

Supplementary Material

An efficient synthesis and antimicrobial evaluation of 5-alkenyl- and 5-styryl-1,2,4-oxadiazoles

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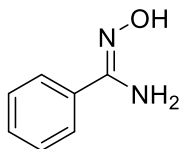
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Preparation and characterization of starting materials

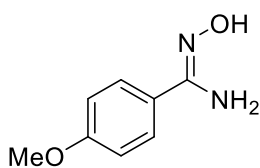
Preparation of amidoximes 2a-f

General procedure¹. To a stirred suspension of corresponding nitrile **1** and hydroxylamine hydrochloride (1.5 equiv.) in EtOH (10 mL per gram of nitrile) NaHCO₃ (1.5 equiv.) was added. The reaction mixture was stirred under reflux for 6 h. After the reaction had completed, the reaction mixture was concentrated under reduced pressure, and the residue was diluted with cold water (200 mL). The resulting precipitate was filtered off and washed with cold water (50 mL).



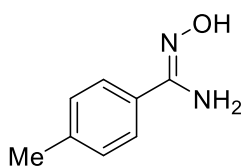
N'-Hydroxybenzimidamide 2a¹

The compound was synthesized from benzonitrile **1a** (15 g, 145 mmol) in 65% (12.87 g) yield; white powder; mp 67-69 °C. ¹H NMR (400 MHz, DMSO-*d*₆): 5.68 (br. s, NH₂, 2H), 7.35 (m, *m*-, *p*- H, 3H), 7.68 (m, *o*-H, 2H), 9.59 (s, OH, 1H).



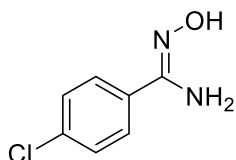
N'-Hydroxy-4-methoxybenzimidamide 2b¹

The compound was synthesized from 4-methoxybenzonitrile **1b** (1 g, 8 mmol) in 78% (0.97 g) yield; white powder; mp 107-109 °C. ¹H NMR (400 MHz, DMSO-*d*₆), δ 3.76 (s, CH₃O, 3H), 5.67 (br. s, NH₂, 2H), 6.92 (d, *J* 7.5 Hz, *m*-H, 2H), 7.08 (d, *J* 7.5 Hz, *o*-H, 2H), 9.43 (s, OH, 1H).



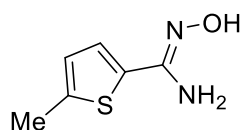
N'-Hydroxy-4-methylbenzimidamide 2c¹

The compound was synthesized from 4-methylbenzonitrile **1c** (5 g, 43 mmol) in 96% (6.15 g) yield; white powder; mp 141-143 °C. ¹H NMR (400 MHz, DMSO-*d*₆), δ 2.32 (s, CH₃, 3H), 5.57 (br. s, NH₂, 2H), 7.15 (d, *J* 7.0 Hz, *o*-H, 2H), 7.56 (d, *J* 7.0 Hz, *m*-H, 2H), 9.45 (s, OH, 1H).



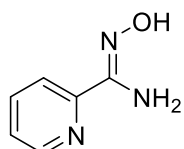
4-Chloro-N'-hydroxybenzimidamide 2d¹

The compound was synthesized from 4-chlorobenzonitrile **1d** (3 g, 22 mmol) in 89% (3.31 g) yield; white powder; mp 128-130 °C. ¹H NMR (400 MHz, DMSO-*d*₆), δ 5.85 (br. s, NH₂, 2H), 7.43 (d, *J* 8.6 Hz, *o*-H, 2H), 7.66 (d, *J* 8.9 Hz, *m*-H, 2H), 9.71 (s, OH, 1H).



***N'*-hydroxy-5-methylthiophene-2-carboximidamide **2e**².**

The compound was synthesized from 5-methylthiophene-2-carbonitrile **1e** (1 g, 8 mmol) in 88% (1.12 g) yield; brown powder; mp 142-144 °C. ¹H NMR (400 MHz, DMSO-*d*₆), δ 2.38 (s, CH₃, 3H), 5.80 (br. s, NH₂, 2H), 6.68-6.75 (m, Th, 1H), 7.23 (d, *J* 3.6 Hz, Th, 1H), 9.50 (s, OH, 1H).



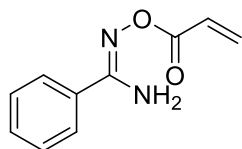
***N'*-hydroxypyridine-2-carboximidamide **2f**².**

The compound was synthesized from 2-picolinonitrile **1f** (1.04 g, 10 mmol) in 86% (1.18 g) yield; white powder; mp 116-118 °C. ¹H NMR (400 MHz, DMSO-*d*₆), δ 5.82 (br. s, NH₂, 2H), 7.38-7.44 (m, Py, 1H), 7.81 (dt, *J* 7.7, 1.6 Hz, Py, 1H), 7.87 (d, *J* 8.0 Hz, Py, 1H), 8.57 (d, *J* 4.8 Hz, Py, 1H), 9.90 (s, OH, 1H).

Synthesis and characterization of *O*-acylamidoximes **3a-p**

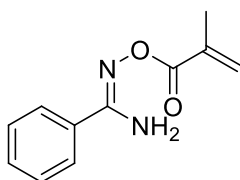
Method A. An ethyl chloroformate (ECF, 3.0 mmol, 0.29 mL) was added, dropwise to a mixture of carboxylic acid (2.5 mmol) and TEA (3.0 mmol, 0.42 mL) in 1,4-dioxane (4 mL). The reaction mixture was stirred at room temperature for 15 min. An amidoxime **2** (2.5 mmol) in 1,4-dioxane (4 mL) was added and resulted mixture was stirred at room temperature for 15 min. The solvent was evaporated at reduced pressure and residue was diluted with water (25 mL). The precipitate was filtered off, washed with cold water (25 mL) and dried in air at room temperature.

Method B. An 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride (EDC, 3.0 mmol, 0.58 g) was added to a mixture of carboxylic acid (2.5 mmol) and acetone (4 mL). The reaction mixture was stirred at room temperature for 30 min, and amidoxime **2** (2.5 mmol) was added. The reaction mixture was stirred at room temperature for 24 h. The solvent was evaporated at reduced pressure and residue was diluted with water (25 mL). The precipitate was filtered off, washed with cold water (25 mL) and dried in air at room temperature.



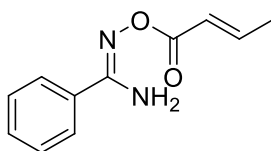
***N'*-(Acryloyloxy)benzenecarboximidamide **3a**³.**

The compound was synthesized by method **A** from *N'*-hydroxybenzimidamide **2a** in 71% (337 mg) yield; white powder. IR, ν, cm⁻¹: 894 (CH=CH₂), 1172 (C-O), 1569 (C=N), 1606 (CH=CH₂), 1737 (C=O), 3062, 3339 (NH₂). ¹H NMR (400 MHz, DMSO-*d*₆), δ 5.96 (dd, *J* 10.1, 1.9 Hz, *cis*-H₂C=CH, 1H), 6.37 (dd, *J* 17.4, 10.1 Hz, H_C=CH₂, 1H), 6.44 (dd, *J* 17.4, 1.9 Hz, *tr*-H₂C=CH, 1H), 6.91 (br. s, NH₂, 2H), 7.41-7.53 (m, *m*, *p*-H, 3H), 7.73 (m, *o*-H, 2H). HRMS (ESI), *m/z*: calcd for C₁₀H₁₁N₂O₂ [M+H]⁺ 191.0815, found 191.0823.



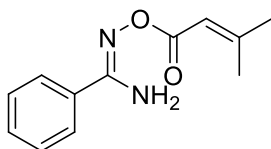
***N'*-(Methacryloyloxy)benzenecarboximidamide 3b.**

The compound was synthesized by method **A** from *N'*-hydroxybenzimidamide **2a** in 58% (296 mg) yield; white powder. IR, ν , cm^{-1} : 1158 (C–O), 1578 (C=N), 1640 (C=CH₂), 1727 (C=O), 3320, 3480 (NH₂). ¹H NMR (400 MHz, CDCl₃), δ 2.08 (s, CH₃, 3H), 5.09 (br.s, NH₂, 2H), 5.63-5.67 (m, C=CH₂, 1H), 6.20 (s, =CH₂, 1H), 7.41-7.54 (m, *m,p*-H, 3H), 7.75 (d, *J* 7.0 Hz, *o*-H, 2H). ¹³C NMR (101 MHz, CDCl₃), δ 18.6 (Me), 125.6 (C(O)C=), 126.8 (*o*-C), 128.7 (*m*-C), 131.0 (*p*-C), 131.2 (*i*-C), 135.6 (C=), 157.1 (N=C-N), 164.7 (C=O). HRMS (ESI), *m/z*: calcd for C₁₁H₁₃N₂O₂ [M+H]⁺ 205.0971, found 205.0970.



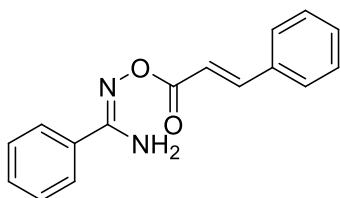
***N'*-((2*E*)-But-2-enyloxy)benzenecarboximidamide 3c⁴.**

The compound was synthesized by method **A** from *N'*-hydroxybenzimidamide **2a** in 75% (382 mg) yield; white powder. IR, ν , cm^{-1} : 970 (*tr*-CH=CH), 1169 (C–O), 1612 (CH=CH), 1657 (C=N), 1723 (C=O), 3328, 3485 (NH₂). ¹H NMR (400 MHz, DMSO-*d*₆), δ 1.90 (dd, *J* 7.0, 1.5 Hz, CH₃, 3H), 6.09 (dd, *J* 15.7, 1.7 Hz, CO-CH=, 1H), 6.82 (br. s, NH₂, 2H), 7.02 (dq, *J* 15.7, 7.0 Hz, CH₃-CH=, 1H), 7.43-7.51 (m, *m,p*-H, 3H), 7.72-7.74 (m, *o*-H, 2H). ¹³C NMR (101 MHz, DMSO-*d*₆), δ 18.3 (Me), 121.9 (CO-CH=), 127.2 (*o*-C), 128.8 (*m*-C), 130.9 (*p*-C), 132.2 (*i*-C), 145.0 (Me-CH=), 157.0 (N=C-N), 164.1 (C=O). HRMS (ESI), *m/z*: calcd for C₁₁H₁₃N₂O₂ [M+H]⁺ 205.0971, found 205.0976.



***N'*-[(3-Methylbut-2-enoyl)oxy]benzenecarboximidamide 3d.**

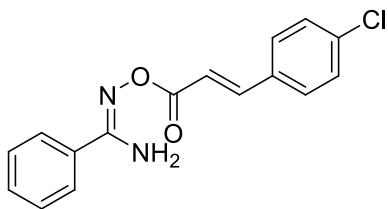
The compound was synthesized by method **A** starting from *N'*-hydroxybenzimidamide **2a** in 70% (382 mg) yield; white powder. IR, ν , cm^{-1} : 1170 (C–O), 1640 (C=C), 1659 (C=N), 1728 (C=O), 3323, 3481 (NH₂). ¹H NMR (400 MHz, DMSO-*d*₆), δ 1.92 (s, CH₃, 3H), 2.14 (s, CH₃, 3H), 5.92 (s, CH=C, 1H), 6.75 (br. s, NH₂, 2H), 7.42-7.49 (m, *m,p*-H, 3H), 7.72 (m, *o*-H, 2H). ¹³C NMR (101 MHz, DMSO-*d*₆), δ 20.3 (CH₃), 27.5 (CH₃), 114.9 (CH=), 127.2 (*o*-C), 127.3 (*m*-C), 128.8 (*p*-C), 130.8 (C=), 132.3 (*i*-C), 156.6 (C=N), 164.1 (C=O). HRMS (ESI), *m/z*: calcd for C₁₂H₁₅N₂O₂ [M+H]⁺ 219.1128, found 219.1137.



***N'*-{[(2*E*)-3-Phenylprop-2-enoyl]oxy}benzenecarboximidamide 3e⁵.**

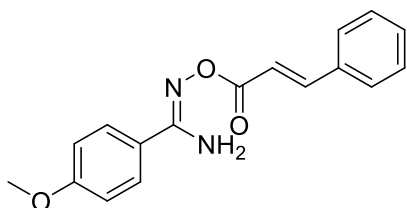
The compound was synthesized by method **A** from *N'*-hydroxybenzimidamide **2a** in 82% (545 mg) yield; white powder. IR, ν , cm^{-1} : 972 (*tr*-CH=CH), 1148 (C–O), 1582 (C=N), 1607 (CH=CH), 1720 (C=O), 3503, 3353 (NH₂). ¹H

NMR (400 MHz, DMSO- d_6), δ 6.80 (d, J 16.2 Hz, C(O)CH=, 1H), 6.93 (br.s, NH₂, 2H), 7.45-7.53 (m, m,p -H, 6H), 7.67-7.85 (m, o -H Ph, Ph-CH=, 5H). ¹³C NMR (101 MHz, DMSO- d_6), δ 117.9 (C(O)CH=), 127.3 (o -C), 128.6 (m -C), 128.8 (o -C), 129.5 (m -C), 130.8 (p -C), 131.0 (p -C), 132.2 (i -C), 134.9 (i -C), 144.3 Ph-CH=), 157.2 (N=C-N), 164.6 (C=O). HRMS (ESI), m/z : calcd for C₁₆H₁₅N₂O₂ [M+H]⁺ 267.1128, found 267.1137.



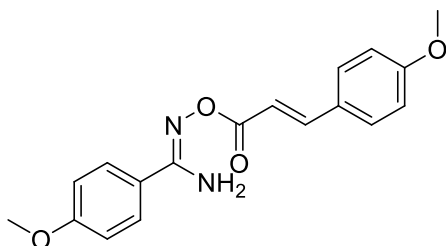
***N'*-{[(2*E*)-3-(4-Chlorophenyl)prop-2-enoyl]oxy}benzenecarboximidamide 3f.**

The compound was synthesized by method **A** from *N'*-hydroxybenzimidamide **2a** in 72% (541 mg) yield; white powder. IR, ν , cm⁻¹: 972 (*tr*-CH=CH), 1167 (C–O), 1584 (C=N), 1609 (CH=CH), 1718 (C=O), 3363, 3506 (NH₂). ¹H NMR (400 MHz, DMSO- d_6), δ 6.80 (d, J 16.2 Hz, C(O)CH=, 1H), 6.94 (br. s, NH₂, 2H), 7.43-7.56 (m, m,p -H, m -H, 5H), 7.72-7.78 (m, o -H, 4H), 7.79 (d, J 16.2 Hz, Ph-CH=, 1H). ¹³C NMR (101 MHz, DMSO- d_6), δ 118.8 (C(O)HC=), 127.3 (o -C), 128.8 (m -C), 129.5 (o -C), 130.3 (m -C), 131.0 (p -C), 132.1 (i -C), 133.9 (i -C), 135.3(p -C), 142.8 (Ph-CH=), 157.3 (N=C-N), 164.4 (C=O). HRMS (ESI), m/z : calcd for C₁₆H₁₆ClN₂O₂ [M+H]⁺ 301.0738, found 301.0747.



4-Methoxy-*N'*-{[(2*E*)-3-phenylprop-2-enoyl]oxy}benzenecarboximidamide 3g.

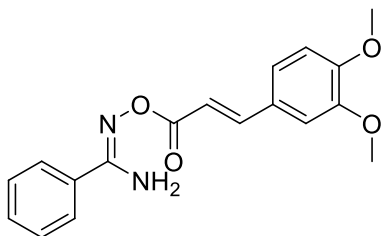
The compound was synthesized by method **A** from *N'*-hydroxy-4-methoxybenzenecarboximidamide **2b** in 80% (592 mg) yield; white powder. IR, ν , cm⁻¹: 981 (*tr*-CH=CH), 1162 (C–O), 1587 (C=N), 1615 (CH=CH), 1721 (C=O), 3367, 3504 (NH₂). ¹H NMR (400 MHz, DMSO- d_6), δ 3.82 (s, OMe, 3H), 6.79 (d, J 16.2 Hz, Ph-CH=, 1H), 6.82 (s, NH₂, 2H), 7.02 (d, J 8.9 Hz, m -H, 2H), 7.45-7.50 (m, m,p -H, 3H), 7.71-7.74 (m, o -H, 4H), 7.78 (d, J 16.2 Hz, C(O)CH=, 1H). ¹³C NMR (101 MHz, DMSO- d_6), δ 55.8 (OMe), 114.2 (m -C), 118.0 (C(O)C=), 124.2 (i -C), 128.6 (m -C), 128.7 (o -C), 129.5 (o -C), 130.8 (p -C), 134.9 (i -C), 144.1 (Ph-CH=), 156.8 (N=C-N), 161.5 (C-OMe), 164.6 (C=O). HRMS (ESI), m/z : calcd for C₁₇H₁₇N₂O₃ [M+H]⁺ 297.1233, found 297.1244.



4-Methoxy-*N'*-{[(2*E*)-3-(4-methoxyphenyl)prop-2-enoyl]oxy}benzenecarboximidamide 3h.

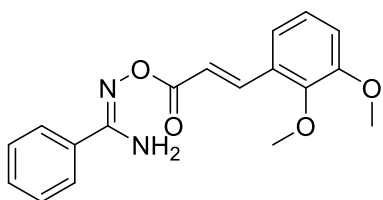
The compound was synthesized by method **A** from *N'*-hydroxy-4-methoxybenzenecarboximidamide **2b** in 80% (652 g) yield; white powder. IR, ν , cm⁻¹: 976 (*tr*-CH=CH), 1028, 1156, 1255 (C–O), 1601 (C=N), 1634 (CH=CH), 1710 (C=O), 3336, 3497 (NH₂). ¹H NMR (400 MHz, DMSO- d_6), δ 3.82 (d, J 0.91 Hz, 2OMe, 6H), 6.63 (d, J 15.9 Hz, C(O)CH=, 1H), 6.78 (br. s, NH₂, 2H), 7.00-7.03 (m, o -H, 4H), 7.63-7.81 (m, m -H, Ph-CH=, 5H). ¹³C NMR (101

MHz, DMSO-*d*₆), δ 55.77 (OMe), 55.82 (OMe), 114.2 (*m*-C), 114.9 (*m*-C), 115.2 (C(O)CH=), 124.3 (*i*-C), 127.5 (*i*-C), 128.6 (*o*-C), 130.3 (*o*-C), 144.0 (Ph-CH=), 156.6 (N=C-N), 161.5 (2 *x p*-C), 164.9 (C=O). HRMS (ESI), *m/z*: calcd for C₁₈H₁₉N₂O₄ [M+H]⁺ 327.1339, found 327.1342.



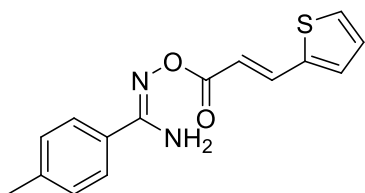
***N'*-{[(2*E*)-3-(3,4-Dimethoxyphenyl)prop-2-enoyl]oxy}benzenecarboximidamide 3i.**

The compound was synthesized by method **A** starting *N'*-hydroxybenzimidamide **2a** in 93% (758 mg) yield; white powder. IR, ν , cm⁻¹: 969 (*tr*-CH=CH), 1157 (C–O), 1569 (C=N), 1612 (CH=CH), 1712 (C=O), 3331, 3468 (NH₂). ¹H NMR (400 MHz, DMSO-*d*₆), δ 3.82 (s, OMe, 3H), 3.84 (s, OMe, 3H), 6.67 (d, *J* 16.2 Hz, C(O)HC=, 1H), 6.89 (br. s, NH₂, 2H), 7.03 (d, *J* 8.2 Hz, *m*-H, 1H), 7.27 (dd, *J* 8.4, 2.0 Hz, *o*-H, 1H), 7.33 (d, *J* 1.8 Hz, *o*-H, 1H), 7.43-7.54 (m, *m,p*-H, 3H), 7.73 (d, *J* 16.0 Hz, Ph-CH=, 1H), 7.74-7.78 (m, *o*-H, 2H). ¹³C NMR (101 MHz, DMSO-*d*₆), δ 56.03 (OMe), 56.06 (OMe), 110.8 (Ar, C-2), 112.1 (Ar, C-5), 115.3 (C(O)CH=), 123.0 (Ar, C-6), 127.2 (*o*-C), 127.7 (Ar, C-1), 128.8 (*m*-C), 130.9 (*p*-C), 132.2 (*i*-C), 144.5 (Ph-CH=), 149.5 (Ar, C-3), 151.4 (Ar, C-4), 157.0 (N=C-N), 164.8 (C=O). HRMS (ESI), *m/z*: calcd for C₁₈H₁₉N₂O₄ [M+H]⁺ 327.1339, found 327.1345.



***N'*-{[(2*E*)-3-(2,3-Dimethoxyphenyl)prop-2-enoyl]oxy}benzenecarboximidamide 3j.**

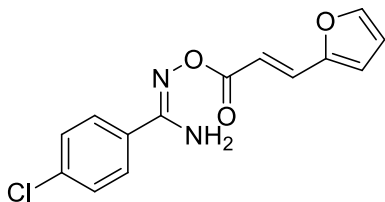
The compound was synthesized by method **A** from *N'*-hydroxybenzimidamide **2a** in 90% (734 mg) yield; white powder. IR, ν , cm⁻¹: 984 (*tr*-CH=CH), 1157 (C–O), 1598 (C=N), 1630 (CH=CH), 1717 (C=O), 3318, 3445 (NH₂). ¹H NMR (400 MHz, DMSO-*d*₆), δ 3.81 (s, OMe, 3H), 3.85 (s, OMe, 3H), 6.84 (d, *J* 16.3 Hz, C(O)CH=, 1H), 6.94 (br. s, NH₂, 2H), 7.14-7.17 (m, *o,p*-H, 2H), 7.30 (m, *m*-H, 1H), 7.45-7.53 (m, *m,p*-H, 3H), 7.76 (d, *J* 8.2 Hz, *o*-H, 2H), 7.89 (d, *J* 16.2 Hz, Ph-CH=, 1H). ¹³C NMR (101 MHz, DMSO-*d*₆), δ 56.3 (OMe), 61.3 (OMe), 115.3 (C(O)CH=), 119.1 (*p*-C), 119.5 (*o*-C), 124.9 (*m*-C), 127.3 (*o*-C), 128.3 (*i*-C), 128.9 (*m*-C), 131.0 (*p*-C), 132.1 (*i*-C), 138.6 (Ph-CH=), 148.3 (*m*-COMe), 153.3 (*o*-COMe), 157.3 (N=C-N), 164.9 (C=O). HRMS (ESI), *m/z*: calcd for C₁₈H₁₉N₂O₄ [M+H]⁺ 327.1339, found 327.1341.



4-Methyl-*N'*-{[(2*E*)-3-(thiophen-2-yl)prop-2-enoyl]oxy}benzenecarboximidamide 3k.

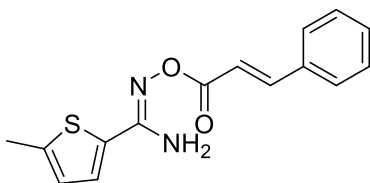
The compound was synthesized by method **A** from *N'*-hydroxy-4-methylbenzimidamide **2c** in 85% (608 mg) yield; white powder. IR, ν , cm⁻¹: 965 (*tr*-CH=CH), 1179 (C–O), 1585 (C=N), 1629 (C=C), 1715 (C=O), 3499, 3369 (NH₂). ¹H NMR (400 MHz, DMSO-*d*₆), δ 2.36 (s, Me, 3H), 6.48 (d, *J* 15.9 Hz, C(O)CH=, 1H), 6.88 (s, NH₂, 2H), 7.18

(dd, J 5.1, 3.5 Hz, Th, H-4, 1H), 7.27 (d, J 8.2 Hz, m -H, 2H), 7.54 (dd, J .7, 0.6 Hz, Th, H-3, 1H), 7.65 (d, J 8.2 Hz, o -H, 2H), 7.73 (d, J 5.2 Hz, Th, H-5, 1H), 7.94 (d, J 15.9 Hz, Th-CH=, 1H). ^{13}C NMR (101 MHz, DMSO- d_6), δ 21.4 (Me), 116.1 (C(O)CH=), 127.1 (o -C), 129.0 (Th, C-3), 129.3 (p -C), 129.4 (m -C), 130.0 (Th, C-4), 132.5 (Th, C-5), 137.1 (Th-CH=), 139.7 (Th, C-2), 140.6 (i -C), 157.0 (N=C-N), 164.4 (C=O). HRMS (ESI), m/z : calcd for $\text{C}_{15}\text{H}_{15}\text{N}_2\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$ 287.0849, found 287.0859.



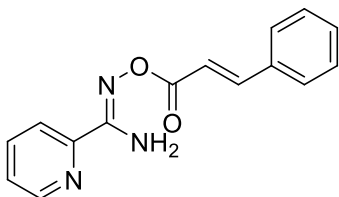
4-Chloro- N' -{[(2E)-3-(furan-2-yl)prop-2-enoyl]oxy}benzenecarboximidamide 3l.

The compound was synthesized by method **A** from N' -hydroxy-4-chlorobenzimidamide **2d** in 89% (646 mg) yield; white powder. IR, ν , cm^{-1} : 979 (tr -CH=CH), 1197 (C–O), 1552 (C=N), 1624 (CH=CH), 1707 (C=O), 3342, 3413 (NH₂). ^1H NMR (400 MHz, DMSO- d_6), δ 6.48 (d, J 15.9 Hz, C(O)CH=, 1H), 6.66 (dd, J 3.4, 1.8 Hz, H-4, 1H), 6.95 (d, J 3.7 Hz, H-3, 1H), 7.01 (s, NH₂, 2H), 7.55 (d, J 8.55 Hz, o -H, 2H), 7.61 (d, J 15.9 Hz, Fur-CH=, 1H), 7.78 (d, J 8.85 Hz, m -H, 2H), 7.88 (d, J 1.2 Hz, H-5, 1H). ^{13}C NMR (101 MHz, DMSO- d_6), δ 113.3 (Fur, C-3), 114.5 (Fur, C-4), 116.4 (C(O)CH=), 128.9 (o -C), 129.0 (i -C), 129.1 (m -C), 131.3 (Fur-CH=), 135.6 (C-Cl), 146.4 (Fur, C-5), 151.0 (Fur, C-2), 156.1 (N=C-N), 164.5 (C=O). HRMS (ESI), m/z : calcd for $\text{C}_{14}\text{H}_{12}\text{ClN}_2\text{O}_3$ $[\text{M}+\text{H}]^+$ 291.0531, found 291.0560.



5-Methyl- N' -{[(2E)-3-phenylprop-2-enoyl]oxy}thiophene-2-carboximidamide 3m.

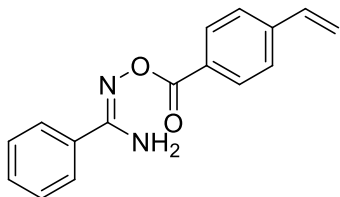
The compound was synthesized by method **A** from N' -hydroxy-5-methylthiophene-2-carboximidamide **2e** in 90% (644 mg) yield; white powder. IR, ν , cm^{-1} : 976 (tr -CH=CH), 1148 (C–O), 1581 (C=N), 1608 (CH=CH), 1721 (C=O), 3367, 3484 (NH₂). ^1H NMR (400 MHz, DMSO- d_6), δ 2.46 (s, Me, 3H), 6.76 (d, J 16.2 Hz, Ph-CH=, 1H), 6.84 (dq, J 3.6 Hz, 1.1, Th, H-4, 1H), 6.93 (s, NH₂, 2H), 7.43-7.50 (m, m,p -H, 3H), 7.53 (d, J 3.6 Hz, Th, H-3, 1H), 7.71 (m, o -H, 2H), 7.78 (d, J 16.2 Hz, Th-CH=, 1H). ^{13}C NMR (101 MHz, DMSO- d_6), δ 15.5 (Me), 117.7 (C(O)CH=), 126.0 (Th, C-3), 128.6 (m,p -C), 129.5 (o -C), 130.9 (Th, C-4), 131.3 (i -C), 134.8 (Th, C-2), 142.8 (Th, C-5), 144.3 (Th-CH=), 153.1 (N=C-N), 164.3 (C=O). HRMS (ESI), m/z : calcd for $\text{C}_{15}\text{H}_{15}\text{N}_2\text{O}_2\text{S}$ $[\text{M}+\text{Na}]^+$ 309.0668, found 309.0676.



N' -{[(2E)-3-Phenylprop-2-enoyl]oxy}pyridine-2-carboximidamide 3n.

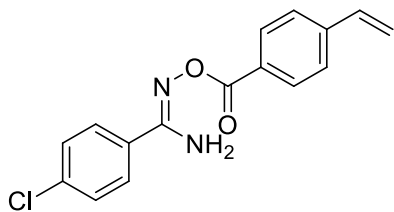
The compound was synthesized by method **A** from N' -hydroxypyridine-2-carboximidamide **2f** in 75% (501 mg) yield; white powder. IR, ν , cm^{-1} : 980 (tr -CH=CH), 1153 (C–O), 1585 (C=N), 1627 (CH=CH), 1724 (C=O), 3366, 3487 (NH₂). ^1H NMR (400 MHz, DMSO- d_6), δ 6.82 (d, J 16.2 Hz, C(O)CH=, 1H), 7.07 (br. s, NH₂, 2H), 7.44-7.51

(m, *m,p*-H, 3H), 7.57 (ddd, *J* 7.3, 4.9, 1.2 Hz, H-5, Py, 1H), 7.73 (m, *o*-H, 2H), 7.84 (d, *J* 16.2 Hz, Ph-CH=, 1H), 7.94 (td, *J* 7.7, 1.7 Hz, H-4, Py, 1H), 7.99-8.08 (d, *J* 7.9 Hz, H-3, Py, 1H), 8.88 (dd, *J* 4.8, 0.8 Hz, H-6, Py, 1H). ¹³C NMR (101 MHz, DMSO-*d*₆), δ 117.7(C(O)CH=), 121.5 (Py, C-3), 126.1 (Py, C-5), 128.6 (*o*-C), 129.5 (*m*-C), 130.9 (*p*-C), 134.8 (Ar, *i*-C), 137.8 (Py, C-4), 144.6 (Ph-CH=), 148.7 (Py, C-2), 149.2 (Py, C-6), 154.8 (N=C-N), 164.4 (C=O). HRMS (ESI), *m/z*: calcd for C₁₅H₁₄N₃O₂ [M+H]⁺ 268.1081, found 268.1092.



***N'*-[(4-Vinylbenzoyl)oxy]benzenecarboximidamide 3o.**

The compound was synthesized by method **B** from *N'*-hydroxybenzimidamide **2a** in 72% (479 mg) yield; white powder. IR, ν , cm⁻¹: 988 (CH=CH₂), 1184 (C–O), 1586 (C=N), 1615 (CH=CH), 1732 (C=O), 3379, 3508 (NH₂). ¹H NMR (400 MHz, DMSO-*d*₆), δ 5.44 (d, *J* 11.1 Hz, *cis*-CH=C, 1H), 6.03 (d, *J* 17.7 Hz, *tr*-CH=C, 1H), 6.85 (dd, *J* 17.7, 11.1 Hz, -CH=, 1H), 6.95 (s, NH₂, 2H), 7.48-7.53 (m, *m,p*-H, 3H), 7.63 (m, H-3,5, 2H), 7.77 (m, *o*-H, 2H), 8.16 (m, H-2,6, 2H). ¹³C NMR (101 MHz, DMSO-*d*₆), δ 117.6 (=CH₂), 126.7 (*m*-C), 127.4 (*o*-C), 128.8 (*m*-C), 129.1 (*p*-C), 130.4 (*o*-C), 131.0 (*i*-C), 132.3 (*i*-C), 136.3 (-CH=), 141.9 (*p*-C), 157.5 (N=C-N), 163.8 (C=O). HRMS (ESI), *m/z*: calcd for C₁₆H₁₅N₂O₂ [M+H]⁺ 267.1128, found 267.1140.

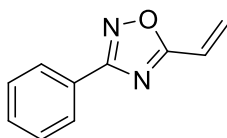


4-Chloro-*N'*-[(4-vinylbenzoyl)oxy]benzenecarboximidamide 3p.

The compound was synthesized by method **B** from 4-chloro-*N'*-hydroxybenzenecarboximidamide **2d** in 77% (578 mg) yield; white powder. IR, ν , cm⁻¹: 776 (C-Cl), 993 (CH=CH₂), 1172 (C–O), 1565 (C=N), 1606 (CH=CH), 1716 (C=O), 3384, 3502 (NH₂). ¹H NMR (400 MHz, DMSO-*d*₆), δ 5.45 (d, *J* 11 Hz, *cis*-CH=CH₂, 1H), 6.03 (d, *J* 18 Hz, *tr*-CH=CH₂, 1H), 6.85 (dd, *J* 18, 11 Hz, CH=CH₂, 1H), 7.04 (s, NH₂, 2H), 7.57 (d, *J* 8.5 Hz, *o*-H, 2H), 7.64 (d, *J* 8.2 Hz, *o*-H, 2H), 7.81 (d, *J* 8.8 Hz, *m*-H, 2H), 8.17 (d, *J* 8.2 Hz, *m*-H, 2H). ¹³C NMR (101 MHz, DMSO-*d*₆), δ 117.7 (=CH₂), 126.7 (*m*-C), 128.9 (*o*-C), 129.1 (*p*-C), 129.2 (*m*-C), 130.4 (*o*-C), 131.1 (*i*-C), 135.7 (*i*-C), 136.3 (CH=), 142.0 (*p*-C), 156.5 (N=C-N), 163.7 (C=O). HRMS (ESI), *m/z*: calcd for C₁₆H₁₄ClN₂O₂ [M+H]⁺ 301.0738, found 301.0747.

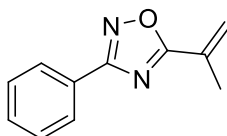
Synthesis and characterization of 1,2,4-oxadiazoles 4a-p

General procedure. An *O*-acylamidoxime **3** (1.5 mmol) was added to a suspension of powdered KOH (1.5 or 0.15 mmol, see Table 1) in DMSO (2 mL). The reaction mixture was stirred at room temperature for a specified time (see Table 1). The reaction mixture was diluted with cold water (20 mL), and resulted precipitate was filtered off, washed with cold water (25 mL) and dried in air at room temperature.



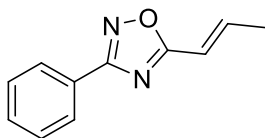
3-Phenyl-5-vinyl-1,2,4-oxadiazole 4a³.

The compound was synthesized using 0.1 equiv of KOH for 0.5 h. Yield after purification by column chromatography (ethyl acetate : hexane 1 : 4) was 11% (28 mg) of yellow oil. IR (microlayer), ν , cm^{-1} : 1215 (C-O), 1593 (C=N), 1647 (CH=CH₂). ¹H NMR (400 MHz, DMSO-*d*₆), δ 6.08 (d, *J* 11 Hz, *cis*-HC=CH₂, 1H), 6.53 (d, *J* 18 Hz, *tr*-HC=CH₂, 1H), 6.88 (dd, *J* 18, 11 Hz, HC=C, 1H), 7.48-7.55 (m, *m,p*-H, 3H), 7.97-8.04 (m, *o*-H, 2H). ¹³C NMR (101 MHz, DMSO-*d*₆), δ 120.7 (=CH₂), 126.6 (*i*-C), 127.4 (*m*-C), 129.5 (*o*-C), 130.2 (-CH=), 131.9 (*p*-C), 168.4 (C-3), 174.9 (C-5). HRMS (ESI), *m/z*: calcd for C₁₀H₉N₂O [M+H]⁺ 173.0709, found 173.0701.



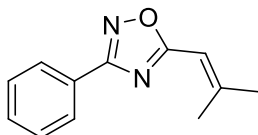
3-Phenyl-5-(prop-1-en-2-yl)-1,2,4-oxadiazole 4b.

The compound was synthesized using 0.1 equiv of KOH for 0.5 h. Total yield after purification by column chromatography (ethyl acetate : hexane 1 : 4) was 15% (41 mg) of yellow oil. IR (microlayer), ν , cm^{-1} : 1158 (C-O), 1578 (C=N), 1643 (CH₂=C). ¹H NMR (400 MHz, DMSO-*d*₆), δ 2.22 (s, Me, 3H), 5.88 (s, =CH₂, 1H), 6.28 (s, =CH₂, 1H), 7.55-7.61 (m, *m,p*-H, 3H), 8.03 (d, *J* 7.9 Hz, *o*-H, 2H). ¹³C NMR (101 MHz, DMSO-*d*₆), δ 18.9 (Me), 125.2 (CH₂=), 125.9 (C=), 126.7 (*i*-C), 127.4 (*m*-C), 129.5 (*o*-C), 131.9 (*p*-C), 168.5 (C-3), 176.5 (C-5). HRMS (ESI), *m/z*: calcd for C₁₁H₁₁N₂O [M+H]⁺ 187.0866, found 187.0860.



(*E*)-3-Phenyl-5-(prop-1-en-1-yl)-1,2,4-oxadiazole 4c⁴.

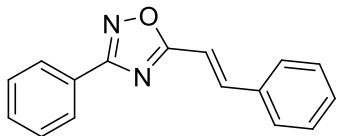
The compound was synthesized using 0.1 equiv of KOH for 0.5 h. Yield 79% (220 mg); yellow oil. IR (microlayer), ν , cm^{-1} : 1120 (C-O), 1562 (C=N), 1665 (CH=CH). ¹H NMR (500 MHz, CDCl₃), δ 2.05 (dd, *J* 7.0, 2 Hz, Me, 3H), 6.50 (dq, *J* 16.2, 2 Hz, Het-CH=, 1H), 7.18 (dq, *J* 16.2, 7.0 Hz, Me-CH=, 1H), 7.49-7.52 (m, *m,p*-H, 3H), 8.11 (d, *J* 8.2 Hz, *o*-H, 2H). ¹³C NMR (125 MHz, CDCl₃), δ 18.8 (Me), 115.0 (Het-CH=), 127.0 (*i*-C), 127.4 (*m*-C), 128.8 (*o*-C), 131.0 (*p*-C), 142.8 (Ph-CH=), 168.4 (C-3), 174.7 (C-5). HRMS (ESI), *m/z*: calcd for C₁₁H₁₁N₂O [M+H]⁺ 187.0866, found 187.0853.



5-(2-Methylprop-1-enyl)-3-phenyl-1,2,4-oxadiazole 4d.

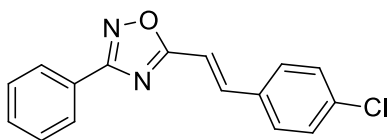
The compound was synthesized using 0.1 equiv of KOH for 0.5 h. Yield 80% (240 mg); beige powder, mp 44-46 °C. IR, ν , cm^{-1} : 841 (C=CH), 1152 (C-O), 1592 (C=N), 1656 (C=CH). ¹H NMR (500 MHz, CDCl₃), δ 2.09 (d, *J* 1.0 Hz, Me, 3H), 2.38 (d, *J* 1.0 Hz, Me, 3H), 6.33 (sept, *J* 1.2 Hz, C=CH, 1H), 7.49-7.52 (m, *m,p*-H, 3H), 8.14 (m, *o*-H, 2H). ¹³C NMR (125 MHz, CDCl₃), δ 21.1 (Me), 27.6 (Me), 108.9 (C=CH), 127.3 (*i*-C), 127.4 (*m*-C), 128.8 (*o*-C), 130.9 (*p*-

C), 154.3 (C=CH), 168.1 (C-3), 175.1 (C-5). HRMS (ESI), m/z : calcd for $C_{12}H_{13}N_2O$ $[M+H]^+$ 201.1022, found 201.1020.



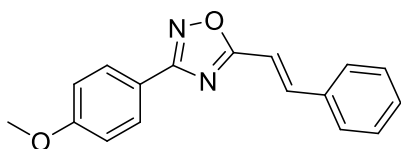
(E)-3-Phenyl-5-(2-phenylethenyl)-1,2,4-oxadiazole 4e ⁶.

The compound was synthesized by following the general procedure in 87% (324 mg) yield; white powder, mp 95-97 °C. IR, ν , cm^{-1} : 971 (*tr*-CH=CH), 1175 (C–O), 1593 (C=N), 1644 (CH=CH). ¹H NMR (400 MHz, DMSO-*d*₆), δ 7.45 (d, *J* 16.4 Hz, Het-CH=, 1H), 7.43-7.49 (m, *m,p*-H, 3H), 7.56-7.63 (m, *m,p*-H, 3H), 7.85 (m, *o*-H, 2H), 7.95 (d, *J* 16.4 Hz, Ph-CH=, 1H), 8.05-8.09 (m, *o*-H, 2H). ¹³C NMR (101 MHz, DMSO-*d*₆), δ 110.7 (Het-CH=), 126.8 (*i*-C, 3-Ph), 127.5 (*o*-C, 5-Ph), 128.9 (*m*-C, 3-Ph), 129.5 (*p*-C, 5-Ph), 129.7 (*m*-C, 5-Ph), 131.1 (*o*-C, 3-Ph), 132.0 (*p*-C, 3-Ph), 134.7 (*i*-C, 5-Ph), 143.3 (Ph-CH=), 168.5 (C-3), 175.9 (C-5). HRMS (ESI), m/z : calcd for $C_{16}H_{13}N_2O$ $[M+H]^+$ 249.1022, found 249.1014.



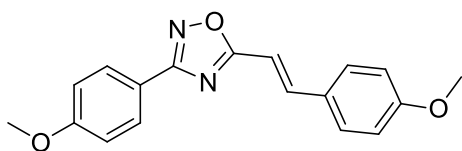
5-[(E)-2-(4-Chlorophenyl)ethenyl]-3-phenyl-1,2,4-oxadiazole 4f ⁶.

