Supporting Information

Koser's Reagent Promoted Synthesis of Substituted Isoxazoles and their Photophysical Properties

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General Information

All reactions, unless specifically mentioned, were carried out using pre-oven-dried glassware equipped with magnetic stirring. Reaction progress was monitored using Merck silica gel 60 F_{254} precoated TLC plates (0.25 mm) with visualization under UV illumination at 254 nm. The crude product was purified by column chromatography on Merck silica gel (100–200 Å mesh), eluting with a gradient of hexane and ethyl acetate. NMR spectra, including ^{1}H (500 MHz), $^{13}C\{^{1}H\}$ (126 MHz), and ^{19}F (471 MHz), were recorded at room temperature employing TMS as an internal standard and $CDCl_3$ or DMSO-d_6 as deuterated solvents. The NMR chemical shifts (δ, ppm) were calibrated against the residual solvent signals: $CDCl_3$ (δ 7.26 for ^{1}H, δ 77.0 for ^{13}C) and DMSO-d_6 (δ 2.50 and 3.30 for ^{1}H, δ 39.52 for ^{13}C), respectively. The NMR parameters are described in the order: δ (ppm) for chemical shift, signal multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet), coupling constant *J* (Hz), followed by the corresponding integration. High-resolution mass spectra (HRMS) were obtained on an Agilent 6545 LC/Q-TOF mass spectrometer employing the electrospray ionization (ESI) technique. FT-IR spectra were recorded for samples in solid state using ATR accessary. The melting points of the compounds were determined on a digitally operated melting point instrument. All chemicals used in this study were acquired from AVRA, GLR, and BLD Pharma and used directly without additional purification.

2.1 Substrates studied in this report

The arylaldoximes were prepared according to the procedures reported in the literature.[1] All other precursors were purchased from commercial sources and used as received.

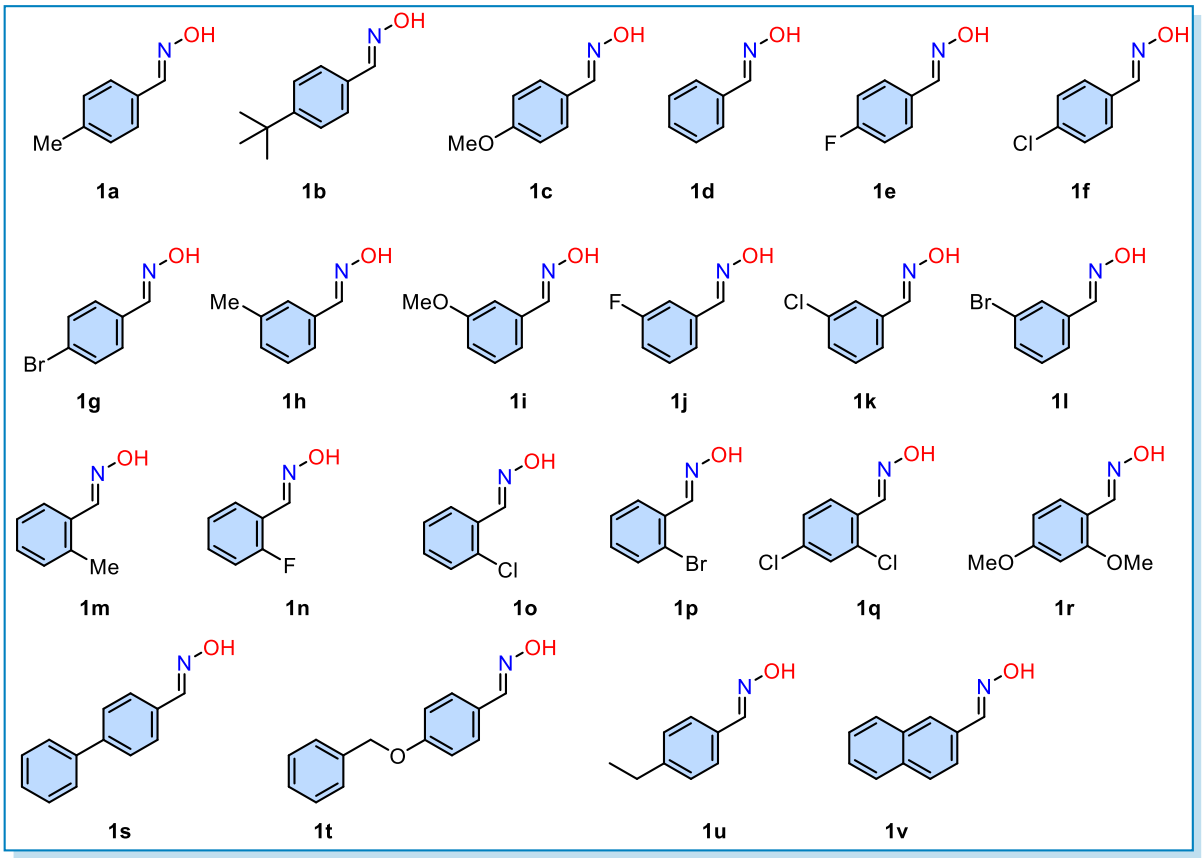


Figure S1. Representative examples of substrates **1**.

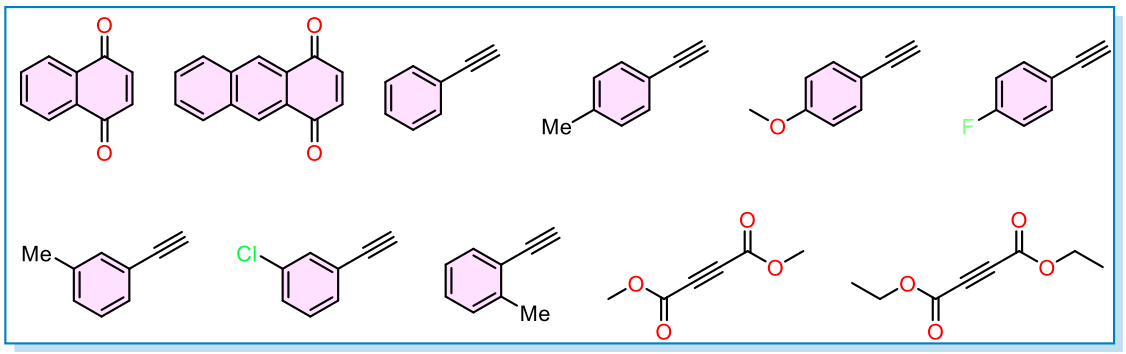


Figure S2. Representative examples of napthoquinone, anthraquinone, arylacetylenes and dialkyl acetylenedicarboxylates.

General Procedure for the Synthesis of 3 and 4

A pre-dried round-bottom flask (10 mL) equipped with a magnetic stir bar was loaded with Koser's reagent [PhI(OH)OTs] (0.70 mmol) to which 1,4-dioxane (2 mL) was subsequently added under open-air conditions. The respective aldoxime (0.60 mmol) was then added to the flask under ambient temperature. Immediately after the addition, the heterogeneous reaction mixture converted into a clear solution. Subsequently, 1,4-naphthoquinone (0.50 mmol) or 1,4-anthraquinone was added to the reaction mixture, and the solution was stirred continuously until the reaction was complete (12 h), as monitored by TLC. The reaction mixture was subsequently diluted with dichloromethane (DCM), washed thoroughly with water, dried over anhydrous sodium sulfate, and concentrated under reduced pressure. The crude mixture obtained was purified by silica gel column chromatography using 2–7% ethyl acetate/hexane as the mobile phase, furnishing the pure isoxazole products.

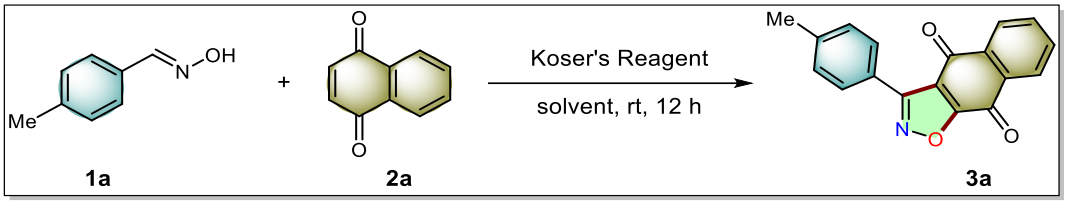
General Procedure for the Synthesis of 5 and 6

A pre-dried round-bottom flask (10 mL) equipped with a magnetic stir bar was loaded with Koser's reagent [PhI(OH)OTs] (0.70 mmol) to which THF (2 mL) was subsequently added under open-air conditions. The respective aldoxime (0.50 mmol) was then added to the flask under ambient temperature. Immediately after the addition, the heterogeneous reaction mixture converted into a clear solution. Subsequently, the derivative of phenylacetylene (0.75 mmol) or dialkyl acetylenedicarboxylate (0.75 mmol) was added to the reaction mixture, and the solution was stirred continuously until the reaction was complete (12 h), as monitored by TLC. The reaction mixture was subsequently diluted with dichloromethane (DCM), washed thoroughly with water, dried over anhydrous sodium sulfate, and concentrated under reduced pressure. The crude mixture obtained was purified by silica gel column chromatography using 2–8% ethyl acetate/hexane as the mobile phase, furnishing the pure isoxazole products.

Genral Procedure for the Synthesis of Koser's Regent [PhI(OH)OTs]

In a 1:1 DCM/Trifluoroethanol solution (15 mL), iodobenzene (2 mmol) was stirred and treated with 2 mmol of *meta*-chloroperbenzoic acid, followed by 2 mmol of *p*-toluenesulfonic acid monohydrate. After maintaining the reaction at room temperature for 30 minutes, the mixture was concentrated. The residue was subsequently washed with diethyl ether (10–15 mL). The solid was collected by filtration and dried *in vacuo* to afford Koser's reagent as a white solid.[2]

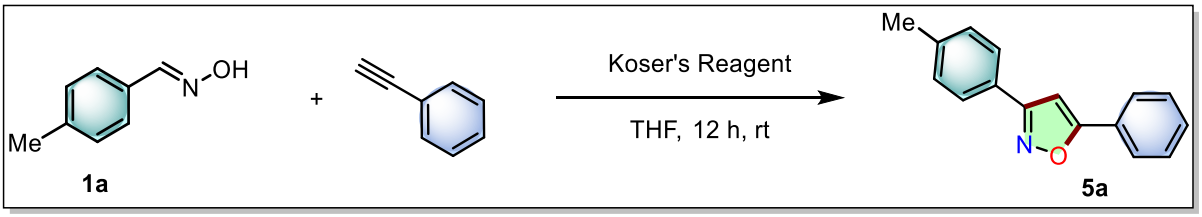
Table S1. Optimization of Reaction Conditions



Entry	Solvent	Yield (%)[b]
1.	without Koser's reagent	nr
2.	reactants in equimolar	71
3.	Reaction time 1 h instead of 12 h	72
4.	Reaction time 24 h instead of 12 h	80

Reaction conditions: [a]aldoxime **1a** (0.6 mmol), 1,4-napthaquinone **2a** (0.5 mmol) Koser's reagent (0.7 mmol), in solvent (2 mL) were stirred at room temperature. [b] Isolated yield of the product after column chromatography.

Table S2. Optimization of Reaction Conditions



Entry	Solvent	Yield (%)[b]
1.	DMSO	52
2.	DCM	42
3.	$CHCl_3$	44
4.	MeOH	70
5.	EtOH	68
6.	DMF	73
7.	DCE	34
8.	EtOAc	58
9.	Acetone	78
10	**THF**	**79**
11.	H_2O	traces
12.	Hexane	traces
13.	Toluene	traces
14.	1,4-Dioxane	77
15.	without Koser's reagent	Nr
16.	reactants in equimolar	70

Reaction conditions*:* All the reactions were performed with arylaldoxime **1a** (0.5 mmol), arylacetylene (0.75 mmol) and Koser's reagent (0.7 mmol), in THF (2 mL) at room temperature for 12 h. [b] Yields correspond to isolated products.

General Procedure for Gram-scale Synthesis of 3a and 5c

For 3a

A pre-dried round-bottom flask (25 mL) equipped with a magnetic stir bar was loaded with Koser's reagent [PhI(OH)OTs] (8.85 mmol) to which 1,4-dioxane (12 mL) was subsequently added under open-air conditions. The respective aldoxime (7.59 mmol, 1.03 g) was then added to the flask under ambient temperature. Immediately after the addition, the heterogeneous reaction mixture converted into a clear solution. Subsequently, 1,4-naphthoquinone (6.32 mmol, 1.00 g) was added to the reaction mixture, and the solution was stirred continuously until the reaction was complete (12 h), as monitored by TLC. The reaction mixture was subsequently diluted with dichloromethane (DCM), washed thoroughly with water, dried over anhydrous sodium sulfate, and concentrated under reduced pressure. The crude mixture obtained was purified by silica gel column chromatography using 3% ethyl acetate/hexane as mobile phase, furnishing the pure isoxazole product in 78% yield (1.42 g).

For 5c

A pre-dried round-bottom flask (25 mL) equipped with a magnetic stir bar was loaded with Koser's reagent [PhI(OH)OTs] (11.54 mmol) to which THF (15 mL) was subsequently added under open-air conditions. The respective aldoxime (8.25 mmol, 1.0 g) was then added to the flask under ambient temperature. Immediately after the addition, the heterogeneous reaction mixture converted into a clear solution. Subsequently, phenyl acetylene (12.37 mmol, 1.26 g) was added to the reaction mixture, and the solution was stirred continuously until the reaction was complete (12 h), as monitored by TLC. The reaction mixture was subsequently diluted with dichloromethane, washed thoroughly with water, dried over anhydrous sodium sulfate, and concentrated under reduced pressure. The crude mixture obtained was purified by silica gel column chromatography using 2% ethyl acetate/hexane as mobile phase, furnishing the pure isoxazole product in 79% yield (1.44 g).

General Procedures and Experimental Details of Synthetic Transformations (7, 8, 9 & 10)

A pre-dried 10 mL round-bottom flask with a stir bar was charged with **3a** (0.115 g, 0.4 mmol), followed by the addition of 3 mL triethylamine and 5 mL acetic anhydride. The mixture was refluxed for 4 hours, and TLC indicated the completion of the reaction. Upon cooling, the crude mixture was washed with water, extracted using DCM, and concentrated. Subsequent purification by flash chromatography (15% hexane/ethyl acetate) afforded compound **7** as a sticky solid in 68% yield.

