

**Ligand-free Cu(II)-mediated aerobic oxidations of aldehyde
hydrazones leading to *N,N'*-diacylhydrazines and 1,3,4-oxadiazoles†**

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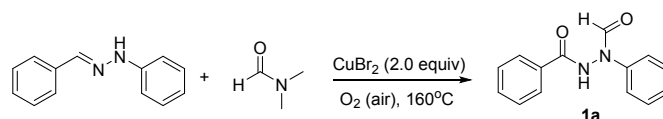
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General Experimental Information

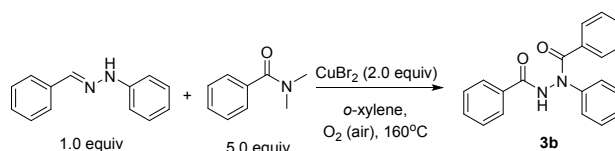
All of the chemicals were obtained from commercial sources or prepared according to standard methods. NMR spectra were recorded with a 400 MHz spectrometer for ^1H NMR, a 101 MHz spectrometer for ^{13}C NMR. TMS was used as an internal standard. Chemical shifts (δ) were reported relative to TMS (^1H) or CDCl_3 (^{13}C). Multiplicities were reported as follows: singlet (s), doublet (d), triplet (t), quartet (q), multiplet (m), dd (doublet of doublets) and dt (doublet of triplets). Coupling constants were reported in Hertz (Hz). Melting points were recorded with a micro melting point apparatus. High resolution mass spectra (HRMS) were recorded on a QTOF mass analyzer with electrospray ionization (ESI).

General procedure using the preparation of *N'*-formyl-*N'*-phenylbenzohydrazide (**1a**) as the example



(E)-1-Benzylidene-2-phenylhydrazine (1.5 mmol, 294 mg), CuBr_2 (2.0 equiv, 670 mg) and DMF (10 mL) were added to a 100 mL round-bottom flask. After the mixture was refluxed at 160°C in air atmosphere for 5 min and TLC indicated the completion of the reaction. The DMF was then distilled off. The residue was dissolved in ethyl acetate (20 mL) and the insoluble residue was filtered. Then the filtrate was washed with water (2 x 5 mL), and dried over Na_2SO_4 . The ethyl acetate was then evaporated and the product was purified by column chromatography on silica gel (petroleum ether/ethyl acetate=5:1) to give **1a** (342 mg, 95%).

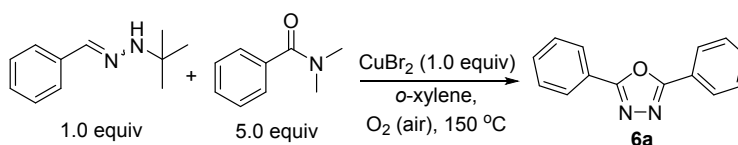
General procedure using the preparation of *N'*-benzoyl-*N'*-phenylbenzohydrazide (**3b**) as the example



(E)-1-Benzylidene-2-phenylhydrazine (1.5 mmol, 294 mg), *N,N*-dimethylbenzamide (5.0 equiv, 1118 mg), CuBr_2 (2.0 equiv, 670 mg) and *o*-xylene (10 mL) were added to a 100 mL round-bottom flask. After the

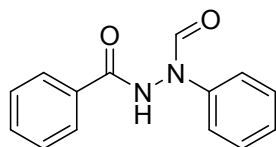
mixture was refluxed at 160 °C in air atmosphere for 5 min and TLC indicated the completion of the reaction. The *N,N*-dimethylbenzamide and *o*-xylene was then distilled off. The residue was dissolved in ethyl acetate (20 mL) and the insoluble residue was filtered. Then the filtrate was washed with water (2 x 5 mL), and dried over Na₂SO₄. The ethyl acetate was then evaporated and the product was purified by column chromatography on silica gel (petroleum ether/ethyl acetate=5:1) to give **3b** (346 mg, 73%).

General procedure using the preparation of 2,5-diphenyl-1,3,4-oxadiazole (6a**) as the example**

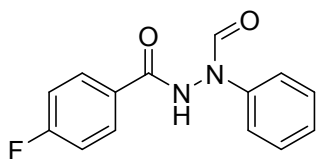


1-Benzylidene-2-*tert*-butylhydrazine (1.5 mmol, 264 mg), *N,N*-dimethylbenzamide (5.0 equiv, 1118 mg), CuBr₂ (1.0 equiv, 335mg) and *o*-xylene (10 mL) were added to a 100 mL round-bottom flask. After the mixture was refluxed at 150 °C in air atmosphere for 0.75 h and TLC indicated the completion of the reaction. The *N,N*-dimethylbenzamide and *o*-xylene was then distilled off. The residue was dissolved in ethyl acetate (20 mL) and the insoluble residue was filtered. Then the filtrate was washed with water (2 x 5 mL), and dried over Na₂SO₄. The ethyl acetate was then evaporated and the product was purified by column chromatography on silica gel (petroleum ether/ethyl acetate=20:1) to give **6a** (283 mg, 85%).

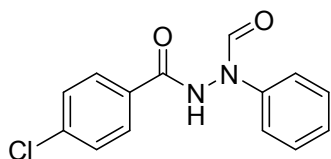
Analytical data for all products



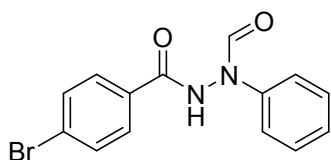
N'-Formyl-N'-phenylbenzohydrazide (1a):¹ 342 mg, 95% yield; white solid; mp: 144-145 °C; ¹H NMR (400 MHz, CDCl₃, two conformers are present, in a 80:20 ratio) δ 9.53 (s, 0.20H), 9.46 (s, 0.80H), 8.64 (s, 0.80H), 8.34 (s, 0.20H), 7.91 (d, *J* = 7.5 Hz, 0.40H), 7.83 (d, *J* = 7.5 Hz, 1.60H), 7.61 – 7.20 (m, 8H). ¹³C NMR (101 MHz, CDCl₃) the major conformer: δ 166.3, 160.6, 140.1, 132.5, 130.9, 129.6, 128.6, 127.6, 127.2, 121.6; the minor conformer: δ 167.4, 164.2, 139.3, 132.8, 131.0, 129.0, 128.8, 127.7, 126.5, 122.2. **HRMS** (ESI) found: *m/z* 263.0795 [M+Na]⁺; calcd. for C₁₄H₁₂N₂O₂Na⁺ 263.0791.



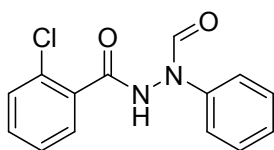
4-Fluoro-N'-formyl-N'-phenylbenzohydrazide (1b): 376 mg, 97% yield; white solid; mp: 139-140 °C; ¹H NMR (400 MHz, CDCl₃, two conformers are present, in a 84:16 ratio) δ 9.88 (s, 0.84H), 9.80 (s, 0.16H), 8.61 (s, 0.84H), 8.29 (s, 0.16H), 7.91 (dd, *J* = 8.1, 5.4 Hz, 0.32H), 7.82 (dd, *J* = 8.5, 5.3 Hz, 1.68H), 7.50 – 7.27 (m, 5H), 7.08 (t, *J* = 8.5 Hz, 0.32H), 6.98 (t, *J* = 8.6 Hz, 1.68H). ¹³C NMR (101 MHz, CDCl₃) the major conformer: δ 166.5, 165.2, 160.7, 140.0, 130.2 - 130.1 (d, *J*_{F-C} = 9.2 Hz), 129.6, 127.4, 127.04 - 127.02 (d, *J*_{F-C} = 1.4 Hz), 121.7, 115.7 - 115.5 (d, *J*_{F-C} = 22.0 Hz); the minor conformer: δ 166.4, 164.2, 164.0, 139.2, 132.7, 130.3, 129.0, 126.6, 122.1, 116.0 - 115.8 (d, *J*_{F-C} = 22.0 Hz). **HRMS** (ESI) found: *m/z* 281.0700 [M+Na]⁺; calcd. for C₁₄H₁₁FN₂O₂Na⁺ 281.0697.



4-Chloro-*N'*-formyl-*N'*-phenylbenzohydrazide (1c): 358 mg, 87% yield; white solid; mp: 152-154 °C; ^1H NMR (400 MHz, CDCl_3 , two conformers are present, in a 89:11 ratio) δ 9.79 (s, 0.89H), 9.51 (s, 0.11H), 8.63 (s, 0.89H), 8.33 (s, 0.11H), 7.83 (d, J = 8.2 Hz, 0.22H), 7.73 (d, J = 8.4 Hz, 1.78H), 7.52 – 7.28 (m, 7H). ^{13}C NMR (101 MHz, CDCl_3) the major conformer: δ 165.2, 160.8, 139.9, 138.9, 129.7, 129.0, 128.8, 127.5, 121.7; the minor conformer: δ 166.5, 164.2, 139.2, 139.1, 132.7, 129.2, 129.1, 126.7, 123.2, 122.1. HRMS (ESI) found: m/z 297.0405 $[\text{M}+\text{Na}]^+$; calcd. for $\text{C}_{14}\text{H}_{11}\text{ClN}_2\text{O}_2\text{Na}^+$ 297.0401.

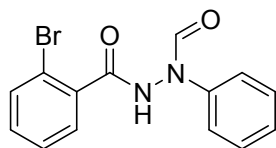


4-Bromo-*N'*-formyl-*N'*-phenylbenzohydrazide (1d): 388 mg, 81% yield; white solid; mp: 175-178 °C; ^1H NMR (400 MHz, CDCl_3 , two conformers are present, in a 89:11 ratio) δ 9.78 (s, 0.89H), 9.41 (s, 0.11H), 8.64 (s, 0.89H), 8.34 (s, 0.11H), 7.76 (d, J = 8.2 Hz, 0.22H), 7.66 (d, J = 8.4 Hz, 1.78H), 7.52 – 7.30 (m, 7H). ^{13}C NMR (101 MHz, CDCl_3) the major conformer: δ 165.2, 160.8, 139.9, 131.8, 129.7, 129.1, 127.54, 127.49, 121.7; the minor conformer: δ 166.6, 164.1, 139.1, 132.0, 129.5, 129.3, 129.0, 127.7, 126.7, 122.2. HRMS (ESI) found: m/z 340.9901 $[\text{M}+\text{Na}]^+$; calcd. for $\text{C}_{14}\text{H}_{11}\text{BrN}_2\text{O}_2\text{Na}^+$ 340.9896.

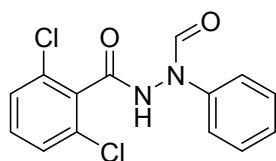


2-Chloro-*N'*-formyl-*N'*-phenylbenzohydrazide (1e): 383 mg, 93% yield; white solid; mp: 137-139 °C; ^1H NMR (400 MHz, CDCl_3 , two conformers are present, in a 79:21 ratio) δ 9.02 (s, 0.21H), 8.64 (s, 0.79H), 8.51 (s, 0.79H), 8.43 (s, 0.21H), 7.78 (d, J = 7.3 Hz, 0.79H), 7.71 (d, J = 7.6 Hz, 0.21H), 7.59 – 7.29 (m, 8H). ^{13}C NMR (101 MHz, CDCl_3) the major conformer: δ 165.9, 159.7, 139.9, 132.2, 131.4, 130.3, 129.6, 127.1, 127.0, 121.1; the minor conformer: δ 166.8, 163.6, 138.9, 132.3, 131.3, 130.2,

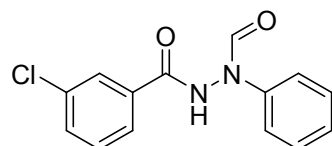
129.8, 128.9, 126.7, 122.3. **HRMS** (ESI) found: m/z 297.0405 $[M+Na]^+$; calcd. for $C_{14}H_{11}ClN_2O_2Na^+$ 297.0401.



2-Bromo-*N'*-formyl-*N'*-phenylbenzohydrazide (1f): 431 mg, 90% yield; white solid; mp: 131-133 °C; **¹H NMR** (400 MHz, $CDCl_3$, two conformers are present, in a 76:24 ratio) δ 8.93 (s, 0.24H), 8.62 (s, 0.76H), 8.45 (s, 0.24H), 8.36 (s, 0.76H), 7.69 – 7.57 (m, 2H), 7.48 – 7.29 (m, 7H). **¹³C NMR** (101 MHz, $CDCl_3$) the major conformer: δ 166.7, 159.7, 139.8, 133.5, 132.2, 129.6, 127.5, 127.1, 122.5, 121.3; the minor conformer: δ 167.6, 163.5, 138.9, 134.7, 132.2, 130.0, 129.0, 126.7, 122.8, 119.8. **HRMS** (ESI) found: m/z 340.9898 $[M+Na]^+$; calcd. for $C_{14}H_{11}BrN_2O_2Na^+$ 340.9896.

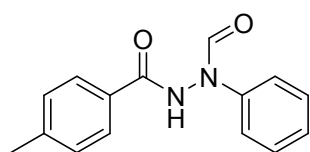


2,6-Dichloro-*N'*-formyl-*N'*-phenylbenzohydrazide (1g): 390 mg, 84% yield; white solid; mp: 125-127 °C; **¹H NMR** (400 MHz, $CDCl_3$, two conformers are present, in a 62:38 ratio) δ 8.97 (s, 0.38H), 8.54 (s, 0.62H), 8.51 (s, 0.62H), 8.46 (s, 0.38H), 7.62 – 7.28 (m, 8H). **¹³C NMR** (101 MHz, $CDCl_3$) the major conformer: δ 163.4, 159.7, 139.5, 132.9, 132.5, 131.6, 128.8, 128.0, 127.3, 122.4; the minor conformer: δ 164.8, 163.5, 138.6, 132.7, 132.6, 131.5, 129.5, 128.1, 126.7, 121.7. **HRMS** (ESI) found: m/z 331.0010 $[M+Na]^+$; calcd. for $C_{14}H_{11}Cl_2N_2O_2Na^+$ 331.0012.

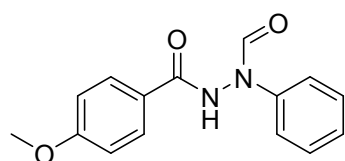


3-Chloro-*N'*-formyl-*N'*-phenylbenzohydrazide (1h): 321 mg, 78% yield; white solid; mp: 168-169 °C; **¹H NMR** (400 MHz, $CDCl_3$, two conformers are present, in a 87:13 ratio) δ 9.80 (s, 0.87H), 9.61 (s,

0.13H), 8.62 (s, 0.87H), 8.32 (s, 0.13H), 7.89 (s, 0.13H), 7.75 (s, 0.87H), 7.70 (d, $J = 7.8$ Hz, 1H), 7.54 – 7.24 (m, 7H). ^{13}C NMR (101 MHz, DMSO) the major conformer: δ 164.2, 159.8, 140.7, 133.7, 135.5, 132.2, 130.7, 129.4, 127.4, 126.4, 125.8, 119.5; the minor conformer: δ 165.4, 164.0, 139.6, 135.5, 133.4, 132.4, 130.7, 128.9, 127.5, 126.5, 125.7, 120.8. **HRMS** (ESI) found: m/z 297.0400 $[\text{M}+\text{Na}]^+$; calcd. for $\text{C}_{14}\text{H}_{11}\text{ClN}_2\text{O}_2\text{Na}^+$ 297.0401.

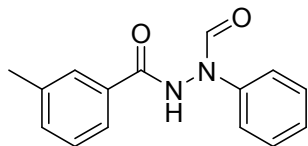


***N'*-Formyl-4-methyl-*N'*-phenylbenzohydrazide (1i):** 271 mg, 71% yield; white solid; mp: 148-149 °C; ^1H NMR (400 MHz, CDCl_3 , two conformers are present, in a 82:18 ratio) δ 9.32 (s, 0.18H), 9.21 (s, 0.82H), 8.64 (s, 0.82H), 8.34 (s, 0.18H), 7.80 (d, $J = 7.8$ Hz, 0.36H), 7.73 (d, $J = 8.0$ Hz, 1.64H), 7.53 – 7.15 (m, 7H), 2.43 (s, 0.54H), 2.39 (s, 2.46H). ^{13}C NMR (101 MHz, CDCl_3) the major conformer: δ 166.4, 160.5, 143.0, 140.3, 129.5, 129.2, 128.2, 127.7, 127.1, 121.5, 21.5; the minor conformer: δ 167.4, 164.2, 143.4, 139.4, 129.4, 128.9, 128.2, 127.7, 126.4, 122.1, 21.6. **HRMS** (ESI) found: m/z 277.0948 $[\text{M}+\text{Na}]^+$; calcd. for $\text{C}_{15}\text{H}_{14}\text{N}_2\text{O}_2\text{Na}^+$ 277.0947.

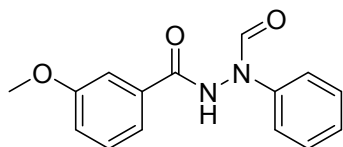


***N'*-Formyl-4-methoxy-*N'*-phenylbenzohydrazide (1j):** 284 mg, 70% yield; white solid; mp: 175-176 °C; ^1H NMR (400 MHz, CDCl_3 , two conformers are present, in a 82:18 ratio) δ 9.30 (m, 1H), 8.65 (s, 0.82H), 8.34 (s, 0.18H), 7.87 (d, $J = 8.6$ Hz, 0.36H), 7.81 (d, $J = 8.8$ Hz, 1.64H), 7.55 – 7.28 (m, 5H), 6.93 (d, $J = 8.7$ Hz, 0.36H), 6.83 (d, $J = 8.8$ Hz, 1.64H), 3.87 (s, 0.54H), 3.84 (s, 2.46H). ^{13}C NMR (101 MHz, DMSO) the major conformer: δ 164.8, 162.4, 159.9, 141.1, 129.6, 129.4, 125.7, 123.8, 119.5, 113.8, 55.4; the minor conformer: δ 166.1, 164.4, 162.6, 139.9, 129.7, 128.8, 125.6, 123.3, 120.8, 114.0, 55.5. **HRMS** (ESI) found: m/z 293.0898 $[\text{M}+\text{Na}]^+$; calcd.

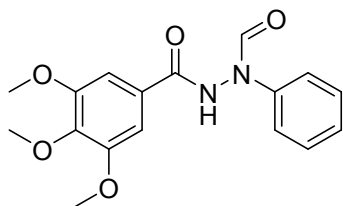
for $C_{15}H_{14}N_2O_3Na^+$ 293.0897.



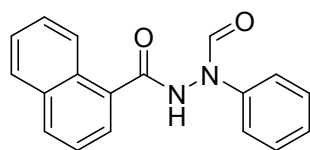
***N'*-Formyl-3-methyl-*N'*-phenylbenzohydrazide (1k):** 290 mg, 76% yield; white solid; mp: 171-174 °C; 1H NMR (400 MHz, $CDCl_3$, two conformers are present, in a 82:18 ratio) δ 9.41 (s, 0.18H), 9.32 (s, 0.82H), 8.63 (s, 0.82H), 8.33 (s, 0.18H), 7.66 (m, 2H), 7.51 – 7.25 (m, 7H), 2.39 (s, 0.54H), 2.34 (s, 2.46H). ^{13}C NMR (101 MHz, DMSO) the major conformer: δ 165.4, 159.9, 141.0, 138.0, 132.9, 131.8, 129.4, 128.5, 128.2, 125.7, 124.8, 119.5, 20.9; the minor conformer: δ 166.8, 164.3, 139.8, 138.1, 133.1, 131.4, 128.8, 128.6, 128.2, 125.6, 124.8, 120.8, 20.9. **HRMS** (ESI) found: m/z 277.0945 $[M+Na]^+$; calcd. for $C_{15}H_{14}N_2O_2Na^+$ 277.0947.



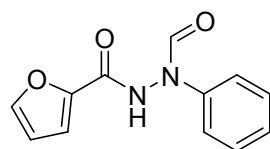
***N'*-Formyl-3-methoxy-*N'*-phenylbenzohydrazide (1l):** 300 mg, 74% yield; white solid; mp: 113-115 °C; 1H NMR (400 MHz, $CDCl_3$, two conformers are present, in a 84:16 ratio) δ 9.64 (s, 1H), 8.62 (s, 0.84H), 8.31 (s, 0.16H), 7.50 – 7.22 (m, 8H), 7.10 (dd, J = 8.2, 1.7 Hz, 0.16H), 7.01 (dd, J = 8.2, 2.3 Hz, 0.84H), 3.82 (s, 0.48H), 3.78 (s, 2.52H). ^{13}C NMR (101 MHz, $CDCl_3$) the major conformer: δ 166.1, 160.7, 159.6, 140.1, 132.2, 129.6, 128.9, 127.2, 121.6, 119.6, 119.1, 112.3, 55.3; the minor conformer: δ 167.3, 164.2, 159.8, 139.3, 132.4, 129.8, 129.6, 126.5, 122.2, 119.6, 112.7, 55.4. **HRMS** (ESI) found: m/z 293.0895 $[M+Na]^+$; calcd. for $C_{15}H_{14}N_2O_3Na^+$ 293.0897.



N'-Formyl-N'-phenyl-3,4,5-trimethoxybenzohydrazide (1m): 292 mg, 59% yield; white solid; mp: 144-145 °C; ¹H NMR (400 MHz, CDCl₃) δ 10.12 (s, 1H), 8.68 (s, 1H), 7.44-7.31 (m, 5H), 7.11 (s, 2H), 3.85 (s, 3H), 3.83 (s, 6H). ¹³C NMR (101 MHz, CDCl₃) the major conformer: δ 165.2, 161.2, 152.8, 140.1, 129.5, 127.4, 125.6, 121.9, 104.8, 60.7, 56.0; the minor conformer: δ 167.0, 164.2, 153.2, 141.4, 128.8, 126.5, 126.1, 122.2, 105.2, 60.9, 56.2. **HRMS** (ESI) found: m/z 353.1109 [M+Na]⁺; calcd. for C₁₇H₁₈N₂O₅Na⁺ 353.1108.

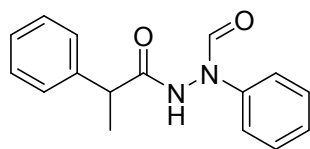


N'-Formyl-N'-phenyl-2-naphthohydrazide (1n): 348 mg, 80% yield; white solid; mp: 138-140 °C; ¹H NMR (400 MHz, CDCl₃, two conformers are present, in a 81:19 ratio) δ 9.19 (s, 0.19H), 8.58 (s, 0.81H), 8.46 (s, 0.81H), 8.39 (dd, *J* = 6.1, 3.4 Hz, 0.81H), 8.34 (s, 0.19H), 8.25 (d, *J* = 8.9 Hz, 0.19H), 7.94 (d, *J* = 8.2 Hz, 1H), 7.87 (dd, *J* = 6.1, 3.2 Hz, 1H), 7.78 (d, *J* = 6.9 Hz, 1H), 7.66 – 7.52 (m, 3H), 7.42 (q, *J* = 7.0 Hz, 2H), 7.35 (d, *J* = 7.3 Hz, 3H). ¹³C NMR (101 MHz, CDCl₃) the major conformer: δ 168.7, 159.9, 140.1, 133.5, 131.6, 129.6, 128.2, 127.5, 127.0, 126.6, 126.1, 125.2, 124.5, 121.2; the minor conformer: δ 169.1, 163.7, 139.2, 133.5, 131.8, 130.4, 130.2, 129.6, 128.9, 128.4, 126.5, 125.0, 124.4, 122.2. **HRMS** (ESI) found: m/z 313.0952 [M+Na]⁺; calcd. for C₁₈H₁₄N₂O₂Na⁺ 313.0947.

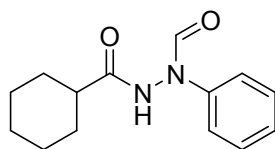


N'-Formyl-N'-phenylfuran-2-carbohydrazide (1o): 128 mg, 37% yield; ¹H NMR (400 MHz, CDCl₃, two conformers are present, in a 77:23 ratio) δ 9.80 (s, 0.23H), 9.57 (s, 0.77H), 8.61 (s, 0.77H), 8.33 (s, 0.23H), 7.55 – 7.23 (m, 6H), 7.21 (d, *J* = 7.4 Hz, 0.23H), 7.16 (d, *J* = 3.4 Hz, 0.77H), 6.52 (dd, *J* = 3.3, 1.5 Hz, 0.23H), 6.44 (dd, *J* = 3.5, 1.7 Hz, 0.77H). ¹³C NMR (101 MHz, CDCl₃) the major conformer: δ 160.4,

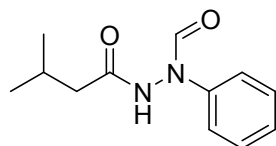
157.2, 145.5, 145.3, 140.2, 129.6, 127.3, 121.8, 116.6, 112.2; the minor conformer: δ 164.0, 158.1, 145.6, 145.3, 139.3, 129.0, 126.8, 122.5, 117.0, 112.4. **HRMS** (ESI) found: m/z 253.0578 $[M+Na]^+$; calcd. for $C_{12}H_{10}N_2O_2Na^+$ 253.0584.



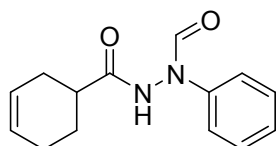
***N'*-Formyl-*N'*,2-diphenylpropionohydrazide (1p)**: 358 mg, 89% yield; white solid; mp: 98-101 °C; **¹H NMR** (400 MHz, $CDCl_3$, two conformers are present, in a 77:23 ratio) δ 8.55 (s, 0.23H), 8.49 (s, 0.77H), 8.11 (s, 0.23H), 8.01 (s, 0.77H), 7.37-7.24 (m, 8H), 7.18-7.10 (m, 2H), 3.76 (m, 1H), 1.57 (t, $J = 5.9$ Hz, 3H). **¹³C NMR** (101 MHz, $CDCl_3$) the major conformer: δ 173.8, 159.8, 140.2, 140.1, 129.5, 128.9, 127.7, 127.5, 126.8, 120.7, 44.7, 18.4; the minor conformer: δ 174.6, 163.8, 140.2, 139.2, 128.9, 127.4, 126.3, 121.5, 44.4, 18.3. **HRMS** (ESI) found: m/z 291.1107 $[M+Na]^+$; calcd. for $C_{16}H_{16}N_2O_2Na^+$ 291.1104.



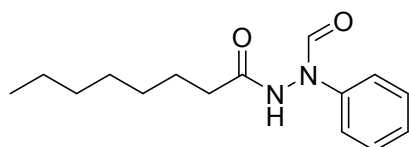
***N'*-Formyl-*N'*-phenylcyclohexanecarbohydrazide (1q)**: 340 mg, 92% yield; white solid; mp: 104-106 °C; **¹H NMR** (400 MHz, $CDCl_3$, two conformers are present, in a 77:23 ratio) δ 8.76 (s, 0.23H), 8.55 (s, 0.77H), 8.21 (s, 0.23H), 8.10 (s, 0.77H), 7.44 – 7.20 (m, 5H), 2.38 – 2.22 (m, 1H), 1.97-1.87 (m, 2H), 1.83 – 1.78 (m, 2H), 1.70 (d, $J = 7.9$ Hz, 1H), 1.60 – 1.48 (m, 2H), 1.33 – 1.20 (m, 3H). **¹³C NMR** (101 MHz, $CDCl_3$) the major conformer: δ 175.9, 159.6, 140.3, 129.5, 126.7, 120.8, 42.9, 29.3, 25.6, 25.4; the minor conformer: δ 176.7, 163.9, 139.3, 128.8, 126.2, 121.6, 42.7, 29.2, 25.5, 25.4. **HRMS** (ESI) found: m/z 269.1264 $[M+Na]^+$; calcd. for $C_{14}H_{18}N_2O_2Na^+$ 269.1260.



N'-Formyl-3-methyl-N'-phenylbutyrohydrazide (1r): 281 mg, 85% yield; white solid; mp: 98-99 °C; ^1H NMR (400 MHz, CDCl_3 , two conformers are present, in a 80:20 ratio) δ 8.62 (s, 0.20H), 8.57 (s, 0.80H), 8.26 (s, 0.20H), 8.08 (s, 0.80H), 7.47 – 7.25 (m, 5H), 2.26 – 2.15 (m, 3H), 1.03 – 0.98 (m, 6H). ^{13}C NMR (101 MHz, CDCl_3) the major conformer: δ 172.4, 159.8, 140.2, 129.5, 126.9, 121.1, 42.9, 26.0, 22.4; the minor conformer: δ 173.2, 163.9, 139.2, 128.9, 126.4, 122.0, 42.7, 25.9, 22.3. **HRMS** (ESI) found: m/z 243.1106 $[\text{M}+\text{Na}]^+$; calcd. for $\text{C}_{12}\text{H}_{16}\text{N}_2\text{O}_2\text{Na}^+$ 243.1104.

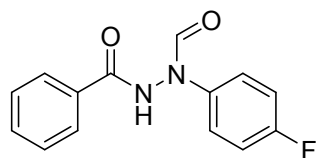


N'-Formyl-N'-phenyl-3-cyclohexenecarbohydrazide (1s): 231 mg, 63% yield; ^1H NMR (400 MHz, CDCl_3 , two conformers are present, in a 79:21 ratio) δ 8.81 (s, 0.21H), 8.56 (s, 0.79H), 8.24 (s, 0.21H), 8.20 (s, 0.79H), 7.45 – 7.24 (m, 5H), 5.81 – 5.62 (m, 2H), 2.64 – 2.52 (m, 1H), 2.33 – 2.03 (m, 4H), 1.95 – 1.63 (m, 2H). ^{13}C NMR (101 MHz, CDCl_3) the major conformer: δ 175.8, 159.7, 140.2, 129.5, 126.8, 126.7, 125.0, 120.9, 38.9, 27.7, 25.4, 24.3; the minor conformer: δ 176.5, 163.9, 139.2, 128.9, 126.7, 126.4, 124.9, 121.8, 38.7, 27.6, 25.3. **HRMS** (ESI) found: m/z 267.1107 $[\text{M}+\text{Na}]^+$; calcd. for $\text{C}_{14}\text{H}_{16}\text{N}_2\text{O}_2\text{Na}^+$ 267.1104.

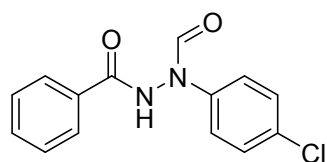


N'-Formyl-N'-phenyl-n-caprylhydrazide (1t): 335 mg, 85% yield; ^1H NMR (400 MHz, CDCl_3 , two conformers are present, in a 80:20 ratio) δ 8.95 (s, 0.20H), 8.54 (s, 0.80H), 8.37 (s, 0.80H), 8.22 (s, 0.20H), 7.46 – 7.24 (m, 5H), 2.33 (t, J = 7.6 Hz, 2H), 1.68 (m, 2H), 1.35 – 1.23 (m, 8H), 0.89 (t, J = 6.6 Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) the major conformer: δ 173.1,

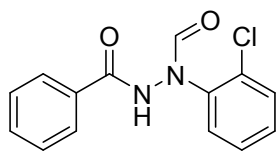
159.9, 140.2, 129.5, 126.9, 121.1 33.9, 31.6, 29.1, 28.9, 25.3, 22.6, 14.0; the minor conformer: δ 173.9, 164.0, 139.3, 128.8, 126.4, 121.9, 33.7, 25.2. **HRMS** (ESI) found: m/z 285.1579 $[M+Na]^+$; calcd. for $C_{15}H_{22}N_2O_2Na^+$ 285.1573.



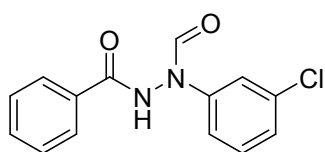
***N'*-(4-Fluorophenyl)-*N'*-formylbenzohydrazide (2a):** 353 mg, 91% yield; white solid; mp: 132-134 °C; **¹H NMR** (400 MHz, $CDCl_3$, two conformers are present, in a 75:25 ratio) δ 9.81 (s, 0.25H), 9.63 (s, 0.75H), 8.49 (s, 0.75H), 8.28 (s, 0.25H), 7.87 (d, $J = 7.4$ Hz, 0.5H), 7.78 (d, $J = 7.4$ Hz, 1.50H), 7.60 – 7.41 (m, 2H), 7.36 - 7.31 (m, 3H), 7.13 – 7.01 (m, 1.50H), 6.95 (t, $J = 8.6$ Hz, 0.50H). **¹³C NMR** (101 MHz, $CDCl_3$) the major conformer: δ 166.5, 162.7 - 160.3 (d, $J_{F-C} = 247.5$ Hz), 160.5, 136.22 - 136.19 (d, $J_{F-C} = 2.6$ Hz), 132.7, 130.8, 128.6, 127.6, 124.4 - 124.3 (d, $J_{F-C} = 8.6$ Hz), 116.5 - 116.3 (d, $J_{F-C} = 23.0$ Hz); the minor conformer: δ 167.6, 164.3, 162.0 - 159.5 (d, $J_{F-C} = 246.7$ Hz), 135.21 – 135.19 (d, $J_{F-C} = 2.3$ Hz), 132.9, 128.8, 127.7, 124.7 - 124.6 (d, $J_{F-C} = 8.4$ Hz), 115.8 - 115.6 (d, $J_{F-C} = 22.8$ Hz). **HRMS** (ESI) found: m/z 281.0702 $[M+Na]^+$; calcd. for $C_{14}H_{11}FN_2O_2Na^+$ 281.0697.



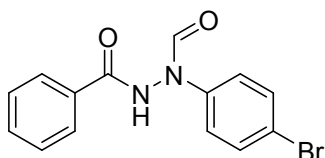
***N'*-(4-Chlorophenyl)-*N'*-formylbenzohydrazide (2b):** 350 mg, 85% yield; white solid; mp: 128-130 °C; **¹H NMR** (400 MHz, $CDCl_3$, two conformers are present, in a 75:25 ratio) δ 9.78 (s, 0.25H), 9.45 (s, 0.75H), 8.59 (s, 0.75H), 8.28 (s, 0.25H), 7.88 (d, $J = 7.6$ Hz, 0.50H), 7.81 (d, $J = 7.5$ Hz, 1.50H), 7.60 – 7.15 (m, 7H). **¹³C NMR** (101 MHz, $CDCl_3$) the major conformer: δ 166.8, 160.0, 141.2, 135.2, 132.8, 130.6, 128.7, 127.7, 127.1, 121.0, 119.0; the minor conformer: δ 167.7, 164.2, 140.3, 134.5, 133.1, 130.0, 128.9, 127.7, 126.5, 121.8, 119.5. **HRMS** (ESI) found: m/z 297.0403 $[M+Na]^+$; calcd. for $C_{14}H_{11}ClN_2O_2Na^+$ 297.0401.



***N'*-(2-Chlorophenyl)-*N'*-formylbenzohydrazide (2c):** 367 mg, 89% yield; white solid; mp: 126-128 °C; ¹H NMR (400 MHz, CDCl₃, two conformers are present, in a 71:29 ratio) δ 9.10 (s, 0.71H), 9.04 (s, 0.29H), 8.43 (s, 0.29H), 8.41 (s, 0.71H), 7.89 – 7.75 (m, 3H), 7.59 – 7.34 (m, 6H). ¹³C NMR (101 MHz, CDCl₃) the major conformer: δ 166.2, 161.7, 137.1, 132.4, 131.5, 130.6, 130.2, 130.0, 128.6, 128.1, 127.7; the minor conformer: δ 167.3, 164.4, 136.3, 132.8, 131.4, 131.0, 130.6, 130.1, 128.8, 127.8. **HRMS** (ESI) found: m/z 297.0399 [M+Na]⁺; calcd. for C₁₄H₁₁ClN₂O₂Na⁺ 297.0401.

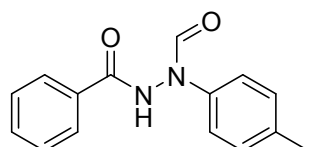


***N'*-(3-Chlorophenyl)-*N'*-formylbenzohydrazide (2d):** 342 mg, 83% yield; white solid; mp: 97-99 °C; ¹H NMR (400 MHz, CDCl₃, two conformers are present, in a 75:25 ratio) δ 9.78 (s, 0.25H), 9.45 (s, 0.75H), 8.59 (s, 0.75H), 8.28 (s, 0.25H), 7.88 (d, *J* = 7.6 Hz, 0.50H), 7.81 (d, *J* = 7.5 Hz, 1.50H), 7.62 – 7.15 (m, 7H). ¹³C NMR (101 MHz, CDCl₃) the major conformer: δ 166.8, 160.0, 141.2, 135.2, 132.8, 130.6, 128.7, 127.7, 127.1, 121.0, 119.0; the minor conformer: δ 167.7, 164.2, 140.3, 134.5, 133.1, 130.0, 128.9, 127.7, 126.5, 121.8, 119.5. **HRMS** (ESI) found: m/z 297.0404 [M+Na]⁺; calcd. for C₁₄H₁₁ClN₂O₂Na⁺ 297.0401.

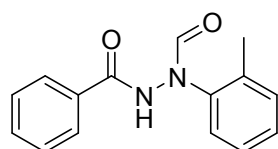


***N'*-(4-Bromophenyl)-*N'*-formylbenzohydrazide (2e):** 388 mg, 81% yield; white solid; mp: 111-113 °C; ¹H NMR (400 MHz, CDCl₃, two conformers are present, in a 74:26 ratio) δ 9.69 (s, 0.26H), 9.42 (s,

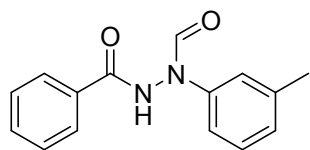
0.74H), 8.55 (s, 0.74H), 8.29 (s, 0.26H), 7.87 (d, $J = 7.6$ Hz, 0.52H), 7.79 (d, $J = 7.5$ Hz, 1.48H), 7.56 – 7.18 (m, 7H). **¹³C NMR** (101 MHz, CDCl₃) the major conformer: δ 166.6, 160.1, 139.2, 132.8, 132.6, 130.7, 128.7, 127.6, 122.8, 120.6; the minor conformer: δ 167.5, 164.1, 138.2, 133.1, 131.9, 128.9, 127.7, 123.4, 119.6. **HRMS** (ESI) found: m/z 340.9897 [M+Na]⁺; calcd. for C₁₄H₁₁BrN₂O₂Na⁺ 340.9896.



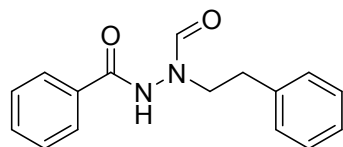
***N'*-Formyl-*N'*-(4-methylphenyl)benzohydrazide (2f)**: 286 mg, 75% yield; white solid; mp: 117-118 °C; **¹H NMR** (400 MHz, CDCl₃, two conformers are present, in a 82:18 ratio) δ 9.56 (s, 0.18H), 9.48 (s, 0.82H), 8.56 (s, 0.82H), 8.31 (s, 0.18H), 7.89 (d, $J = 7.5$ Hz, 0.36H), 7.81 (d, $J = 7.5$ Hz, 1.64H), 7.49 – 7.17 (m, 7H), 2.36 (s, 2.46H), 2.31 (s, 0.54H). **¹³C NMR** (101 MHz, CDCl₃) the major conformer: δ 166.4, 160.7, 137.7, 137.2, 132.4, 131.0, 130.1, 128.5, 127.7, 122.0, 21.0; the minor conformer: δ 167.6, 164.3, 136.8, 136.4, 132.7, 131.1, 129.5, 128.7, 127.8, 122.6, 21.1. **HRMS** (ESI) found: m/z 277.0948 [M+Na]⁺; calcd. for C₁₅H₁₄N₂O₂Na⁺ 277.0947.



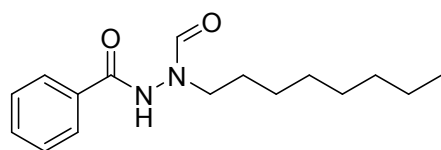
***N'*-Formyl-*N'*-(2-methylphenyl)benzohydrazide (2g)**: 275 mg, 72% yield; white solid; mp: 119-120 °C; **¹H NMR** (400 MHz, CDCl₃, two conformers are present, in a 82:18 ratio) δ 9.85 (s, 0.82H), 9.54 (s, 0.18H), 8.35 (s, 0.82H), 8.34 (s, 0.18H), 7.81 (d, $J = 7.3$ Hz, 0.36H), 7.73 (d, $J = 7.3$ Hz, 1.64H), 7.60 – 7.24 (m, 7H), 2.46 (s, 2.46H), 2.36 (s, 0.54H). **¹³C NMR** (101 MHz, CDCl₃) the major conformer: δ 166.0, 162.2, 138.3, 135.1, 132.3, 131.5, 130.9, 128.7, 128.5, 127.6, 127.1, 18.2; the minor conformer: δ 167.4, 164.2, 138.1, 136.0, 132.3, 131.3, 129.0, 128.2, 127.7, 126.9, 126.8, 18.3. **HRMS** (ESI) found: m/z 277.0945 [M+Na]⁺; calcd. for C₁₅H₁₄N₂O₂Na⁺ 277.0947.



N'-Formyl-N'-(3-methylphenyl)benzohydrazide (2h): 305 mg, 80% yield; white solid; mp: 116-118 °C; ¹H NMR (400 MHz, CDCl₃, two conformers are present, in a 83:17 ratio) δ 9.59 (s, 0.17H), 9.49 (s, 0.83H), 8.60 (s, 0.83H), 8.31 (s, 0.17H), 7.90 (d, *J* = 7.4 Hz, 0.34H), 7.82 (d, *J* = 7.5 Hz, 1.66H), 7.55 – 7.07 (m, 7H), 2.36 (s, 2.49H), 2.30 (s, 0.51H). ¹³C NMR (101 MHz, CDCl₃) the major conformer: δ 166.2, 160.6, 140.1, 139.7, 132.4, 129.4, 128.6, 128.1, 127.6, 122.3, 118.8, 21.4; the minor conformer: δ 167.2, 164.1, 139.2, 138.9, 132.7, 131.0, 128.8, 127.7, 127.5, 123.1, 119.5, 21.4. **HRMS** (ESI) found: *m/z* 277.0945 [M+Na]⁺; calcd. for C₁₅H₁₄N₂O₂Na⁺ 277.0947.