The compound was synthesized by following the general procedure in 88% (373 mg) yield; white powder, mp 158-160 °C. IR, ν , cm^{-1} : 975 (*tr*-CH=CH), 1174 (C–O), 1573 (C=N), 1648 (CH=CH). ¹H NMR (400 MHz, DMSO-*d*₆), δ 7.50 (d, *J* 16.5 Hz, Het-HC=, 1H), 7.55 (d, *J* 8.5 Hz, *m*-H, 2H), 7.58-7.63 (m, *m,p*-H, 3H), 7.90 (d, *J* 8.5 Hz, *o*-H, 2H), 7.96 (d, *J* 16.5 Hz, Ph-HC=, 1H), 8.05-8.08 (m, *o*-H, 2H). ¹³C NMR (101 MHz, DMSO-*d*₆), δ 111.5 (Het-CH=), 126.7 (*i*-C, 3-Ph), 127.5 (*m*-C, 3-Ph), 129.5 (*o*-C, 3-Ph), 129.7 (*m*-C, 5-Ph), 130.6 (*o*-C, 5-Ph), 132.1 (*p*-C, 3-Ph), 133.7 (*i*-C, 5-Ph), 135.7 (*p*-C, 5-Ph), 141.9 (Ph-CH=), 168.5 (C-3), 175.7 (C-5). HRMS (ESI), m/z : calcd for $C_{16}H_{12}ClN_2O$ $[M+H]^+$ 283.0633, found 283.0632.



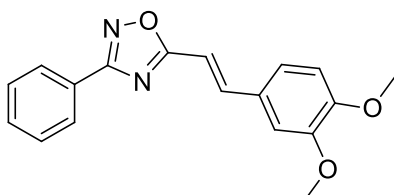
3-(4-Methoxyphenyl)-5-[(E)-2-phenylethenyl]-1,2,4-oxadiazole 4g ⁶.

The compound was synthesized by following the general procedure in 80% (333 mg) yield; white powder, mp 122-123 °C. IR, ν , cm^{-1} : 975 (*tr*-CH=CH), 1177, 1255 (C–O), 1556 (C=N), 1637 (CH=CH). ¹H NMR (400 MHz, DMSO-*d*₆), δ 3.85 (s, OMe, 3H), 7.14 (d, *J* 8.9 Hz, *m*-H, 2H), 7.43 (d, *J* 16.5 Hz, Het-CH=, 1H), 7.46-7.50 (m, *m,p*-H, 3H), 7.85-7.87 (m, *o*-H, 2H), 7.94 (d, *J* 16.5 Hz, Ph-CH=, 1H), 8.00 (d, *J* 8.8 Hz, *o*-H, 2H). ¹³C NMR (101 MHz, DMSO-*d*₆), δ 55.9 (OMe), 110.8 (Het-CH=), 115.1 (*m*-C, 3-Ph), 119.1 (*i*-C, 3-Ph), 128.8 (*o*-C, 5-Ph), 129.2 (*o*-C, 3-Ph), 129.5 (*m*-C, 5-Ph), 131.1 (*p*-C, 5-Ph), 134.8 (*i*-C, 5-Ph), 143.1 (Ph-CH=), 162.2 (*p*-C, 3-Ph), 168.2 (C-3), 175.6 (C-5). HRMS (ESI), m/z : calcd for $C_{17}H_{15}N_2O_2$ $[M+H]^+$ 279.1128, found 279.1133.



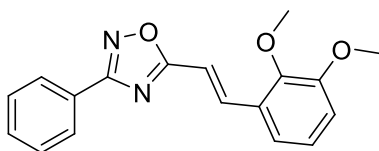
3-(4-Methoxyphenyl)-5-[(E)-2-(4-methoxyphenyl)ethenyl]-1,2,4-oxadiazole 4h [6].

The compound was synthesized by following the general procedure in 82% (379 mg) yield; white powder, mp 112-114 °C. IR, ν , cm^{-1} : 970 (*tr*-CH=CH), 1030, 1172, 1252 (C–O), 1598 (C=N), 1642 (CH=CH). ^1H NMR (400 MHz, $\text{DMSO-}d_6$), δ 3.83 (d, *J* 8.2 Hz, OMe, 6H), 7.03 (d, *J* 8.5 Hz, *m*-H, 5-Ph, 2H), 7.12 (d, *J* 8.9 Hz, *m*-H, 3-Ph, 2H), 7.24 (d, *J* 16.4 Hz, Het-CH=, 1H), 7.80 (d, *J* 8.8 Hz, *o*-H, 5-Ph, 2H), 7.86 (d, *J* 16.4 Hz, Ph-CH=, 1H), 7.98 (d, *J* 8.8 Hz, *o*-H, 3-Ph, 2H). ^{13}C NMR (101 MHz, $\text{DMSO-}d_6$), δ 55.9 (2 OMe), 108.1 (Het-CH=), 115.0 (*m*-C, 3-Ph), 115.1 (*m*-C, 5-Ph), 119.2 (*i*-C, 3-Ph), 127.4 (*i*-C, 5-Ph), 129.1 (*o*-C, 3-Ph), 130.6 (*o*-C, 5-Ph), 142.9 (Ph-CH=), 161.8 (*p*-C, 5-Ph), 162.1 (*p*-C, 3-Ph), 168.1 (C-3), 175.9 (C-5). HRMS (ESI), *m/z*: calcd for $\text{C}_{18}\text{H}_{17}\text{N}_2\text{O}_3$ $[\text{M}+\text{H}]^+$ 309.1234, found 309.1231.



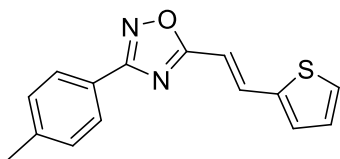
5-[(E)-2-(3,4-Dimethoxyphenyl)ethenyl]-3-phenyl-1,2,4-oxadiazole 4i.

The compound was synthesized by following the general procedure in 80% (369 mg) yield; white powder, mp 118-119 °C. IR, ν , cm^{-1} : 966 (*tr*-CH=CH), 1039, 1266 (C–O), 1582 (C=N), 1646 (CH=CH). ^1H NMR (400 MHz, $\text{DMSO-}d_6$), δ 3.82 (s, OMe, 3H), 3.86 (s, OMe, 3H), 7.03 (d, *J* 8.2 Hz, H-6, 5-Ph, 1H), 7.35 (d, *J* 8.2 Hz, H-5, 5-Ph, 1H), 7.36 (d, *J* 16.5 Hz, Ar-CH=, 1H), 7.51 (s, H-2, 5-Ph, 1H), 7.60 (m, *m,p*-H, Ph, 3H), 7.87 (d, *J* 16.5 Hz, Ph-CH=, 1H), 8.06 (m, *o*-H, Ph, 2H). ^{13}C NMR (101 MHz, $\text{DMSO-}d_6$), δ 56.1 (OMe), 56.2 (OMe), 108.2 (Het-CH=), 110.8 (CH, Ar), 112.1 (CH, Ar), 123.7 (CH, Ar), 126.9 (*i*-C, Ph), 127.5 (*m*-C, Ph), 127.6 (*i*-C, Ar), 129.7 (*o*-C, Ph), 131.9 (*p*-C, Ph), 143.5 (Ar-CH=), 149.6 (C, Ar), 151.7 (C, Ar), 168.4 (C-3), 176.3 (C-5). HRMS (ESI) calcd for $\text{C}_{18}\text{H}_{17}\text{N}_2\text{O}_3$ $[\text{M}+\text{H}]^+$ 309.1234, found 309.1238.



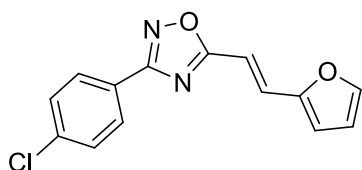
5-[(E)-2-(2,3-Dimethoxyphenyl)ethenyl]-3-phenyl-1,2,4-oxadiazole 4j.

The compound was synthesized by following the general procedure in 79% (365 mg) yield; white powder, mp 106-108 °C. IR, ν , cm^{-1} : 975 (*tr*-CH=CH), 1071, 1269 (C–O), 1557 (C=N), 1630 (CH=CH). ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 3.85 (s, 2Me, 6H), 7.17 (m, H-4,6, Ar, 2H), 7.41 (d, *J* 16.5 Hz, Het-CH=, 1H), 7.51 (m, H-5, Ar, 1H), 7.55-7.63 (m, *m,p*-H, 3H), 8.05-8.10 (m, *o*-H, Ph-CH=, 3H). ^{13}C NMR (101 MHz, $\text{DMSO-}d_6$), δ 56.3 (OMe), 61.4 (OMe), 111.7 (Het-CH=), 115.6 (CH, Ar), 119.5 (CH, Ar), 124.9 (CH, Ar), 126.8 (*i*-C, Ph), 127.5 (*m*-C, Ph), 128.1 (*i*-C, Ar), 129.7 (*o*-C, Ph), 132.0 (*p*-C, Ph), 137.4 (Ar-CH=), 148.3 (C, Ar), 153.2 (C, Ar), 168.5 (C-3), 176.0 (C-5). HRMS (ESI), *m/z*: calcd for $\text{C}_{18}\text{H}_{17}\text{N}_2\text{O}_3$ $[\text{M}+\text{K}]^+$ 347.0793, found 347.0794.



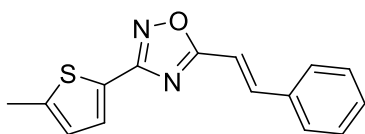
3-(4-Methylphenyl)-5-[(E)-2-(thiophen-2-yl)ethenyl]-1,2,4-oxadiazole 4k.

The compound was synthesized by following the general procedure in 85% (342 mg) yield; white powder, mp 102-104 °C. IR, ν , cm^{-1} : 954 (*tr*-CH=CH), 1160 (C–O), 1550 (C=N), 1629 (CH=CH). ^1H NMR(400 MHz, DMSO- d_6), δ 2.35 (s, Me, 3H), 6.98 (d, *J* 15.8 Hz, Het-CH=, 1H), 7.17 (dd, *J* 5.0,3.3 Hz, Th, H-4, 1H), 7.33 (d, *J* 7.9 Hz, *m*-H, 2H), 7.63 (d, *J* 3.3 Hz, Th, H-3, 1H), 7.77 (d, *J* 5.0 Hz, Th, H-5, 1H), 7.90 (d, *J* 7.9 Hz, *o*-H, 2H), 8.04 (d, *J* 16.2 Hz, Th-CH=, 1H). ^{13}C NMR (101 MHz, DMSO- d_6), δ 21.5 (Me), 108.7 (Het-CH=), 124.0 (Th, C-4), 127.4 (*o*-C), 129.1 (Th, C-3), 130.1 (*m*-C), 130.8 (*i*-C, Ph), 132.5 (Th, C-5), 135.8 (Th, C-2), 139.5 (*p*-C), 141.8 (Het-CH=), 168.4 (C-3), 175.3 (C-5). HRMS (ESI), *m/z*: calcd for $\text{C}_{15}\text{H}_{13}\text{N}_2\text{OS}$ [$\text{M}+\text{H}$] $^+$ 269.0743, found 269.0751.



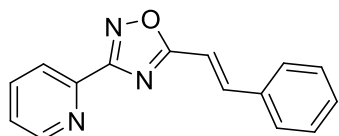
3-(4-Chlorophenyl)-5-[(E)-2-(furan-2-yl)ethenyl]-1,2,4-oxadiazole 4l.

The compound was synthesized by following the general procedure in 78% (319 mg) yield; white powder, mp 115-116 °C. IR, ν , cm^{-1} : 964 (*tr*-CH=CH), 1091, 1272 (C–O), 1528 (C=N), 1653 (CH=CH). ^1H NMR (400 MHz, DMSO- d_6), δ 6.71 (dd, *J* 3.4, 1.8 Hz, Fur, H-4, 1H), 6.97 (d, *J* 15.9 Hz, Het-CH=, 1H), 7.09 (d, *J* 3.4 Hz, Fur, H-3, 1H), 7.66 (d, *J* 8.5 Hz, *m*-H, 2H), 7.79 (d, *J* 16.2 Hz, Fur-CH=, 1H), 7.95 (m, Fur, H-5, 1H), 8.05 (d, *J* 8.5 Hz, *o*-H, 5H). ^{13}C NMR (101 MHz, DMSO- d_6), δ 107.0 (Het-CH=), 113.6 (Fur, C-3), 117.2 (Fur, C-4), 125.6 (*i*-C, Ph), 129.3 (*m*-C), 129.9 (*o*-C), 130.1 (Fur-CH=), 136.8 (*p*-C), 147.0 (Fur, C-5), 150.7 (Fur, C-2), 167.7 (C-3), 175.9 (C-5). HRMS (ESI), *m/z*: calcd for $\text{C}_{14}\text{H}_{10}\text{ClN}_2\text{O}_2$ [$\text{M}+\text{H}$] $^+$ 273.0425, found 273.0427.



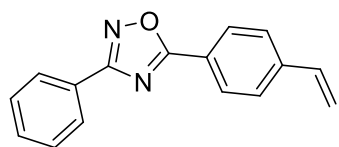
3-(5-Methylthiophen-2-yl)-5-[(E)-2-phenylethenyl]-1,2,4-oxadiazole 4m.

The compound was synthesized by following the general procedure in 95% (382 mg) yield; white powder, mp 113-115 °C. IR, ν , cm^{-1} : 974 (*tr*-CH=CH), 1098 (C–O), 1572 (C=N), 1643 (CH=CH). ^1H NMR (400 MHz, DMSO- d_6), δ 2.53 (s, Me, 3H), 6.98 (d, *J* 3 Hz, H-4, Th, 1H), 7.41 (d, *J* 16.4 Hz, Het-HC=, 1H), 7.45-7.50 (m, *m,p*-H, 3H), 7.64 (d, *J* 3.4 Hz, H-3, Th, 1H), 7.84-7.87 (m, *o*-H, 2H), 7.91 (d, *J* 16.4 Hz, Ph-HC=, 1H). ^{13}C NMR (101 MHz, DMSO- d_6), δ 15.6 (Me), 110.5 (Het-CH=), 125.5 (Th, C-5), 127.5 (*p*-C), 128.9 (*m*-C), 129.5 (*o*-C), 130.5 (Th, C-3), 131.1 (Th, C-4), 134.7 (*i*-C), 143.4 (Ph-CH=), 145.0 (Th, C-2), 164.5 (C-3), 175.6 (C-5). HRMS (ESI), *m/z*: calcd for $\text{C}_{15}\text{H}_{13}\text{N}_2\text{OS}$ [$\text{M}+\text{H}$] $^+$ 269.0743, found 269.0748.



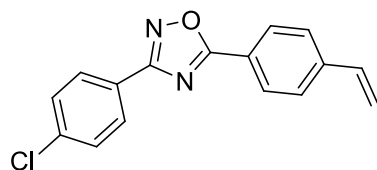
2-{5-[(E)-2-Phenylethenyl]-1,2,4-oxadiazol-3-yl}pyridine 4n.

The compound was synthesized by following the general procedure in 74% (276 mg) yield; white powder, mp 114-116 °C. IR, ν , cm^{-1} : 980 (*tr*-CH=CH), 1071 (C–O), 1572 (C=N), 1644 (CH=CH). ^1H NMR(400 MHz, DMSO- d_6), δ 7.46 - 7.50 (m, *m,p*-H, Ph, Het-CH=, 4H), 7.63 (ddd, *J* 7.6, 4.9, 1.2 Hz, H-5, Py, 1H), 7.86-7.88 (m, *o*-H, Ph, 2H), 7.99 (d, *J* 16.5 Hz, Ph-CH=, 1H), 8.05 (td, *J* 7.7, 1.7 Hz, H-4, Py, 1H), 8.13 (d, *J* 7.9 Hz, H-3, Py, 1H), 8.78 (d, *J* 4.5 Hz, H-6, Py, 1H). ^{13}C NMR (101 MHz, DMSO- d_6), δ 110.7 (Het-CH=), 123.8 (Py, C-3), 126.6 (Py, C-5), 128.9 (*o*-C), 129.5 (*m*-C), 131.3 (*p*-C), 134.7 (*i*-C, Ph), 138.2 (Ph-CH=), 143.6 (Py, C-4), 146.3 (Py, C-2), 150.8 (Py, C-6), 168.6 (C-3), 176.2 (C-5). HRMS (ESI), *m/z*: calcd for $\text{C}_{15}\text{H}_{12}\text{N}_3\text{O}$ [$\text{M}+\text{H}$] $^+$ 250.0974, found 250.0979.



3-Phenyl-5-(4-vinylphenyl)-1,2,4-oxadiazole 4o.

The compound was synthesized by following the general procedure in 88% (327 g) yield; white powder, mp 75-77 °C. IR, ν , cm^{-1} : 991 (CH=CH $_2$), 1276 (C–O), 1594 (C=N), 1627 (CH=CH). ^1H NMR (400 MHz, DMSO- d_6), δ 5.47 (d, *J* 10.9 Hz, *cis*-CH=CH $_2$, 1H), 6.05 (d, *J* 17.5 Hz, *tr*-CH=CH $_2$, 1H), 6.86 (dd, *J* 17.5 Hz, 10.9 Hz, CH=CH $_2$, 1H), 7.60 (m, *m,p*-H, Ph, 3H), 7.74 (d, *J* 7.9 Hz, Ar, 2H), 8.08-8.15 (m, *o*-H, Ph, Ar, 4H). ^{13}C NMR (101 MHz, DMSO- d_6), δ 118.1 (=CH $_2$), 122.9 (*i*-C), 126.7 (*p*-C), 127.6 (*o*-C), 128.7 (*m*-C), 129.7 (*m*-C), 132.1 (*i*-C), 136.1 (-CH=), 142.2 (*p*-C), 168.7 (C-3), 175.6 (C-5). HRMS (ESI), *m/z*: calcd for $\text{C}_{16}\text{H}_{13}\text{N}_2\text{O}$ [$\text{M}+\text{H}$] $^+$ 249.1022, found 249.1018.



3-(4-Chlorophenyl)-5-(4-ethenylphenyl)-1,2,4-oxadiazole 4p.

The compound was synthesized by following the general procedure in 85% (360 mg) yield; white powder, mp 110-112 °C. IR, ν , cm^{-1} : 992 (CH=CH $_2$), 1278 (C–O), 1589 (C=N), 1629 (CH=CH). ^1H NMR (400 MHz, DMSO- d_6), δ 5.46 (d, *J* 10.9 Hz, *cis*-CH=CH $_2$, 1H), 6.00 (d, *J* 17.5 Hz, *tr*-CH=CH $_2$, 1H), 6.86 (dd, *J* 17.5, 10.9 Hz, CH=CH $_2$, 1H), 7.58-7.72 (m, 4H), 8.01-8.14 (m, 4H). ^{13}C NMR (101 MHz, DMSO- d_6), δ 117.9 (=CH $_2$), 126.2 (*i*-C), 127.2 (*p*-C), 127.5 (*o*-C), 128.7 (*m*-C), 131.5 (*m*-C), 131.8 (*i*-C), 134.5 (-CH=), 136.2 (*p*-C), 142.5 (*p*-C), 167.8 (C-3), 176.0 (C-5). HRMS (ESI), *m/z*: calcd for $\text{C}_{16}\text{H}_{12}\text{ClN}_2\text{O}$ [$\text{M}+\text{H}$] $^+$ 283.0633, found 283.0622.

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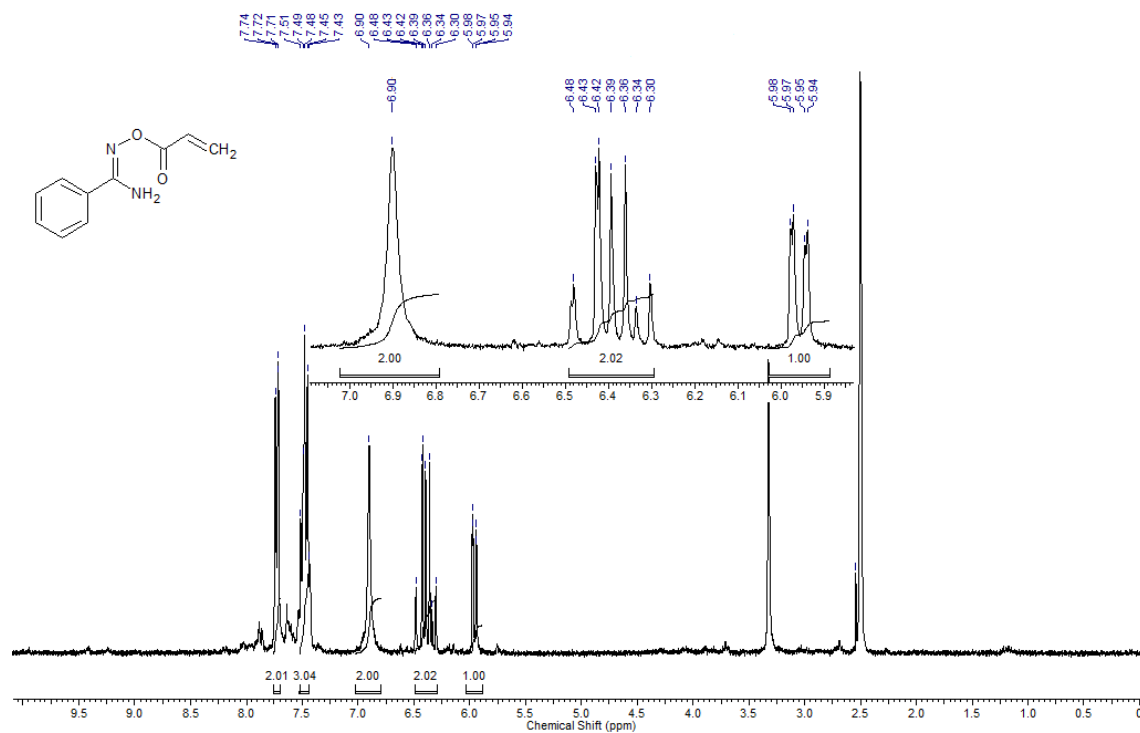
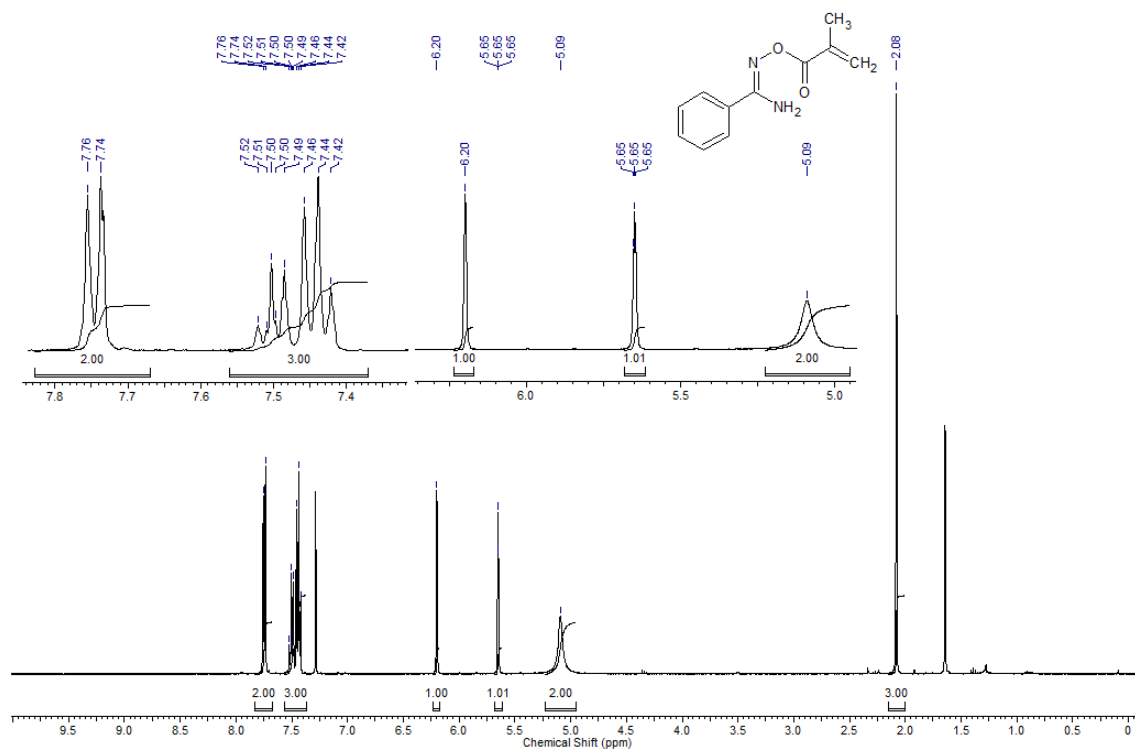
^1H , ^{13}C , and ^{13}C DEPT NMR spectra of *O*-acryloyloxime 3a-p and 1,2,4-oxadiazoles 4a-pFigure S1. ^1H NMR spectra of *N'*-(acryloyloxy)benzenecarboximidamide 3aFigure S2. ^1H NMR spectra of *N'*-(methacryloyloxy)benzenecarboximidamide 3b

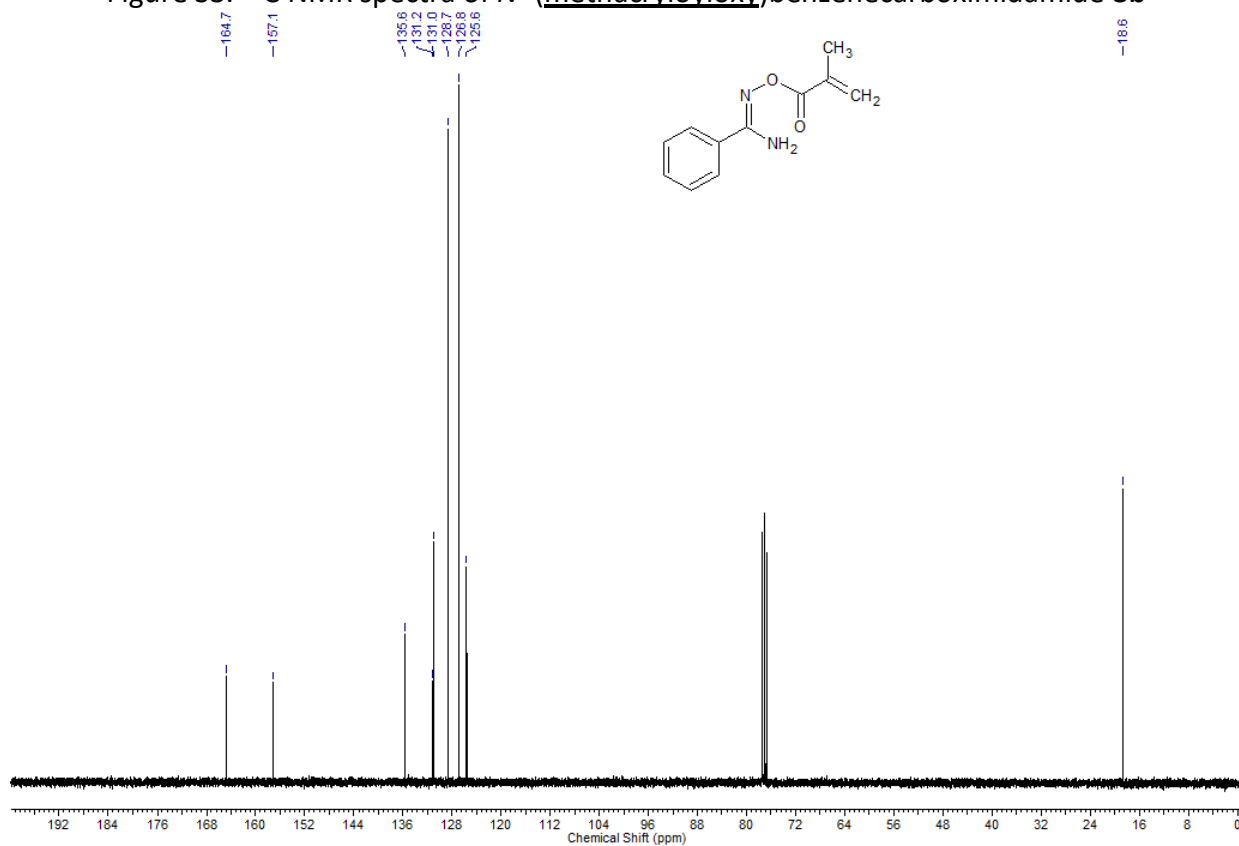
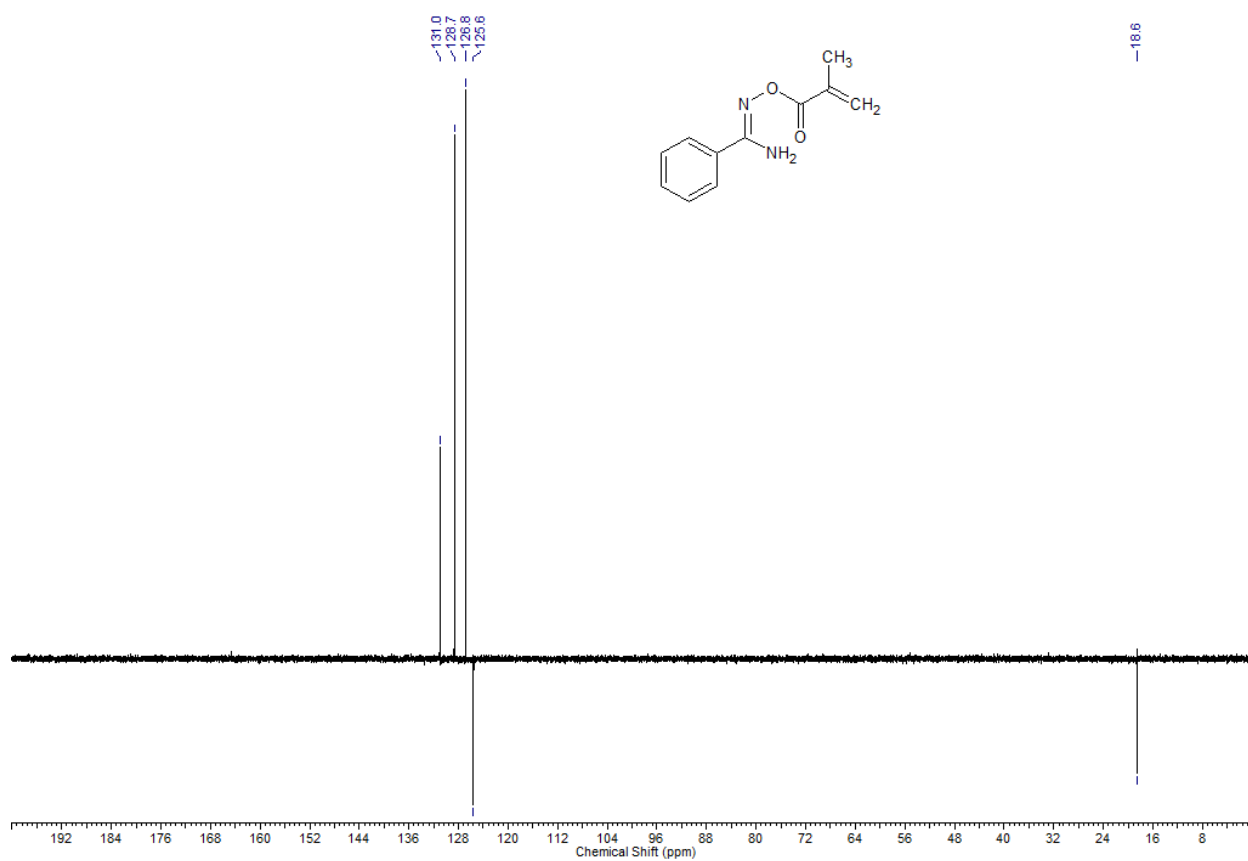
Figure S3. ^{13}C NMR spectra of *N'*-(methacryloyloxy)benzenecarboximidamide **3b**Figure S4. ^{13}C DEPT NMR spectra of *N'*-(methacryloyloxy)benzenecarboximidamide **3b**

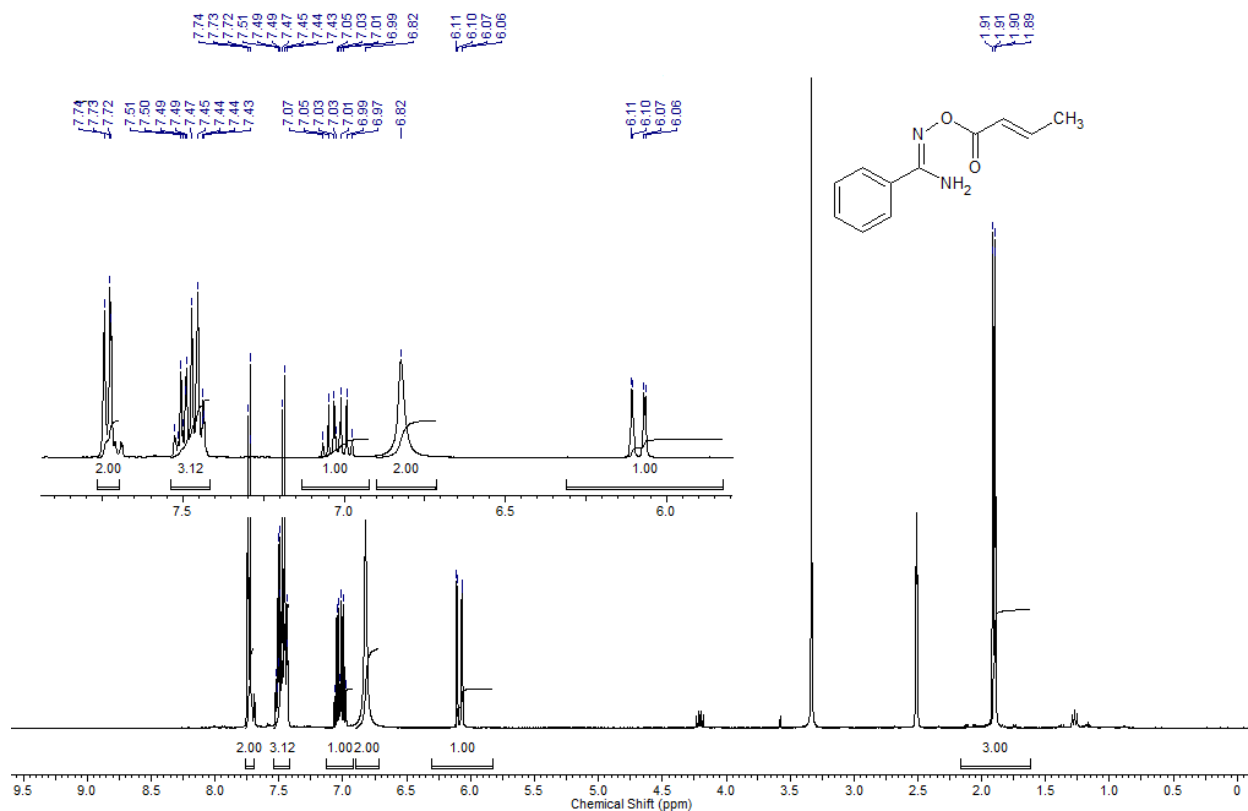
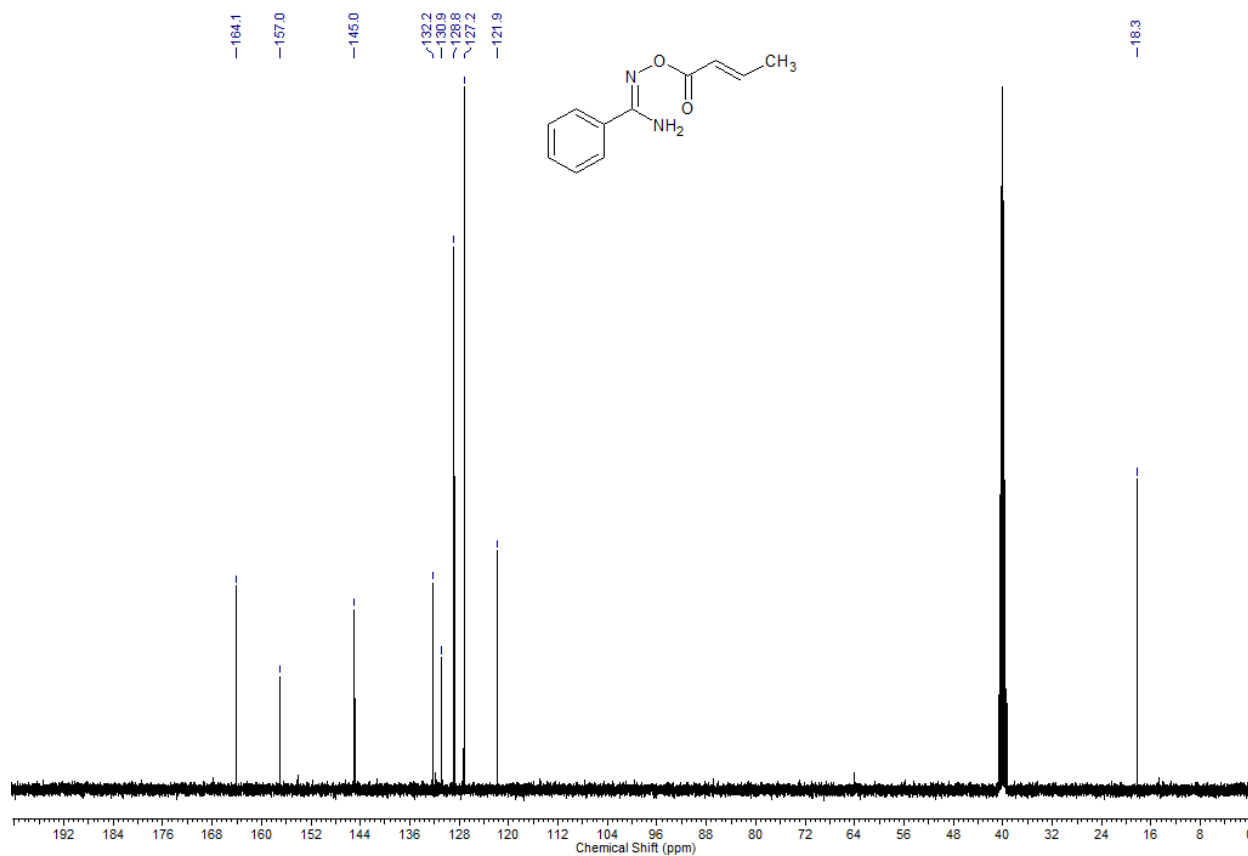
Figure S5. ^1H NMR spectra of N' -[($2E$)-but-2-enoyloxy]benzenecarboximidamide **3c**Figure S6. ^{13}C NMR spectra of N' -[($2E$)-but-2-enoyloxy]benzenecarboximidamide **3c**

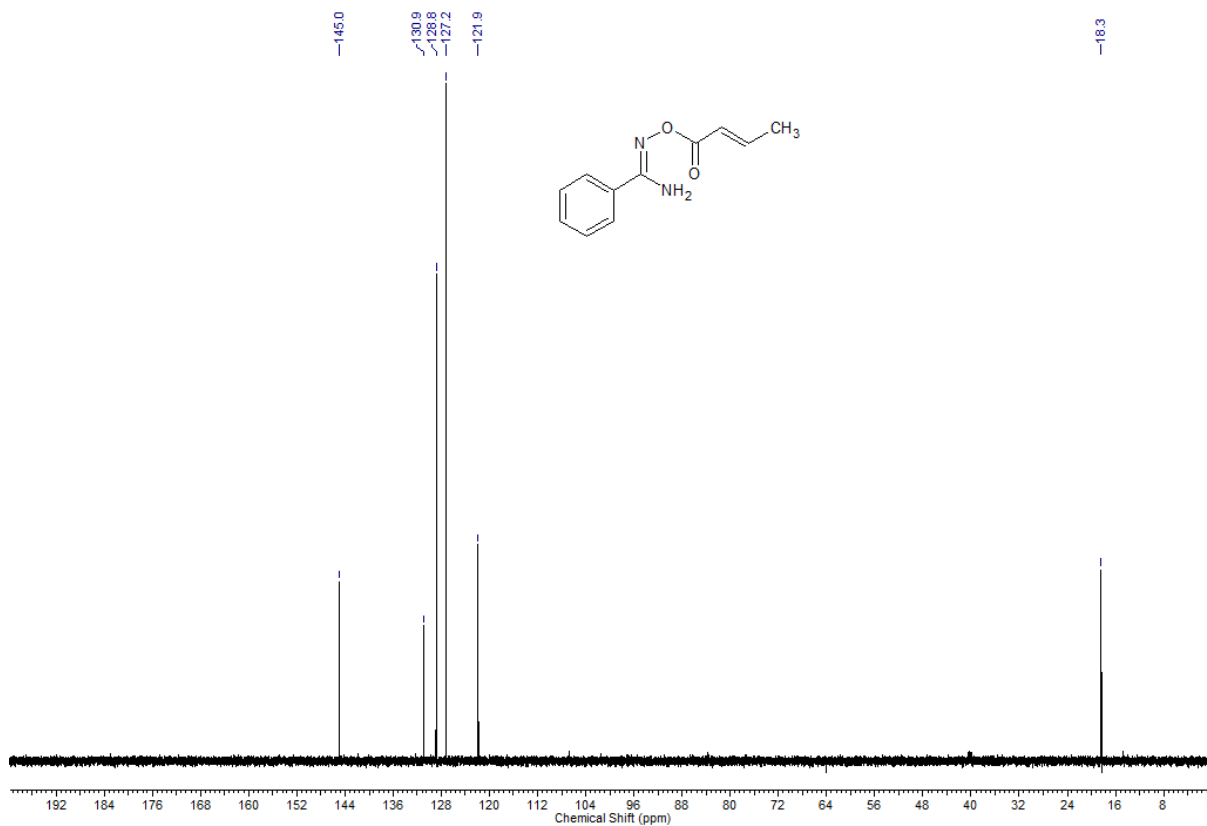
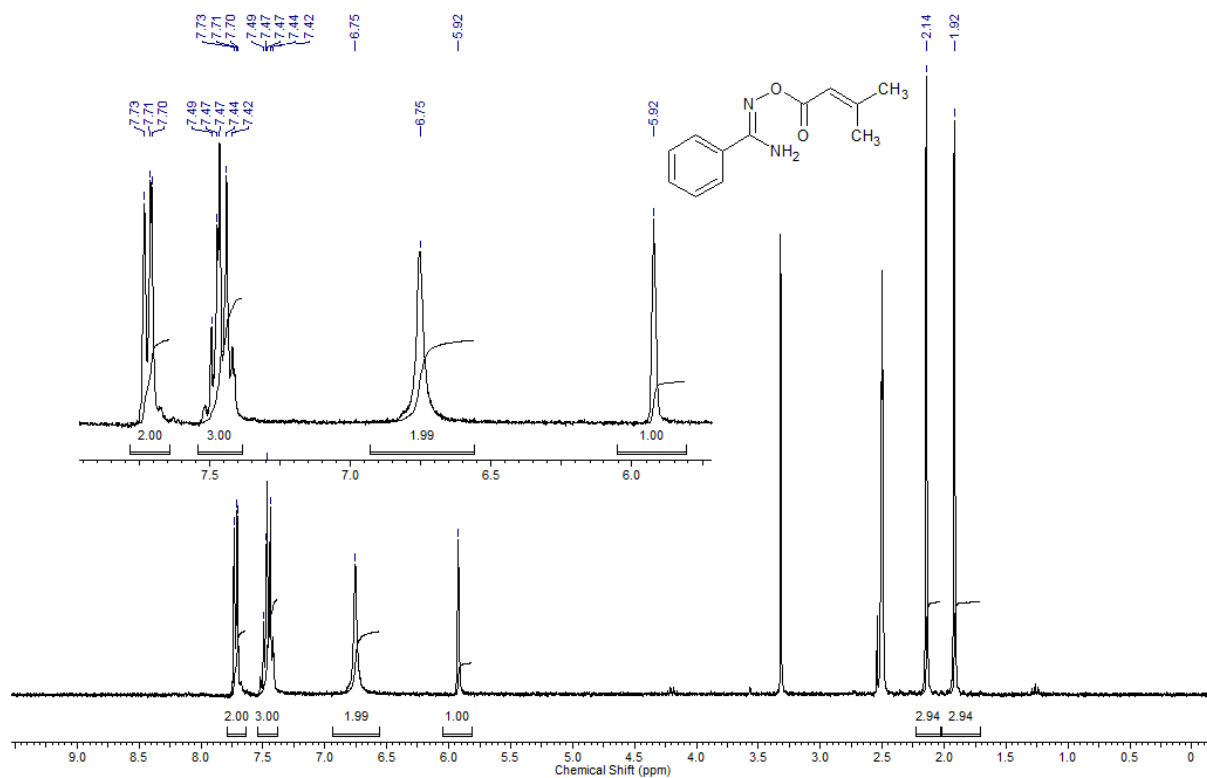
Figure S7. ^{13}C DEPT NMR spectra of *N'-[(2*E*)-but-2-enoyloxy]benzenecarboximidamide **3c***Figure S8. ^1H NMR spectra of *N'-[(3-methylbut-2-enoyl)oxy]benzenecarboximidamide **3d***