In a 10 mL oven-dried round-bottom flask, Compound **3c** (0.071 g, 0.23 mmol) was dissolved in 2 mL of 35% HBr in acetic acid. Then the reaction mixture was heated at reflux for 5 h. After completing the reaction, as monitored by thin layer chromatography. The reaction mixture was cooled to room temperature. The reaction mixture was treated with saturated sodium bicarbonate solution and extracted with DCM. Then the organic layer was washed with water and dried over anhydrous sodium sulfate. Subsequent solvent removal under reduced pressure produced a crude product that was purified by flash chromatography (12% ethyl acetate/hexane) to afford compound **8** as an orange viscous product in 74% yield.

Compound **9** was synthesized according to the following protocol. An oven-dried 10 mL Schlenk tube fitted with a magnetic stir bar was charged with dibromo compound **5s** (0.035 g, 0.106 mmol, 1.0 equiv), phenylboronic acid (0.019 g, 0.16 mmol, 1.5 equiv), and K_2CO_3 (0.037 g, 0.265 mmol,

2.5 equiv). A solvent mixture of H_2O:1,4-dioxane (1:3, 2 mL) was added under a nitrogen atmosphere, and the reaction mixture was purged with nitrogen for 5 min. Subsequently, $Pd(PPh_3)_4$ (0.005 g, 5 mol%) was introduced, followed by an additional nitrogen purge for 5 min. The reaction was heated at 100 °C in an oil bath for 24 h. After completion was confirmed by TLC, the mixture was filtered through a Celite pad and washed with ethyl acetate. Solvent removal under reduced pressure afforded a crude residue that was purified by silica gel column chromatography (hexane/ethyl acetate) to give compound **9** in 79% yield.

In an oven-dried 10 mL round-bottom flask, compound **5a** (0.43 mmol) was combined with *N*-iodosuccinimide (0.86 mmol), followed by the addition of 4 mL acetic acid. The reaction mixture was then heated to 130 °C. After 6 h, progress was assessed by TLC. Upon completion, the reaction mixture was washed sequentially with sodium thiosulfate solution, water, and DCM. The crude residue was purified by column chromatography (hexane/ethyl acetate) to give the desired product **10** as a white solid.

X-Ray Crystallographic Data: Crystals of **3r**/**3t**/**5a** were obtained by dissolving the compounds in an appropriate solvent and enabling slow solvent evaporation at 25 °C. A well-formed crystal was isolated, mounted on a glass fiber using paraffin oil and subjected to data collection at 100 K on a Bruker Kappa (D8 QUEST) Apex-II CCD system with graphite-monochromated Mo-Kα radiation (λ = 0.71073 Å). The structures were solved using APEX4 and Olex2 software. The finalized crystallographic results have been deposited with the **CCDC** under the assigned deposition number.

Compound 3r

The crystallization of **3r** was accomplished through dissolution in $CDCl_3$, with the solvent left to evaporate slowly at 25 °C.

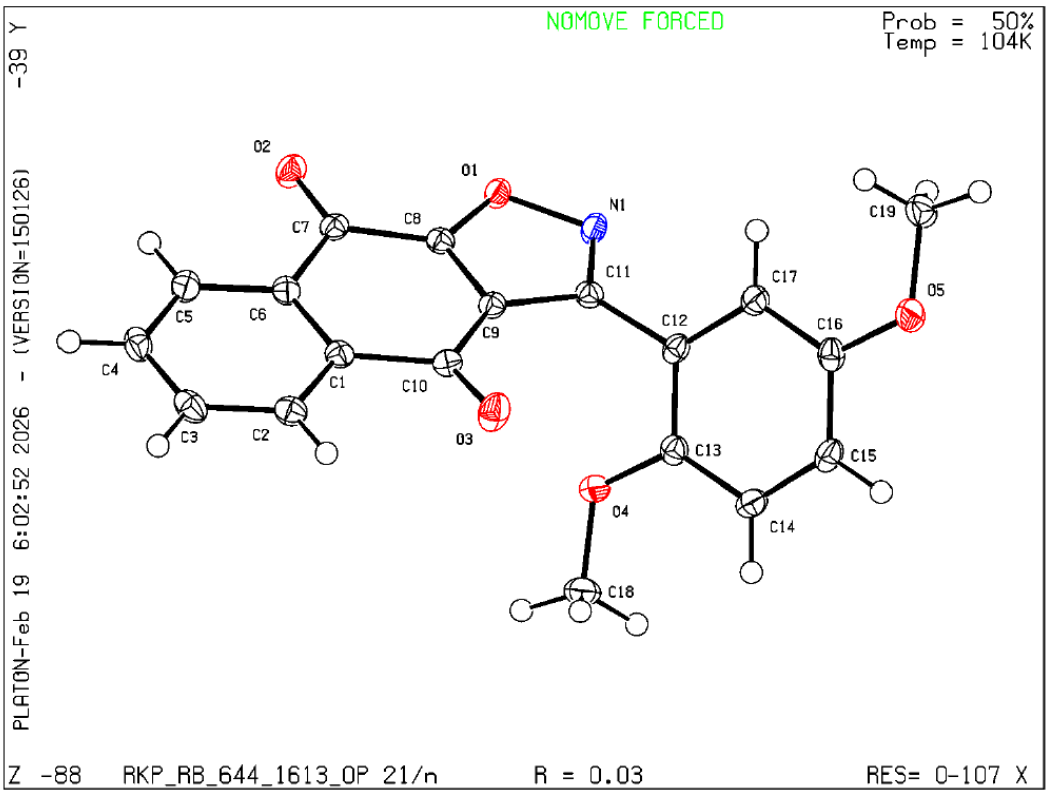


Figure S3. The ORTEP plot and crystallographic data for compound **3r**.

Table S3. X-Ray crystallographic data of **3r**

CCDC	2513848
Formula	$C_{19}H_{13}NO_5$
Formula weight	335.30
Crystal system	monoclinic
Space group	P 21/n
a (Å)	12.7597(5)
b (Å)	6.7156(2)
c (Å)	17.4401(6)
α (°)	90
β (°)	95.4980(10)
γ (°)	90
Volume ($Å^3$)	1487.55(9)
Z	4
Density (g/cm^3)	1.497
Absorption coefficient (mm^{-1})	0.110
Temp. (K)	104 K
Total reflns.	24150
Indepnt. reflns.	2728
Final R indices [I > 2σ(I)]	$R_1 = 0.0333$, $wR_2 = 0.0911$
R indices (all data)	$R_1 = 0.0359$, $wR_2 = 0.0934$

Compound 3t

The crystallization of **3t** was accomplished through dissolution in $CDCl_3$, with the solvent left to evaporate slowly at 25 °C.

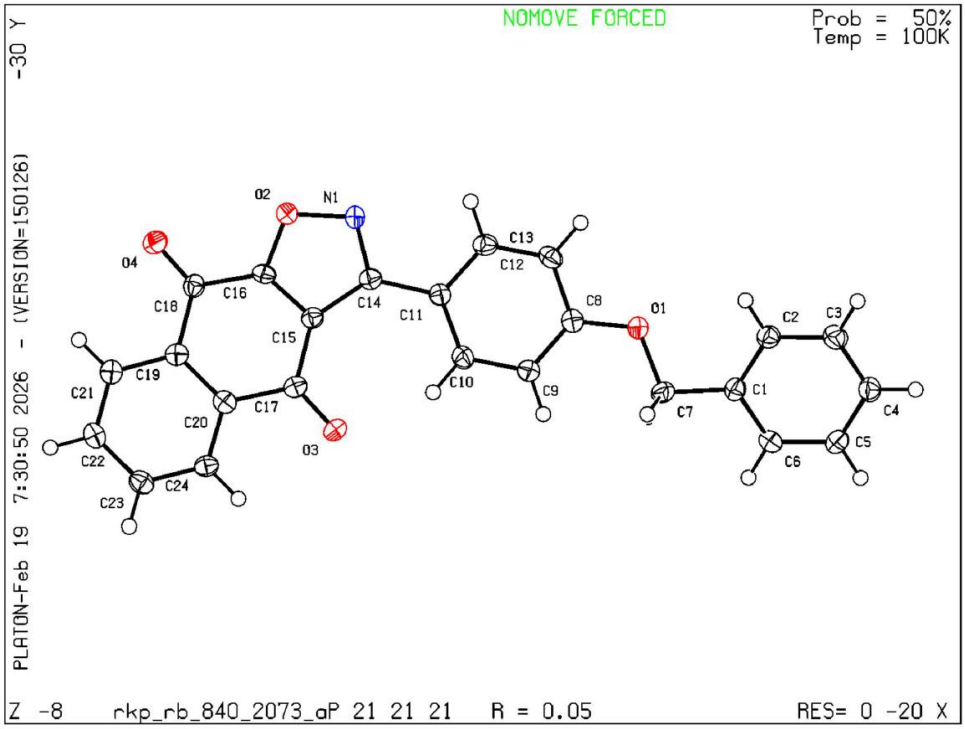


Figure S4. The ORTEP plot and crystallographic data for compound **3t**.

Table S4. X-Ray crystallographic data of **3t**

CCDC	2513849
Formula	$C_{24}H_{15}NO_4$
Formula weight	381.37
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a (Å)	6.684(3)
b (Å)	13.176(6)
c (Å)	19.701(9)
α (°)	90
β (°)	90
γ (°)	90
Volume (Å^3)	1735.0(13)
Z	4
Density (g/cm^3)	1.460
Absorption coefficient (mm^{-1})	0.100
Temp. (K)	100 K
Total reflns.	21461
Indepnt. reflns.	3050
Final R indices [I > 2σ(I)]	R_1 = 0.0454, wR_2 = 0.1026
R indices (all data)	R_1 = 0.0534, wR_2 = 0.1101

Compound 5a

The crystallization of **5a** was accomplished through dissolution in $CDCl_3$, with the solvent left to evaporate slowly at 25 °C.

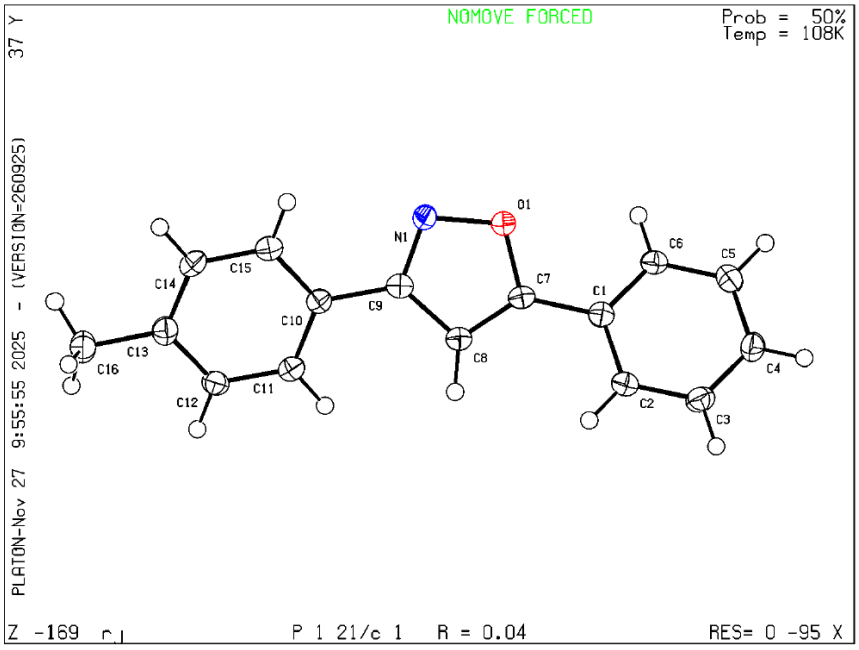


Figure S5. The ORTEP plot and crystallographic data for compound **5a**.

Table S5. X-Ray crystallographic data of **5a**

CCDC	2513852
Formula	$C_{16}H_{13}NO$
Formula weight	941.09
Crystal system	monoclinic
Space group	$P2_1/c$
a (Å)	12.0197(5)
b (Å)	17.7856(8)
c (Å)	12.4927(6)
α (°)	90
β (°)	152.9491(10)
γ (°)	90
Volume (Å^3)	1214.57(10)
Z	4
Density (g/cm^3)	1.287
Absorption coefficient (mm^{-1})	0.080
Temp. (K)	108 K
Total reflns.	46846
Indepnt. reflns.	2128
Final R indices [I > 2σ(I)]	R_1 = 0.0405, wR_2 = 0.0978
R indices (all data)	R_1 = 0.0429, wR_2 = 0.1000

Emission spectra of Compound 3a

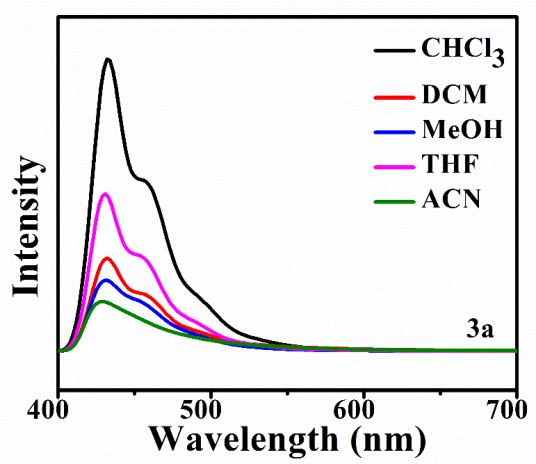


Figure S6. Emission spectra of compound **3a**.

Compound	Solvent	λ_{ex} (nm)	λ_{emi} (nm)	Strokes shift (cm^{-1})
3a	$CHCl_3$	340.0	432	6260
	ACN	337.0	428	6310
	MeOH	337.0	431	6470
	THF	335.0	430	6610
	DCM	341.0	431	6120

Table S6. Photophysical data for compound **3a** in solvents of different polarity.