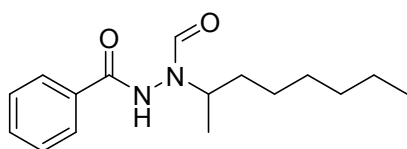


N'-Formyl-N'-(2-phenylethyl)benzohydrazide (2i): 298 mg, 74% yield; white solid; mp: 80-82 °C; ¹H NMR (400 MHz, CDCl₃, two conformers are present, in a 53:47 ratio) δ 9.15 (br s, 0.47H), 8.32 (br s, 0.53H), 8.06 (s, 0.53H), 7.88 (s, 0.47H), 7.71 (dd, *J* = 8.2, 1.1 Hz, 0.94H), 7.58 (dt, *J* = 8.5, 1.6 Hz, 1.06H), 7.55 – 7.17 (m, 8H), 3.90 (t, *J* = 7.1 Hz, 0.94H), 3.83 (t, *J* = 6.9 Hz, 1.06H), 2.92 (t, *J* = 7.1 Hz, 2H). ¹³C NMR (101 MHz, CDCl₃) the major conformer: δ 167.1, 165.2, 137.8, 132.7, 131.2, 128.8, 128.6, 127.4, 126.7, 47.7, 33.6; the minor conformer: δ 166.3, 161.2, 138.7, 132.4, 131.2, 128.8, 128.5, 127.5, 126.9, 51.4, 34.4. **HRMS** (ESI) found: *m/z* 291.1107 [M+Na]⁺; calcd. for C₁₅H₁₄N₂O₂Na⁺ 291.1104.

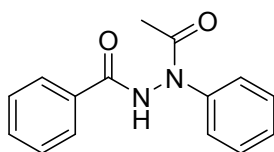


N'-Formyl-N'-(n-octyl)benzohydrazide

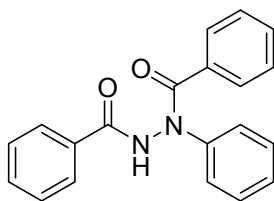
(2j): 286 mg, 69% yield; $^1\text{H NMR}$ (400 MHz, CDCl_3 , two conformers are present, in a 56:44 ratio) δ 9.36 (s, 0.56H), 8.97 (s, 0.44H), 8.13 (s, 1H), 7.87 (d, $J = 7.4$ Hz, 0.88H), 7.74 (d, $J = 7.3$ Hz, 1.12H), 7.61 – 7.31 (m, 3H), 3.59 (m, 2H), 1.66 – 1.54 (m, 2H), 1.31 – 1.25 (m, 10H), 0.88 (q, $J = 6.8$ Hz, 3H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) the major conformer: δ 167.5, 165.3, 132.6, 131.4, 128.7, 127.6, 46.2, 31.7, 29.20, 29.17, 26.83, 26.78, 22.6, 14.0; the minor conformer: δ 166.0, 161.3, 132.2, 131.1, 128.4, 127.5, 49.9, 31.7, 29.2, 29.1, 27.6, 26.4, 22.6, 14.0. **HRMS** (ESI) found: m/z 299.1735 $[\text{M}+\text{Na}]^+$; calcd. for $\text{C}_{16}\text{H}_{24}\text{N}_2\text{O}_2\text{Na}^+$ 299.1730.



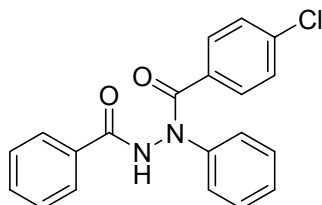
***N'*-Formyl-*N'*-(sec-octyl)benzohydrazide (2k)**: 253 mg, 61% yield; $^1\text{H NMR}$ (400 MHz, CDCl_3 , two conformers are present, in a 57:43 ratio) δ 8.60 (s, 0.57H), 8.44 (s, 0.43H), 8.16 (s, 0.57H), 8.08 (s, 0.43H), 7.83 (d, $J = 7.2$ Hz, 0.86H), 7.76 (d, $J = 7.2$ Hz, 1.14H), 7.60 – 7.31 (m, 3H), 4.57 – 4.52 (m, 0.43H), 3.85 – 3.72 (m, 0.57H), 1.78 – 1.15 (m, 13H), 0.88 (q, $J = 6.9$ Hz, 3H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) the major conformer: δ 167.0, 161.1, 132.1, 131.7, 128.4, 127.6, 57.1, 34.5, 31.7, 28.9, 26.3, 22.6, 18.9, 14.0; the minor conformer: δ 168.0, 165.2, 132.5, 131.4, 128.7, 127.6, 51.3, 33.7, 29.1, 26.4, 22.6, 17.4, 14.0. **HRMS** (ESI) found: m/z 299.1733 $[\text{M}+\text{Na}]^+$; calcd. for $\text{C}_{16}\text{H}_{24}\text{N}_2\text{O}_2\text{Na}^+$ 299.1730.



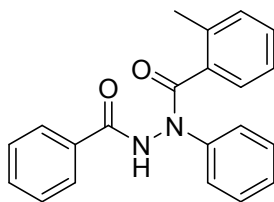
***N'*-Acetyl-*N'*-phenylbenzohydrazide (3a)**:² 328 mg, 86% yield; $^1\text{H NMR}$ (400 MHz, CDCl_3 , two conformers are present, in a 68:32 ratio) δ 9.74 (s, 0.32H), 9.45 (s, 0.68H), 7.85 – 7.24 (m, 10H), 2.22 (s, 0.96H), 2.07 (s, 2.04H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) the major conformer: δ 170.3, 166.6, 141.2, 132.6, 131.5, 128.7, 127.6, 124.8, 21.7; the minor conformer: δ 173.0, 166.6, 142.1, 132.1, 129.5, 128.5, 126.8, 22.2. **HRMS** (ESI) found: m/z 277.0943 $[\text{M}+\text{Na}]^+$; calcd. for $\text{C}_{15}\text{H}_{14}\text{N}_2\text{O}_2\text{Na}^+$ 277.0947.



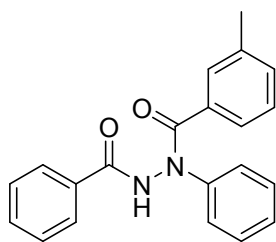
***N'*-Benzoyl-*N'*-phenylbenzohydrazide (3b):**³ 346 mg, 73% yield; white solid; mp: 175-177 °C; ¹H NMR (400 MHz, CDCl₃) δ 9.43 (s, 1H), 7.78 (d, *J* = 7.2 Hz, 2H), 7.33 (m, 13H); ¹³C NMR (101 MHz, DMSO) δ 165.9, 135.8, 132.7, 132.3, 130.8, 129.2, 129.1, 128.3, 128.0, 127.8, 126.7.



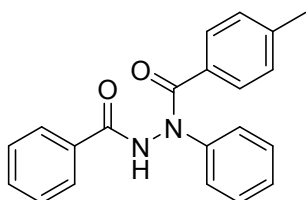
***N'*-(4-Chlorobenzoyl)-*N'*-phenylbenzohydrazide (3c):**³ 405 mg, 77% yield; ¹H NMR (400 MHz, DMSO) δ 11.59 (s, 1H), 7.73 (s, 2H), 7.63 – 7.55 (m, 3H), 7.51 – 7.37 (m, 8H), 7.26 (t, *J* = 6.5 Hz, 1H); ¹³C NMR (101 MHz, DMSO) δ 165.9, 135.6, 134.6, 132.8, 132.1, 130.0, 129.3, 129.1, 128.5, 127.8, 126.9.



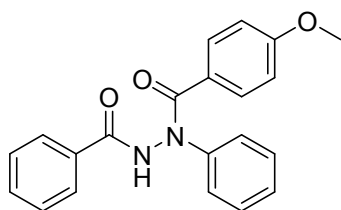
***N'*-(2-Methylbenzoyl)-*N'*-phenylbenzohydrazide (3d):** 282 mg, 57% yield; ¹H NMR (400 MHz, DMSO) δ 11.39 (s, 1H), 7.90 – 6.96 (m, 14H), 2.41 (s, 3H); ¹³C NMR (101 MHz, DMSO) δ 166.4, 136.2, 135.4, 132.6, 132.5, 130.7, 129.6, 129.2, 129.0, 127.8, 125.4, 124.1, 19.4. **HRMS** (ESI) found: *m/z* 353.1259 [M+Na]⁺; calcd. for C₂₁H₁₈N₂O₂Na⁺ 353.1260.



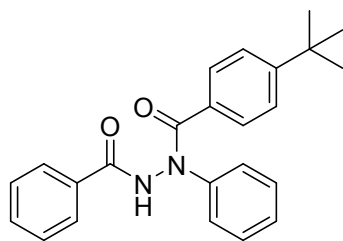
***N'*-(3-Methylbenzoyl)-*N'*-phenylbenzohydrazide (3e):** 352 mg, 71% yield; **¹H NMR** (400 MHz, DMSO) δ 11.52 (s, 1H), 7.71 (s, 2H), 7.57 (t, J = 7.3 Hz, 1H), 7.51 – 7.32 (m, 8H), 7.29 – 7.19 (m, 3H), 2.28 (s, 3H); **¹³C NMR** (101 MHz, DMSO) δ 166.0, 142.6, 137.6, 135.7, 132.7, 132.4, 131.5, 129.2, 129.1, 128.7, 128.2, 127.8, 126.7, 125.2, 124.8, 21.3. **HRMS** (ESI) found: m/z 353.1259 [M+Na]⁺; calcd. for C₂₁H₁₈N₂O₂Na⁺ 353.1260.



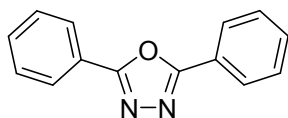
***N'*-(4-Methylbenzoyl)-*N'*-phenylbenzohydrazide (3f):**⁴ 327 mg, 66% yield; white solid; mp: 158-159 °C; **¹H NMR** (400 MHz, DMSO) δ 11.52 (s, 1H), 7.76 (d, J = 6.8 Hz, 2H), 7.57 (t, J = 7.3 Hz, 1H), 7.48 (t, J = 7.6 Hz, 4H), 7.38 (d, J = 5.8 Hz, 4H), 7.21 (m, 3H), 2.28 (s, 3H); **¹³C NMR** (101 MHz, DMSO) δ 165.8, 140.8, 132.8, 132.7, 132.3, 129.2, 129.1, 128.9, 128.3, 127.8, 126.7, 124.8, 21.40.



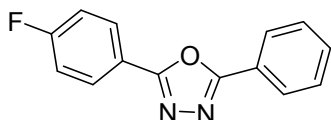
***N'*-(4-Methoxybenzoyl)-*N'*-phenylbenzohydrazide (3g):**³ 223 mg, 43% yield; white solid; mp: 191-193 °C; **¹H NMR** (400 MHz, DMSO) δ 11.52 (s, 1H), 7.78 (d, J = 7.2 Hz, 2H), 7.57 (d, J = 7.2 Hz, 3H), 7.49 (t, J = 7.5 Hz, 2H), 7.37 (d, J = 4.0 Hz, 4H), 7.27 – 7.16 (m, 1H), 6.92 (d, J = 8.6 Hz, 2H), 3.75 (s, 3H); **¹³C NMR** (101 MHz, DMSO) δ 165.8, 161.4, 143.0, 132.7, 132.3, 130.5, 129.2, 129.1, 127.8, 127.5, 126.5, 124.7, 113.7, 55.7.



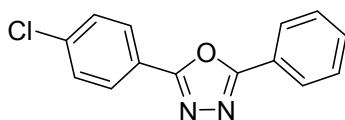
***N'*-(4-*tert*-Butylbenzoyl)-*N'*-phenylbenzohydrazide (3h):** 330 mg, 59% yield; white solid; ^1H NMR (400 MHz, DMSO) δ 11.50 (s, 1H), 7.69 (d, J = 6.3 Hz, 2H), 7.58 – 7.52 (m, 3H), 7.49 – 7.35 (m, 8H), 7.23 (t, J = 6.8 Hz, 1H), 1.24 (s, 9H); ^{13}C NMR (101 MHz, DMSO) δ 166.1, 153.7, 132.9, 132.6, 132.5, 129.2, 129.0, 128.2, 127.8, 127.4, 126.6, 125.4, 125.1, 124.8, 35.0, 31.3. **HRMS** (ESI) found: m/z 395.1728 $[\text{M}+\text{Na}]^+$; calcd. for $\text{C}_{24}\text{H}_{24}\text{N}_2\text{O}_3\text{Na}^+$ 395.1730.



2,5-Diphenyl-1,3,4-oxadiazole (6a):⁵ 283 mg, 85% yield; ^1H NMR (400 MHz, CDCl_3) δ 8.20 – 8.05 (m, 4H), 7.56 – 7.47 (m, 6H); ^{13}C NMR (101 MHz, CDCl_3) δ 164.5, 131.7, 129.0, 126.9, 123.9.

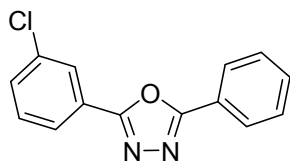


2-(4-Fluorophenyl)-5-phenyl-1,3,4-oxadiazole (6b):⁵ 238 mg, 66% yield; ^1H NMR (400 MHz, CDCl_3) δ 8.16 - 8.11 (m, 4H), 7.56 – 7.51 (m, 3H), 7.23 (t, J = 8.6 Hz, 2H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.0 - 163.8 (d, $J_{\text{F-C}}$ = 230.4 Hz), 164.6, 163.5, 131.8, 129.24 - 129.15 (d, $J_{\text{F-C}}$ = 8.9 Hz), 129.1, 126.9, 123.8, 120.30 - 120.27 (d, $J_{\text{F-C}}$ = 3.2 Hz), 116.5 - 116.3 (d, $J_{\text{F-C}}$ = 22.3 Hz).

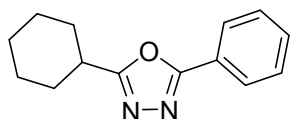


2-(4-Chlorophenyl)-5-phenyl-1,3,4-oxadiazole (6c and 6c'):⁵ 277 mg, 72% yield;

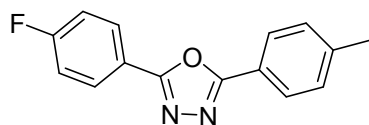
¹H NMR (400 MHz, CDCl₃) δ 8.16 (dd, *J* = 7.8, 1.8 Hz, 2H), 8.11 (d, *J* = 8.6 Hz, 2H), 7.62 – 7.52 (m, 5H); **¹³C NMR** (101 MHz, CDCl₃) δ 164.7, 163.7, 137.9, 131.9, 129.4, 129.1, 128.1, 126.9, 123.7, 122.3.



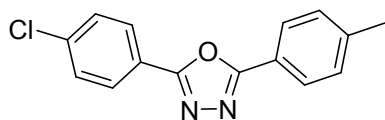
2-(3-Chlorophenyl)-5-phenyl-1,3,4-oxadiazole (6d):⁶ 320 mg, 83% yield; **¹H NMR** (400 MHz, CDCl₃) δ 8.23 – 8.12 (m, 3H), 8.07 (dt, *J* = 7.5, 1.4 Hz, 1H), 7.62 – 7.48 (m, 5H); **¹³C NMR** (101 MHz, CDCl₃) δ 164.8, 163.4, 135.2, 132.0, 131.7, 130.5, 129.1, 127.0, 126.8, 125.5, 125.0, 123.6.



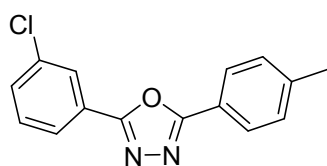
2-Cyclohexyl-5-phenyl-1,3,4-oxadiazole (6e):⁷ 253 mg, 74% yield; **¹H NMR** (400 MHz, CDCl₃) δ 8.04 (dd, *J* = 7.4, 1.7 Hz, 2H), 7.54 – 7.46 (m, 3H), 3.03 – 2.96 (m, 1H), 2.19 – 2.09 (m, 2H), 1.91 – 1.84 (m, 2H), 1.77 - 1.64 (m, 3H), 1.49 – 1.28 (m, 3H); **¹³C NMR** (101 MHz, CDCl₃) δ 170.0, 164.4, 131.5, 129.0, 126.8, 124.2, 35.3, 30.2, 25.6, 25.4.



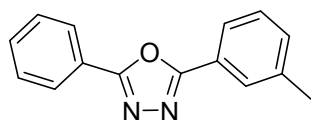
2-(4-Fluorophenyl)-5-(4-methylphenyl)-1,3,4-oxadiazole (6f): 278 mg, 73% yield; **¹H NMR** (400 MHz, CDCl₃) δ 8.19 – 8.09 (m, 2H), 8.01 (d, *J* = 8.2 Hz, 2H), 7.33 (d, *J* = 8.0 Hz, 2H), 7.28 – 7.20 (m, 2H), 2.44 (s, 3H); **¹³C NMR** (101 MHz, CDCl₃) δ 166.0 - 163.5 (d, *J*_{F-C} = 249.8 Hz), 164.7, 163.4, 142.3, 129.8, 129.2 - 129.1 (d, *J*_{F-C} = 8.8 Hz), 126.8, 121.0, 120.39 - 120.35 (d, *J*_{F-C} = 3.4 Hz), 116.5 - 116.2 (d, *J*_{F-C} = 22.3 Hz), 21.6.



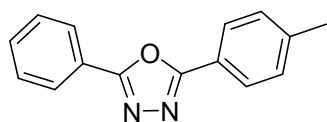
2-(4-Chlorophenyl)-5-(4-methylphenyl)-1,3,4-oxadiazole (6g):⁸ 329 mg, 81% yield; ¹H NMR (400 MHz, CDCl₃) δ 8.10 (d, *J* = 8.6 Hz, 2H), 8.04 (d, *J* = 8.2 Hz, 2H), 7.54 (d, *J* = 8.6 Hz, 2H), 7.36 (d, *J* = 8.0 Hz, 2H), 2.47 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 164.8, 163.5, 142.5, 137.8, 129.8, 129.4, 128.1, 126.9, 122.5, 120.9, 21.7.



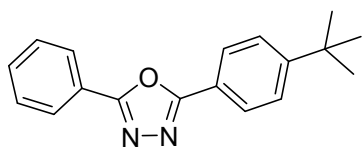
2-(3-Chlorophenyl)-5-(4-methylphenyl)-1,3,4-oxadiazole (6h): 345 mg, 85% yield; ¹H NMR (400 MHz, CDCl₃) δ 8.14 (t, *J* = 1.7 Hz, 1H), 8.07 – 8.04 (m, 3H), 7.56 – 7.48 (m, 2H), 7.37 (d, *J* = 7.9 Hz, 2H), 2.47 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 165.0, 163.1, 142.6, 135.2, 131.6, 130.4, 129.8, 126.9, 126.8, 125.6, 125.0, 120.8, 21.71.



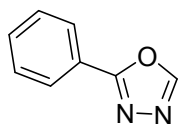
2-(3-Methylphenyl)-5-phenyl-1,3,4-oxadiazole (6i):⁶ 276 mg, 78% yield; ¹H NMR (400 MHz, CDCl₃) δ 8.22 – 8.14 (m, 2H), 8.00 (s, 1H), 7.97 (d, *J* = 7.6 Hz, 1H), 7.61 – 7.53 (m, 3H), 7.44 (d, *J* = 7.6 Hz, 1H), 7.39 (d, *J* = 7.6 Hz, 1H), 2.49 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 164.7, 164.5, 139.0, 132.5, 131.7, 129.1, 129.0, 127.4, 126.9, 124.1, 124.0, 123.8, 21.4.



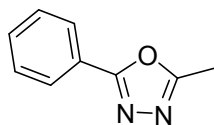
2-(4-Methylphenyl)-5-phenyl-1,3,4-oxadiazole (6j):⁷ 287 mg, 81% yield; ¹H NMR (400 MHz, CDCl₃) δ 8.21 – 8.13 (m, 2H), 8.06 – 8.04 (m, 2H), 7.61 – 7.52 (m, 3H), 7.36 (dd, *J* = 6.7, 1.8 Hz, 2H), 2.47 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 164.7, 164.3, 142.3, 131.6, 129.8, 129.0, 126.9, 126.8, 124.0, 121.1, 21.6.



2-(4-*tert*-Butylphenyl)-5-phenyl-1,3,4-oxadiazole (6k):⁵ 380 mg, 91% yield; ¹H NMR (400 MHz, CDCl₃) δ 8.21 – 8.14 (m, 2H), 8.10 (d, *J* = 8.6 Hz, 2H), 7.61 – 7.53 (m, 5H), 1.40 (s, 9H); ¹³C NMR (101 MHz, CDCl₃) δ 164.6, 164.3, 155.3, 131.6, 129.0, 126.9, 126.8, 126.1, 123.9, 121.0, 35.1, 31.1.

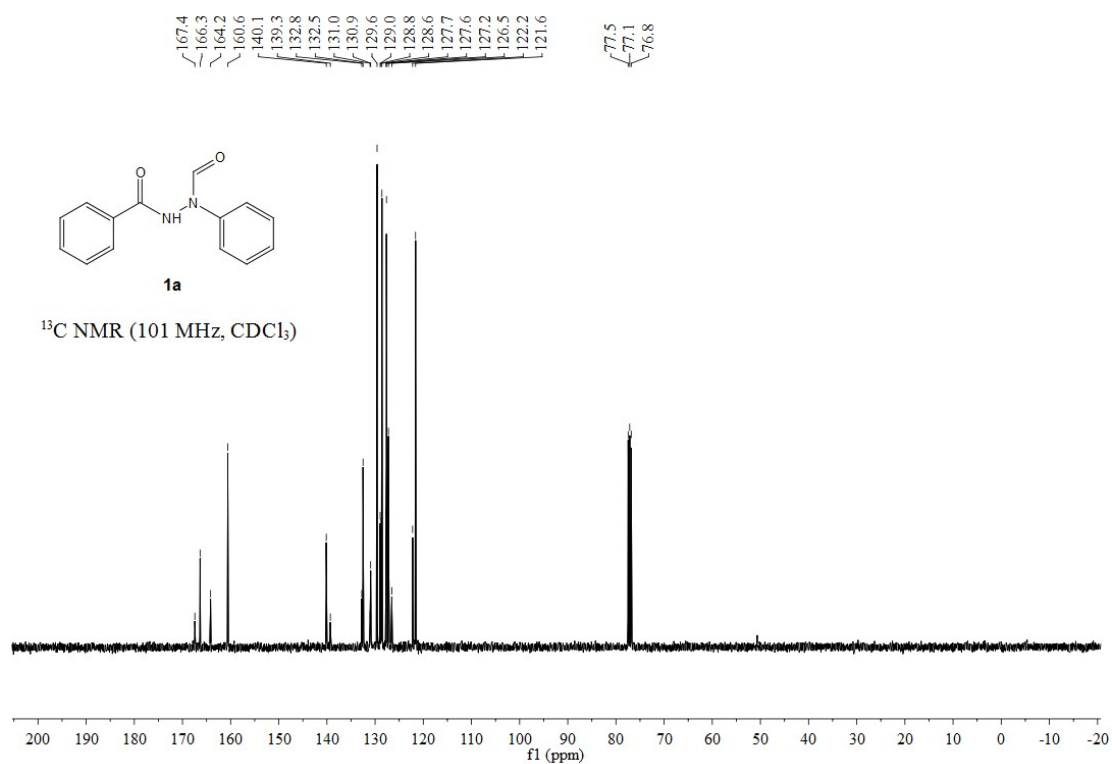
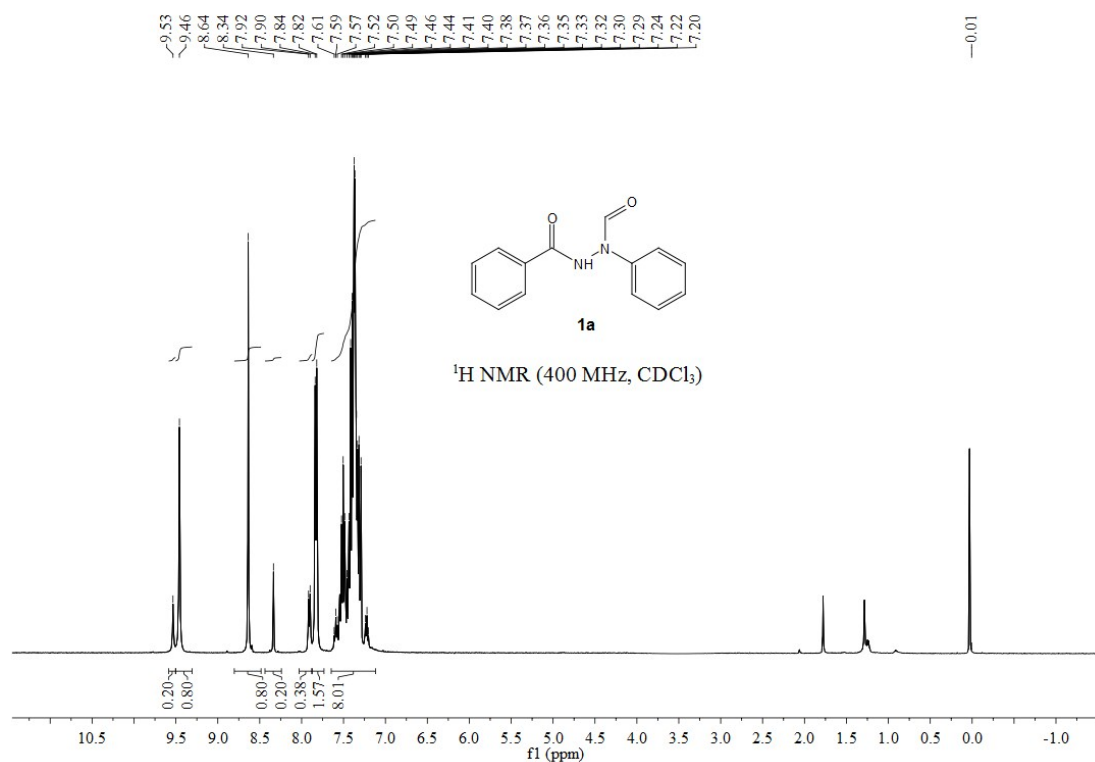


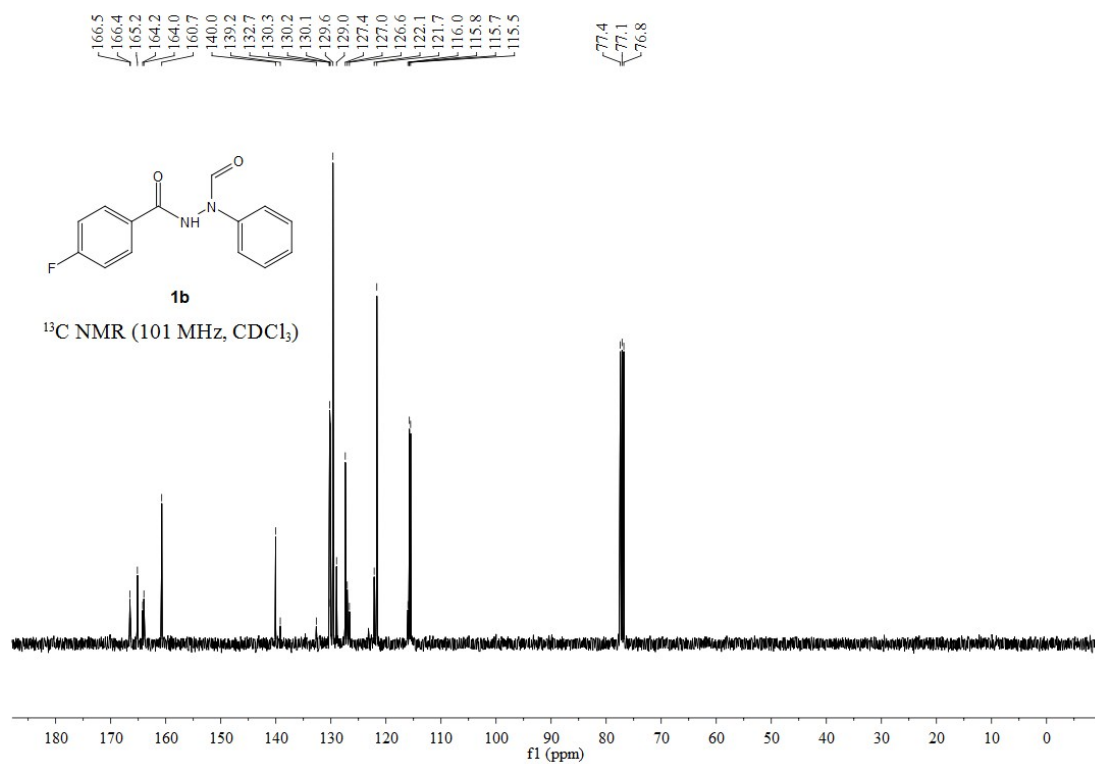
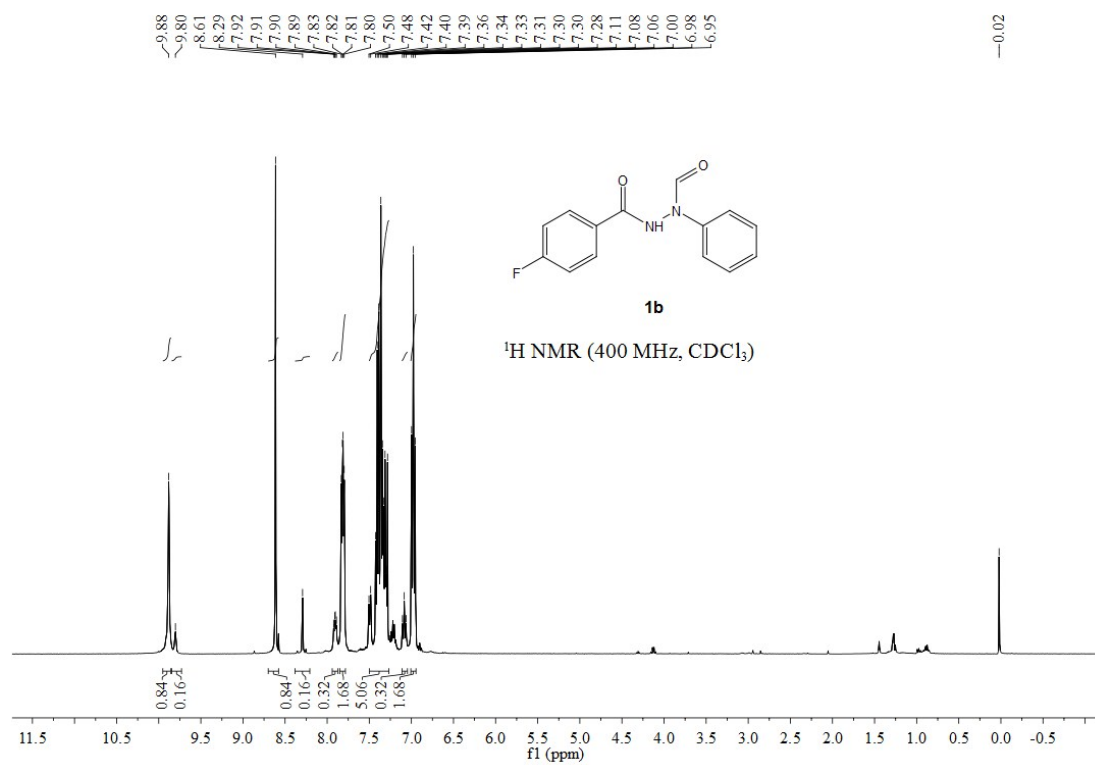
2-Phenyl-1,3,4-oxadiazole (6l):⁹ 195 mg, 89% yield; ¹H NMR (400 MHz, CDCl₃) δ 8.51 (s, 1H), 8.12 (dd, *J* = 8.1, 1.5 Hz, 2H), 7.61 – 7.53 (m, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 164.8, 152.7, 132.0, 129.2, 127.1, 123.5.

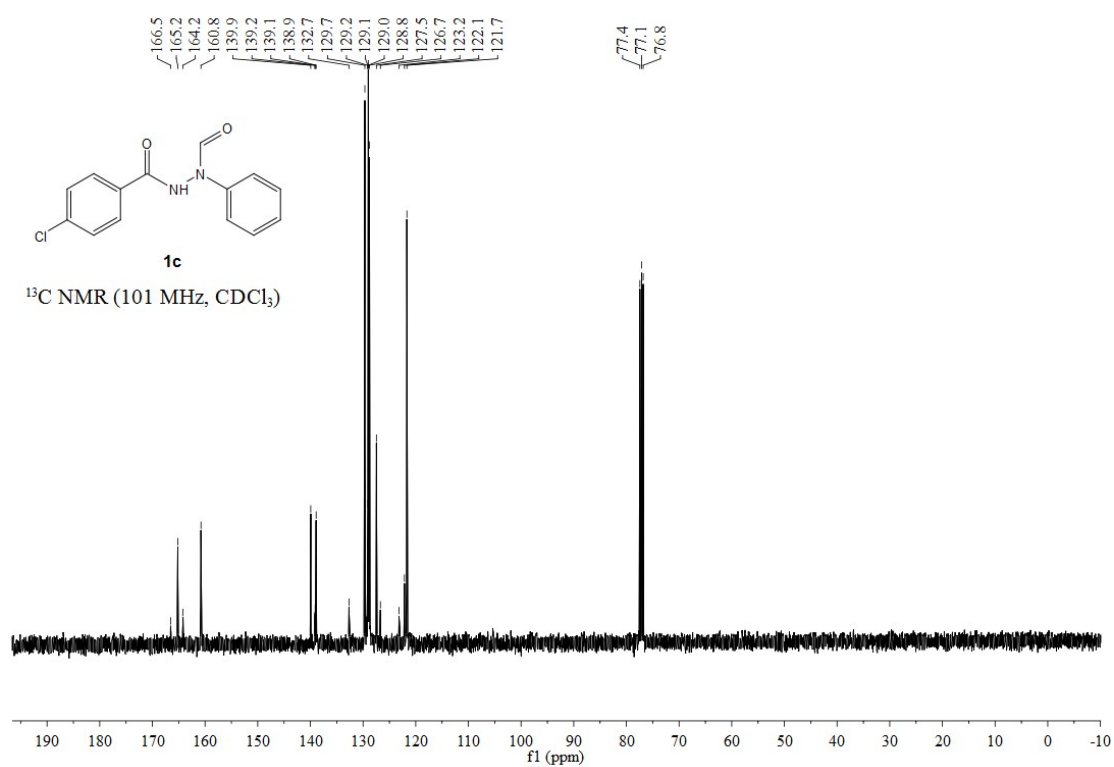
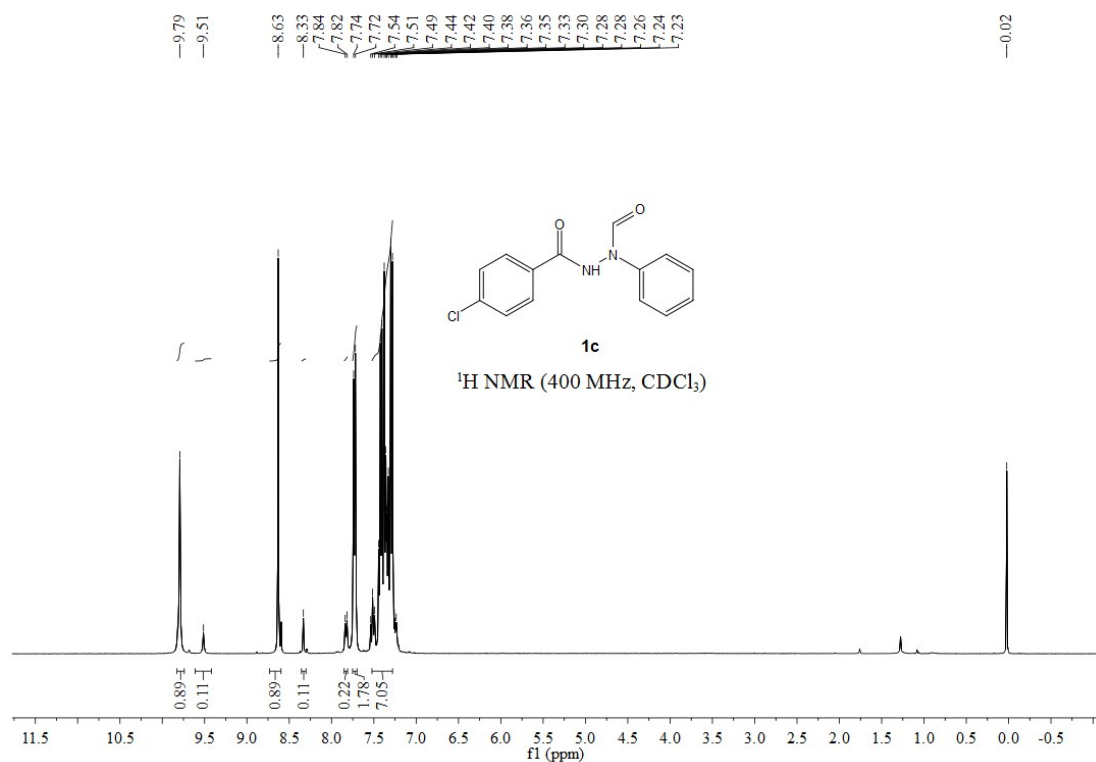


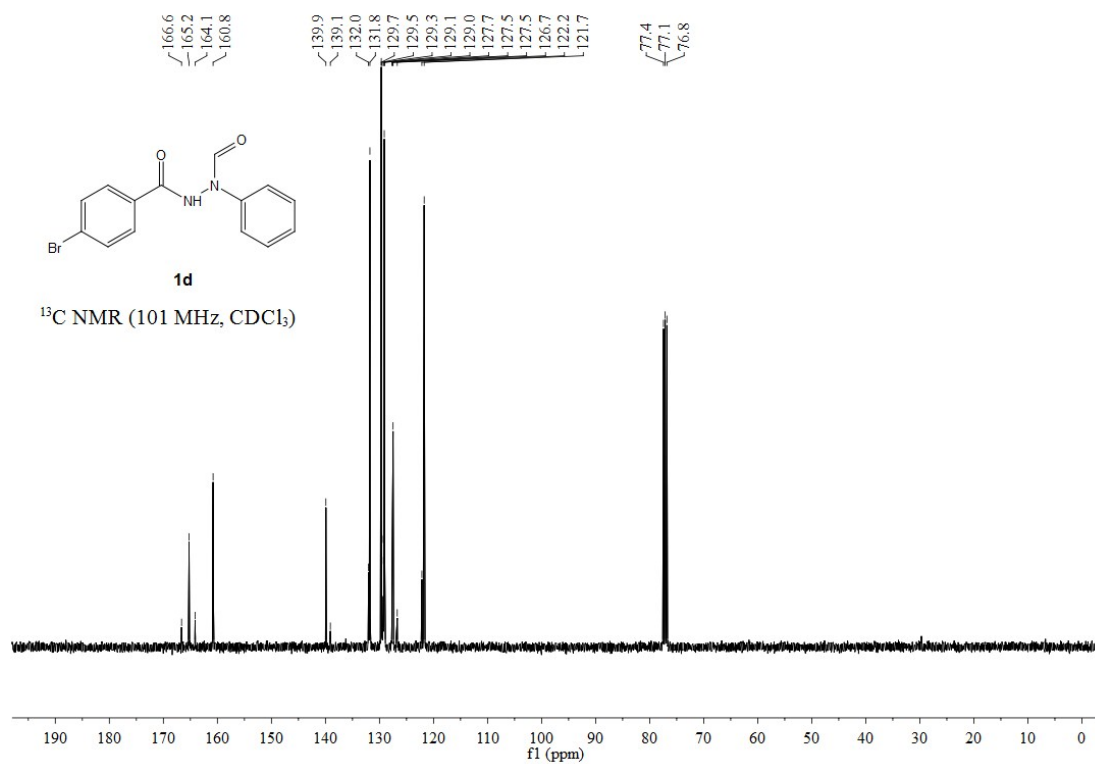
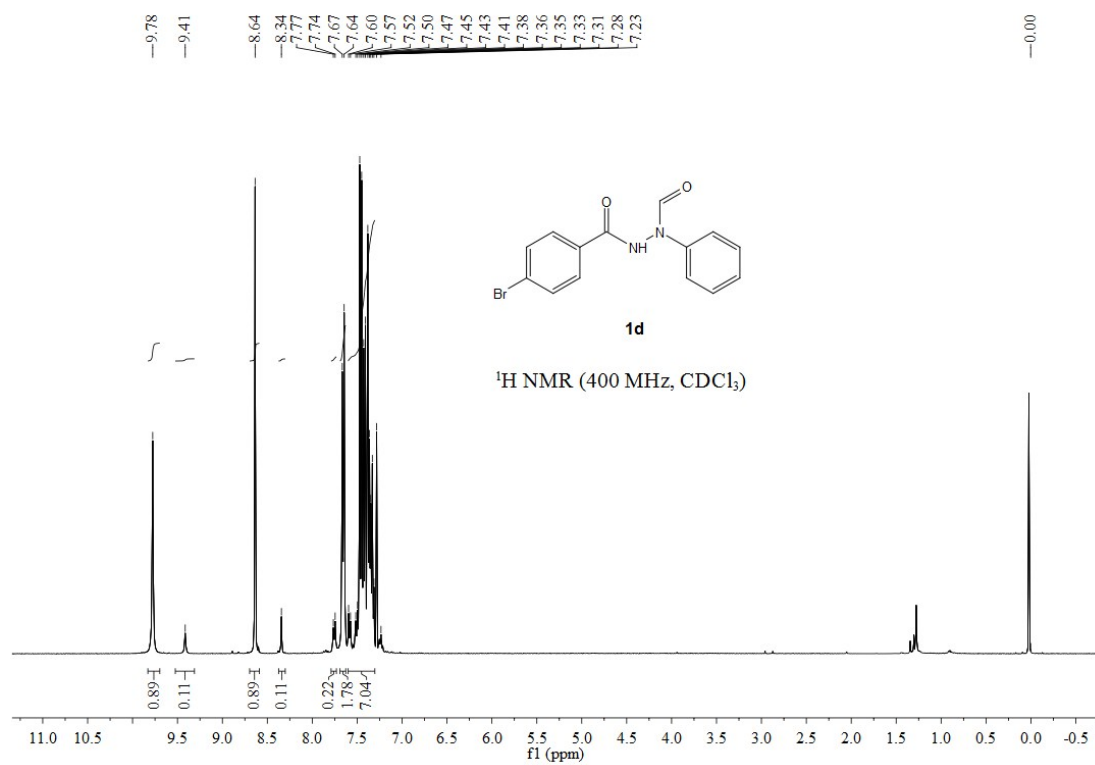
2-Methyl-5-phenyl-1,3,4-oxadiazole (6m):¹⁰ 207 mg, 86% yield; ¹H NMR (400 MHz, CDCl₃) δ 8.03 (dd, *J* = 7.7, 1.7 Hz, 2H), 7.54 – 7.48 (m, 3H), 2.63 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 164.9, 163.7, 131.6, 129.0, 126.7, 123.9, 11.10.