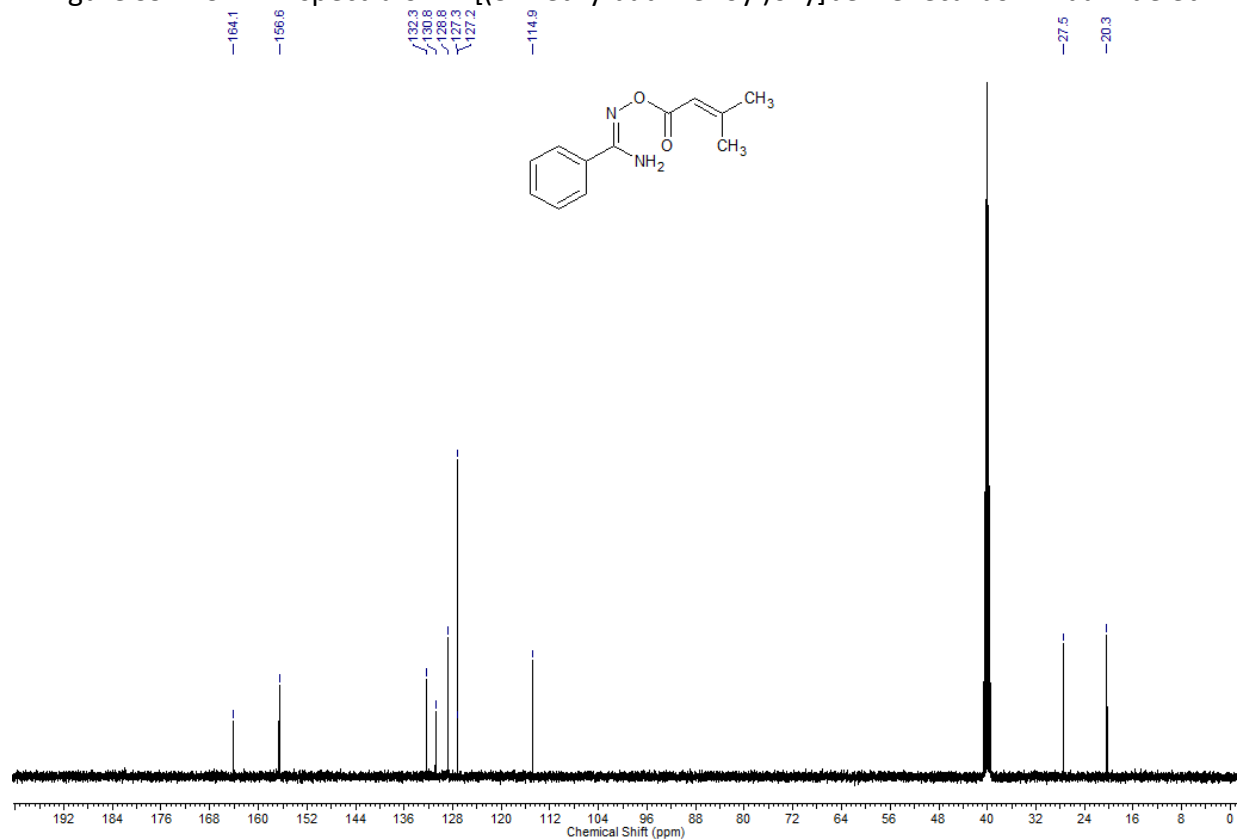
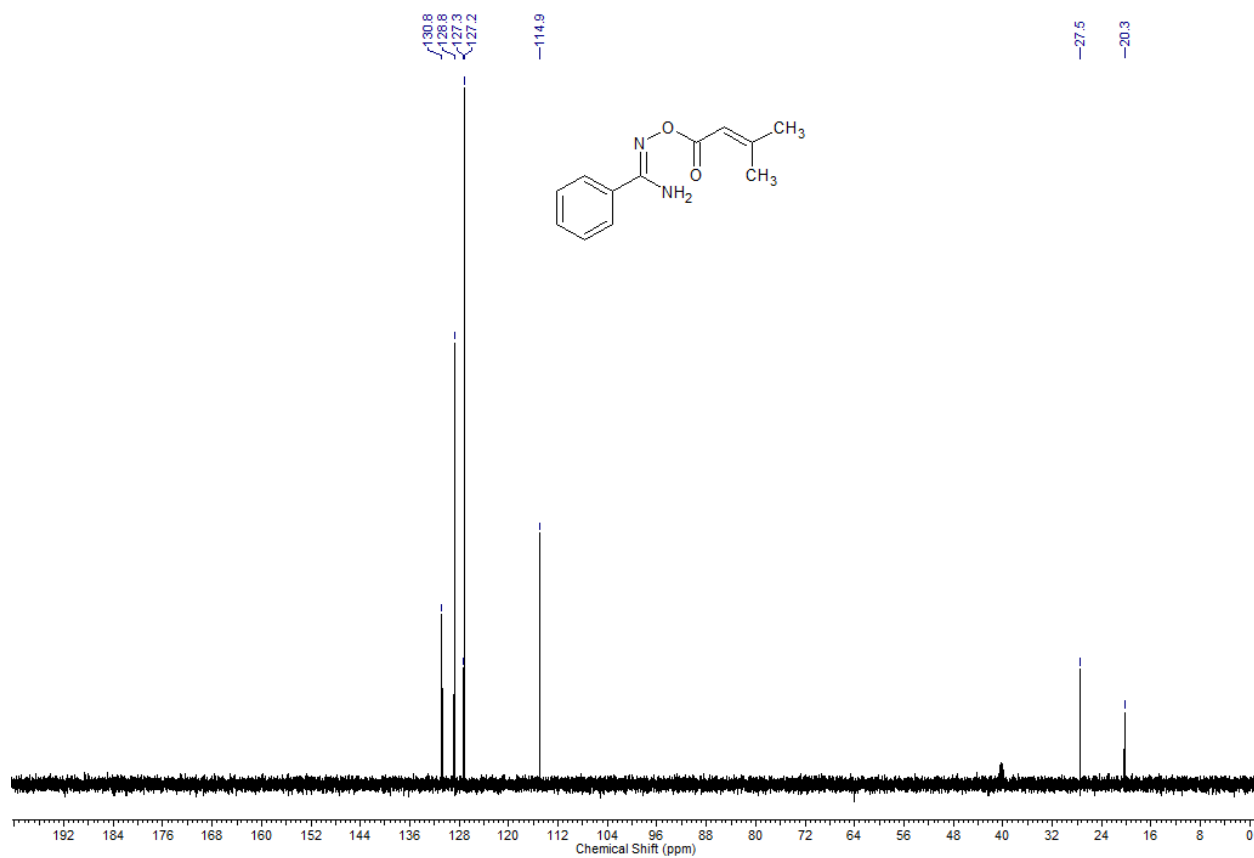
Figure S9. ^{13}C NMR spectra of *N'*-[(3-methylbut-2-enyl)oxy]benzenecarboximidamide **3d**Figure S10. ^{13}C DEPT NMR spectra of *N'*-[(3-methylbut-2-enyl)oxy]benzenecarboximidamide **3d**

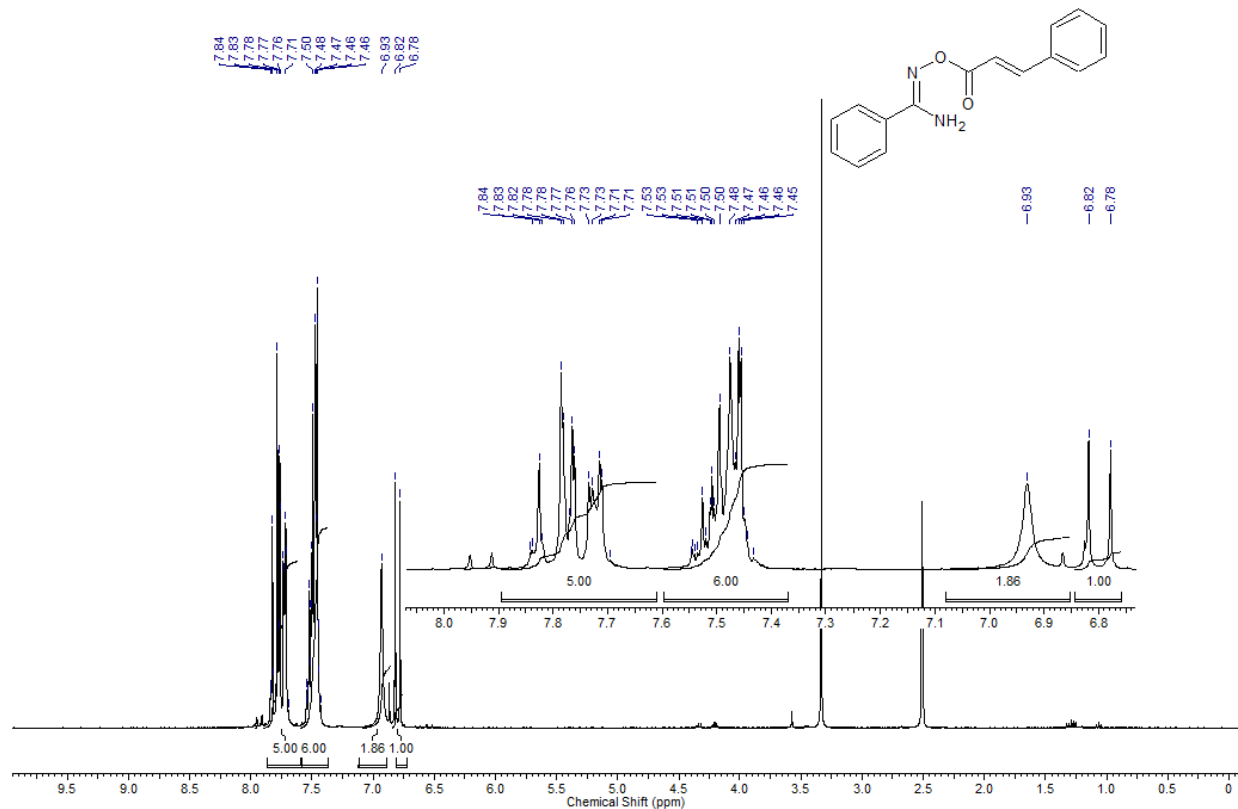
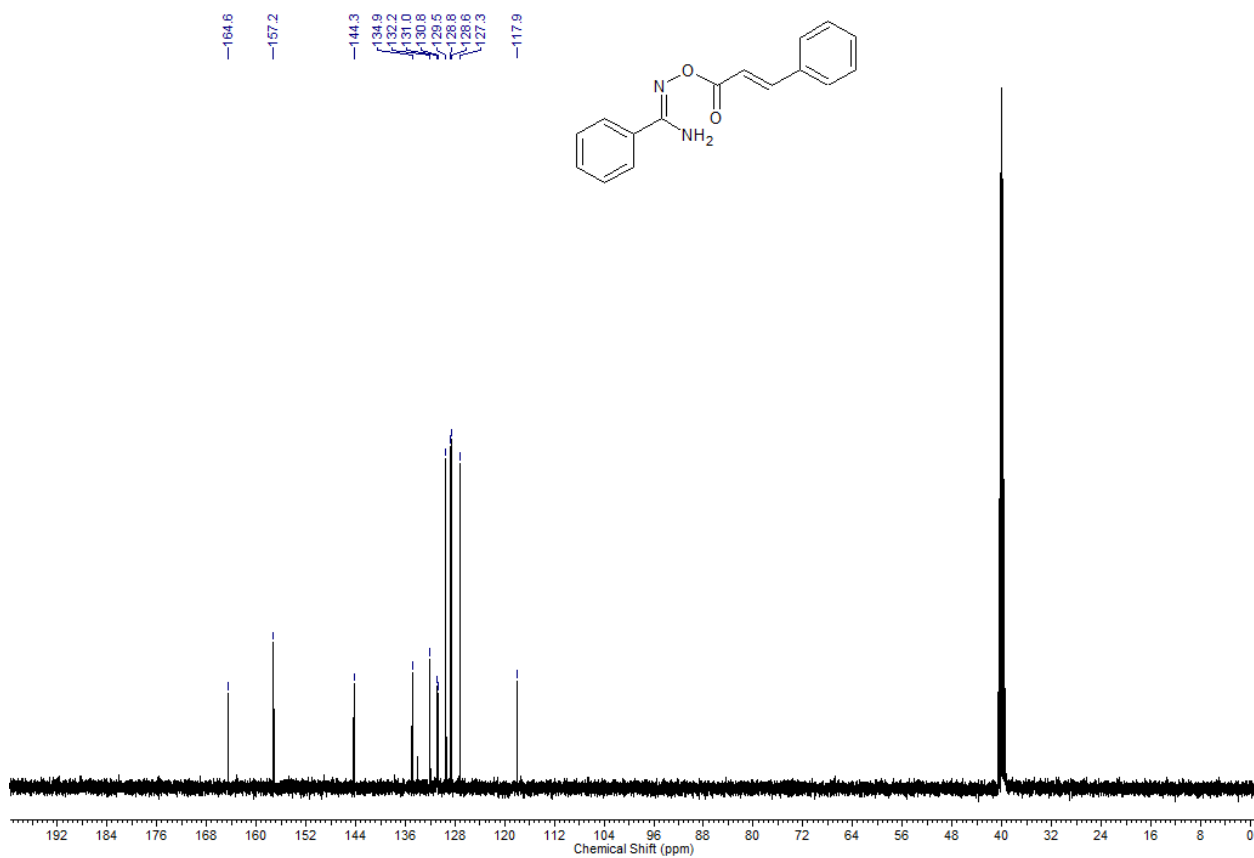
Figure S11. ^1H NMR spectra of N' -{[(2*E*)-3-phenylprop-2-enoyl]oxy}benzenecarboximidamide **3e**Figure S12. ^{13}C NMR spectra of N' -{[(2*E*)-3-phenylprop-2-enoyl]oxy}benzenecarboximidamide **3e**

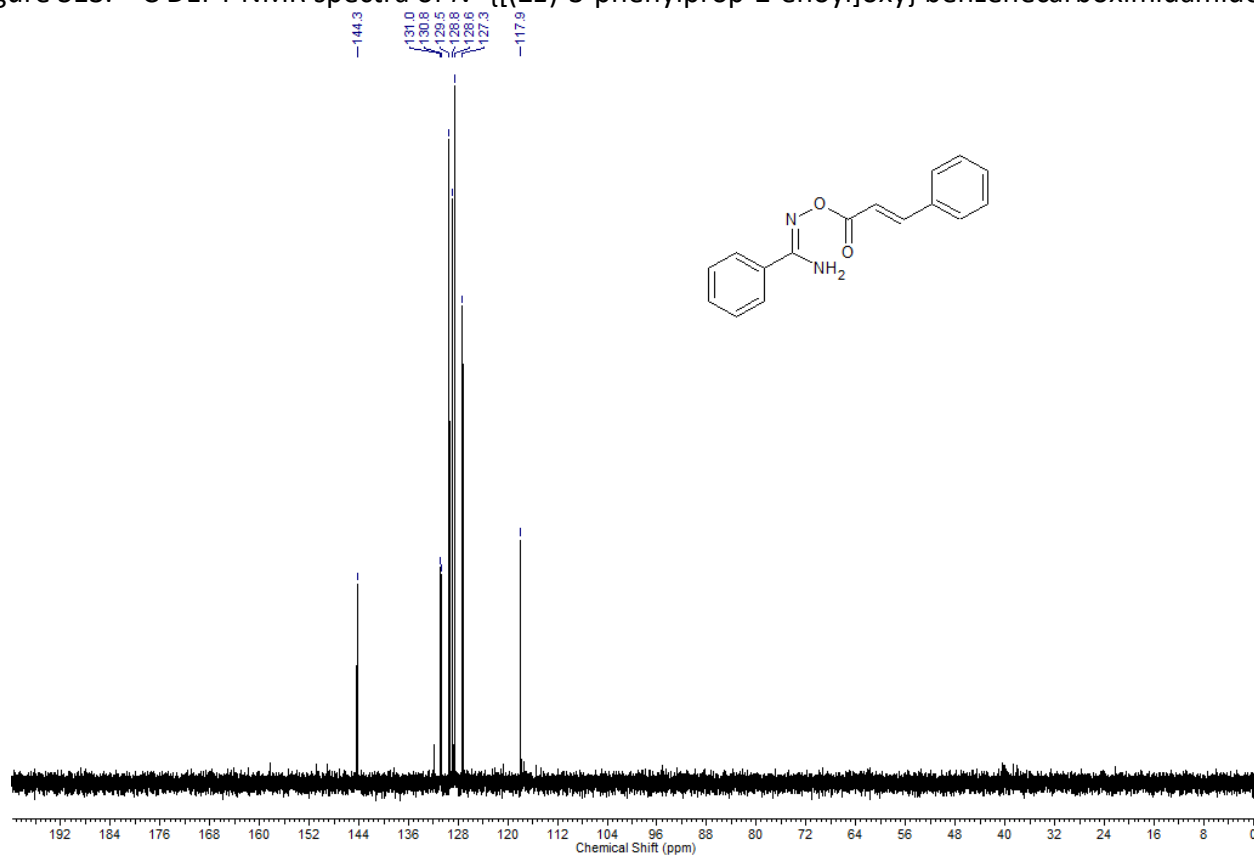
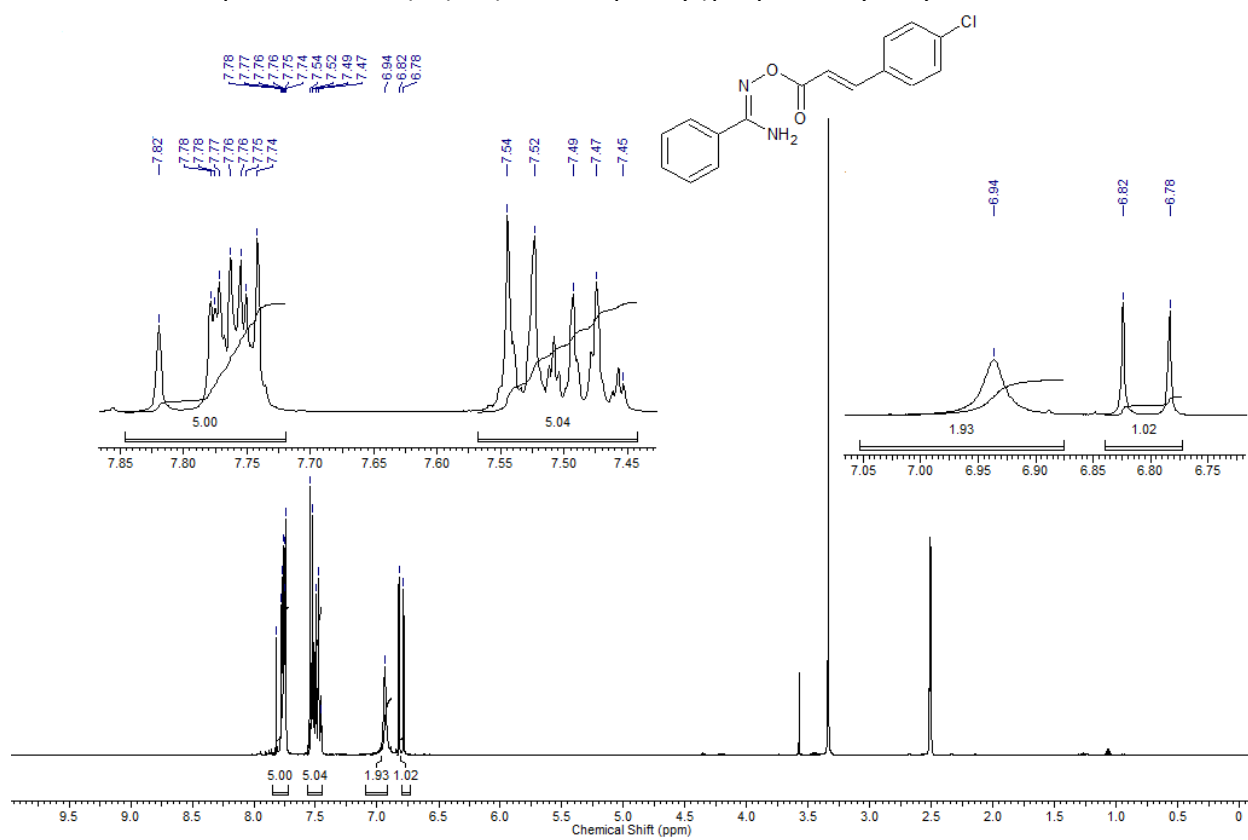
Figure S13. ^{13}C DEPT NMR spectra of N' -{[(*E*)-3-phenylprop-2-enyl]oxy} benzenecarboximidamide **3e**Figure S14. ^1H NMR spectra of N' -{[(*E*)-3-(4-Chlorophenyl)prop-2-enyl]oxy} benzenecarboximidamide **3f**

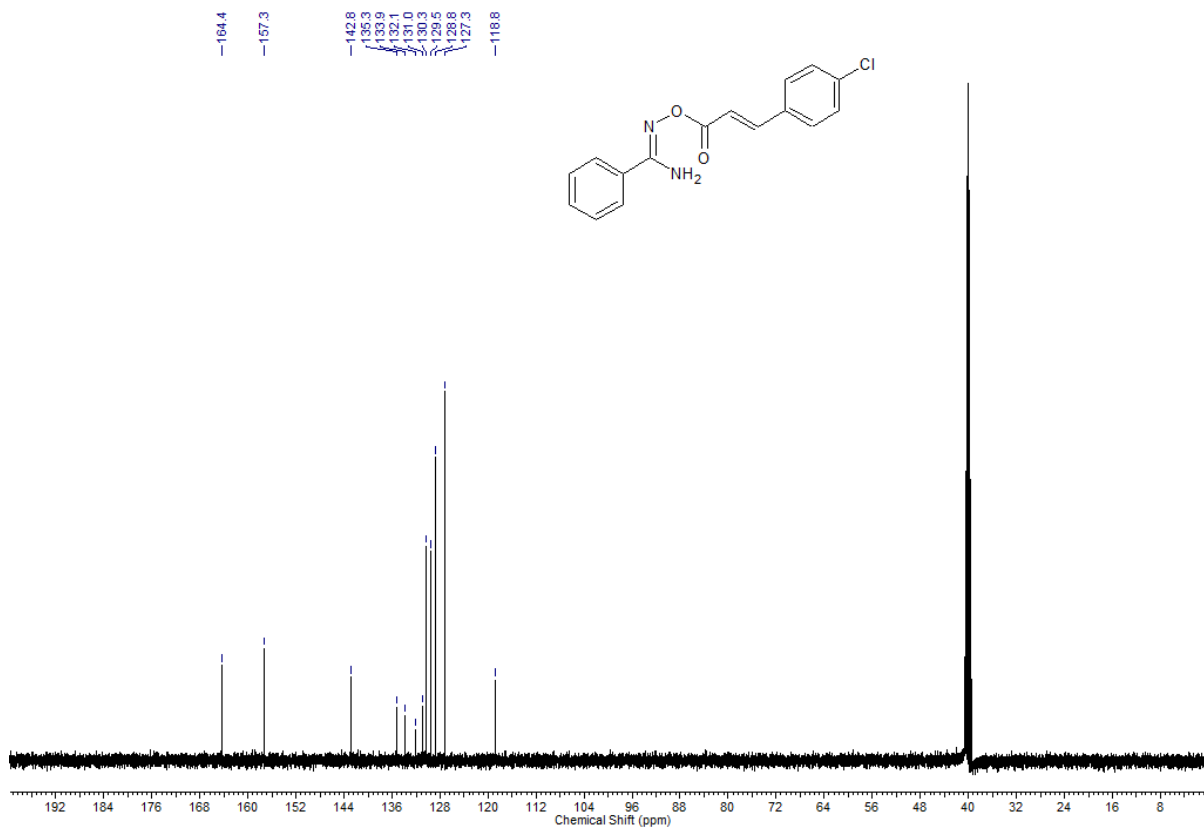
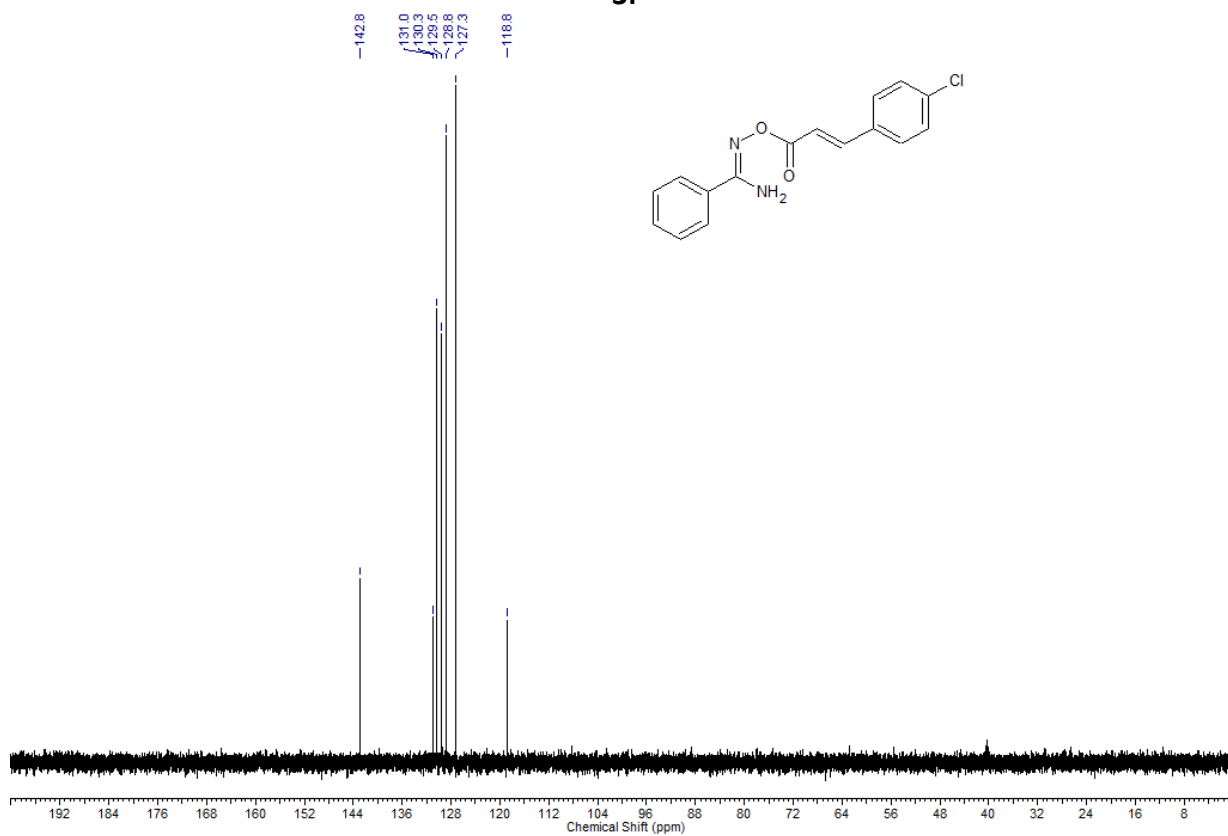
Figure S15 ^{13}C NMR spectra of *N'*-{[(*E*)-3-(4-Chlorophenyl)prop-2-enyl]oxy} benzenecarboximidamide **3f**Figure S16. ^{13}C DEPT NMR spectra of *N'*-{[(*E*)-3-(4-Chlorophenyl)prop-2-enyl]oxy} benzenecarboximidamide **3f**

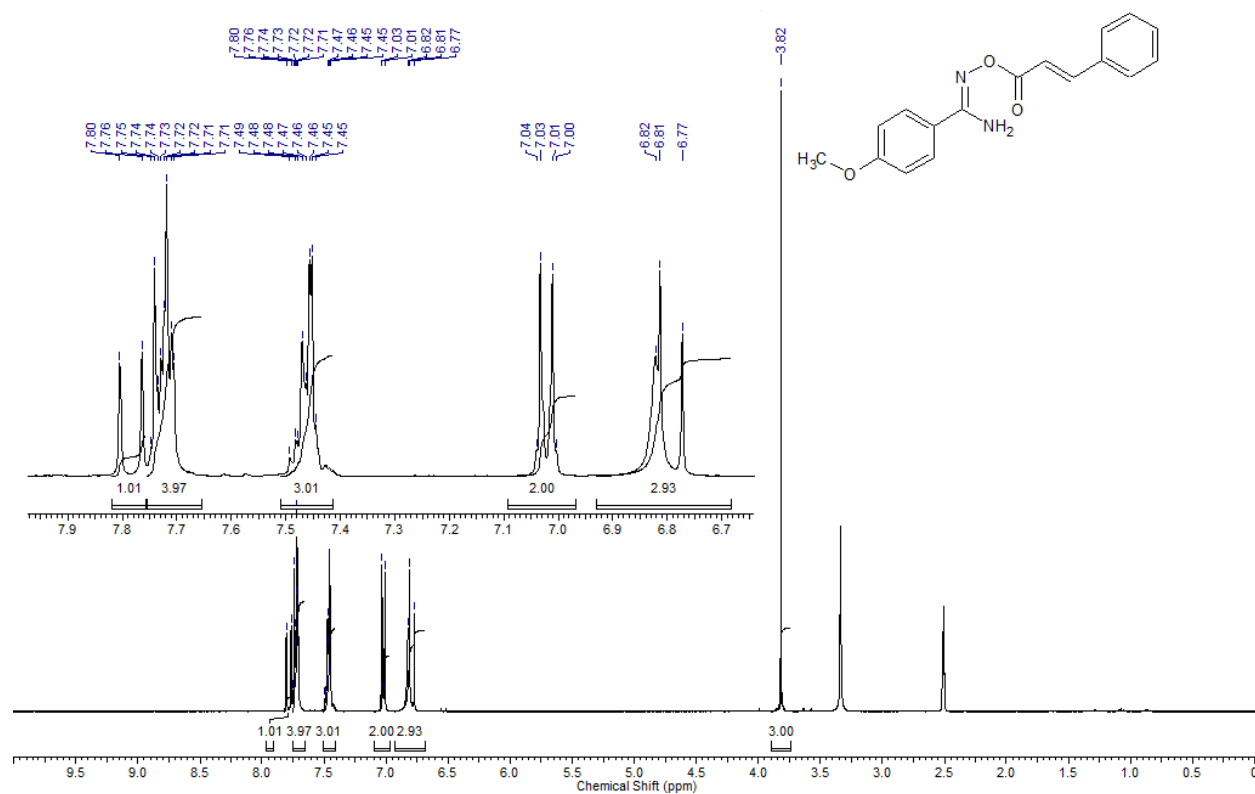
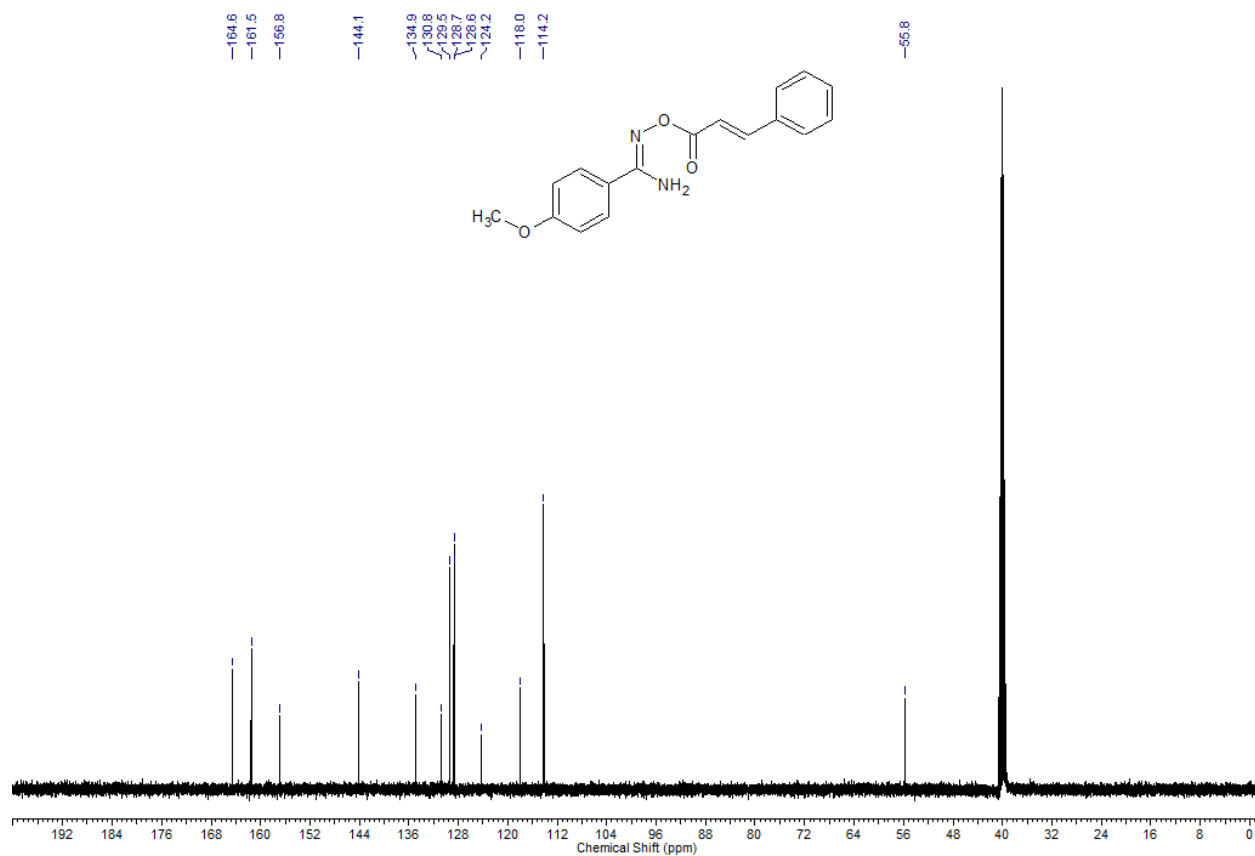
Figure S17. ^1H NMR spectra of 4-methoxy- N' -{[(2*E*)-3-phenylprop-2-enyl]oxy} benzenecarboximidamide **3g**Figure S18. ^{13}C NMR spectra of 4-methoxy- N' -{[(2*E*)-3-phenylprop-2-enyl]oxy} benzenecarboximidamide **3g**

Figure S19. ^{13}C DEPT NMR spectra of 4-methoxy- N' -{[(E)-3-phenylprop-2-enoyl]oxy}benzenecarboximidamide **3g**

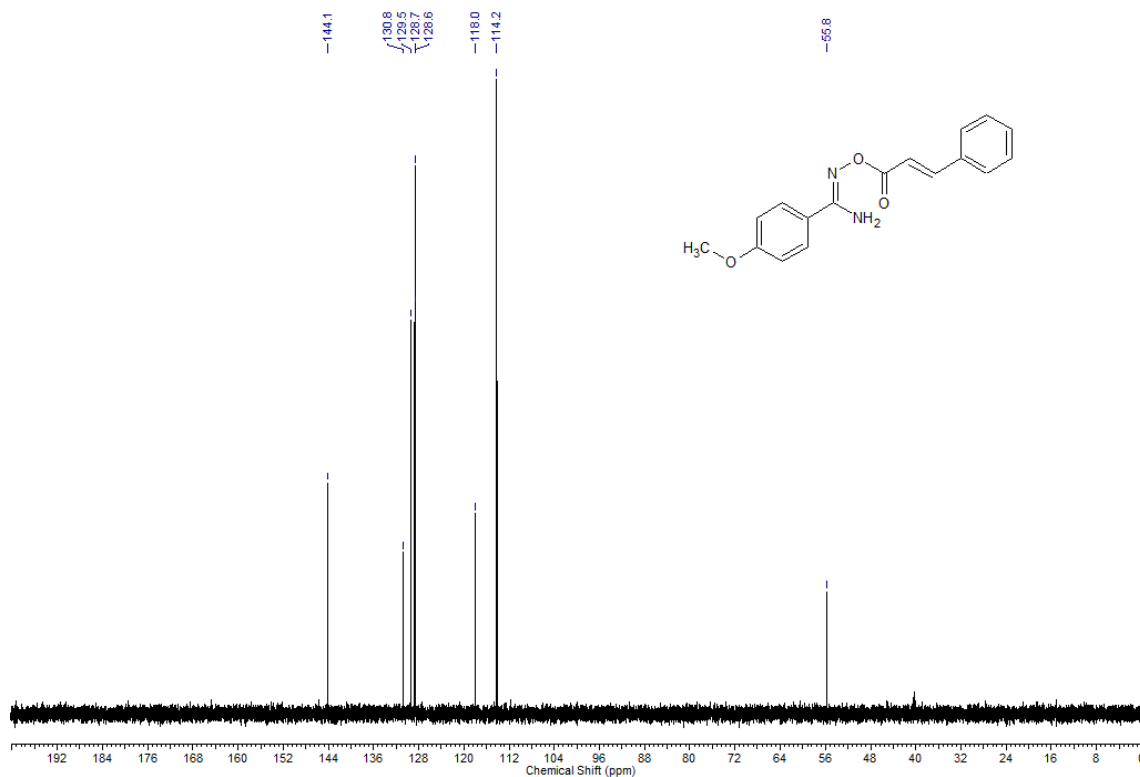


Figure S20. ^1H NMR spectra of 4-methoxy- N' -{[(E)-3-(4-methoxyphenyl)prop-2-enoyl]oxy}benzenecarboximidamide **3h**

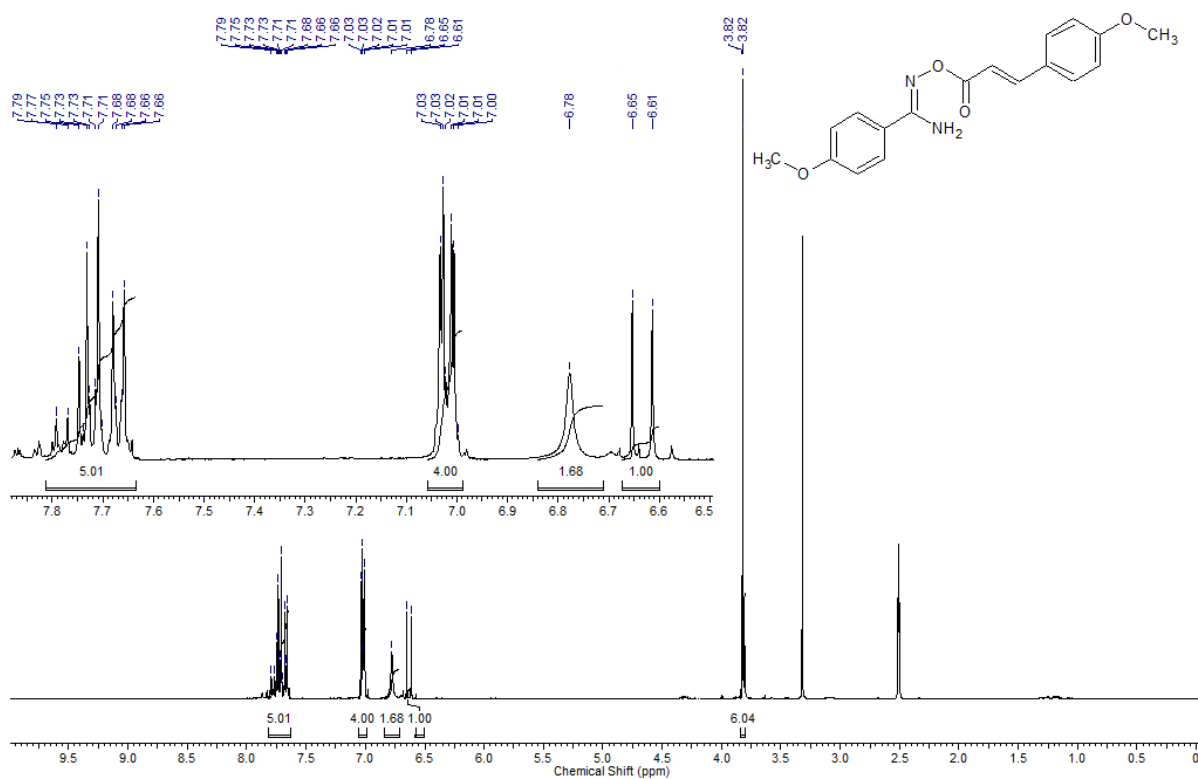


Figure S21. ^{13}C NMR spectra of 4-methoxy- N' -{[(2*E*)-3-(4-methoxyphenyl)prop-2-enoyl]oxy}benzenecarboximidamide **3h**