Cyclic Voltammogram of Compound 3a

Electrochemical characterization was carried out using a Multi Autolab/M204 potentiostat/galvanostat (Metrohm Autolab B.V., The Netherlands) under a three-electrode arrangement, where Ag/AgCl and Pt wire served as the reference and counter electrodes, respectively. The working electrodes were fabricated by a drop-casting method. Specifically, a slurry consisting of 20 mg active material, 2.5 mg PVDF, and 2.5 mg carbon black was dispersed in 300 µL *N*-methyl-2-pyrrolidone (NMP). After uniform mixing, the slurry was deposited onto a pre-treated nickel foam (1 × 1 cm^2) and dried at 60 °C overnight. The final catalyst loading was adjusted to approximately 3.96 mg cm^{-2}. Cyclic voltammetry experiments were conducted in 2.0 M KOH electrolyte over a potential range of −0.0 to 0.5 V vs Ag/AgCl at a scan rate of 50 mV s^{-1}.

Optimized Structure of Compound 3a

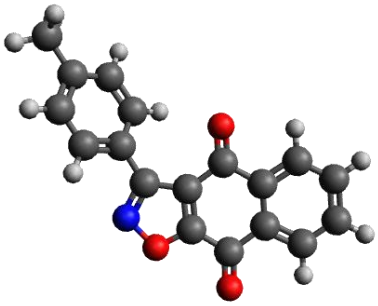


Figure S7. Optimised structure of the compound **3a** obtained by DFT calculations in DCM solution.

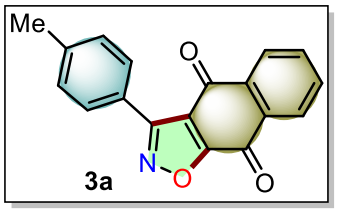
XYZ Coordinates of 3a in S_0 optimized geometry

C	-1.96449950620771	-0.69173316139548	1.95741176935663
C	-0.62874998260064	-1.04013412830837	1.79108406316096
C	0.18190956597566	-0.33352350457000	0.90693924537423
C	-0.36815451668217	0.74389467444323	0.18040078152210
C	-1.70768320546017	1.08689677582308	0.35546789658530
C	-2.50477374313396	0.37198538402098	1.24007199371539
H	-2.58348754131427	-1.25048484820111	2.64771552487206
H	-0.20192511487556	-1.86480539227174	2.34567652617200

C	1.61716412361867	-0.75166971873913	0.76614677792570
C	0.45098291973923	1.53589864139834	-0.77349873437974
H	-2.11309925731553	1.91664979028043	-0.20804316259842
H	-3.54439973739806	0.64378397087469	1.36999184182840
C	1.84361080285030	1.06344184580054	-0.88159246101310
C	2.39593838964786	0.01004341675860	-0.21807141053980
O	2.09148919819609	-1.65115310649238	1.43786123771060
O	0.03754805485483	2.48454251153435	-1.41362930529106
C	3.76213204351337	-0.00041961529845	-0.66518331609129
N	3.95677270288045	0.97619283821729	-1.52523322311248
O	2.73976367783260	1.65813696362994	-1.66052345337967
C	4.87925076181897	-0.88693185940442	-0.31392982821338
C	6.17598394462471	-0.37161612377753	-0.20976266190820
C	4.67958556157094	-2.25667492681843	-0.12509530362558
C	7.24208164024359	-1.20993591817508	0.08154192103947
H	6.34332971573180	0.68857078709580	-0.34861446770355
C	5.75441635605445	-3.08768995783699	0.15751161342609
H	3.68519846717252	-2.67168718381119	-0.20461565336048
C	7.05186751390423	-2.58156159314320	0.27161687346781
H	8.23904428296438	-0.79296482265916	0.16455672883169
H	5.58276371530778	-4.14940727027223	0.29132913169222
C	8.20642534271792	-3.48114532353359	0.62044858009822
H	9.13719953759501	-3.12074338608747	0.17973629815242
H	8.34972068131897	-3.51640616048727	1.70477620333110
H	8.03102861485360	-4.50259560859402	0.27994777295435

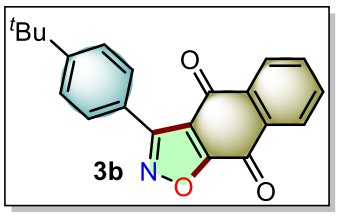
Spectroscopic Data of Compounds

1. 3-(*p*-Tolyl)naphtho[2,3-*d*]isoxazole-4,9-dione (3a)



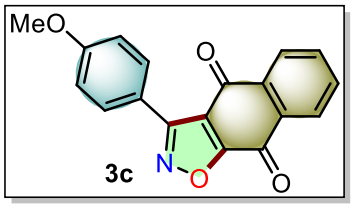
Compound **3a** was synthesized according to the general procedure through the treatment of 4-methylbenzaldehyde oxime (0.081 g, 0.60 mmol) and 1,4-naphthoquinone (0.079 g, 0.50 mmol) with Koser's reagent (0.275 g, 0.70 mmol) in 2 mL of 1,4-dioxane at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **3a** (0.115 g, 80%) as a light yellow solid. **MP**: 152.4–153.2 °C; **^{1}H NMR (500 MHz, CDCl$_3$)**: δ 8.26 (dd, *J* = 7.2, 6.0 Hz, 2H), 8.07–8.03 (m, 2H), 7.88–7.79 (m, 2H), 7.36–7.31 (m, 2H), 2.44 (s, 3H). **^{13}C NMR (126 MHz, CDCl$_3$)**: δ 178.6, 173.3, 166.2, 160.9, 141.7, 135.2, 134.2, 133.8, 131.8, 129.4, 129.3, 127.7, 127.2, 123.2, 119.5, 21.6; **HRMS (ESI)**: m/z calcd for $C_{18}H_{12}NO_3^+$ $[M+H]^+$ 290.0812; found: 290.0811; **IR (cm^{-1})**: ν_{max} 3089, 3028, 2959, 2917, 2857, 1680, 1578, 1438, 1341, 1298, 1256, 1207, 1164, 1008, 718.

2. 3-(4-(*tert*-Butyl)phenyl)naphtho[2,3-*d*]isoxazole-4,9-dione (3b)



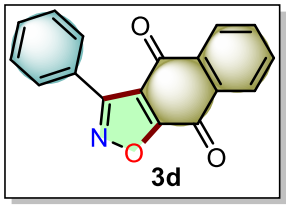
Compound **3b** was synthesized according to the general procedure through the treatment of 4-(*tert*-butyl)benzaldehyde oxime (0.106 g, 0.6 mmol) and 1,4-naphthoquinone (0.079 g, 0.5 mmol) with Koser's reagent (0.275 g, 0.7 mmol) in 2 mL of 1,4-dioxane at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **3b** (0.129 g, 78%) as a light yellow solid. **MP**: 112.5–113.3 °C; **^{1}H NMR (500 MHz, CDCl$_3$)**: δ 8.30–8.25 (m, 2H), 8.12–8.10 (m, 1H), 8.09 (d, *J* = 2.0 Hz, 1H), 7.85 (m, 2H), 7.58 (s, 1H), 7.56 (s, 1H), 1.39 (s, 9H); **^{13}C NMR (126 MHz, CDCl$_3$)**: δ 178.7, 173.4, 166.2, 160.9, 154.7, 135.3, 134.3, 133.8, 131.8, 129.1, 127.7, 127.2, 125.7, 123.2, 119.6, 35.0, 31.2. **HRMS (ESI)**: m/z calcd for $C_{21}H_{18}NO_3^+$ $[M+H]^+$ 332.1281; found: 332.1281; **IR (cm^{-1})**: ν_{max} 2953, 2903, 2864, 1678, 1587, 1433, 1339, 1262, 1202, 1178, 719.

3. 3-(4-Methoxyphenyl)naphtho[2,3-*d*]isoxazole-4,9-dione (3c)



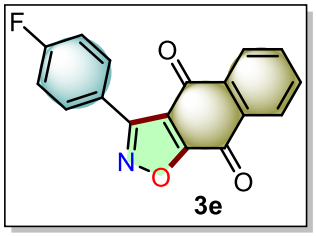
Compound **3c** was synthesized according to the general procedure through the treatment of 4-methoxybenzaldehyde oxime (0.091 g, 0.6 mmol) and 1,4-naphthoquinone (0.079 g, 0.5 mmol) with Koser's reagent (0.275 g, 0.7 mmol) in 2 mL of 1,4-dioxane at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **3c** (0.105 g, 69%) as a light yellow solid. **MP**: 132.6–133.4; **^{1}H NMR (500 MHz, CDCl$_3$)**: δ 8.28 (d, *J* = 6.3 Hz, 2H), 8.18 (d, *J* = 8.6 Hz, 2H), 7.90–7.81 (m, 2H), 7.06 (d, *J* = 8.6 Hz, 2H), 3.90 (s, 3H); **^{13}C NMR (126 MHz, CDCl$_3$)**: δ 178.8, 173.4, 166.2, 162.0, 160.6, 135.3, 134.2, 133.8, 131.8, 131.0, 130.2, 129.8, 128.3, 127.7, 127.2, 119.5, 118.5, 114.1, 55.4. **HRMS (ESI)**: m/z calcd for $C_{18}H_{12}NO_4^+$ $[M + H]^+$ 306.0761; found: 306.0758; **IR (cm^{-1})**: ν_{max} 3077, 3011, 2972, 2929, 2838, 1680, 1596, 1518, 1429, 1336, 1299, 1254, 1209, 1168, 1031, 721.

4. 3-Phenylnaphtho[2,3-*d*]isoxazole-4,9-dione (3d)



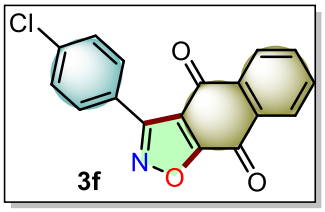
Compound **3d** was synthesized according to the general procedure through the treatment of benzaldehyde oxime (0.073 g, 0.6 mmol) and 1,4-naphthoquinone (0.079 g, 0.5 mmol) with Koser's reagent (0.275 g, 0.7 mmol) in 2 mL of 1,4-dioxane at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **3d** (0.109 g, 79%) as a light yellow solid. **MP**: 130.8–131.6 °C; **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 8.28 (m, 2H), 8.16 (dd, *J* = 7.8, 1.7 Hz, 2H), 7.89–7.81 (m, 2H), 7.58–7.53 (m, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 178.7, 173.4, 166.3, 161.0, 138.7, 135.3, 134.3, 133.8, 131.8, 131.3, 129.4, 128.7, 127.7, 127.3, 126.1, 119.6; **HRMS (EI)**: m/z: calcd for $C_{17}H_{10}NO_3^+$ $[M+H]^+$ 276.0655, found 276.0659; **IR (cm^{-1})**: ν_{max} 3070, 2922, 2852, 1682, 1585, 1426, 1339, 1308, 1262, 1203, 1173, 718.

5. 3-(4-Fluorophenyl)naphtho[2,3-*d*]isoxazole-4,9-dione (3e)



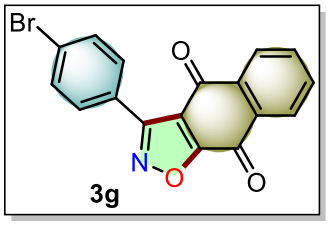
Compound **3e** was synthesized according to the general procedure through the treatment of 4-fluorobenzaldehyde oxime (0.083 g, 0.6 mmol) and 1,4-naphthoquinone (0.079 g, 0.5 mmol) with Koser's reagent (0.275 g, 0.7 mmol) in 2 mL of 1,4-dioxane at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **3e** (0.123 g, 84%) as a light yellow solid. **MP**: 164.9–165.6; **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 8.28–8.23 (m, 2H), 8.23–8.18 (m, 2H), 7.89–7.80 (m, 2H), 7.24–7.19 (m, 2H). **^{13}C NMR (126 MHz, $CDCl_3$)**: 178.7, 173.2, 166.3, 165.6, 163.6, 160.0, 135.4, 134.4, 133.6, 131.6 131.6, 127.7, 127.3, 122.3, 122.3, 119.4, 116.0, 115.8. **^{19}F NMR (471 MHz, $CDCl_3$)**: δ –107.97 to –107.92 (m, 1F); **HRMS (EI)**: m/z: calcd for $C_{17}H_9FNO_3^+$ $[M+H]^+$ 294.0561, found 294.0563; **IR (cm^{-1})**: ν_{max} 3084, 3032, 1684, 1599, 1584, 1519, 1431, 1340, 1303, 1235, 1205, 1167, 1005, 714.

6. 3-(4-Chlorophenyl)naphtho[2,3-*d*]isoxazole-4,9-dione (3f)



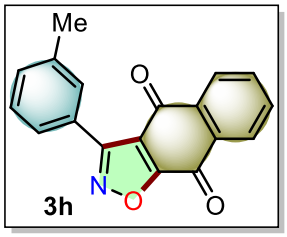
Compound **3f** was synthesized according to the general procedure through the treatment of 4-chlorobenzaldehyde oxime (0.093 g, 0.6 mmol) and 1,4-naphthoquinone (0.079 g, 0.5 mmol) with Koser's reagent (0.275 g, 0.7 mmol) in 2 mL of 1,4-dioxane at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **3f** (0.126 g, 82%) as a light yellow solid. **MP:** 160.2–161.0; **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 8.29–8.25 (m, 2H), 8.17–8.14 (m, 2H), 7.89–7.82 (m, 2H), 7.53–7.50 (m, 2H). **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 178.7, 173.2, 166.4, 160.0, 137.6, 135.4, 134.4, 133.6, 131.7, 130.7, 129.0, 127.8, 127.3, 124.6, 119.4; **HRMS (EI)**: m/z: calcd for $C_{17}H_9ClNO_3^+$ $[M+H]^+$ 310.0265, found 310.0266; **IR (cm^{-1})**: ν_{max} 3082, 2921, 2855, 1680, 1595, 1581, 1442, 1339, 1266, 1212, 1194, 1094, 1006, 718.

