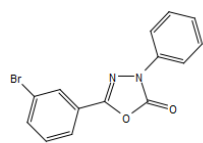
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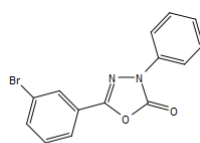
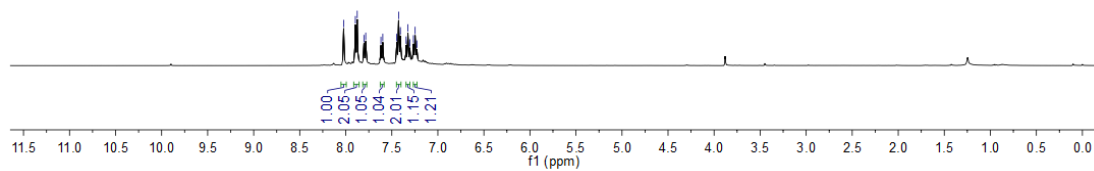
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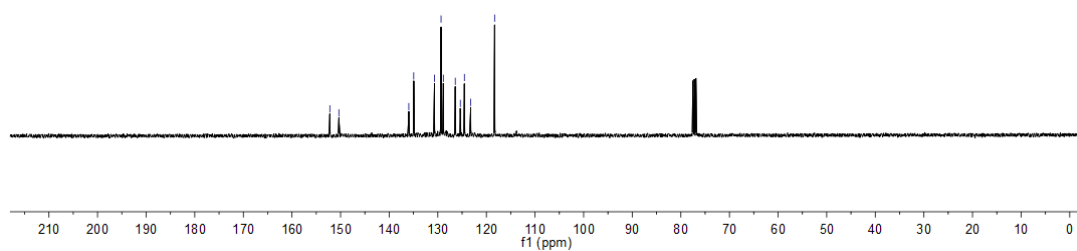
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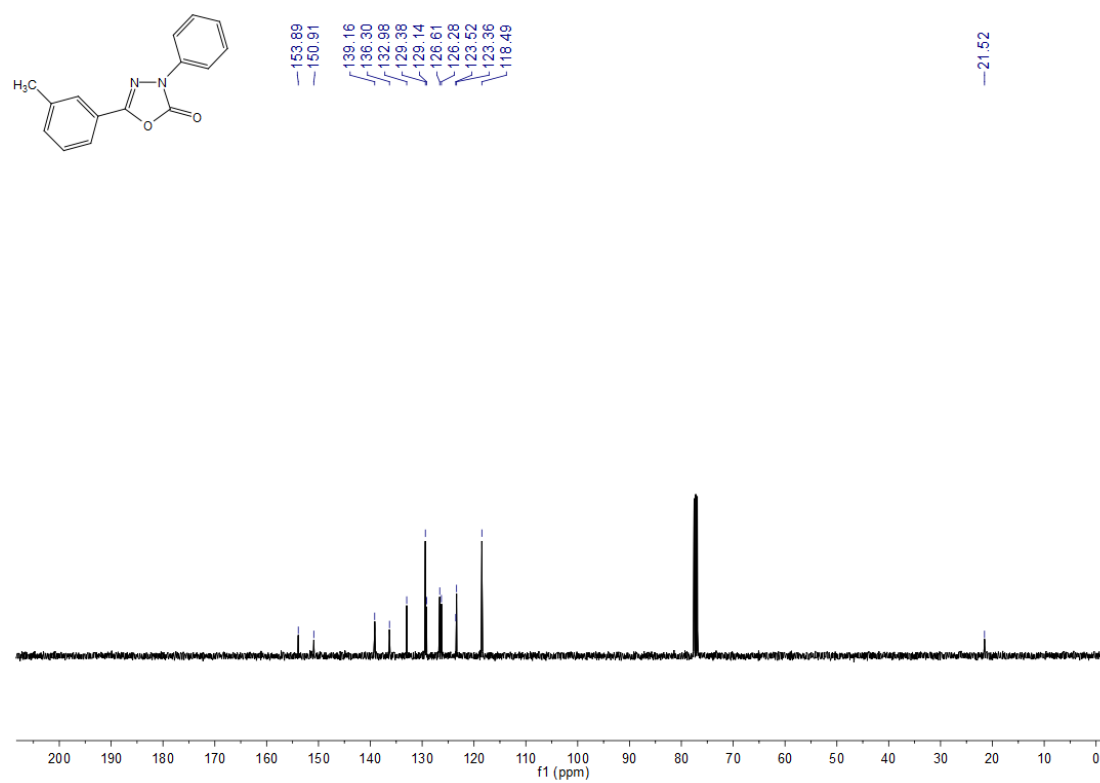
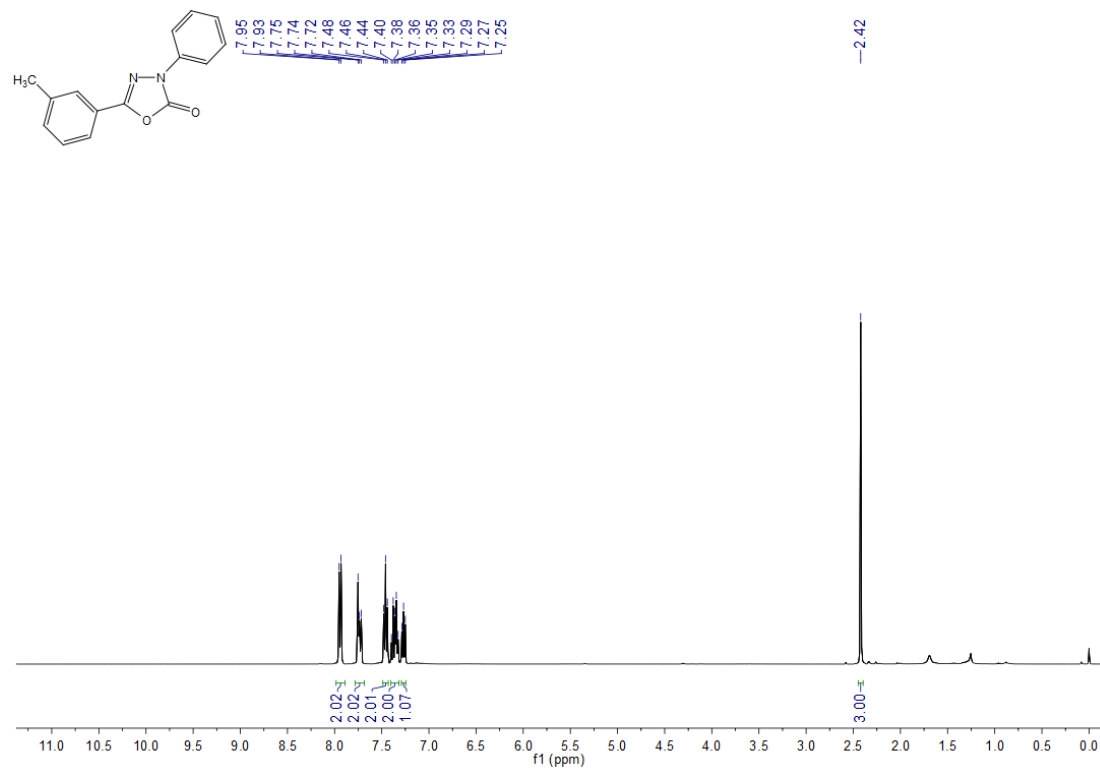
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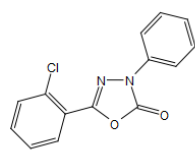
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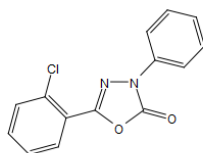