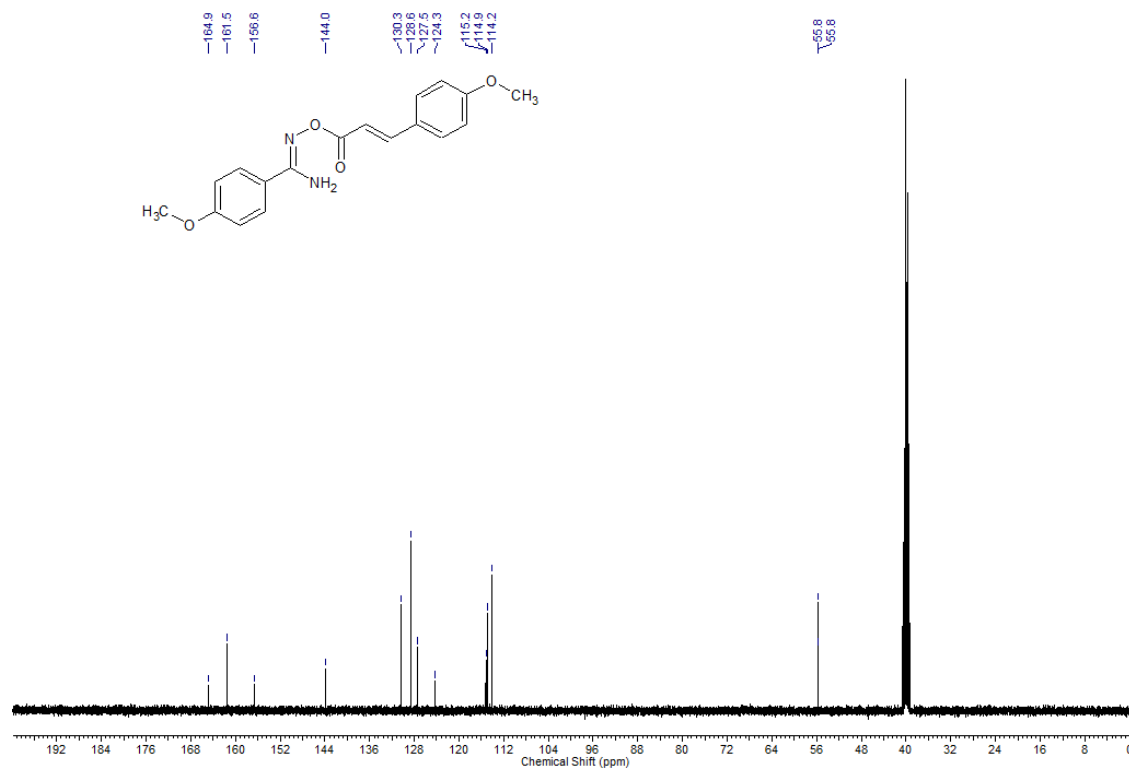


Figure S22. ^{13}C DEPT NMR spectra of 4-methoxy- N' -{[(2*E*)-3-(4-methoxyphenyl)prop-2-enoyl]oxy}benzenecarboximidamide **3h**

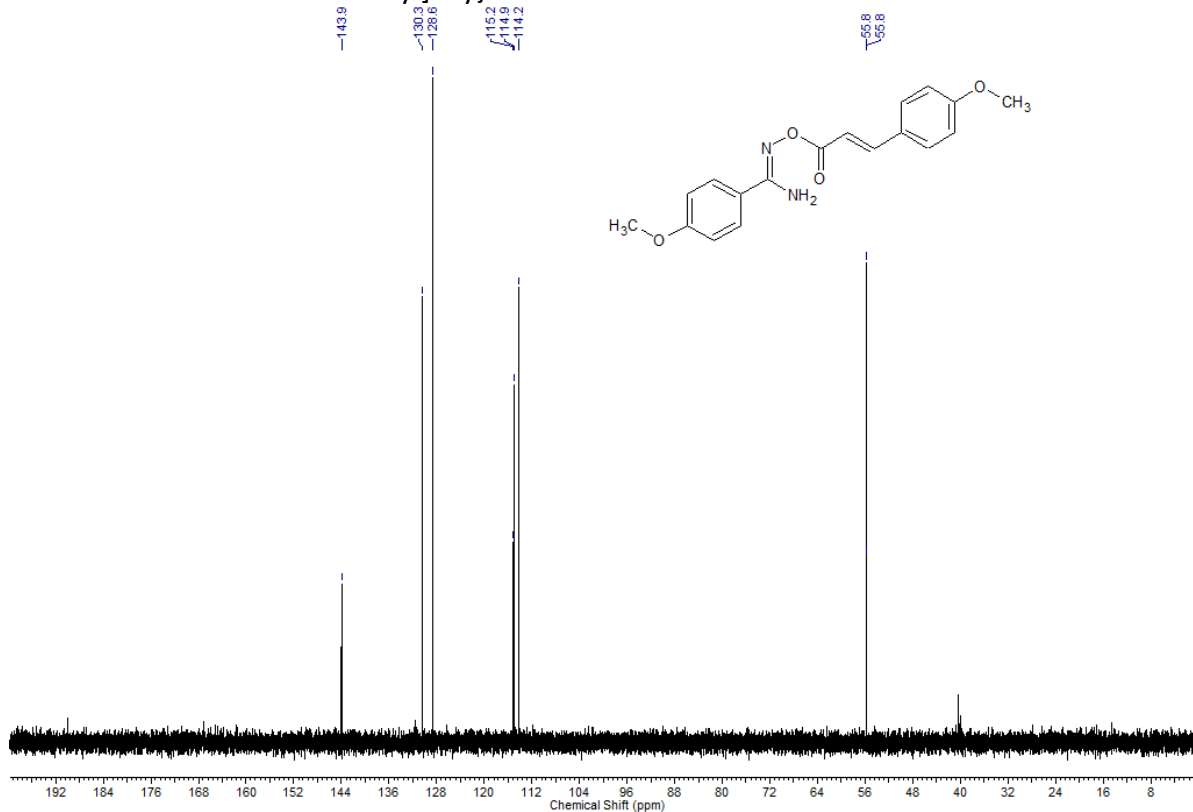


Figure S23. ^1H NMR spectra of N' -{[(*2E*)-3-(3,4-dimethoxyphenyl)prop-2-enoyl]oxy} benzenecarboximidamide **3i**

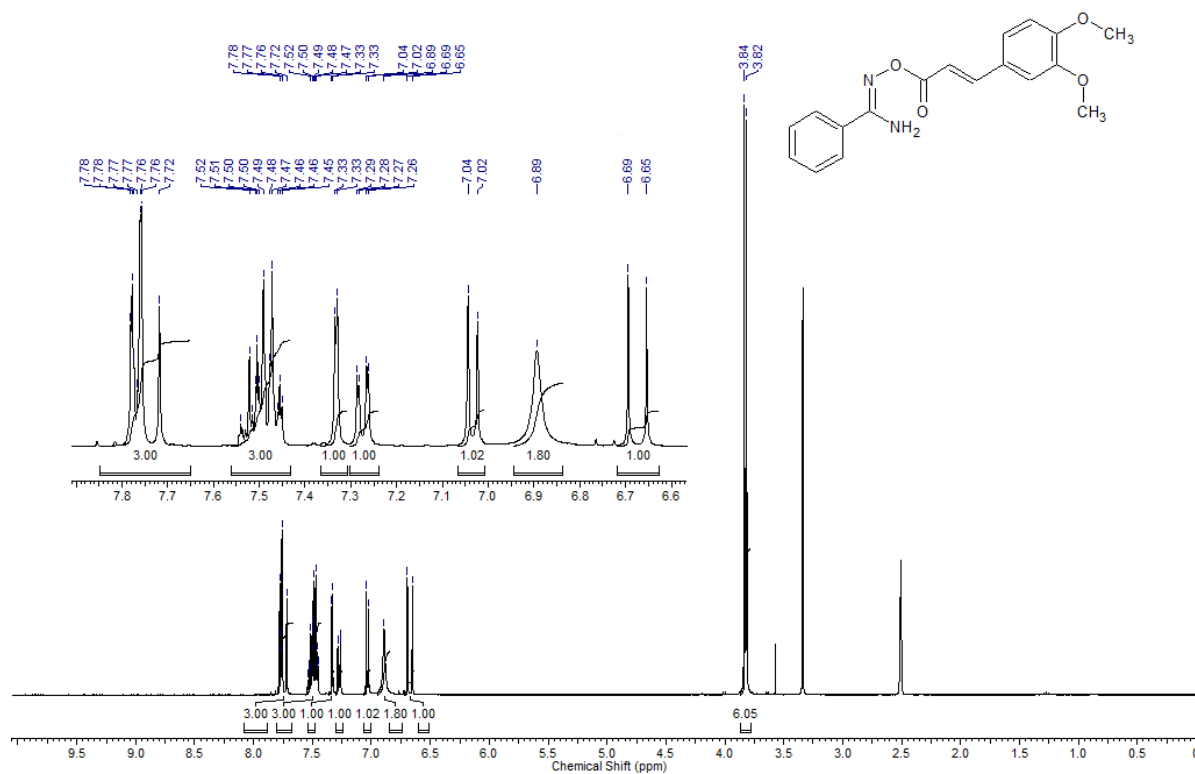


Figure S24. ^{13}C NMR spectra of N' -{[(*2E*)-3-(3,4-dimethoxyphenyl)prop-2-enoyl]oxy} benzenecarboximidamide **3i**

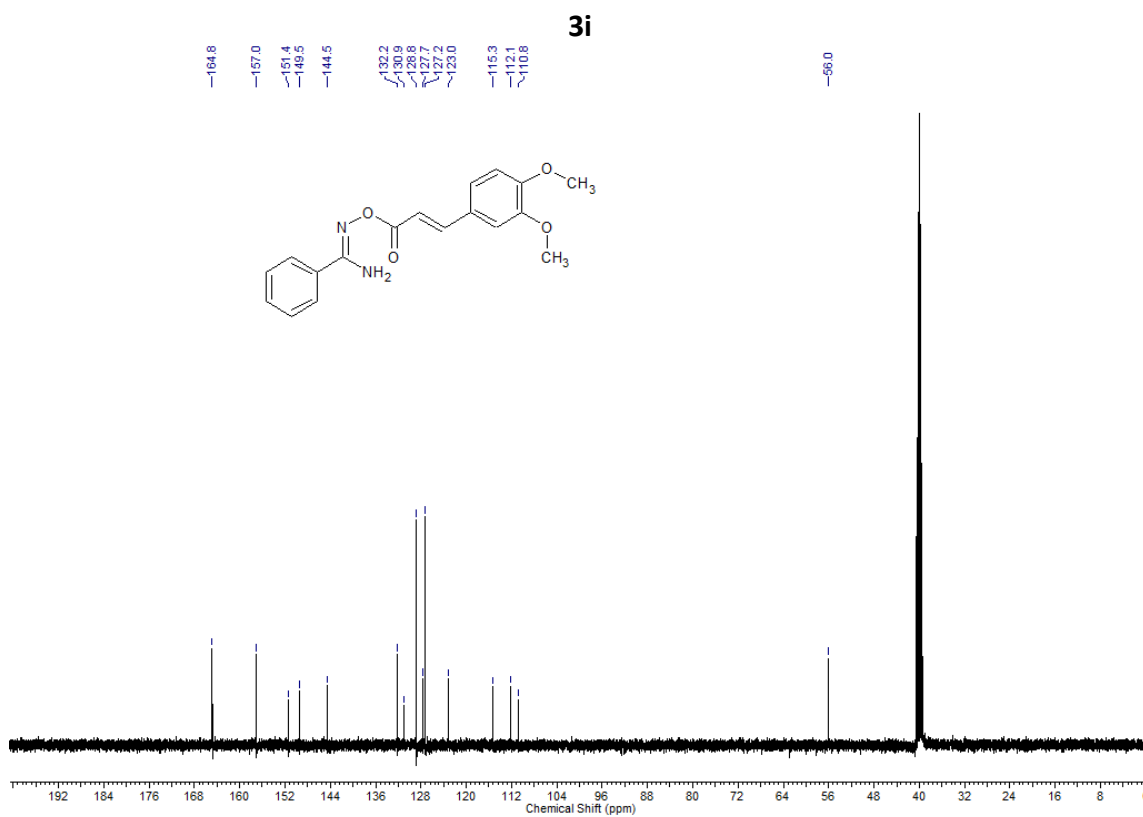


Figure S25. ^{13}C DEPT NMR spectra of *N'*-{[(*E*)-3-(3,4-dimethoxyphenyl)prop-2-enoyl]oxy} benzenecarboximidamide **3i**

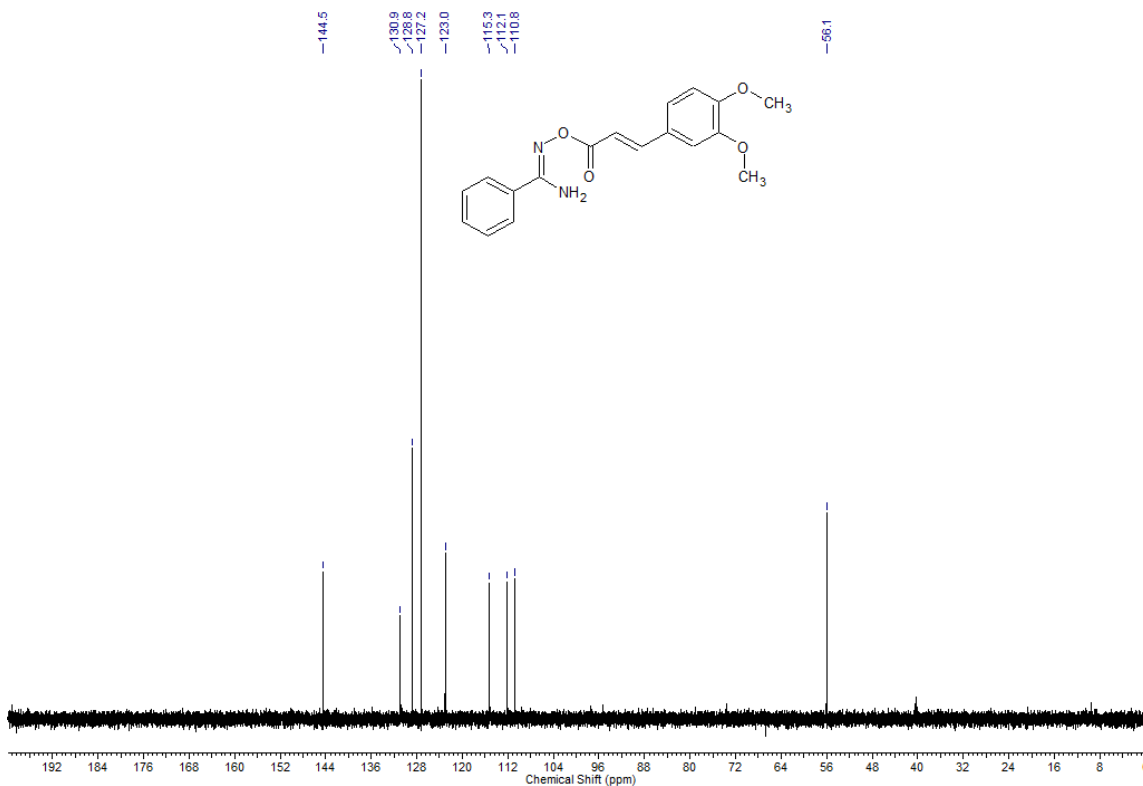


Figure S26. ^1H NMR spectra of *N'*-{[(*E*)-3-(2,3-dimethoxyphenyl)prop-2-enoyl]oxy} benzenecarboximidamide **3j**

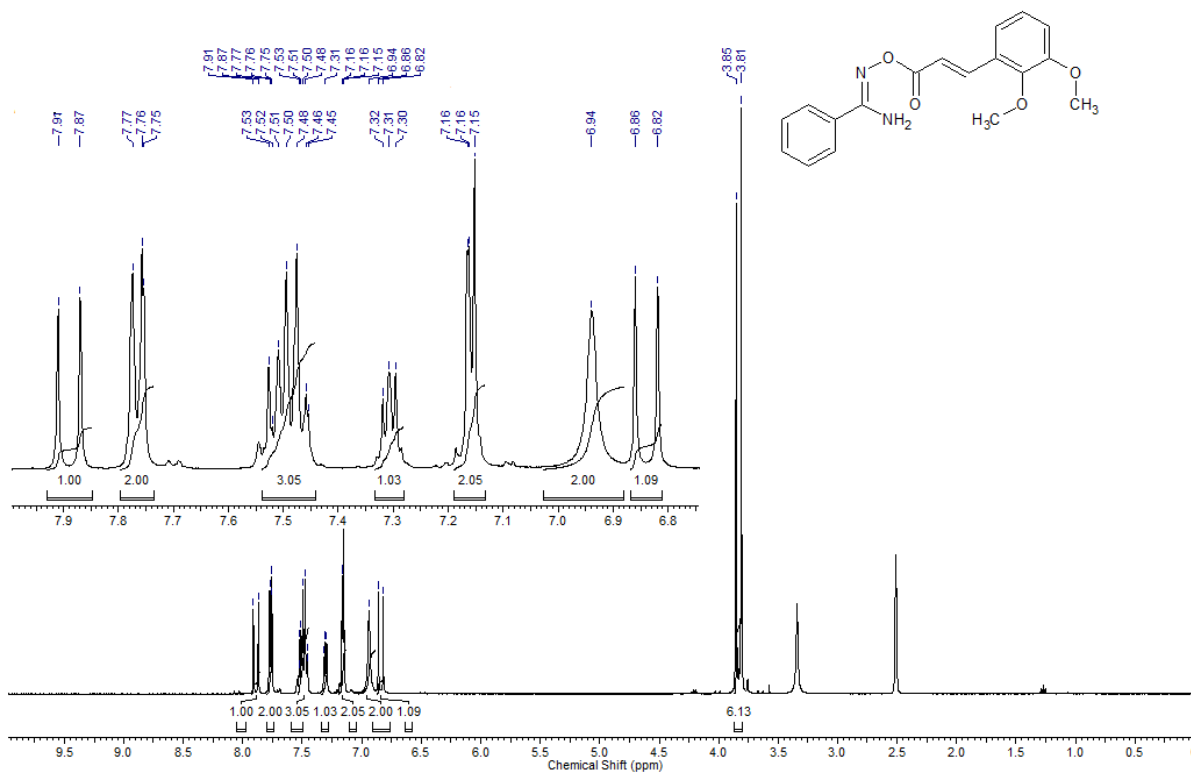


Figure S27. ^{13}C NMR spectra of N' -{[(2E)-3-(2,3-dimethoxyphenyl)prop-2-enoyl]oxy} benzenecarboximidamide **3j**

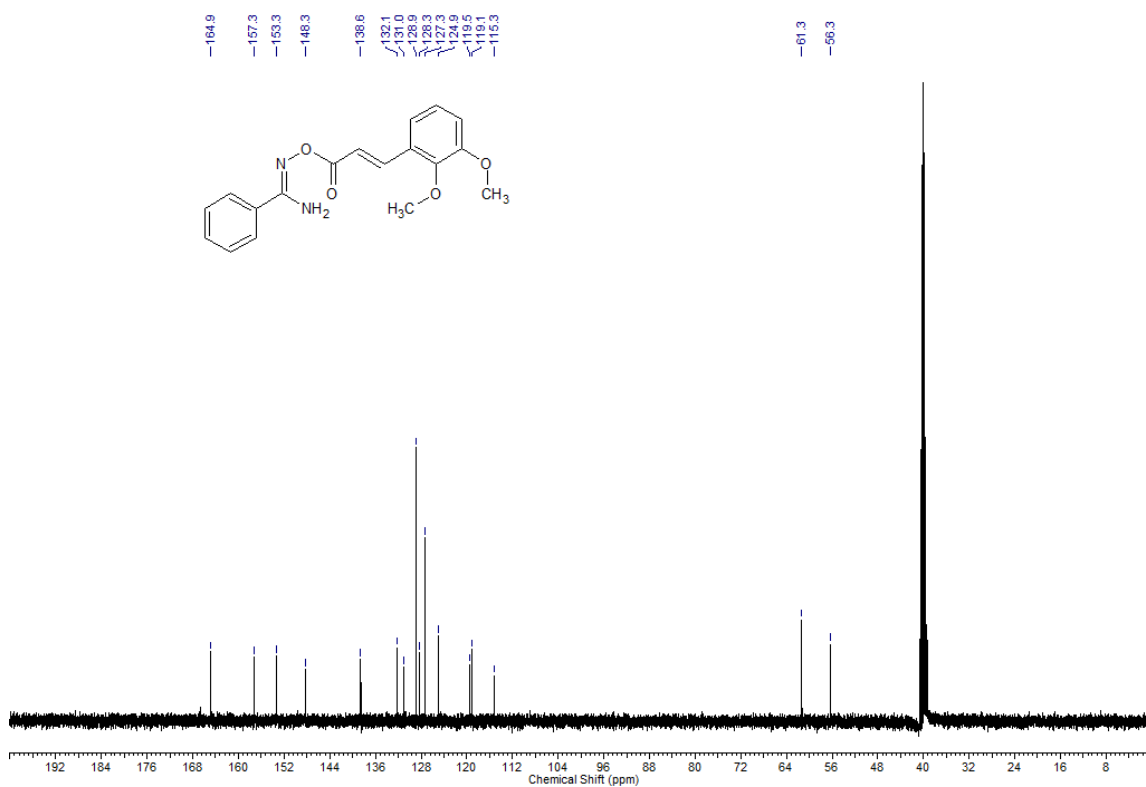


Figure S28. ^{13}C DEPT NMR spectra of N' -{[(2E)-3-(2,3-dimethoxyphenyl)prop-2-enoyl]oxy} benzenecarboximidamide **3j**

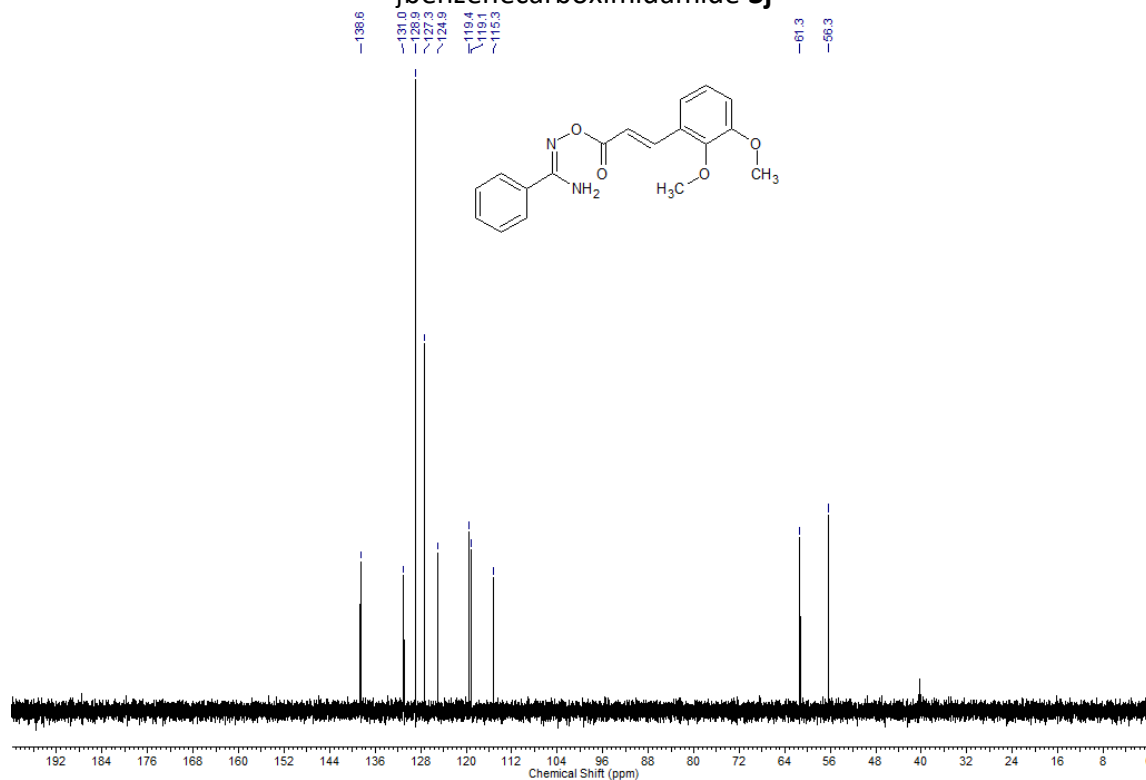


Figure S29. ^1H NMR spectra of 4-methyl- N' -{[($2E$)-3-(thiophen-2-yl)prop-2-enoyl]oxy} benzenecarboximidamide **3k**

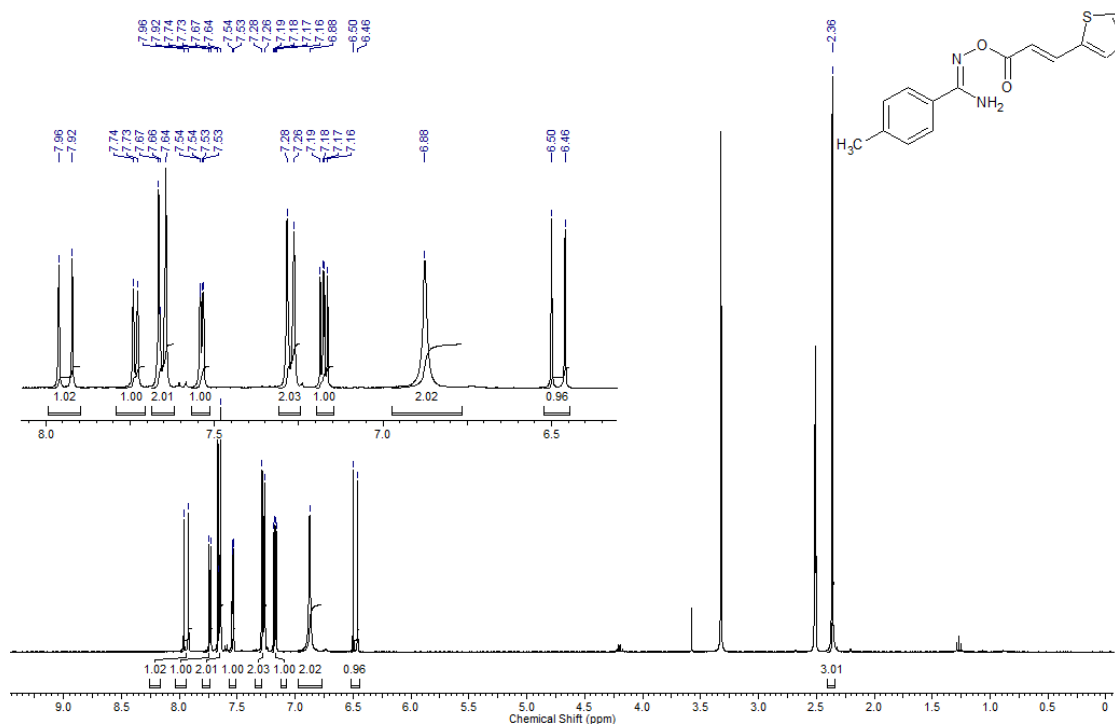


Figure S30. ^{13}C NMR spectra of 4-methyl- N' -{[($2E$)-3-(thiophen-2-yl)prop-2-enoyl]oxy} benzenecarboximidamide **3k**

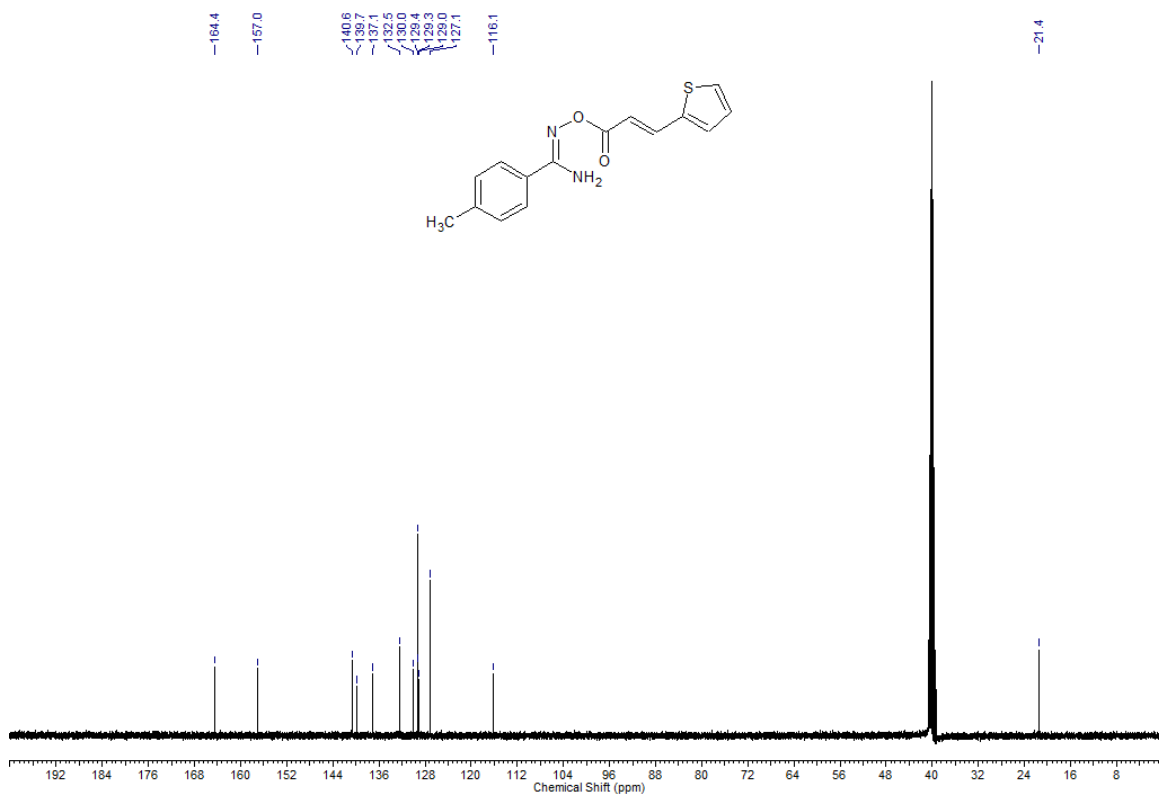


Figure S31. ^{13}C DEPT NMR spectra of 4-methyl- N' -{[($2E$)-3-(thiophen-2-yl)prop-2-enoyl]oxy} benzenecarboximidamide **3k**

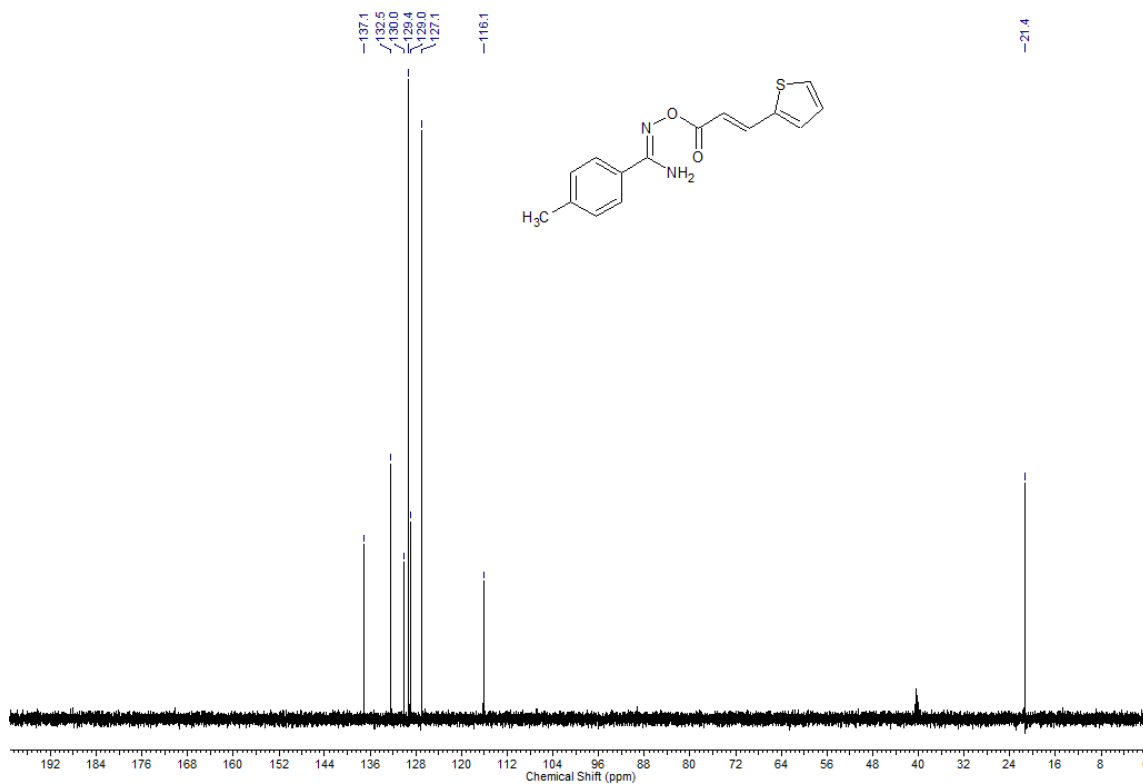


Figure S32. ^1H NMR spectra of 4-chloro- N' -{[($2E$)-3-(furan-2-yl)prop-2-enoyl]oxy} benzenecarboximidamide **3l**

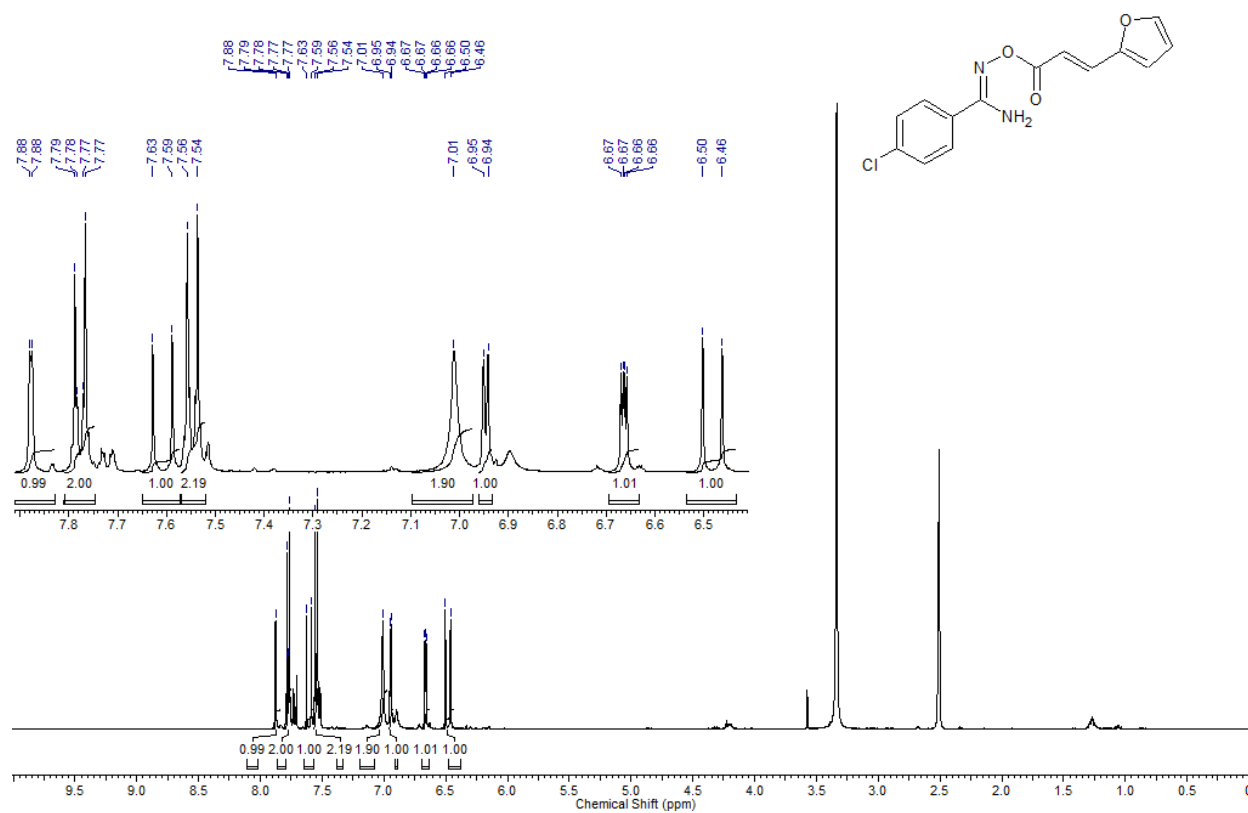


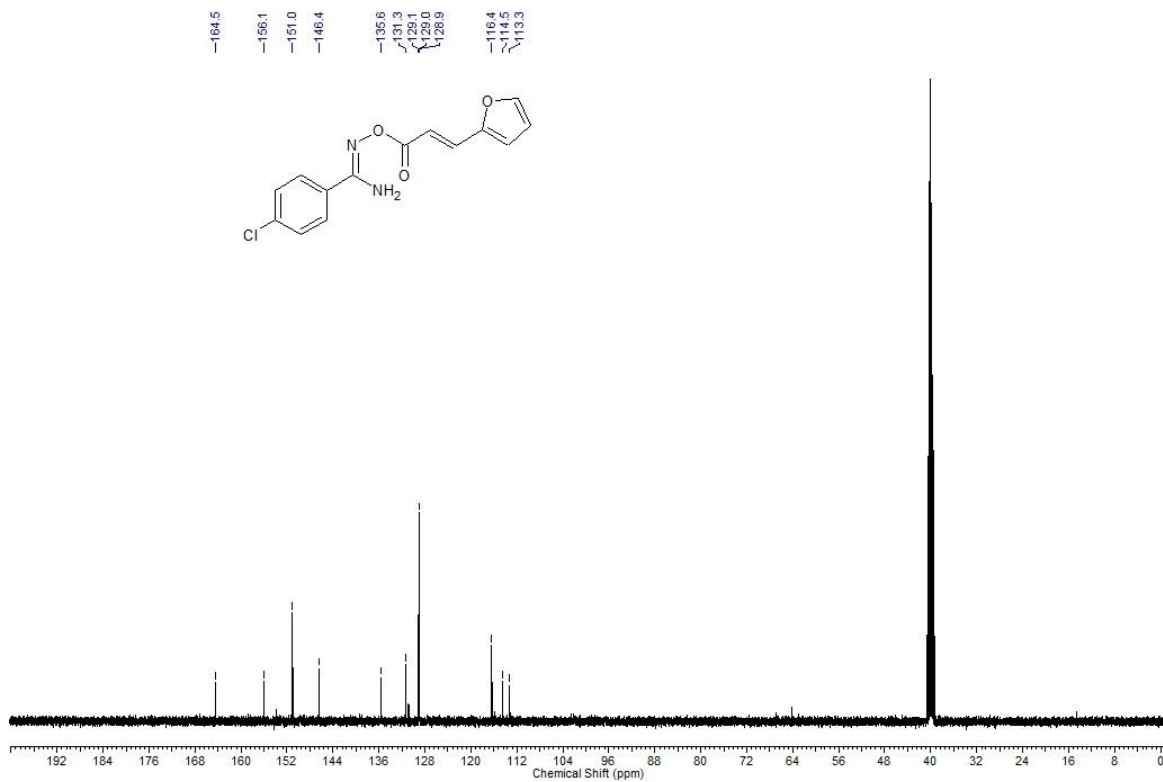
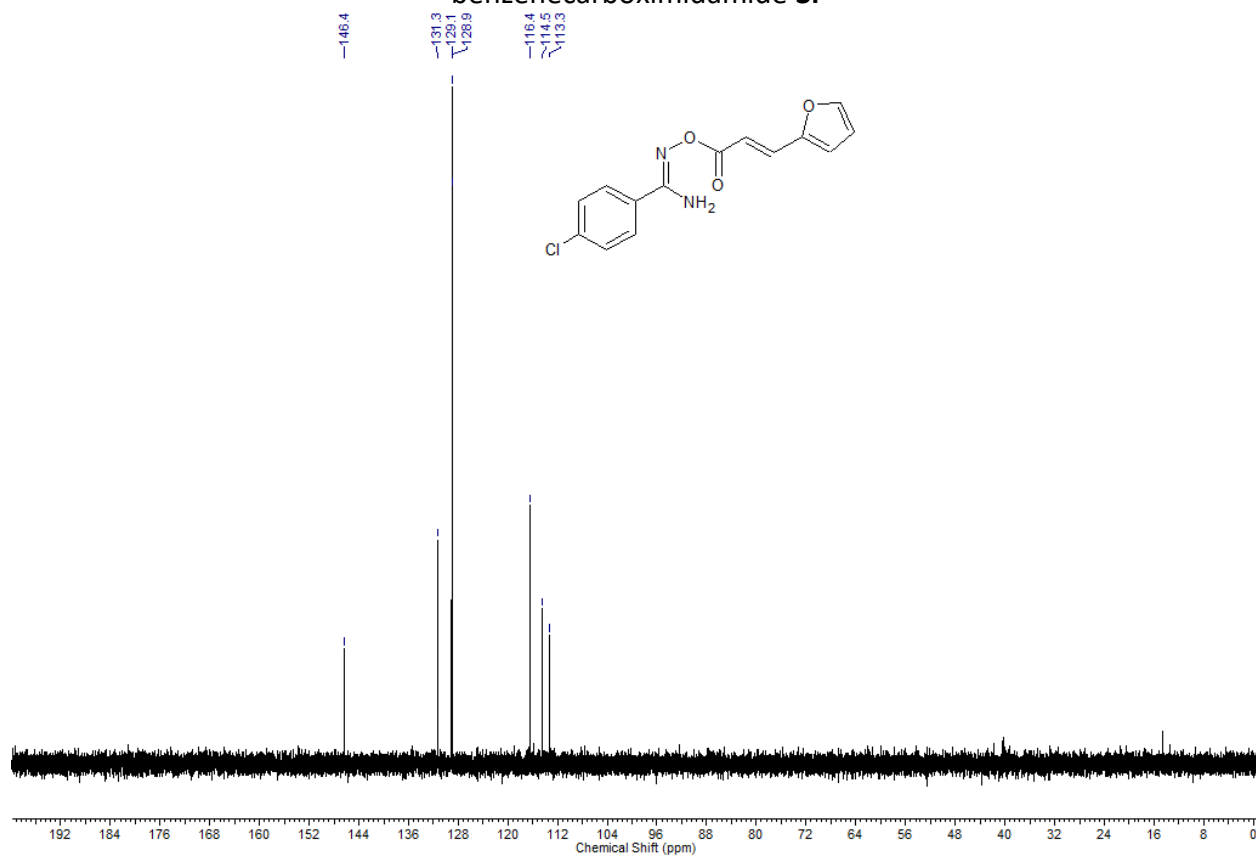
Figure S33. ^{13}C NMR spectra of 4-chloro- N' -{[(2*E*)-3-(furan-2-yl)prop-2-enoyl]oxy} benzenecarboximidamide **3I**Figure S34. ^{13}C DEPT NMR spectra of 4-chloro- N' -{[(2*E*)-3-(furan-2-yl)prop-2-enoyl]oxy} benzenecarboximidamide **3I**