7. 3-(4-Bromophenyl)naphtho[2,3-*d*]isoxazole-4,9-dione (3g)



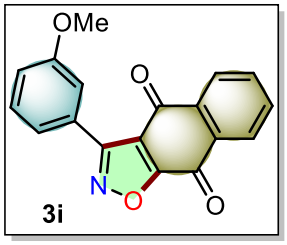
Compound **3g** was synthesized according to the general procedure through the treatment of (4-bromobenzaldehyde oxime (0.120 g, 0.6 mmol) and 1,4-naphthoquinone (0.079 g, 0.5 mmol) with Koser's reagent (0.275 g, 0.7 mmol) in 2 mL of 1,4-dioxane at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **3g** (0.124 g, 70%) as a light yellow solid. **MP**: 177.3–178.1; **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 8.27–8.22 (m, 2H), 8.06 (d, J = 8.5 Hz, 2H), 7.85 (m, 2H), 7.66 (d, J = 8.4 Hz, 2H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 178.6, 173.1, 166.4, 160.1, 135.4, 134.4, 133.6, 131.9, 131.7, 130.8, 127.8, 127.3, 126.1, 125.1, 119.4. ; **HRMS (EI)**: m/z: calcd for $C_{17}H_9BrNO_3^+$ $[M+H]^+$ 353.9760, found 353.9755; **IR (cm^{-1})**: ν_{max} 2920, 2844, 1683, 1587, 1566, 1441, 1333, 1300, 1261, 1200, 1177, 1044, 1005, 715.

8. 3-(*m*-Tolyl)naphtho[2,3-*d*]isoxazole-4,9-dione (3h)



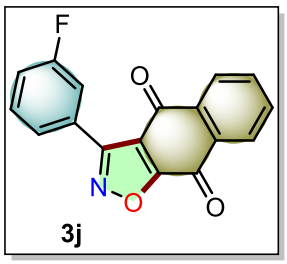
Compound **3h** was synthesized according to the general procedure through the treatment of 3-methylbenzaldehyde oxime (0.081 g, 0.60 mmol) and 1,4-naphthoquinone (0.079 g, 0.5 mmol) with Koser's reagent (0.275 g, 0.7 mmol) in 2 mL of 1,4-dioxane at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **3h** (0.113 g, 78%) as a light yellow solid. **MP**: 142.4–143.2 °C; **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 8.30–8.24 (m, 2H), 7.95 (d, J = 9.2 Hz, 2H), 7.89–7.81 (m, 2H), 7.43 (t, J = 7.6 Hz, 1H), 7.38 (d, J = 7.6 Hz, 1H), 2.47 (s, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 178.6, 173.4, 166.2, 161.1, 138.5, 135.3, 134.3, 133.8, 132.1, 131.8, 129.8, 128.5, 127.7, 127.2, 126.6, 126.0, 119.6, 21.4; **HRMS (ESI)**: m/z calcd for $C_{18}H_{12}NO_3^+$ $[M + H]^+$ 290.0812; found: 290.0816; **IR (cm^{-1})**: ν_{max} 3070, 1683, 1585, 1424, 1383, 1335, 1303, 1267, 1206, 1169, 719.

9. 3-(3-Methoxyphenyl)naphtho[2,3-*d*]isoxazole-4,9-dione (3i)



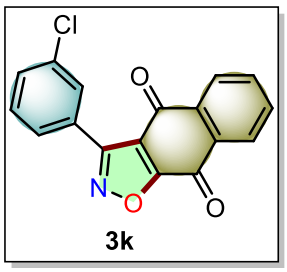
Compound **3i** was synthesized according to the general procedure through the treatment of 3-methoxybenzaldehyde oxime (0.091 g, 0.6 mmol) and 1,4-naphthoquinone (0.079 g, 0.5 mmol) with Koser's reagent (0.275 g, 0.7 mmol) in 2 mL of 1,4-dioxane at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **3i** (0.80 g, 53%) as a light yellow solid. **MP**: 172.8–173.6 °C; **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 8.30–8.24 (m, 2H), 7.88–7.81 (m, 2H), 7.79–7.75 (m, 2H), 7.44 (t, J = 8.2 Hz, 1H), 7.10 (m, 1H), 3.92 (s, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 178.6, 173.3, 166.3, 160.9, 159.6, 135.3, 134.3, 133.8, 131.7, 129.7, 127.8, 127.2, 121.7, 119.6, 117.6, 114.3, 55.5; **HRMS (ESI)**: m/z calcd for $C_{18}H_{12}NO_4^+$ $[M + H]^+$ 306.0761; found: 306.0764; **IR (cm^{-1})**: ν_{max} 3089, 2921, 2848, 1675, 1585, 1565, 1467, 1334, 1272, 1206, 1173, 1010, 721.

10. 3-(3-Fluorophenyl)naphtho[2,3-*d*]isoxazole-4,9-dione (3j)



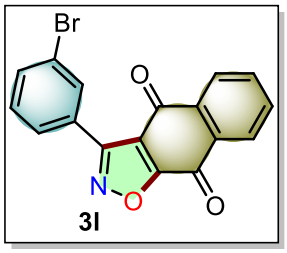
Compound **3e** was synthesized according to the general procedure through the treatment of 3-fluorobenzaldehyde oxime (0.083 g, 0.6 mmol) and 1,4-naphthoquinone (0.079 g, 0.5 mmol) with Koser's reagent (0.275 g, 0.7 mmol) in 2 mL of 1,4-dioxane at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **3j** (0.117 g, 80%) as a light yellow solid. **MP**: 161.5–162.3; **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 8.28–8.24 (m, 2H), 8.01–7.99 (m, 1H), 7.89–7.82(m, 1H), 7.89–7.82 (m, 2H), 7.51 (m, 1H), 7.28–7.23 (m, 1H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 178.5, 173.2, 166.4, 162.6 (d, J = 246.6 Hz), 159.9, 135.4, 134.4, 133.6, 131.7, 130.3 (d, J = 7.5 Hz), 128.1 (d, J = 7.0 Hz), 127.8, 127.3, 125.1, 119.4, 118.3 (d, J = 21.5 Hz), 116.6, 116.4; **^{19}F NMR (500 MHz, $CDCl_3$)**: δ –111.52 to –111.57 (m, 1F). **HRMS (EI)**: m/z: calcd for $C_{17}H_9FNO_3^+$ $[M+H]^+$ 294.0561, found 294.0556; **IR (cm^{-1})**: ν_{max} 3084, 3065, 1690, 1673, 1583, 1464, 1453, 1339, 1269, 1204, 729.

11. 3-(3-Chlorophenyl)naphtho[2,3-*d*]isoxazole-4,9-dionedione (3k)



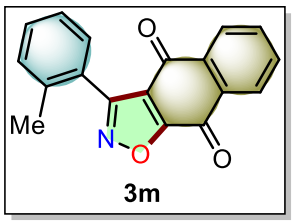
Compound **3k** was synthesized according to the general procedure through the treatment of 3-chlorobenzaldehyde oxime (0.093 g, 0.6 mmol) and 1,4-naphthoquinone (0.079 g, 0.5 mmol) with Koser's reagent (0.275 g, 0.7 mmol) in 2 mL of 1,4-dioxane at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **3k** (0.115 g, 74%) as a beige solid. **MP**: 148.2–149.0 °C; **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 8.28 – 8.26 (m, 2H), 8.22–8.19 (m, 1H), 8.11–8.08 (m, 1H), 7.89–7.83 (m, 2H), 7.55–7.52 (m, 1H), 7.48 (t, J = 7.9 Hz, 1H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 178.5, 173.1, 166.4, 159.8, 135.4, 134.7, 134.5, 133.6, 131.7, 131.4, 130.0, 129.3, 127.8, 127.5, 127.3, 119.4; **HRMS (EI)**: m/z: calcd for $C_{17}H_9ClNO_3^+$ $[M+H]^+$ 310.0265, found 310.0261; **IR (cm^{-1})**: ν_{max} 3084, 2919, 1676, 1591, 1551, 1418, 1377, 1340, 1299, 1208, 1165, 1079, 1005, 718.

12. 3-(3-Bromophenyl)naphtho[2,3-*d*]isoxazole-4,9-dione (3l)



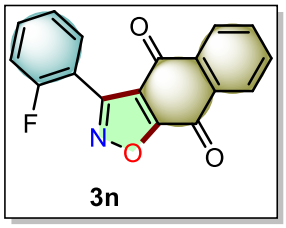
Compound **3l** was synthesized according to the general procedure through the treatment of (3-bromobenzaldehyde oxime (0.120 g, 0.6 mmol) and 1,4-naphthoquinone (0.079 g, 0.5 mmol) with Koser's reagent (0.275 g, 0.7 mmol) in 2 mL of 1,4-dioxane at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **3l** (0.145 g, 82%) as a light yellow solid. **MP**: 168.6–169.4 °C; **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 8.37 (t, J = 1.7 Hz, 1H), 8.30–8.26 (m, 2H), 8.16–8.13 (m, 1H), 7.90–7.82 (m, 2H), 7.71–7.68 (m, 1H), 7.42 (t, J = 7.9 Hz, 1H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 178.5, 173.2, 166.4, 159.8, 135.4, 134.5, 134.3, 133.6, 132.2, 131.7, 130.2, 128.1, 128.0, 127.8, 127.3, 122.7, 119.4; **HRMS (EI)**: m/z: calcd for $C_{17}H_9BrNO_3^+$ $[M+H]^+$ 353.9760, found 353.9754; **IR (cm^{-1})**: ν_{max} 3080, 2918, 2853, 1672, 1585, 1551, 1420, 1378, 1300, 1259, 1203, 1166, 1112, 1072, 1001, 717.

13. 3-(*o*-Tolyl)naphtho[2,3-*d*]isoxazole-4,9-dione (3m)



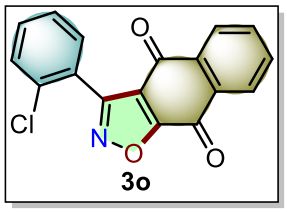
Compound **3m** was synthesized according to the general procedure through the treatment of 2-methylbenzaldehyde oxime (0.081 g, 0.60 mmol) and 1,4-naphthoquinone (0.079 g, 0.5 mmol) with Koser's reagent (0.275 g, 0.7 mmol) in 2 mL of 1,4-dioxane at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **3m** (0.094 g, 65%) as a light yellow solid. **MP**: 183.1–183.9 °C; **^{1}H NMR (500 MHz, CDCl$_3$)**: δ 8.30–8.25 (m, 1H), 8.20–8.16 (m, 1H), 7.84–7.81 (m, 2H), 7.45 (ddd, *J* = 8.9, 7.5, 1.7 Hz, 2H), 7.39–7.30 (m, 2H), 2.33 (s, 3H); **^{13}C NMR (126 MHz, CDCl$_3$)**: δ 178.5, 173.4, 165.4, 160.8, 137.6, 135.2, 134.3, 133.5, 132.0, 130.6, 130.2, 127.4, 127.4, 125.8, 125.5, 120.6, 20.1; **HRMS (ESI)**: m/z calcd for $C_{18}H_{12}NO_3^+$ $[M+H]^+$ 290.0812; found: 290.0814; **IR (cm^{-1})**: ν_{max} 3070, 2920, 2854, 1680, 1584, 1452, 1336, 1268, 1195, 1081, 1036, 723.

14. 3-(2-Fluorophenyl)naphtho[2,3-*d*]isoxazole-4,9-dione (3n)



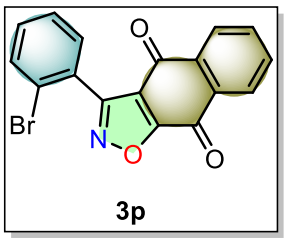
Compound **3n** was synthesized according to the general procedure through the treatment of 2-fluorobenzaldehyde oxime (0.083 g, 0.6 mmol) and 1,4-naphthoquinone (0.079 g, 0.5 mmol) with Koser's reagent (0.275 g, 0.7 mmol) in 2 mL of 1,4-dioxane at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **3n** (0.130 g, 89%) as a light yellow solid. **MP**: 191.5–192.3 °C; **^{1}H NMR (500 MHz, CDCl$_3$)**: δ 8.31–8.28 (m, 1H), 8.23–8.20 (m, 1H), 7.87–7.81 (m, 2H), 7.72–7.68 (m, 1H), 7.67–7.56(m, 1H), 7.35–7.27 (m, 2H); **^{13}C NMR (126 MHz, CDCl$_3$)**: δ 178.1, 173.2, 165.5, 160.5 (d, *J* = 253.2 Hz), 156.3, 135.3, 134.3, 133.6, 133.0 (d, *J* = 8.2 Hz), 132.0, 131.1, 127.5 (d, *J* = 8.0 Hz), 124.4, 120.6, 116.2 (d, *J* = 21.2 Hz), 114.7, 114.6; **^{19}F NMR (471 MHz, CDCl$_3$)**: δ –111.10 to –111.15 (m, 1F); **HRMS (EI)**: m/z: calcd for $C_{17}H_9FNO_3^+$ $[M+H]^+$ 294.0561, found 294.0561; **IR (cm^{-1})**: ν_{max} 2923, 2852, 1683, 1584, 1464, 1437, 1334, 1259, 1226, 1199, 1159, 1120, 1083, 1005, 762.

15. 3-(2-Chlorophenyl)naphtho[2,3-*d*]isoxazole-4,9-dione (3o)



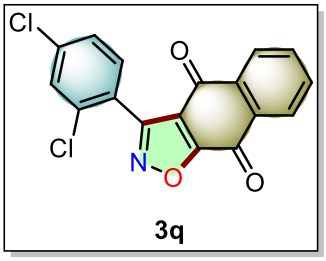
Compound **3o** was synthesized according to the general procedure through the treatment of 2-chlorobenzaldehyde oxime (0.093 g, 0.6 mmol) and 1,4-naphthoquinone (0.079 g, 0.5 mmol) with Koser's reagent (0.275 g, 0.7 mmol) in 2 mL of 1,4-dioxane at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **3o** (0.134 g, 87%) as a peach yellow solid. **MP**: 188.3–189.1 °C; **^{1}H NMR (500 MHz, CDCl$_3$)**: δ 8.29 (dd, *J* = 4.7, 2.3 Hz, 1H), 8.21–8.17 (m, 1H), 7.84 (dd, *J* = 5.2, 3.1 Hz, 2H), 7.61–7.51 (m, 3H), 7.43 (t, *J* = 7.4 Hz, 1H); **^{13}C NMR (126 MHz, CDCl$_3$)**: δ 178.1, 173.2, 165.2, 158.9, 135.2, 134.4, 134.1, 133.4, 131.9, 131.3, 129.9, 127.4, 126.9, 125.7, 120.9; **HRMS (EI)**: m/z: calcd for $C_{17}H_9ClNO_3^+$ $[M+H]^+$ 310.0265, found 310.0265; **IR (cm^{-1})**: ν_{max} 2954, 2922, 2852, 1683, 1590, 1501, 1435, 1407, 1333, 1303, 1199, 1159, 1106, 1034, 1000, 713.