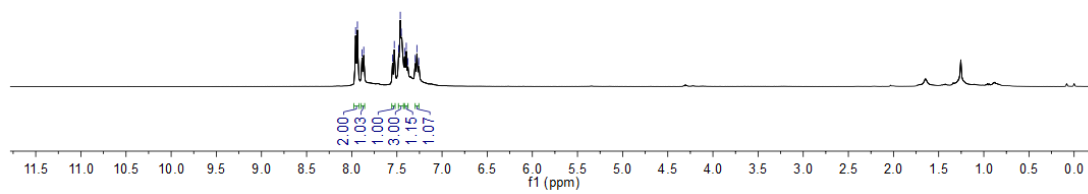
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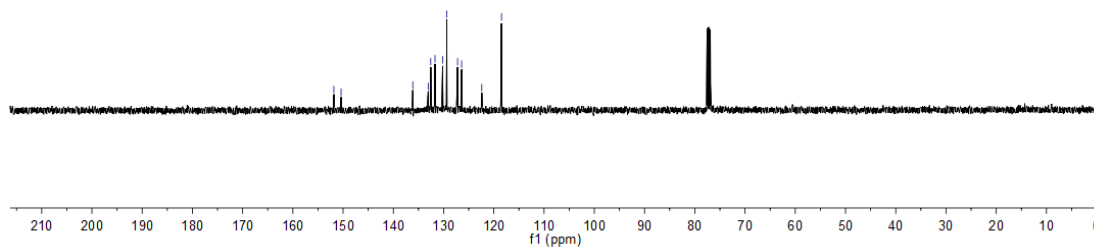
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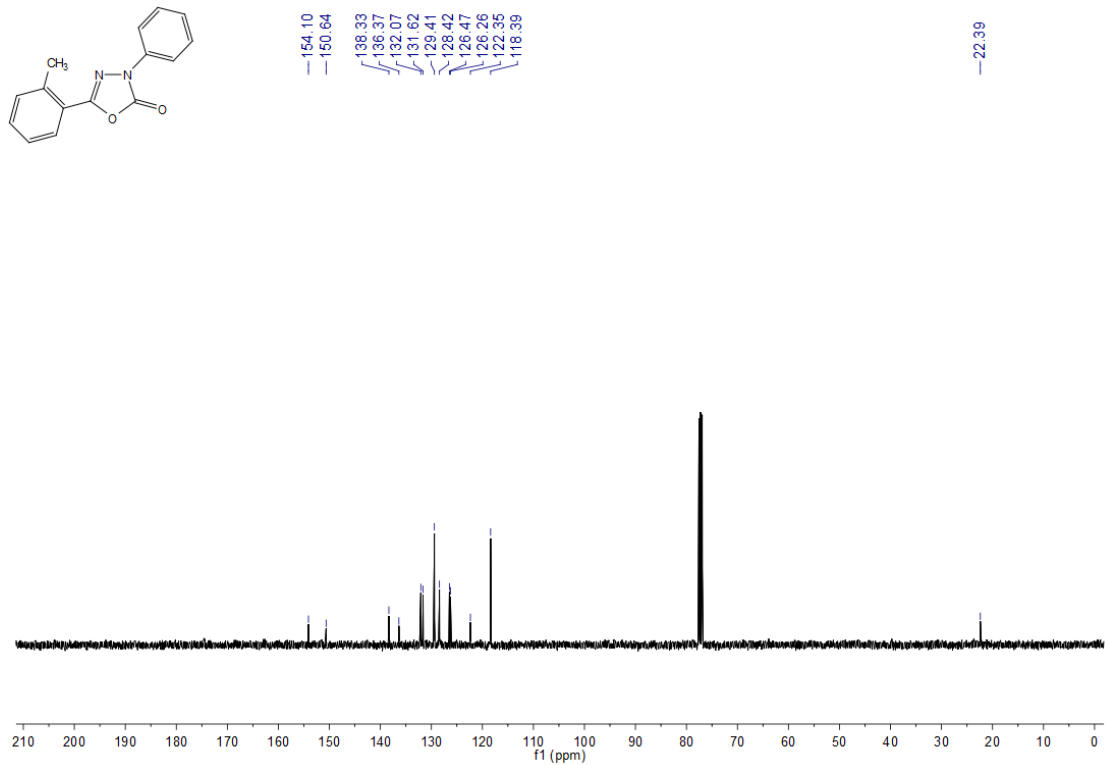
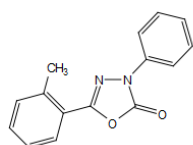
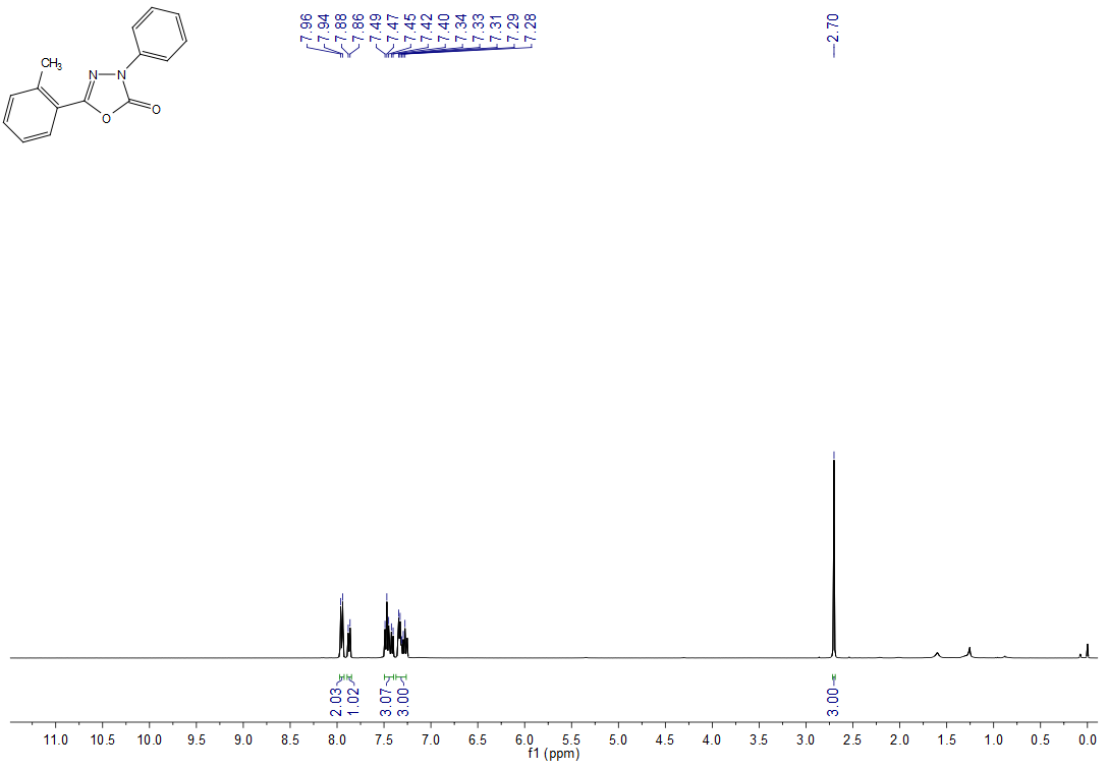
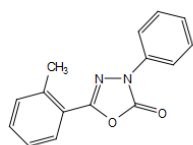
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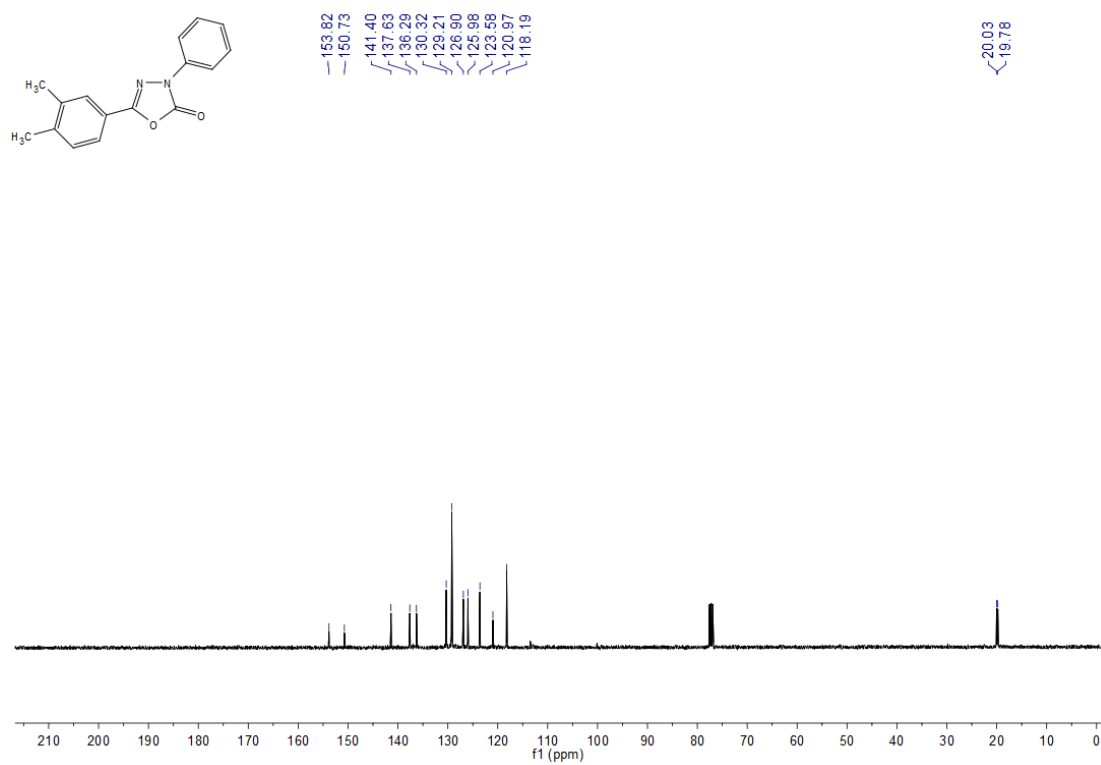
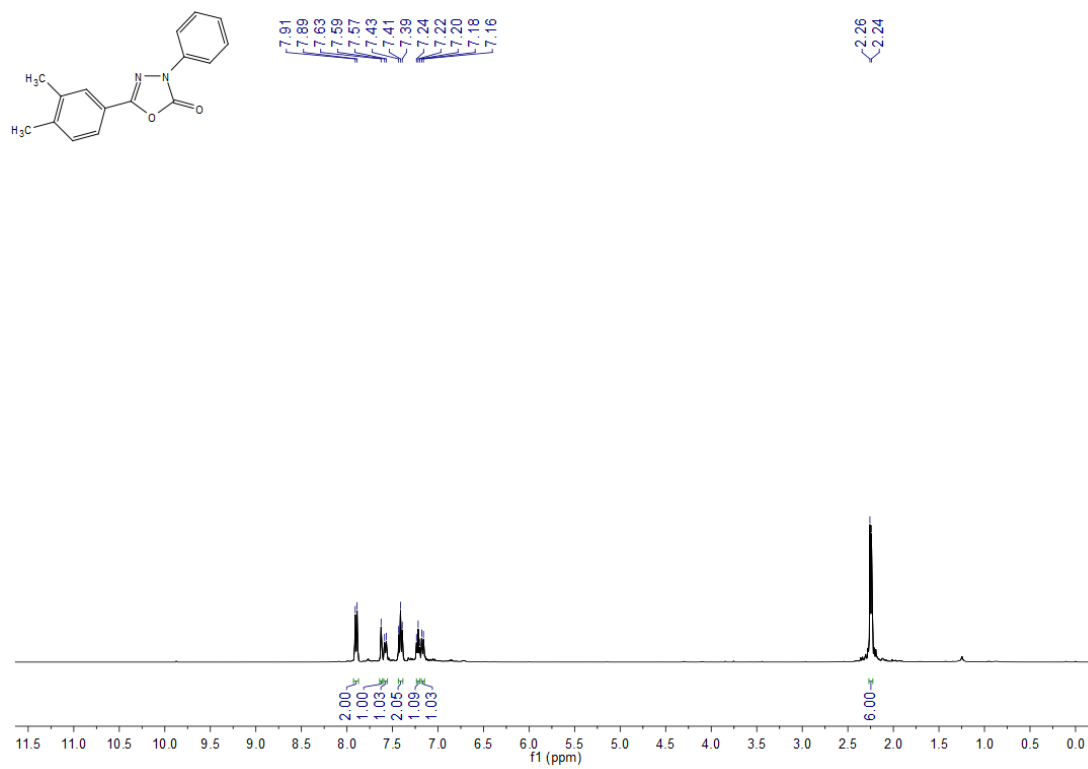
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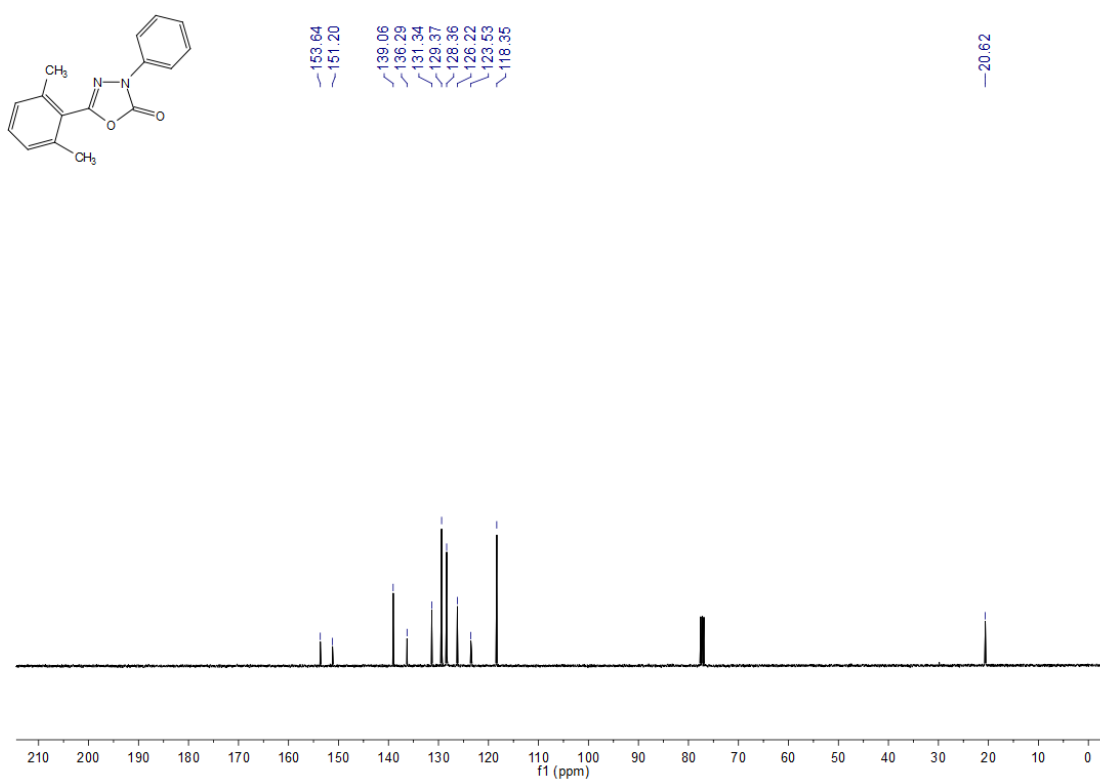
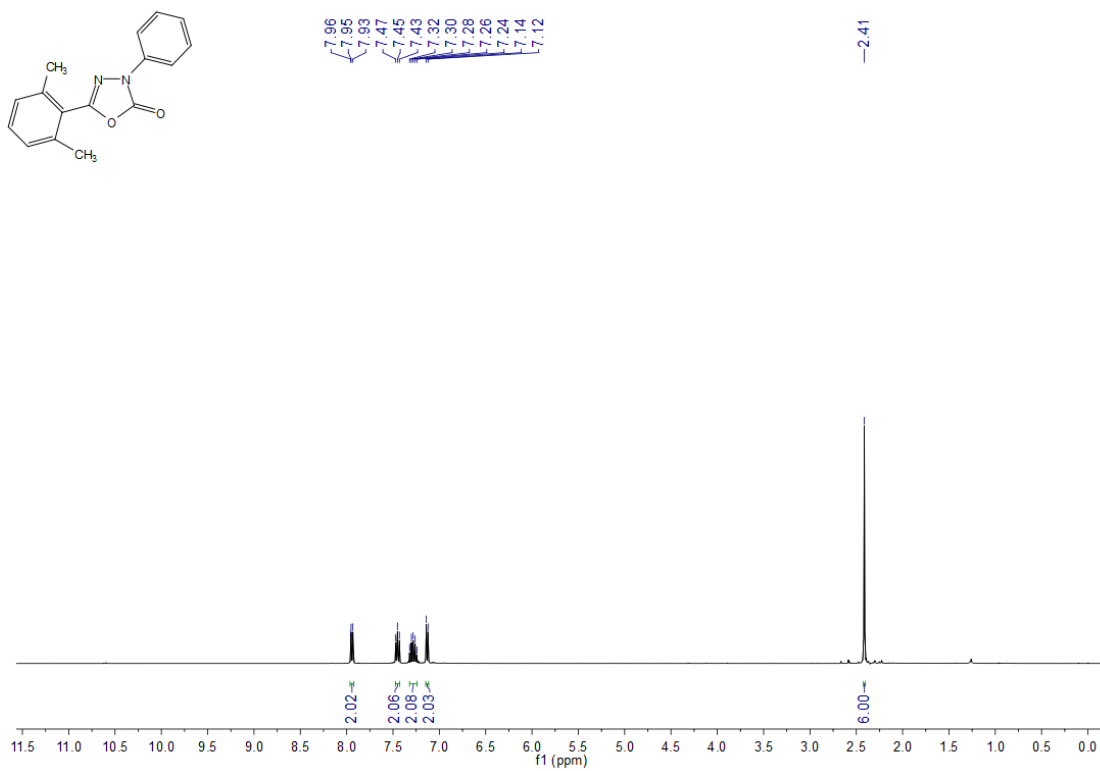