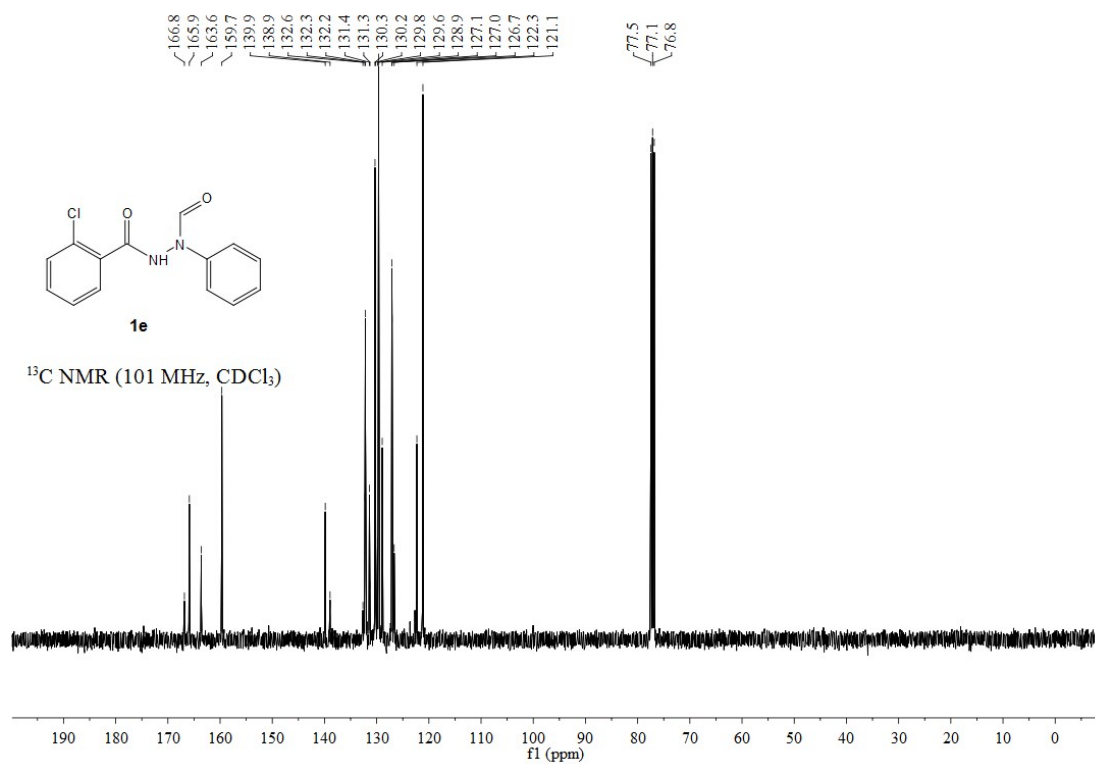
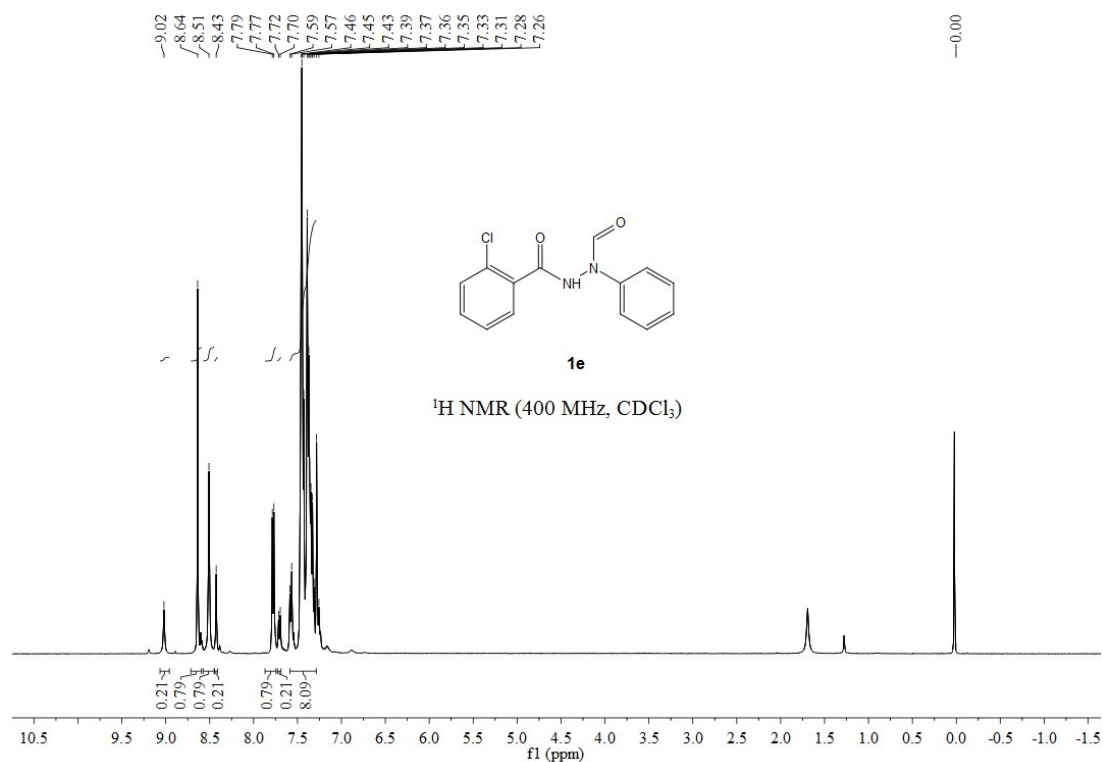
¹H NMR and ¹³C NMR spectra for all compounds

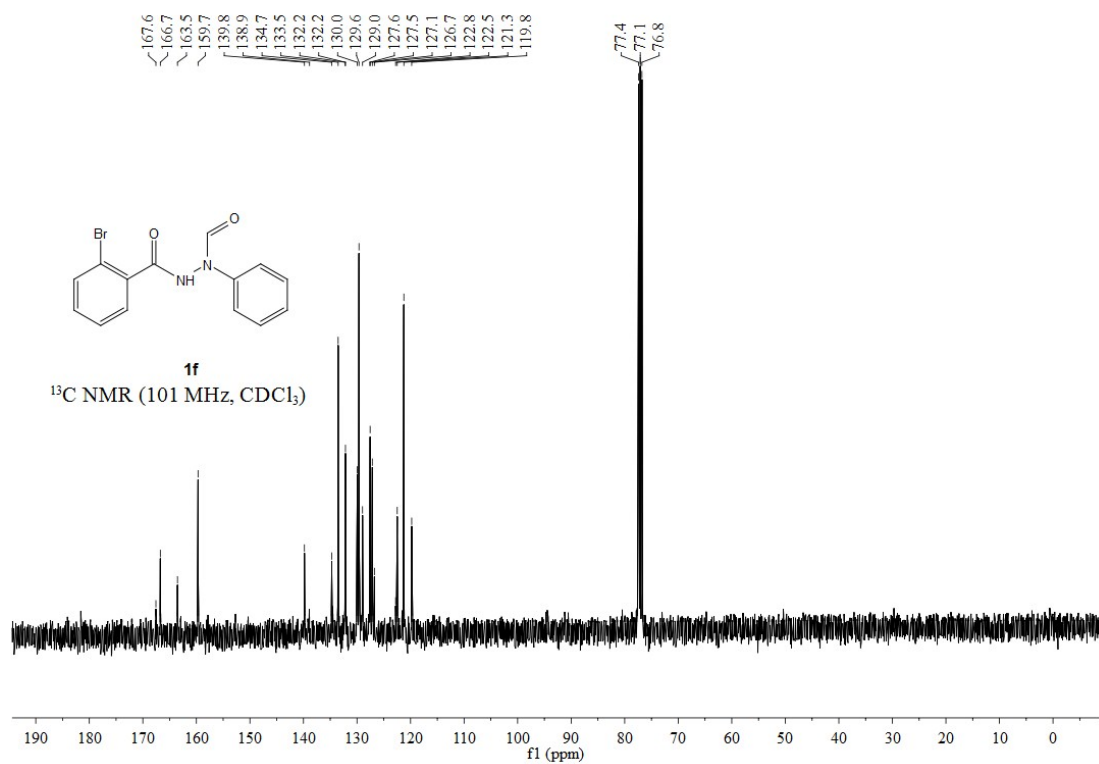
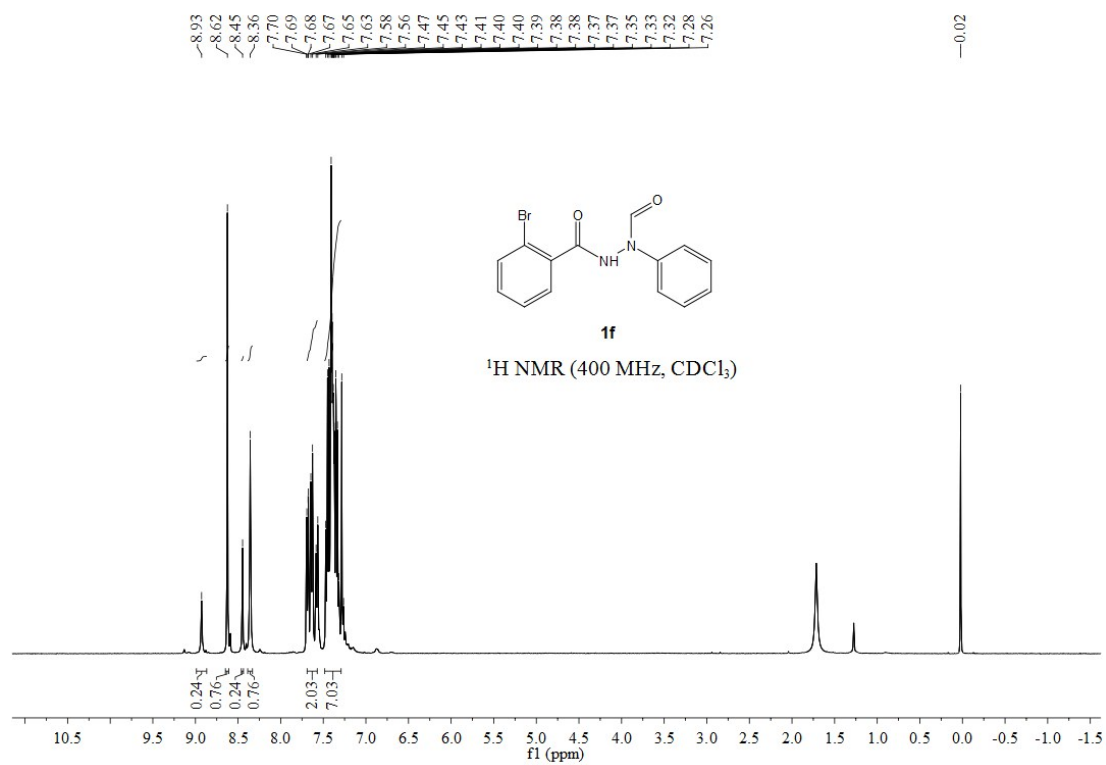


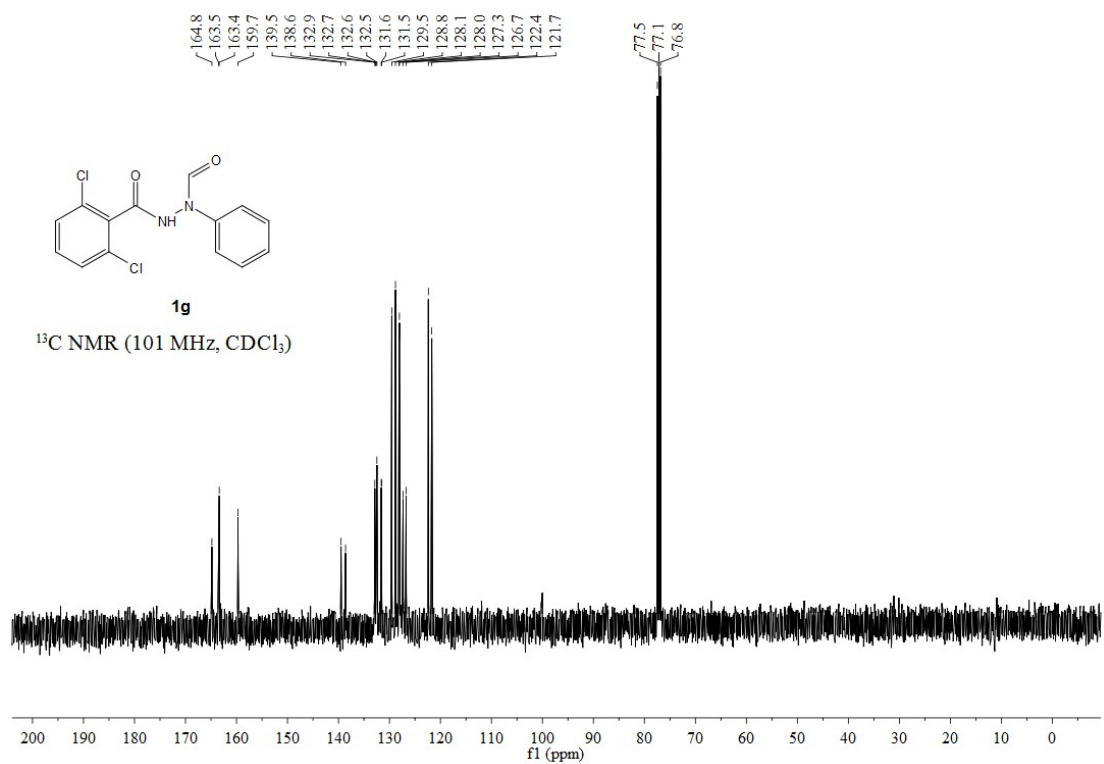
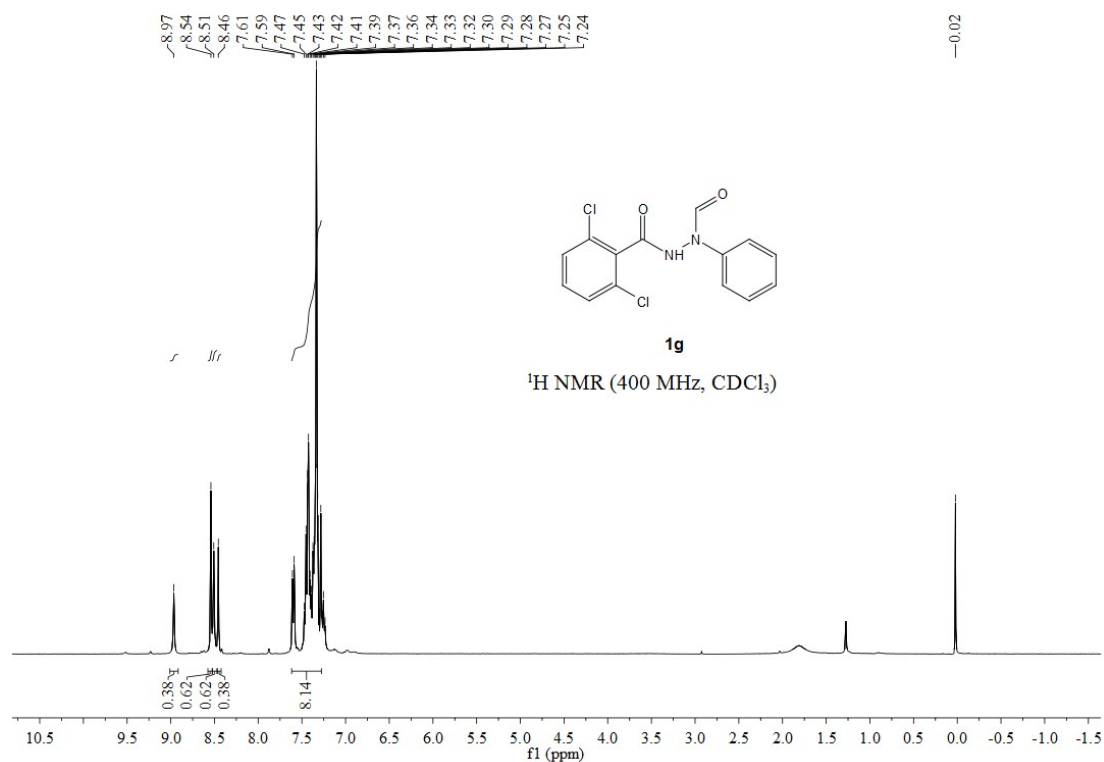


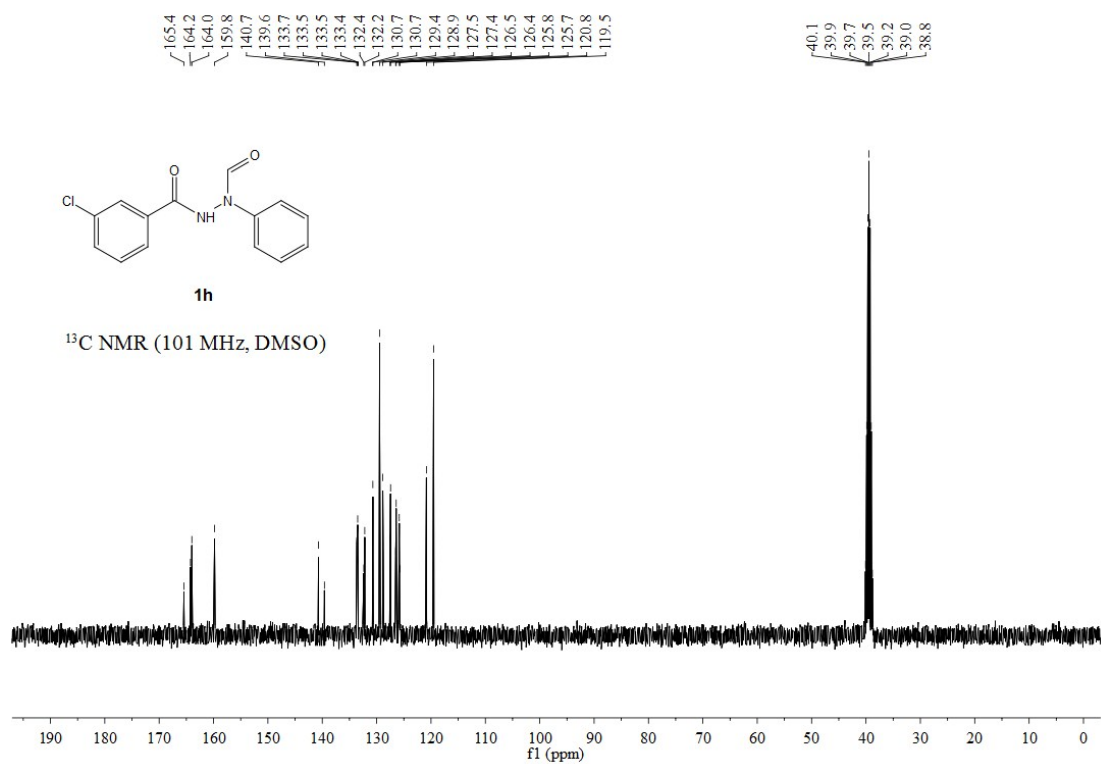
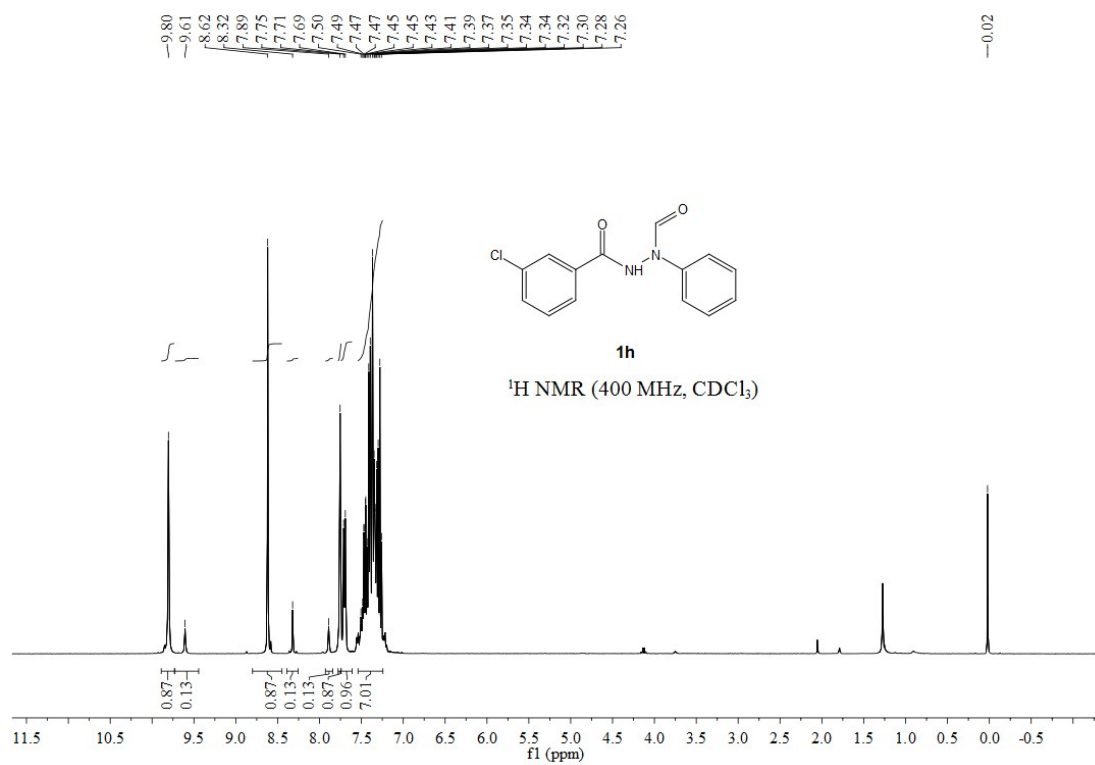


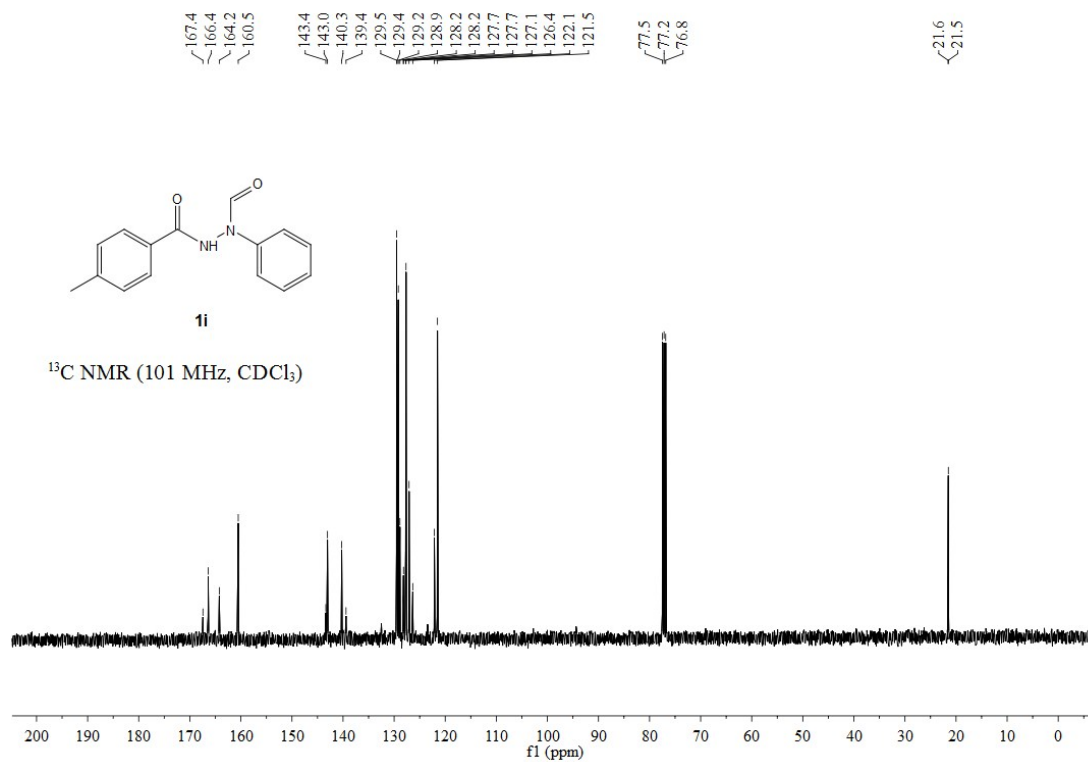
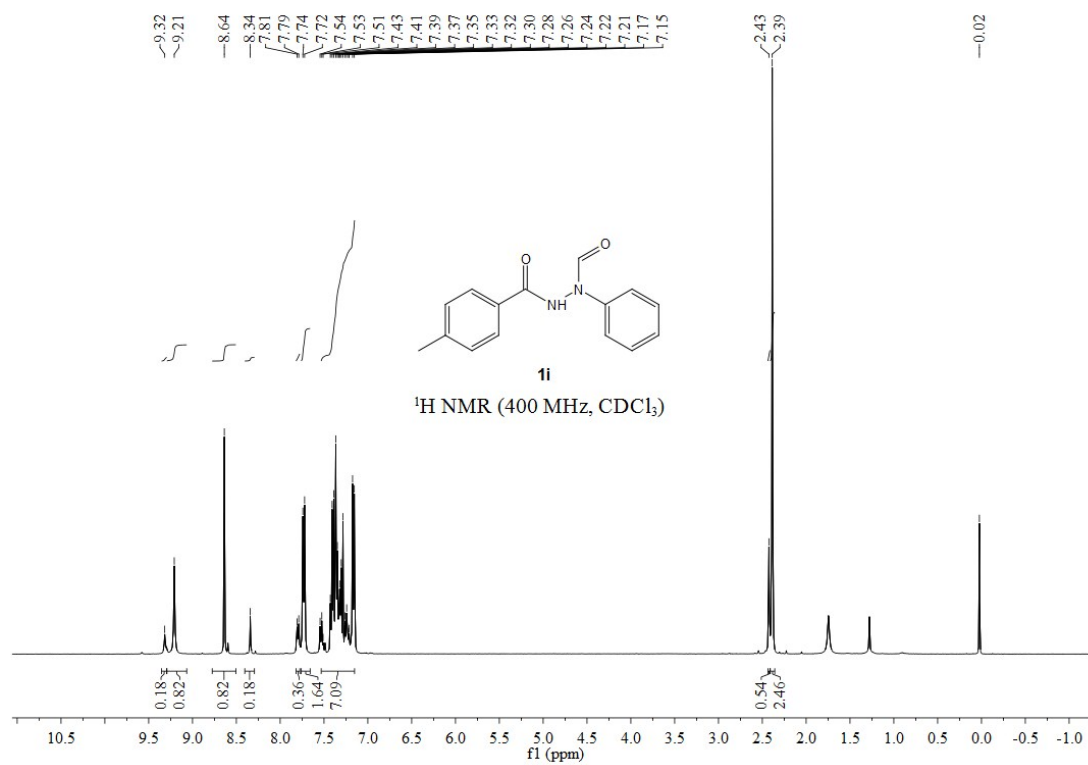


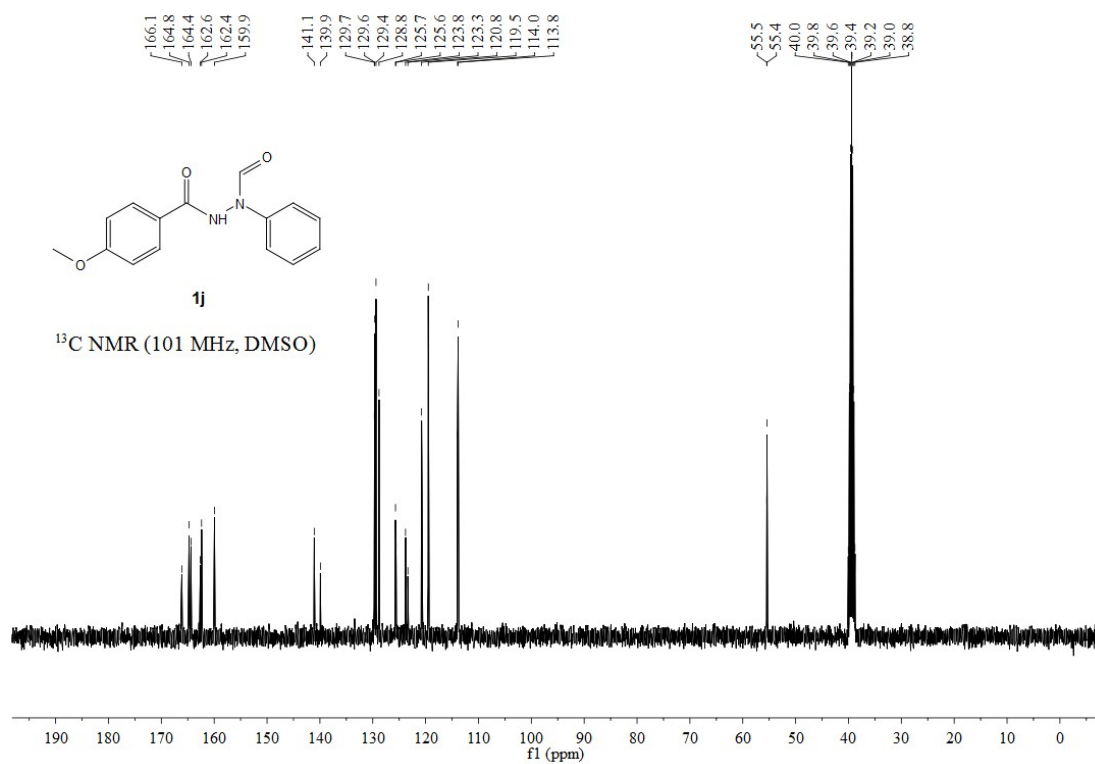
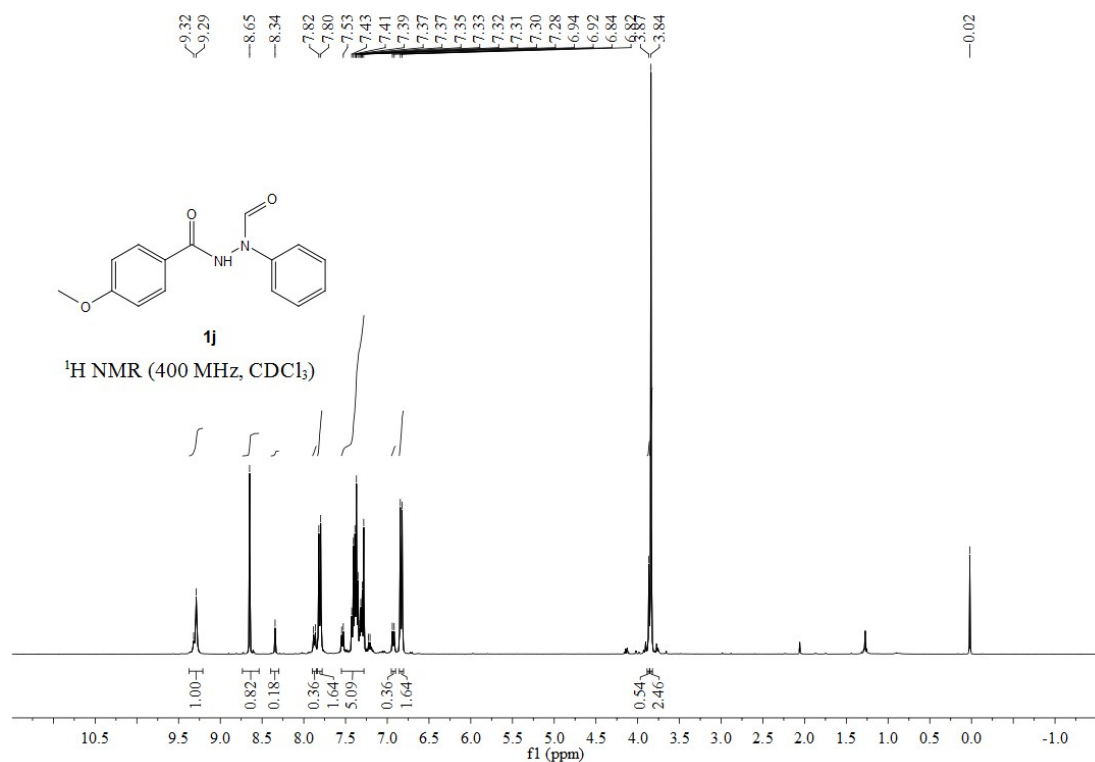


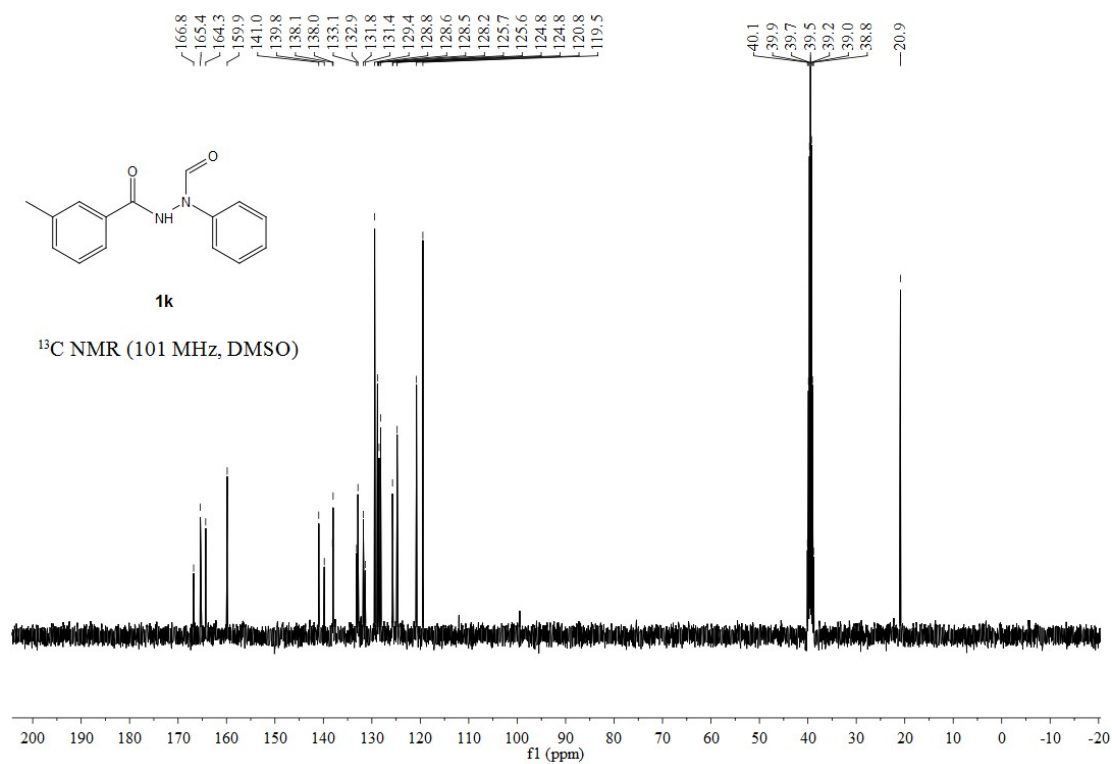
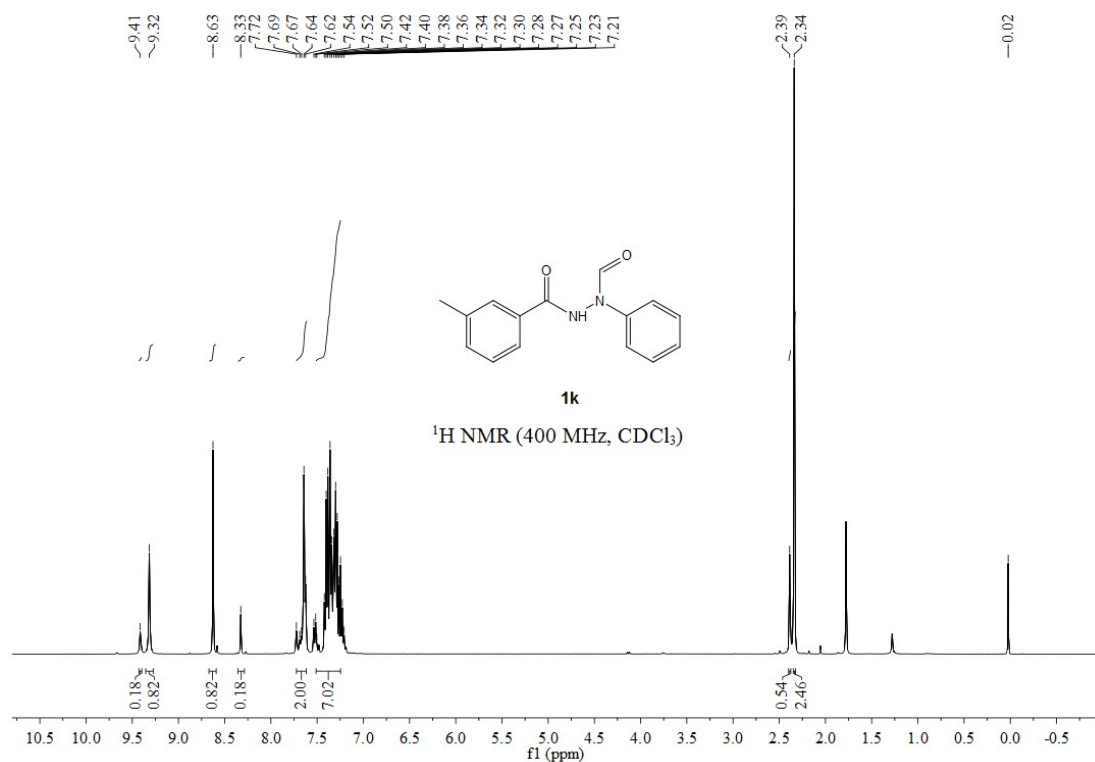


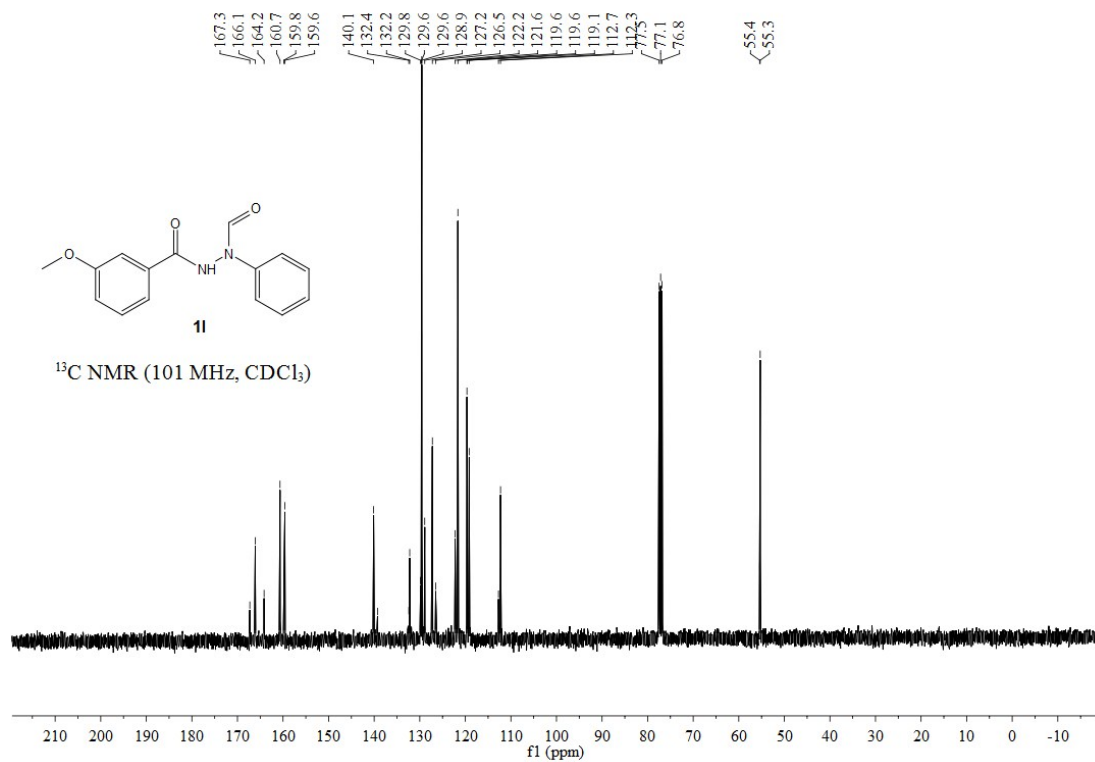
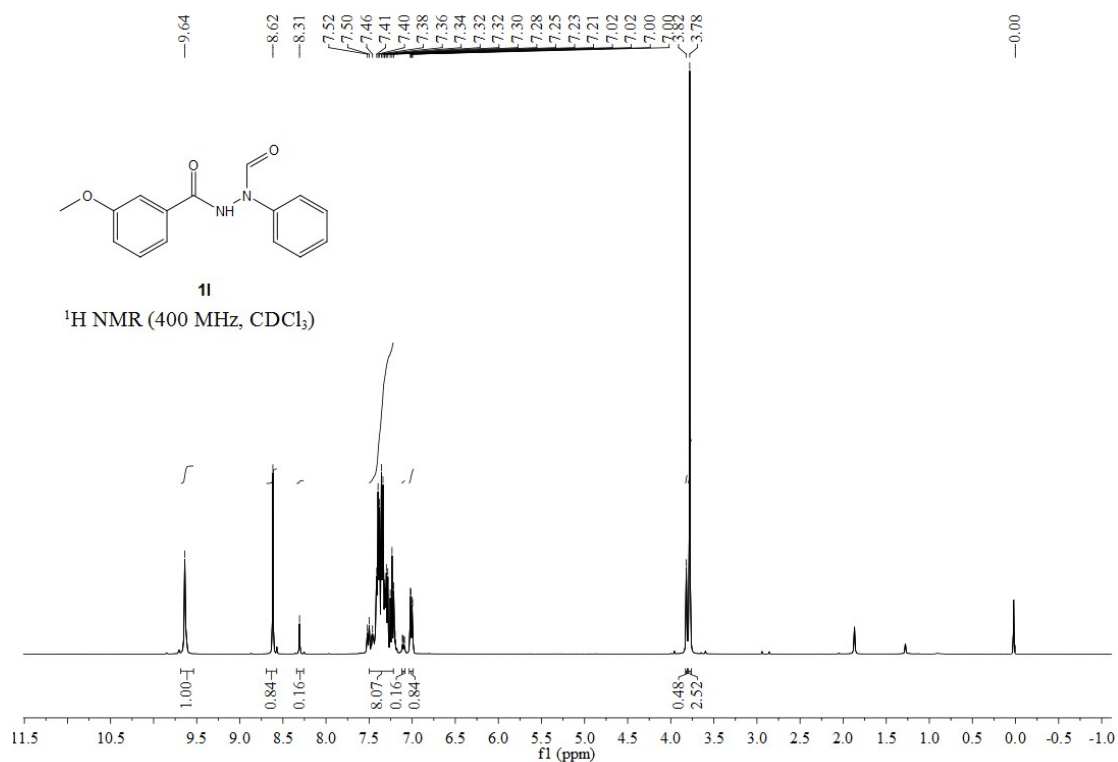