16. 3-(2-Bromophenyl)naphtho[2,3-*d*]isoxazole-4,9-dione (3p)



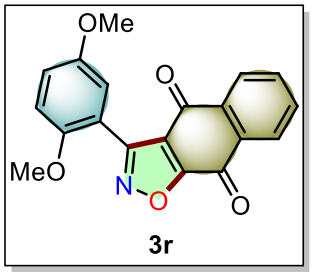
Compound **3p** was synthesized according to the general procedure through the treatment of 2-bromobenzaldehyde oxime (0.120 g, 0.6 mmol) and 1,4-naphthoquinone (0.079 g, 0.5 mmol) with Koser's reagent (0.275 g, 0.7 mmol) in 2 mL of 1,4-dioxane at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **3p** (0.152 g, 86%) as a peach colour solid. **MP**: 179.3–180.1 °C; **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 8.31–8.27 (m, 1H), 8.20–8.16 (m, 1H), 7.85–7.82 (m, 2H), 7.78–7.74 (m, 1H), 7.51–7.43 (m, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 178.1, 173.2, 170.5, 165.2, 160.2, 135.2, 134.47, 133.8, 133.1, 132.0, 131.3, 130.2, 129.8, 128.3, 127.7, 127.5, 123.4, 120.8; **HRMS (EI)**: m/z: calcd for $C_{17}H_9BrNO_3^+$ $[M+H]^+$ 353.9760, found 353.9760; **IR (cm^{-1})**: ν_{max} 2920, 2852, 1680, 1591, 1571, 1500, 1616, 1327, 1301, 1258, 1196, 1141, 1000, 716.

17. 3-(2,4-Dichlorophenyl)naphtho[2,3-*d*]isoxazole-4,9-dione (3q)



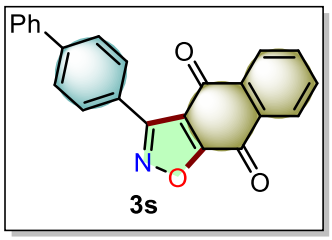
Compound **3q** was synthesized according to the general procedure through the treatment of 2,4-dichlorobenzaldehyde oxime (0.114 g, 0.6 mmol) and 1,4-naphthoquinone (0.079 g, 0.5 mmol) with Koser's reagent (0.275 g, 0.7 mmol) in 2 mL of 1,4-dioxane at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **3q** (0.100 g, 58%) as a light yellow solid. **MP**: 234.3–235.1 °C; **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 8.32–8.29 (m, 1H), 8.22–8.19 (m, 1H), 7.88–7.83 (m, 2H), 7.62 (d, J = 2.0 Hz, 1H), 7.50 (d, J = 8.2 Hz, 1H), 7.43 (dd, J = 8.2, 2.0 Hz, 1H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 178.1, 173.1, 165.4, 158.2, 137.7, 135.4, 135.1, 134.5, 133.3, 132.1, 130.1, 127.6, 127.4, 124.3, 120.9; **HRMS (EI)**: m/z: calcd for $C_{17}H_8Cl_2NO_3^+$ $[M+H]^+$ 343.9876, found 343.9875; **IR (cm^{-1})**: ν_{max} 3069, 2922, 2851, 1678, 1589, 1507, 1431, 1335, 1300, 1202, 1177, 1099, 1001, 716.

18. 3-(2,5-Dimethoxyphenyl)naphtho[2,3-*d*]isoxazole-4,9-dione (3r)



Compound **3r** was synthesized according to the general procedure through the treatment of 2,5-dimethoxybenzaldehyde oxime (0.109 g, 0.6 mmol) and 1,4-naphthoquinone (0.079 g, 0.5 mmol) with Koser's reagent (0.275 g, 0.7 mmol) in 2 mL of 1,4-dioxane at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **3r** (0.100 g, 66%) as a light yellow solid. **MP**: 187.4–188.2 °C; **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 8.29–8.26 (m, 1H), 8.20–8.17 (m, 1H), 7.83–7.80 (m, 2H), 7.10–7.07 (m, 2H), 7.02–6.99 (m, 1H), 3.81 (s, 3H), 3.76 (s, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 177.9, 173.5, 165.0, 158.4, 153.3, 152.2, 135.1, 134.0, 133.7, 132.1, 127.3, 127.3, 121.3, 117.8, 115.8, 115.7, 112.5, 56.2, 55.9; **HRMS (EI)**: m/z: calcd for $C_{19}H_{14}NO_5^+$ $[M+H]^+$ 336.0866, found 336.0870; **IR (cm^{-1})**: ν_{max} 2996, 2947, 1684, 1595, 1475, 1434, 1323, 1277, 1214, 1184, 1030, 712.

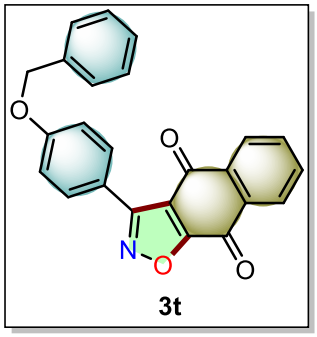
19. 3-([1,1'-Biphenyl]-4-yl)naphtho[2,3-*d*]isoxazole-4,9-dione (3s)



3s

Compound **3s** was synthesized according to the general procedure through the treatment of [1,1'-biphenyl]-4-carbaldehyde oxime (0.118 g, 0.6 mmol) and 1,4-naphthoquinone (0.079 g, 0.5 mmol) with Koser's reagent (0.275 g, 0.7 mmol) in 2 mL of 1,4-dioxane at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **3s** (0.125 g, 71%) as a light yellow solid. **MP**: 190.1–190.9 °C; **^{1}H NMR (500 MHz, CDCl$_3$)**: δ 8.33–8.24(m, 4H), 7.91–7.83 (m, 2H), 7.78 (d, *J* = 8.4 Hz, 2H), 7.69–7.66 (m, 2H), 7.49 (t, *J* = 7.6 Hz, 2H), 7.43–7.39 (m, 1H); **^{13}C NMR (126 MHz, CDCl$_3$)**: δ 178.8, 173.4, 166.3, 160.8, 144.1, 140.1, 135.4, 134.4, 133.8, 131.8, 129.8, 128.9, 128.0, 127.8, 127.3, 127.2, 125.0, 119.6; **HRMS (EI)**: m/z: calcd for $C_{23}H_{14}NO_3^+$ $[M+H]^+$ 352.0968, found 352.0971; **IR (cm^{-1})**: ν_{max} 2920, 2851, 1683, 1587, 1442, 1337, 1266, 1201, 1172, 1002, 717.

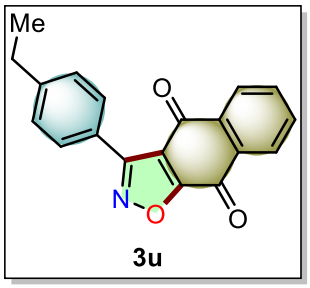
20. 3-(4-(Benzyloxy)phenyl)naphtho[2,3-*d*]isoxazole-4,9-dione (3t)



3t

Compound **3t** was synthesized according to the general procedure through the treatment of 4-(benzyloxy)benzaldehyde oxime (0.136 g, 0.6 mmol) and 1,4-naphthoquinone (0.079 g, 0.5 mmol) with Koser's reagent (0.275 g, 0.7 mmol) in 2 mL of 1,4-dioxane at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **3t** (0.124 g, 65%) as a light yellow solid. **MP**: 170.9–171.7 °C; **^{1}H NMR (500 MHz, CDCl$_3$)**: δ 8.30–8.26 (m, 2H), 8.18 (d, *J* = 9.0 Hz, 2H), 7.89–7.81 (m, 2H), 7.47 (dd, *J* = 7.9, 1.0 Hz, 2H), 7.43–7.39 (m, 2H), 7.36 (dt, *J* = 9.6, 4.3 Hz, 1H), 7.15–7.11 (m, 2H), 5.16 (s, 2H); **^{13}C NMR (126 MHz, CDCl$_3$)**: δ 178.8, 173.4, 166.3, 161.2, 160.6, 136.4, 135.3, 134.3, 133.8, 131.8, 131.1, 128.7, 128.2, 127.8, 127.5, 127.2, 119.5, 118.7, 115.0, 70.1; **HRMS (EI)**: m/z: calcd for $C_{24}H_{16}NO_4^+$ $[M+H]^+$ 382.1074, found 382.1077; **IR (cm^{-1})**: ν_{max} 3064, 2921, 2852, 1672, 1585, 1519, 1427, 1336, 1249, 1182, 1024, 738.

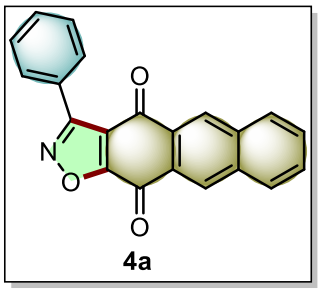
21. 3-(4-Ethoxyphenyl)naphtho[2,3-*d*]isoxazole-4,9-dione (3u)



3u

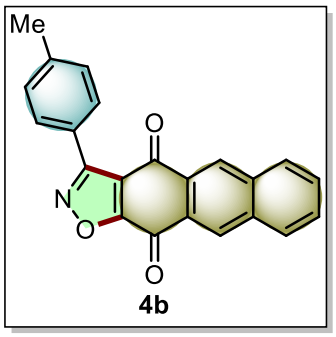
Compound **3u** was synthesized according to the general procedure through the treatment of 4-ethylbenzaldehyde oxime (0.089 g, 0.6 mmol) and 1,4-naphthoquinone (0.079 g, 0.5 mmol) with Koser's reagent (0.275 g, 0.7 mmol) in 2 mL of 1,4-dioxane at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **3u** (0.106 g, 70%) as a light yellow solid. **MP**: 138.7–139.5 °C; **^{1}H NMR (500 MHz, CDCl$_3$)**: δ 8.25–8.19 (m, 2H), 8.04 (d, *J* = 8.3 Hz, 2H), 7.84–7.77 (m, 2H), 7.33 (d, *J* = 8.0 Hz, 2H), 2.71 (q, *J* = 7.6 Hz, 2H), 1.28 (t, *J* = 7.6 Hz, 3H); **^{13}C NMR (126 MHz, CDCl$_3$)**: δ 178.6, 173.3, 166.1, 160.8, 147.9, 135.2, 134.2, 133.7, 131.7, 129.3, 128.1, 127.6, 127.1, 123.4, 119.5, 28.8, 15.2; ; **HRMS (EI)**: m/z: calcd for $C_{19}H_{14}NO_3^+$ $[M+H]^+$ 304.0968, found 304.0956; **IR (cm^{-1})**: ν_{max} 2959, 2952, 1680, 1581, 1434, 1335, 1202, 1165, 719.

22. 3-Phenylanthra[2,3-*d*]isoxazole-4,11-dione (4a)



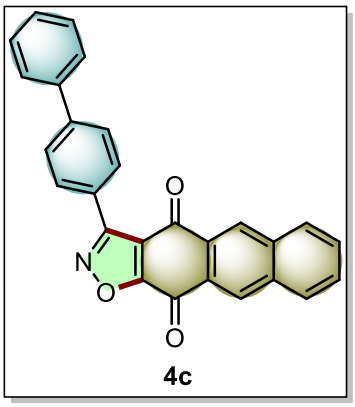
Compound **4a** was synthesized according to the general procedure through the treatment of benzaldehyde oxime (0.073 g, 0.6 mmol) and anthracene-1,4-dione (0.104 g, 0.5 mmol) with Koser's reagent (0.275 g, 0.7 mmol) in 2 mL of 1,4-dioxane at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **4a** (0.146 g, 90%) as a yellow solid. **MP**: 234.6–235.4 °C; **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 8.75 (d, *J* = 26.9 Hz, 2H), 8.18 (dd, *J* = 7.6, 1.8 Hz, 2H), 8.07 (t, *J* = 8.2 Hz, 2H), 7.72 (dd, *J* = 5.7, 2.9 Hz, 2H), 7.61–7.52 (m, 3H). **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 178.3, 173.0, 167.2, 161.2, 135.3, 134.6, 131.3, 130.5, 130.4, 130.4, 130.1, 129.9, 129.5, 128.6, 128.4, 126.3, 120.7; **HRMS (EI)**: m/z: calcd for $C_{21}H_{12}NO_3^+$ $[M+H]^+$ 326.0812, found 326.0803; **IR (cm^{-1})**: ν_{max} 3052, 1677, 1578, 1498, 1220, 1394, 1342, 1281, 1162, 1028, 763.

23. 3-(*p*-Tolyl)anthra[2,3-*d*]isoxazole-4,11-dione (4b)



Compound **4b** was synthesized according to the general procedure through the treatment of benzaldehyde oxime (0.081 g, 0.6 mmol) and anthracene-1,4-dione (0.104 g, 0.5 mmol) with Koser's reagent (0.275 g, 0.7 mmol) in 2 mL of 1,4-dioxane at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **4b** (0.139 g, 82%) as a yellow solid. **MP**: 220.6–221.4 °C; **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 8.82 (s, 1H), 8.77 (s, 1H), 8.13–8.07 (m, 4H), 7.78–7.72 (m, 2H), 7.37 (d, *J* = 7.9 Hz, 2H), 2.47 (s, 3H);**^{13}C NMR (126 MHz, $CDCl_3$)**: δ 178.5, 173.2, 167.3, 161.3, 141.8, 135.4, 134.8, 130.6, 130.2, 129.5, 128.6, 123.5, 120.9, 21.7; **HRMS (EI)**: m/z: calcd for $C_{22}H_{14}NO_3^+$ $[M+H]^+$ 340.0968, found 340.0958; **IR (cm^{-1})**: ν_{max} 3055, 2919, 2858, 1677, 1621, 1578, 1440, 1393, 1223, 1165, 1021, 755.