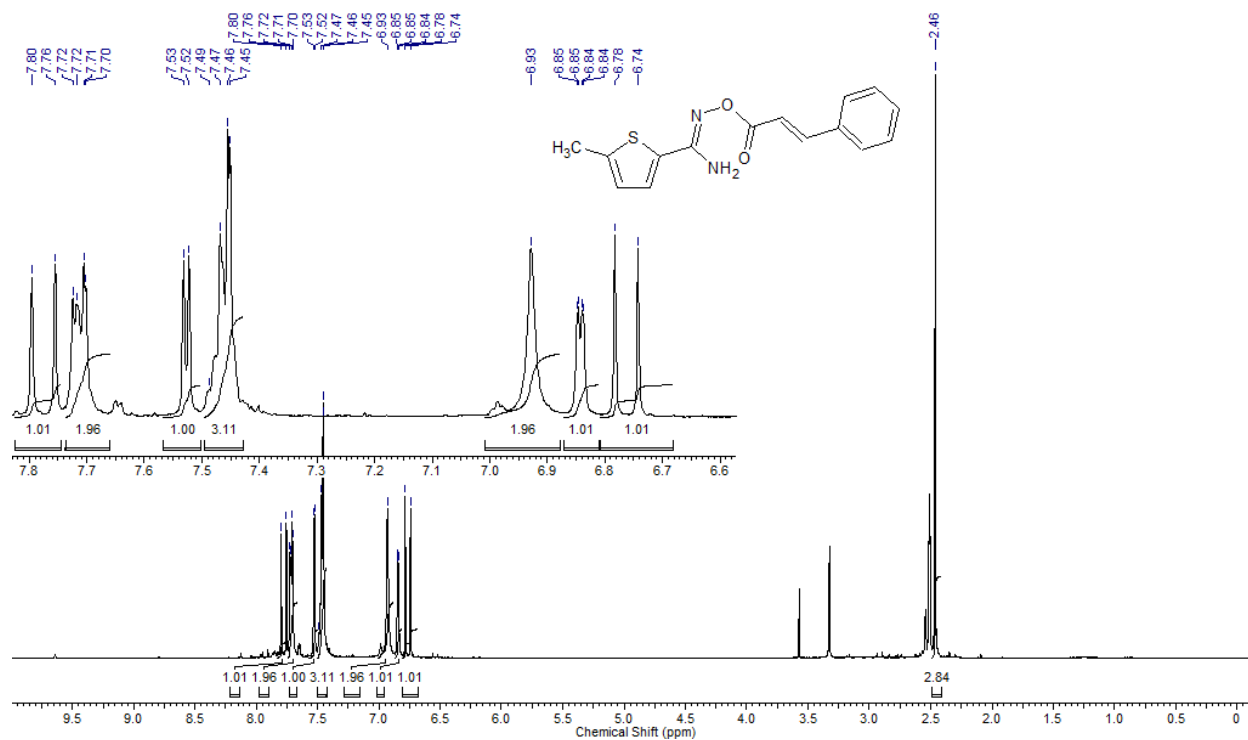
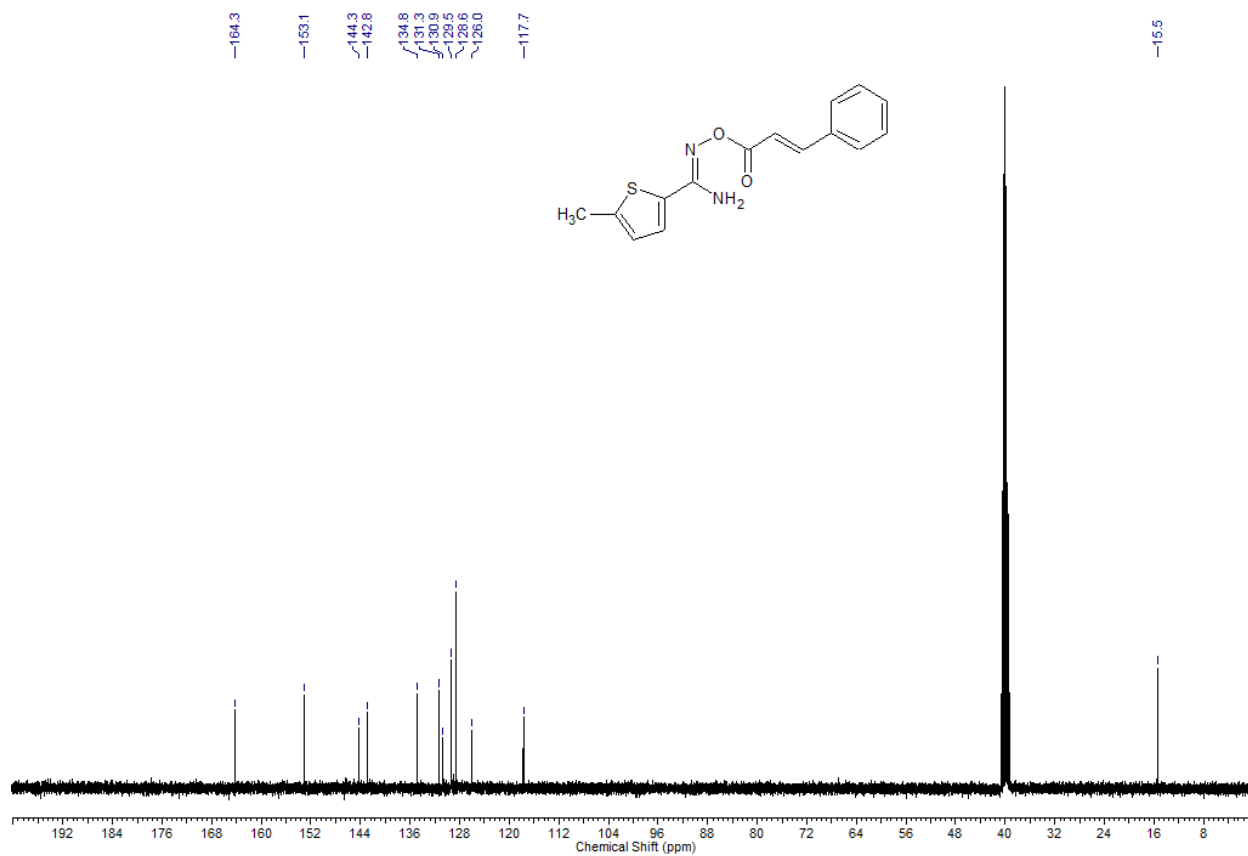
Figure S35. ^1H NMR spectra of 5-methyl- N' -{[(*E*)-3-phenylprop-2-enoyl]oxy}thiophene-2-carboximidamide **3m**Figure S36. ^{13}C NMR spectra of 5-methyl- N' -{[(*E*)-3-phenylprop-2-enoyl]oxy}thiophene-2-carboximidamide **3m**

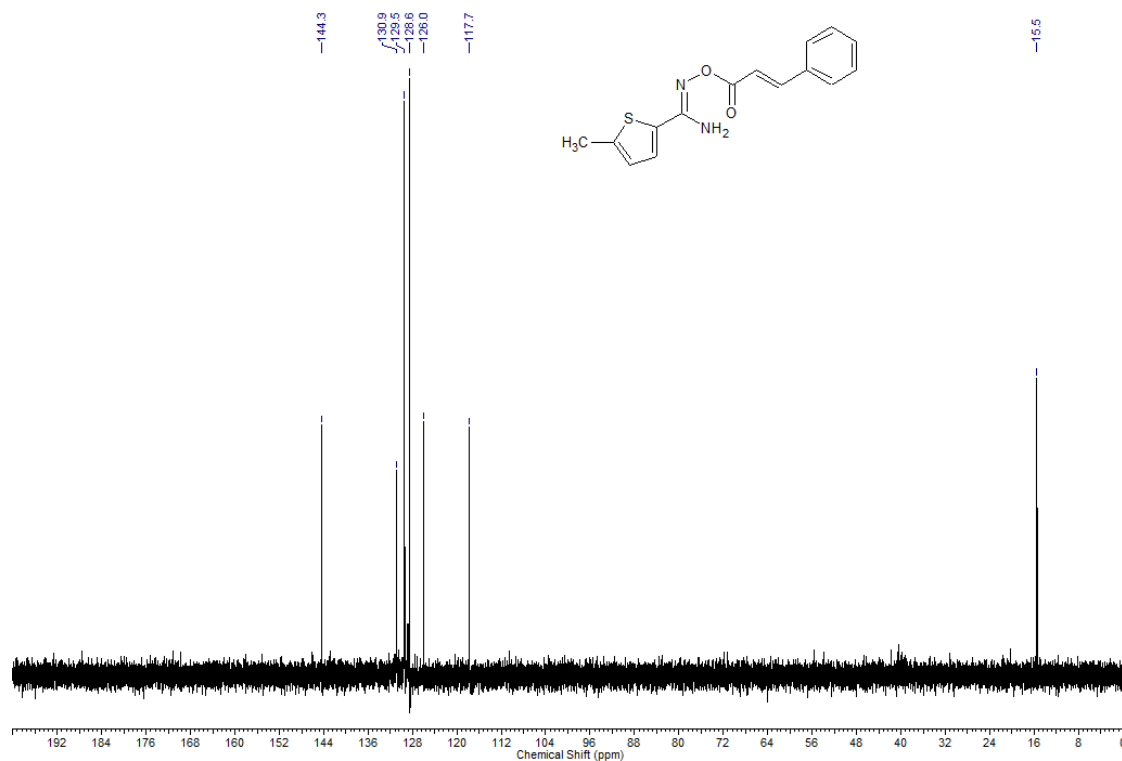
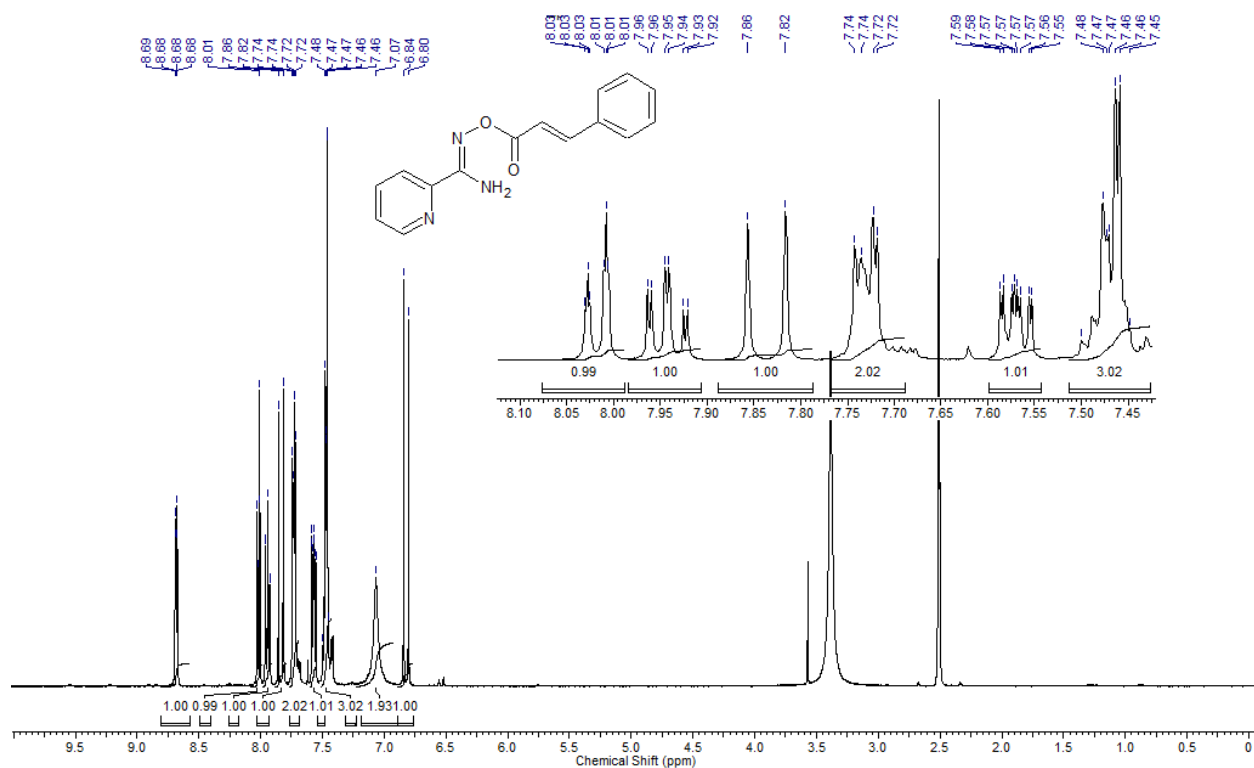
Figure S37. ^{13}C DEPT NMR spectra of 5-methyl-*N'*-[[(*E*)-3-phenylprop-2-enoyl]oxy]thiophene-2-carboximidamide **3m**Figure S38. ^1H NMR spectra of *N'*-[[(*E*)-3-phenylprop-2-enoyl]oxy]pyridine-2-carboximidamide **3n**

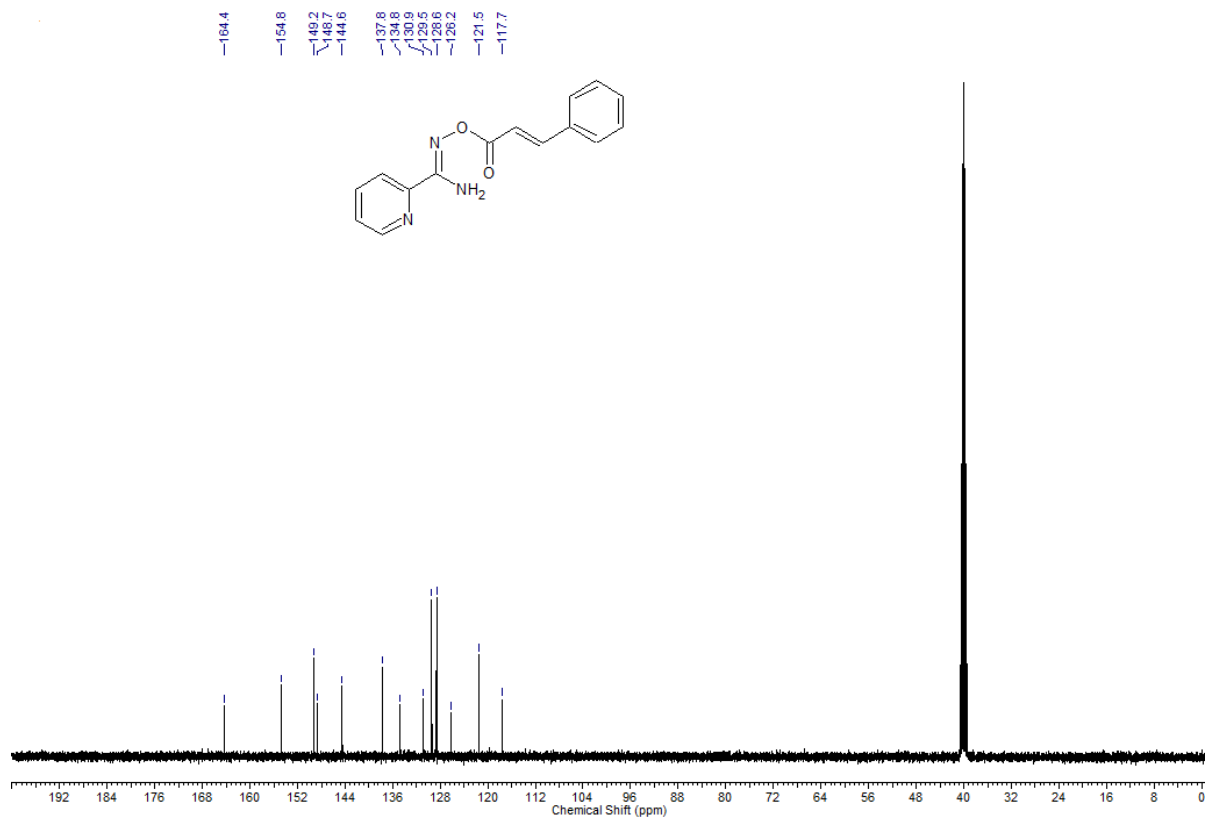
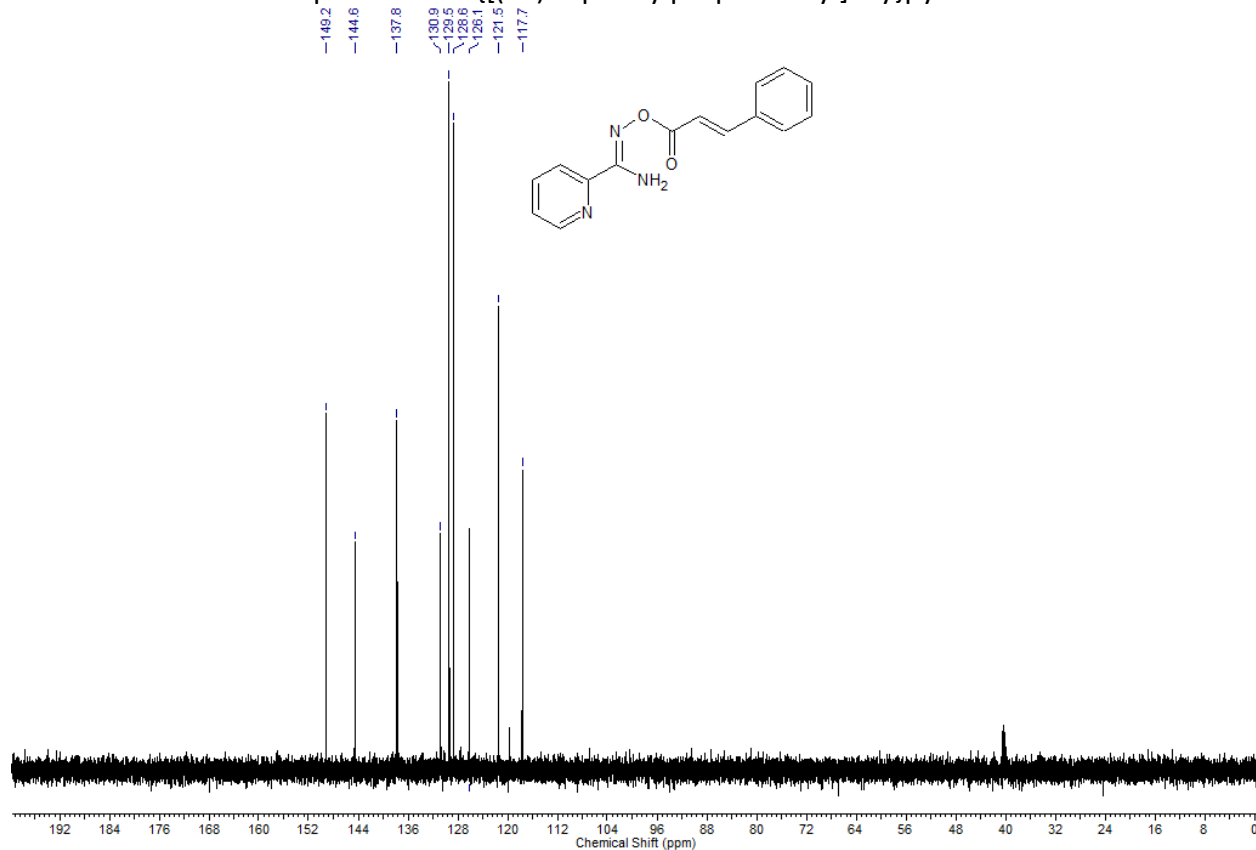
Figure S39. ^{13}C NMR spectra of *N'*-{[(*E*)-3-phenylprop-2-enoyl]oxy}pyridine-2-carboximidamide **3n**Figure S40. ^{13}C DEPT NMR spectra of *N'*-{[(*E*)-3-phenylprop-2-enoyl]oxy}pyridine-2-carboximidamide **3n**

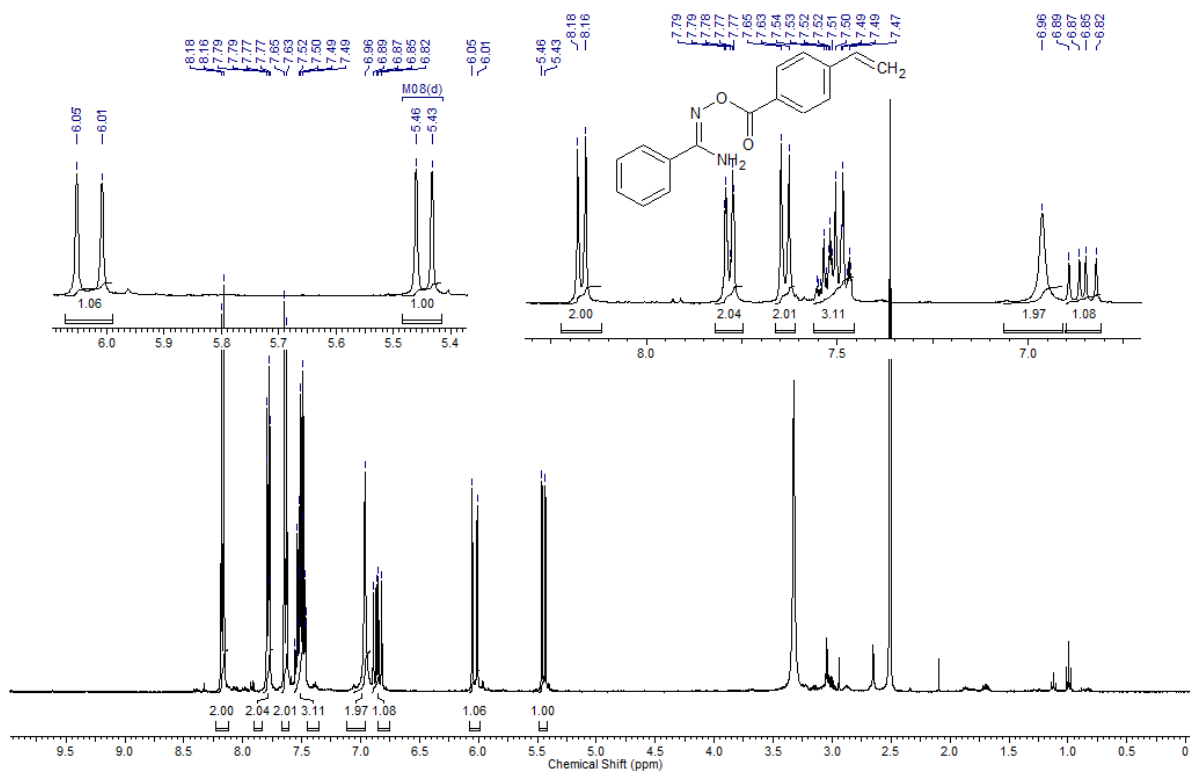
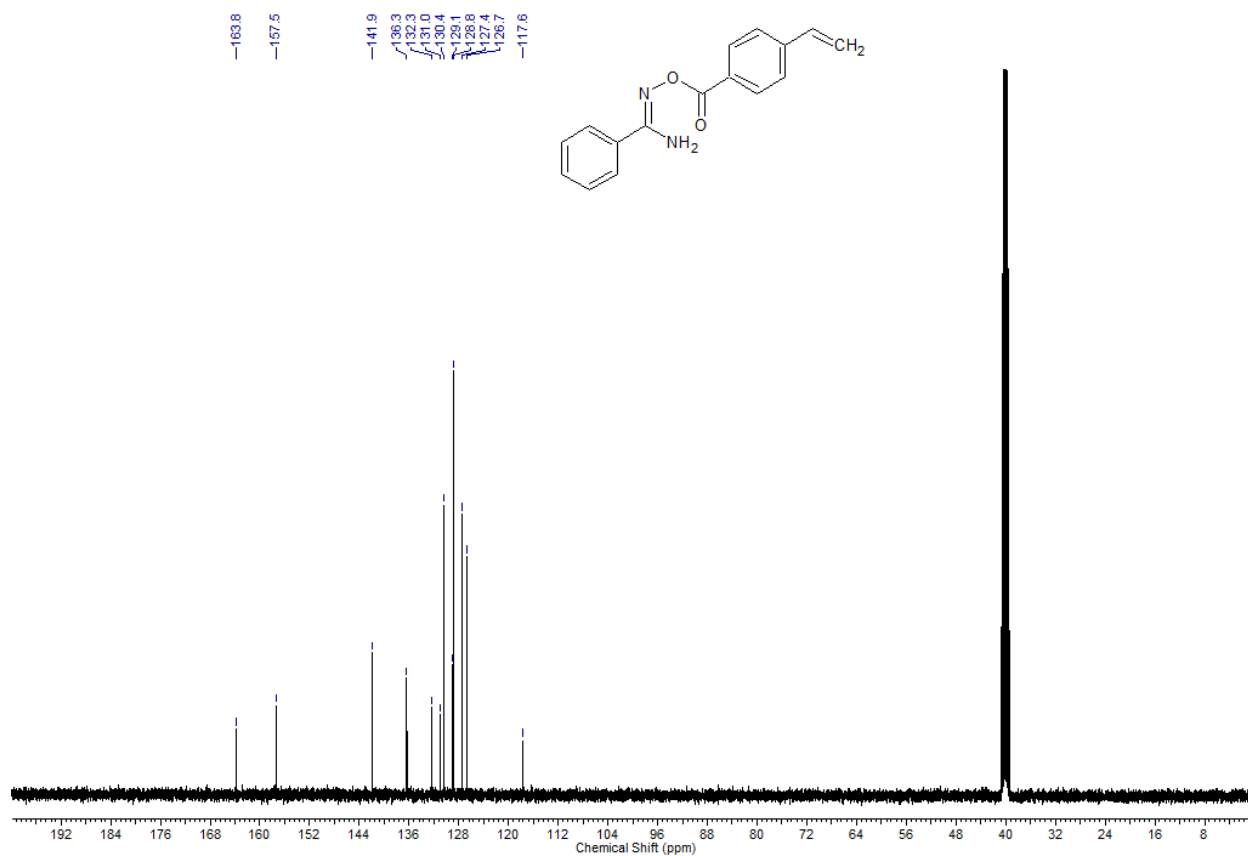
Figure S41. ^1H NMR spectra of N' -[(4-vinylbenzoyl)oxy] benzenecarboximidamide **3o**.Figure S42. ^{13}C NMR spectra of N' -[(4-vinylbenzoyl)oxy] benzenecarboximidamide **3o**.

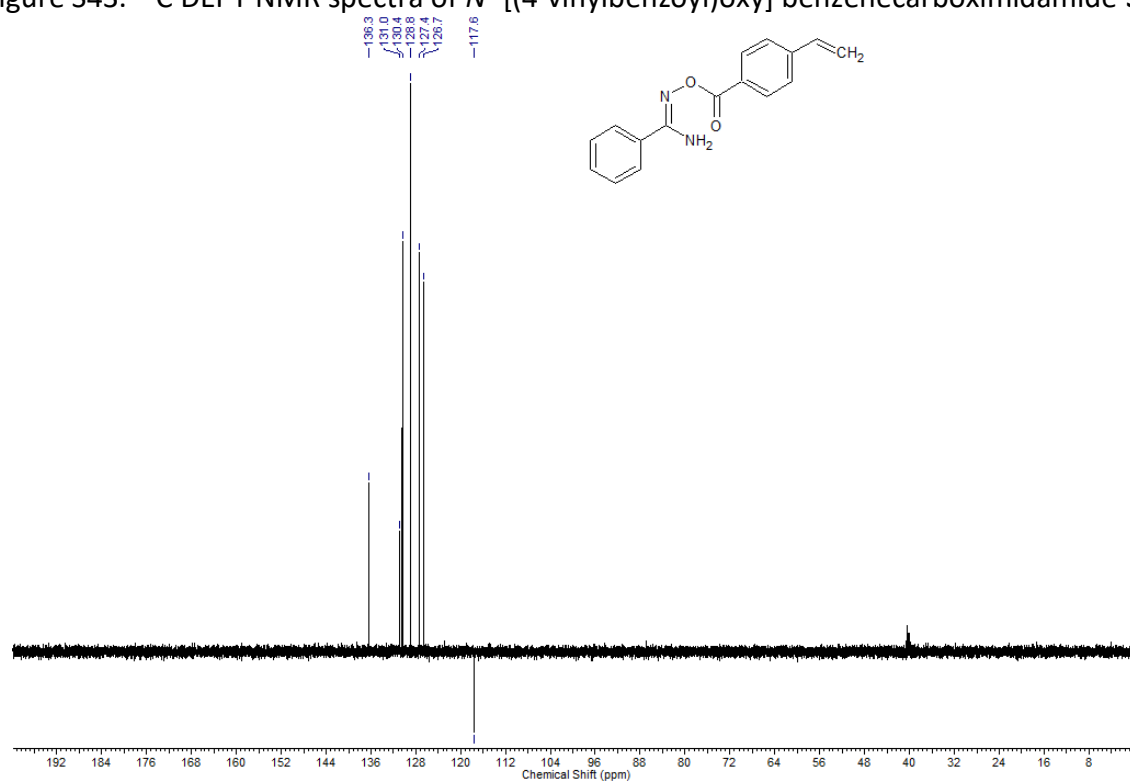
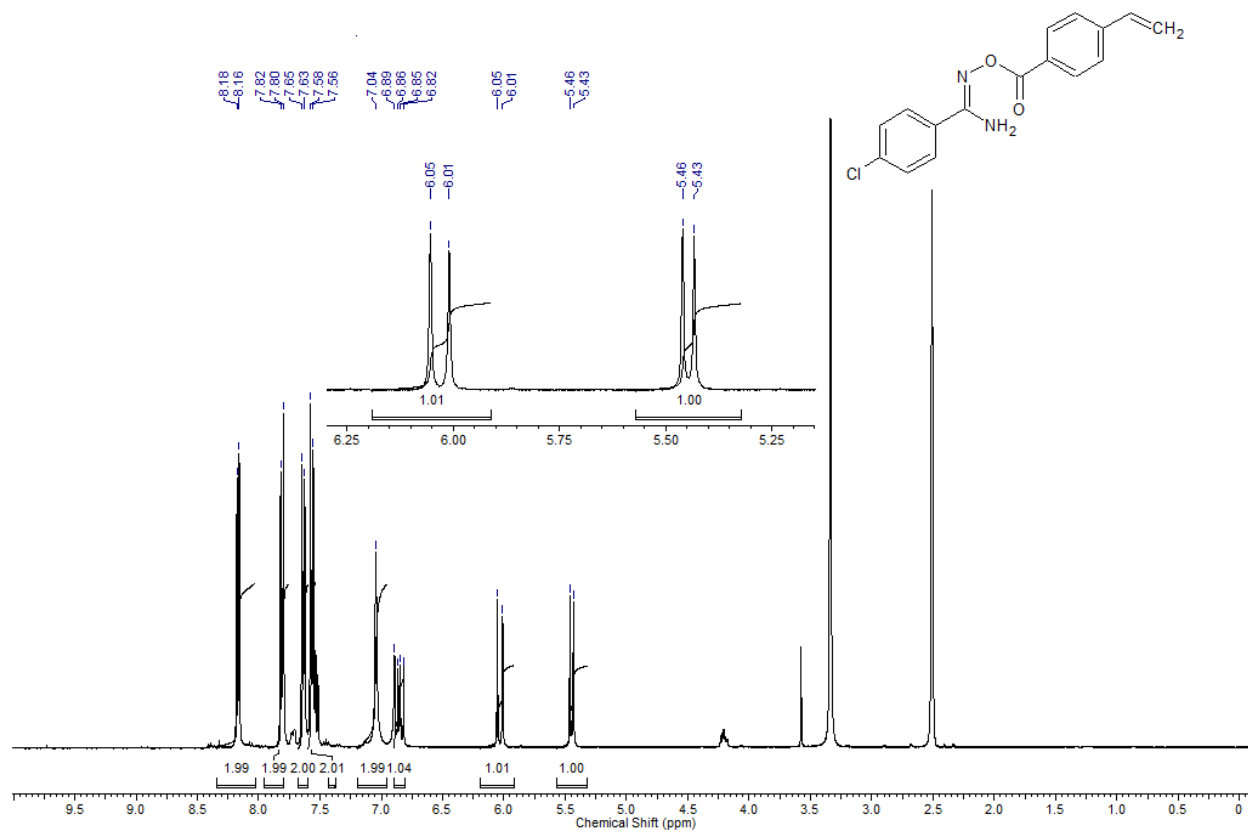
Figure S43. ^{13}C DEPT NMR spectra of *N'*-[(4-vinylbenzoyl)oxy] benzenecarboximidamide **3o**.Figure S44. ^1H NMR spectra of 4-chloro-*N'*-[(4-vinylbenzoyl)oxy] benzenecarboximidamide **3p**

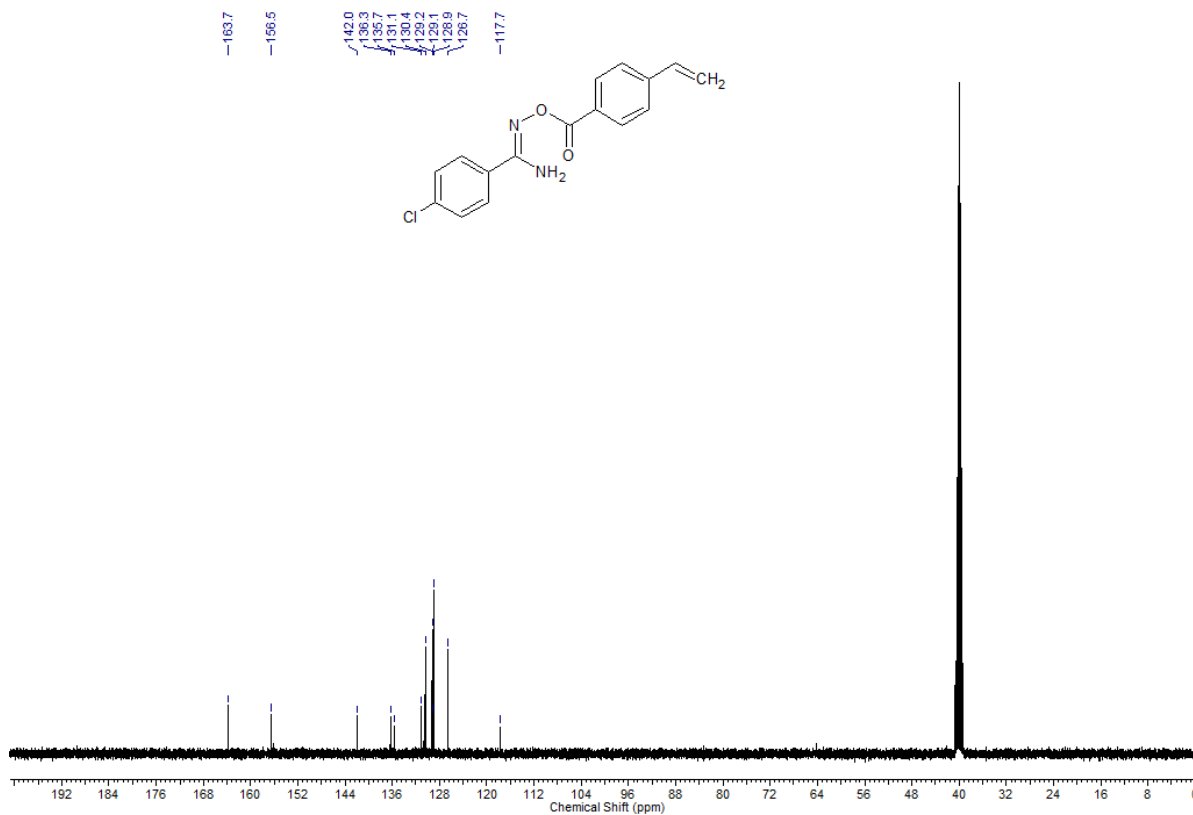
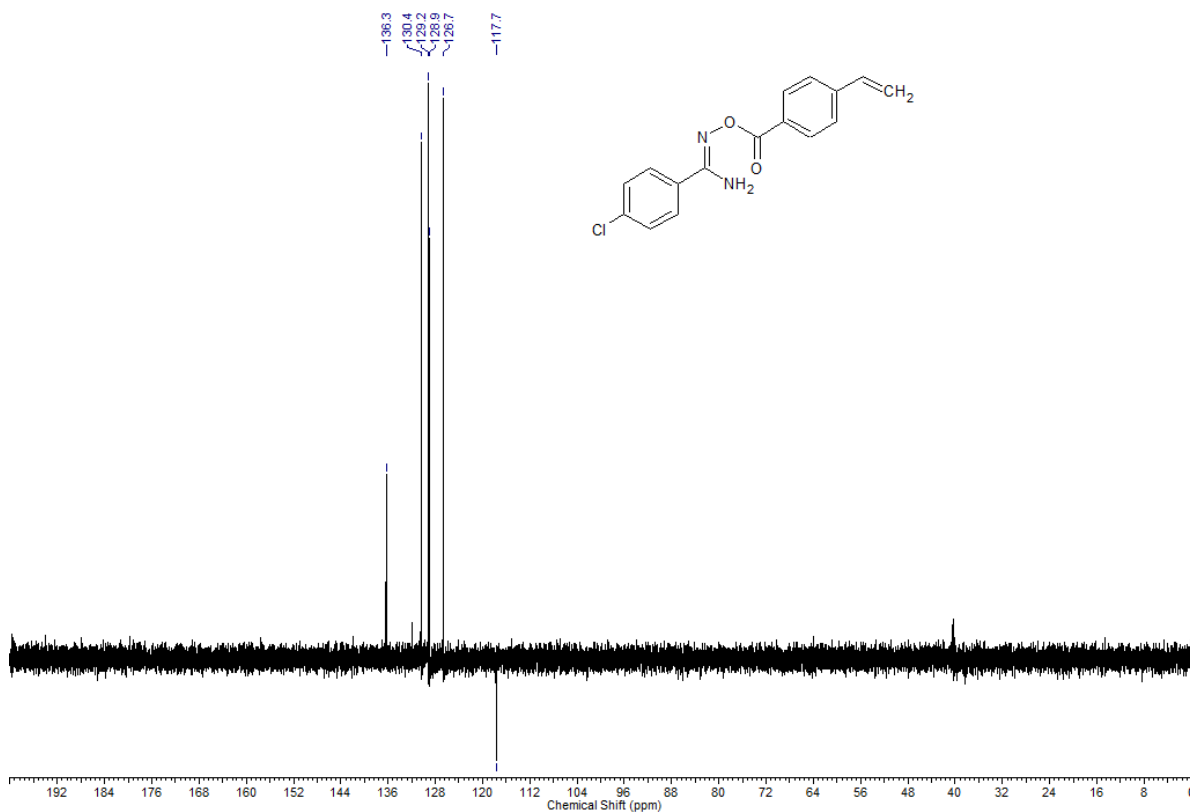
Figure S45. ^{13}C NMR spectra of 4-chloro-*N'*-[(4-vinylbenzoyl)oxy] benzenecarboximidamide **3p**Figure S46. ^{13}C DEPT NMR spectra of 4-chloro-*N'*-[(4-vinylbenzoyl)oxy] benzenecarboximidamide **3p**