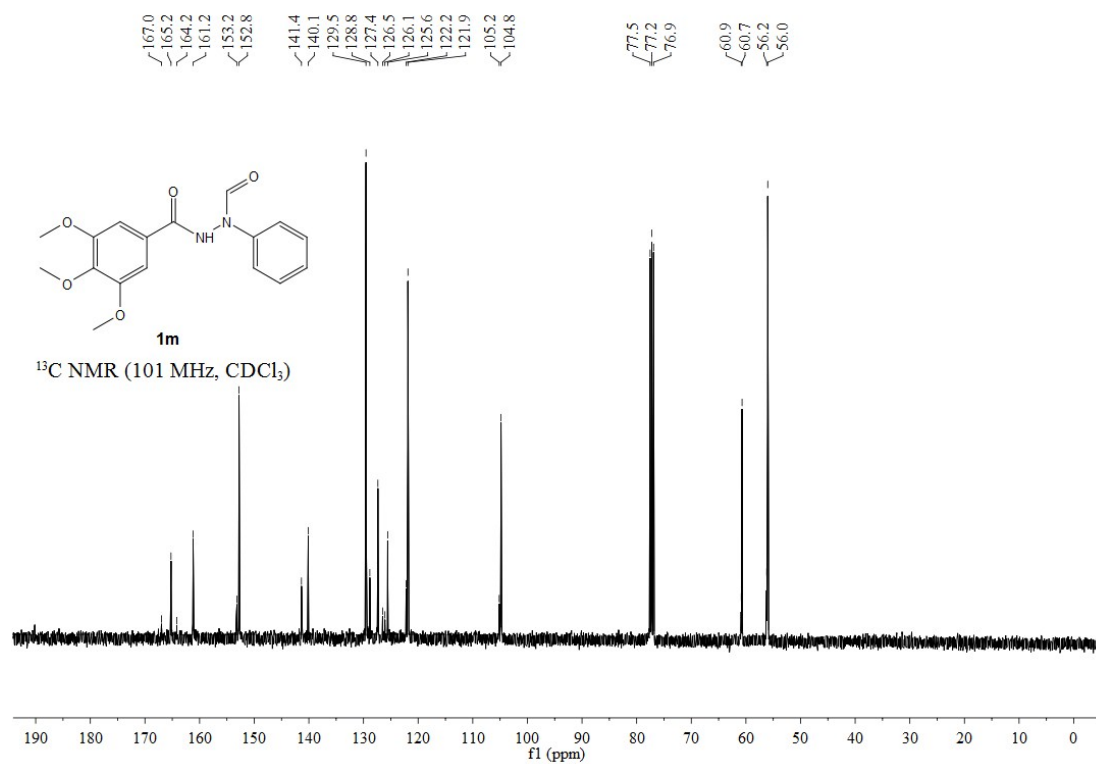
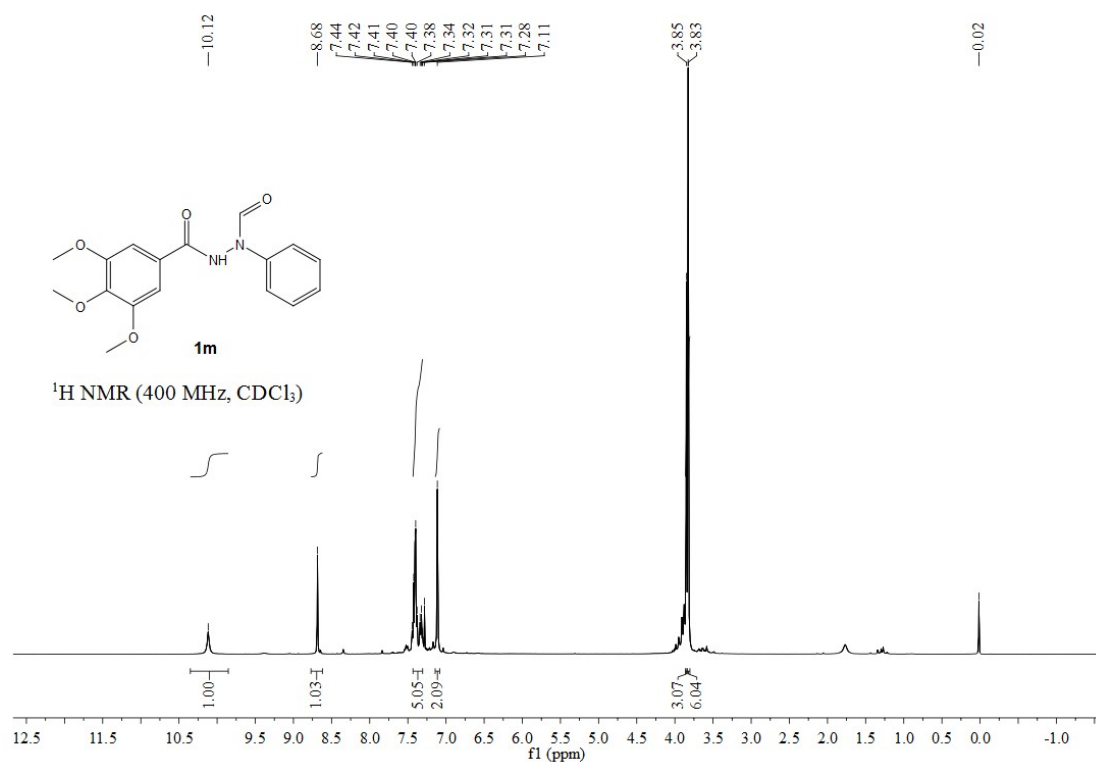


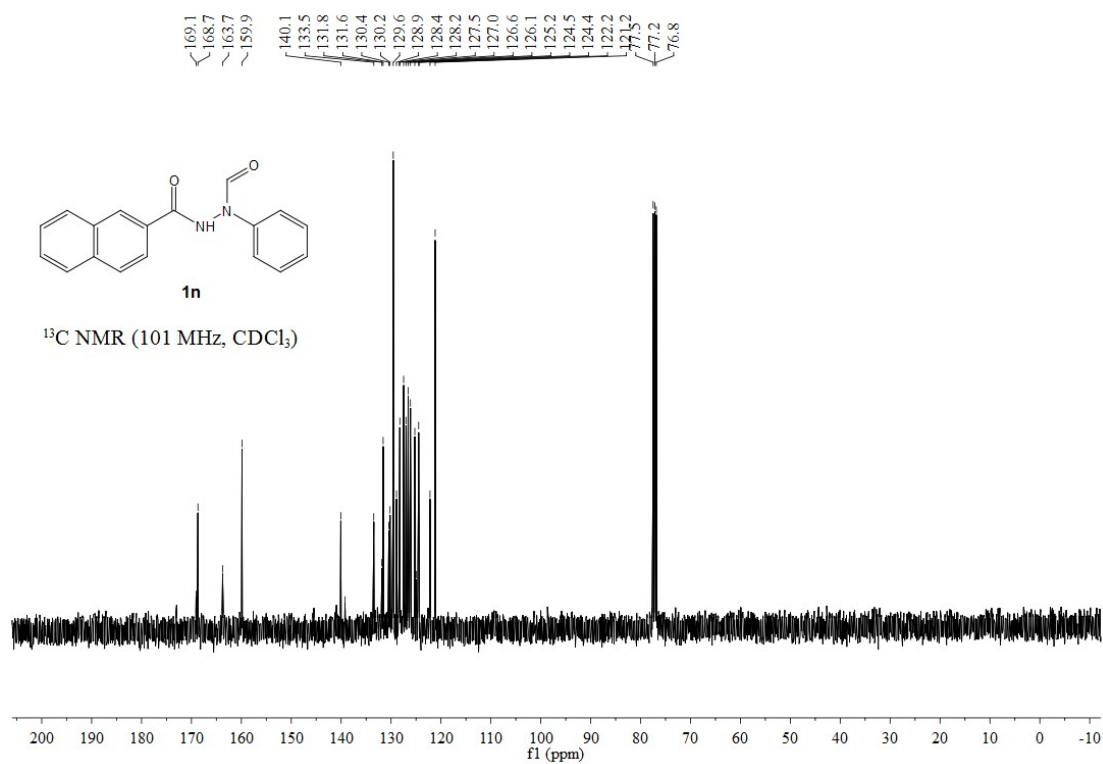
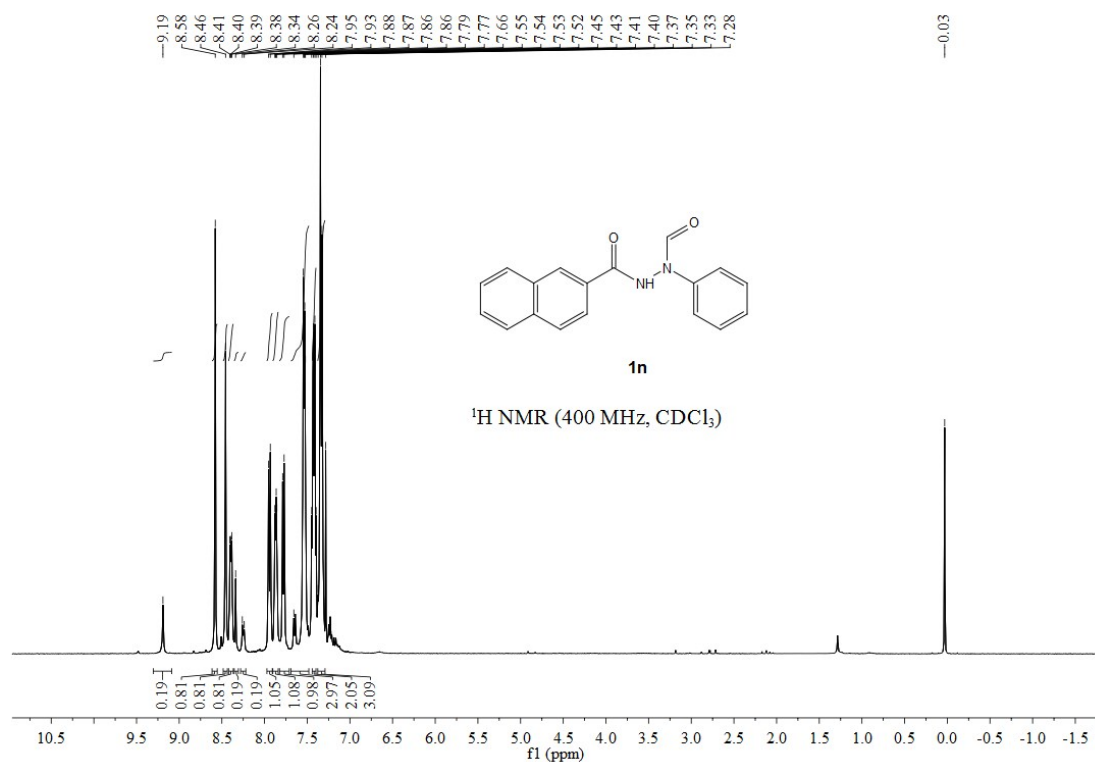


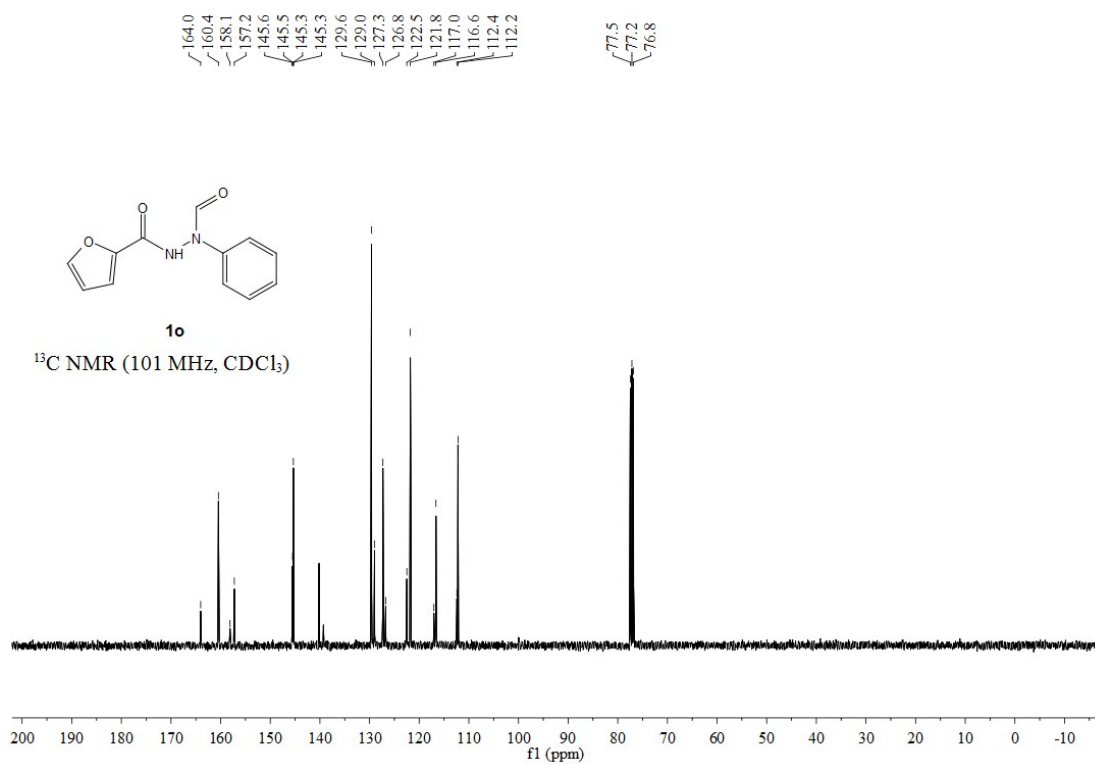
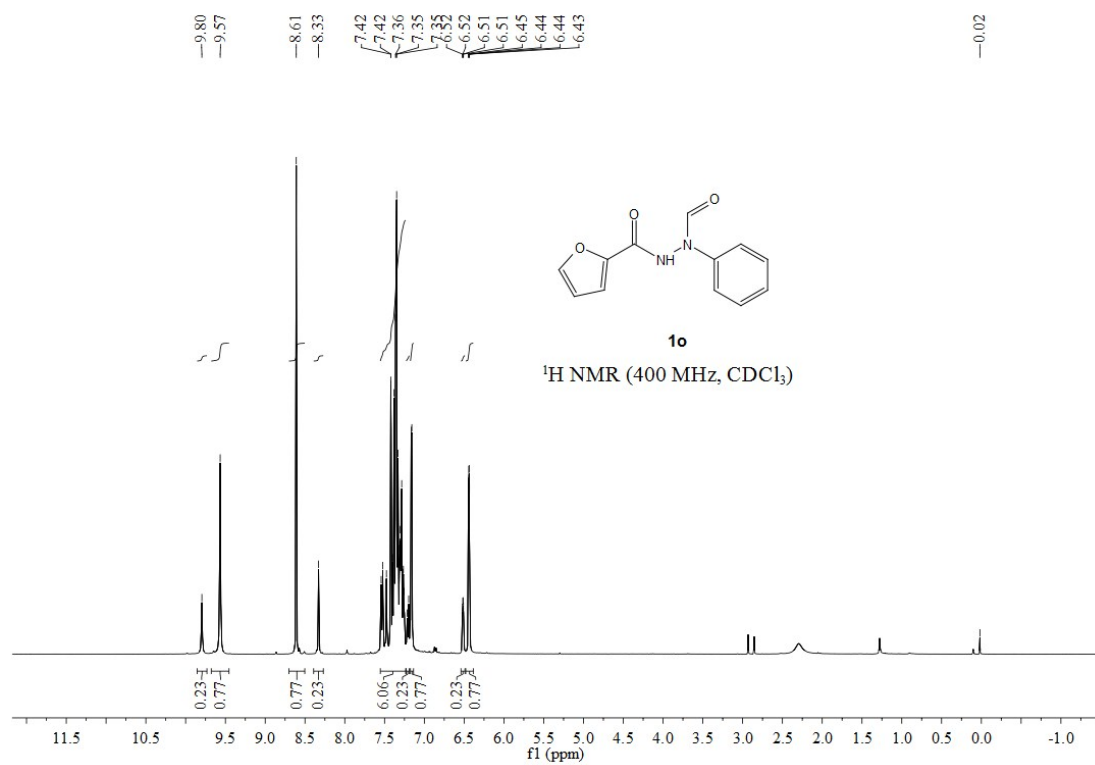


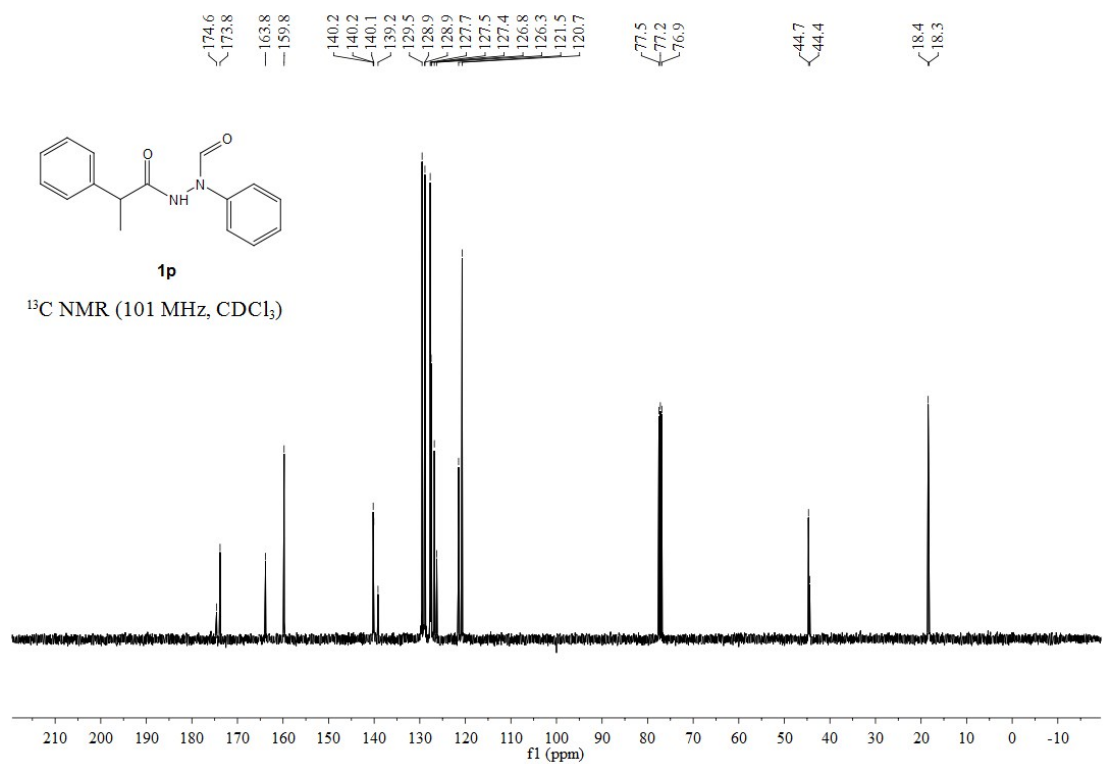
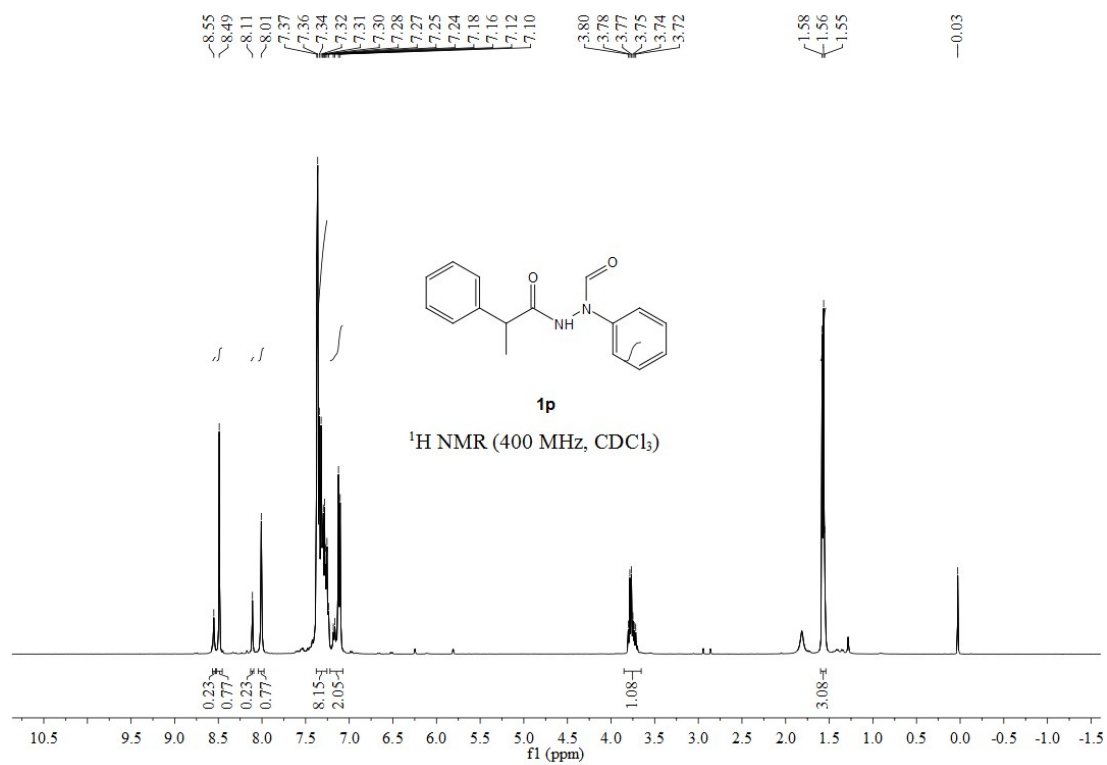


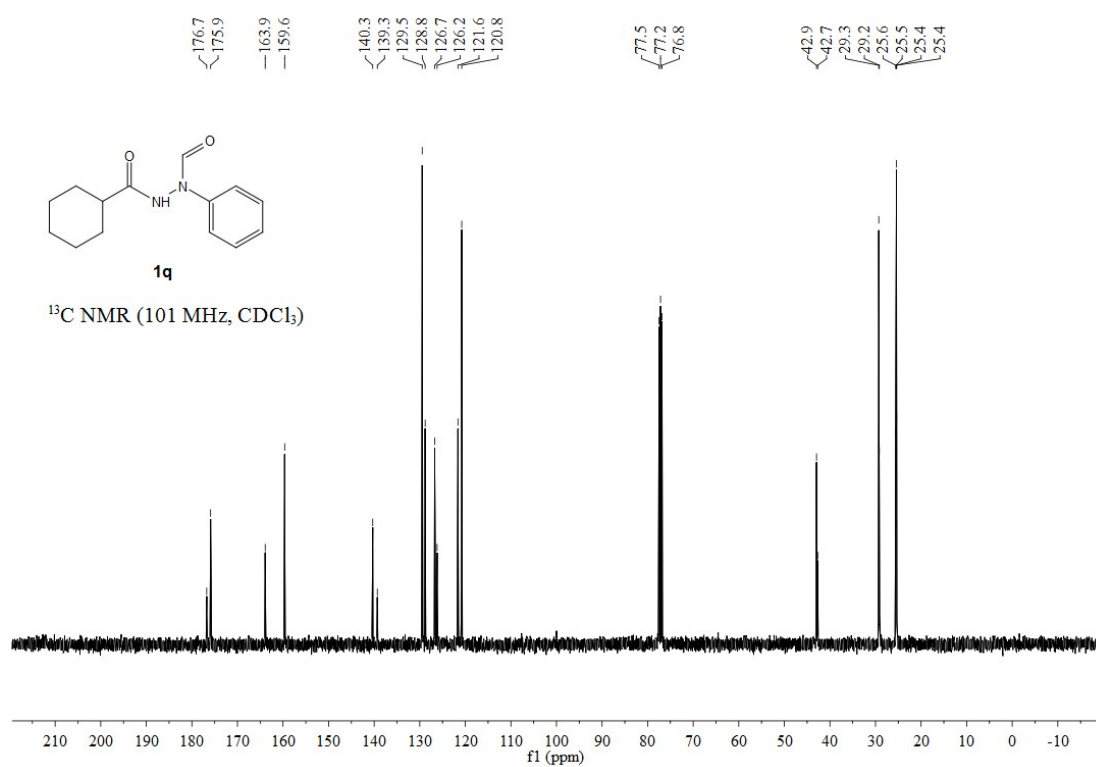
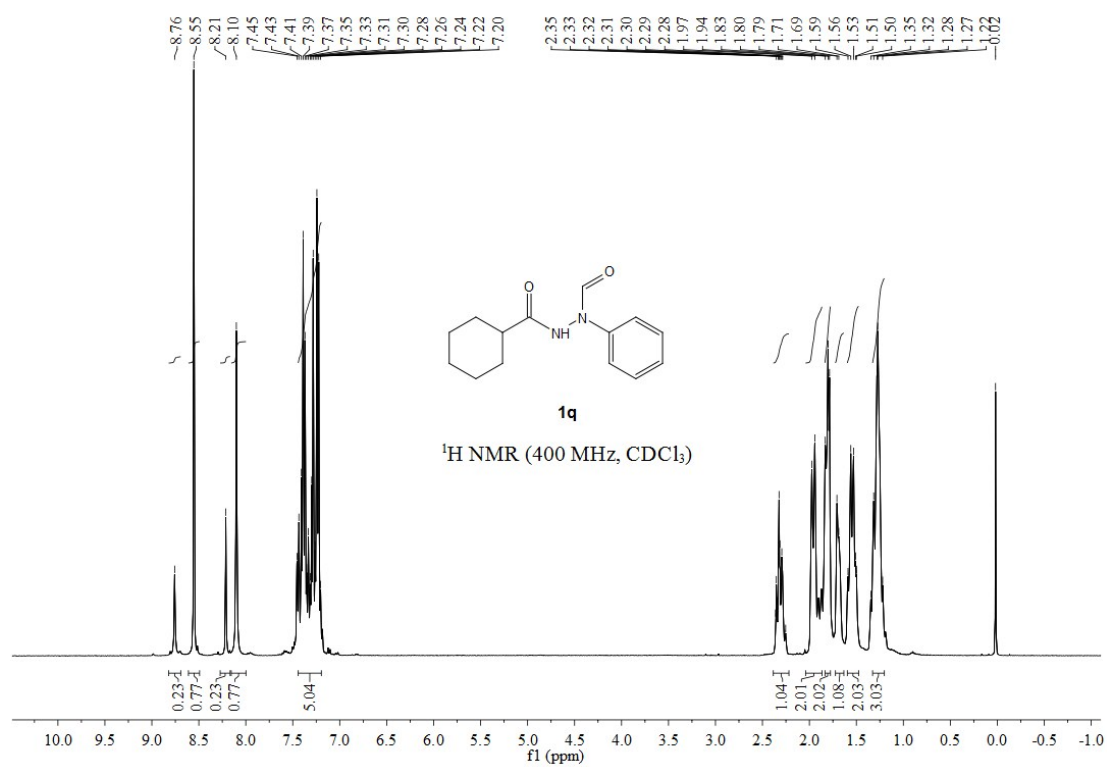


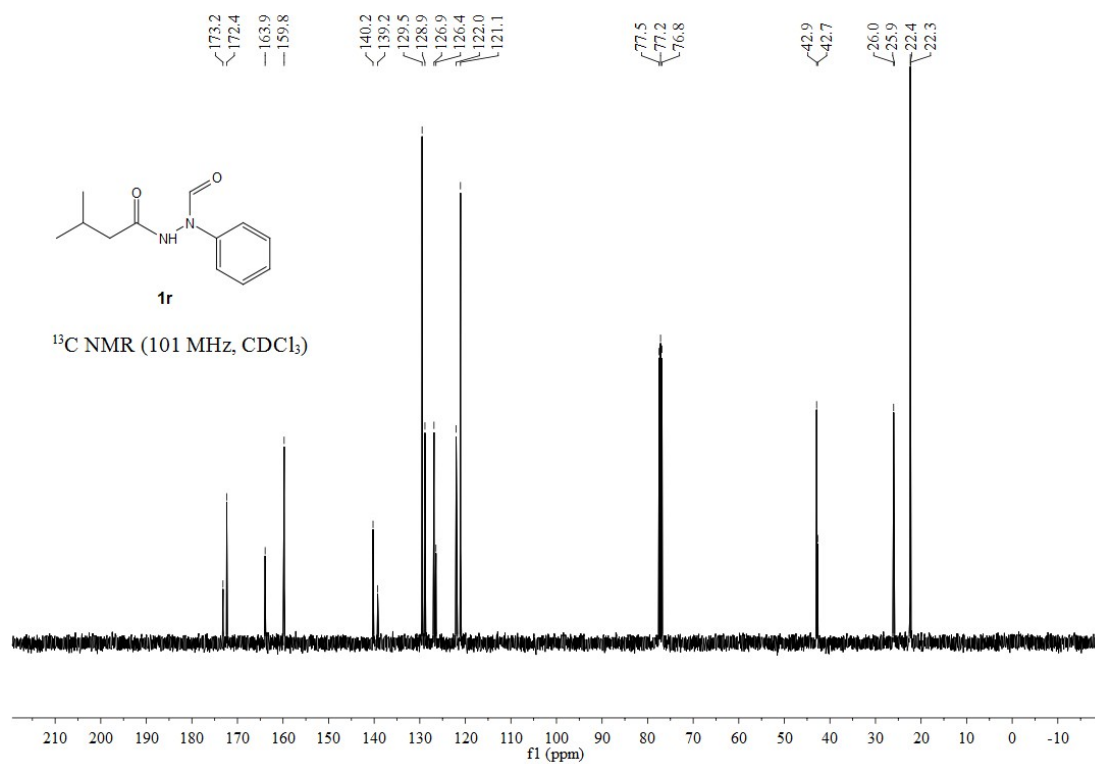
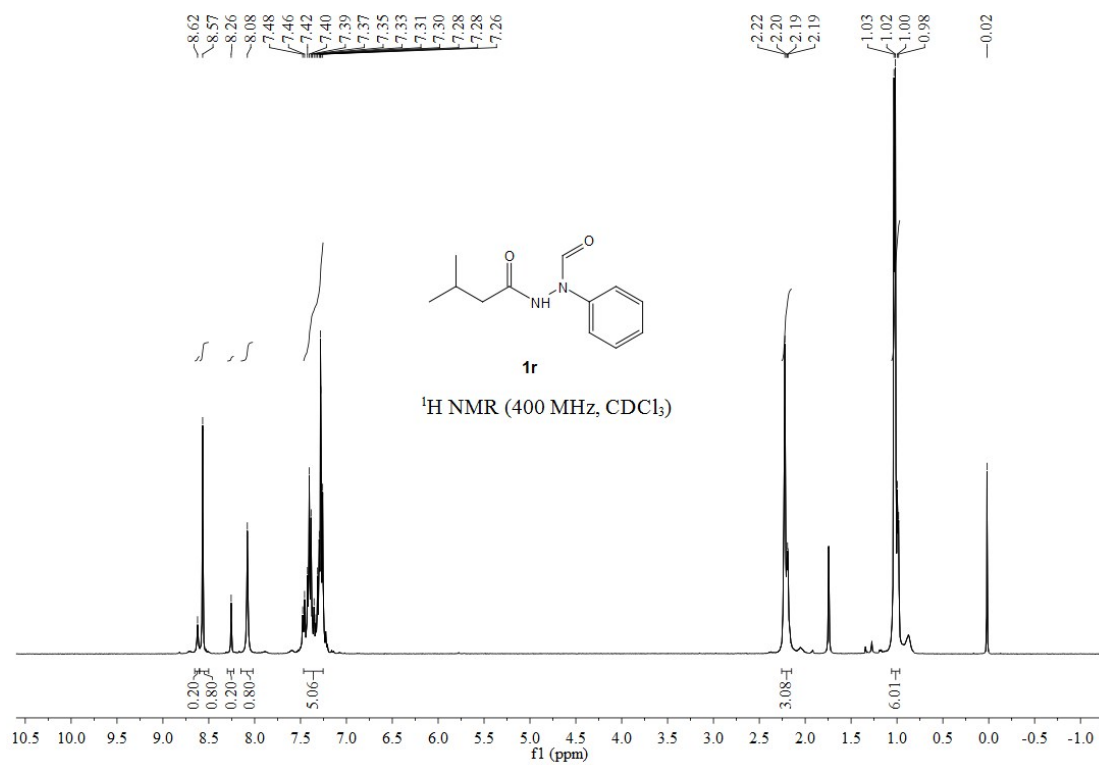


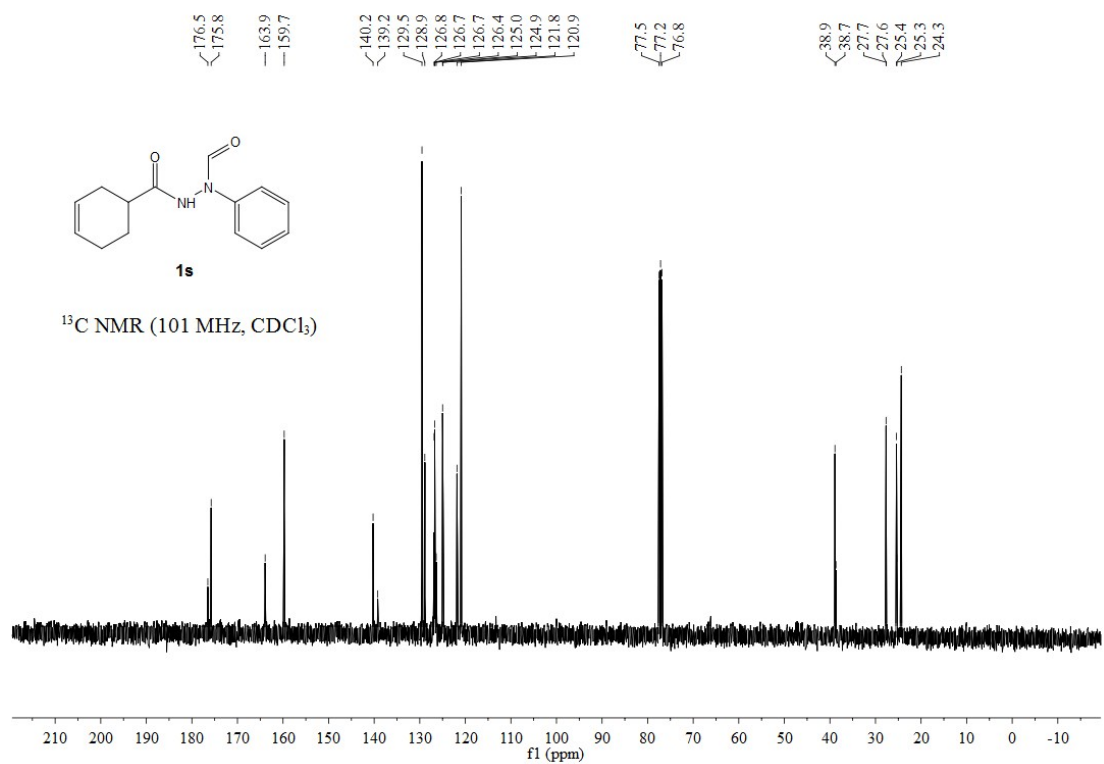
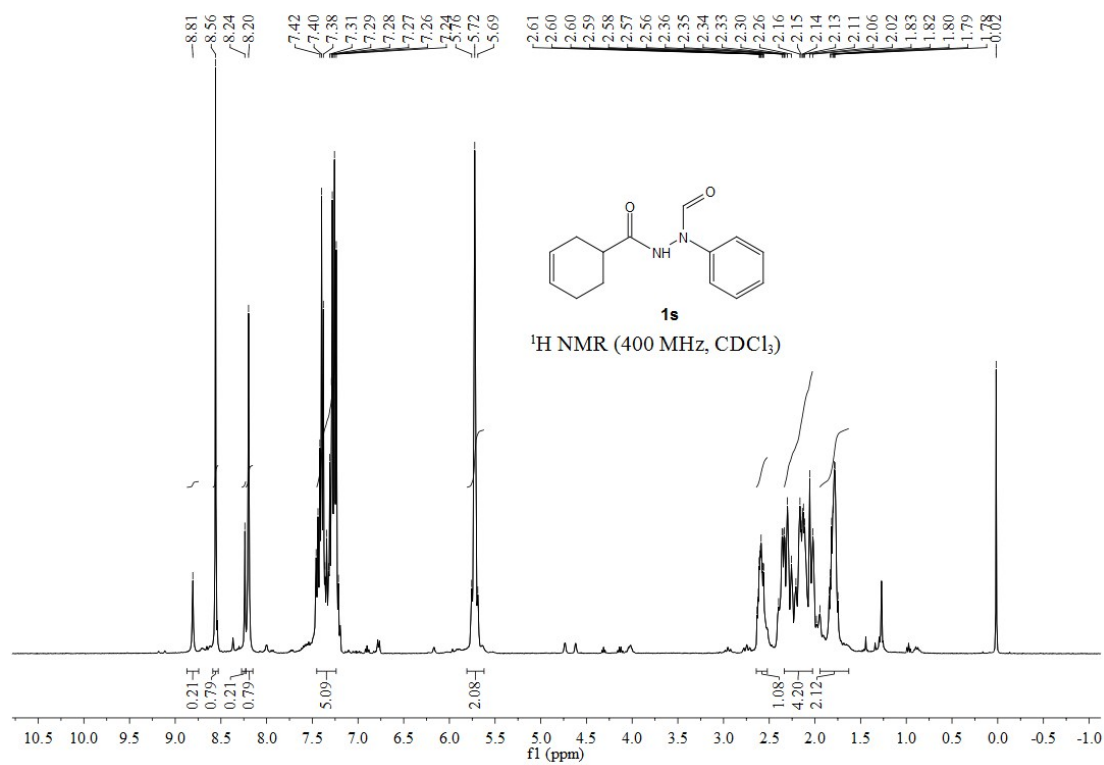


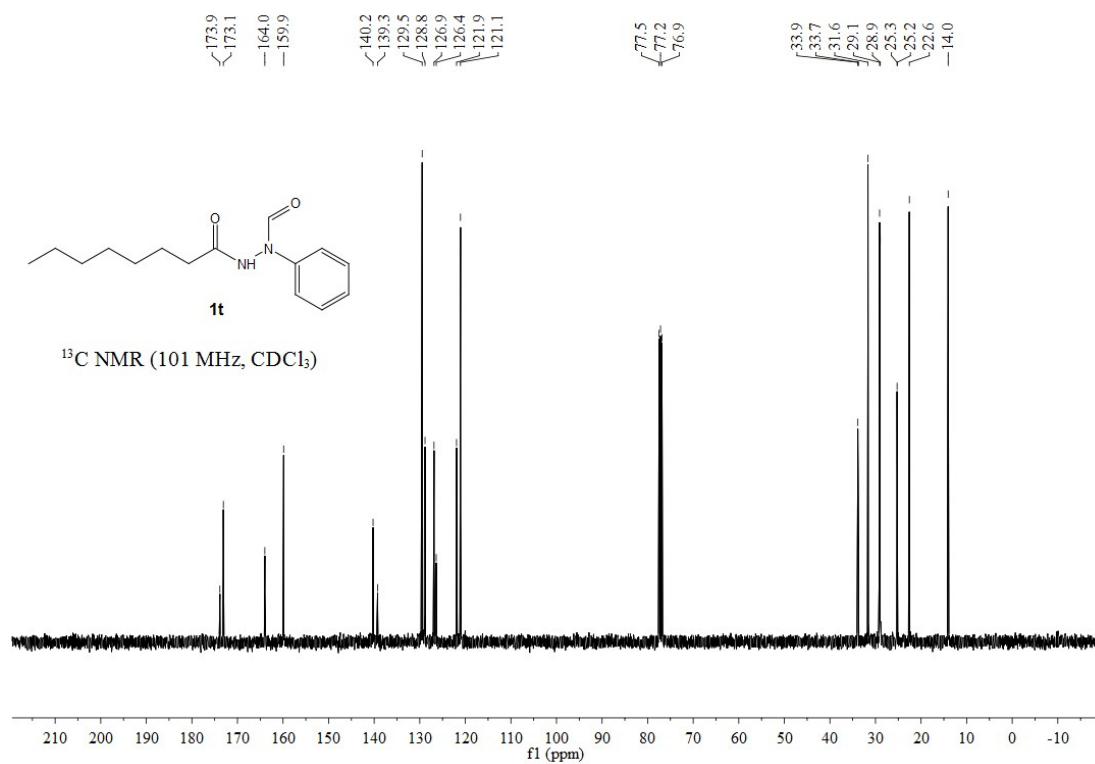
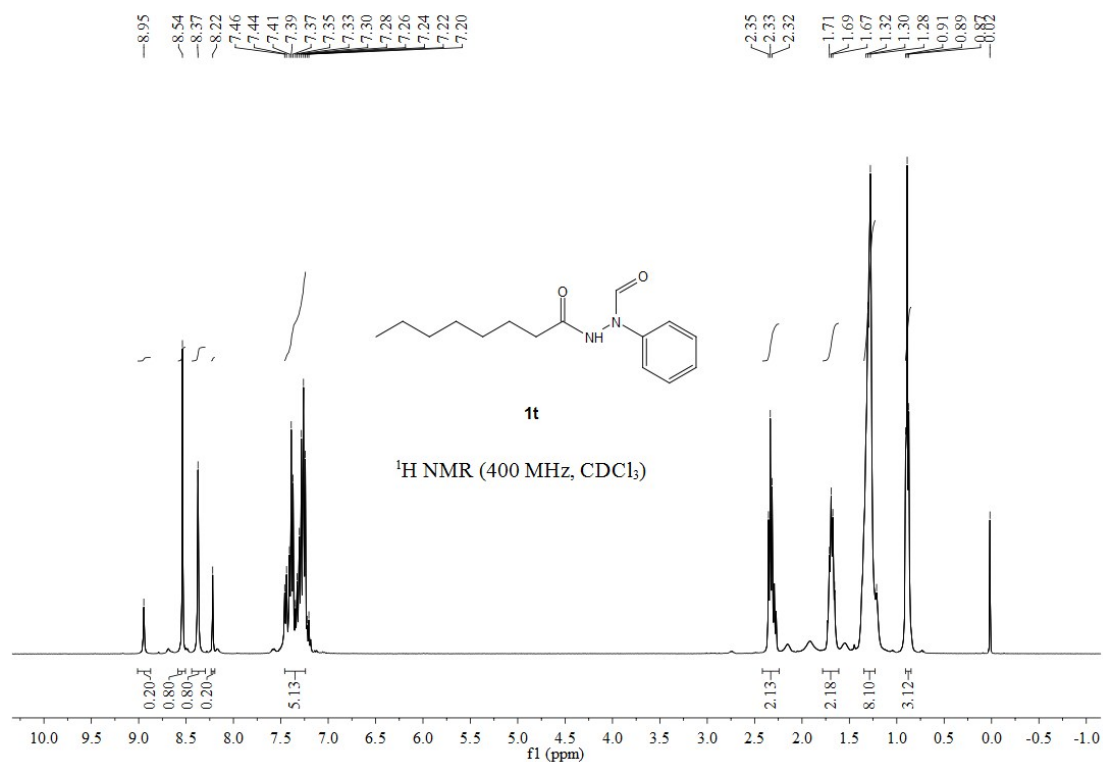