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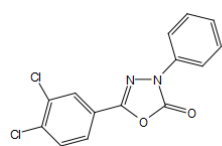
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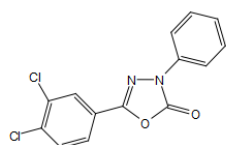
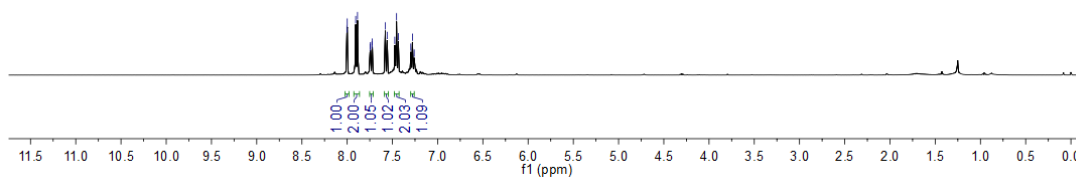
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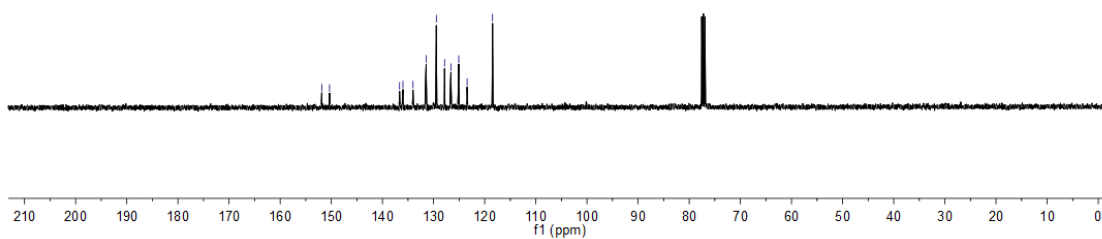
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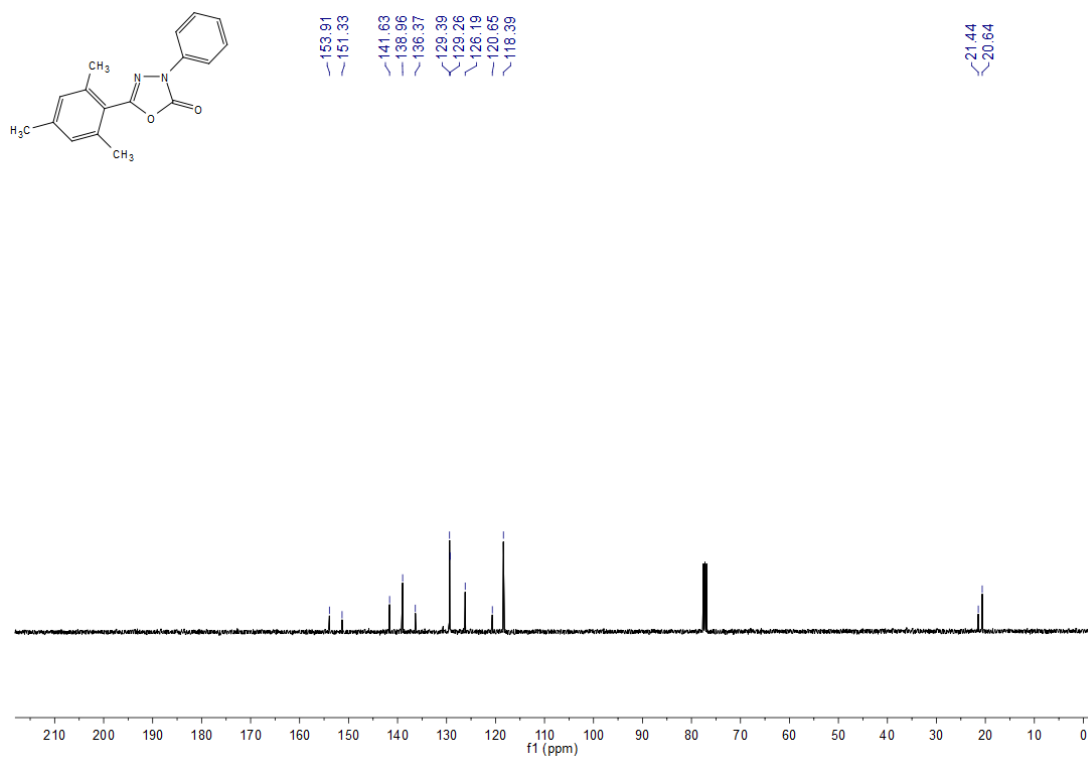
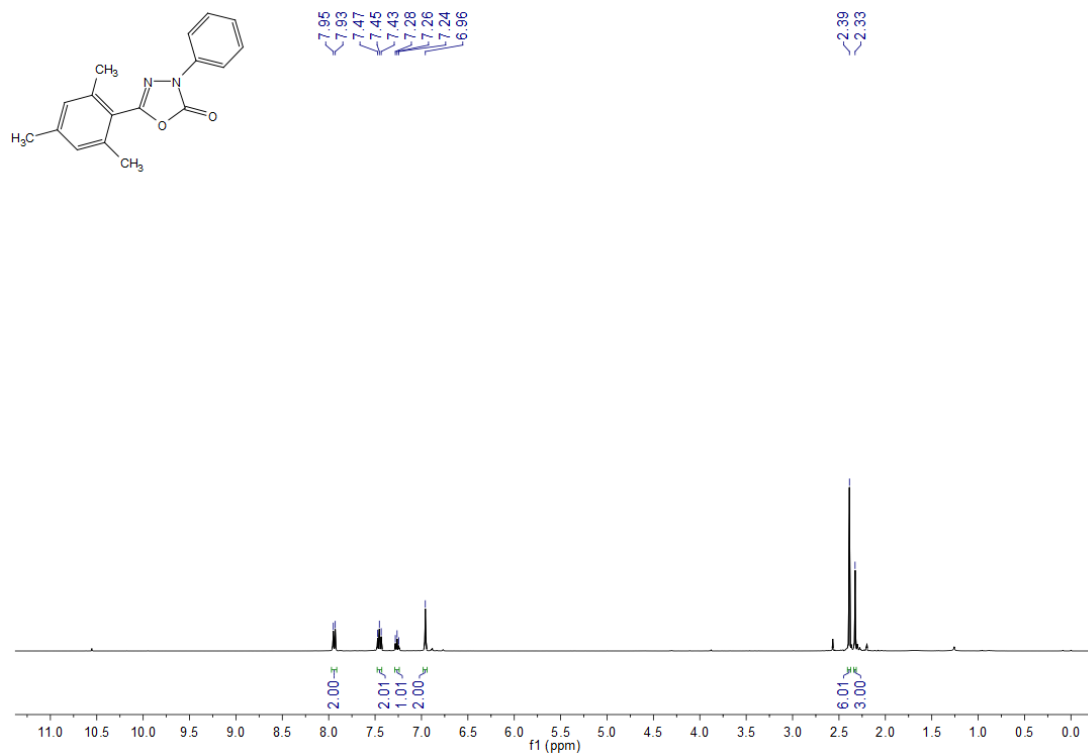
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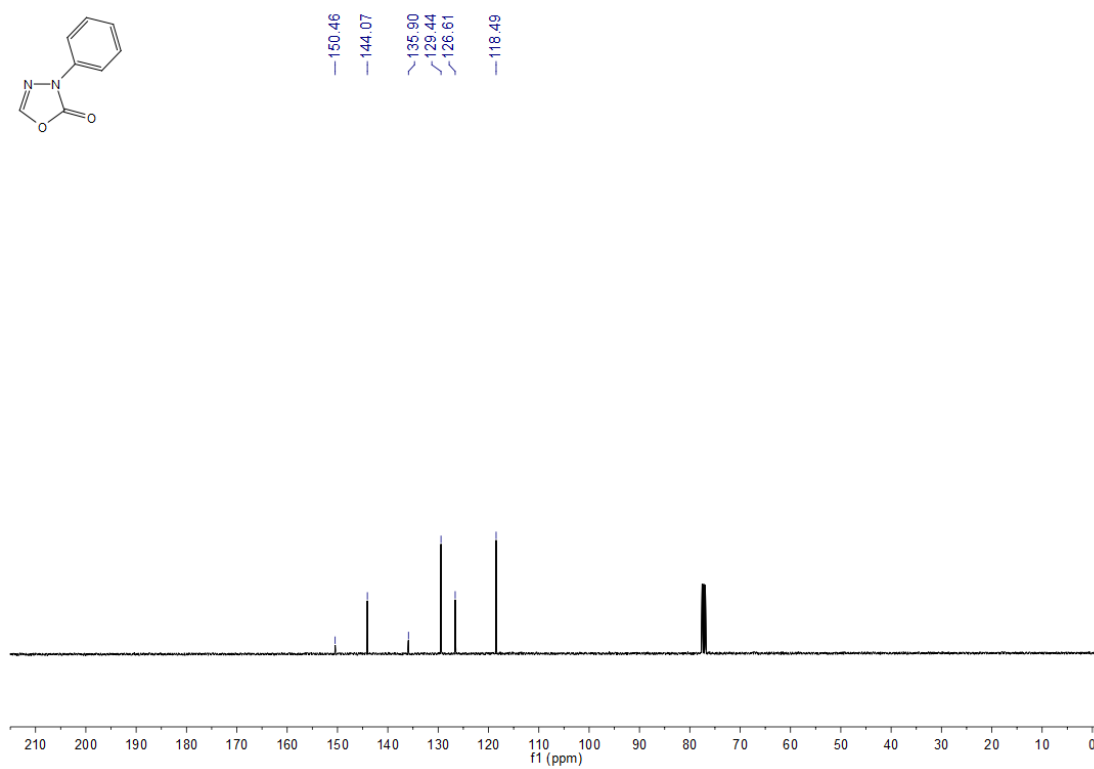
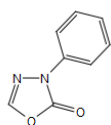