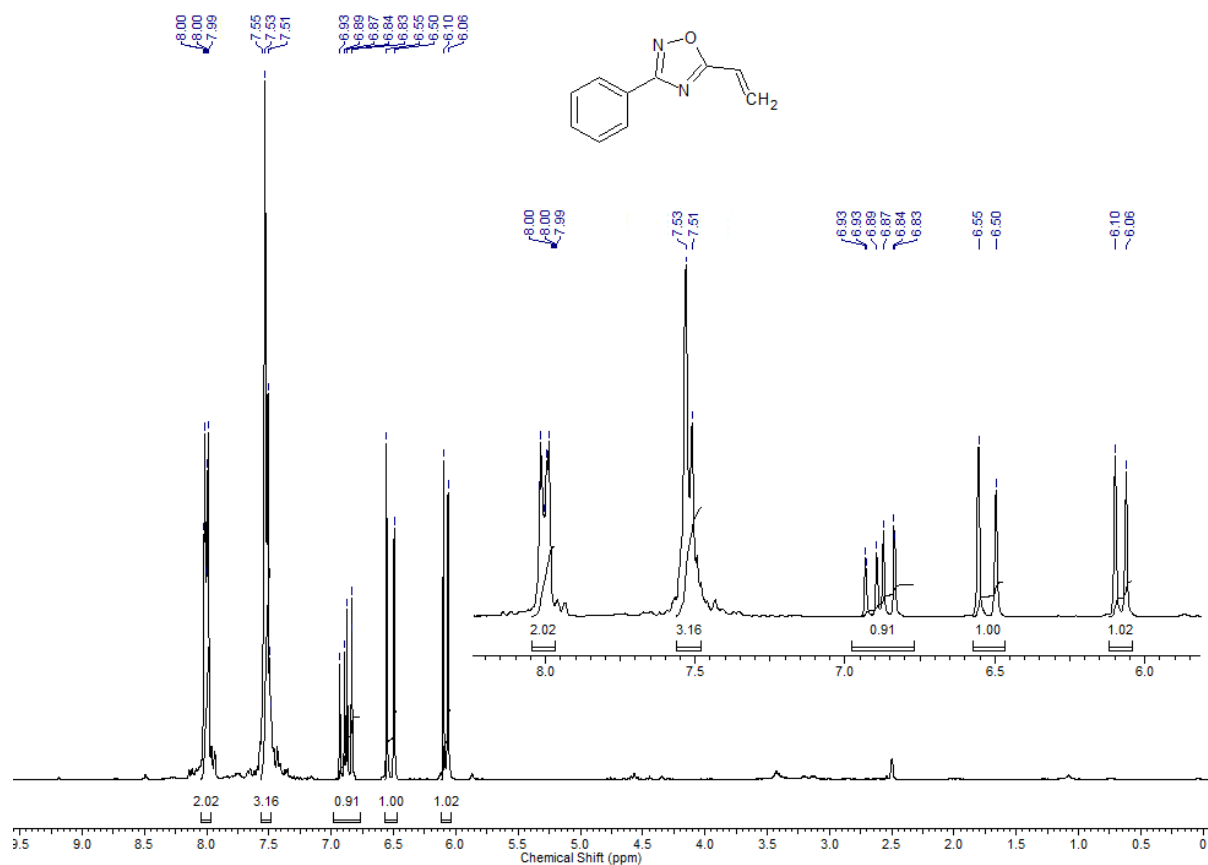
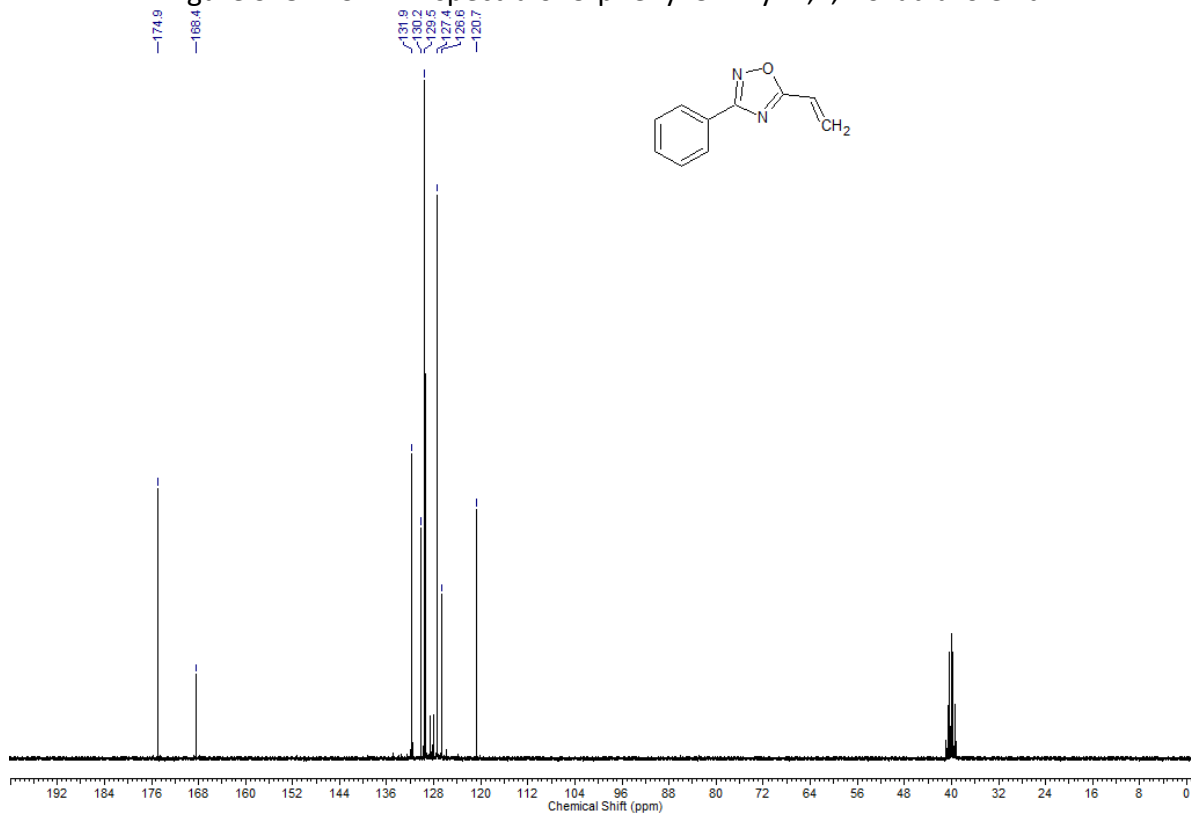
Figure S47. ^1H NMR spectra of 3-phenyl-5-vinyl-1,2,4-oxadiazole **4a**Figure S48. ^{13}C NMR spectra of 3-phenyl-5-vinyl-1,2,4-oxadiazole **4a**

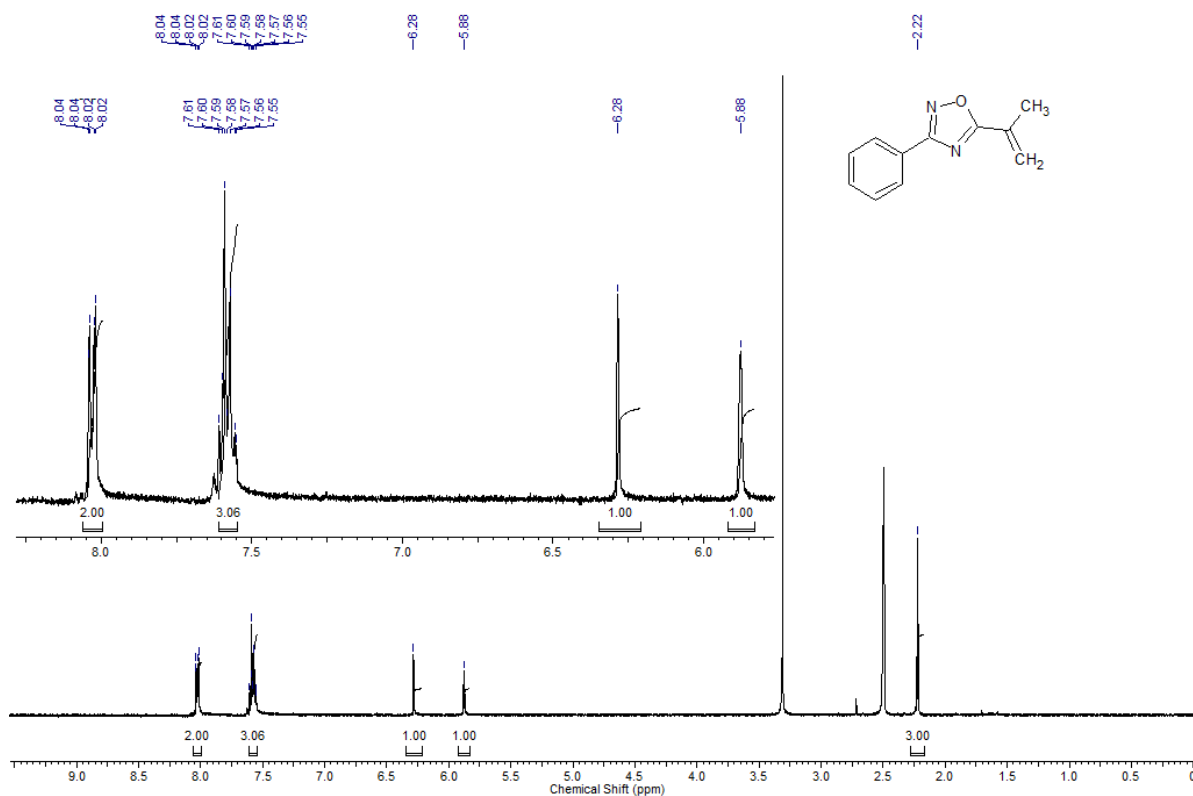
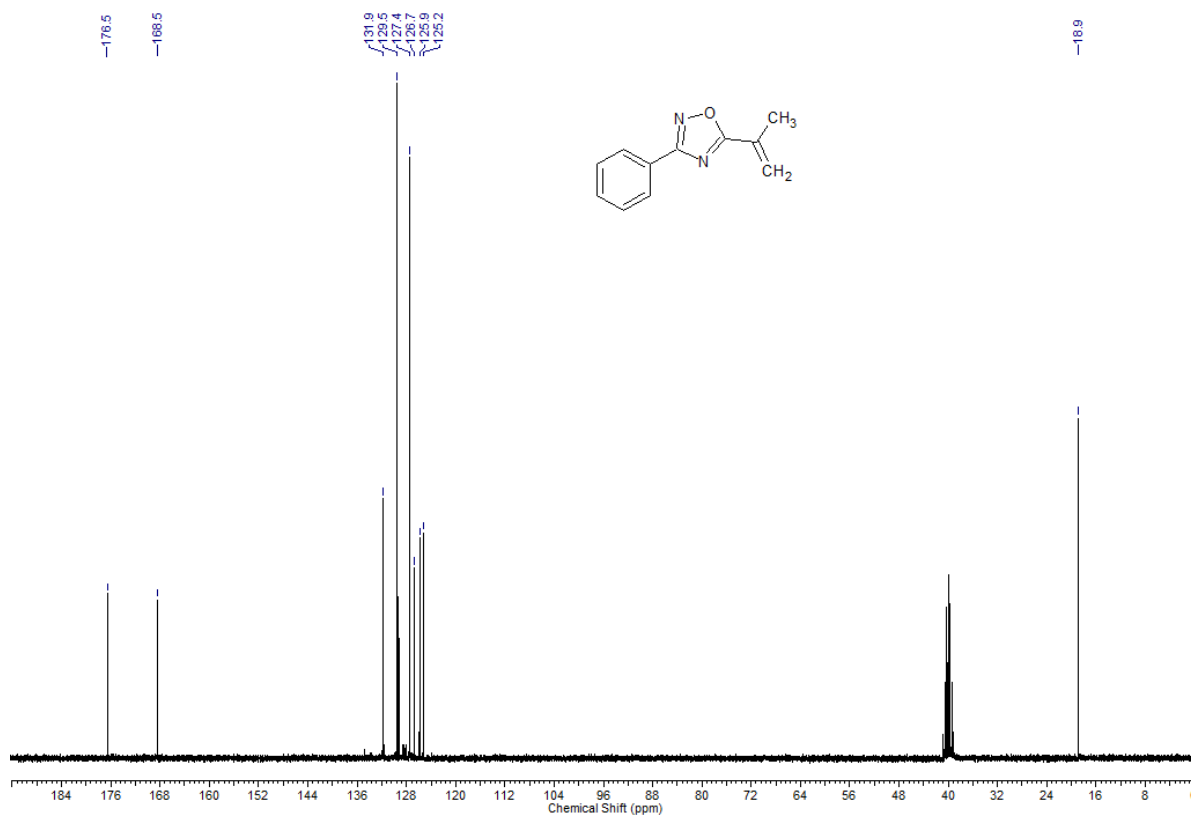
Figure S49. ^1H NMR spectra of 3-phenyl-5-(prop-1-en-2-yl)-1,2,4-oxadiazole **4b**Figure S50. ^{13}C NMR spectra of 3-phenyl-5-(prop-1-en-2-yl)-1,2,4-oxadiazole **4b**

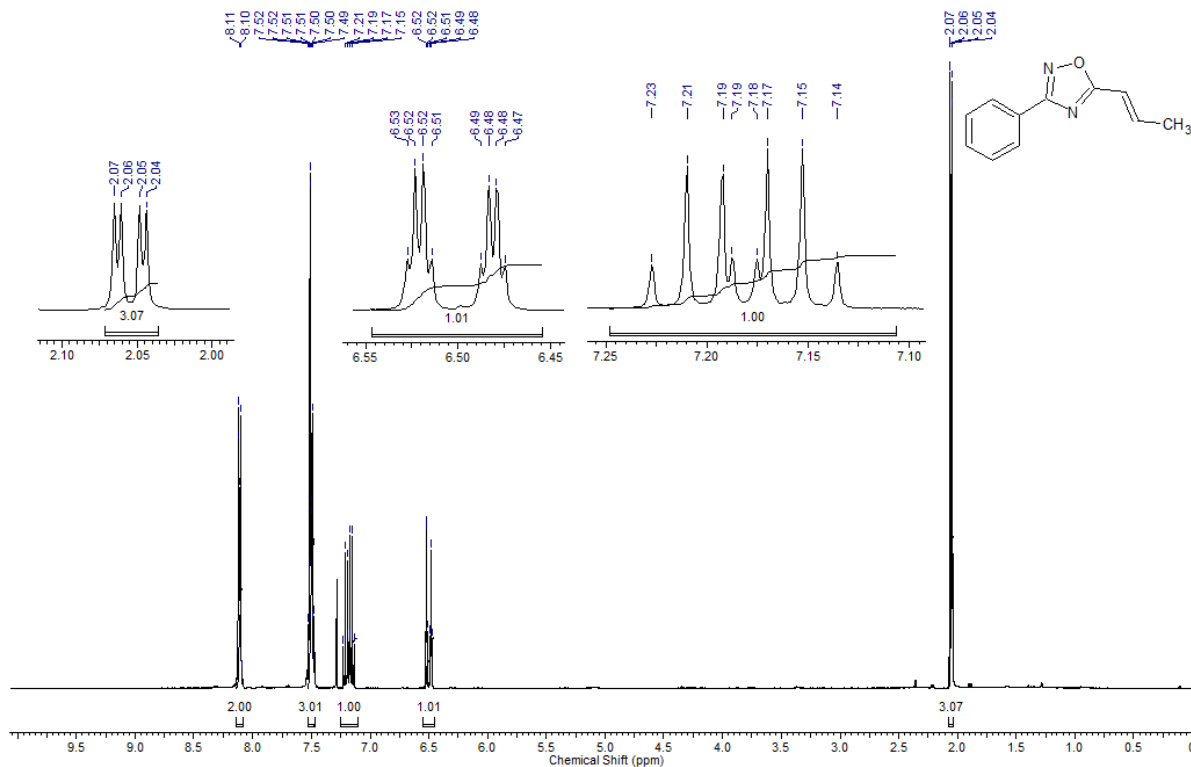
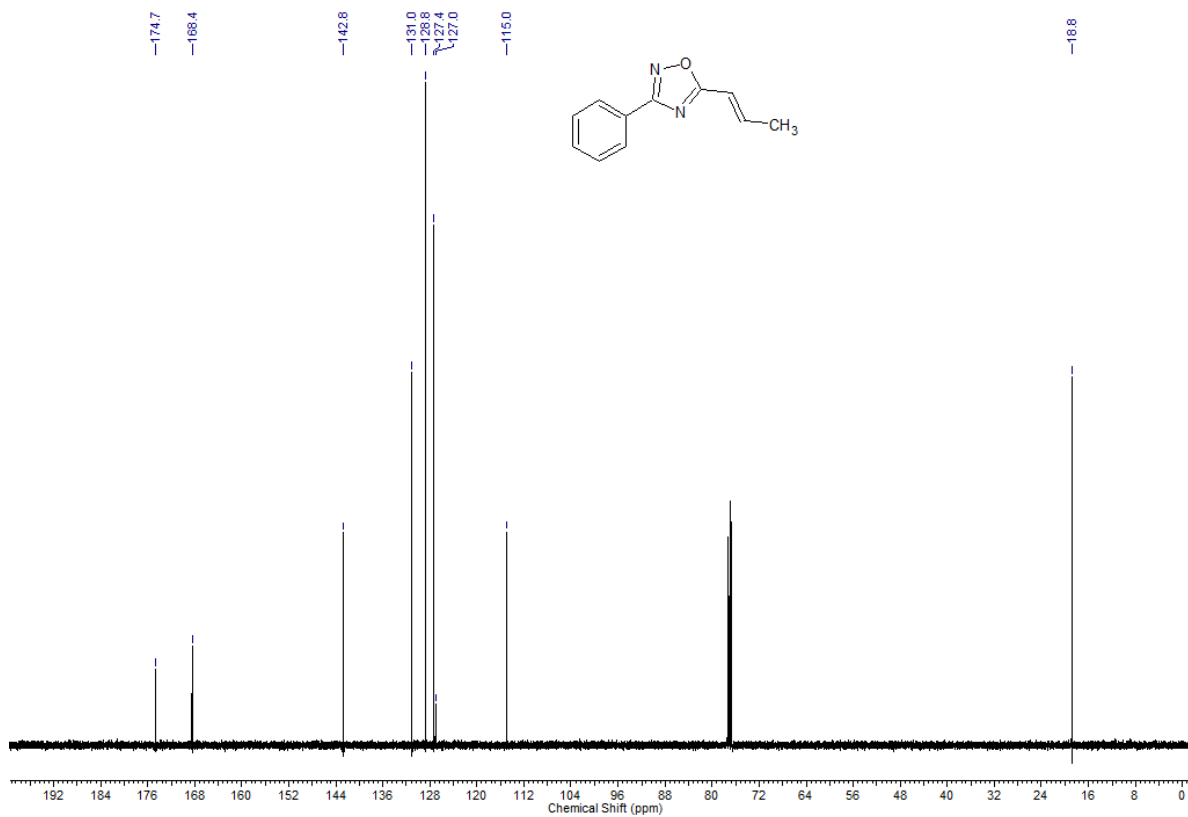
Figure S51. ^1H NMR spectra of (*E*)-3-phenyl-5-(prop-1-en-1-yl)-1,2,4-oxadiazole **4c**Figure S52. ^{13}C NMR spectra of (*E*)-3-phenyl-5-(prop-1-en-1-yl)-1,2,4-oxadiazole **4c**

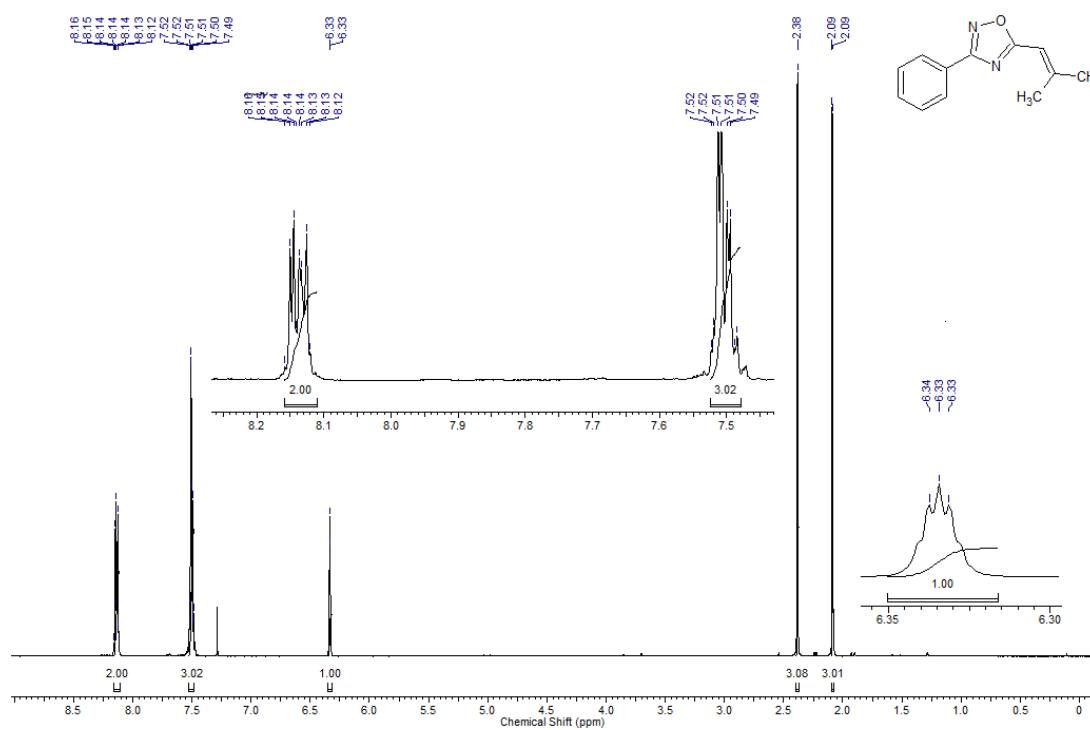
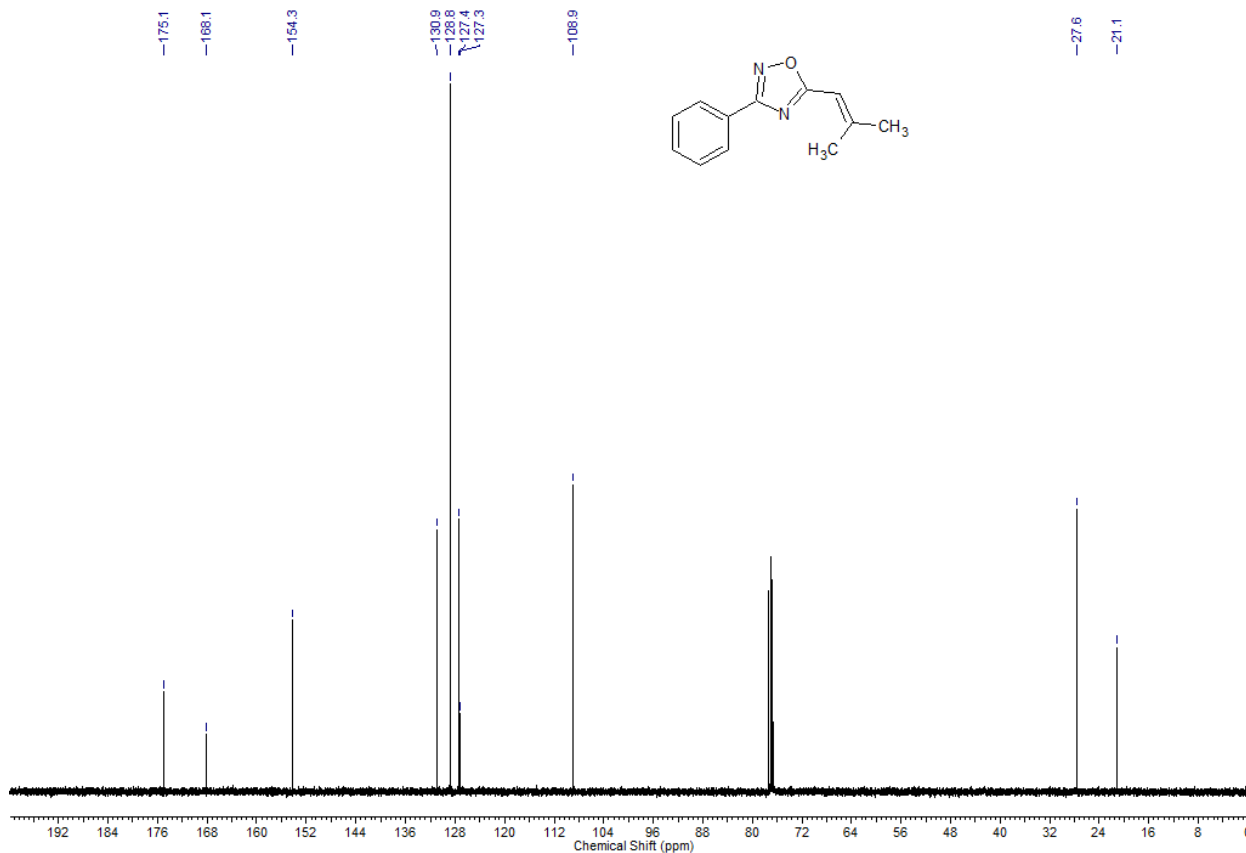
Figure S53. ^1H NMR spectra of 5-(2-methylprop-1-enyl)-3-phenyl-1,2,4-oxadiazole **4d**Figure S54. ^{13}C NMR spectra of 5-(2-methylprop-1-enyl)-3-phenyl-1,2,4-oxadiazole **4d**

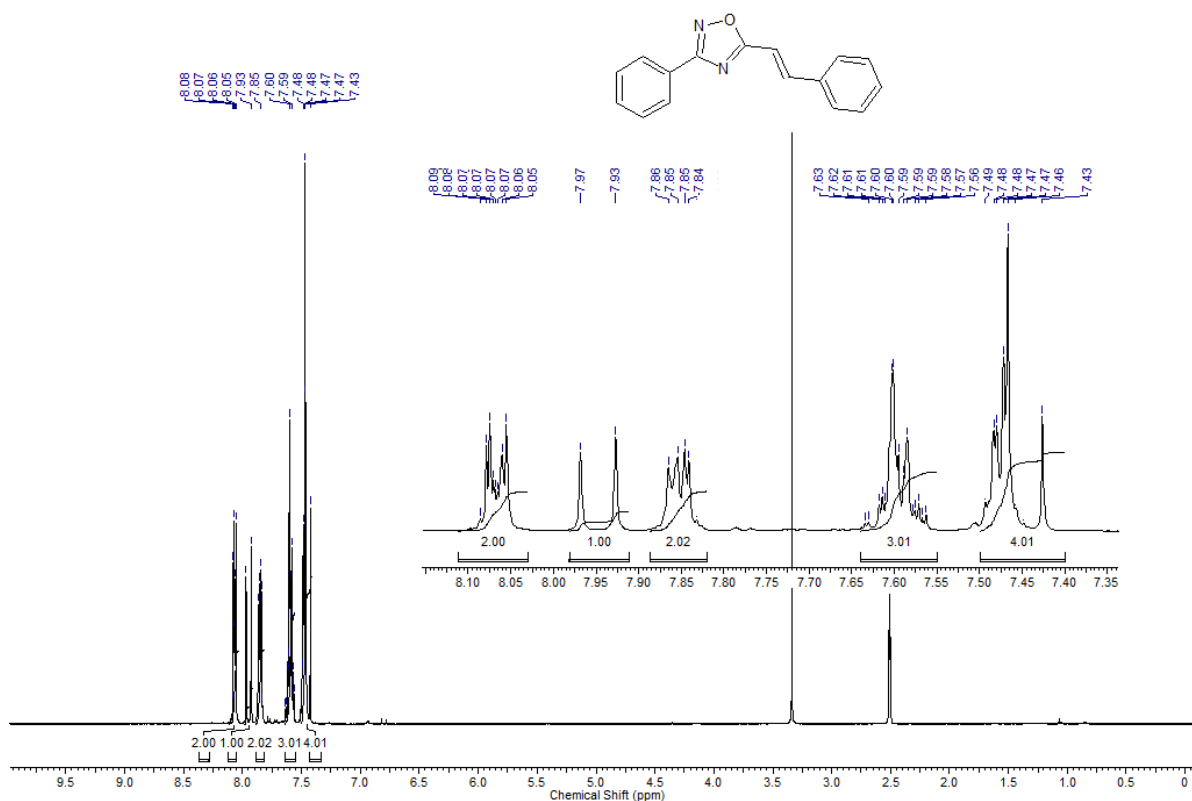
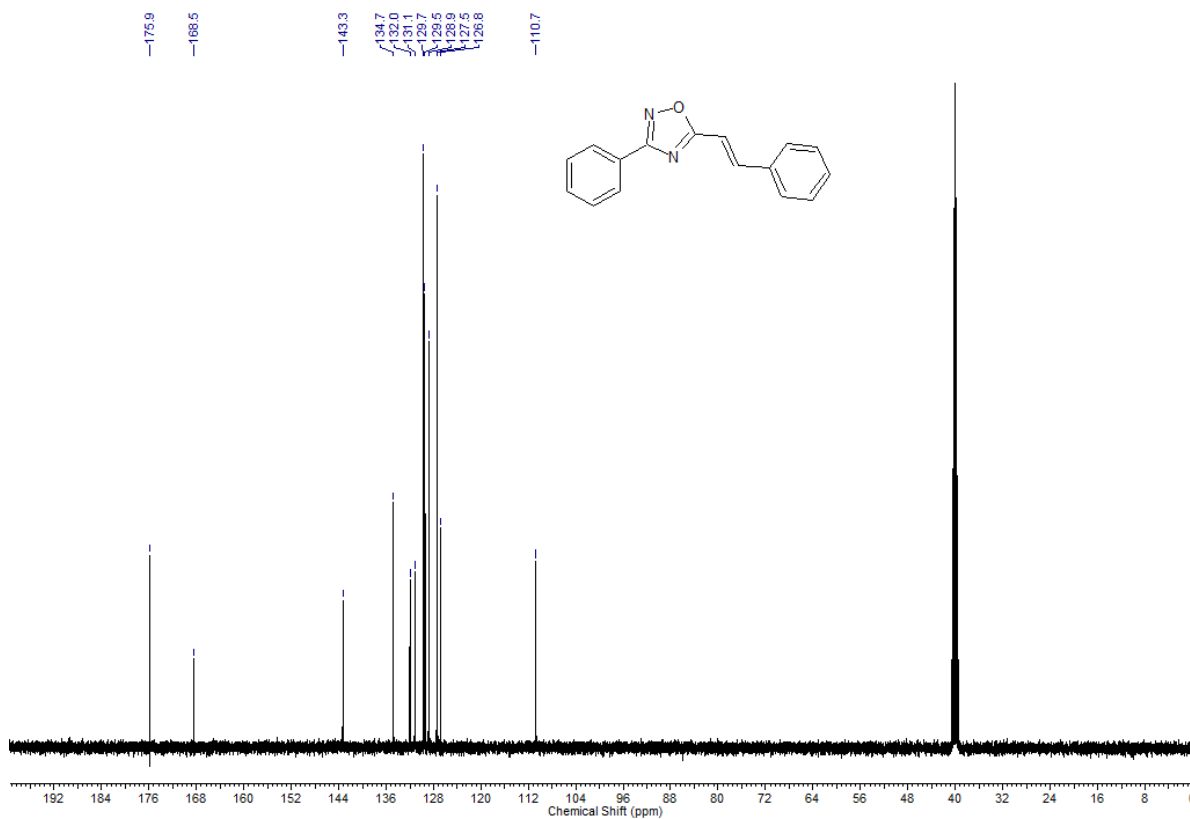
Figure S55. ^1H NMR spectra of (*E*)-3-phenyl-5-(2-phenylethenyl)-1,2,4-oxadiazole **4e**Figure S56. ^{13}C NMR spectra of (*E*)-3-phenyl-5-(2-phenylethenyl)-1,2,4-oxadiazole **4e**

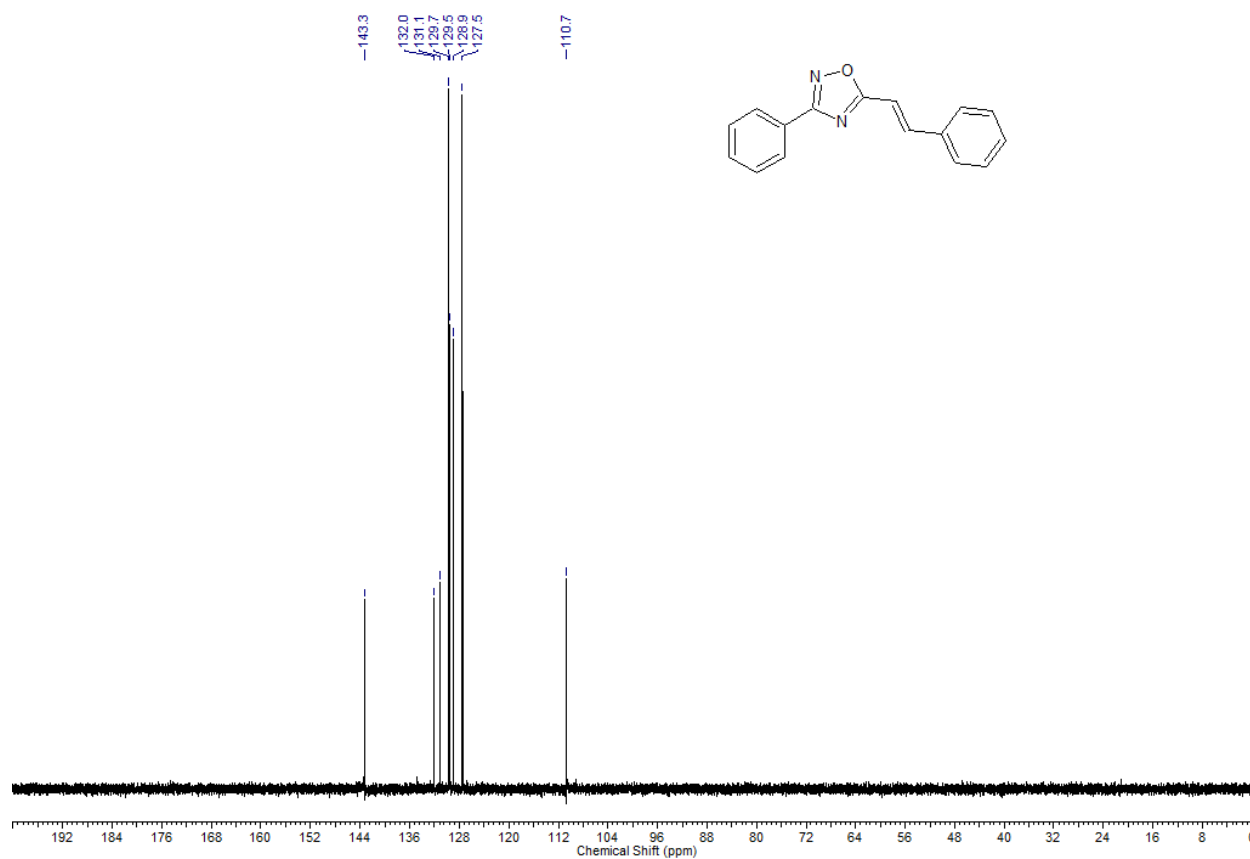
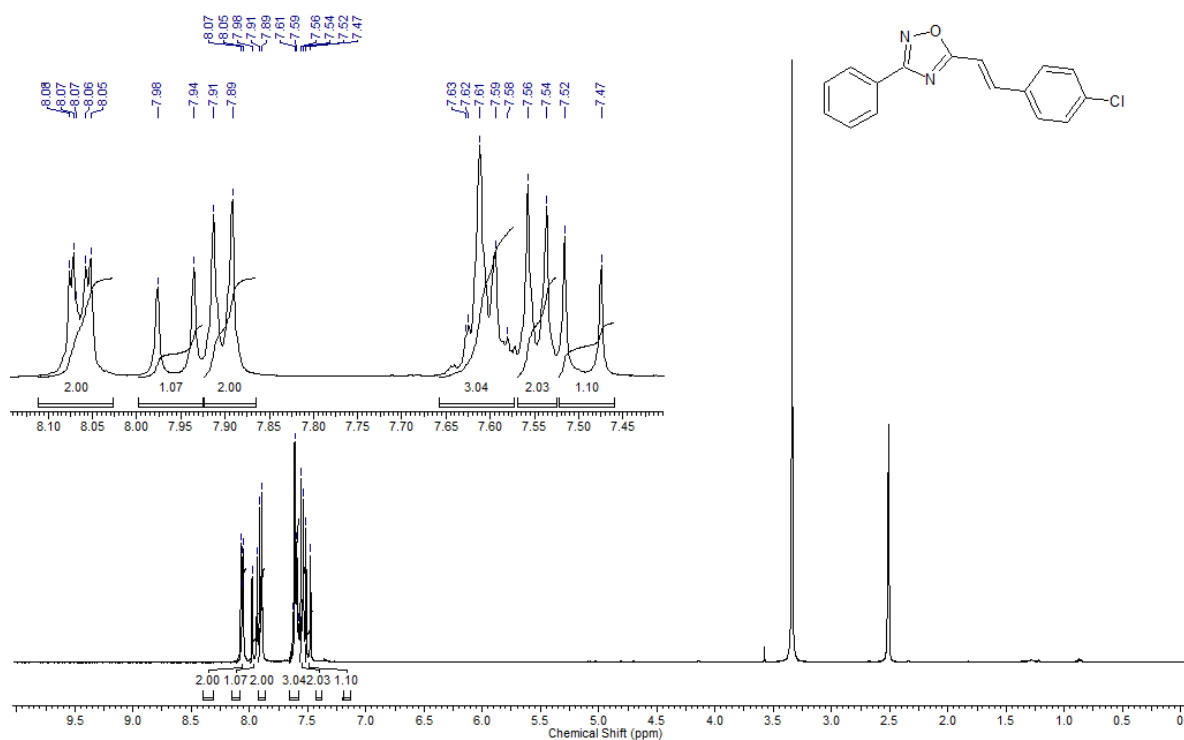
Figure S57. ^{13}C DEPT NMR spectra of (*E*)-3-phenyl-5-(2-phenylethenyl)-1,2,4-oxadiazole **4e**Figure S58. ^1H NMR spectra of 5-[(*E*)-2-(4-chlorophenyl)ethenyl]-3-phenyl-1,2,4-oxadiazole **4f**

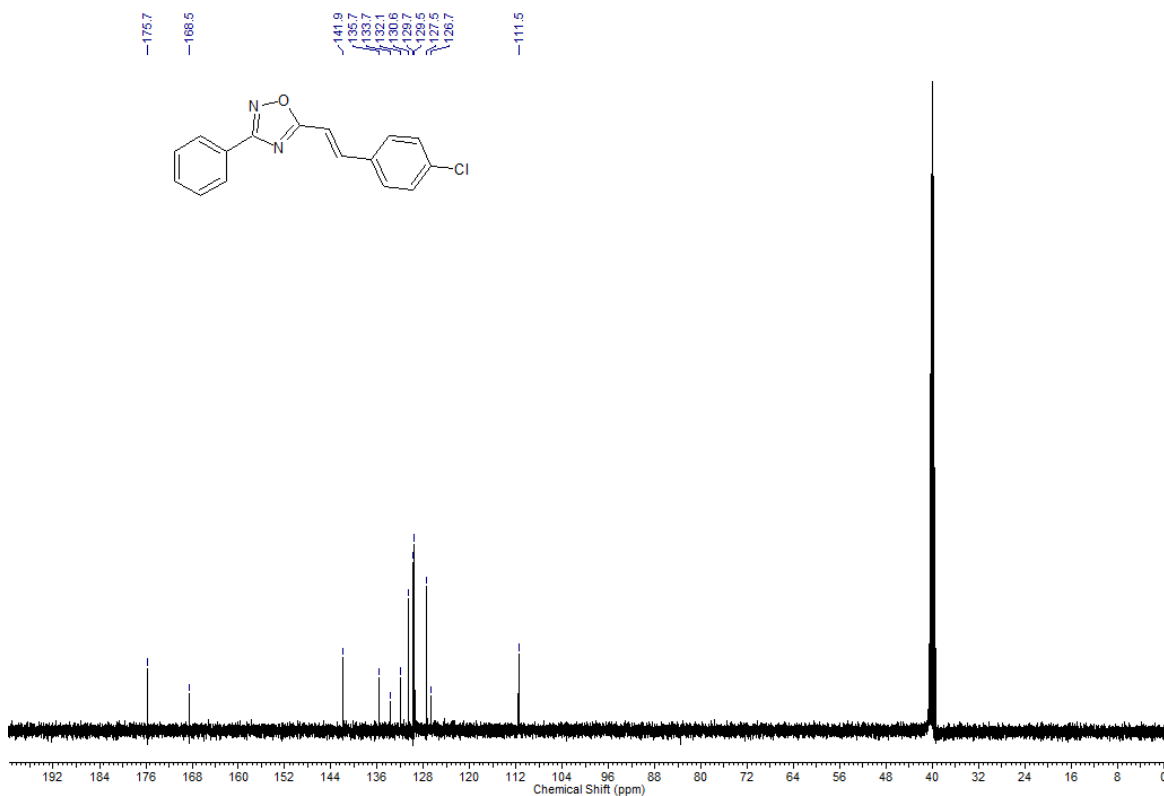
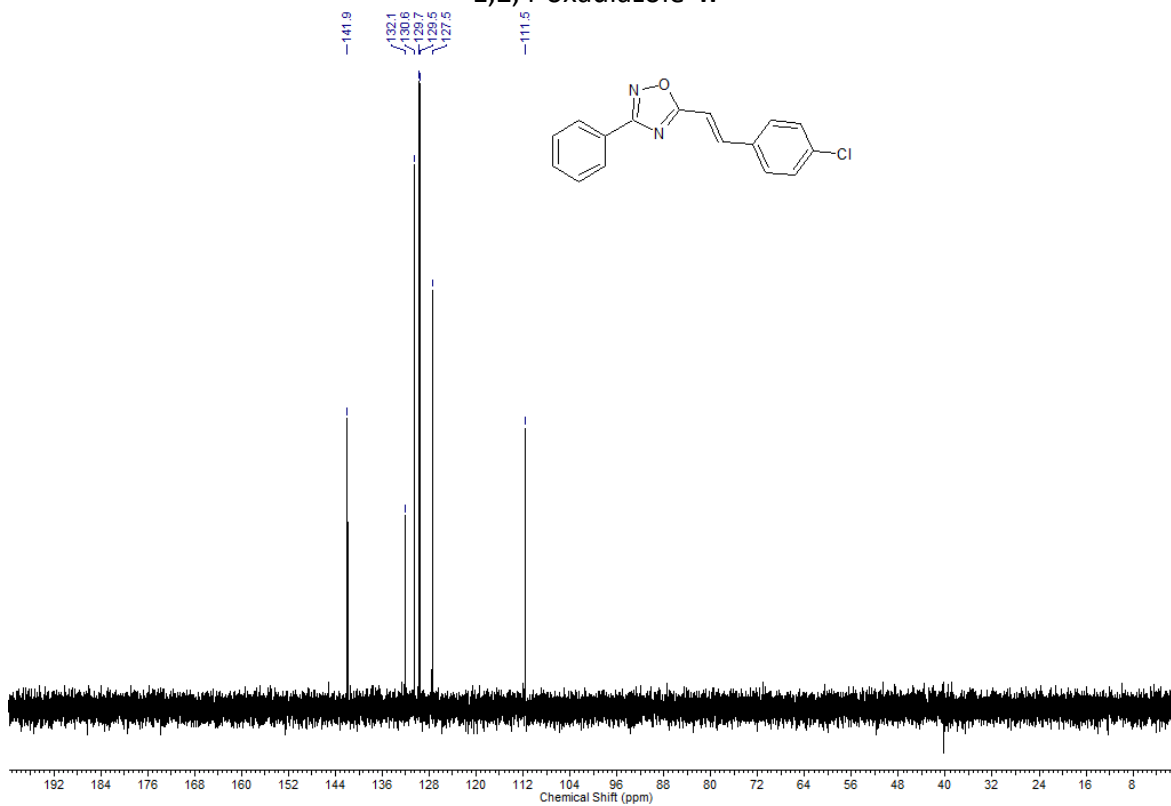
Figure S59. ^{13}C NMR spectra of 5-[(*E*)-2-(4-chlorophenyl)ethenyl]-3-phenyl-1,2,4-oxadiazole **4f**Figure S60. ^{13}C DEPT NMR spectra of 5-[(*E*)-2-(4-chlorophenyl)ethenyl]-3-phenyl-1,2,4-oxadiazole **4f**

Figure S61. ^1H NMR spectra of 3-(4-methoxyphenyl)-5-[(*E*)-2-phenylethenyl]-1,2,4-oxadiazole **4g**.