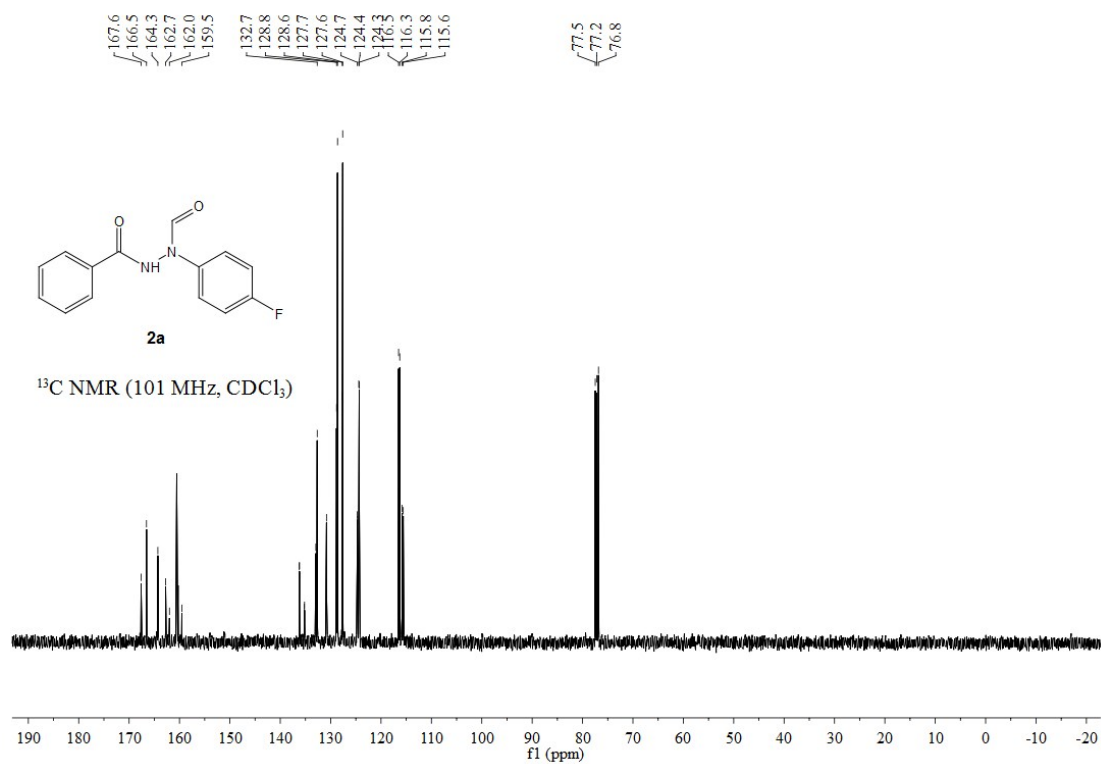
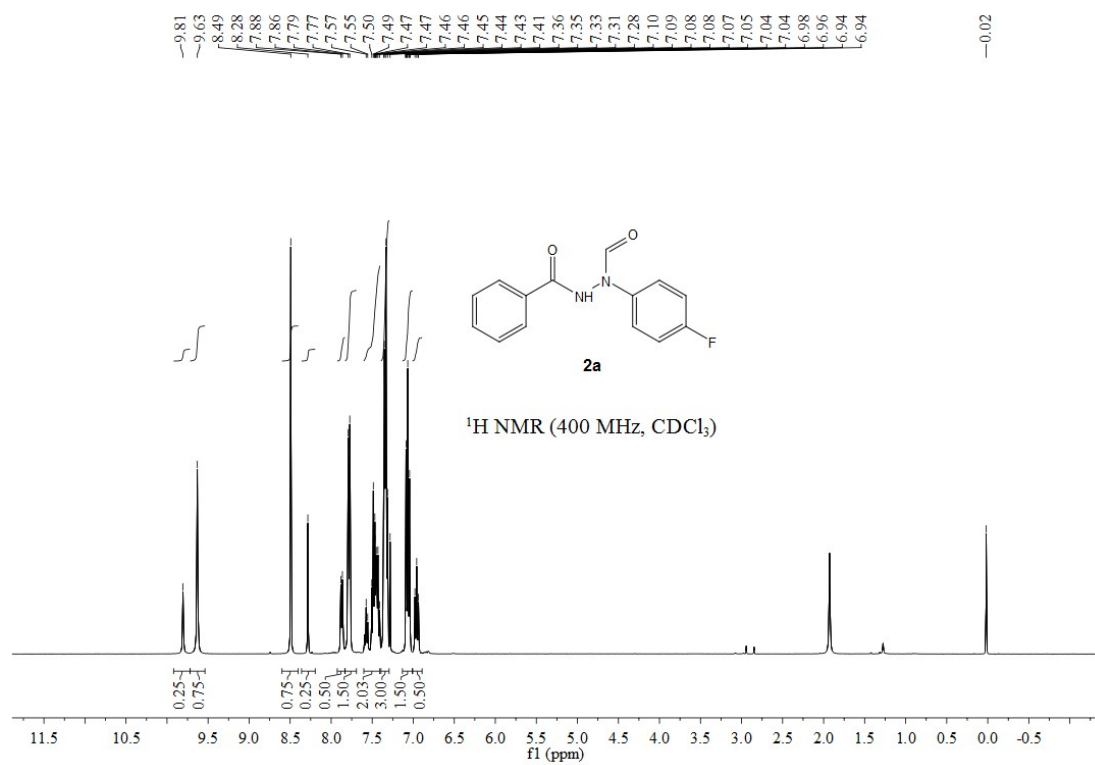


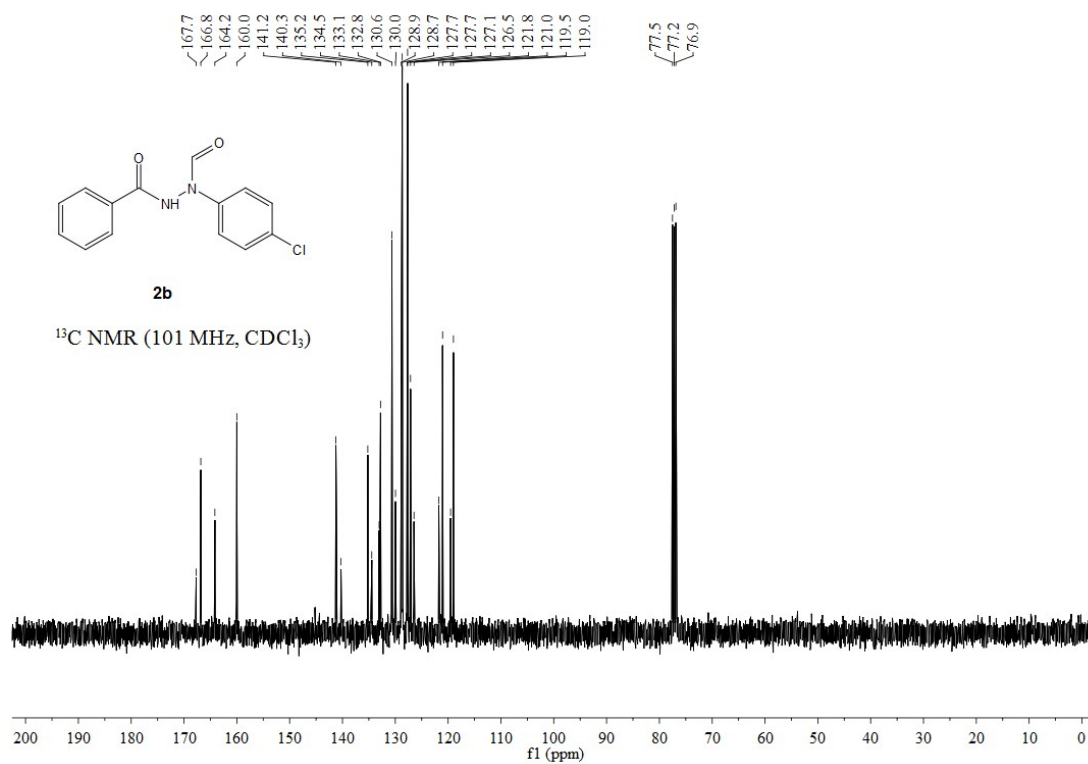
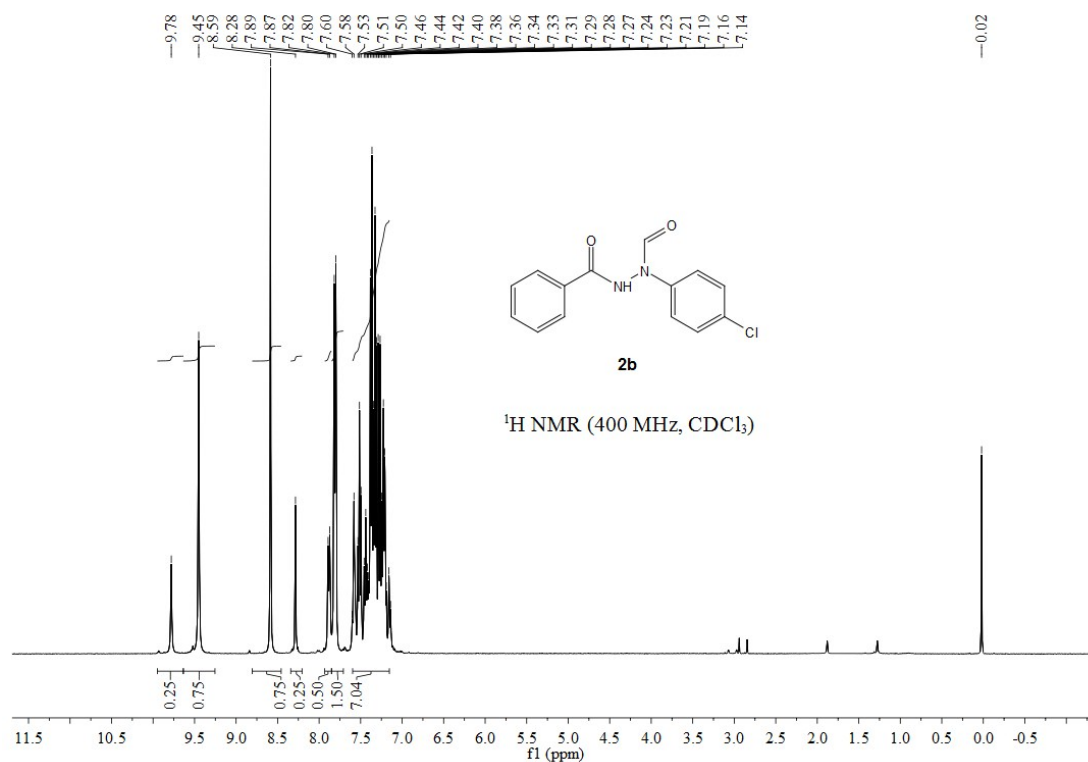


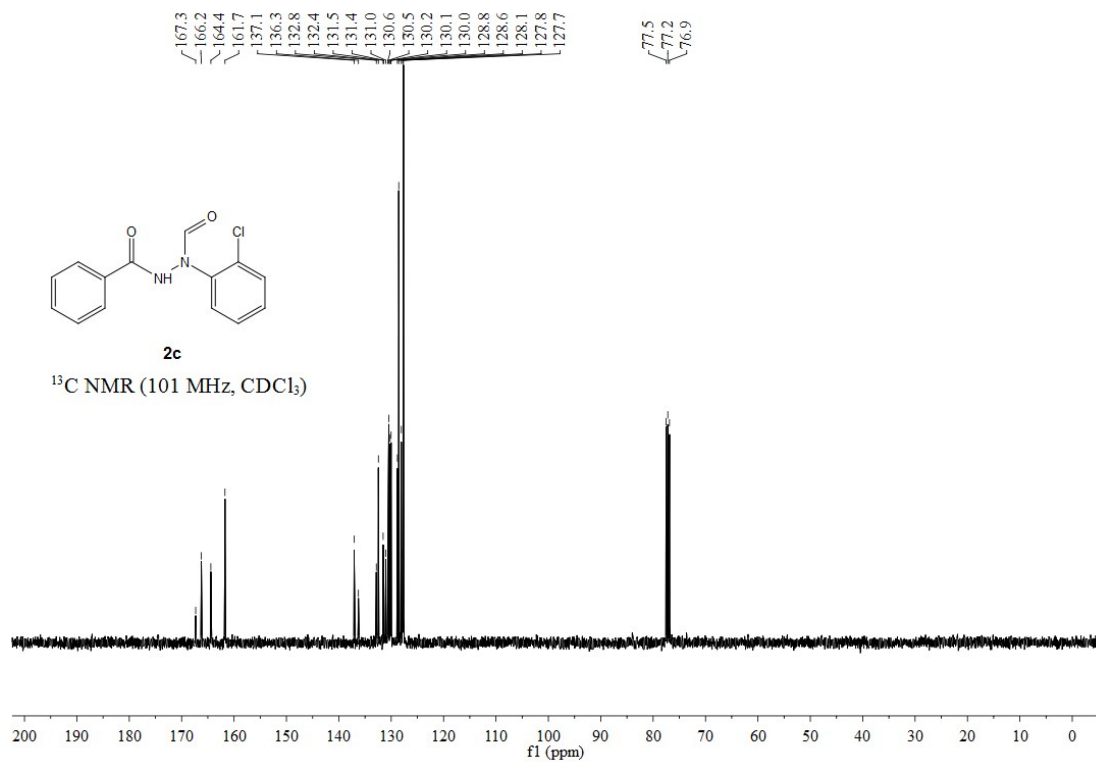
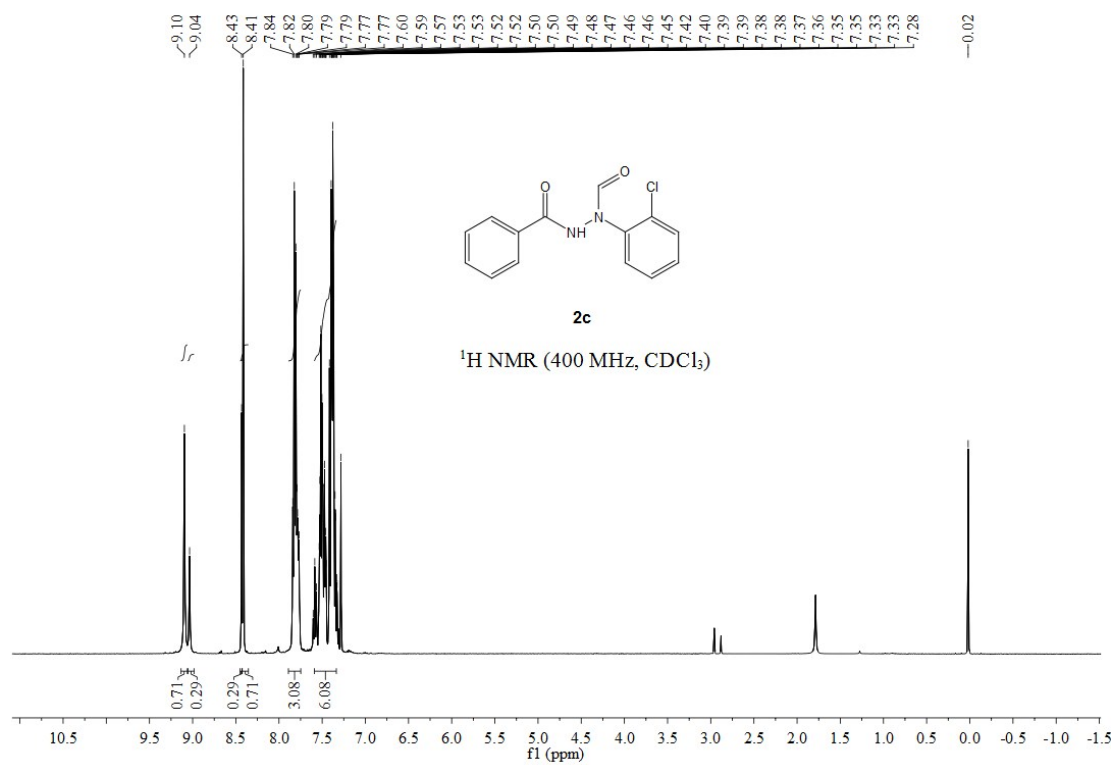


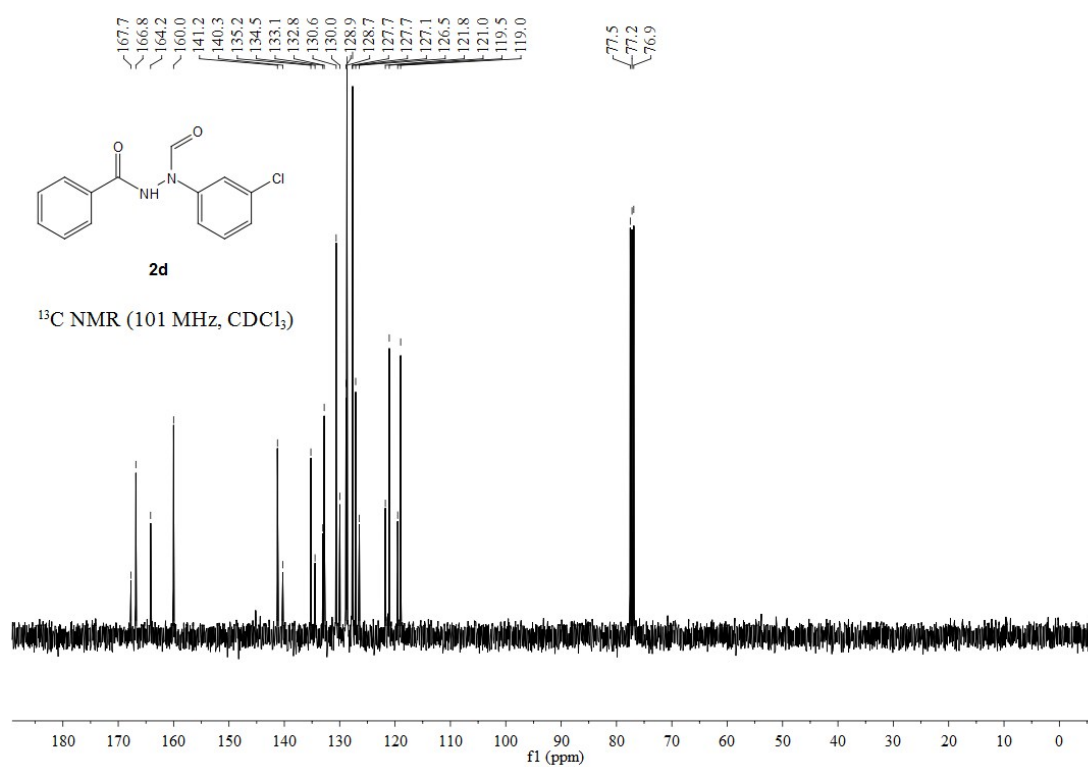
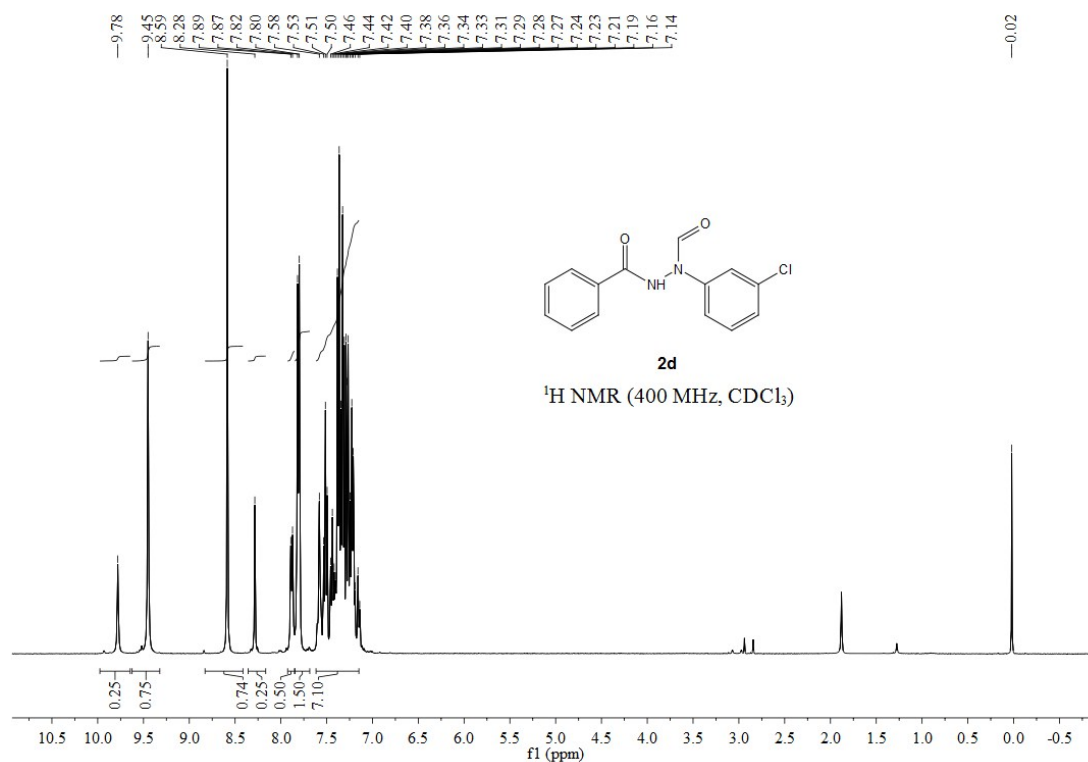


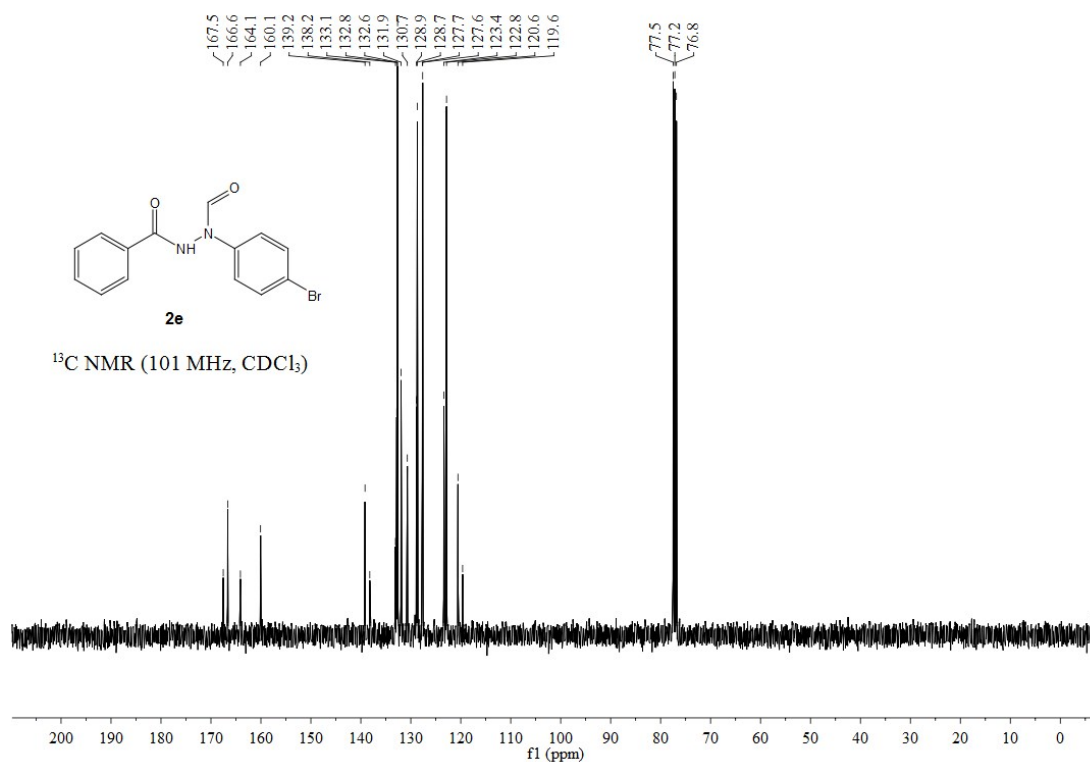
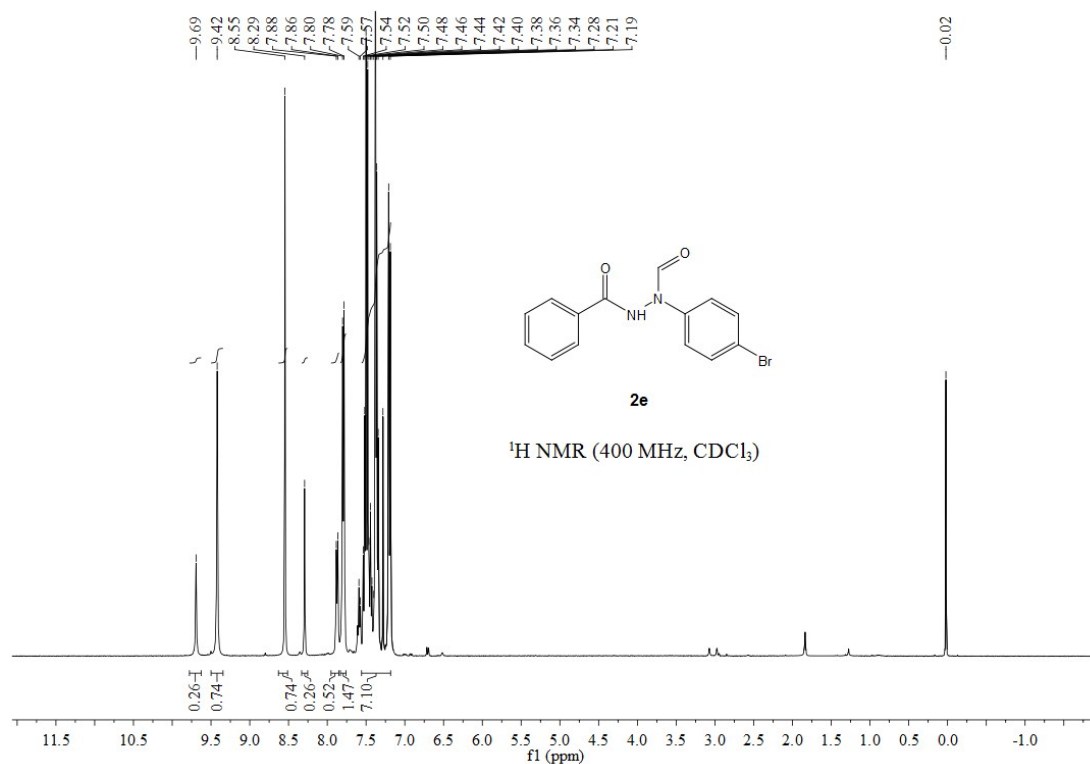


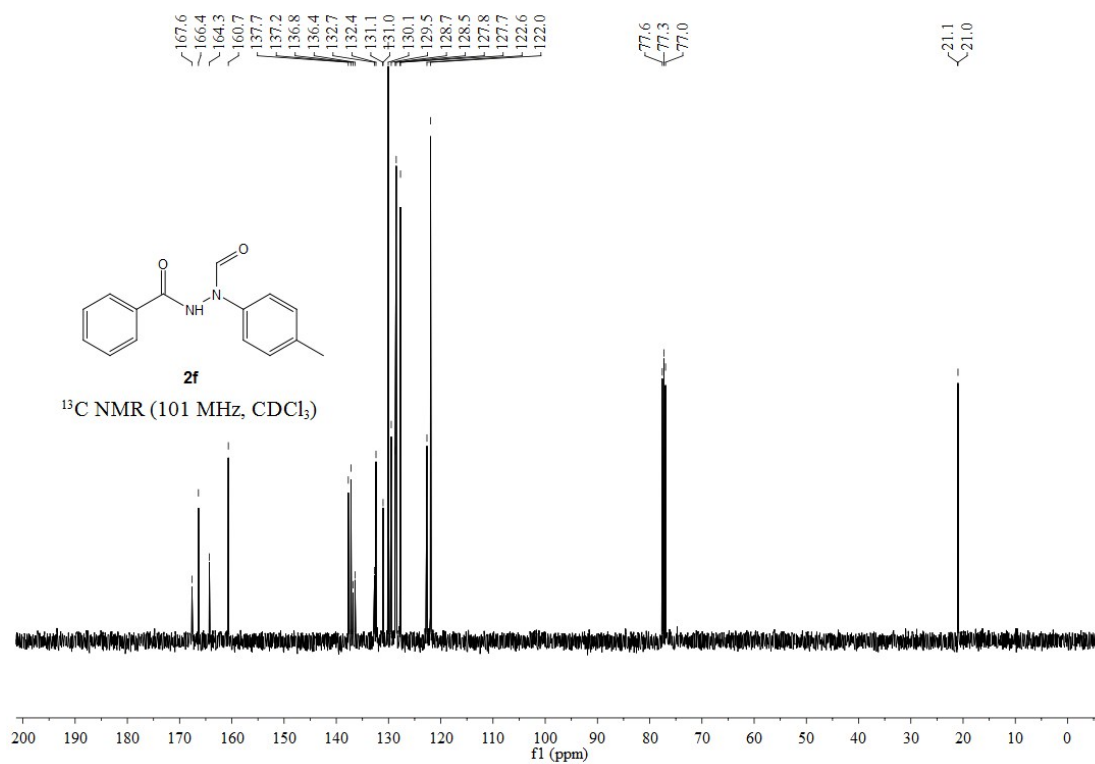
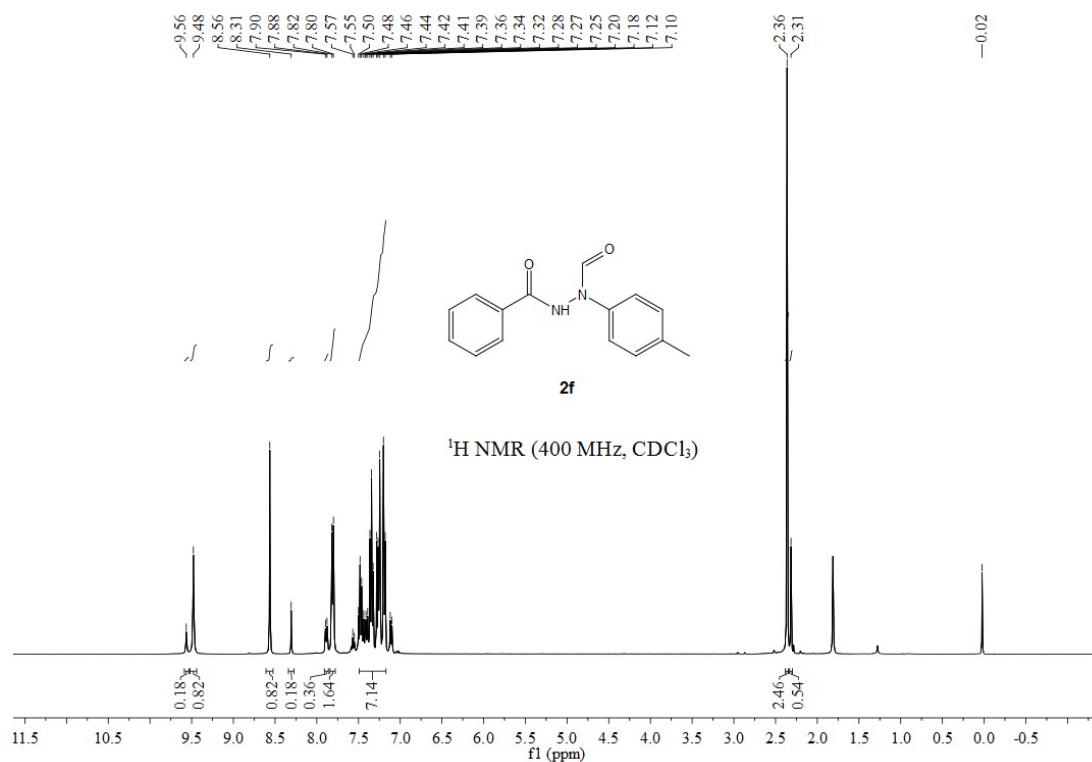


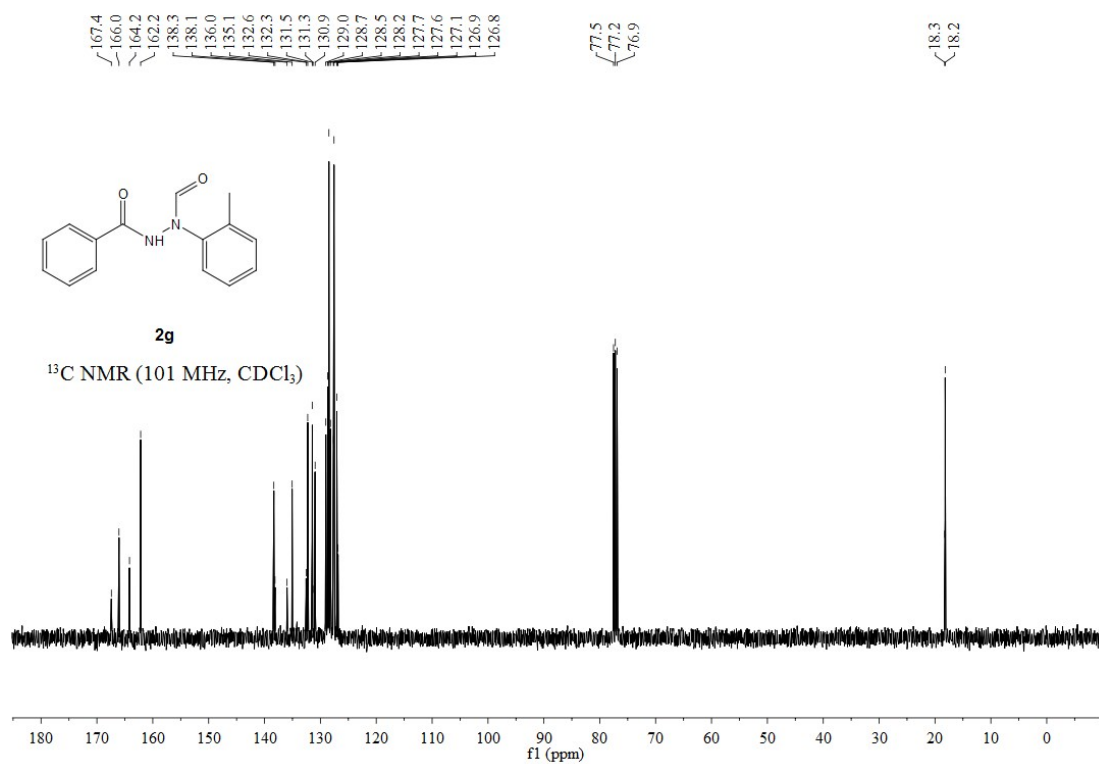
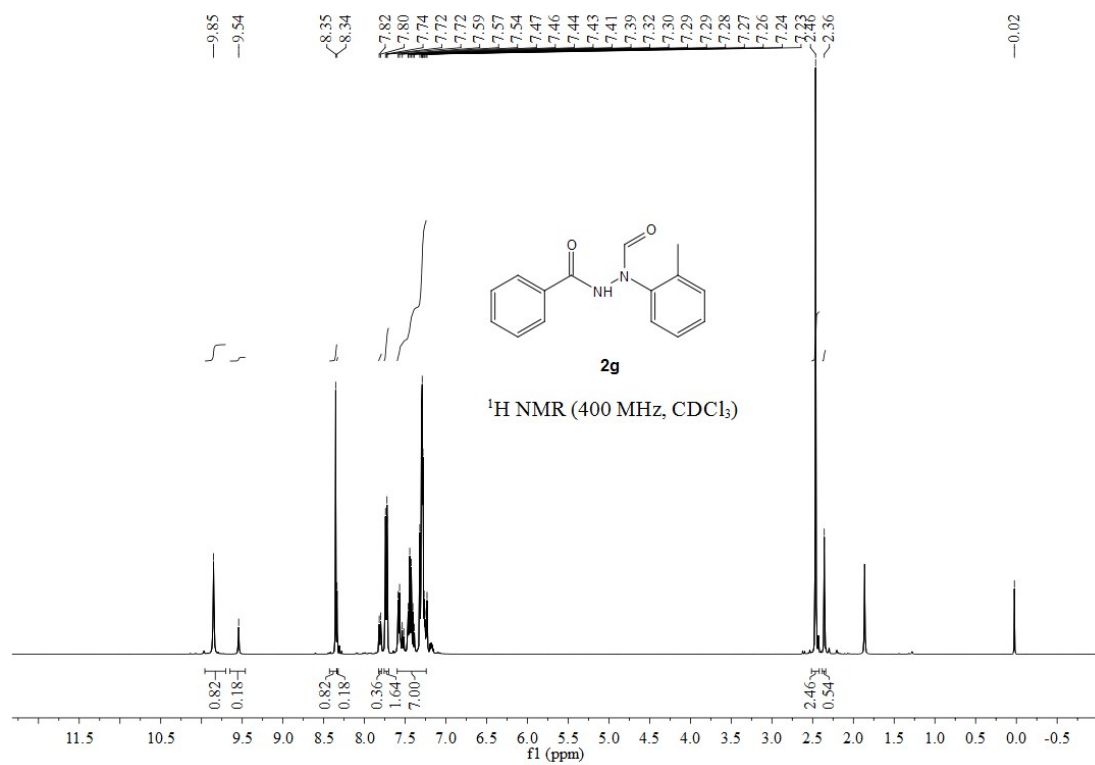


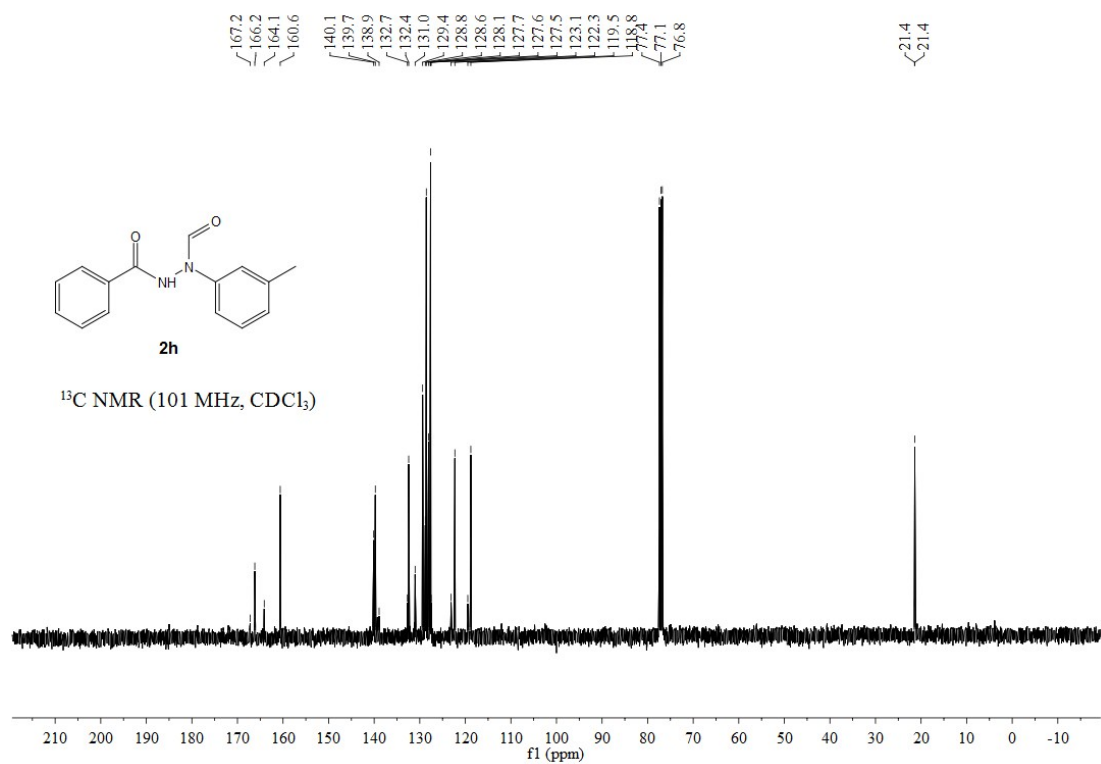
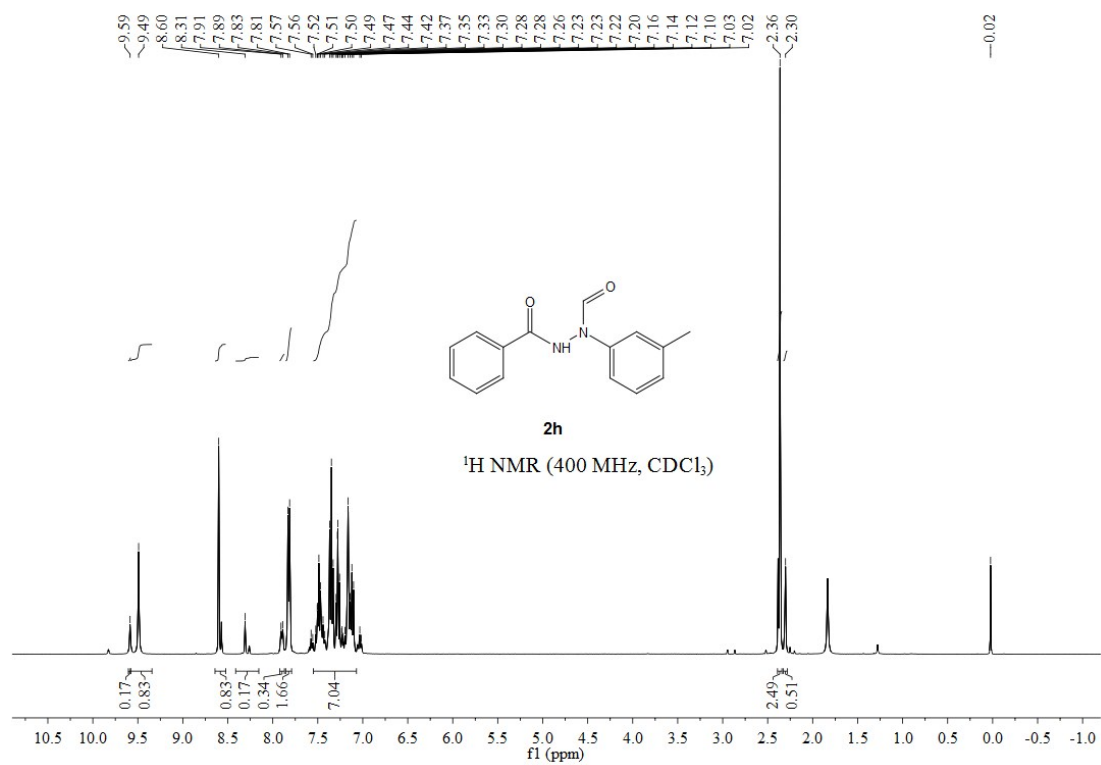