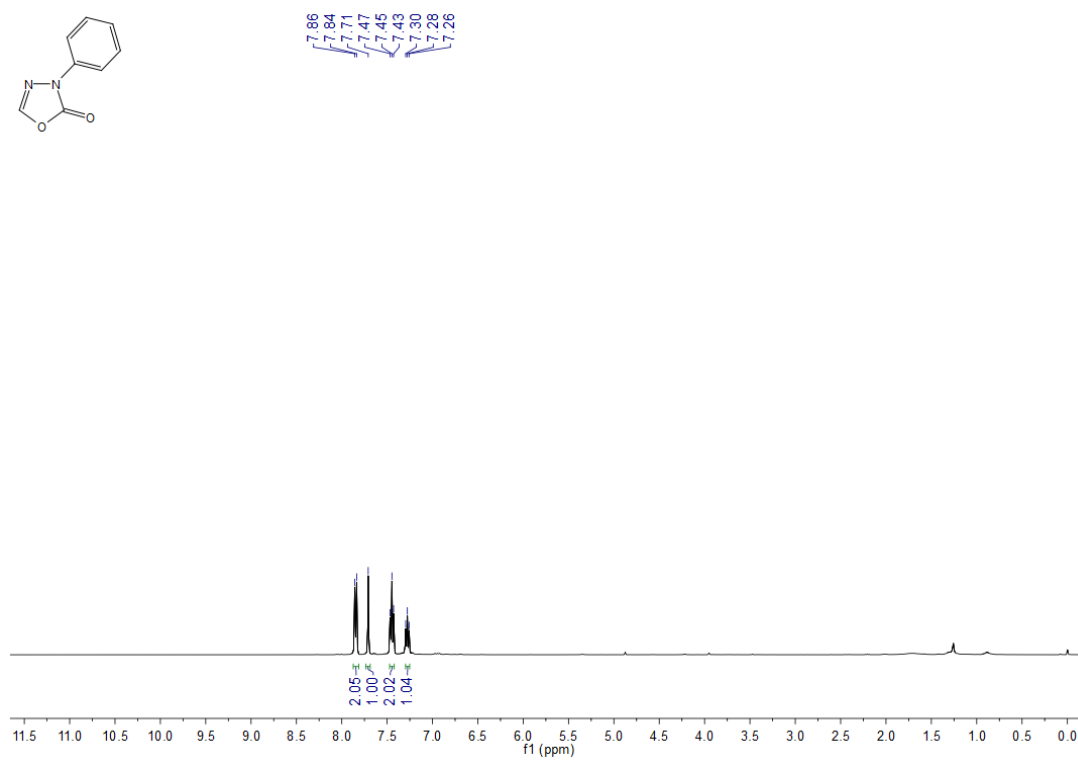
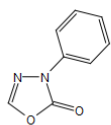
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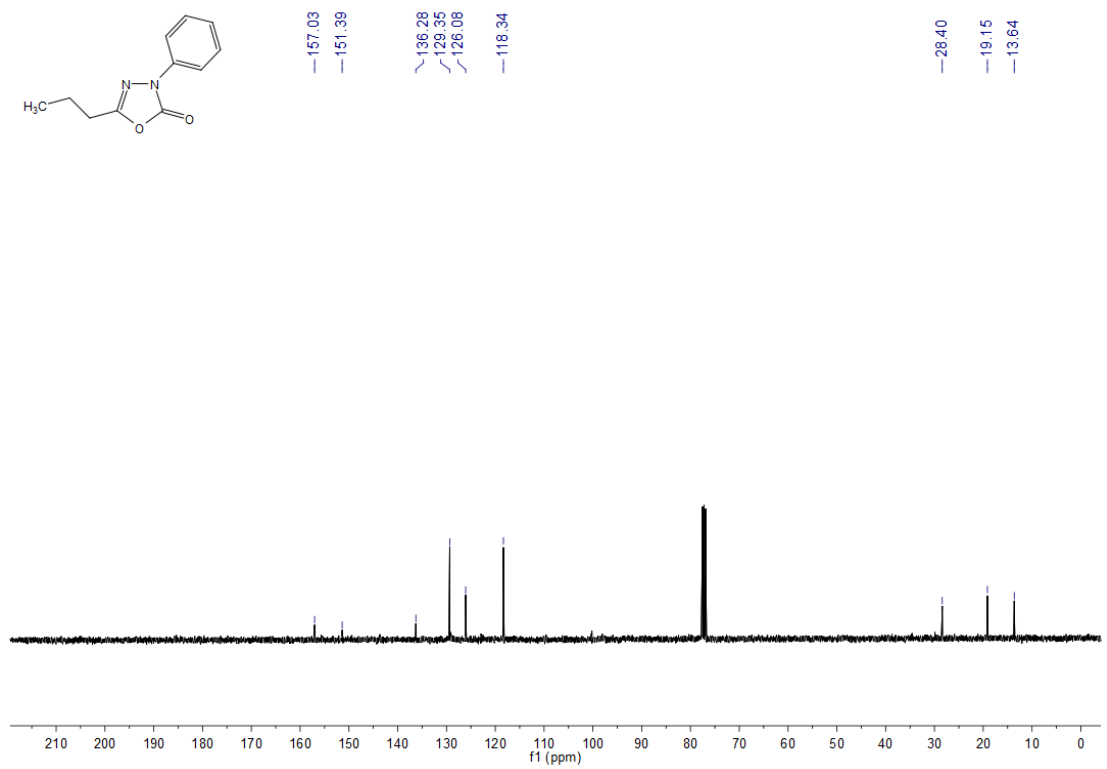
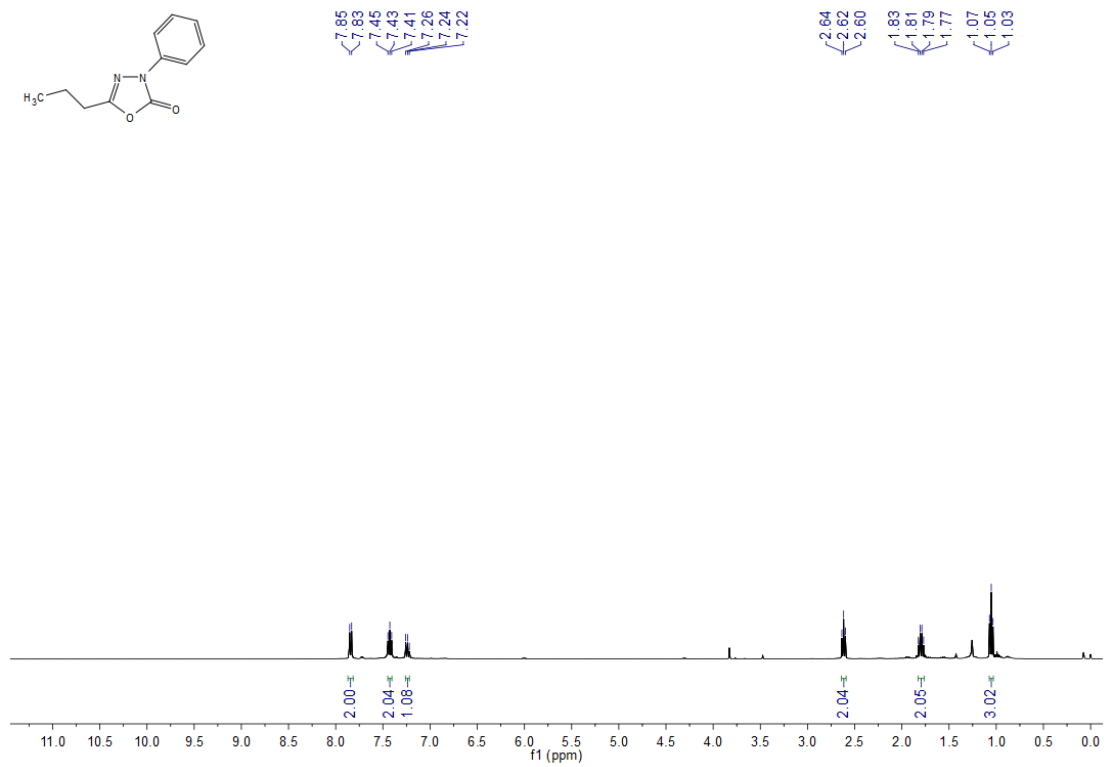
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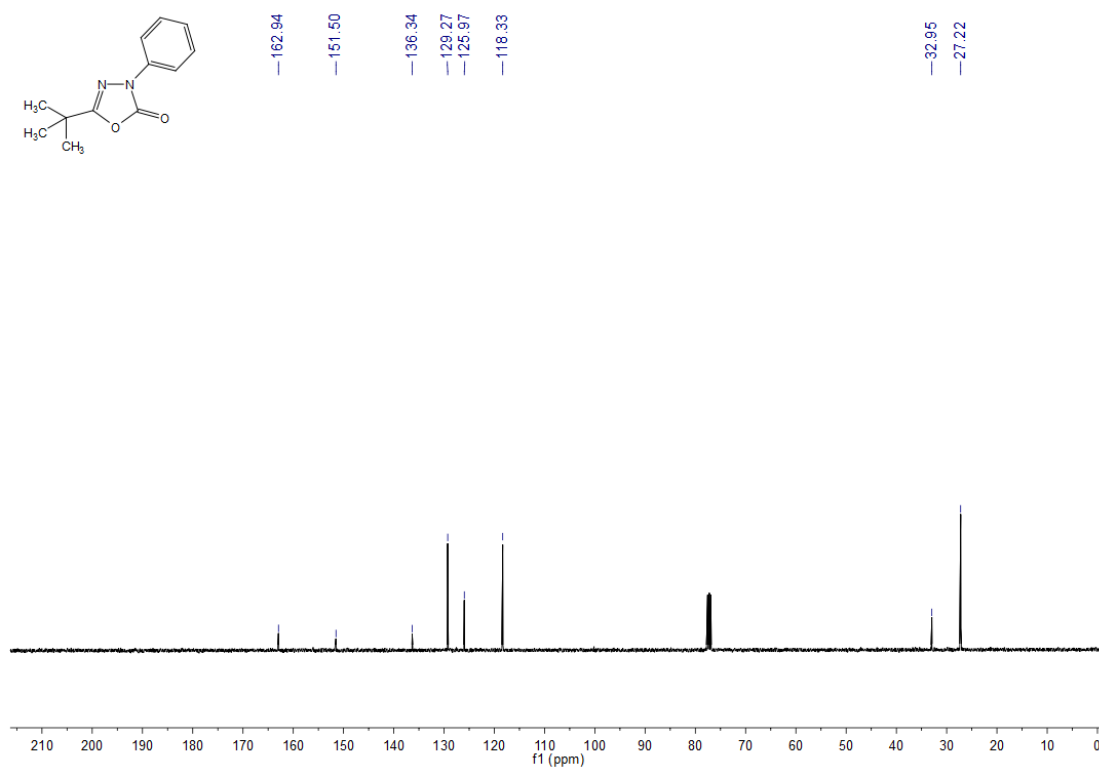
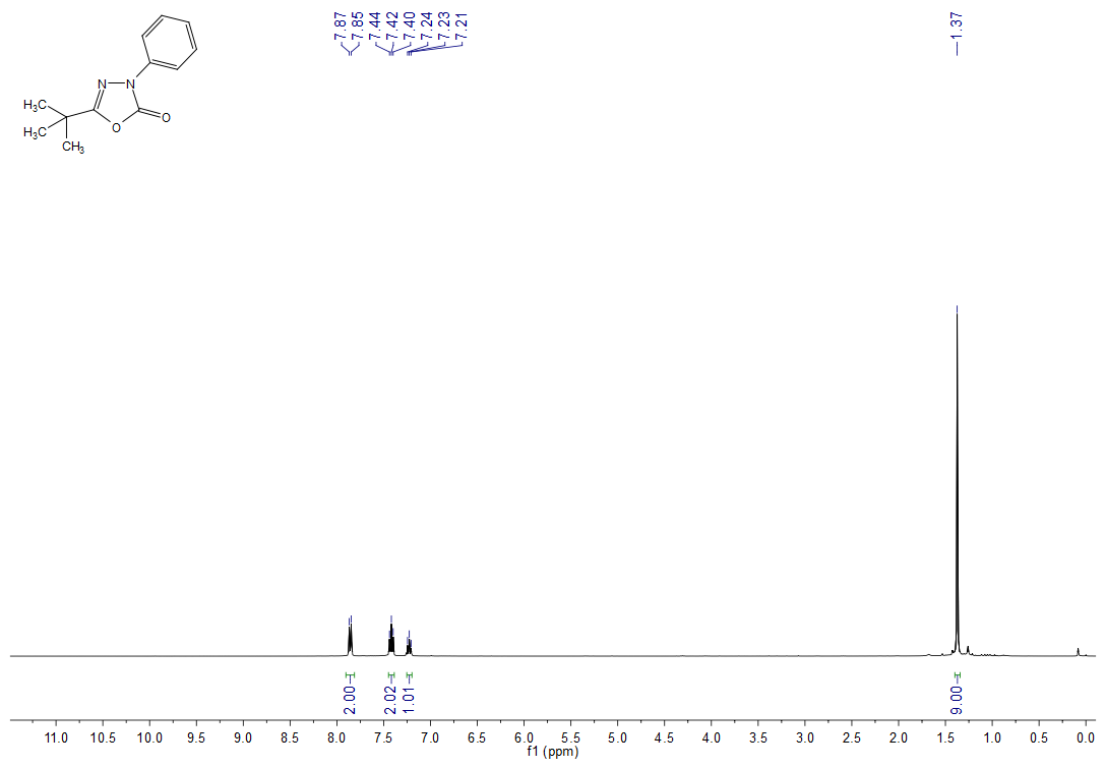
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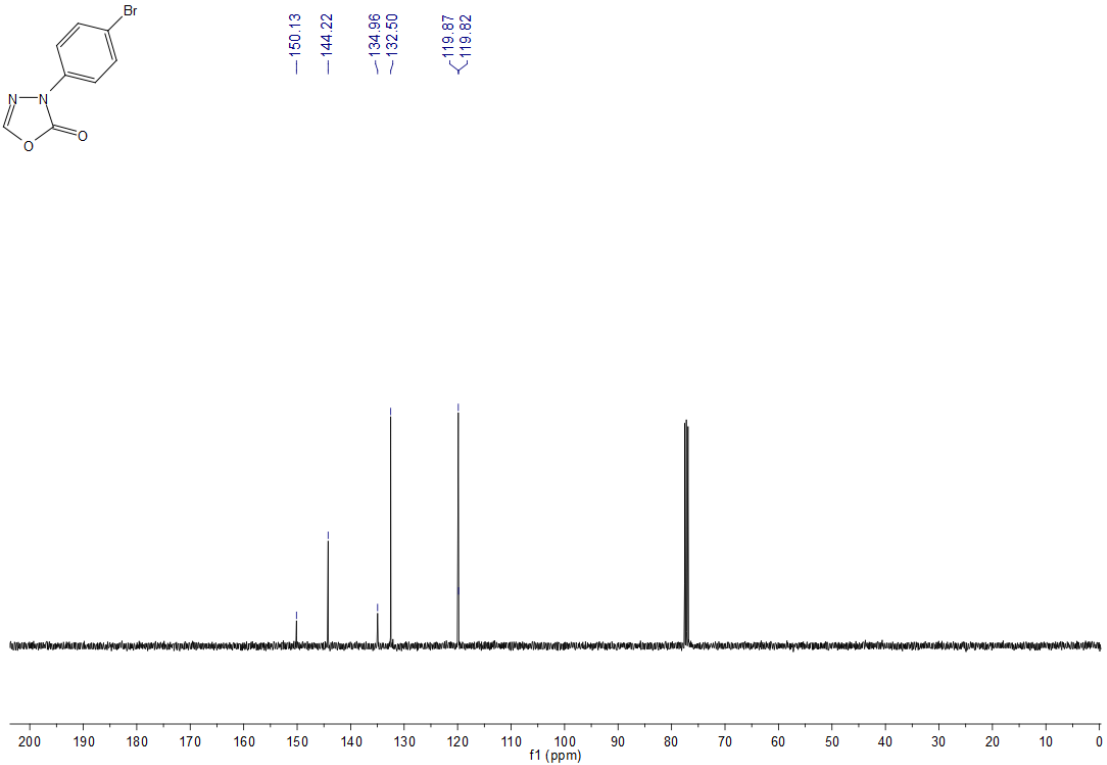
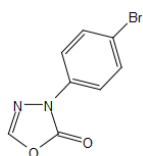
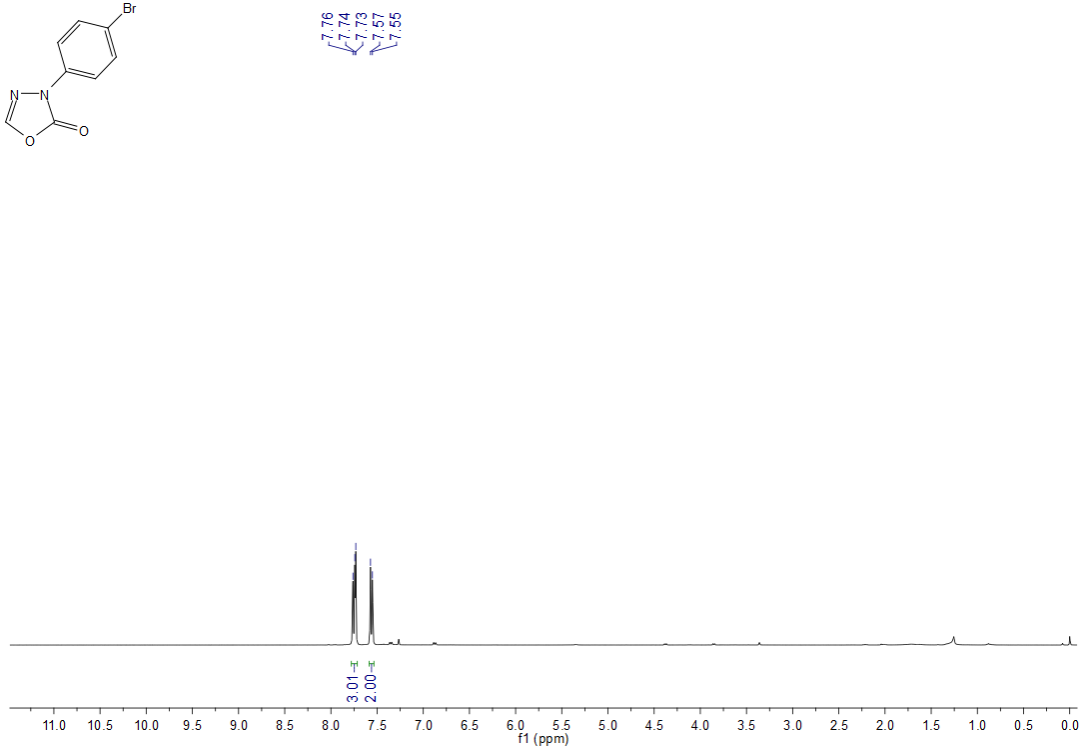
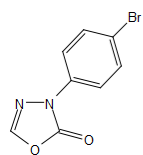
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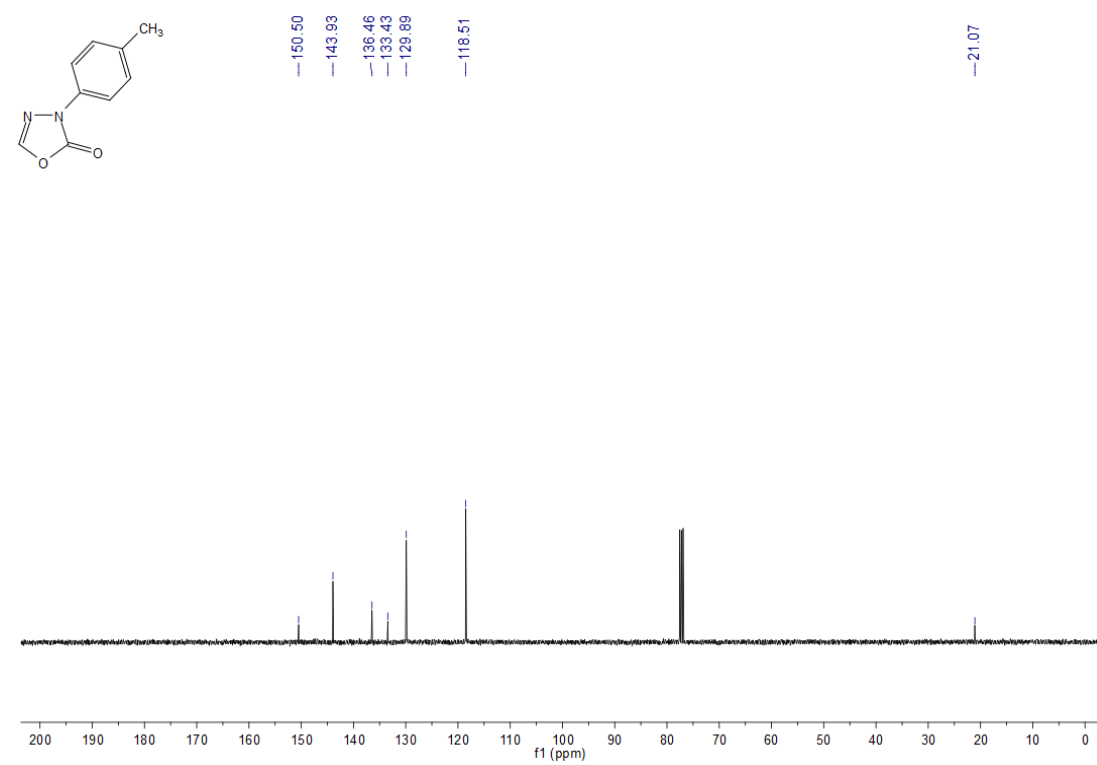