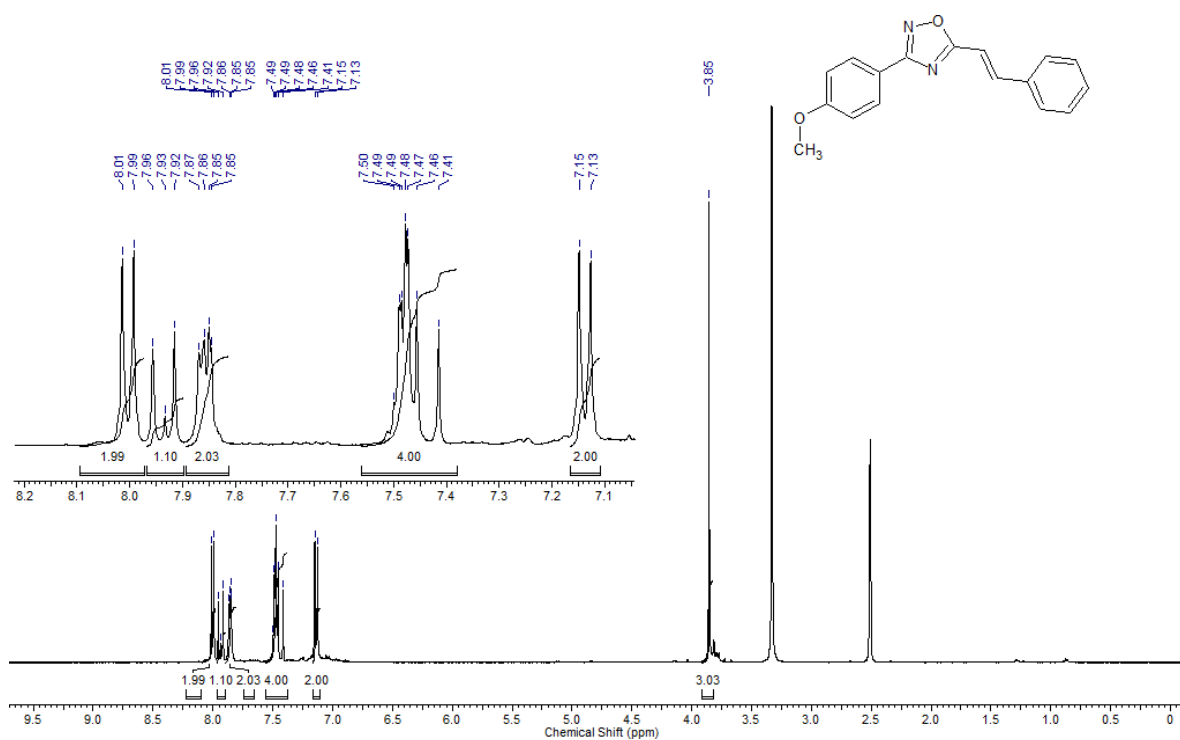


Figure S62. ^{13}C NMR spectra of 3-(4-methoxyphenyl)-5-[(*E*)-2-phenylethenyl]-1,2,4-oxadiazole **4g**.

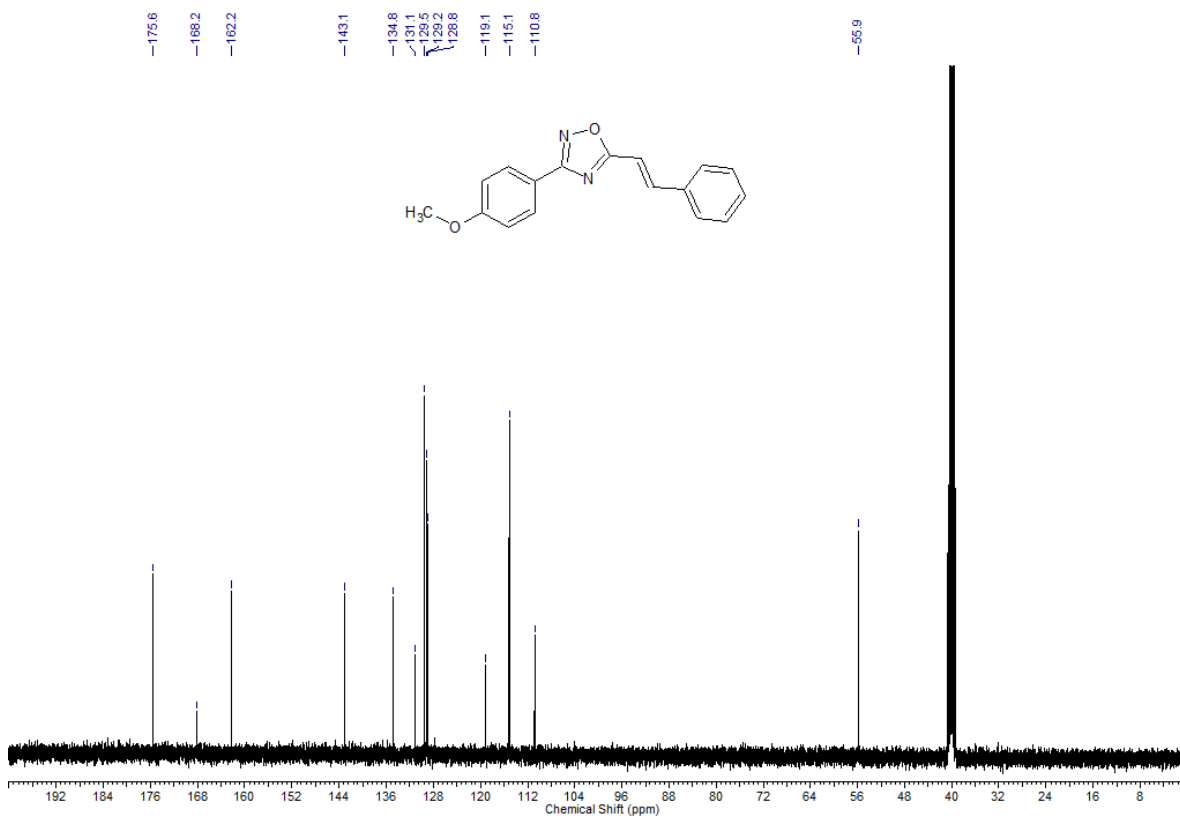


Figure S63. ^{13}C DEPT NMR spectra of 3-(4-methoxyphenyl)-5-[(*E*)-2-phenylethenyl]-1,2,4-oxadiazole **4g**.

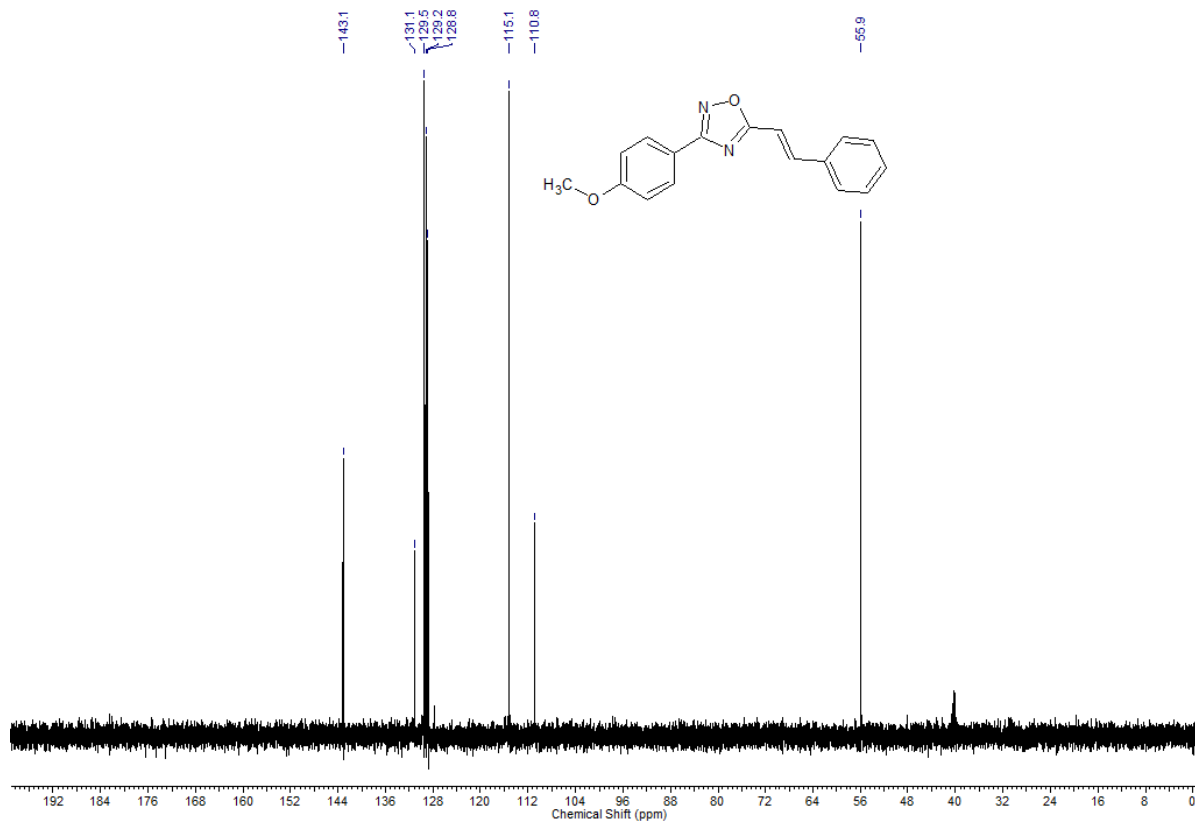


Figure S64. ^1H NMR spectra of 3-(4-methoxyphenyl)-5-[(*E*)-2-(4-methoxyphenyl)ethenyl]-1,2,4-oxadiazole **4h**

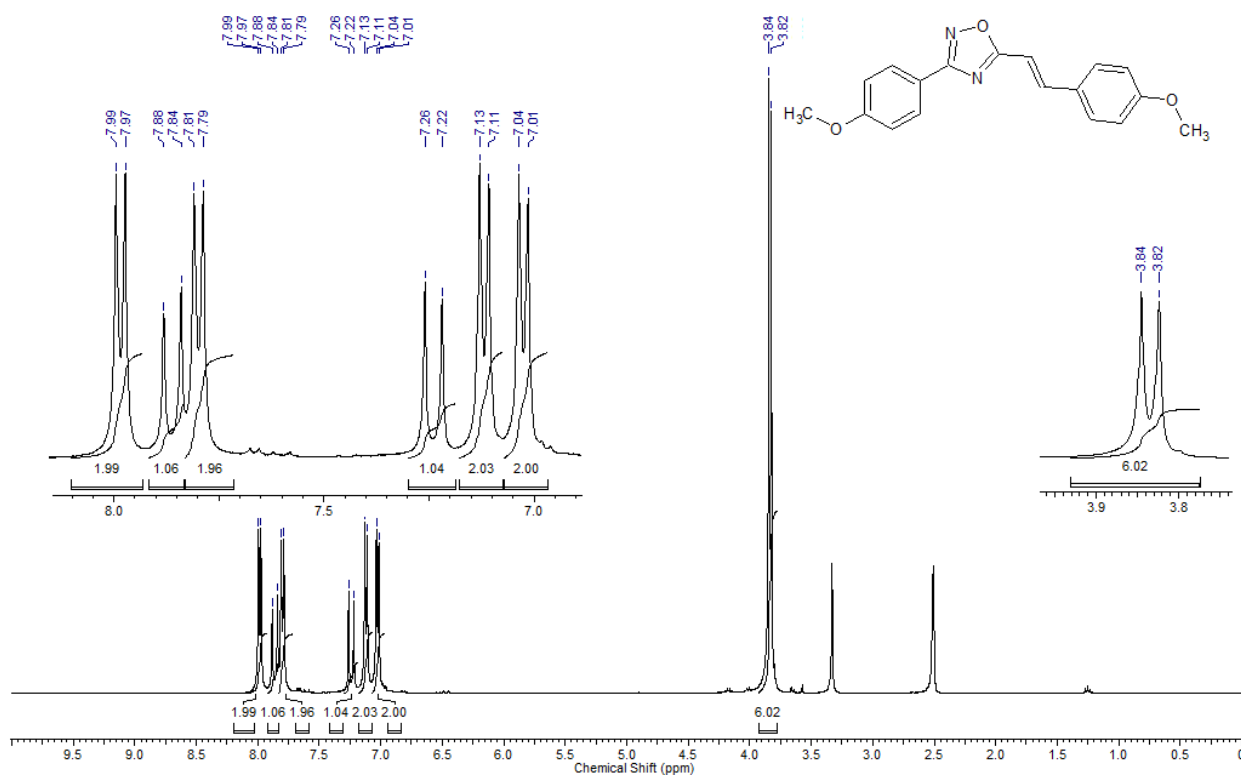


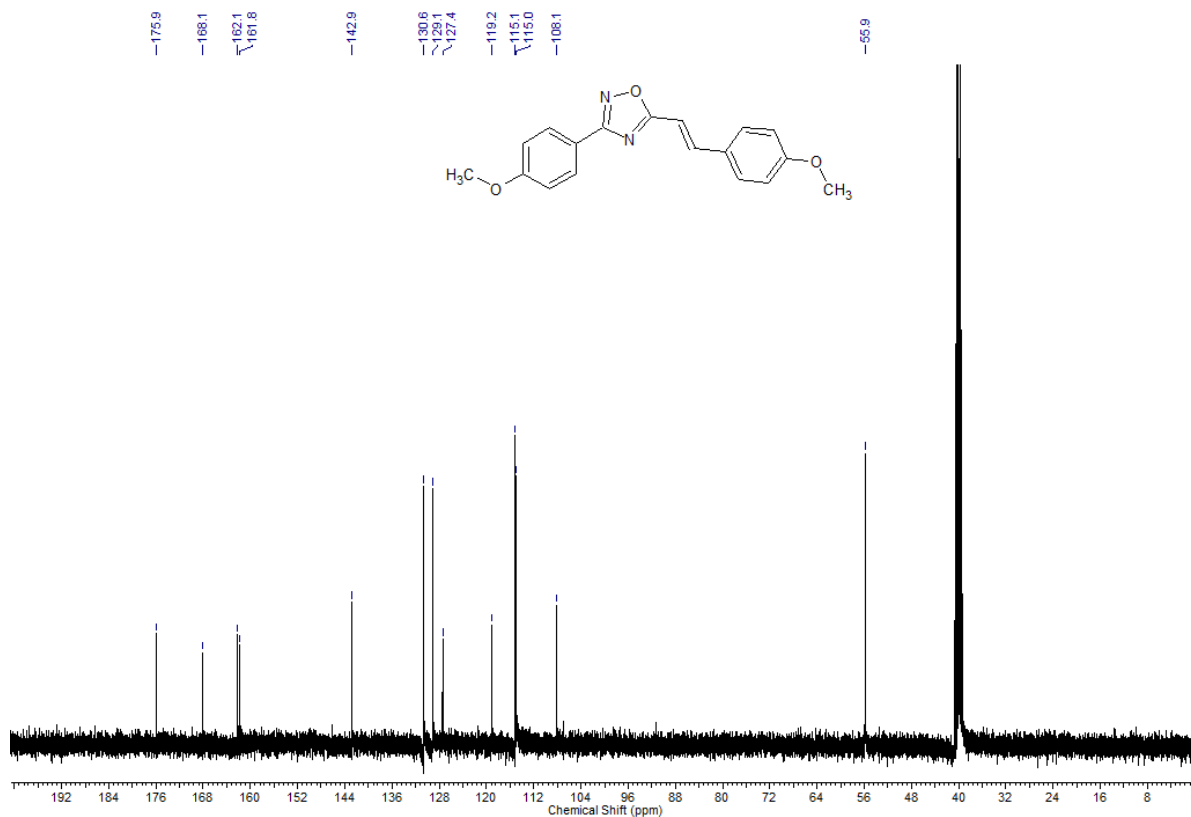
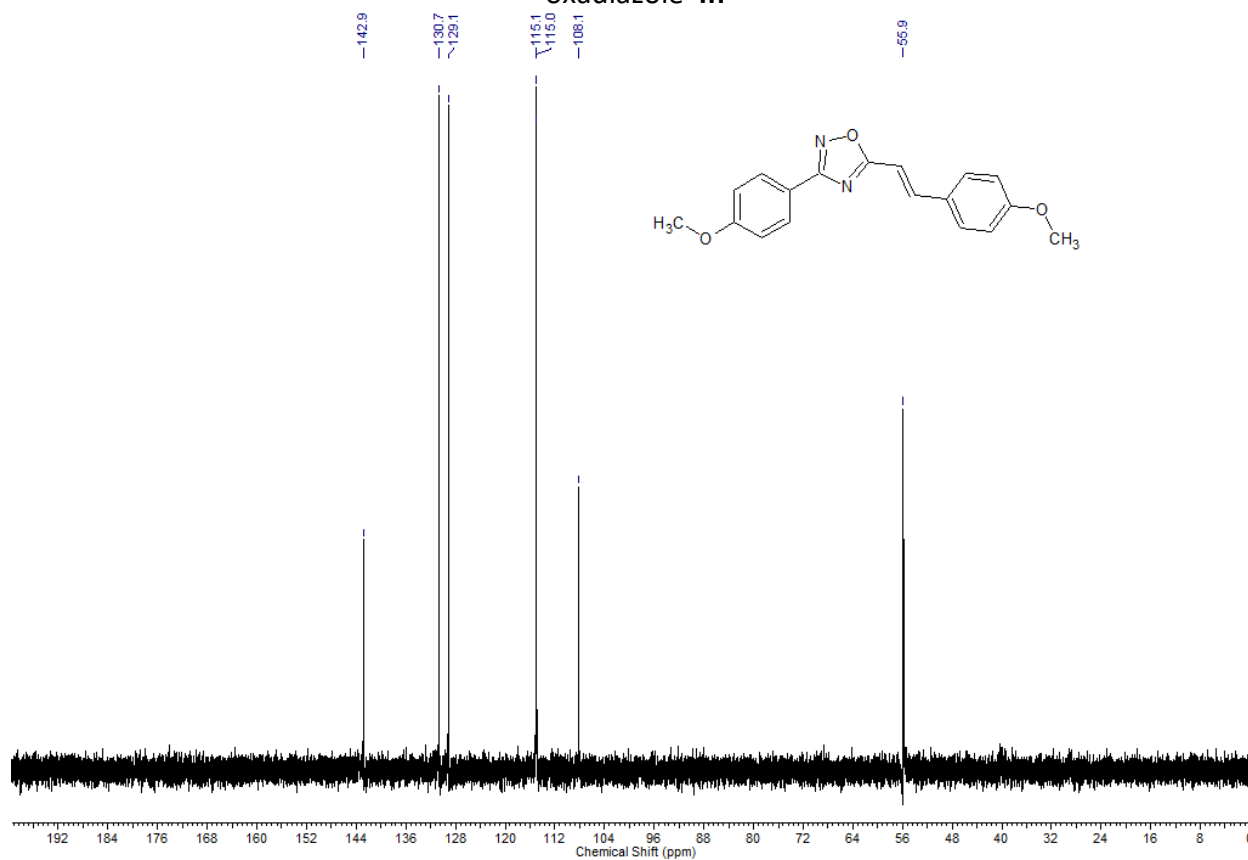
Figure S65. ^{13}C NMR spectra of 3-(4-methoxyphenyl)-5-[(*E*)-2-(4-methoxyphenyl)ethenyl]-1,2,4-oxadiazole **4h**Figure S66. ^{13}C DEPT NMR spectra of 3-(4-methoxyphenyl)-5-[(*E*)-2-(4-methoxyphenyl)ethenyl]-1,2,4-oxadiazole **4h**

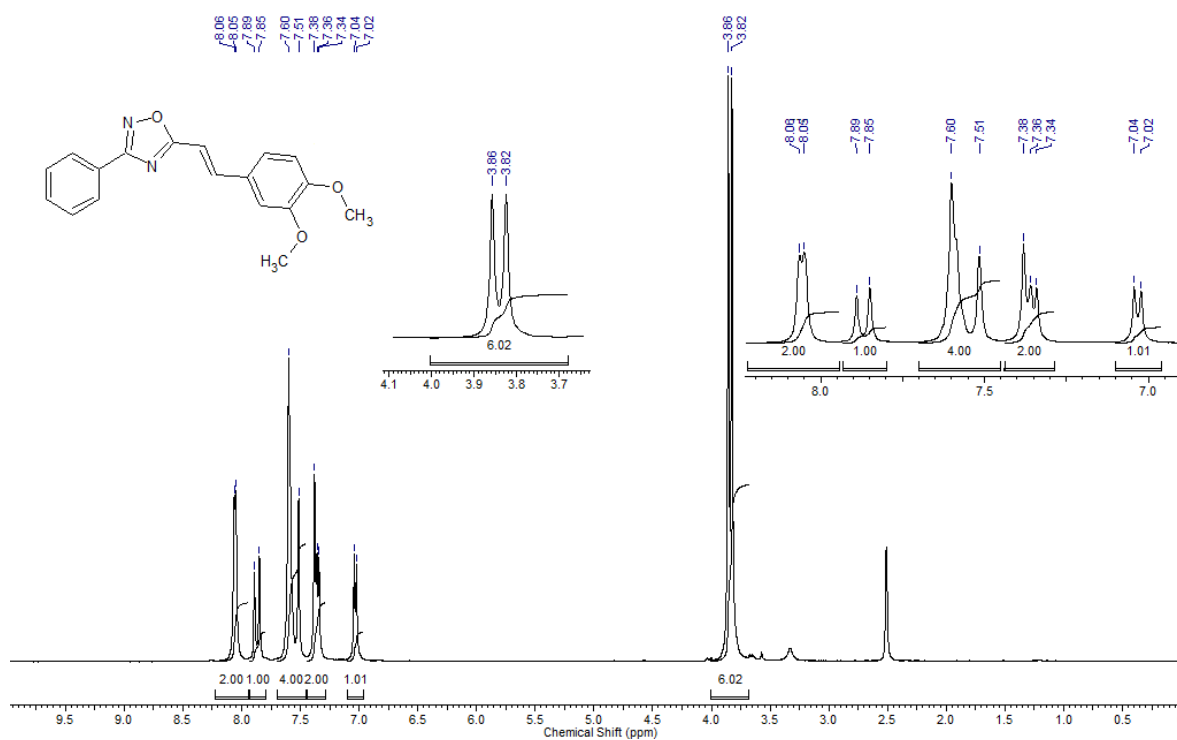
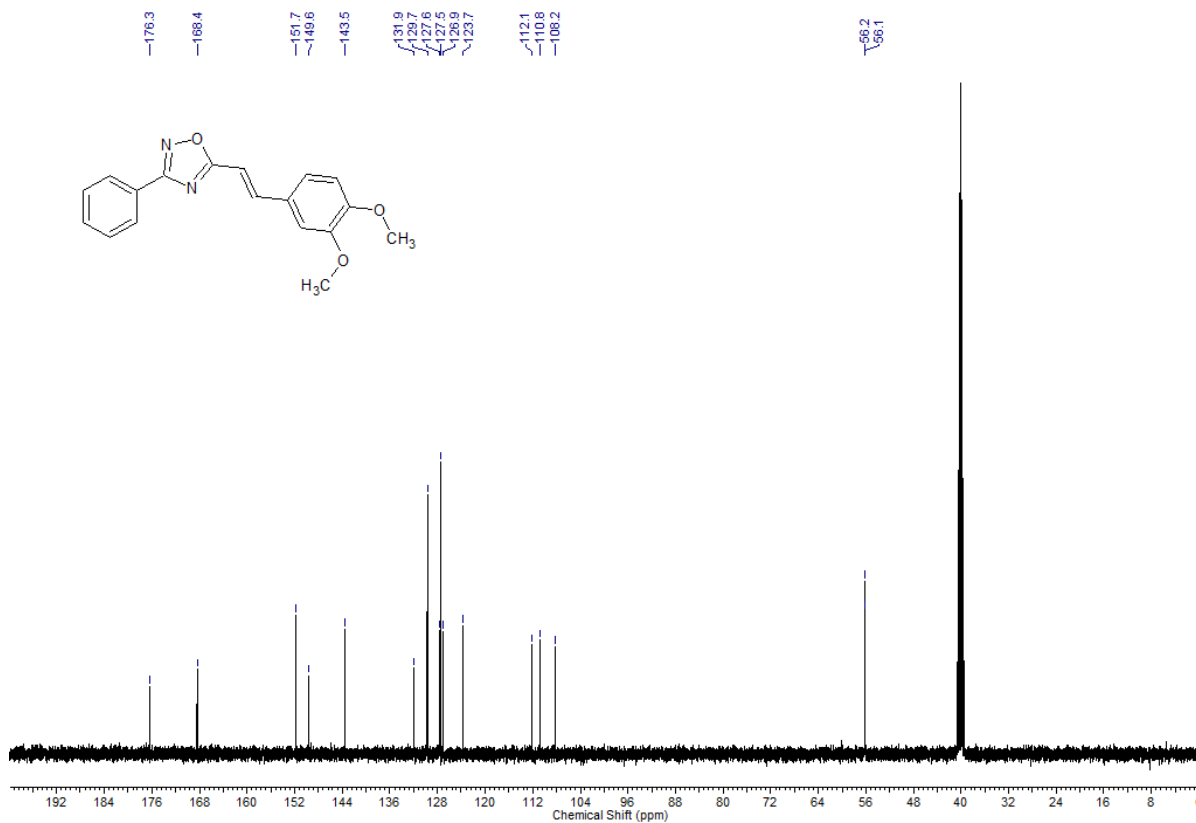
Figure S67. ¹H NMR spectra of 5-[(*E*)-2-(3,4-dimethoxyphenyl)ethenyl]-3-phenyl-1,2,4-oxadiazole **4i**Figure S68. ¹³C NMR spectra of 5-[(*E*)-2-(3,4-dimethoxyphenyl)ethenyl]-3-phenyl-1,2,4-oxadiazole **4i**

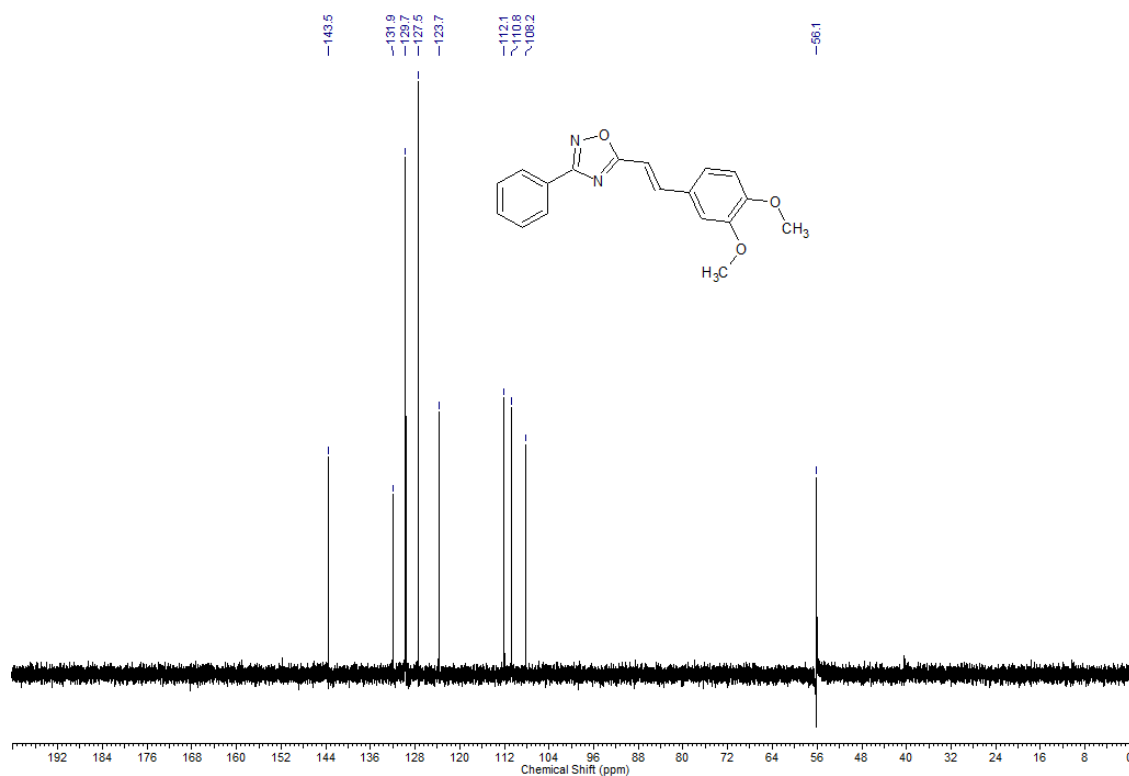
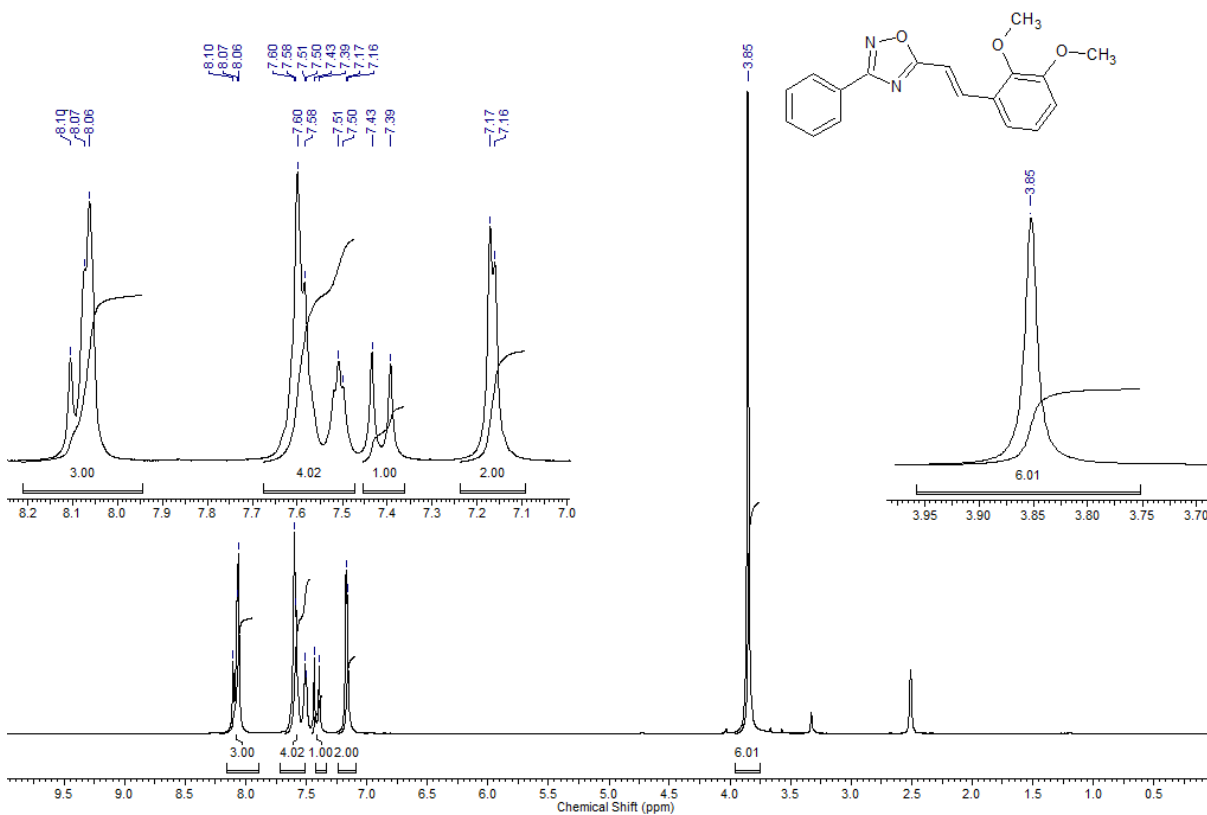
Figure S69. ^{13}C DEPT NMR spectra of 5-[(*E*)-2-(3,4-dimethoxyphenyl)ethenyl]-3-phenyl-1,2,4-oxadiazole **4i**Figure S70. ^1H NMR spectra of 5-[(*E*)-2-(2,3-dimethoxyphenyl)ethenyl]-3-phenyl-1,2,4-oxadiazole **4j**

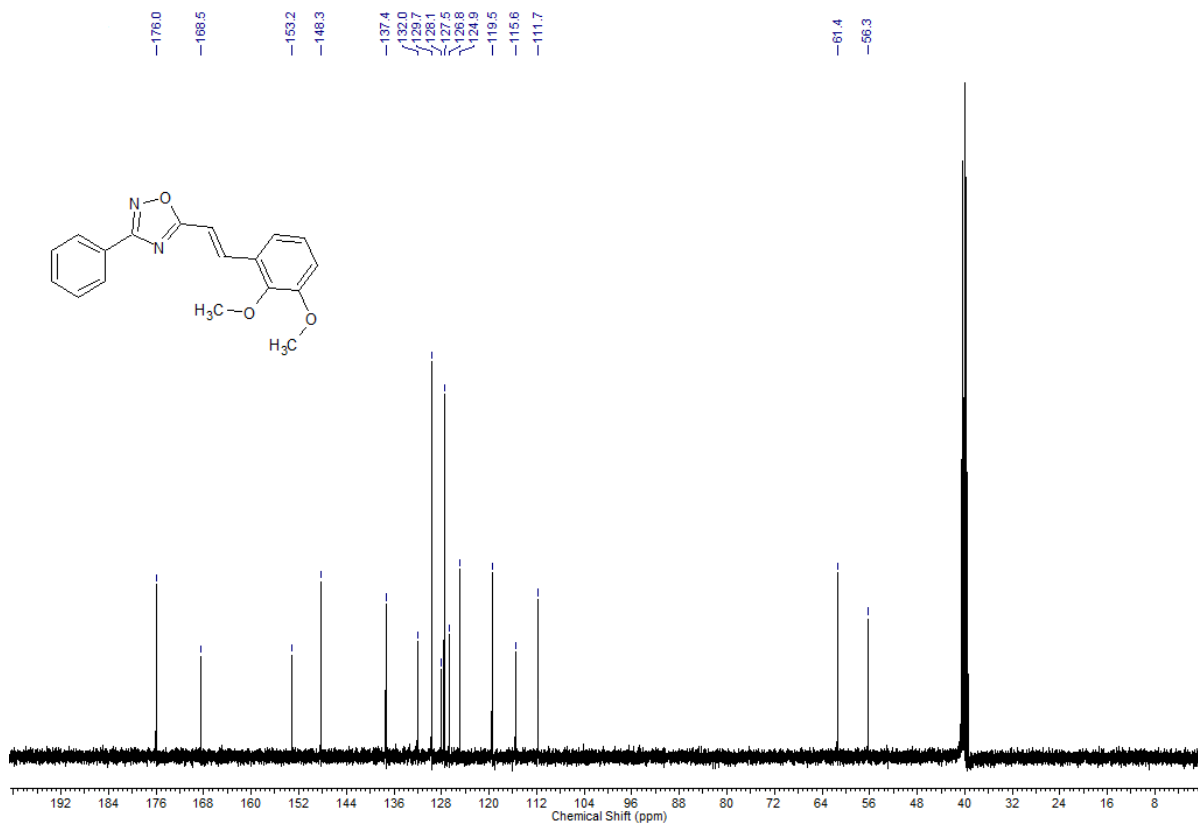
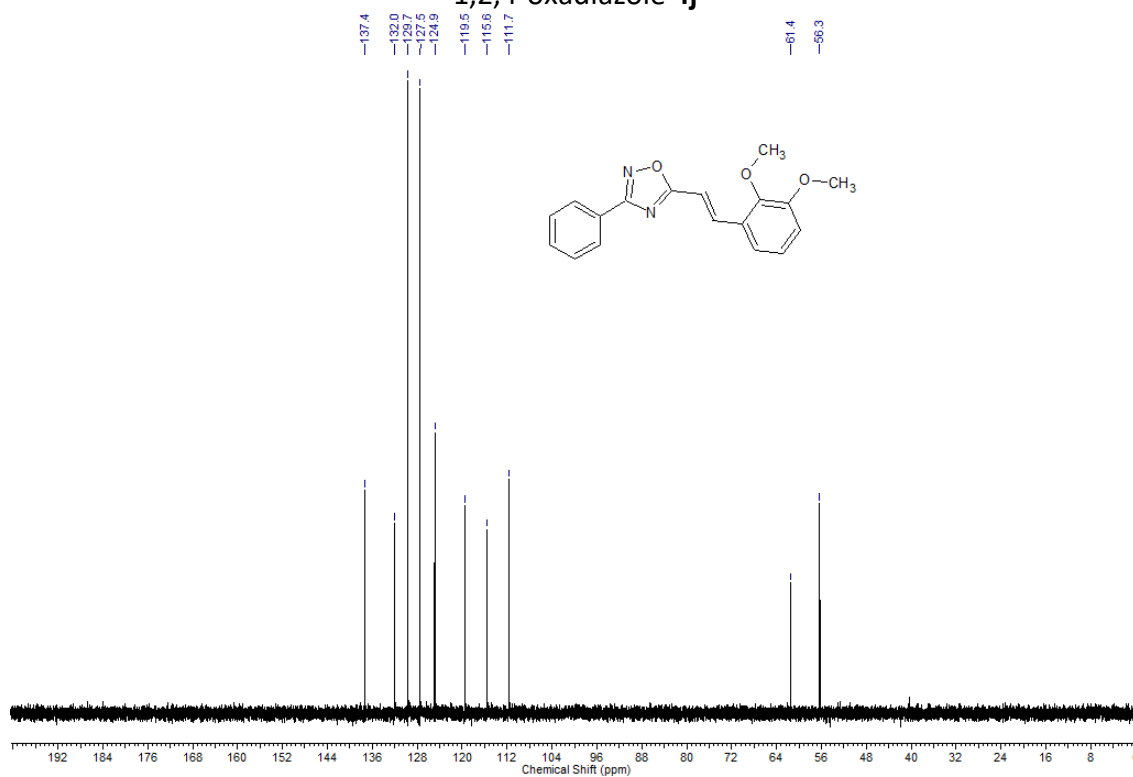
Figure S71. ^{13}C NMR spectra of 5-[(*E*)-2-(2,3-dimethoxyphenyl)ethenyl]-3-phenyl-1,2,4-oxadiazole **4j**Figure S72. ^{13}C DEPT NMR spectra of 5-[(*E*)-2-(2,3-dimethoxyphenyl)ethenyl]-3-phenyl-1,2,4-oxadiazole **4j**

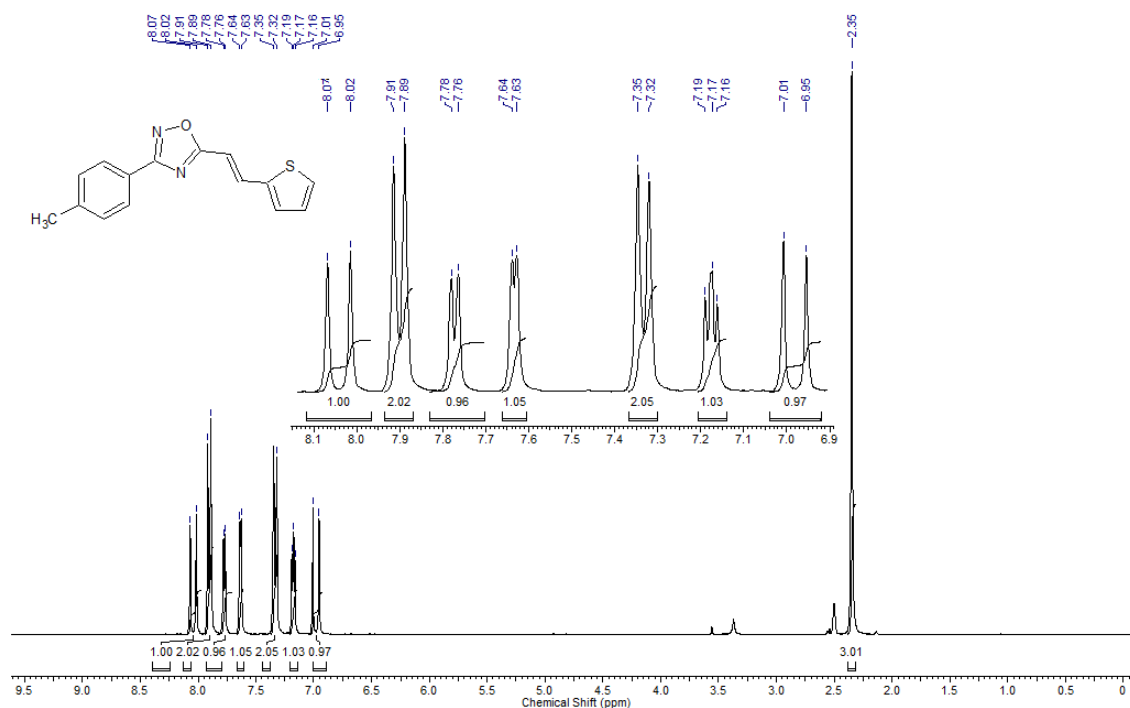
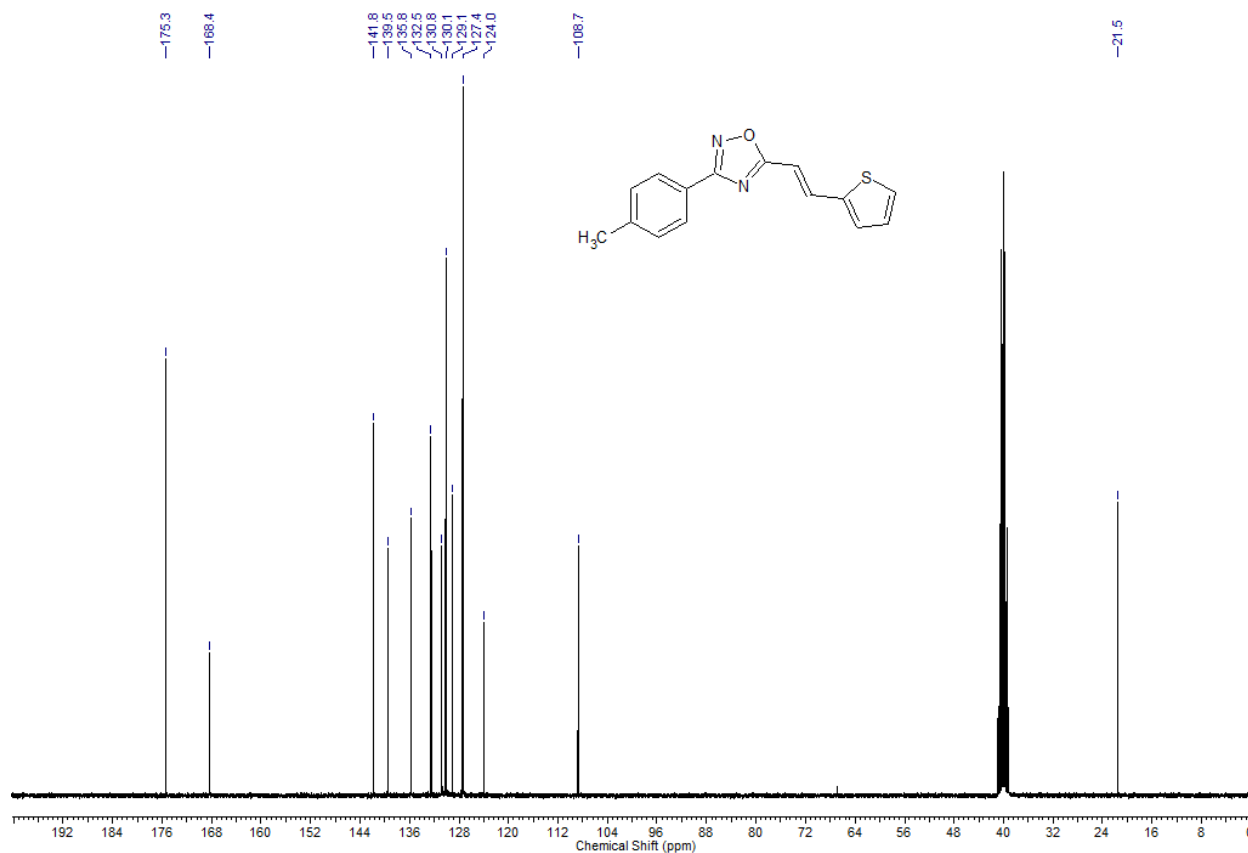
Figure S73. ^1H NMR spectra of 3-(4-Methylphenyl)-5-[(*E*)-2-(thiophen-2-yl)ethenyl]-1,2,4-oxadiazole **4k**.Figure S74. ^{13}C NMR spectra of 3-(4-Methylphenyl)-5-[(*E*)-2-(thiophen-2-yl)ethenyl]-1,2,4-oxadiazole **4k**.