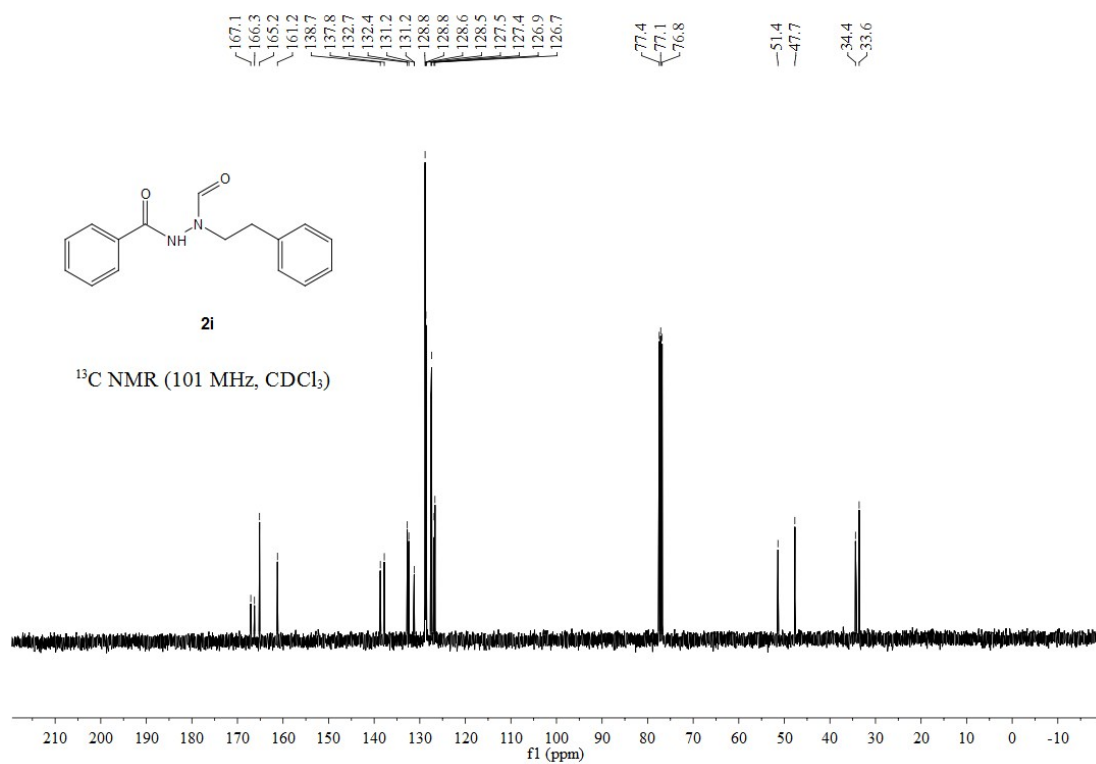
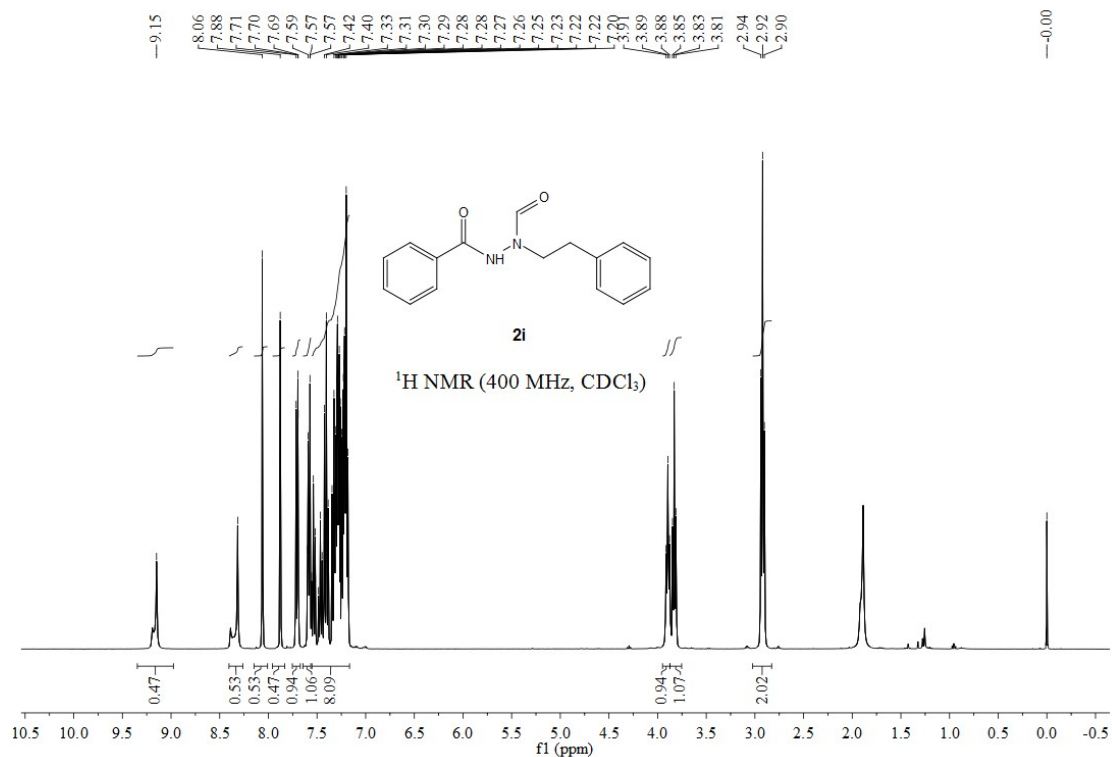


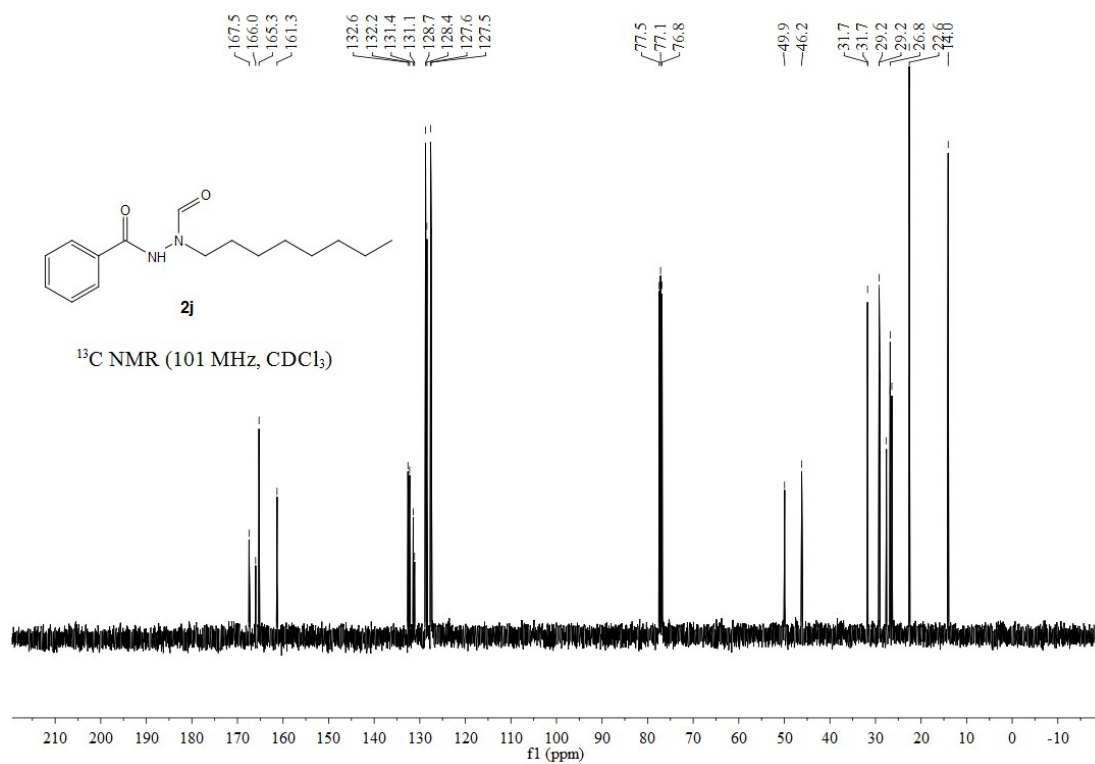
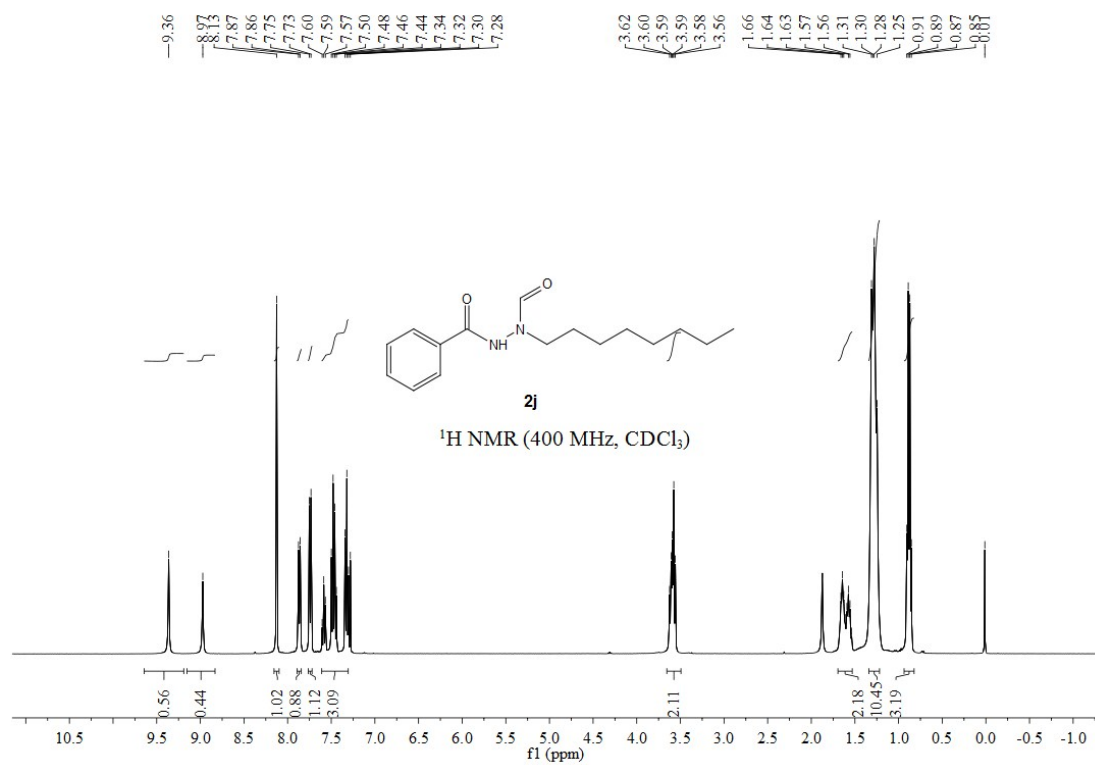


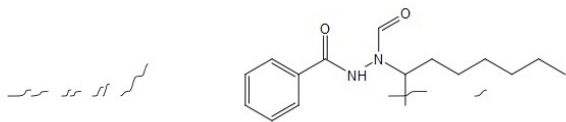
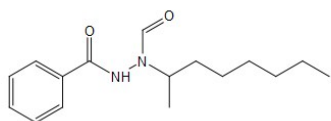


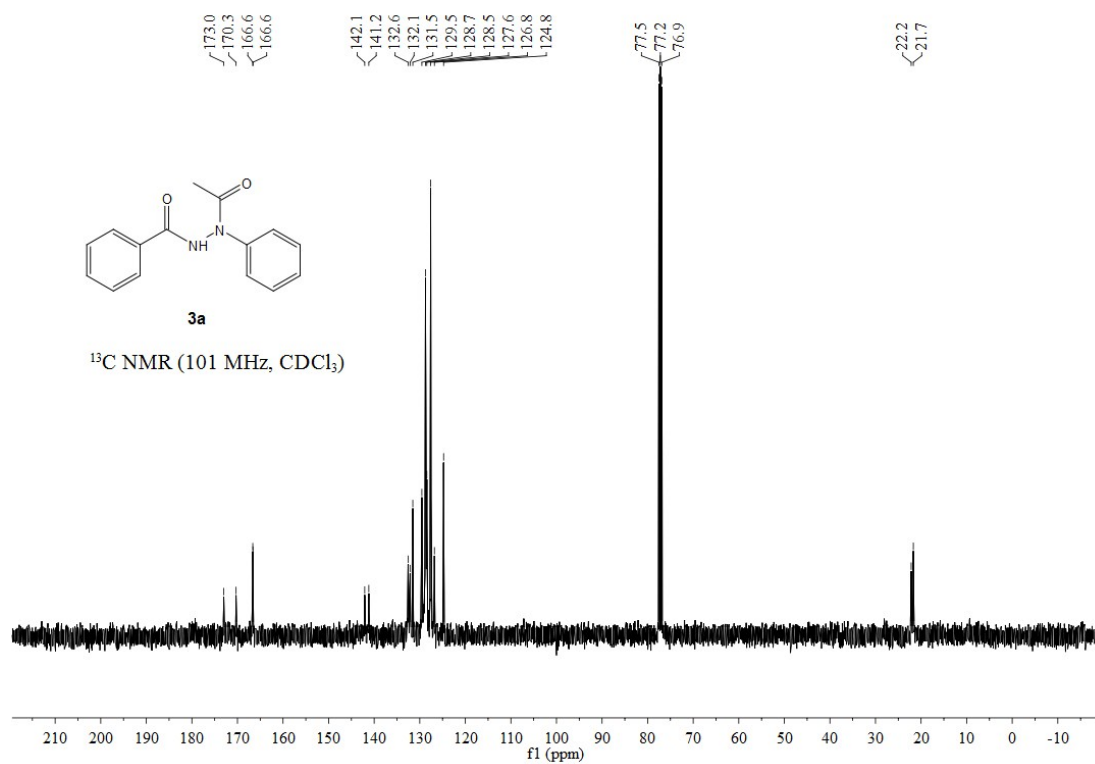
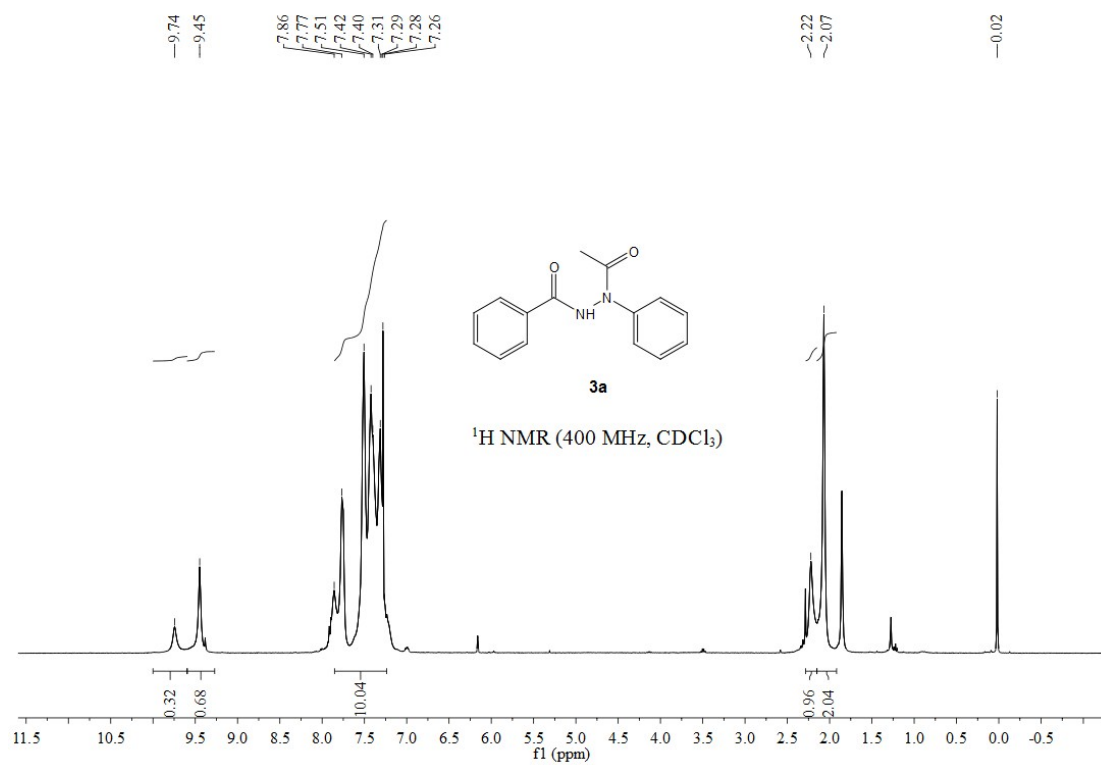


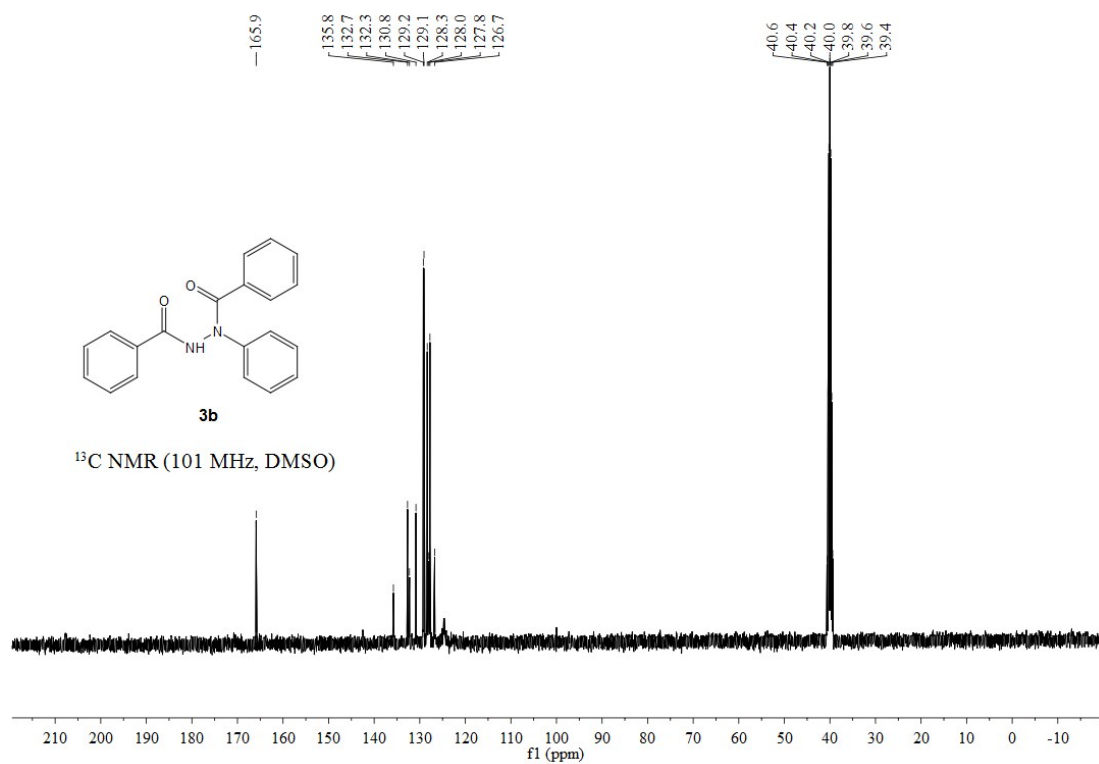
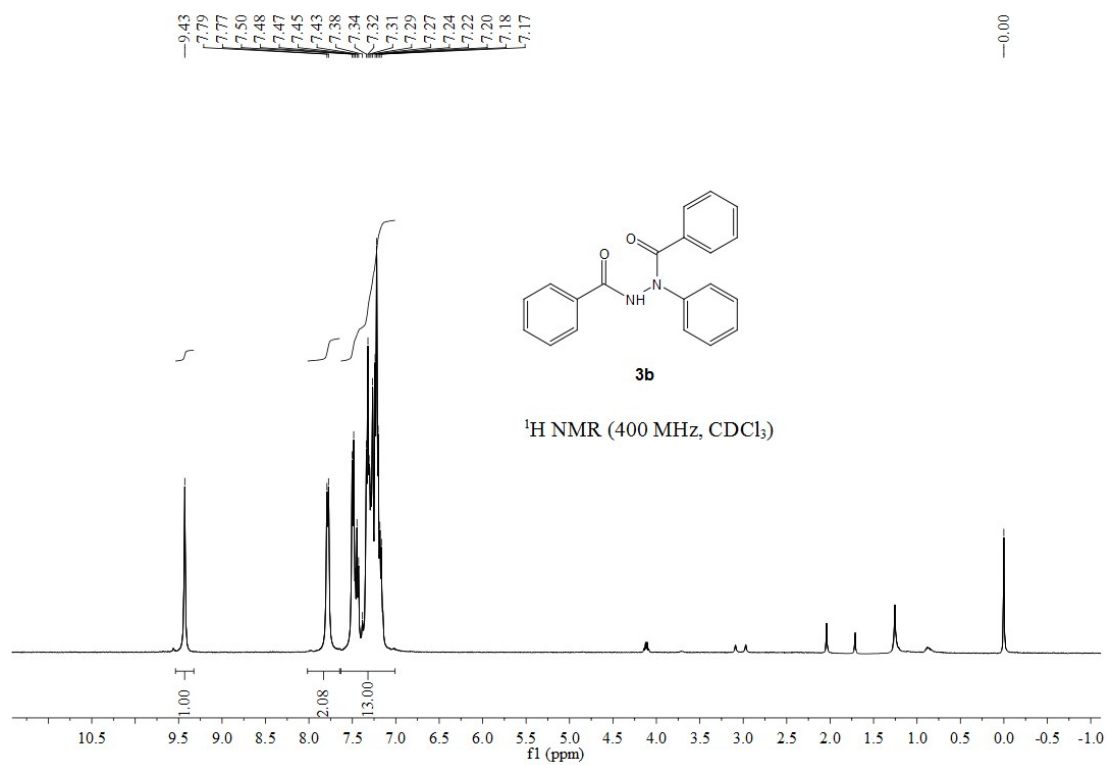


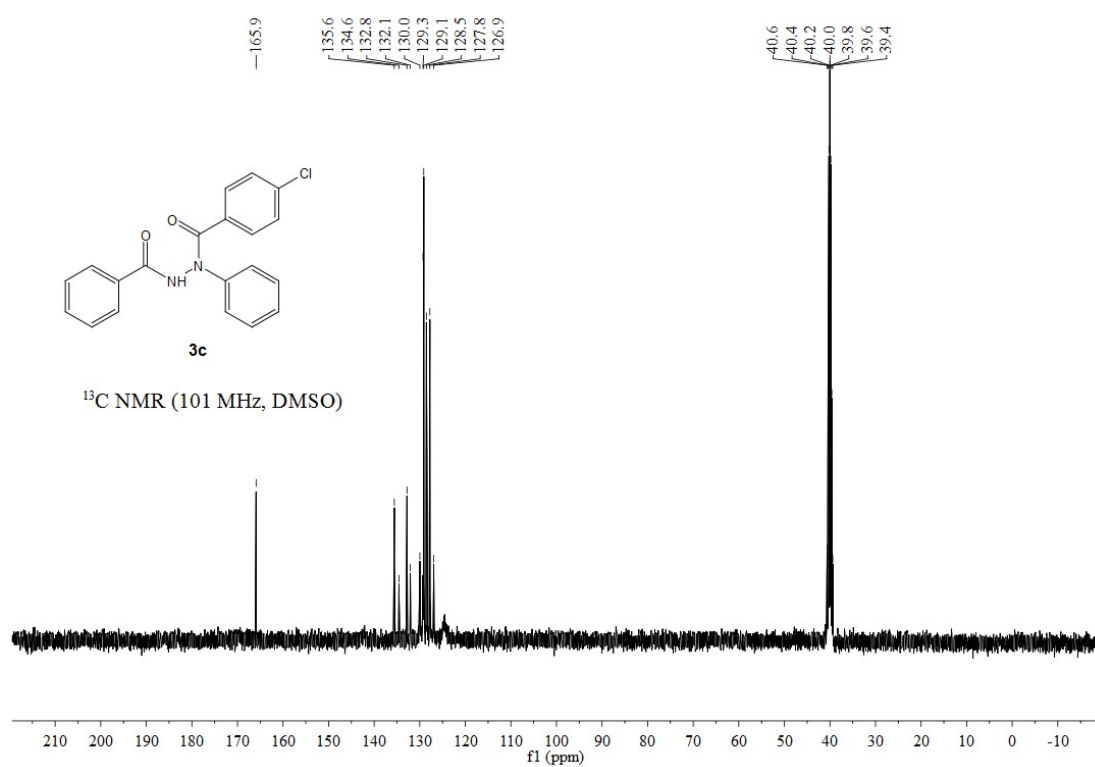
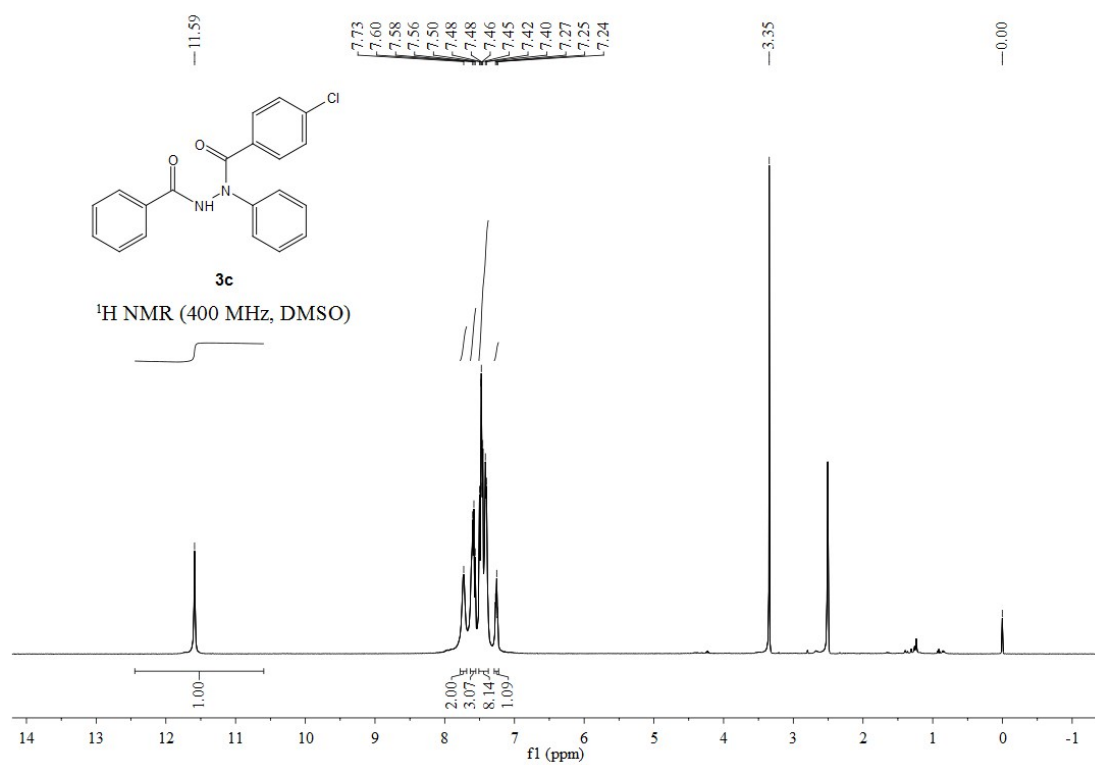


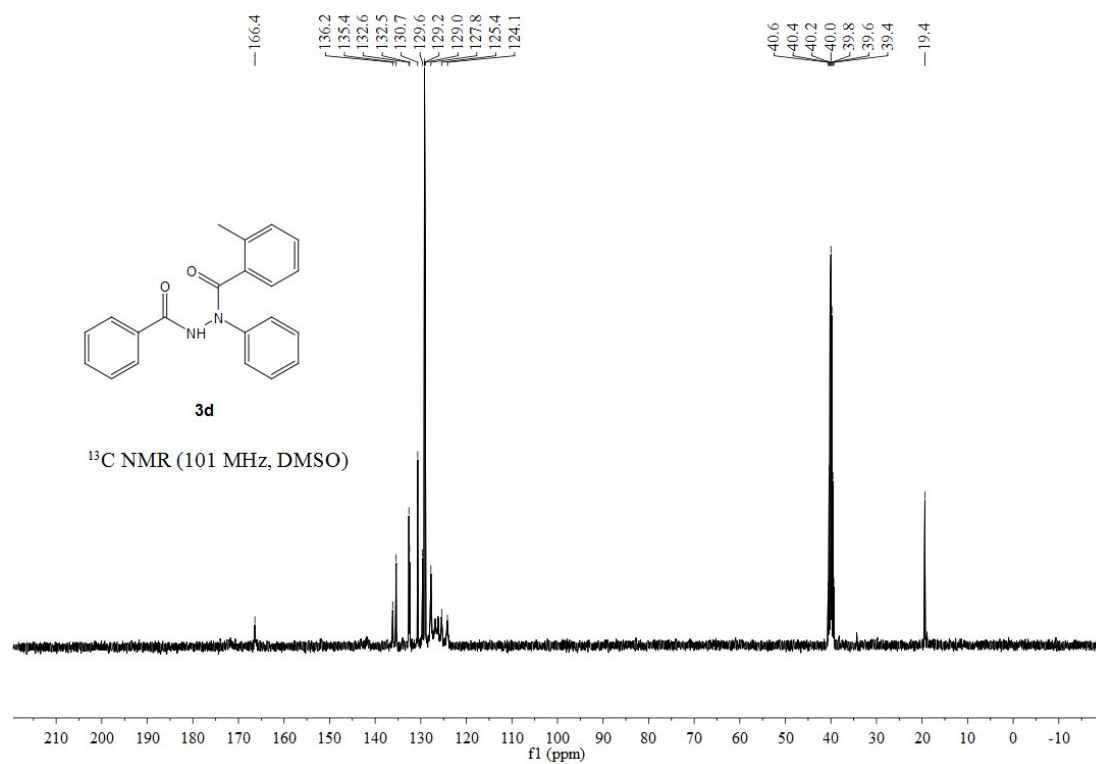
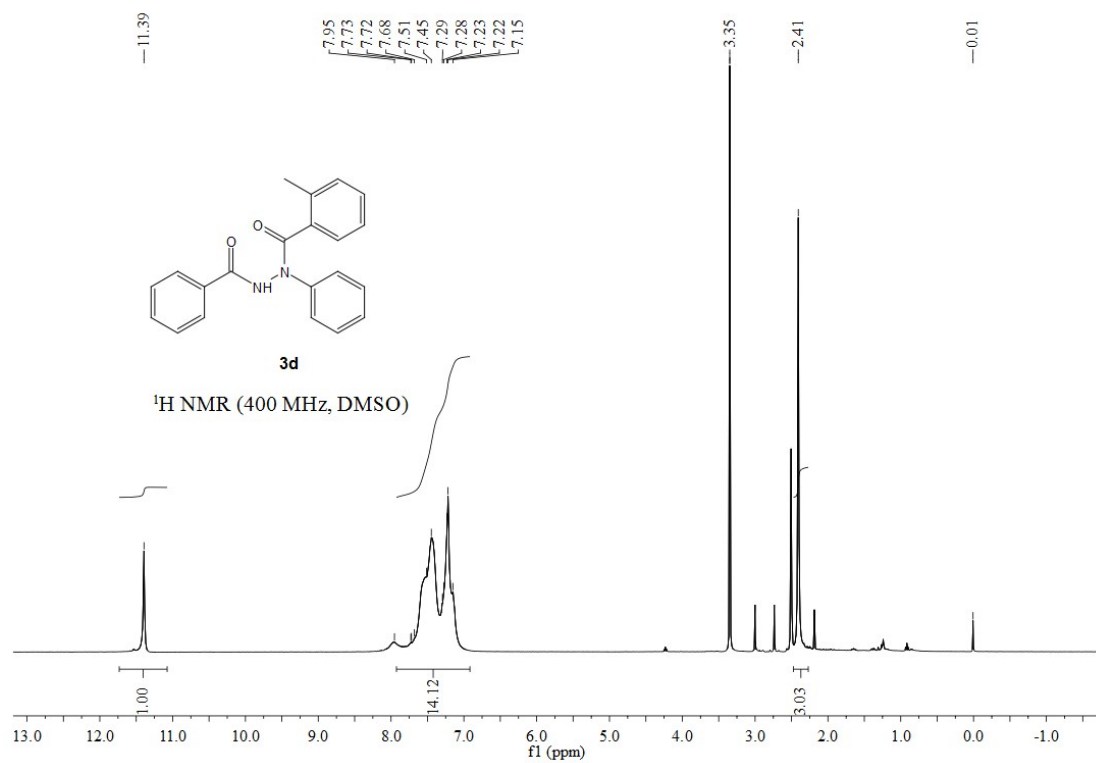


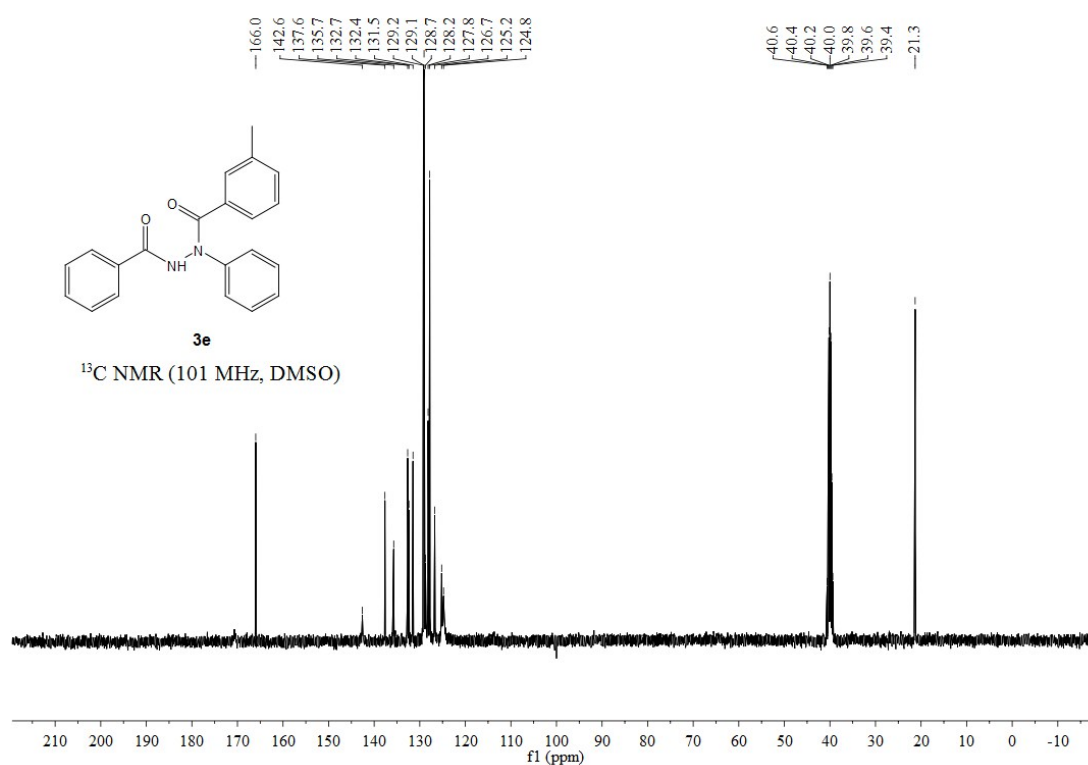
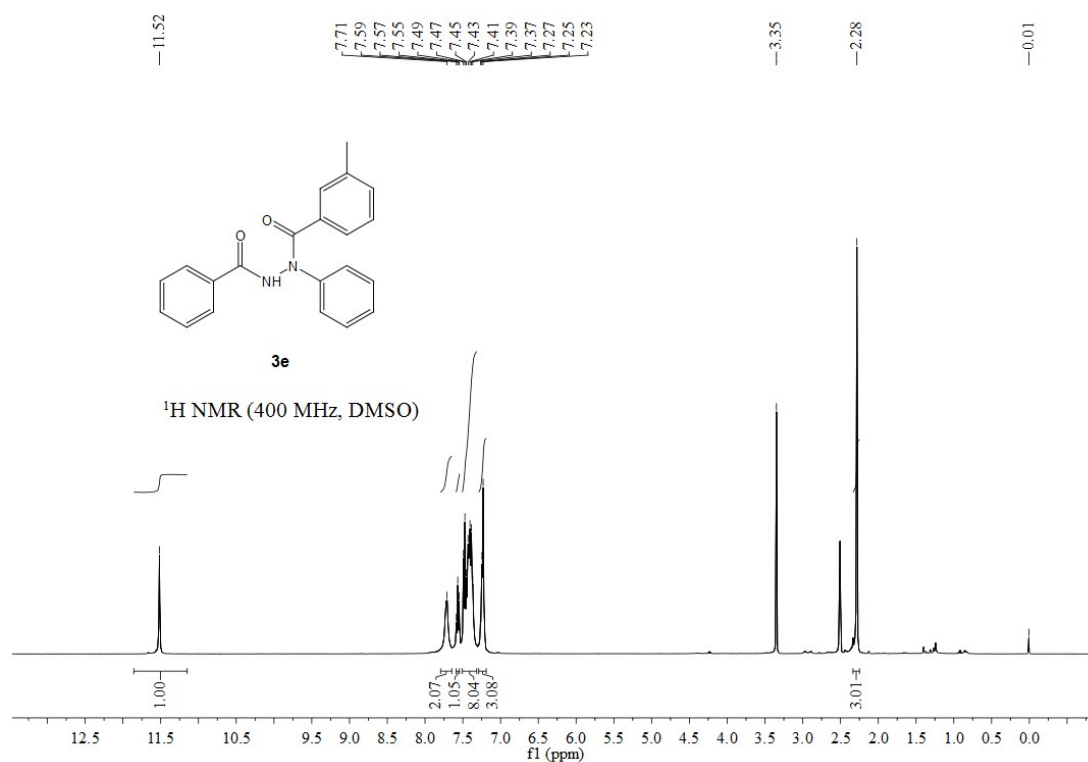
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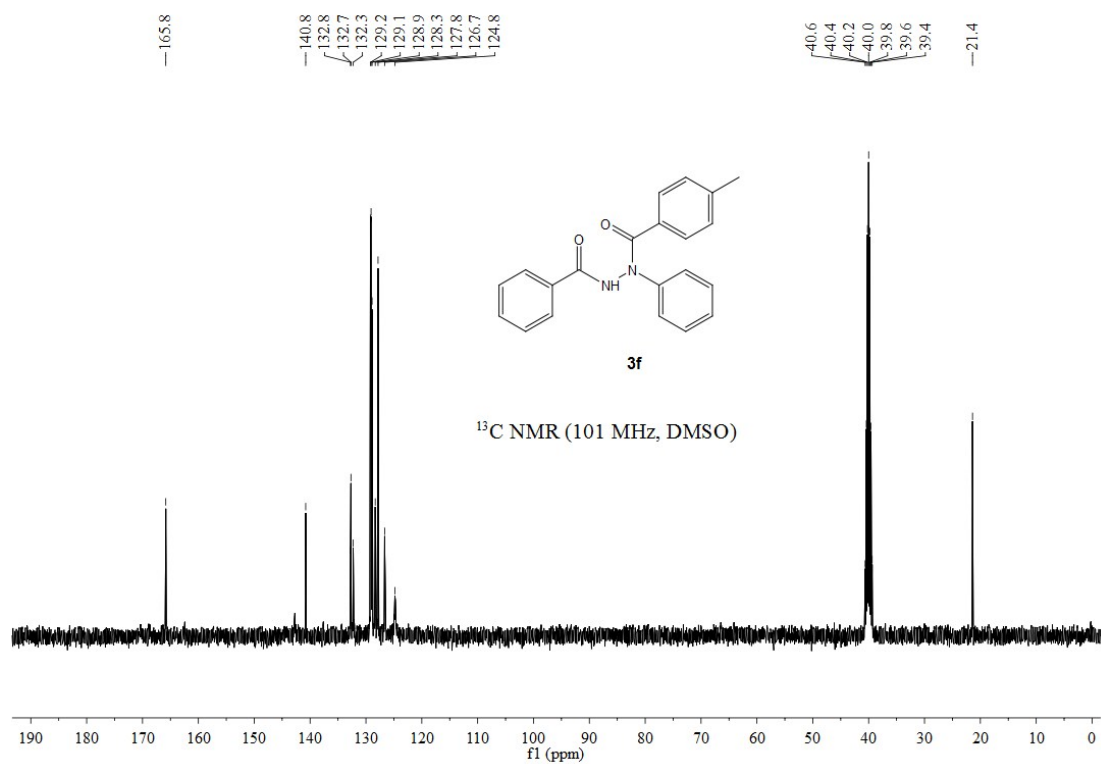
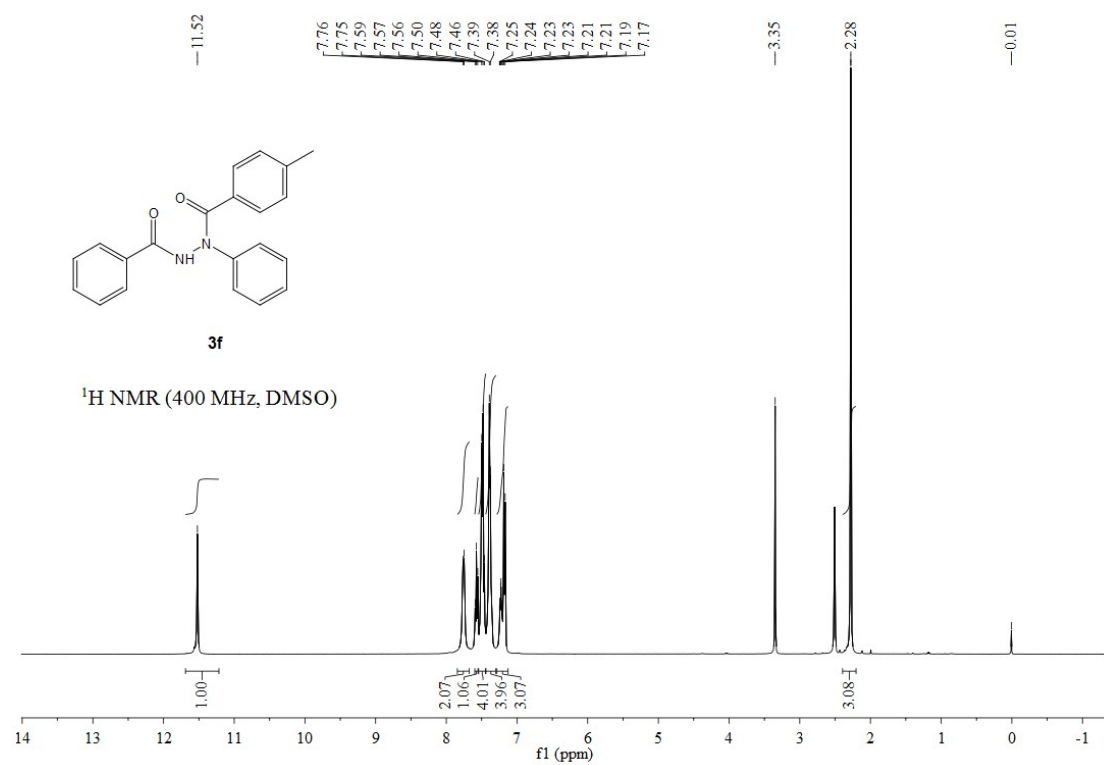