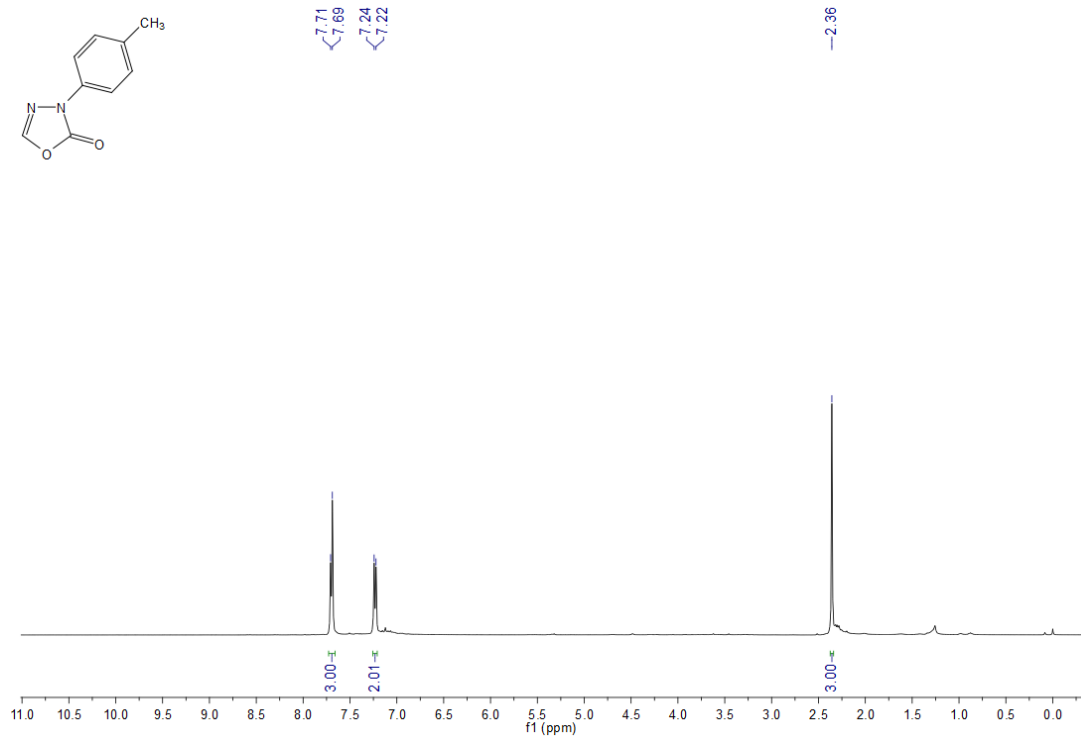
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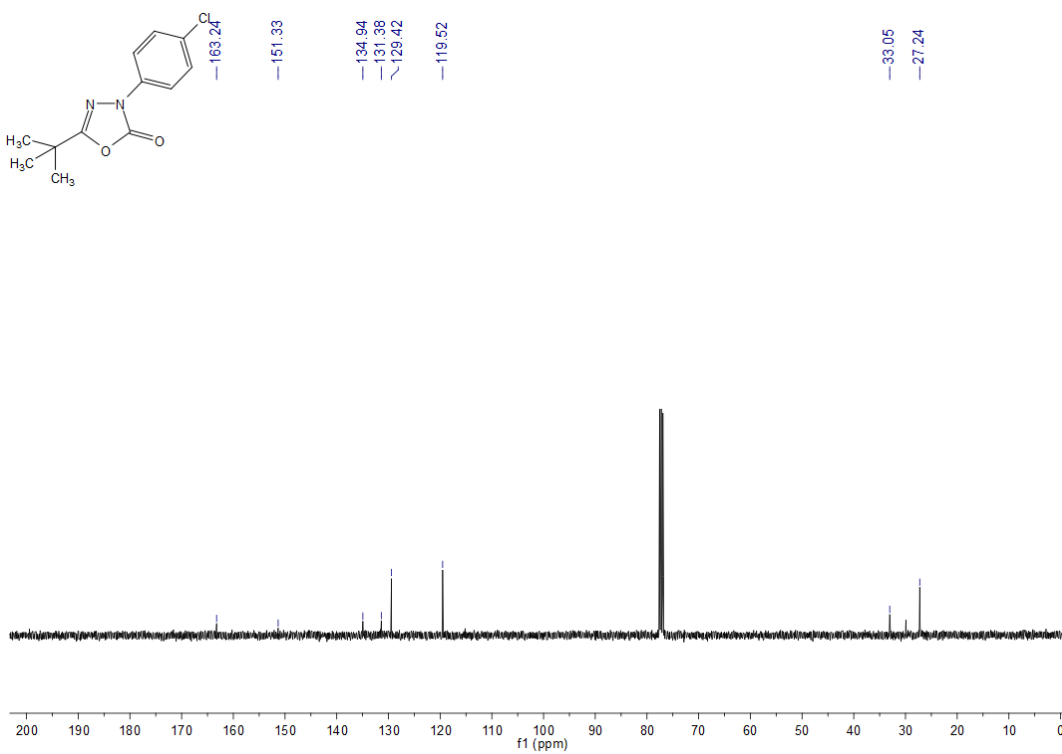
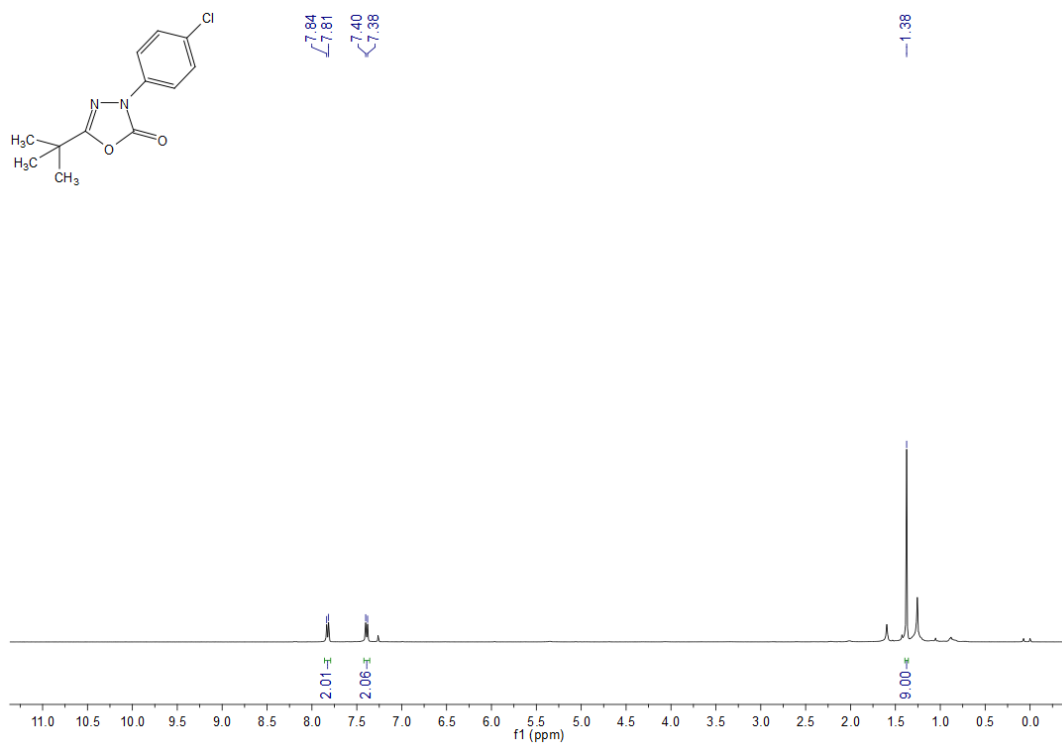
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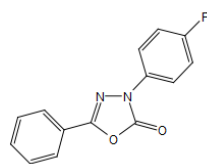
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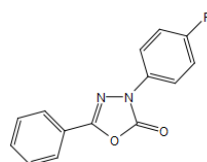
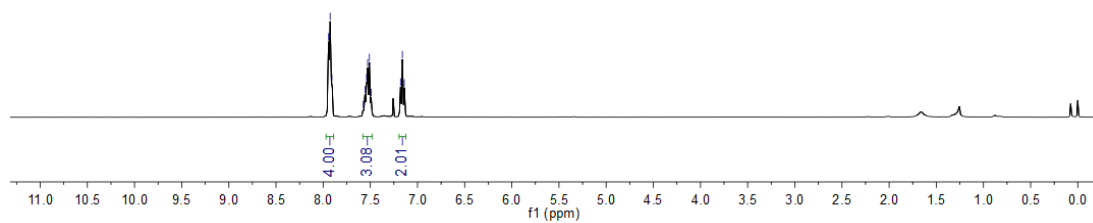
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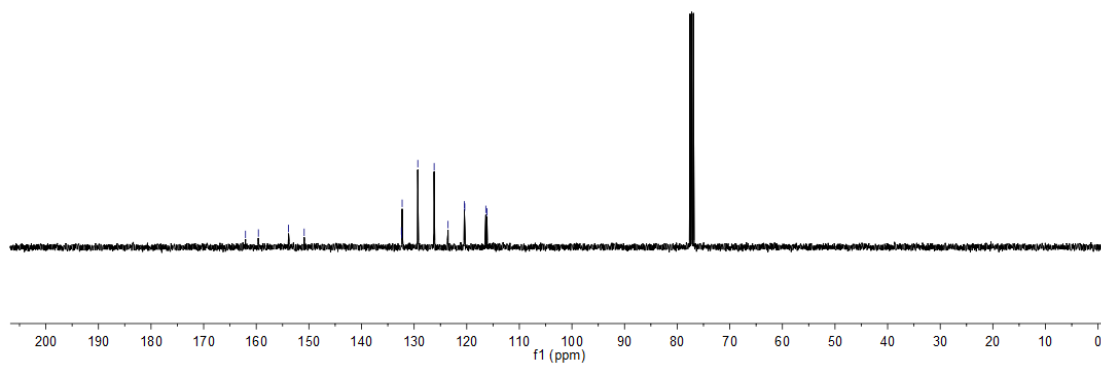
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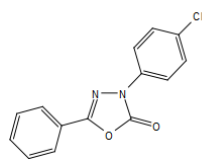