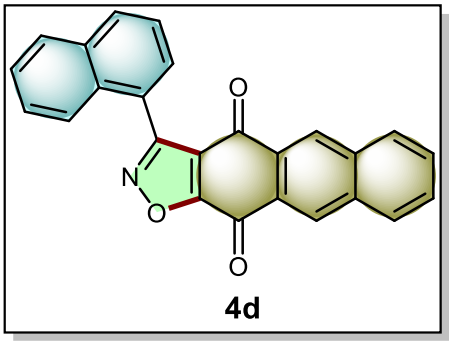
24. 3-([1,1'-Biphenyl]-4-yl)anthra[2,3-*d*]isoxazole-4,11-dione (4c)



Compound **4c** was synthesized according to the general procedure through the treatment of [1,1'-biphenyl]-4-carbaldehyde oxime (0.118 g, 0.6 mmol) and anthracene-1,4-dione (0.104 g, 0.5 mmol) with Koser's reagent (0.275 g, 0.7 mmol) in 2 mL of 1,4-dioxane at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **4c** (0.148 g, 74%) as an orange solid. **MP**: 168.8–169.6 °C; **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 8.81 (d, *J* = 18.4 Hz, 1H), 8.30 (d, *J* = 8.5 Hz, 1H), 8.13–8.08 (m, 2H), 8.02–7.99 (m, 1H), 7.80–7.77 (m, 1H, 7.76–7.73 (m, 1H), 7.70–7.67 (m, 1H), 7.64 (d, *J* = 2.8 Hz, 1H), 7.63–7.58 (m, 2H), 7.52–7.37 (m, 4H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 178.4, 173.1, 170.5, 167.3, 160.9, 149.6, 144.0, 143.1, 140.2, 135.3, 134.7, 133.8, 131.0, 130.5, 130.3, 129.9, 129.8, 128.9, 128.3 128.0, 127.6, 127.3,

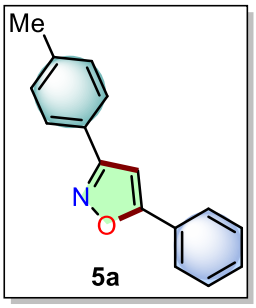
127.2, 127.0, 125.1, 120.8; **HRMS (EI)**: m/z: calcd for $C_{27}H_{16}NO_3^+$ $[M+H]^+$ 402.1125, found 402.1108; **IR (cm^{-1})**: ν_{max} 3020, 2871, 1680, 1580, 1433, 1297, 1161, 1071, 754.

25. 3-(Naphthalen-1-yl)anthra[2,3-*d*]isoxazole-4,11-dione (4d)



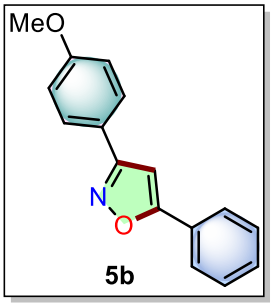
Compound **4d** was synthesized according to the general procedure through the treatment of naphthaldehyde oxime (0.103 g, 0.6 mmol) and anthracene-1,4-dione (0.104 g, 0.5 mmol) with Koser's reagent (0.275 g, 0.7 mmol) in 2 mL of 1,4-dioxane at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **4d** (0.127 g, 68%) as an orange solid. MP: 208.9–209.7 °C; **^{1}H NMR (500 MHz, CDCl$_3$)**: δ 8.86 (s, 1H), 8.65 (s, 1H), 8.14–8.10 (m, 1H), 8.08 (d, *J* = 8.3 Hz, 1H), 8.06–8.02 (m, 1H), 7.97 (d, *J* = 8.0 Hz, 1H), 7.92 (d, *J* = 8.4 Hz, 1H), 7.83 (dd, *J* = 7.1, 1.0 Hz, 1H), 7.77–7.71 (m, 2H), 7.64 (dd, *J* = 8.2, 7.2 Hz, 1H), 7.54 (m, 2H); **^{13}C NMR (126 MHz, CDCl$_3$)**: δ 177.9, 173.1, 166.6, 160.4, 135.3, 134.7, 133.6, 131.3, 131.3, 130.6, 130.5, 130.4, 130.2, 130.1, 129.9, 129.2, 128.7, 128.6, 127.1, 126.5, 125.1, 124.9, 123.4, 122.2; **HRMS (EI)**: m/z: calcd for $C_{25}H_{14}NO3^+$ $[M+H]^+$ 376.0968, found 376.0964; **IR (cm^{-1})**: ν_{max} 3054, 2919, 2853, 1678, 1619, 1577, 1509, 1442, 1400, 1164, 756.

26. 5-Phenyl-3-(*p*-tolyl)isoxazole (5a)



Compound **5a** was synthesized according to the general procedure through the treatment of 4-methylbenzaldehyde oxime (0.068 g, 0.5 mmol) and phenylacetylene (0.076 g, 0.75 mmol) with Koser's reagent (0.275 g, 0.70 mmol) in 2 mL of THF at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **5a** (0.090 g, 77%) as a white solid. **MP**:134.1–134.9 °C; **IR (cm^{-1})**: ^{1}H **NMR (500 MHz, CDCl$_3$)**: δ 7.86–7.83 (m, 2H), 7.76 (d, *J* = 8.1 Hz, 2H), 7.51–7.44 (m, 3H), 7.31– 7.28 (m, 2H), 6.81 (s, 1H), 2.42 (s, 3H); **^{13}C NMR (126 MHz, CDCl$_3$)**: δ 170.3, 163.0 140.3, 130.3, 129.7, 129.1, 127.6, 126.8, 126.3, 125.9, 97.5, 21.5; **HRMS (EI)**: m/z: calcd for $C_{16}H_{14}NO^+$ $[M+H]^+$ 236.1070, found 236.1063; **IR (cm^{-1})**: ν_{max} 3113, 3016, 2917, 1609, 1573, 1487, 1382, 1034, 685.

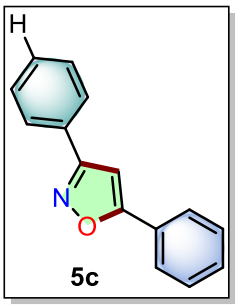
27. 3-(4-Methoxyphenyl)-5-phenylisoxazole (5b)



Compound **5b** was synthesized according to the general procedure through the treatment of 4-methoxybenzaldehyde oxime (0.076 g, 0.5 mmol) and phenylacetylene (0.076 g, 0.75 mmol) with Koser's reagent (0.275 g, 0.70 mmol) in 2 mL of THF at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **5b** (0.065 g, 52%) as a white solid. **MP**: 119.3–120.1 °C; **^{1}H NMR (500 MHz, CDCl$_3$)**: δ 7.85–7.79 (m, 4H), 7.51–7.43 (m, 3H), 7.00 (d, *J* = 8.9 Hz, 2H), 6.78 (s, 1H), 3.87 (s, 3H); **^{13}C NMR (126 MHz, CDCl$_3$)**: δ 170.1, 162.6, 161.0, 130.1, 128.9, 128.2, 127.5, 125.8, 121.6, 114.3,

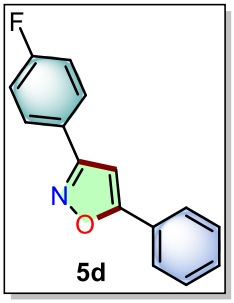
97.3, 55.4; **HRMS (EI)**: m/z: calcd for $C_{16}H_{14}NO_2^+$ $[M+H]^+$ 252.1019, found 252.1017; **IR (cm^{-1})**: ν_{max} 3108, 3043, 2931, 2842, 1603, 1568, 1522, 1481, 1432, 1377, 1291, 1235, 1018, 682.

28. 3,5-Diphenylisoxazole (5c)



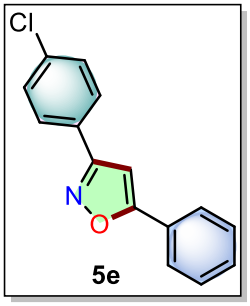
Compound **5c** was synthesized according to the general procedure through the treatment of benzaldehyde oxime (0.061 g, 0.5 mmol) and phenylacetylene (0.076 g, 0.75 mmol) with Koser's reagent (0.275 g, 0.70 mmol) in 2 mL of THF at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **5c** (0.089 g, 81%) as a white solid. **MP**: 139.5–140.3 °C; **IR**: **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 7.89–7.83 (m, 4H), 7.52–7.44 (m, 6H), 6.84 (s, 1H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 170.4, 162.9, 130.2, 130.0, 129.1, 129.0, 128.9, 127.4, 126.8, 125.8, 97.5; **HRMS (EI)**: m/z: calcd for $C_{15}H_{12}NO^+$ $[M+H]^+$ 222.0913, found 222.0913; **IR (cm^{-1})**: ν_{max} 3111, 3040, 2919, 1603, 1560, 1446, 1387, 914, 684.

29. 3-(4-Fluorophenyl)-5-phenylisoxazole (5d)



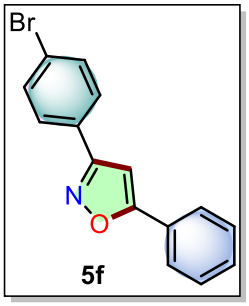
Compound **5d** was synthesized according to the general procedure through the treatment of 4-fluorobenzaldehyde oxime (0.069 g, 0.5 mmol) and phenylacetylene (0.076 g, 0.75 mmol) with Koser's reagent (0.275 g, 0.70 mmol) in 2 mL of THF at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **5d** (0.095 g, 79%) as a white solid. **MP**: 165.6–166.2 °C; **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 7.88–7.82 (m, 4H), 7.51–7.44 (m, 3H), 7.20–7.14 (m, 2H), 6.79 (s, 1H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 170.6, 163.8 (d, J = 249.9 Hz), 162.0, 130.3, 129.0, 128.7 (d, J = 8.5 Hz), 127.3, 125.8, 125.3, 125.3, 116.1, 115.9, 97.3; **^{1}H NMR (471 MHz, $CDCl_3$)**: δ -110.43 to -110.46 (m, 1F); **HRMS (EI)**: m/z: calcd for $C_{15}H_{11}FNO^+$ $[M+H]^+$ 240.0819, found 240.0818; **IR (cm^{-1})**: ν_{max} 3108, 3044, 1600, 1519, 1483, 1430, 1416, 1374, 1216, 913, 687.

30. 3-(4-Chlorophenyl)-5-phenylisoxazole (5e)



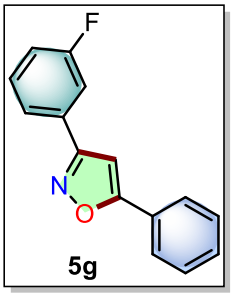
Compound **5e** was synthesized according to the general procedure through the treatment of 4-chlorobenzaldehyde oxime (0.078 g, 0.5 mmol) and phenylacetylene (0.076 g, 0.75 mmol) with Koser's reagent (0.275 g, 0.70 mmol) in 2 mL of THF at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **5e** (0.100 g, 78%) as a white solid. **MP**: 177.1–177.9 °C; **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 7.85–7.79 (m, 4H), 7.52–7.44 (m, 5H), 6.81 (s, 1H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 170.7, 162.0, 136.0, 130.4, 129.2, 129.0, 128.1, 127.6, 127.3, 125.8, 97.3; **HRMS (EI)**: m/z: calcd for $C_{15}H_{11}ClNO^+$ $[M+H]^+$ 256.0524, found 256.0521; **IR (cm^{-1})**: ν_{max} 3109, 3052, 2922, 2854, 1597, 1562, 1480, 1433, 1411, 1369, 1260, 1077, 913, 685.

31. 3-(4-Bromophenyl)-5-phenylisoxazole (5f)



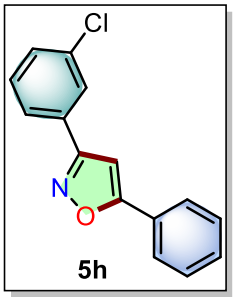
Compound **5f** was synthesized according to the general procedure through the treatment of 4-bromobenzaldehyde oxime (0.100 g, 0.5 mmol) and phenylacetylene (0.076 g, 0.75 mmol) with Koser's reagent (0.275 g, 0.70 mmol) in 2 mL of THF at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **5f** (0.120 g, 80%) as a white solid. **MP**: 180.4–181.2 °C; **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 7.84 (dd, *J* = 8.1, 1.5 Hz, 2H), 7.75 (d, *J* = 8.7 Hz, 2H), 7.62 (d, *J* = 8.7 Hz, 2H), 7.52–7.46 (m, 3H), 6.81 (s, 1H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 170.7, 162.1, 132.2, 130.4, 129.1, 128.3, 128.0, 127.2, 125.8, 124.3, 97.3; **HRMS (EI)**: m/z: calcd for $C_{15}H_{11}BrNO^+$ $[M+H]^+$ 300.0019, found 300.0013; **IR (cm^{-1})**: ν_{max} 3109, 3041, 1595, 1556, 1477, 1431, 1409, 1367, 1260, 1059, 914, 682.

32. 3-(3-Fluorophenyl)-5-phenylisoxazole (5g)



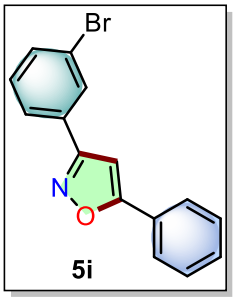
Compound **5g** was synthesized according to the general procedure through the treatment of 3-fluorobenzaldehyde oxime (0.069 g, 0.5 mmol) and phenylacetylene (0.076 g, 0.75 mmol) with Koser's reagent (0.275 g, 0.70 mmol) in 2 mL of THF at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **5g** (0.084 g, 70%) as a white solid. **MP**: 84.6–85.6 °C; **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 7.84 (dd, *J* = 8.1, 1.6 Hz, 2H), 7.66–7.63 (m, 1H), 7.59 (ddd, *J* = 9.6, 2.5, 1.6 Hz, 1H), 7.51–7.42 (m, 4H), 7.18–7.13 (m, 1H), 6.81 (s, 1H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 170.7, 163.0 (d, *J* = 245.9 Hz), 131.2 (d, *J* = 8.2 Hz), 130.6 (d, *J* = 8.3 Hz), 130.4, 129.0, 127.2, 125.8, 122.5, 122.5, 116.9 (d, *J* = 21.2 Hz), 113.9, 113.7, 97.4; **HRMS (EI)**: m/z: calcd for $C_{15}H_{11}FNO^+$ $[M+H]^+$ 240.0819, found 240.0822; **IR (cm^{-1})**: ν_{max} 3110, 2924, 2856, 1580, 1451, 1232, 1169, 681.