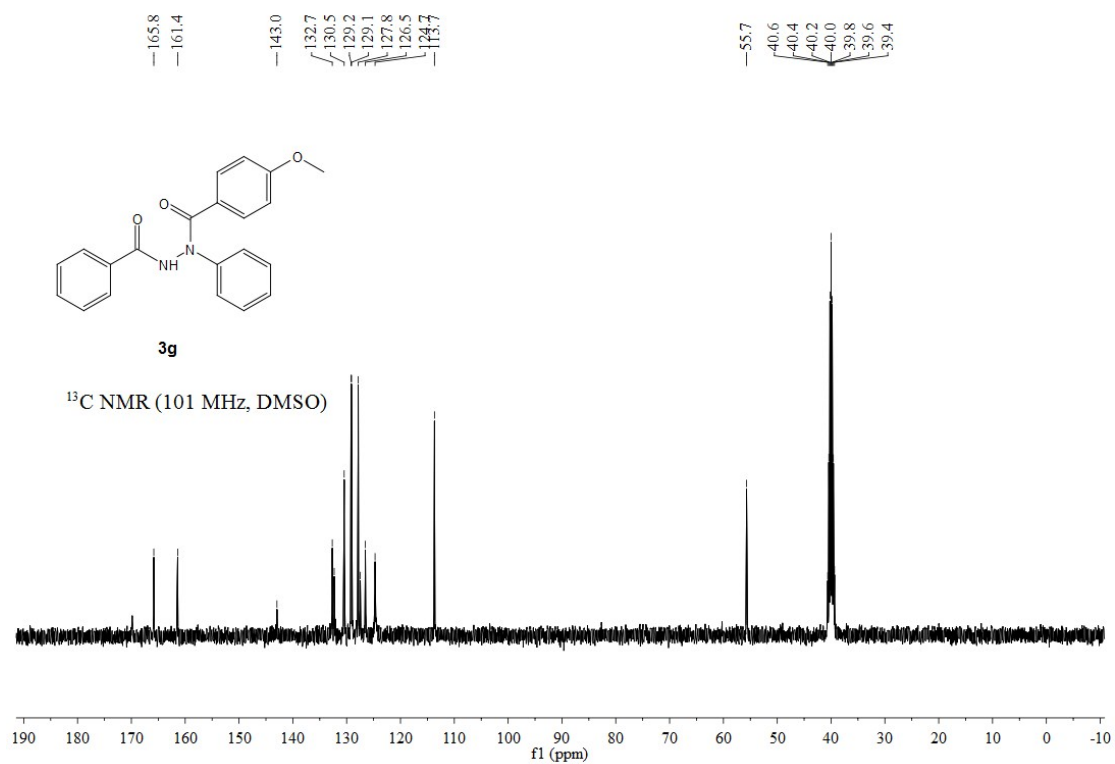
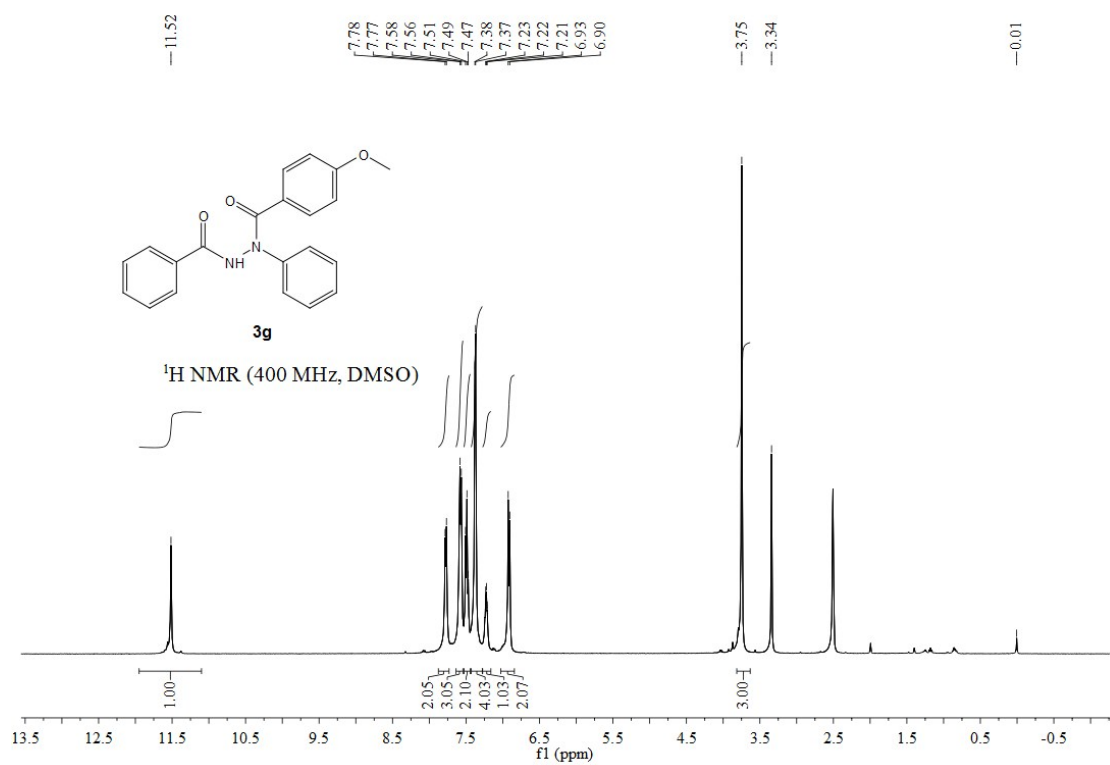


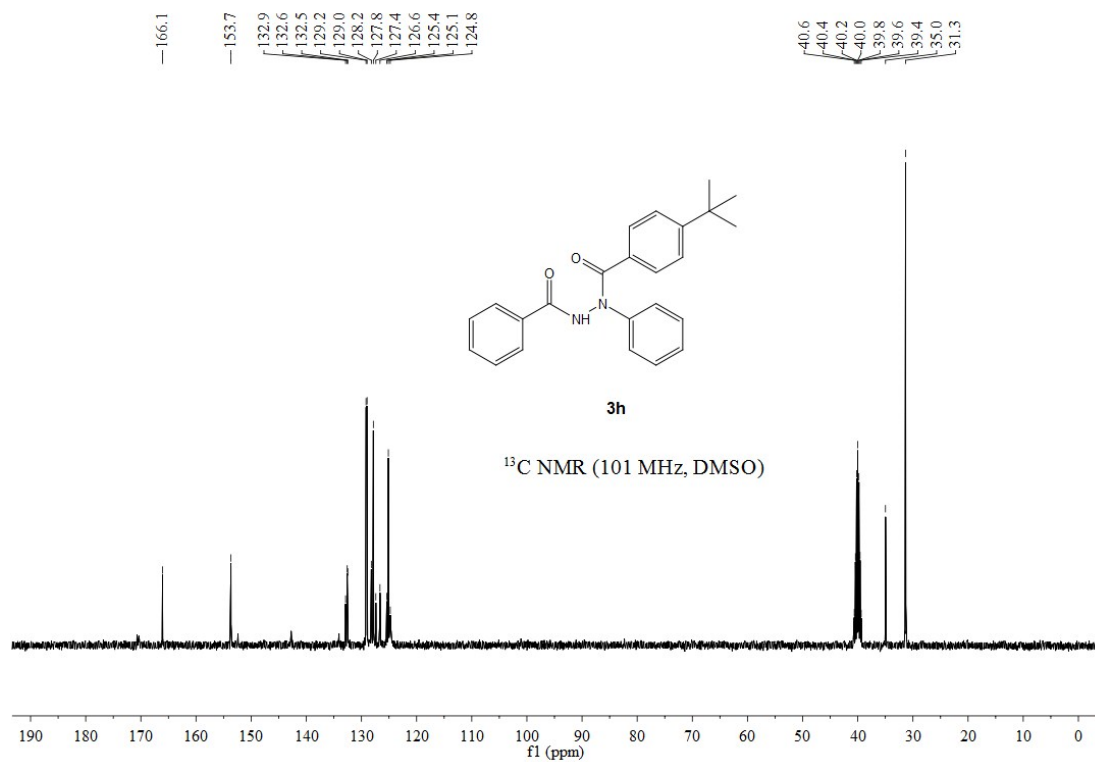
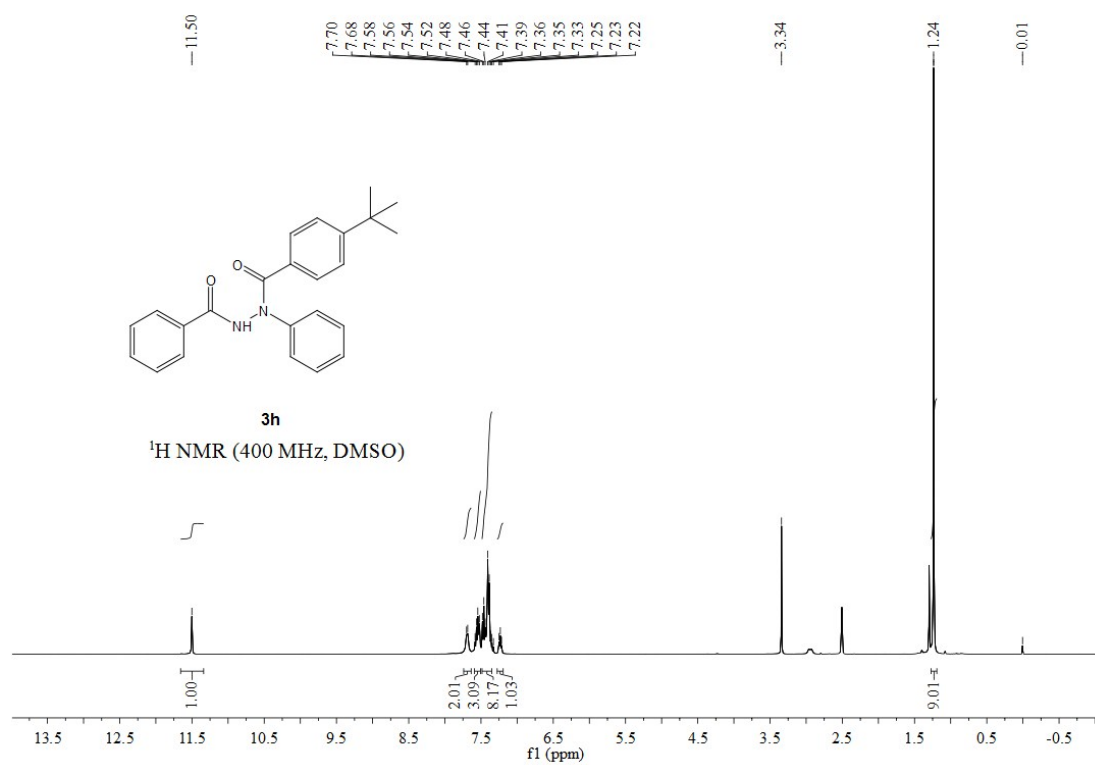


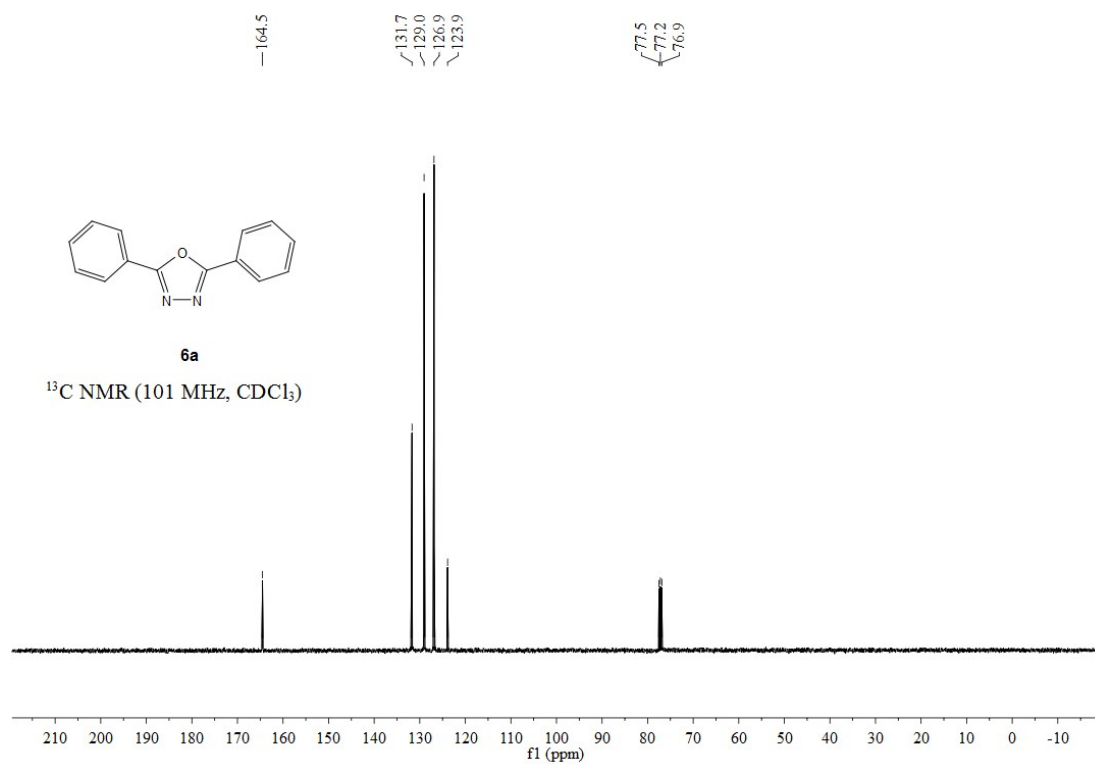
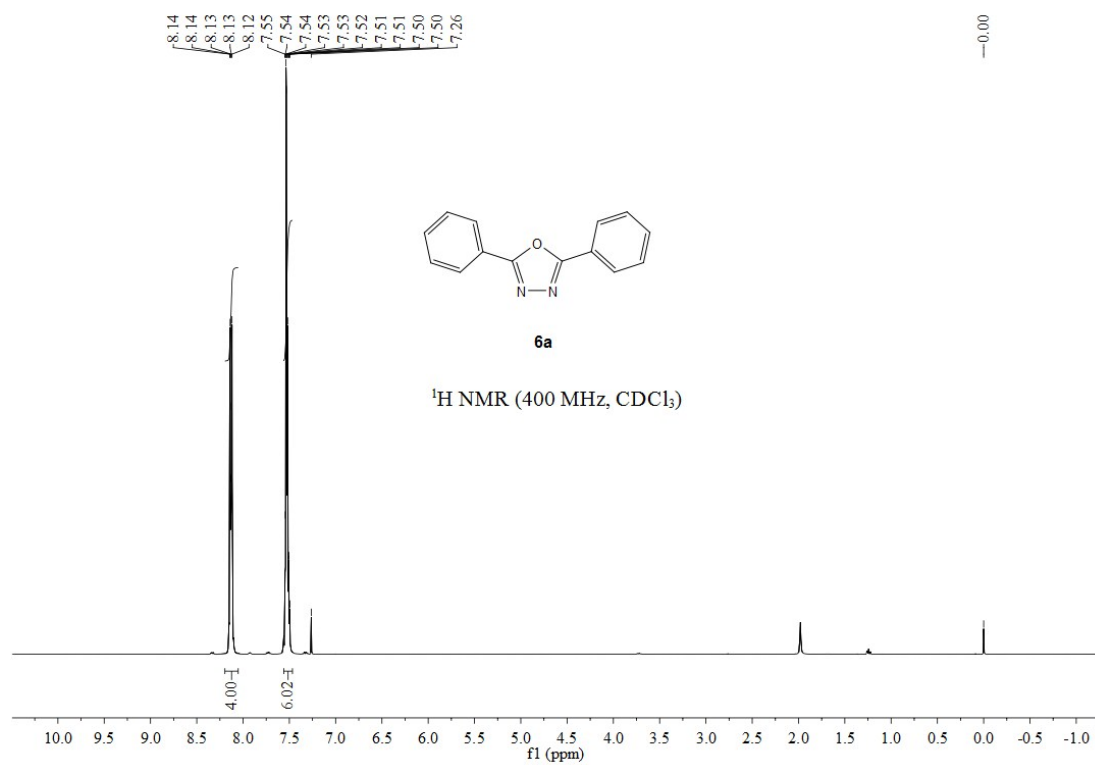


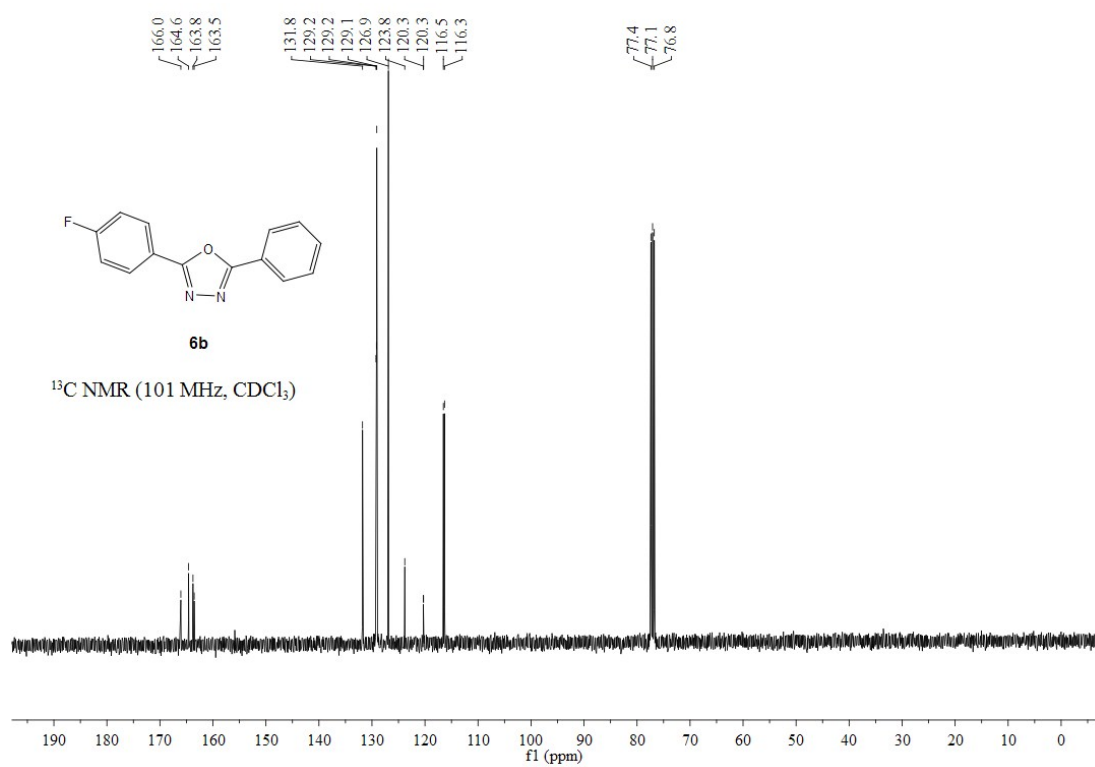
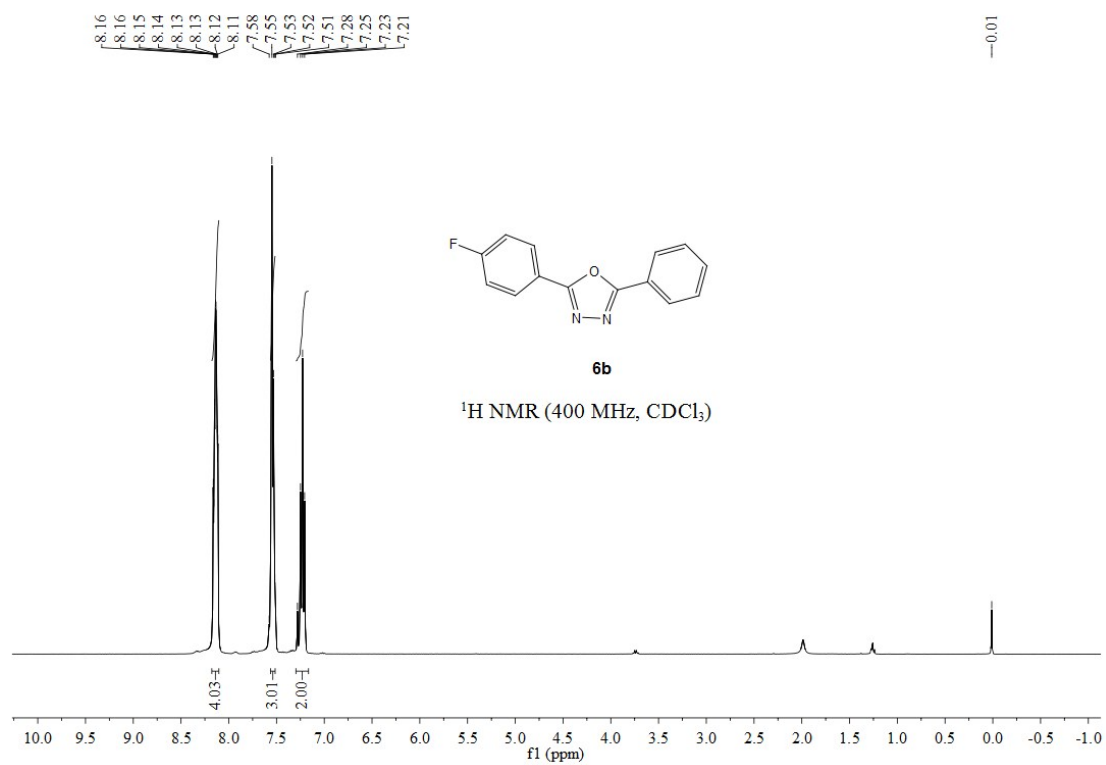


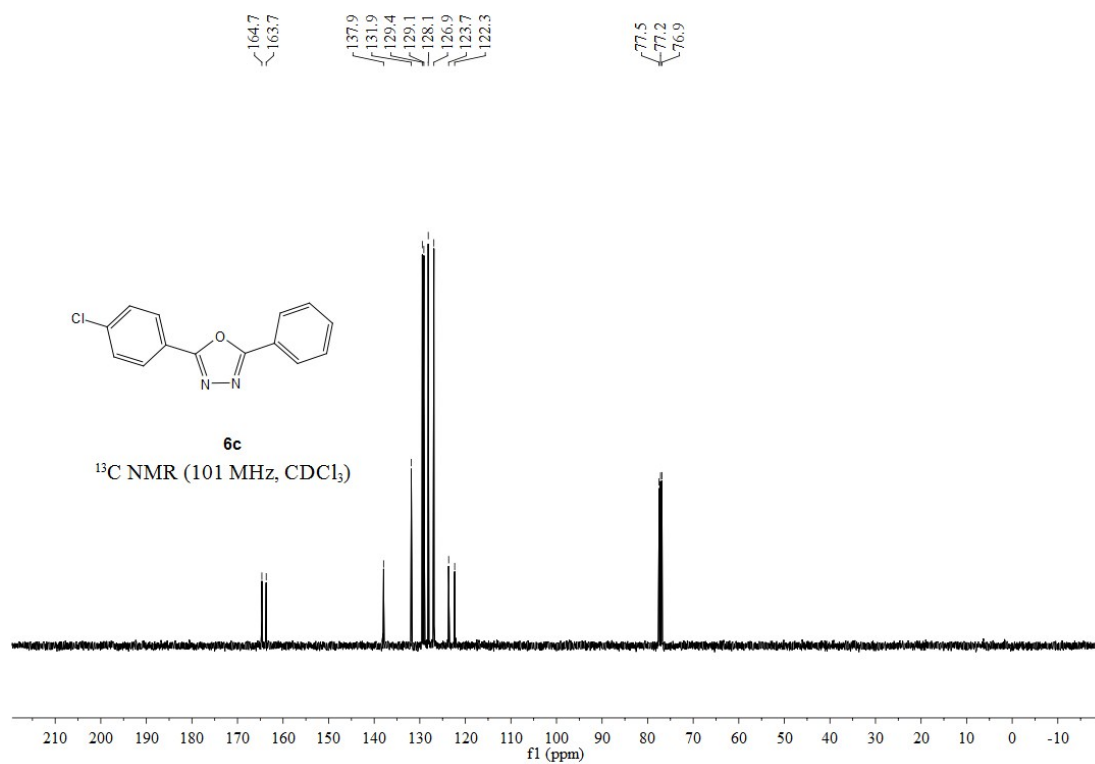
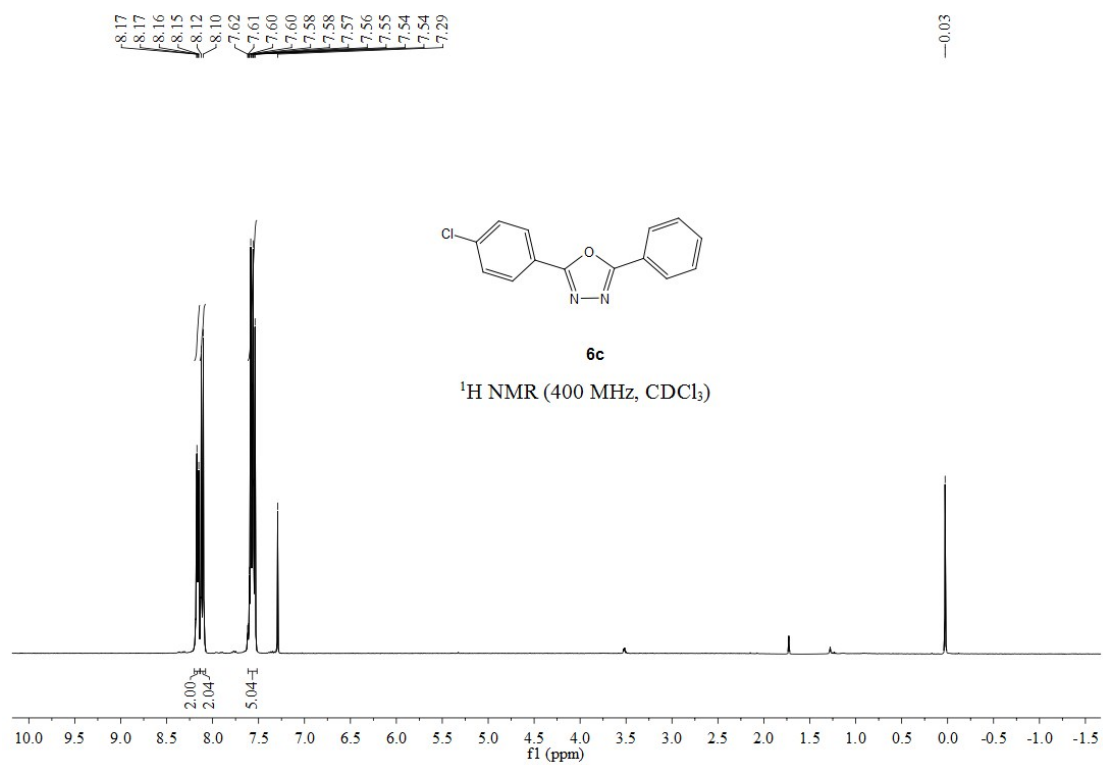


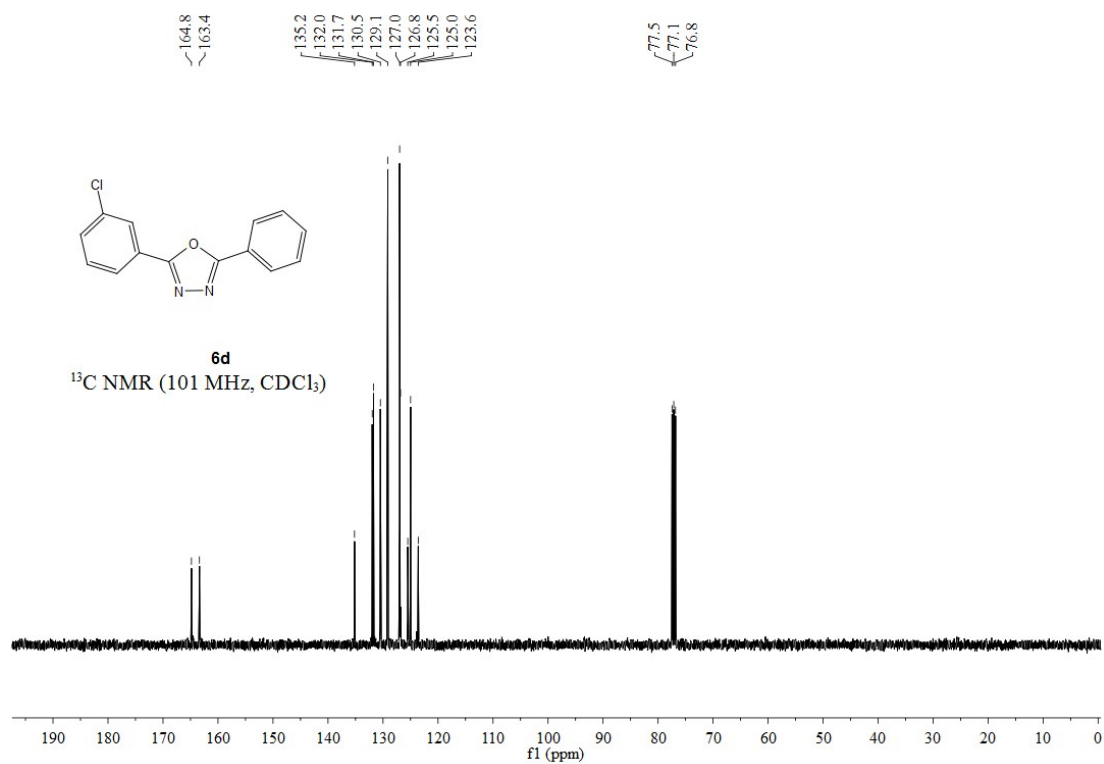
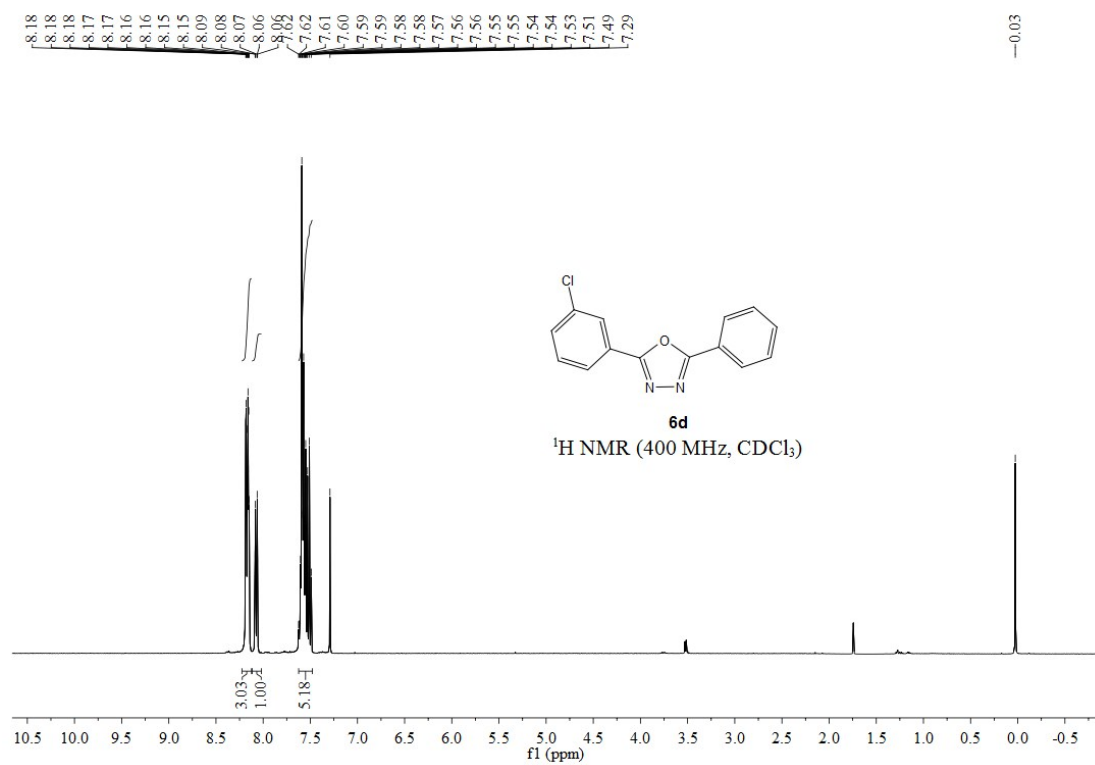


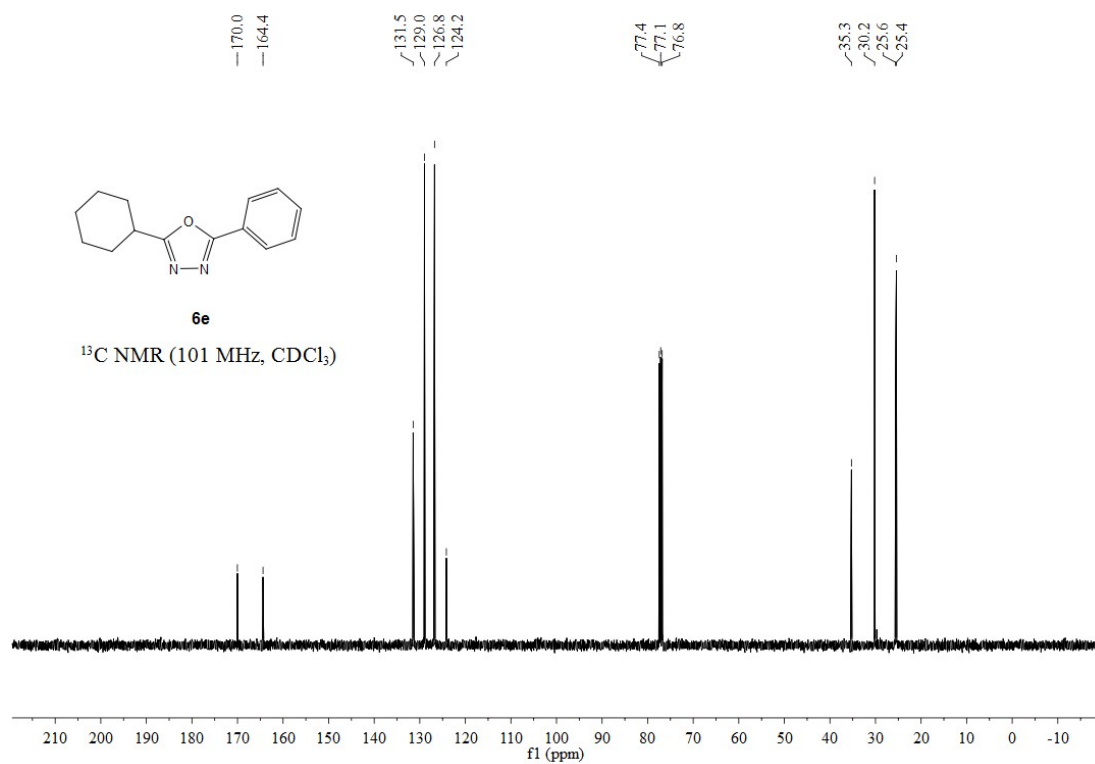
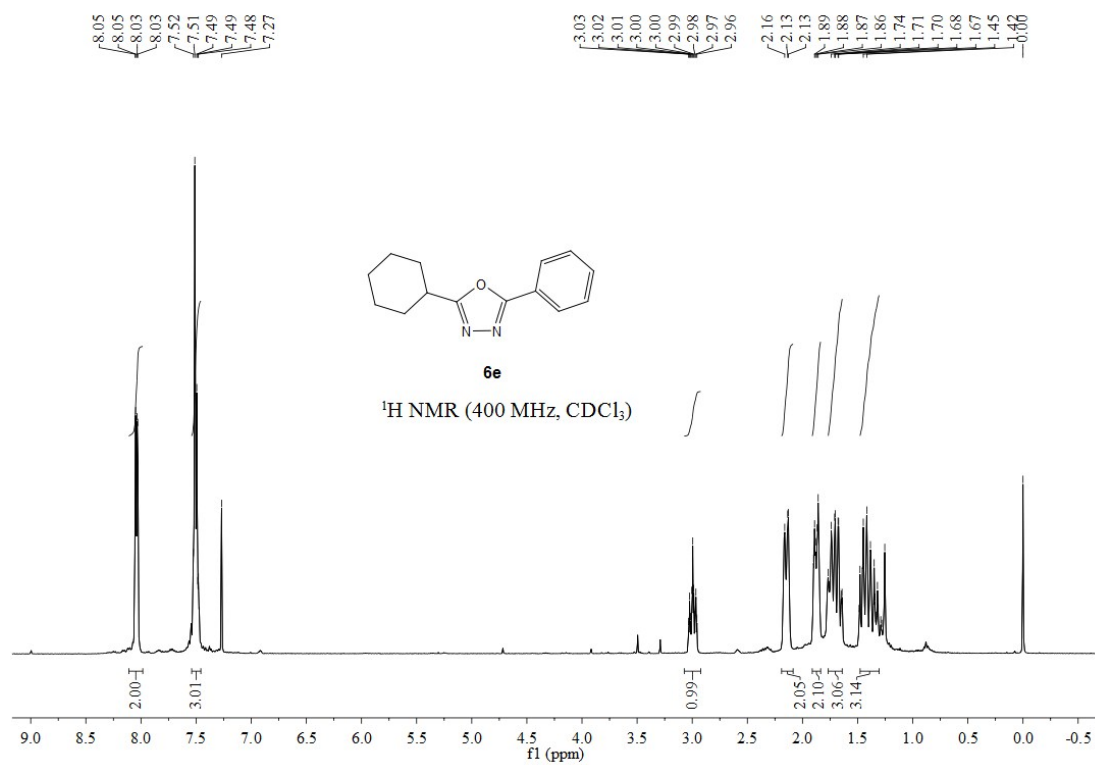