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7.54
7.53
7.51
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7.14



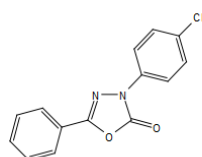
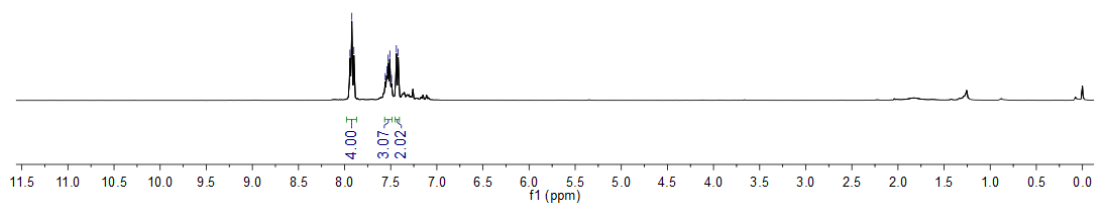
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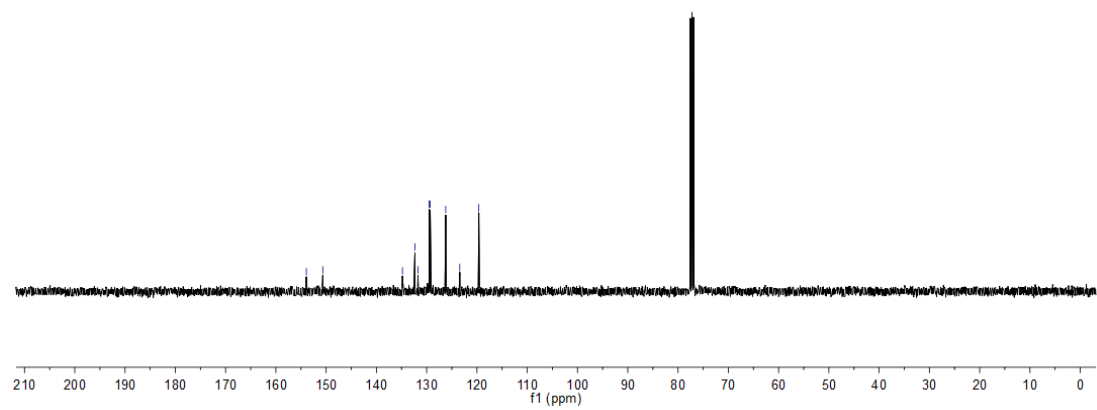
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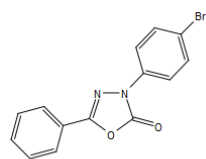
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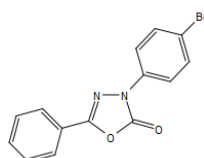
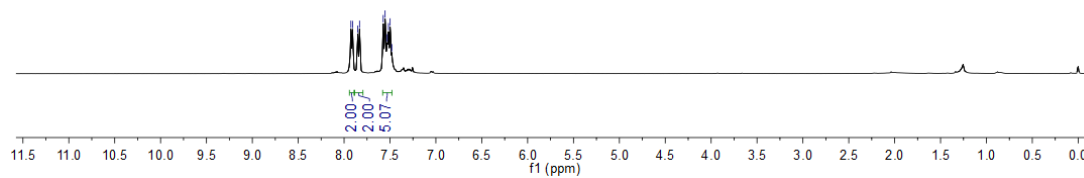
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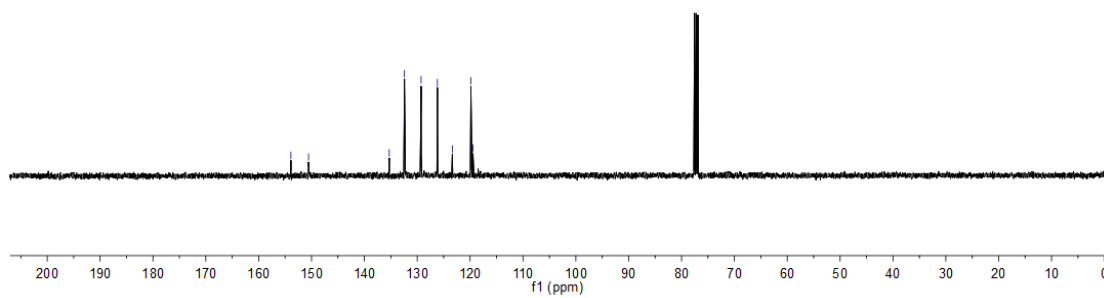