33. 3-(3-Chlorophenyl)-5-phenylisoxazole (5h)



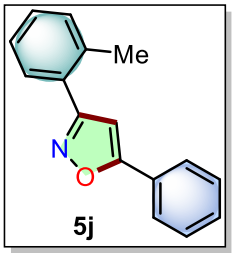
Compound **5h** was synthesized according to the general procedure through the treatment of 3-chlorobenzaldehyde oxime (0.078 g, 0.5 mmol) and phenylacetylene (0.076 g, 0.75 mmol) with Koser's reagent (0.275 g, 0.70 mmol) in 2 mL of THF at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **5h** (0.72 g, 56%) as a white solid. MP: 134.2–135.0; **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 7.88–7.82 (m, 3H), 7.76 (dt, *J* = 6.8, 1.8 Hz, 1H), 7.52–7.46 (m, 3H), 7.45–7.40 (m, 2H), 6.81 (s, 1H); **^{13}C NMR (126 MHz, $CDCl_3$)**: 170.9, 161.9, 135.04, 130.9, 130.5, 130.3, 130.1, 129.2, 127.3, 127.0, 125.9, 125.0, 97.4; **HRMS (EI)**: m/z: calcd for $C_{15}H_{11}ClNO^+$ $[M+H]^+$ 256.0524, found 256.0522; **IR (cm^{-1})**: ν_{max} 3112, 3058, 2922, 2855, 1601, 1572, 1438, 1365, 1068, 682.

34. 3-(3-Bromophenyl)-5-phenylisoxazole (5i)



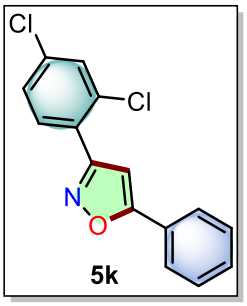
Compound **5i** was synthesized according to the general procedure through the treatment of 3-bromobenzaldehyde oxime (0.100 g, 0.5 mmol) and phenylacetylene (0.076 g, 0.75 mmol) with Koser's reagent (0.275 g, 0.70 mmol) in 2 mL of THF at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **5i** (0.120 g, 80%) as a white solid. **MP**: 102.6–103.2 °C; **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 8.02 (d, *J* = 1.4 Hz, 1H), 7.86–7.78 (m, 3H), 7.59 (dd, *J* = 8.0, 0.9 Hz, 1H), 7.53–7.44 (m, 3H), 7.36 (t, *J* = 7.9 Hz, 1H), 6.81 (s, 1H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 170.8, 161.7, 132.9, 131.1, 130.5, 130.4, 129.8, 129.1, 127.2, 125.8, 125.3, 123.0, 97.3; **HRMS (EI)**: m/z: calcd for $C_{15}H_{11}BrNO^+$ $[M+H]^+$ 300.0019, found 300.0017; **IR (cm^{-1})**: ν_{max} 3115, 3057, 1604, 1567, 1064, 903, 680.

35. 5-Phenyl-3-(*o*-tolyl)isoxazole (5j)



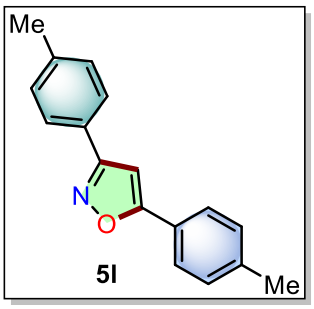
Compound **5j** was synthesized according to the general procedure through the treatment of 2-methylbenzaldehyde oxime (0.068 g, 0.5 mmol) and phenylacetylene (0.076 g, 0.75 mmol) with Koser's reagent (0.275 g, 0.822 mmol) in 2 mL of THF at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **5j** (0.076 g, 70%) as a white solid. **MP**: 67.3– 68.1 °C; **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 7.85 (dd, *J* = 8.2, 1.5 Hz, 2H), 7.56 (dd, *J* = 7.5, 1.3 Hz, 1H), 7.52–7.44 (m, 3H), 7.39–7.28 (m, 3H), 6.70 (s, 1H), 2.53 (s, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 169.5, 163.6, 136.9, 131.1, 130.2, 129.5, 129.4, 129.0, 128.8, 127.4, 126.0, 125.8, 100.2, 21.1; **HRMS (EI)**: m/z: calcd for $C_{16}H_{14}NO^+$ $[M+H]^+$ 236.1070, found 236.1069; **IR (cm^{-1})**: ν_{max} 3051, 2922, 2856, 1603, 1564, 1452, 1387, 1270, 909, 680.

36. 3-(2,4-Dichlorophenyl)-5-phenylisoxazole (5k)



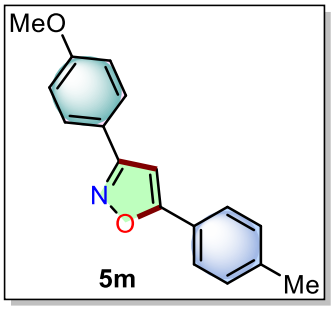
Compound **5k** was synthesized according to the general procedure through the treatment of 2,4-dichlorobenzaldehyde oxime (0.094 g, 0.5 mmol) and phenylacetylene (0.076 g, 0.75 mmol) with Koser's reagent (0.275 g, 0.70 mmol) in 2 mL of THF at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **5k** (0.126 g, 87%) as a white solid. **MP**: 105.6–106.2 °C; **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 7.86–7.83 (m, 2H), 7.75 (d, *J* = 8.4 Hz, 1H), 7.54 (d, *J* = 2.1 Hz, 1H), 7.52–7.45 (m, 3H), 7.37 (dd, *J* = 8.4, 2.1 Hz, 1H), 6.98 (s, 1H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 170.0, 160.7, 136.3, 133., 131.7, 130.4, 130.3, 129.0, 127.6, 127.2, 126.9, 125.8, 100.5; **HRMS (EI)**: m/z: calcd for $C_{15}H_{10}Cl_2NO^+$ $[M+H]^+$ 290.0134, found 290.0133; **IR (cm^{-1})**: ν_{max} 3054, 2961, 1593, 1552, 1484, 1363, 1259, 1022, 680.

37. 3,5-di-*p*-Tolylisoxazole (5l)



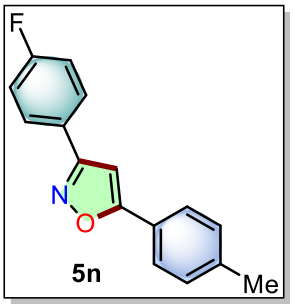
Compound **5l** was synthesized according to the general procedure through the treatment of 4-methylbenzaldehyde oxime (0.068 g, 0.5 mmol) and 1-ethynyl-4-methylbenzene (0.087 g, 0.75 mmol) with Koser's reagent (0.275 g, 0.70 mmol) in 2 mL of THF at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **5l** (0.087 g, 70%) as a white solid. MP: 148.3–149.1 °C; **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 7.74 (dd, *J* = 13.9, 8.1 Hz, 4H), 7.30–7.27 (m, 4H), 6.76 (s, 1H), 2.41 (s, 6H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 170.5, 162.9, 140.5, 140.2, 129.8, 129.70, 126.8, 126.4, 125.9, 124.9, 96.9, 21.6, 21.5; **HRMS (EI)**: m/z: calcd for $C_{17}H_{16}NO^+$ $[M+H]^+$ 250.1226, found 250.1224; **IR (cm^{-1})**: ν_{max} 3114, 3024, 2917, 2852, 1612, 1596, 1564, 1501, 1425, 1381, 1258, 905, 719.

38. 3-(4-Methoxyphenyl)-5-(*p*-tolyl)isoxazole (5m)



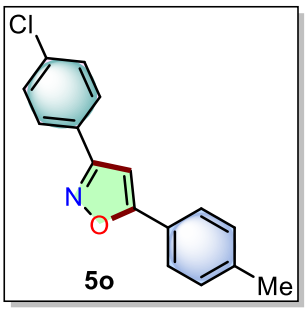
Compound **5m** was synthesized according to the general procedure through the treatment of 4-methoxybenzaldehyde oxime (0.076 g, 0.5 mmol) and 1-ethynyl-4-methylbenzene (0.087 g, 0.75 mmol) with Koser's reagent (0.275 g, 0.70 mmol) in 2 mL of THF at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **5m** (0.077 g, 58%) as a white solid. MP: 154.2–155.0; **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 7.80 (d, *J* = 8.9 Hz, 2H), 7.72 (d, *J* = 8.2 Hz, 2H), 7.28 (dd, *J* = 8.5, 0.6 Hz, 2H), 6.99 (d, *J* = 8.9 Hz, 2H), 6.73 (s, 1H), 3.86 (s. 3H), 2.41 (s, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 170.3, 162.5, 160.9, 140.4, 129.6, 128.2, 125.7, 124.8, 121.7, 114.3, 96.7, 55.3, 21.5; **HRMS (EI)**: m/z: calcd for $C_{17}H_{16}NO_2^+$ $[M+H]^+$ 266.1176, found 266.1173; **IR (cm^{-1})**: ν_{max} 3105, 3032, 2957, 2922, 2853, 1605, 1527, 1500, 1453, 1425, 1383, 1297, 1250, 807.

39. 3-(4-Fluorophenyl)-5-(*p*-tolyl)isoxazole (5n)



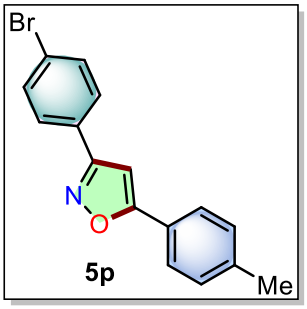
Compound **5n** was synthesized according to the general procedure through the treatment of 4-fluorobenzaldehyde oxime (0.069 g, 0.5 mmol) and 1-ethynyl-4-methylbenzene (0.087 g, 0.75 mmol) with Koser's reagent (0.275 g, 0.70 mmol) in 2 mL of THF at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **5n** (0.104 g, 82%) as a white solid. **MP**: 161.8–163.6 °C; **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 7.87–7.82 (m, 2H), 7.72 (d, *J* = 8.1 Hz, 2H), 7.29 (dd, *J* = 8.5, 0.6 Hz, 2H), 7.19–7.14 (m, 2H), 6.74 (s, 1H), 2.42 (s, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 170.8, 163.8 (d, *J* = 249.8 Hz), 162.0, 140.6, 129.7, 128.7 (d, *J* = 8.6 Hz), 125.8, 125.4, 125.4, 124.6, 116.0 (d, *J* = 22.0 Hz), 96.7, 21.5; **^{19}F NMR (471 MHz, $CDCl_3$)**: δ –110.52 to –110.57 (m, 1F); **HRMS (EI)**: m/z: calcd for $C_{16}H_{13}FNO^+$ $[M+H]^+$ 254.0976, found 254.0973; **IR (cm^{-1})**: ν_{max} 3072, 2921, 2852, 1604, 1502, 1430, 1380, 1217, 1123, 808, 684.

40. 3-(4-Chlorophenyl)-5-(*p*-tolyl)isoxazole (5o)



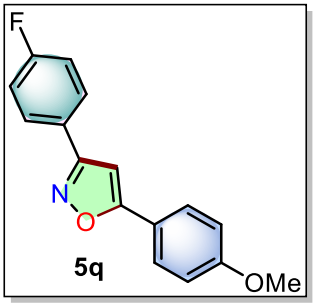
Compound **5o** was synthesized according to the general procedure through the treatment of 4-chlorobenzaldehyde oxime (0.078 g, 0.5 mmol) and 1-ethynyl-4-methylbenzene (0.087 g, 0.75 mmol) with Koser's reagent (0.275 g, 0.70 mmol) in 2 mL of THF at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **5o** (0.141 g, 86%) as a white solid. **MP**: 194.6–195.4 °C; **^{1}H NMR (500 MHz, CDCl$_3$)**: δ 7.80 (d, *J* = 8.5 Hz, 2H), 7.72 (d, *J* = 8.2 Hz, 2H), 7.45 (d, *J* = 8.5 Hz, 2H), 7.29 (d, *J* = 7.9 Hz, 2H), 6.75 (s, 1H), 2.42 (s, 3H); **^{13}C NMR (126 MHz, CDCl$_3$)**: δ 170.89, 161.94, 140.70, 135.94, 129.71, 129.17, 128.05, 127.68, 125.76, 124.55, 96.68, 21.50; **HRMS (EI)**: m/z: calcd for $C_{16}H_{13}ClNO^+$ $[M+H]^+$ 270.0680, found 270.0679; **IR (cm^{-1})**: ν_{max} 3109, 2914, 2858, 1603, 1486, 1417, 1368, 1082, 804.

41. 3-(4-Bromophenyl)-5-(*p*-tolyl)isoxazole (5p)



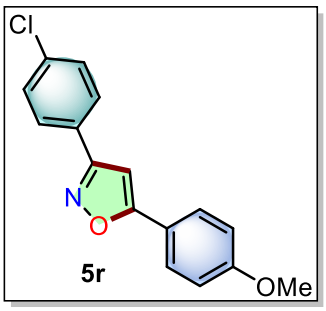
Compound **5p** was synthesized according to the general procedure through the treatment of 4-bromobenzaldehyde oxime (0.100 g, 0.5 mmol) and 1-ethynyl-4-methylbenzene (0.087 g, 0.75 mmol) with Koser's reagent (0.275 g, 0.70 mmol) in 2 mL of THF at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **5p** (0.122 g, 78%) as a white solid. **MP**: 211.0–211.8 °C; **^{1}H NMR (500 MHz, CDCl$_3$)**: δ 7.76–7.70 (m, 4H), 7.61 (d, *J* = 8.7 Hz, 2H), 7.29 (d, *J* = 7.9 Hz, 2H), 6.75 (s, 1H), 2.42 (s, 3H); **^{13}C NMR (126 MHz, CDCl$_3$)**: δ 170.9, 162.0, 140.7, 132.1, 129.7, 128.3, 128.1, 125.8, 124.5, 124.2, 96.7, 21.5; **HRMS (EI)**: m/z: calcd for $C_{16}H_{13}BrNO^+$ $[M+H]^+$ 314.0175, found 314.0175; **IR (cm^{-1})**: ν_{max} 3109, 2915, 1601, 1483, 1417, 1366, 1260, 1068, 806.