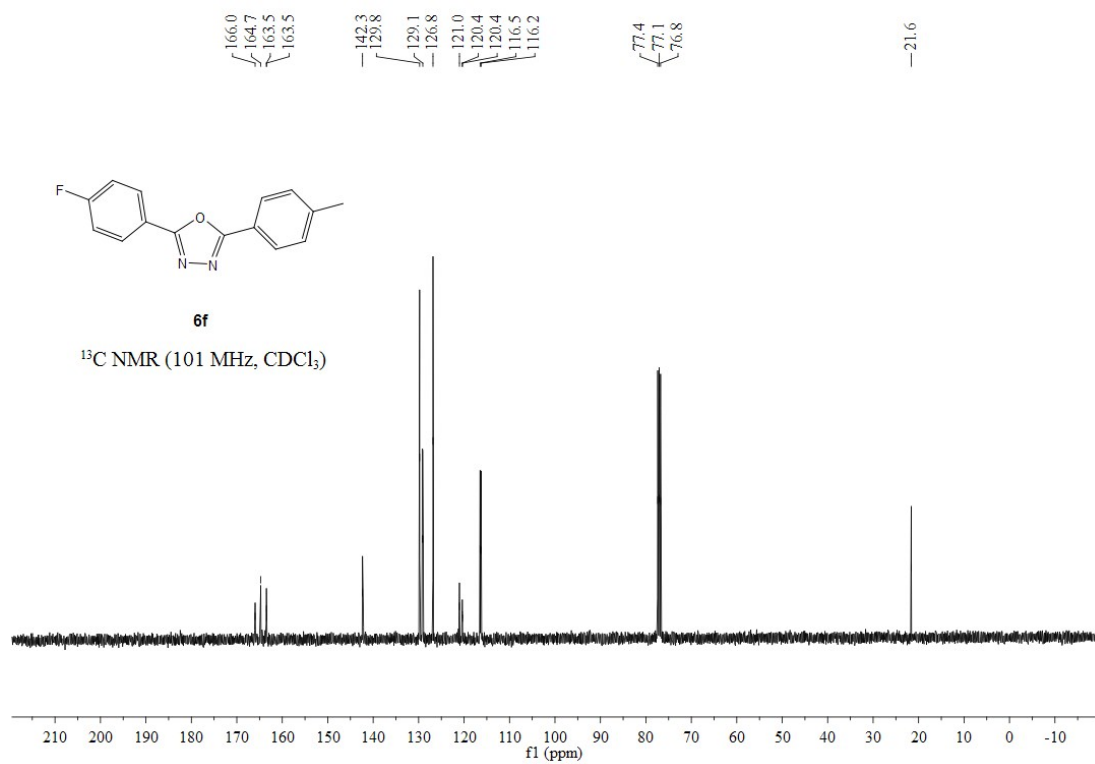
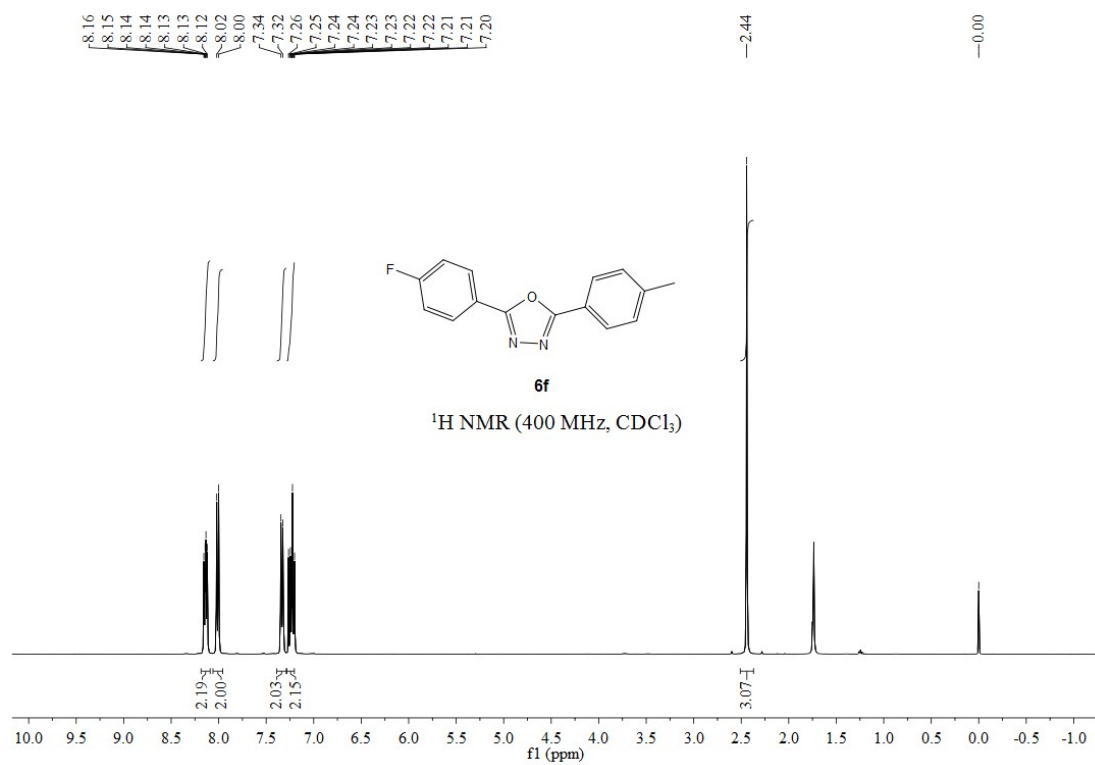


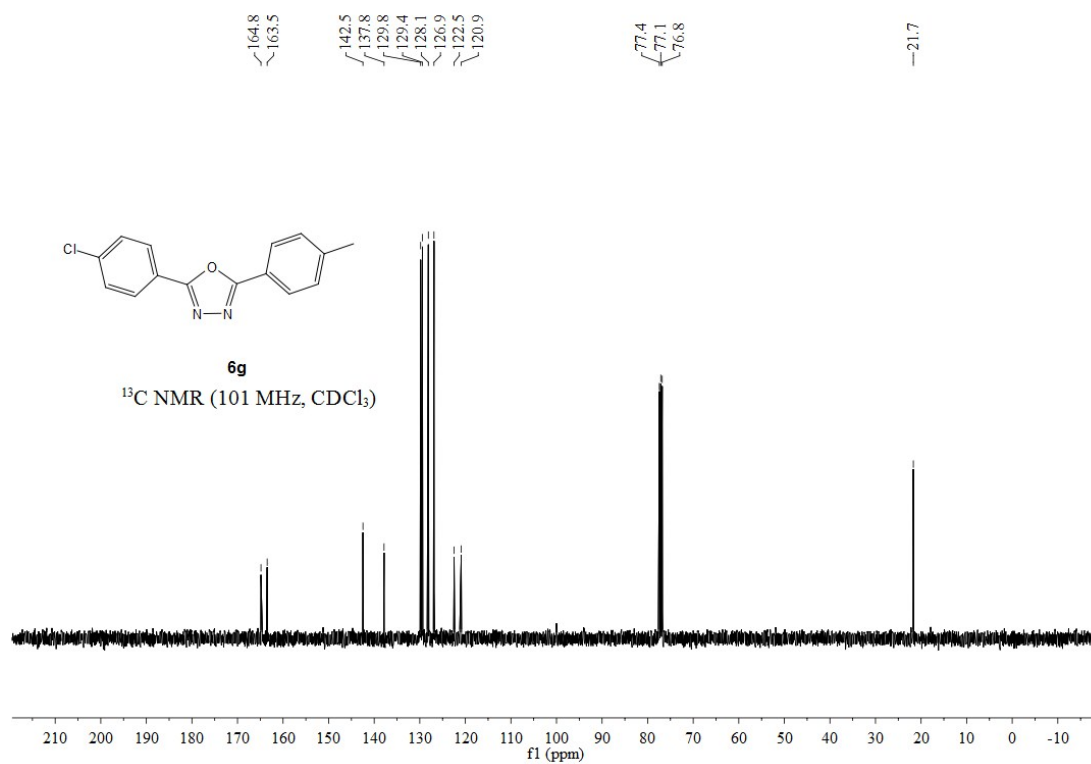
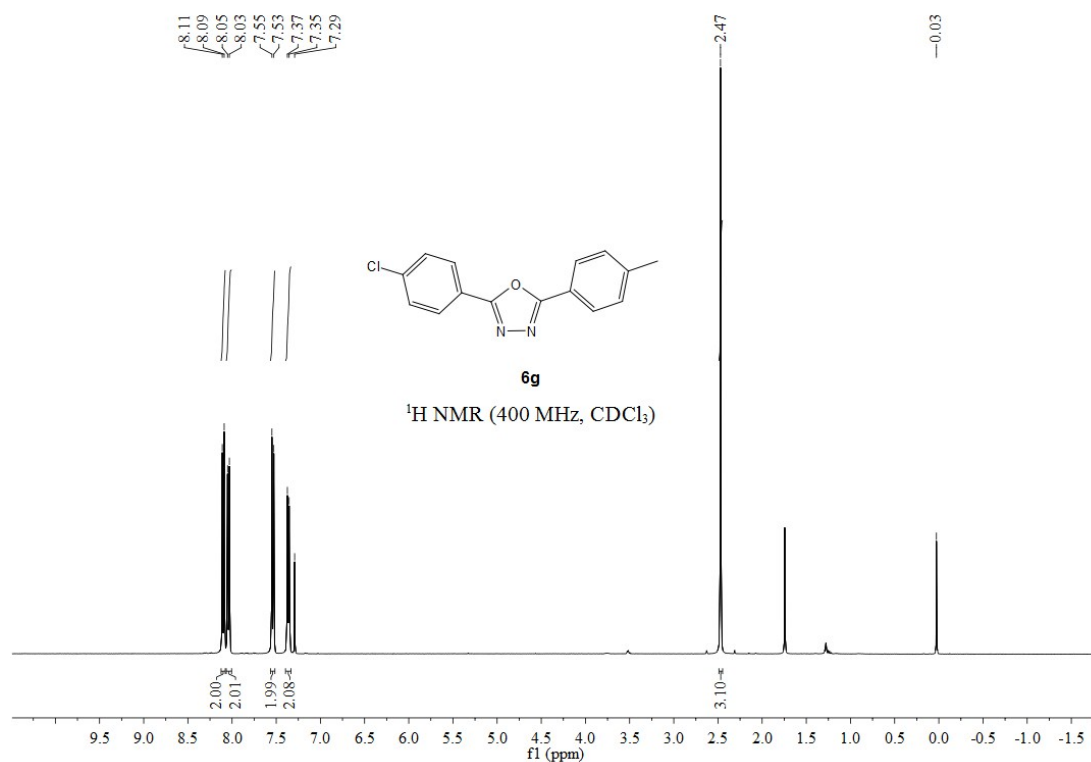


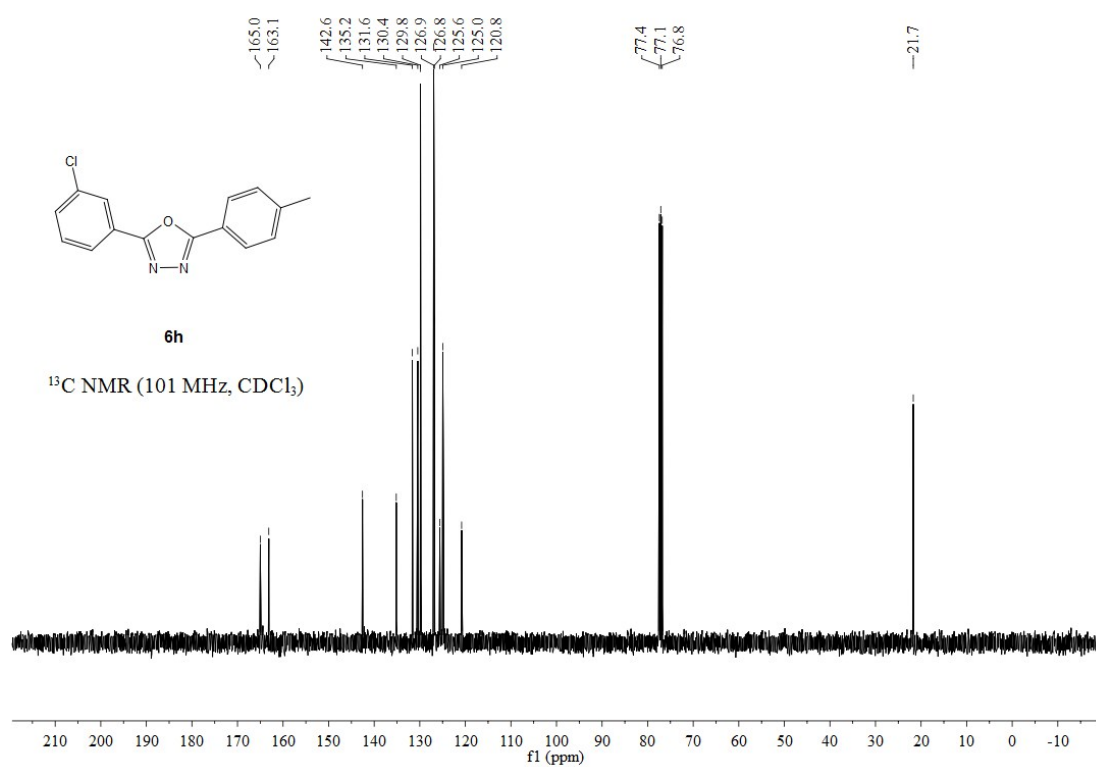
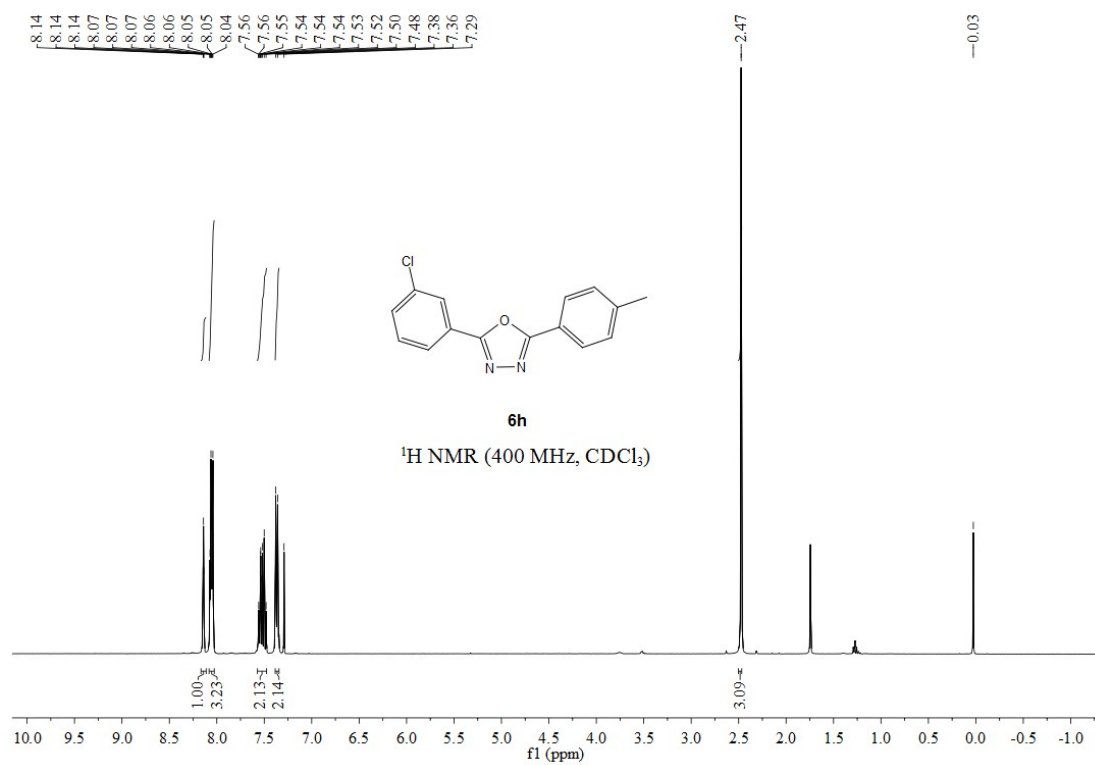


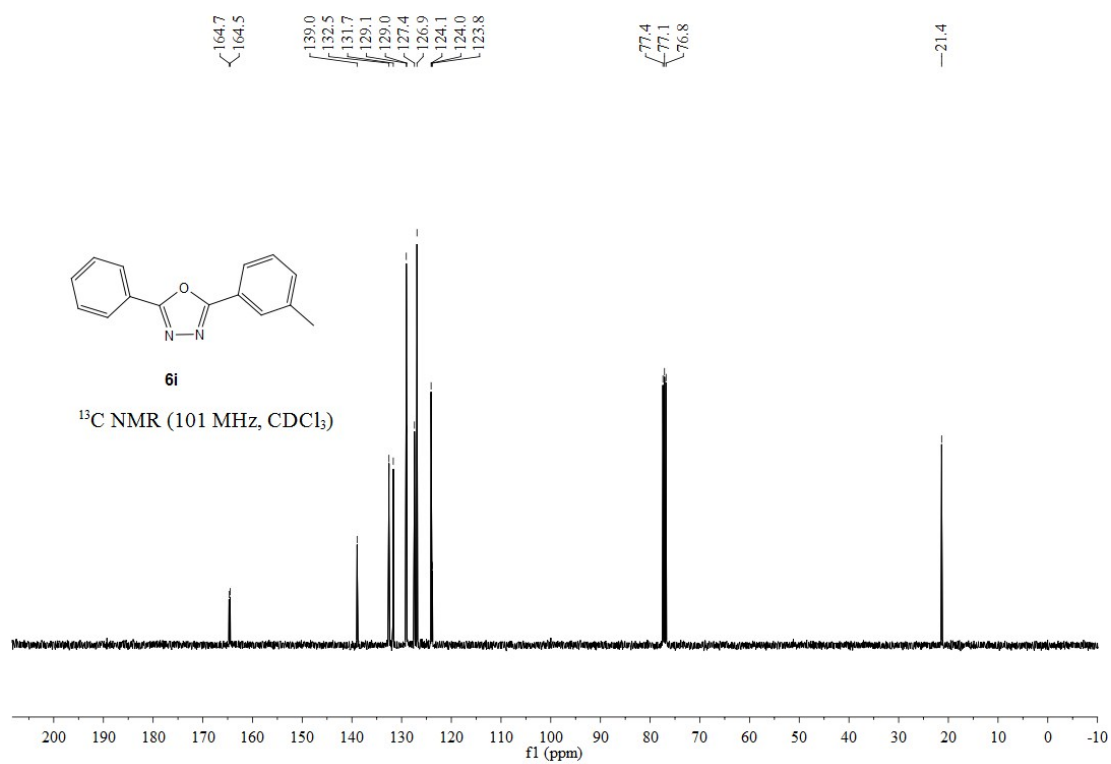
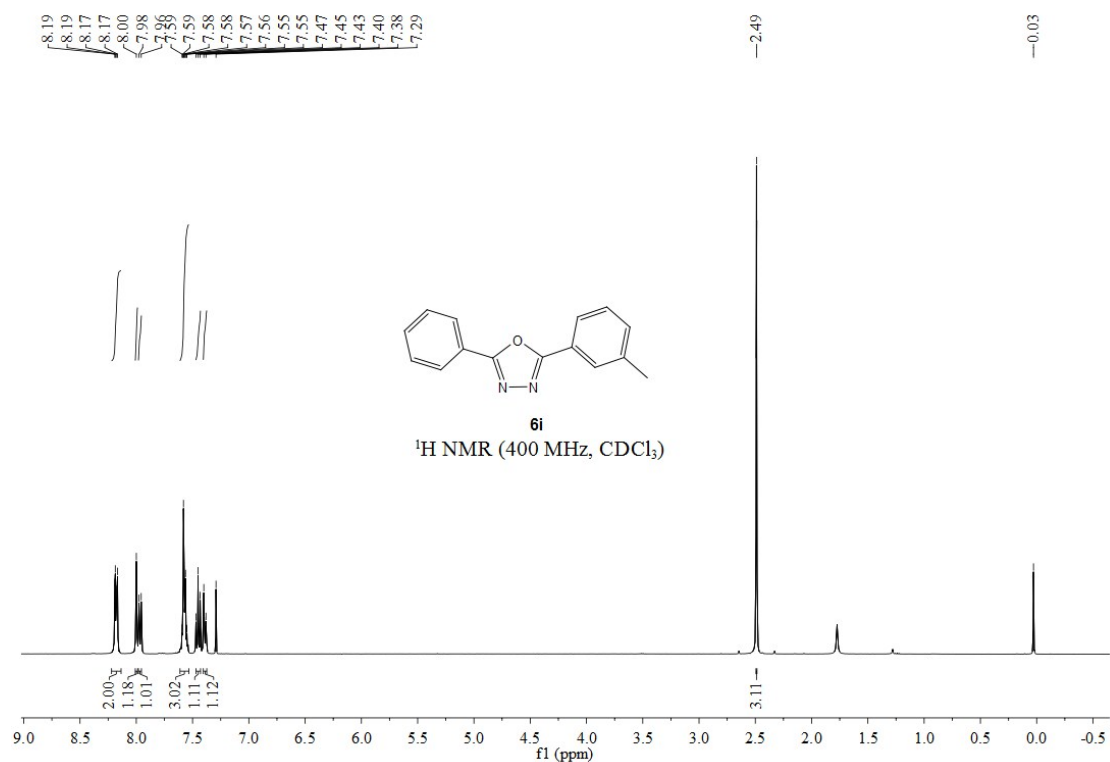


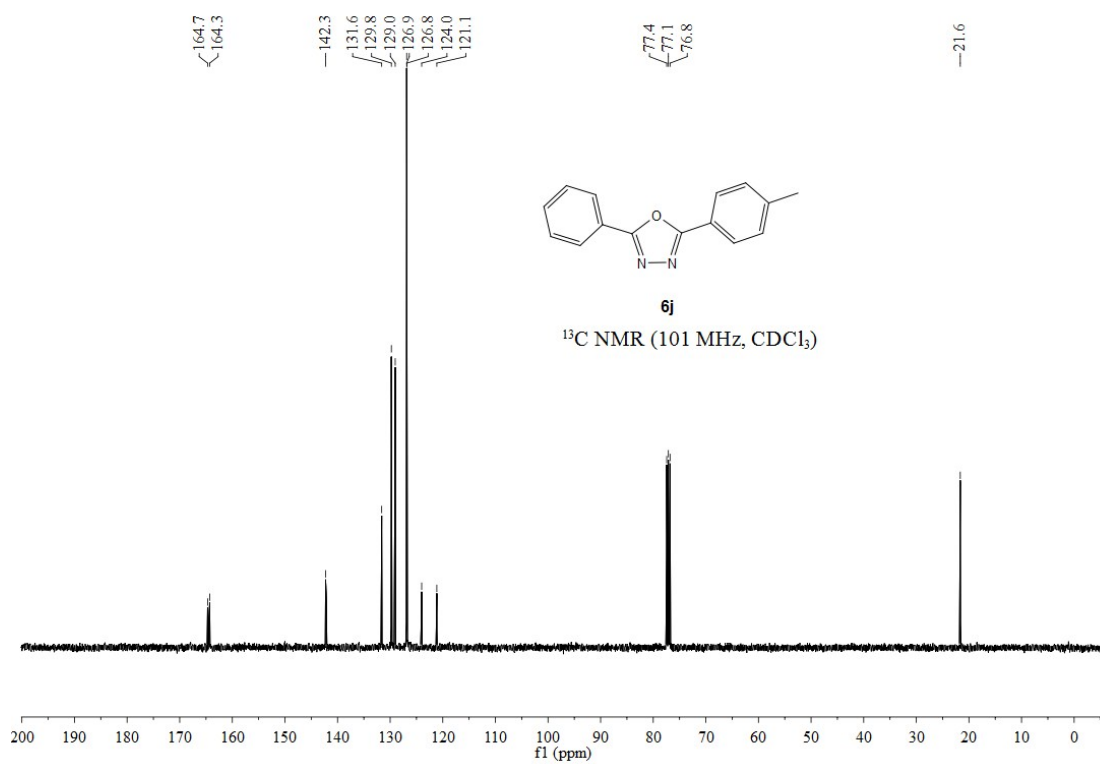
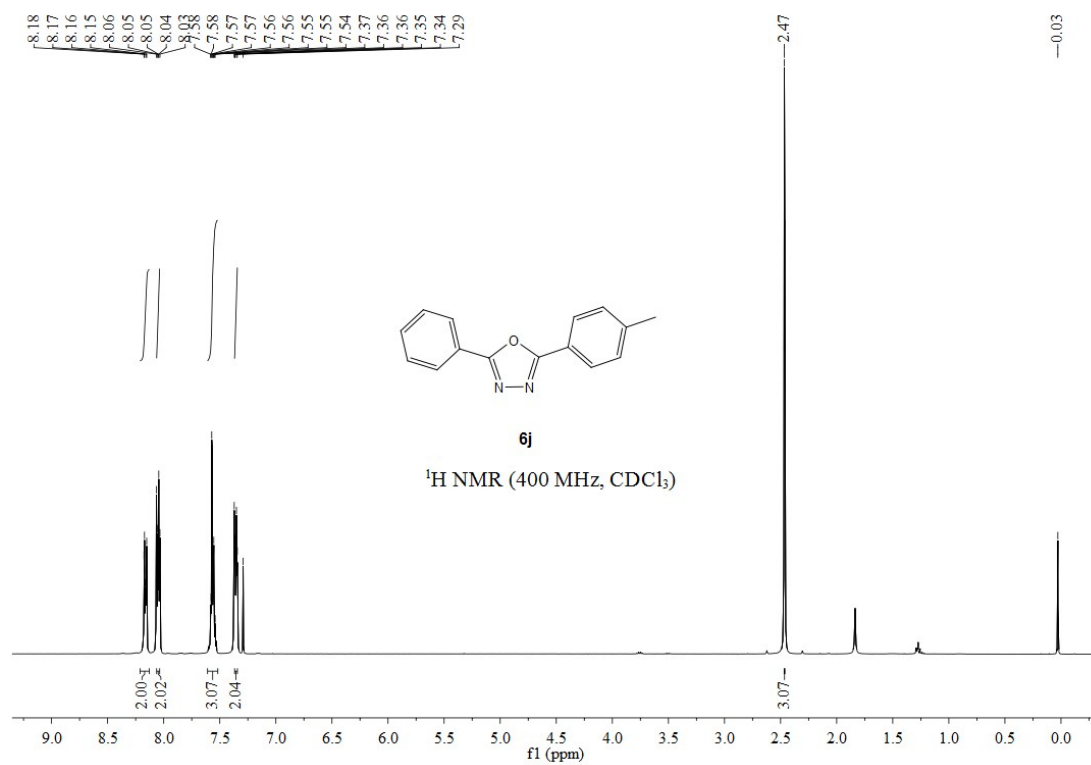


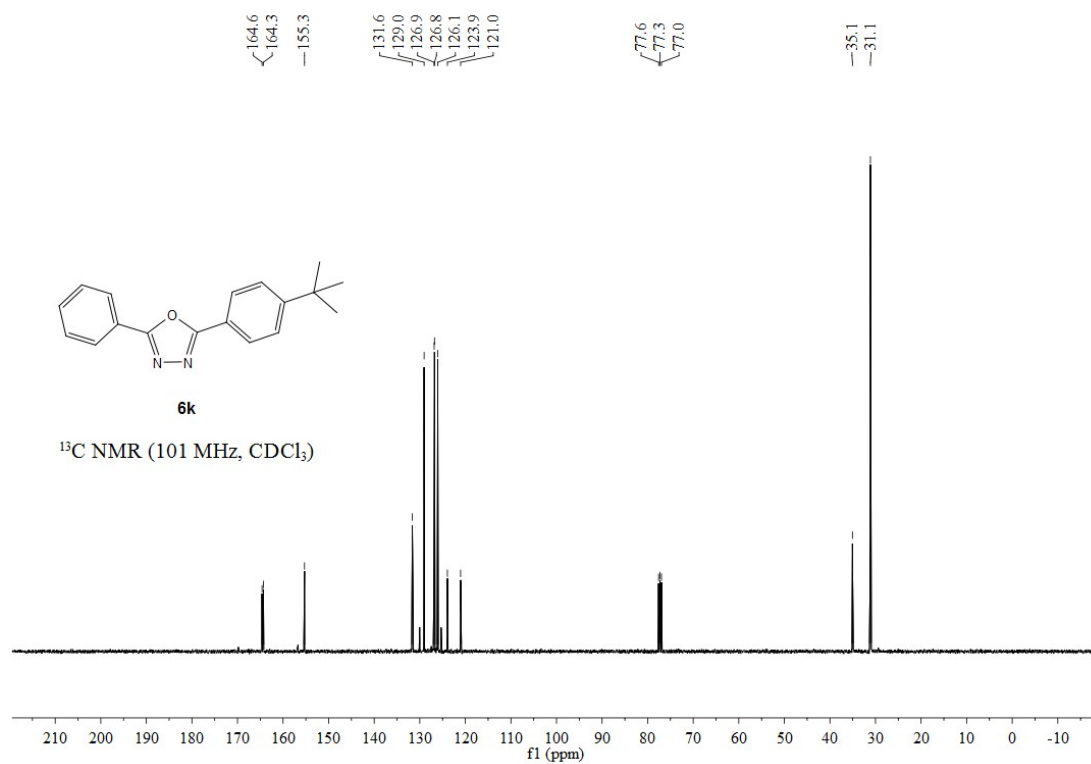
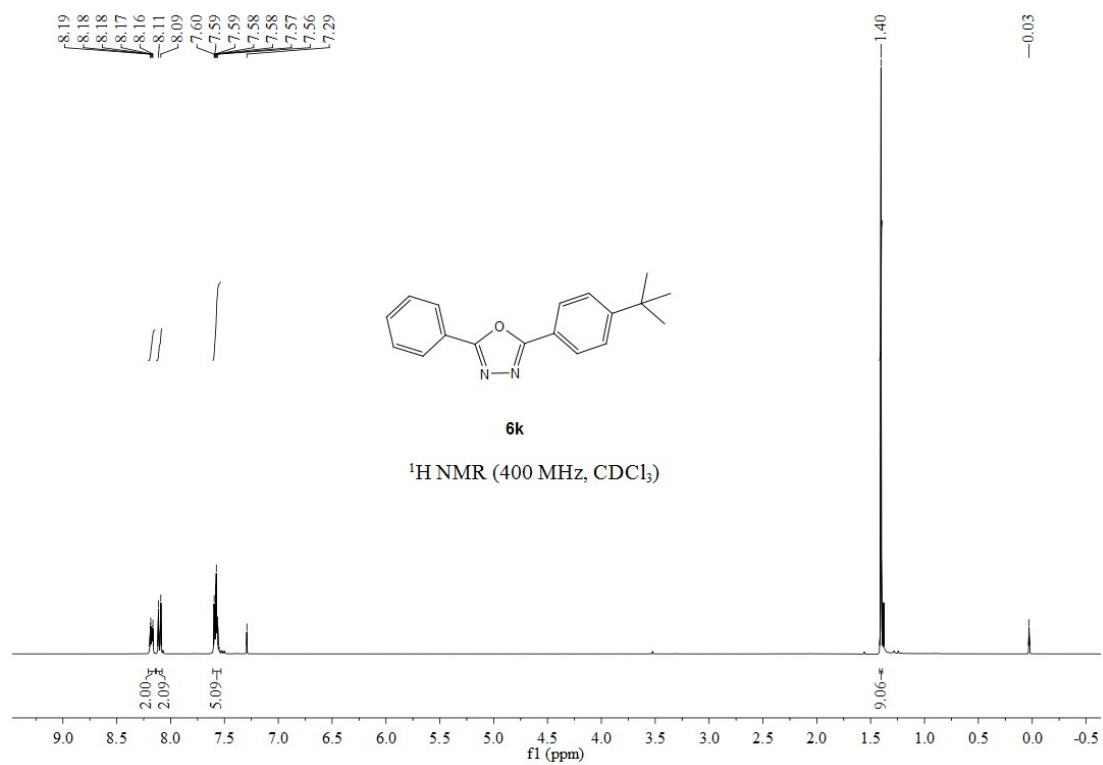


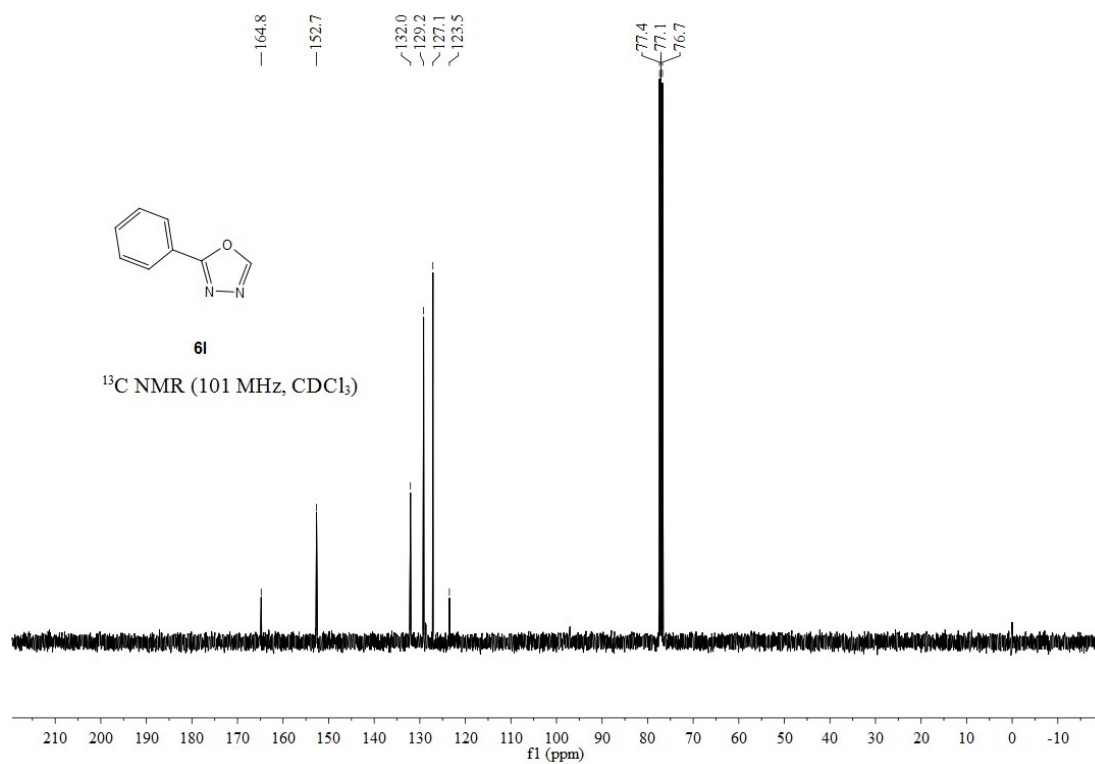
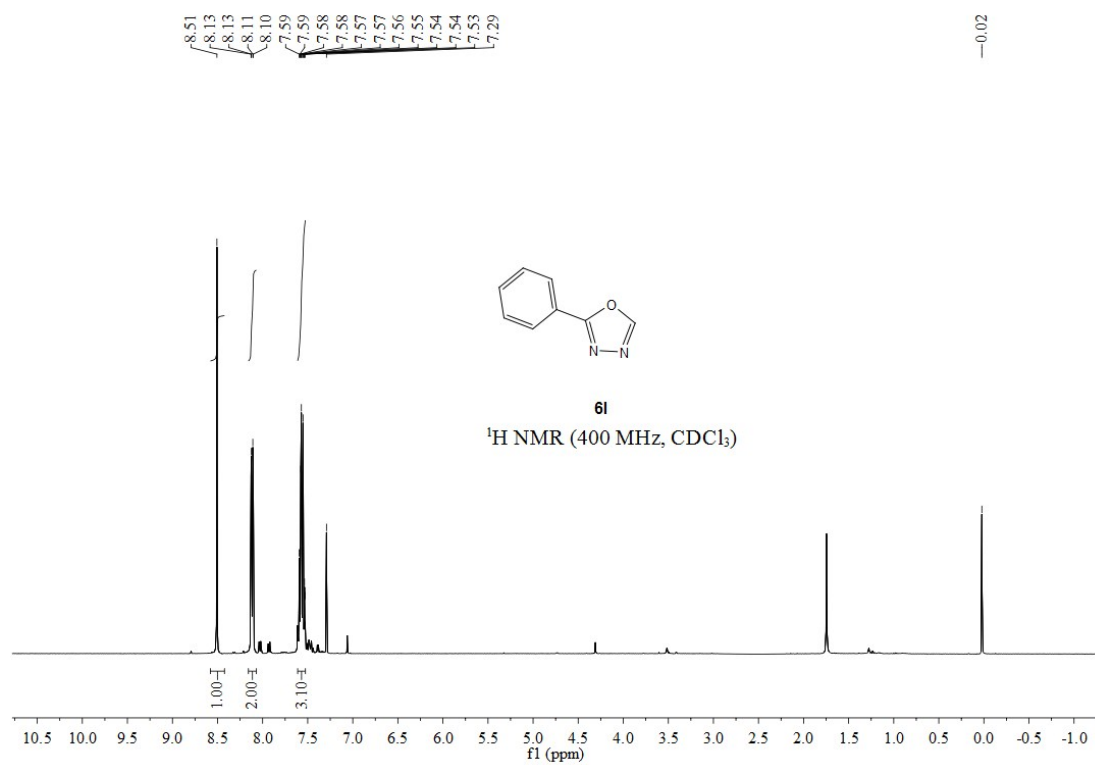


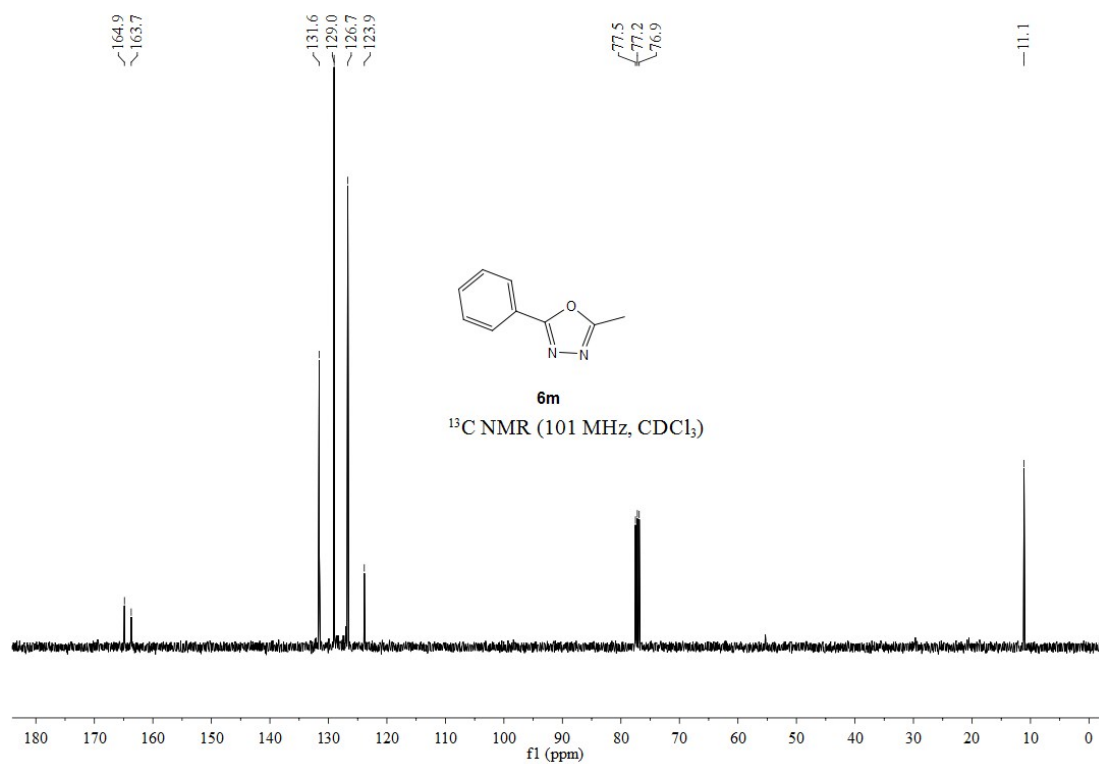
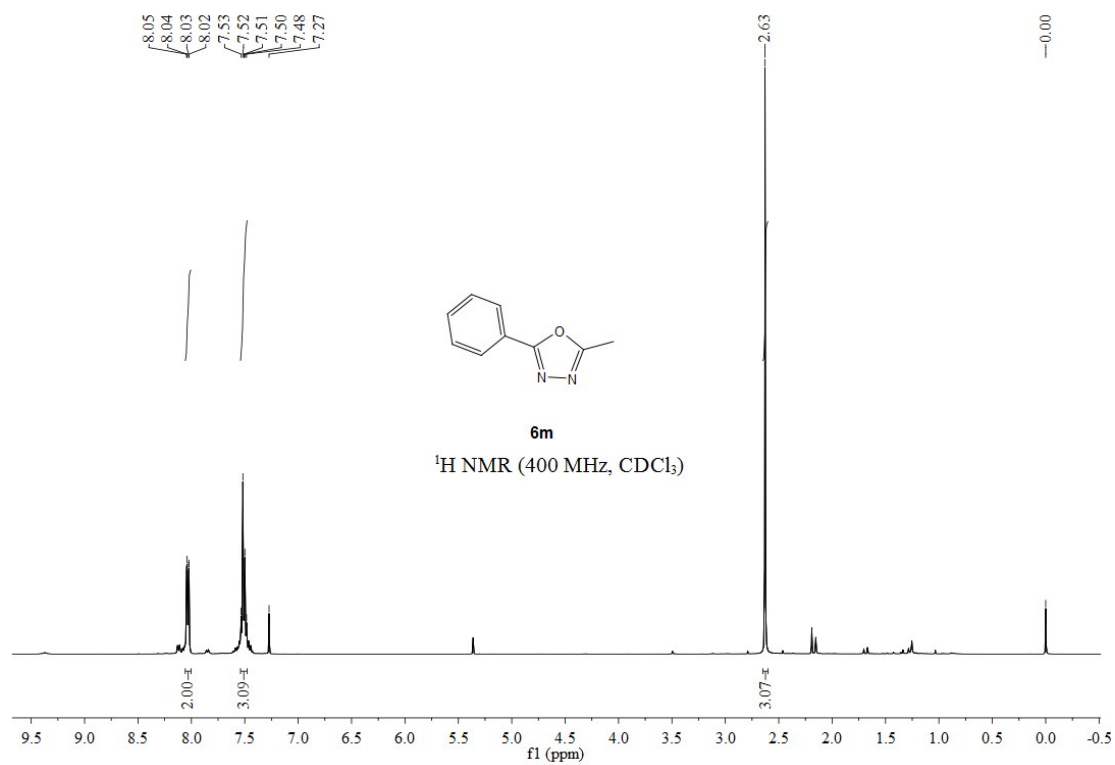












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