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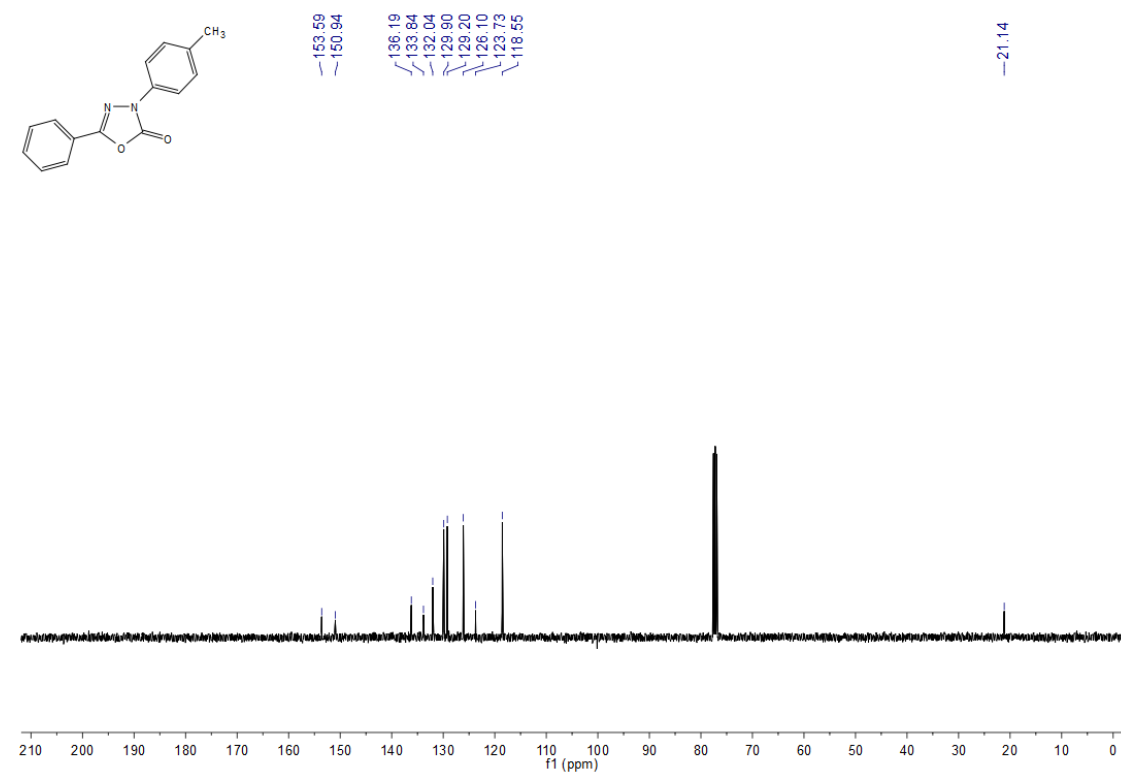
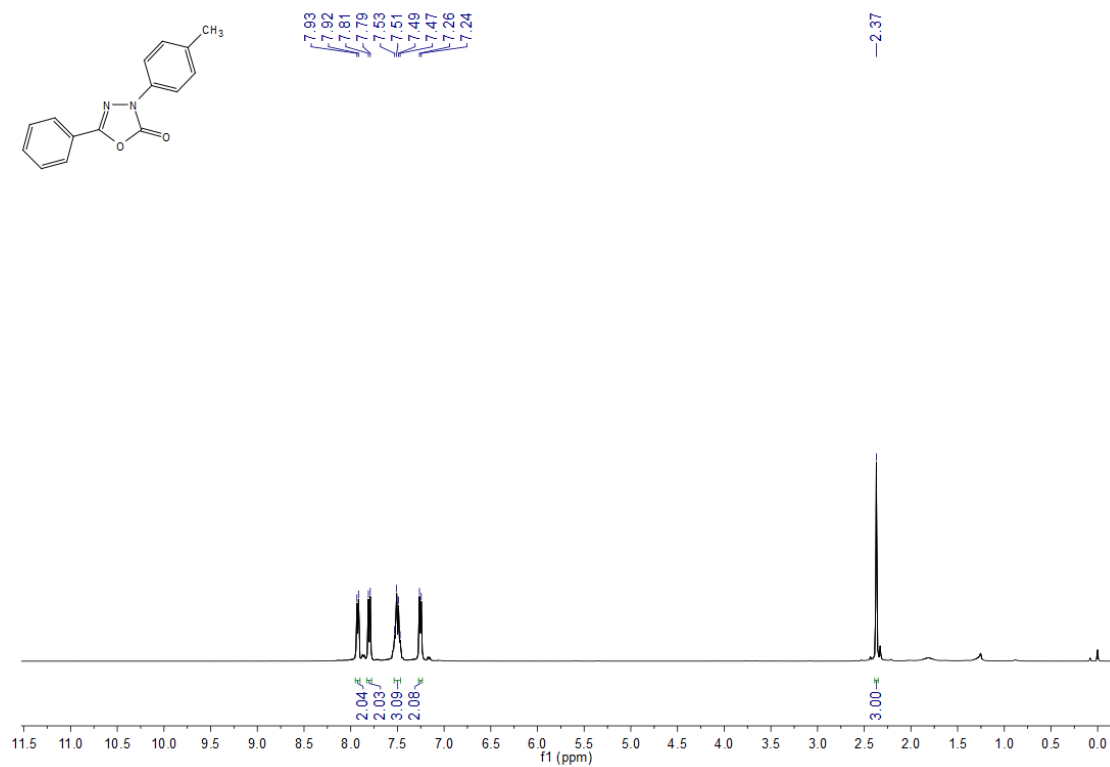
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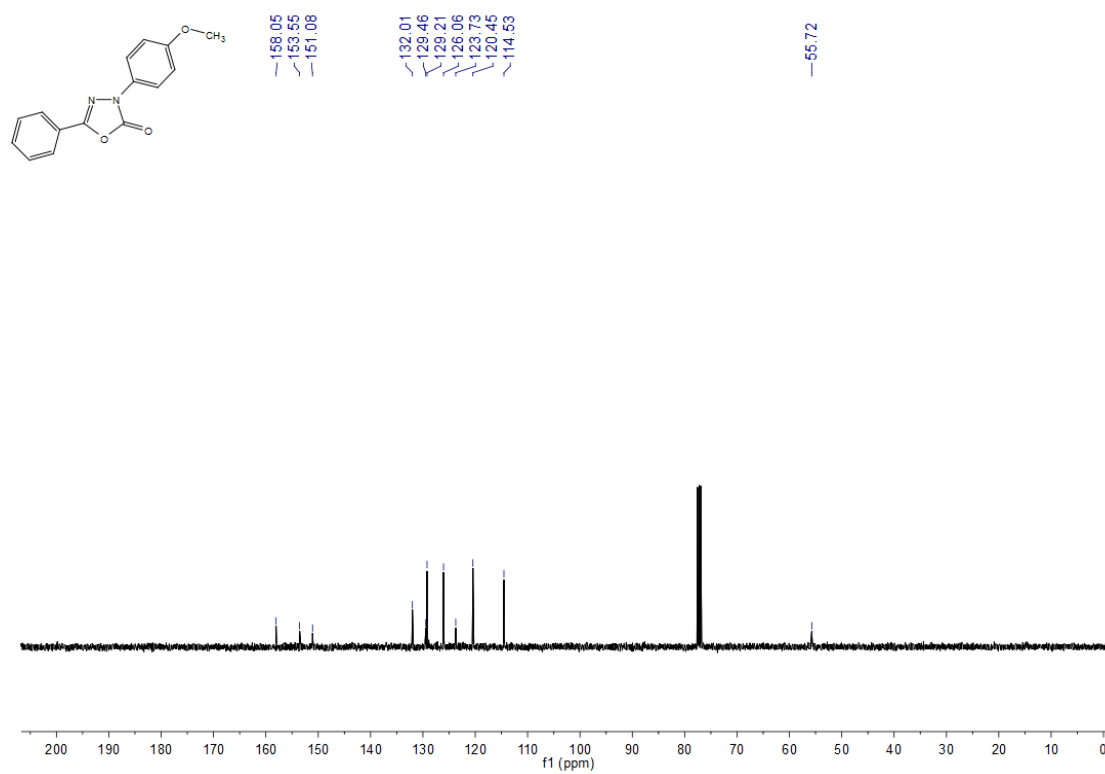
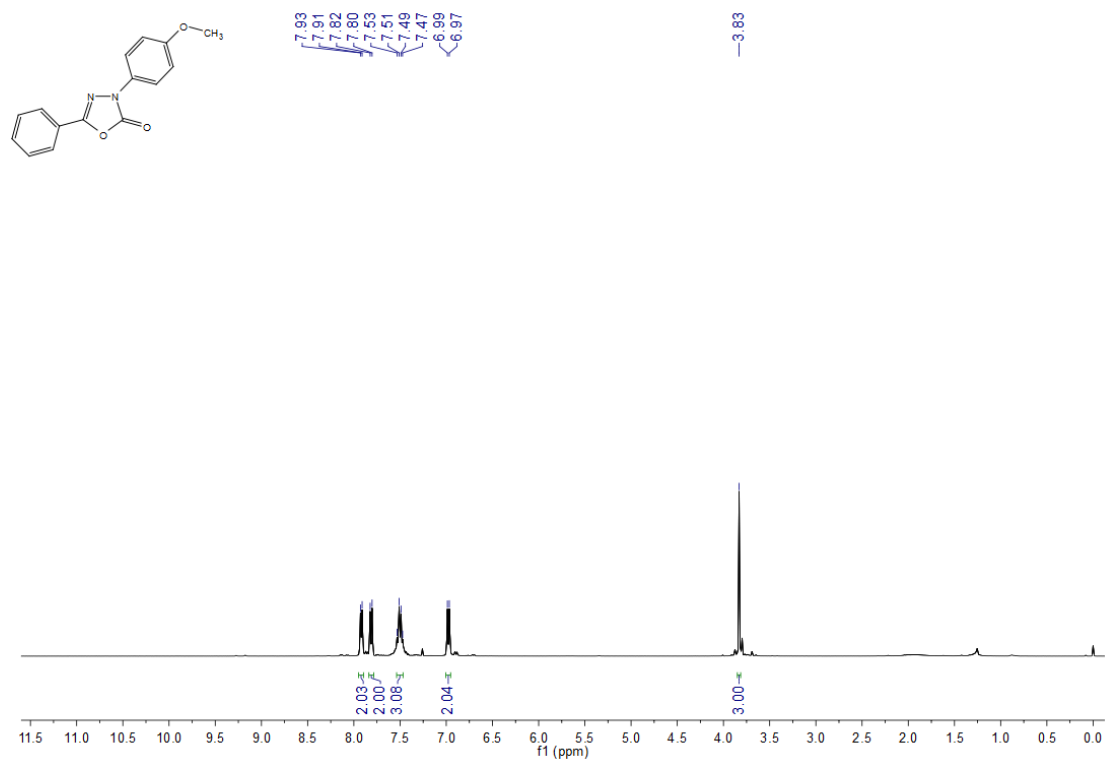
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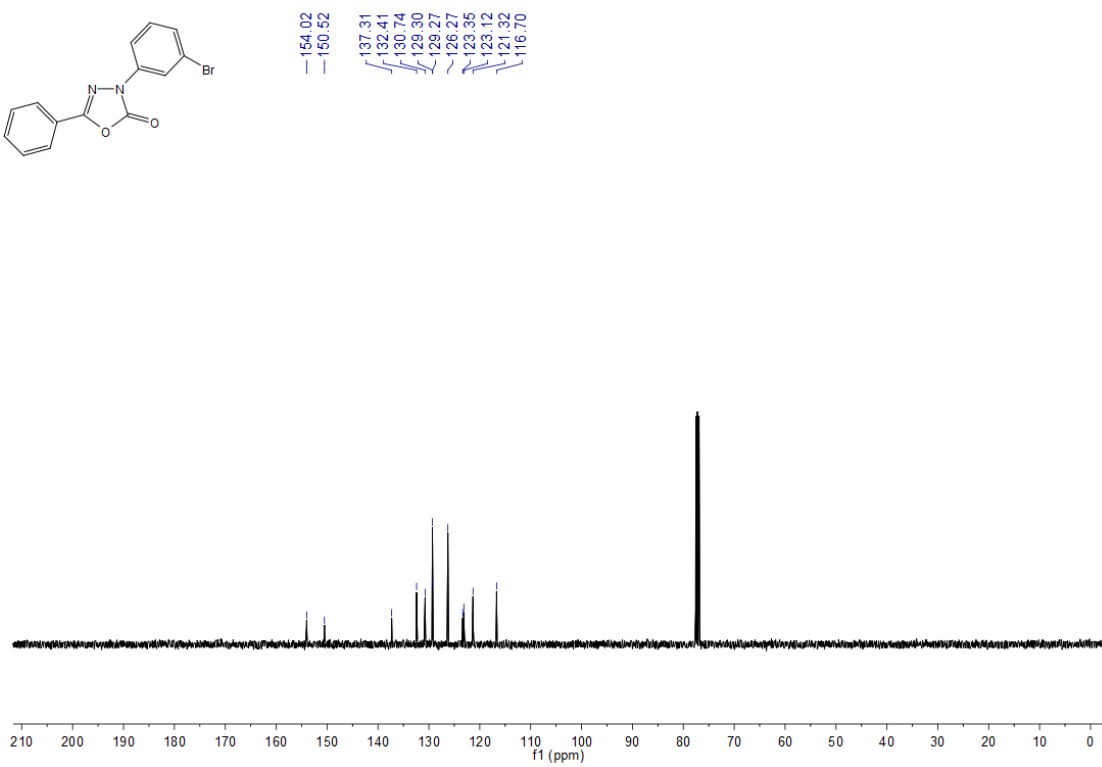
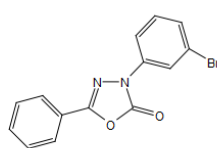
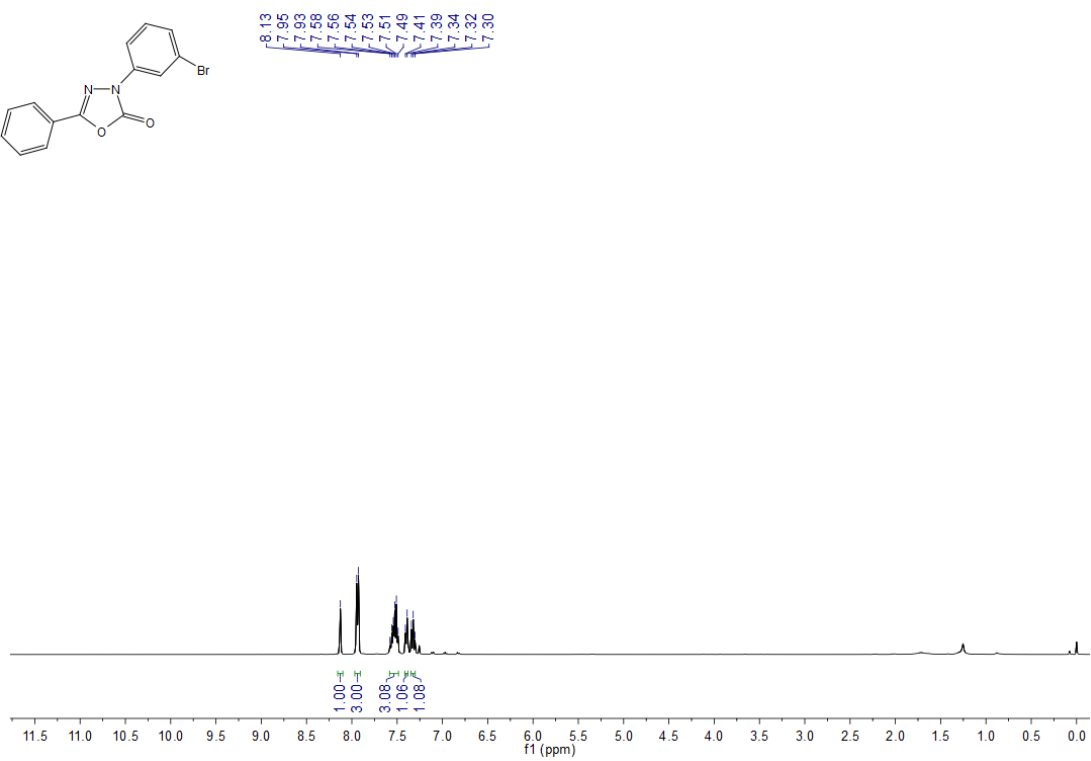
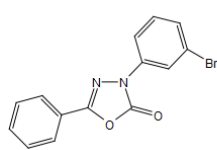
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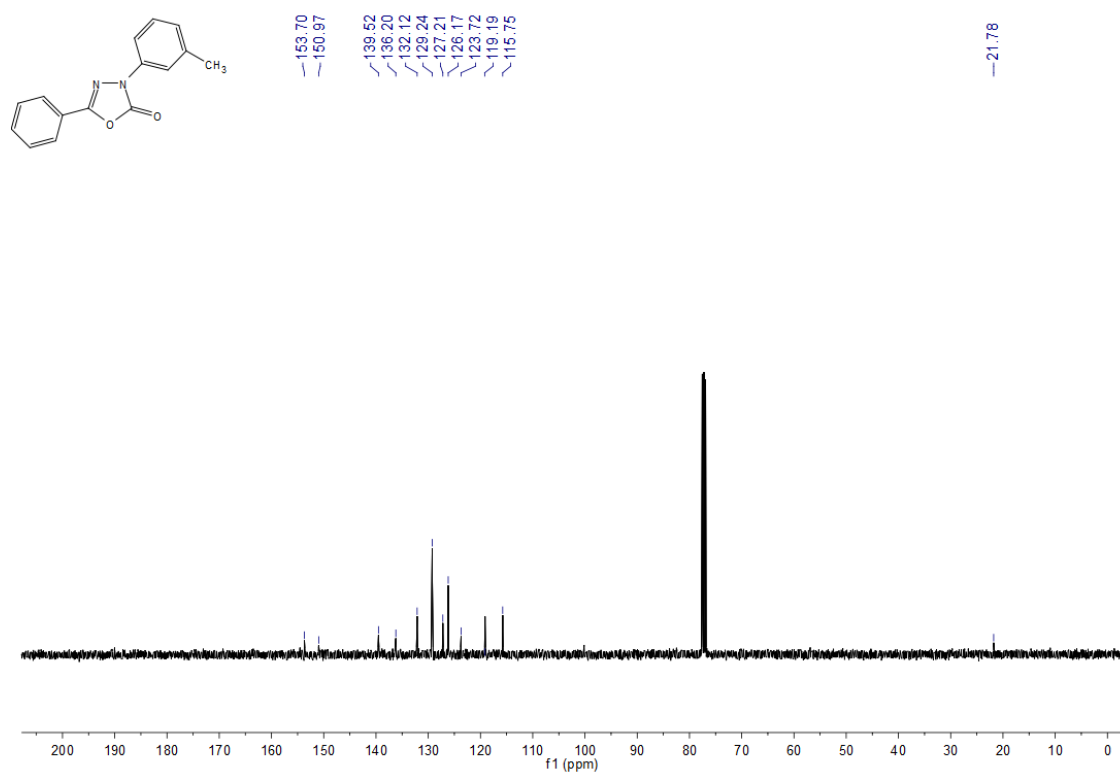