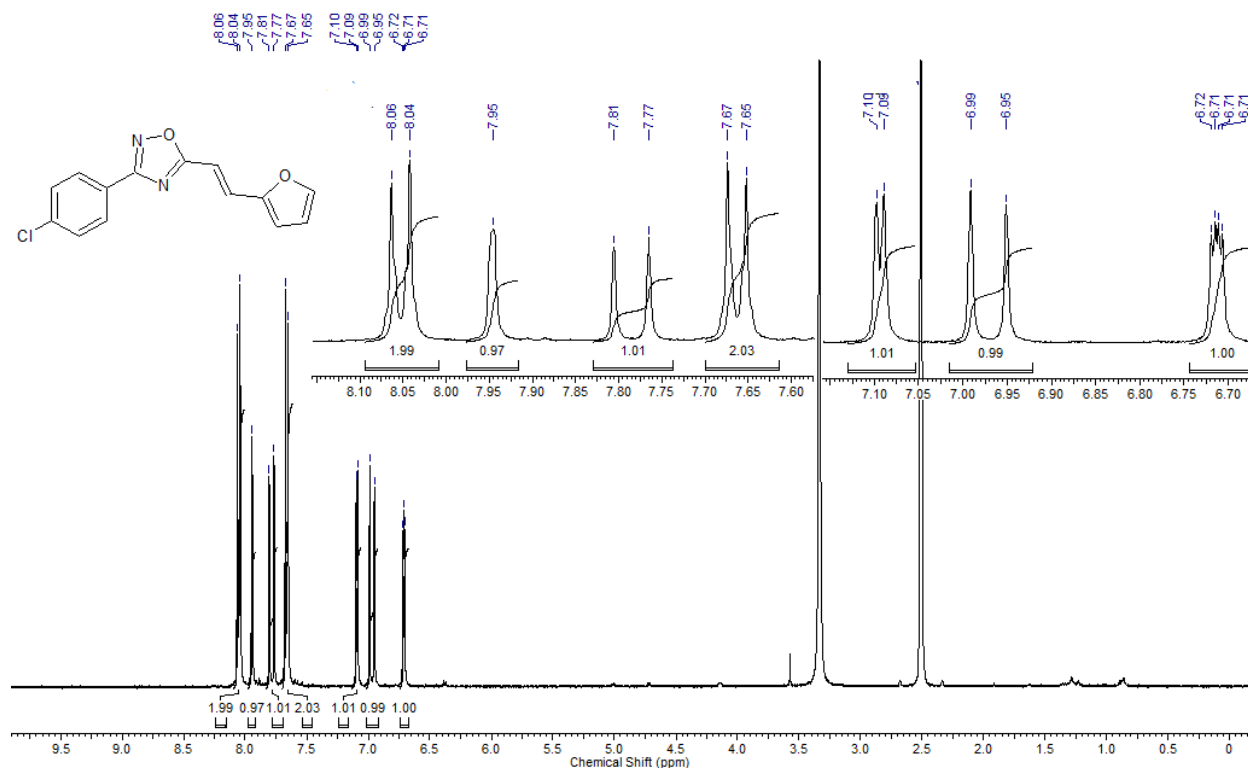
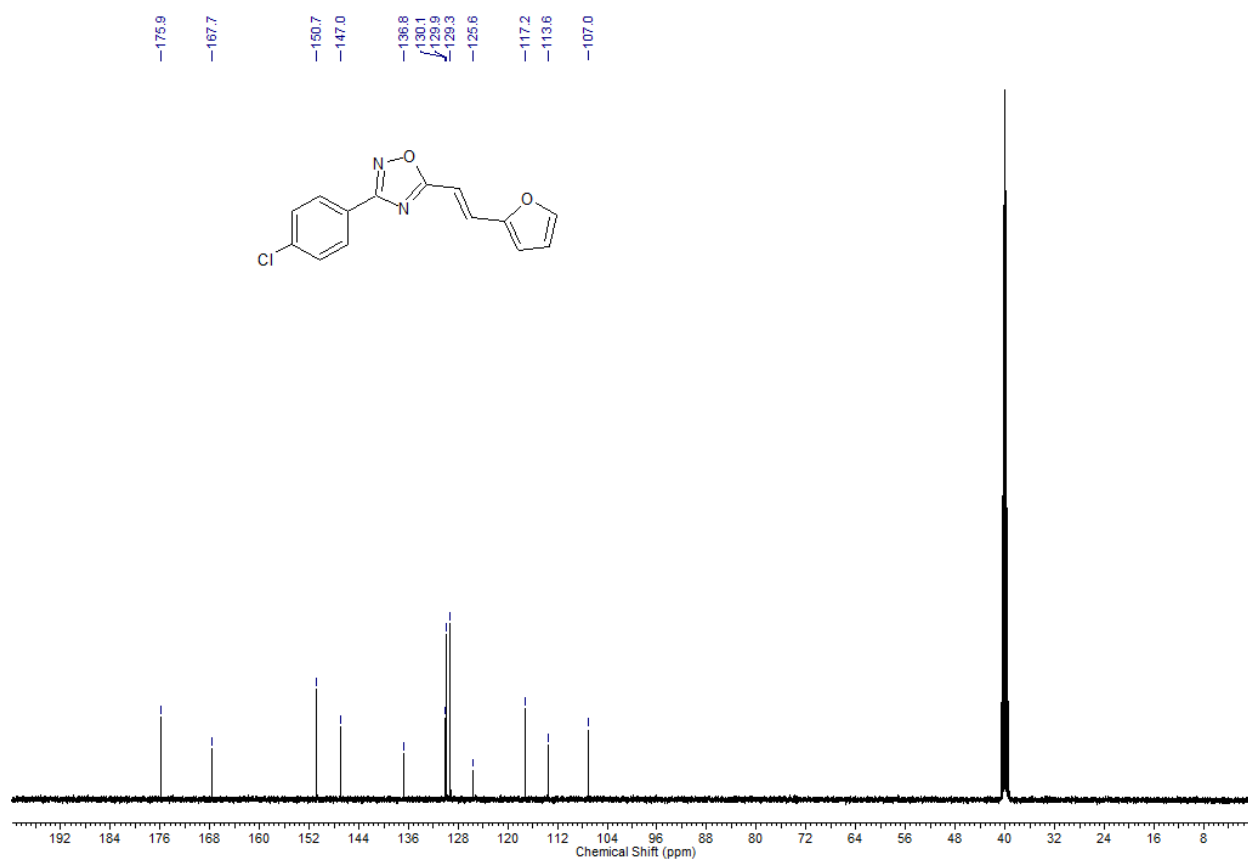
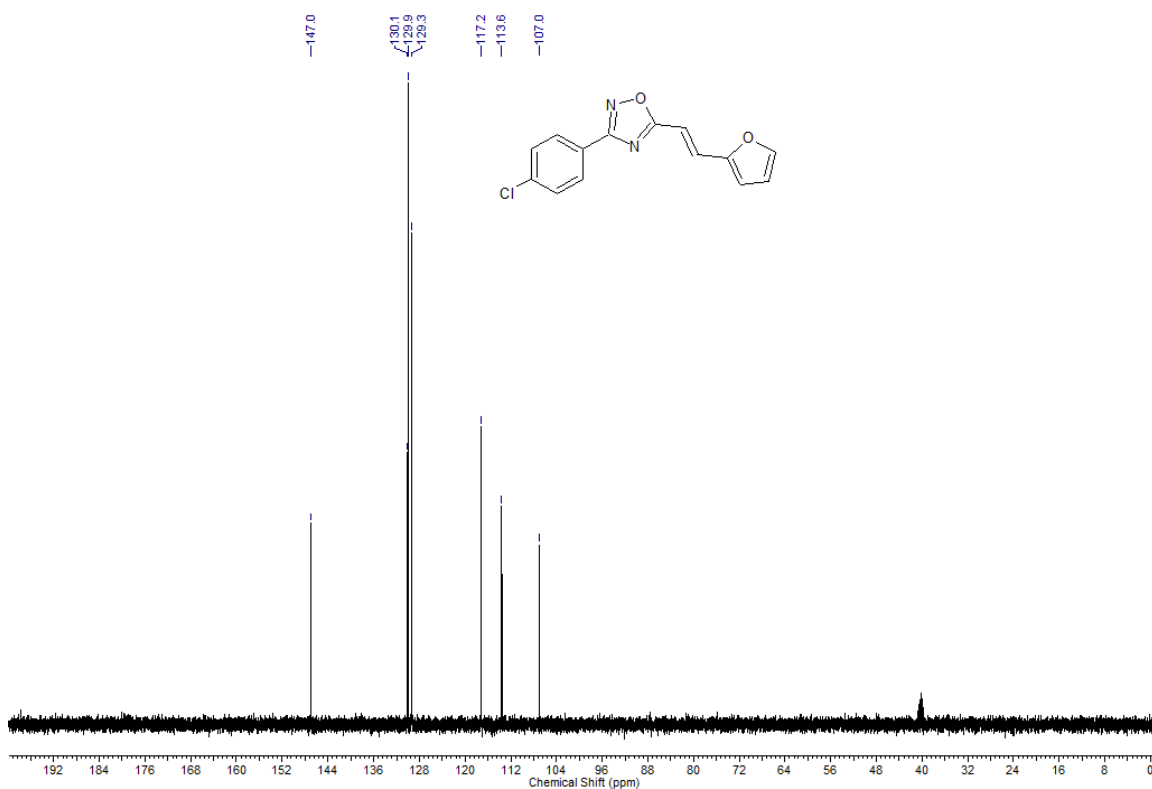
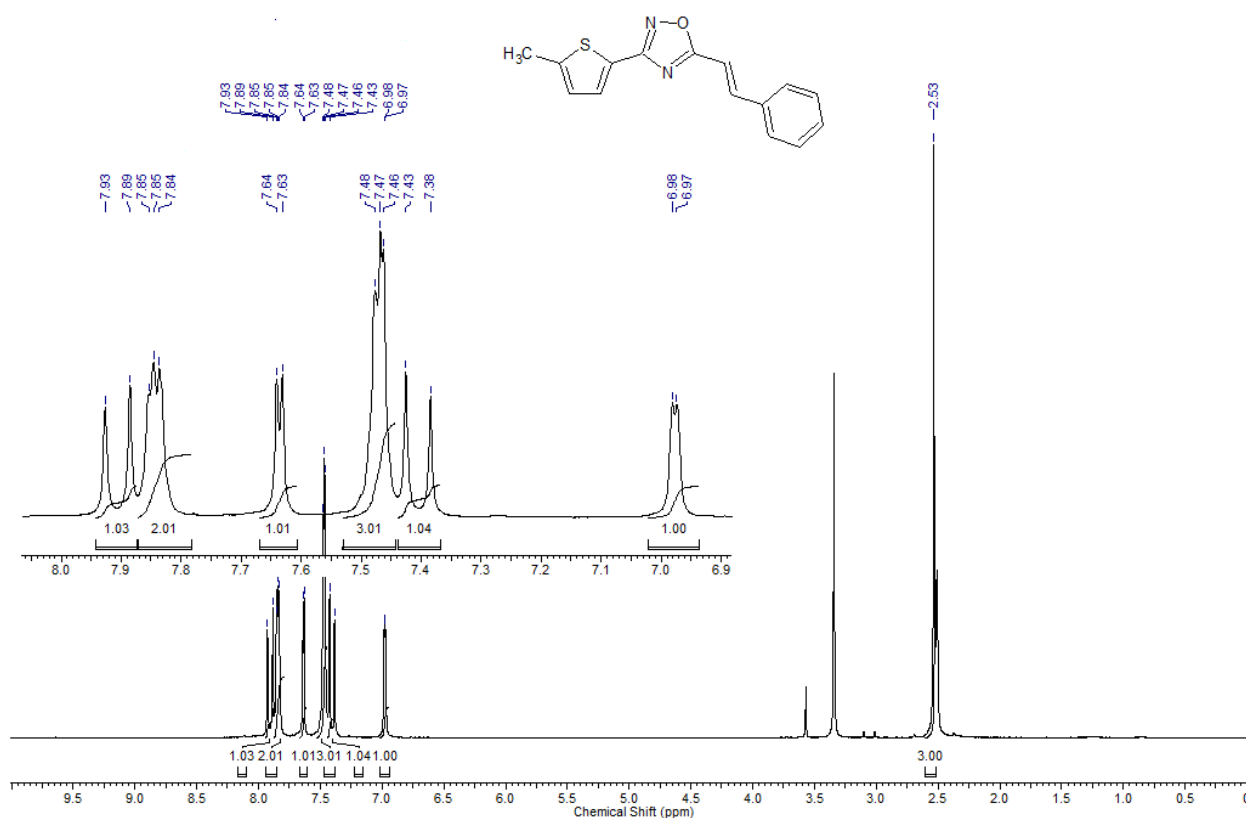
Figure S75. ^1H NMR spectra of 3-(4-Chlorophenyl)-5-[(*E*)-2-(furan-2-yl)ethenyl]-1,2,4-oxadiazole **4I**Figure S76. ^{13}C NMR spectra of 3-(4-Chlorophenyl)-5-[(*E*)-2-(furan-2-yl)ethenyl]-1,2,4-oxadiazole **4I**

Figure S77. ^{13}C DEPT NMR spectra of 3-(4-Chlorophenyl)-5-[(*E*)-2-(furan-2-yl)ethenyl]-1,2,4-oxadiazole **4l**Figure S78. ^1H NMR spectra of 3-(5-methylthiophen-2-yl)-5-[(*E*)-2-phenylethenyl]-1,2,4-oxadiazole **4m**Figure S79. ^{13}C NMR spectra of 3-(5-methylthiophen-2-yl)-5-[(*E*)-2-phenylethenyl]-1,2,4-oxadiazole **4m**

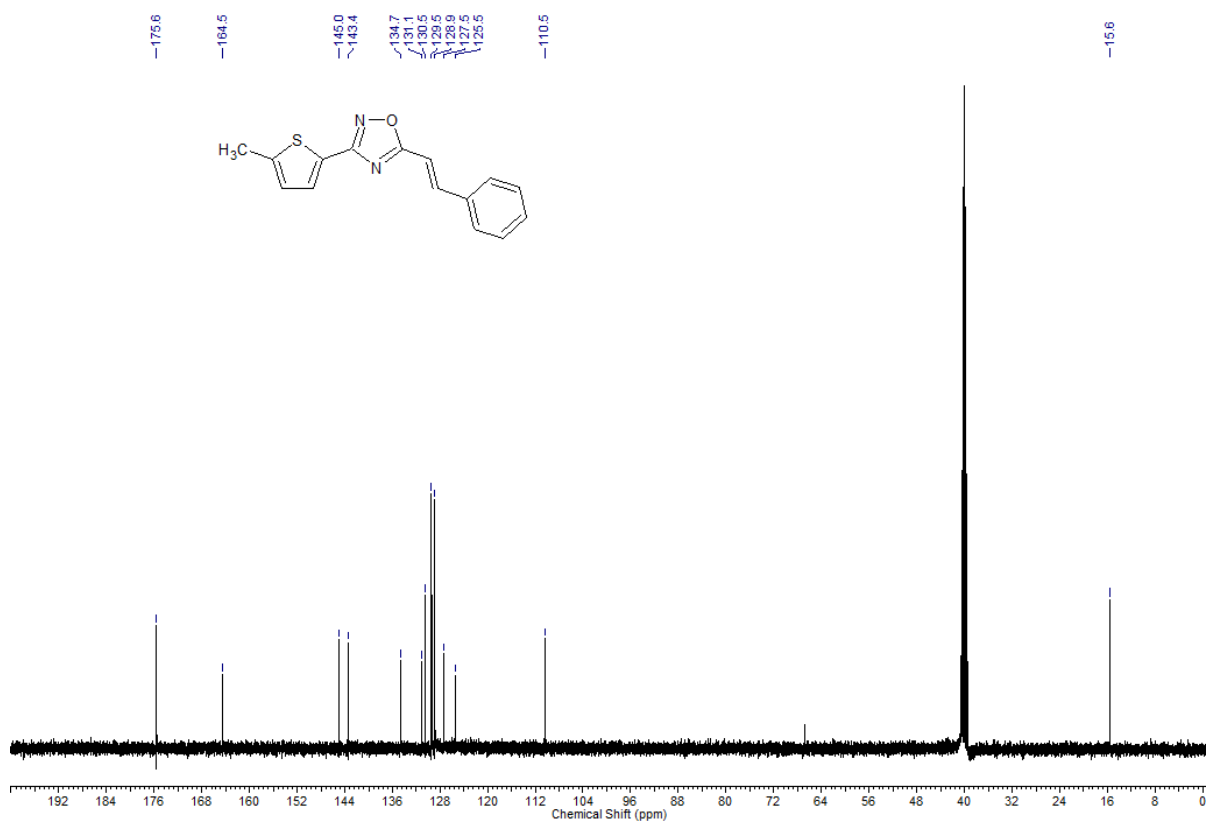


Figure S80. ¹³C DEPT NMR spectra of 3-(5-methylthiophen-2-yl)-5-[(*E*)-2-phenylethenyl]-1,2,4-oxadiazole **4m**

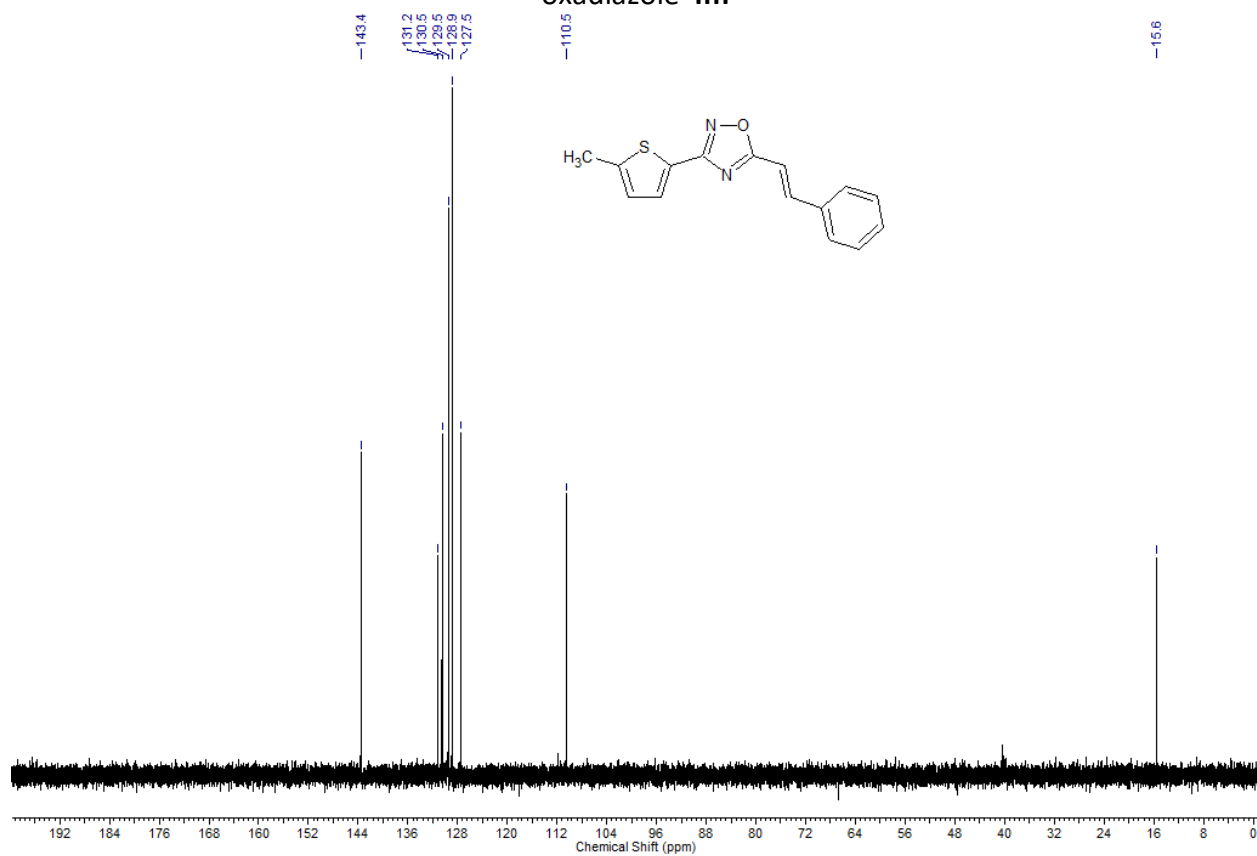
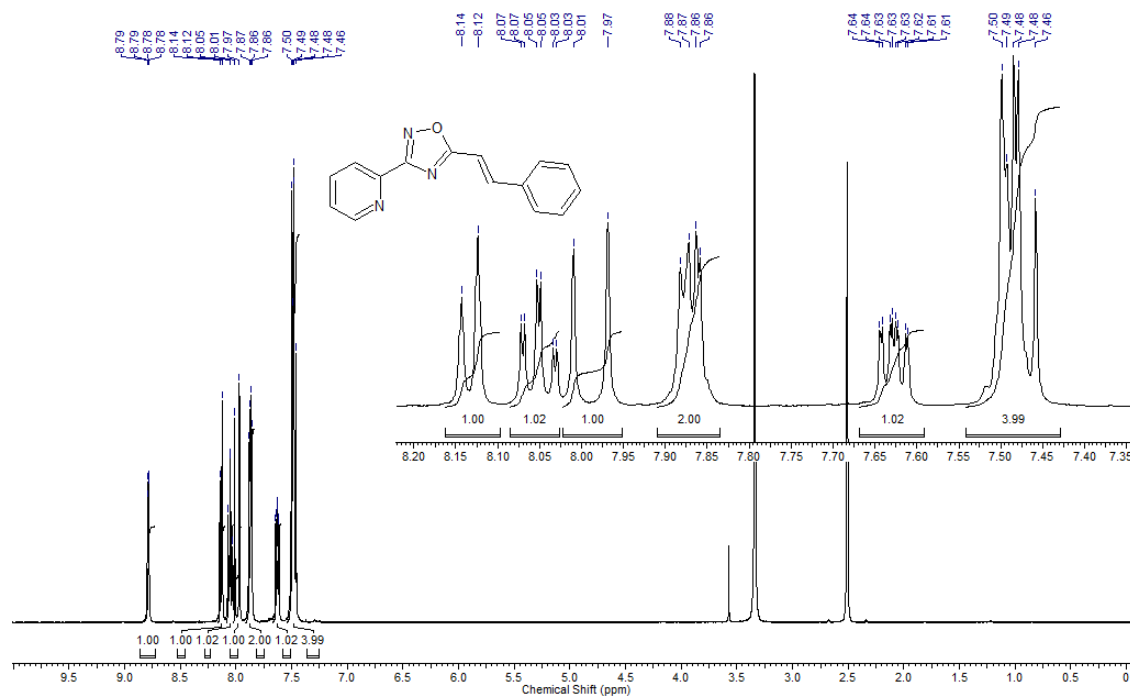
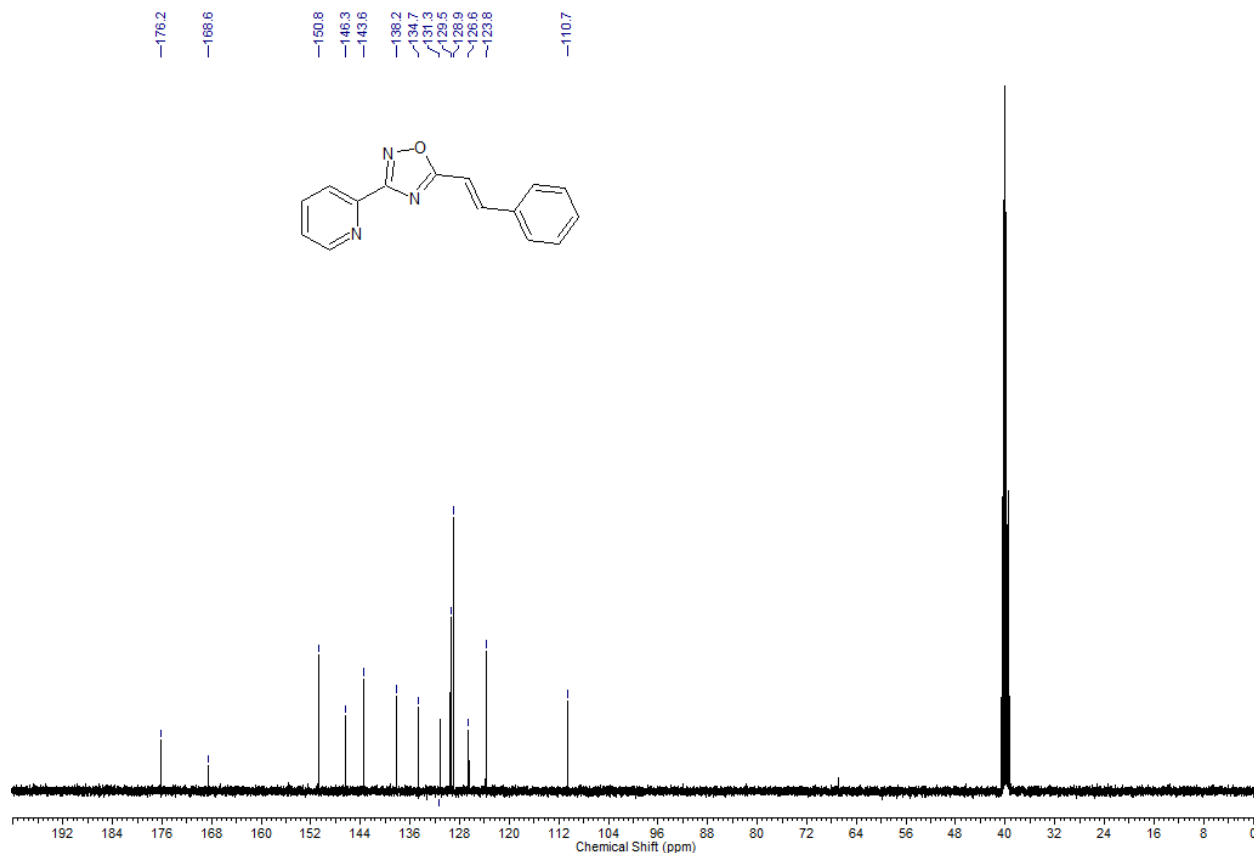


Figure S81. ^1H NMR spectra of 2-{5-[(*E*)-2-phenylethenyl]-1,2,4-oxadiazol-3-yl}pyridine **4n**Figure S82. ^{13}C NMR spectra of 2-{5-[(*E*)-2-phenylethenyl]-1,2,4-oxadiazol-3-yl}pyridine **4n**Figure S83. ^{13}C DEPT NMR spectra of 2-{5-[(*E*)-2-phenylethenyl]-1,2,4-oxadiazol-3-yl}pyridine **4n**

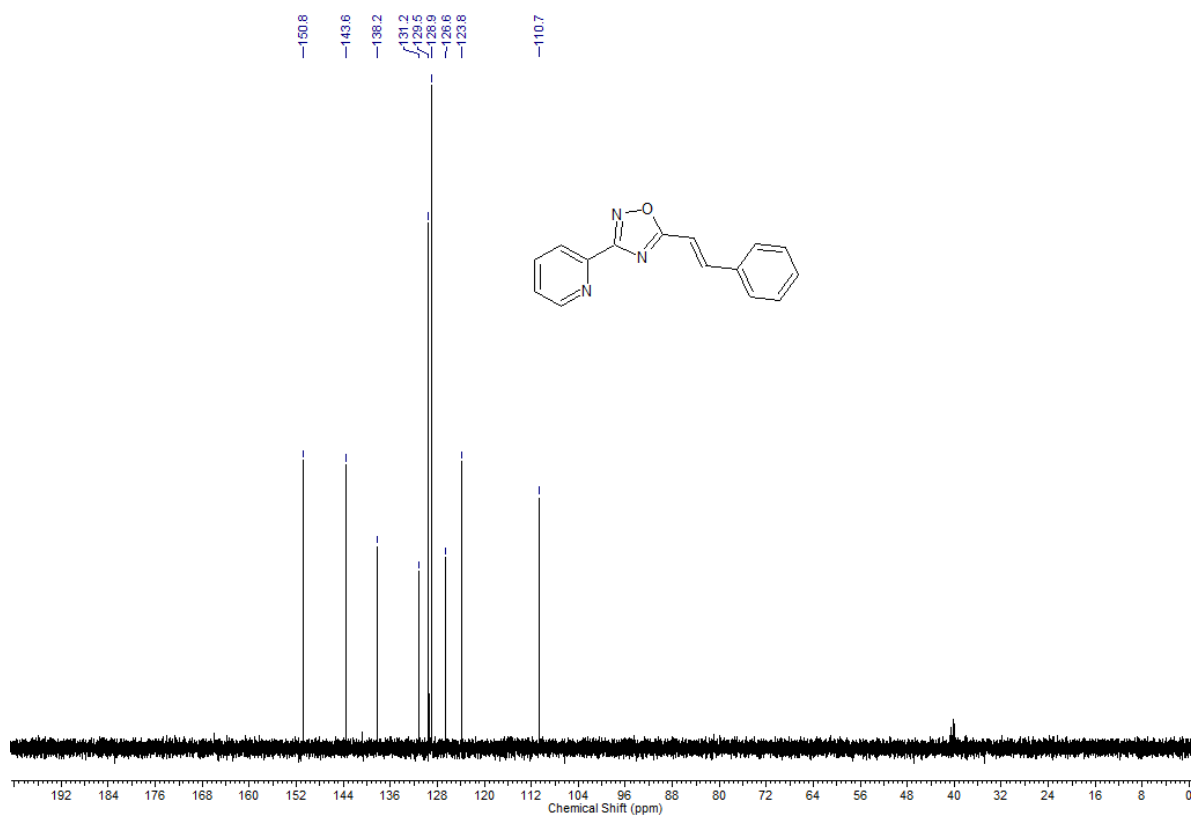
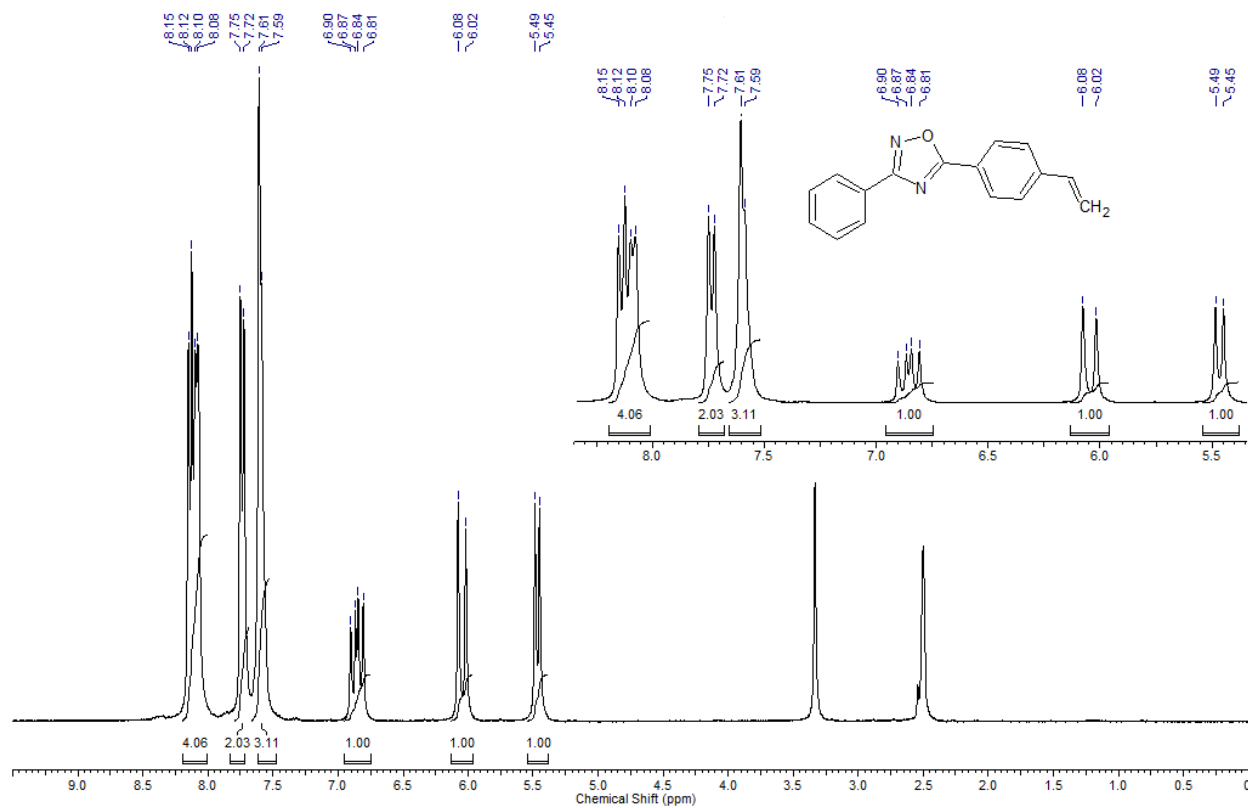
Figure S84. ¹H NMR spectra of 3-phenyl-5-(4-vinylphenyl)-1,2,4-oxadiazole **4o**

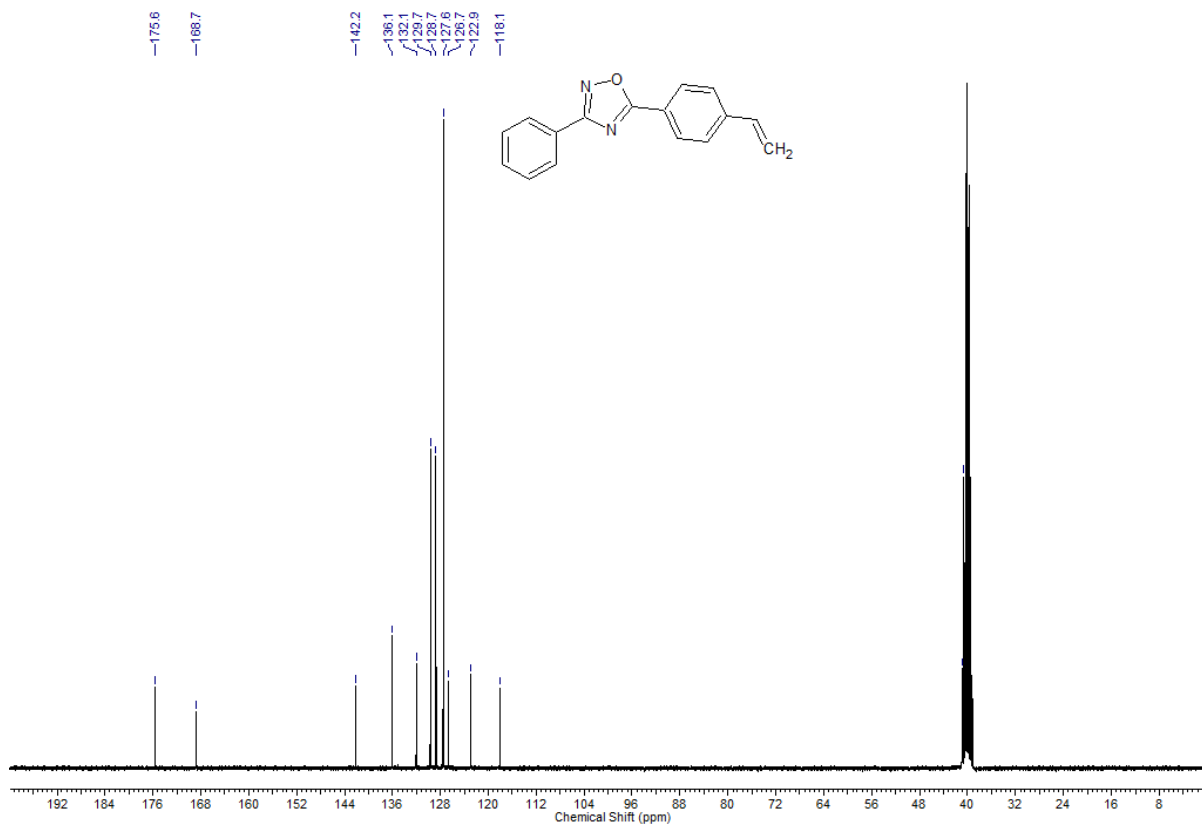
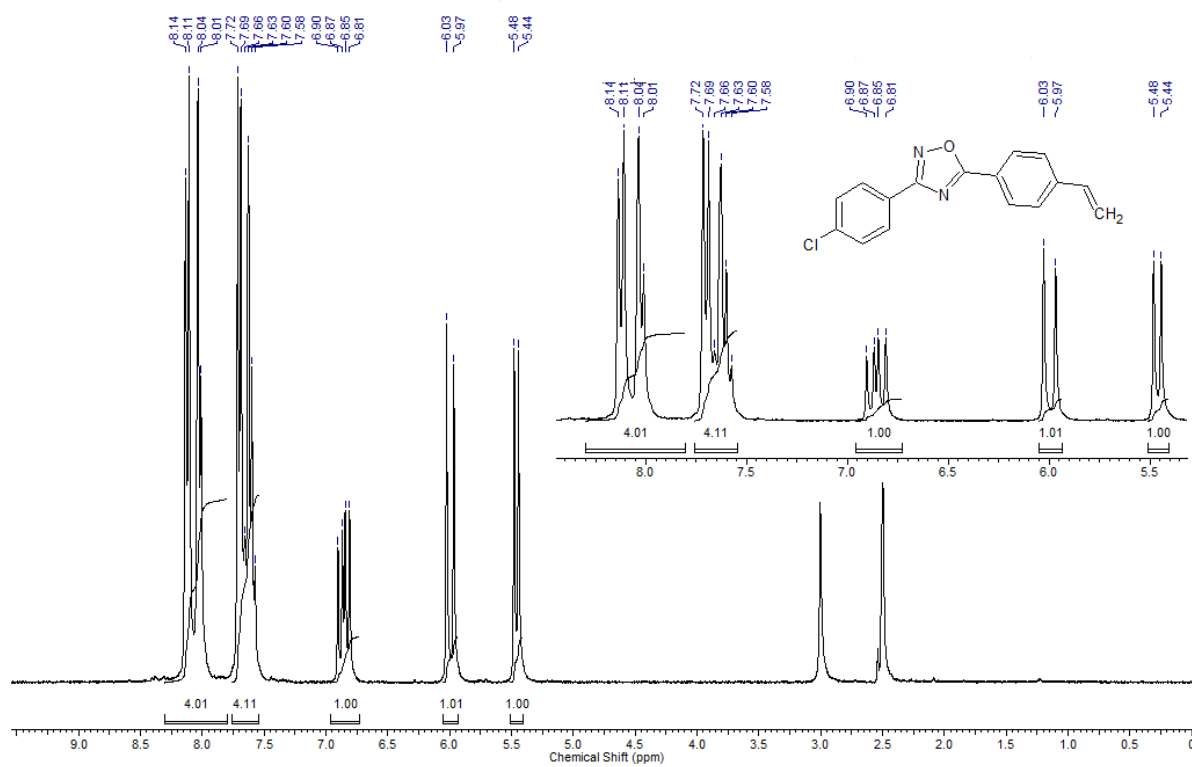
Figure S85. ^{13}C NMR spectra of 3-phenyl-5-(4-vinylphenyl)-1,2,4-oxadiazole **4o**Figure S86. ^1H NMR spectra of 3-(4-chlorophenyl)-5-(4-ethenylphenyl)-1,2,4-oxadiazole **4p**

Figure S87. ^{13}C NMR spectra of 3-(4-chlorophenyl)-5-(4-ethenylphenyl)-1,2,4-oxadiazole **4p**