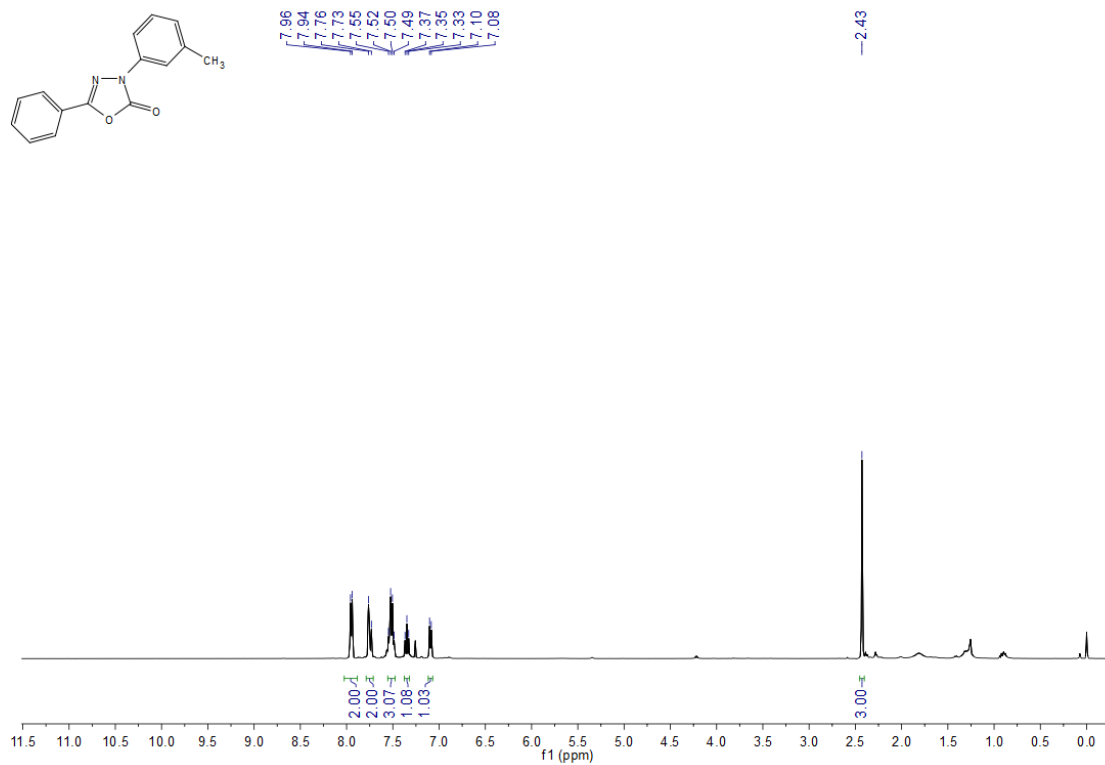
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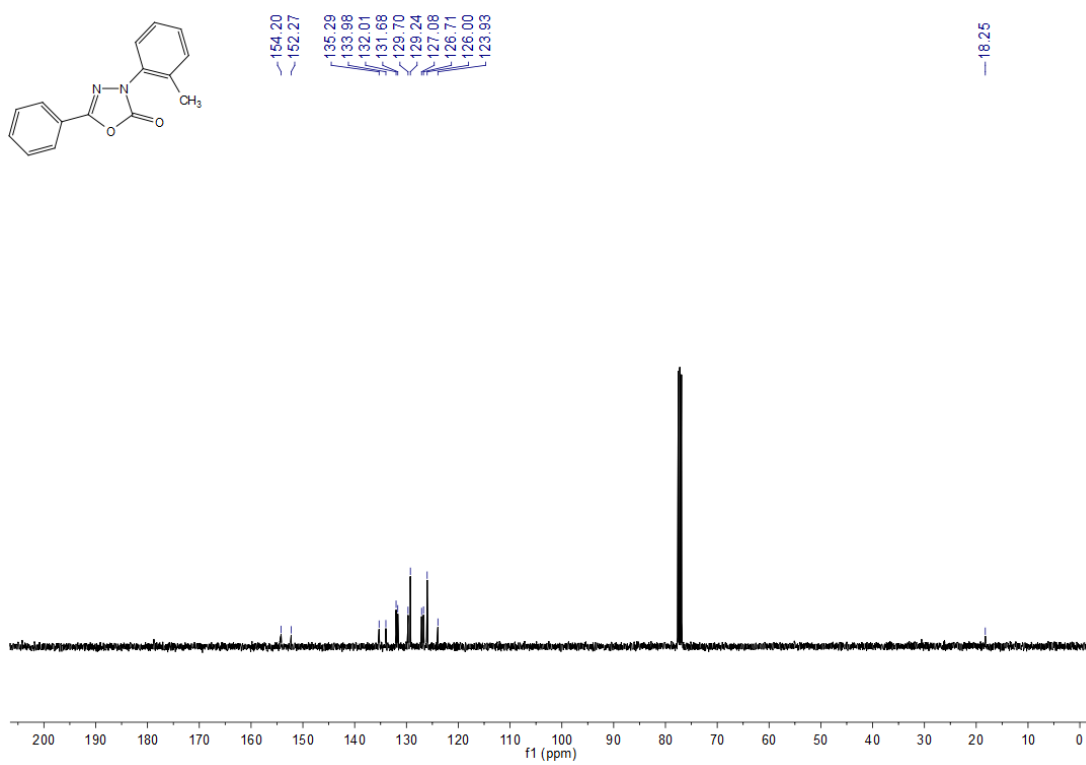
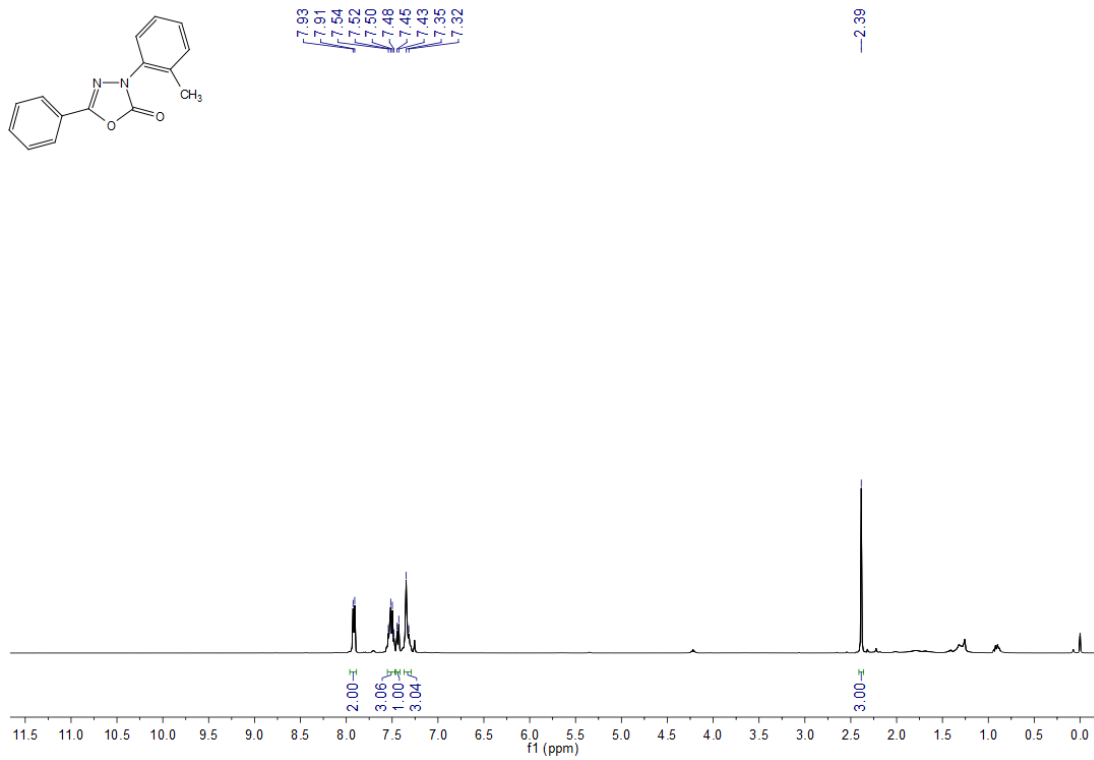
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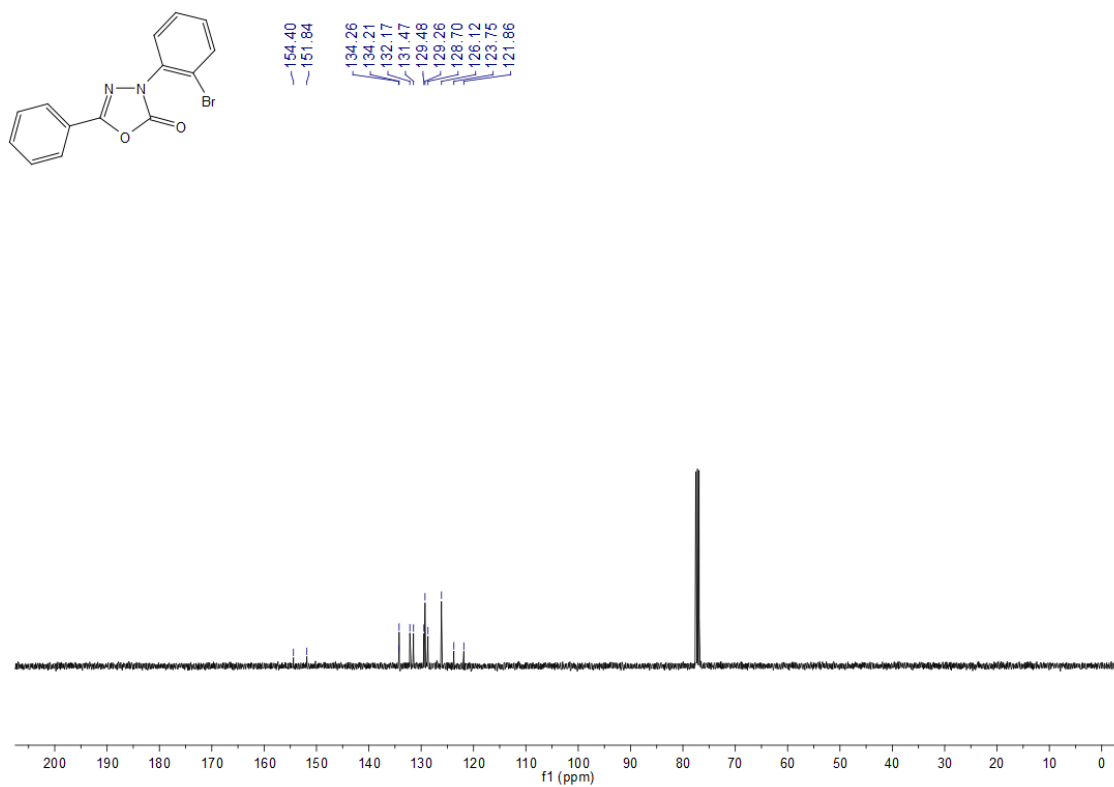
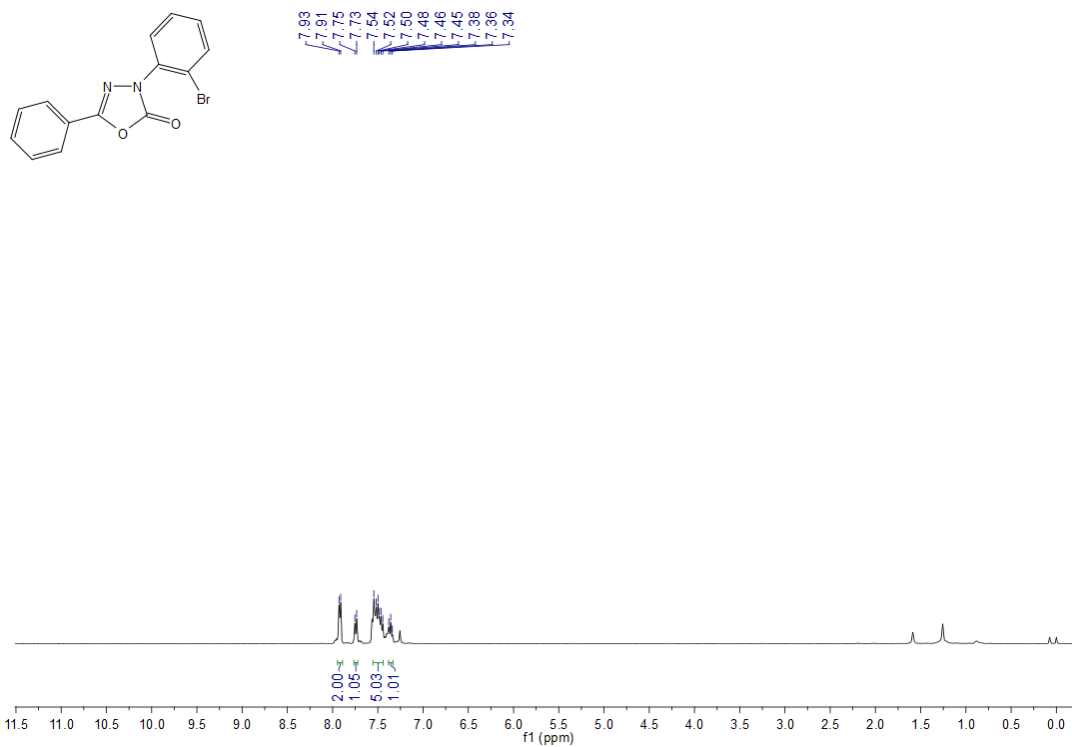
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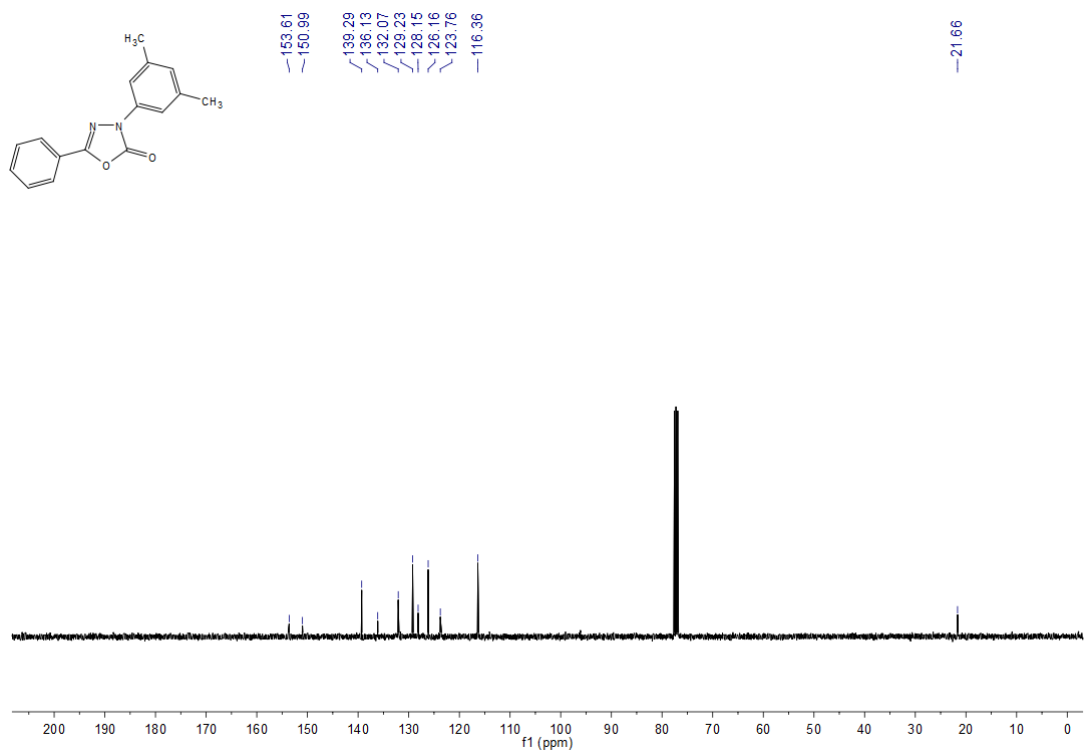
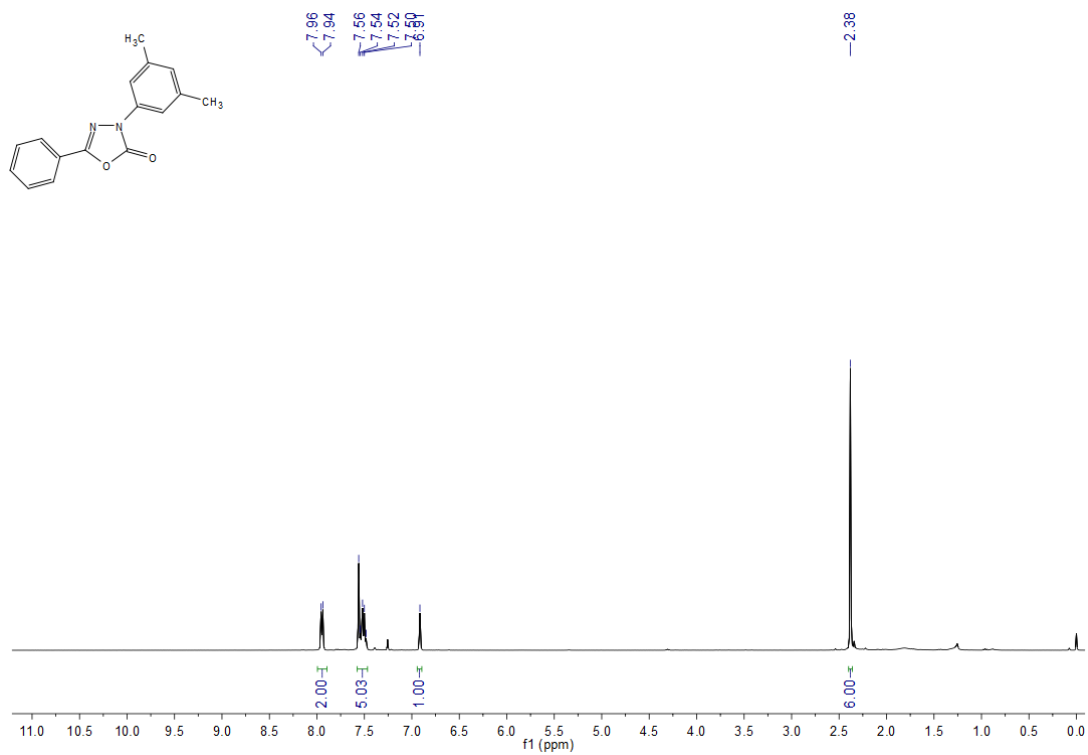
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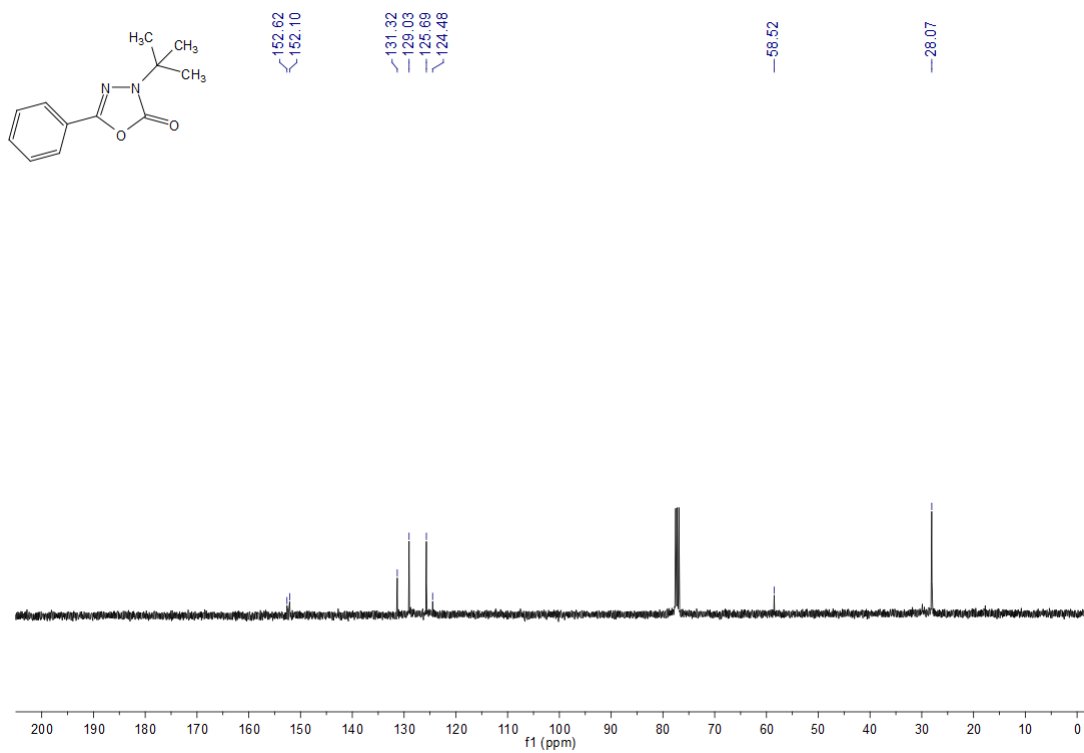
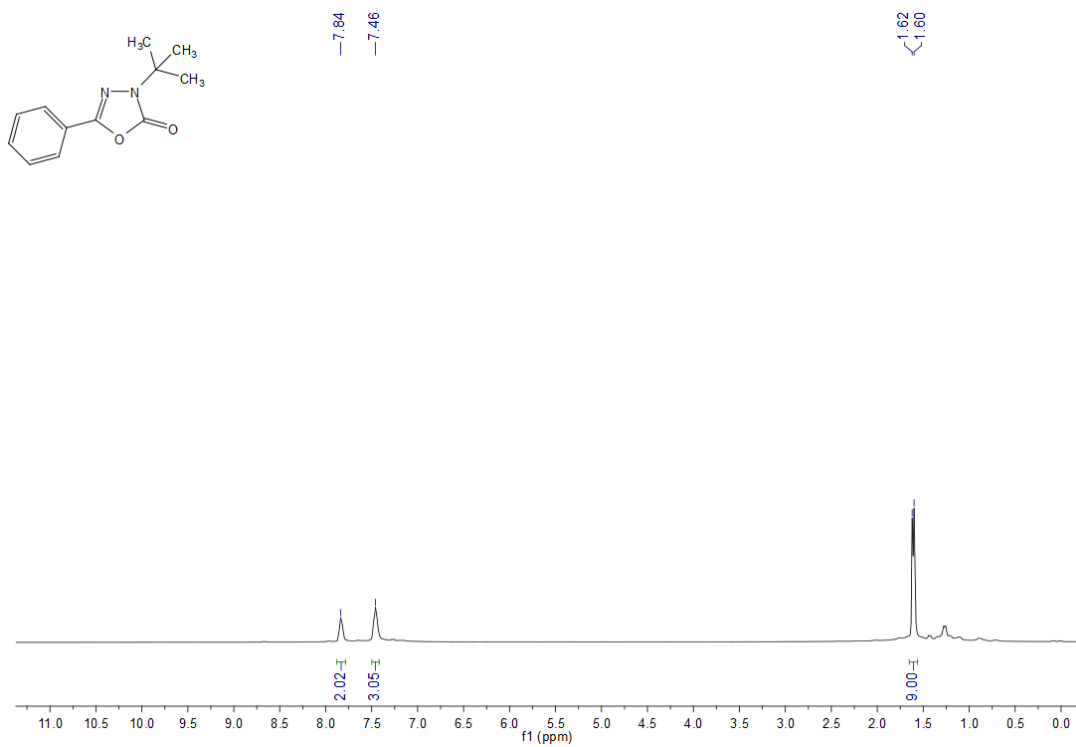
4i



4j



4k



5a