42. 3-(4-Fluorophenyl)-5-(4-methoxyphenyl)isoxazole (5q)



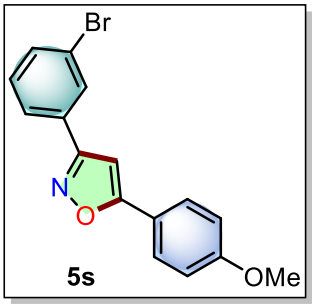
Compound **5q** was synthesized according to the general procedure through the treatment of 4-fluorobenzaldehyde oxime (0.069 g, 0.5 mmol) and 1-ethynyl-4-methoxybenzene (0.099 g, 0.75 mmol) with Koser's reagent (0.275 g, 0.70 mmol) in 2 mL of THF at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **5q** (0.105 g, 78%) as a white solid. MP: 140.7–141.3 °C; **^{1}H NMR (500 MHz, CDCl$_3$)**: δ 7.86–7.82 (m, 2H), 7.77 (d, *J* = 8.9 Hz, 2H), 7.16 (t, *J* = 8.7 Hz, 2H), 7.00 (d, *J* = 8.9 Hz, 2H), 6.66 (s, 1H), 3.87 (s, 3H); **^{13}C NMR (126 MHz, CDCl$_3$)**: δ 170.5, 164.7, 162.7, 162.0, 161.1, 128.7, 128.6, 127.4, 125.5, 120.1, 116.1, 115.9, 114.4, 95.9, 55.4; **^{19}F NMR (471 MHz, CDCl$_3$)**: δ –110.59 to –110.65 (m, 1F); **HRMS (EI)**: m/z: calcd for $C_{16}H_{13}FNO_2^+$ $[M+H]^+$ 270.0925, found 270.0922; **IR (cm^{-1})**: ν_{max} 2922, 2853, 1602, 1496, 1425, 1375, 1302, 1249, 1217, 1165, 1102, 1018, 800.

43. 3-(4-chlorophenyl)-5-(4-methoxyphenyl)isoxazole (5r)



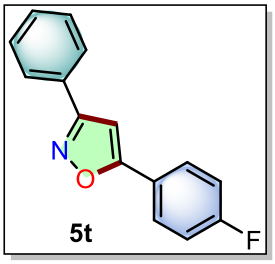
Compound **5r** was synthesized according to the general procedure through the treatment of 4-chlorobenzaldehyde oxime (0.078 g, 0.5 mmol) and 1-ethynyl-4-methoxybenzene (0.099 g, 0.75 mmol) with Koser's reagent (0.275 g, 0.70 mmol) in 2 mL of THF at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **5r** (0.093 g, 65%) as a white solid. MP: 175.3–176.1 °C; **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 7.82–7.75 (m, 4H), 7.45 (d, J = 8.7 Hz, 2H), 7.00 (d, J = 8.9 Hz, 2H), 6.68 (s, 1H), 3.87 (s, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 170.7, 161.9, 161.2, 135.9, 129.2, 128.1, 127.7, 127.5, 120.1, 114.4, 95.9, 55.4; **HRMS (EI)**: m/z: calcd for $C_{16}H_{13}ClNO_2^+$ $[M+H]^+$ 286.0629, found 286.0627; **IR (cm^{-1})**: ν_{max} 3114, 3016, 2936, 2837, 1604, 1493, 1451, 1425, 1379, 1302, 1254, 1171, 803.

44. 3-(3-Bromophenyl)-5-(4-methoxyphenyl)isoxazole (5s)



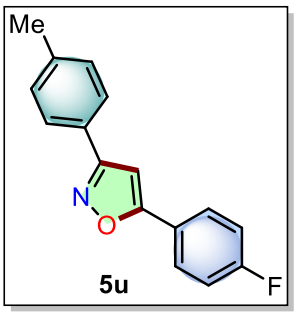
Compound **5s** was synthesized according to the general procedure through the treatment of 3-bromobenzaldehyde oxime (0.100 g, 0.5 mmol) and 1-ethynyl-4-methoxybenzene (0.099 g, 0.75 mmol) with Koser's reagent (0.275 g, 0.70 mmol) in 2 mL of THF at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **5s** (0.132 g, 80%) as a white solid. MP: 120.1–121.9 °C; **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 8.00 (s, 1H), 7.81–7.74 (m, 3H), 7.58 (ddd, J = 7.9, 1.8, 0.9 Hz, 1H), 7.34 (t, J = 7.9 Hz, 1H), 7.00 (d, J = 8.9 Hz, 2H), 6.68 (s, 1H), 3.87 (s, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 170.8, 161.7, 161.3, 132.8, 131.3, 130.4, 129.8, 127.5, 125.3, 122.9, 120.1, 114.5, 95.9, 55.4; **HRMS (EI)**: m/z: calcd for $C_{16}H_{13}BrNO_2^+$ $[M+H]^+$ 330.0124, found 330.0119; **IR (cm^{-1})**: ν_{max} 3111, 2930, 2834, 1605, 1501, 1483, 1438, 1364, 1242, 1168, 1018, 788.

45. 5-(4-Fluorophenyl)-3-phenylisoxazole (5t)



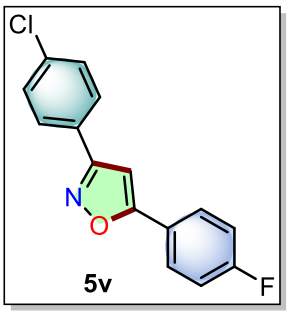
Compound **5t** was synthesized according to the general procedure through the treatment of benzaldehyde oxime (0.061 g, 0.5 mmol) and 1-ethynyl-4-fluorobenzene (0.090 g, 0.75 mmol) with Koser's reagent (0.275 g, 0.70 mmol) in 2 mL of THF at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **5t** (0.088 g, 74%) as a white solid. MP: 154.4–144.2 °C; **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 7.88–7.81 (m, 4H), 7.51–7.46 (m, 3H), 7.19 (t, J = 8.7 Hz, 2H), 6.79 (s, 1H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 169.4, 163.8 (d, J = 251.1 Hz), 163.1, 130.1, 129.0, 127.9 (d, J = 8.5 Hz), 126.8, 123.8, 116.2 (d, J = 22.1 Hz), 97.3; **^{19}F NMR (471 MHz, $CDCl_3$)**: δ –109.30 to –109.36 (m, 1F); **HRMS (EI)**: m/z: calcd for $C_{15}H_{11}FNO^+$ $[M+H]^+$ 240.0819, found 330.0818; **IR (cm^{-1})**: ν_{max} 3112, 3056, 2920, 1609, 1493, 1458, 1391, 1222, 692.

46. 5-(4-Fluorophenyl)-3-(*p*-tolyl)isoxazole (5u)



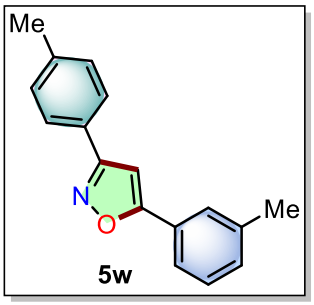
Compound **5u** was synthesized according to the general procedure through the treatment of 4-methylbenzaldehyde oxime (0.068 g, 0.5 mmol) and 1-ethynyl-4-fluorobenzene (0.090 g, 0.75 mmol) with Koser's reagent (0.275 g, 0.70 mmol) in 2 mL of THF at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **5u** (0.077 g, 66%) as a white solid. MP: 173.6–174.8 °C;**^{1}H NMR (500 MHz, CDCl$_3$)**: δ 7.83 (dd, *J* = 8.9, 5.2 Hz, 2H), 7.75 (d, *J* = 8.1 Hz, 2H), 7.29 (d, *J* = 7.9 Hz, 2H), 7.18 (t, *J* = 8.7 Hz, 2H), 6.76 (s, 1H), 2.42 (s, 3H); **^{13}C NMR (126 MHz, CDCl$_3$)**: δ 169.2, 163.7 (d, *J* = 251.1 Hz), 163.0, 140.3, 129.6, 127.9 (d, *J* = 8.6 Hz), 126.7, 126.1, 123.9, 116.2 (d, *J* = 22.1 Hz), 97.2, 21.4; **^{19}F NMR (471 MHz, CDCl$_3$)**: δ –109.43 to –109.49 (m, 1F); **HRMS (EI)**: m/z: calcd for $C_{16}H_{14}FNO^+$ $[M+H]^+$ 254.0976, found 254.0968; **IR (cm^{-1})**: ν_{max} 3109, 3020, 1612, 1498, 1457, 1424, 1388, 1217, 807.

47. 3-(4-Chlorophenyl)-5-(4-fluorophenyl)isoxazole (5v)



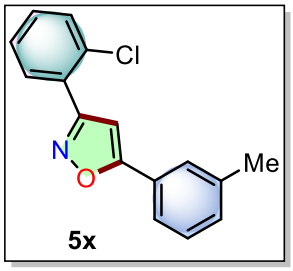
Compound **5v** was synthesized according to the general procedure through the treatment of 4-chlorobenzaldehyde oxime (0.078 g, 0.5 mmol) and 1-ethynyl-4-fluorobenzene (0.090 g, 0.75 mmol) with Koser's reagent (0.275 g, 0.70 mmol) in 2 mL of THF at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **5v** (0.101 g, 74%) as a white solid. MP: 177.1–177.9 °C; **^{1}H NMR (500 MHz, CDCl$_3$)**: δ 7.907–7.763 (m, 4H), 7.46 (d, *J* = 8.3 Hz, 2H), 7.19 (t, *J* = 8.5 Hz, 2H), 6.75 (s, 1H); **^{13}C NMR (126 MHz, CDCl$_3$)**: δ 169.7, 163.9 (d, *J* = 249.5 Hz), 162.9, 136.1, 129.2, 128.1, 127.9, 127.9 (d, *J* = 8.3 Hz), 116.3 (d, *J* = 22.2 Hz), 97.1; **^{19}F NMR (471 MHz, CDCl$_3$)**: δ –108.99 to –109.03 (m, 1F); **HRMS (EI)**: m/z: calcd for $C_{16}H_{14}FNO^+$ $[M+H]^+$ 274.0429, found 274.0429; **IR (cm^{-1})**: ν_{max} 3109, 1676, 1696, 1492, 1453, 1423, 1379, 1227, 1094, 809.

48. 5-(*m*-Tolyl)-3-(*p*-tolyl)isoxazole (5w)



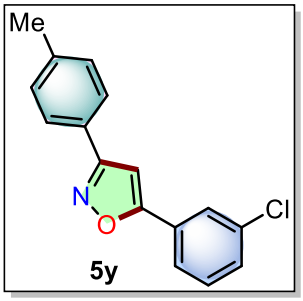
Compound **5w** was synthesized according to the general procedure through the treatment of 4-methylbenzaldehyde oxime (0.068 g, 0.5 mmol) and 1-ethynyl-3-methylbenzene (0.087 g, 0.75 mmol) with Koser's reagent (0.275 g, 0.70 mmol) in 2 mL of THF at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **5w** (0.093 g, 73%) as a white solid. MP: 124.4 l– 125.0 °C; **^{1}H NMR (500 MHz, CDCl$_3$)**: δ 7.76 (d, *J* = 8.1 Hz, 2H), 7.68–7.62 (m, 2H), 7.37 (t, *J* = 7.6 Hz, 1H), 7.30–7.25 (m, 3H), 6.79 (s, 1H), 2.44 (s, 3H), 2.42 (s, 3H); **^{13}C NMR (126 MHz, CDCl$_3$)**: δ 170.4, 162.9, 140.1, 138.7, 129.6, 128.9, 127.4, 126.7, 126.4, 126.3, 123.0, 97.3, 21.4; **HRMS (EI)**: m/z: calcd for $C_{17}H_{16}NO^+$ $[M+H]^+$ 250.1226, found 250.1229; **IR (cm^{-1})**: ν_{max} 3099, 3025, 2914, 2855, 1574, 1507, 1429, 1378, 1269, 1111, 805.

49. 3-(2-Chlorophenyl)-5-(m-tolyl)isoxazole (5x)



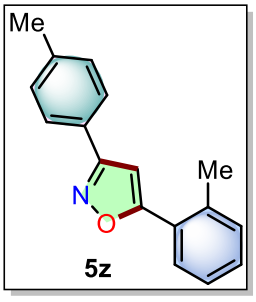
Compound **5x** was synthesized according to the general procedure through the treatment of 2-chlorobenzaldehyde oxime (0.078 g, 0.5 mmol) and 1-ethynyl-3-methylbenzene (0.087 g, 0.75 mmol) with Koser's reagent (0.275 g, 0.70 mmol) in 2 mL of THF at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **5x** (0.097 g, 72%) as a white solid. MP: 58.6–57.4 °C; **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 7.82–7.78 (m, 1H), 7.68–7.64 (M, 2H), 7.53–7.50 (m, 1H), 7.429–7.35 (m, 3H), 7.29–7.26 (m, 1H), 6.98 (s, 1H), 2.44 (s, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 169.9, 161.5, 138.8, 132.9, 131.0, 130.9, 130.8, 130.4, 128.9, 128.4, 127.3, 127.1, 126.4, 123.0, 100.7, 21.4; **HRMS (EI)**: m/z: calcd for $C_{16}H_{13}NOCl^+$ $[M+H]^+$ 270.0680, found 270.0684; **IR (cm^{-1})**: ν_{max} 2957, 2924, 2857, 1600, 1565, 1445, 1391, 1264, 1124, 1038, 753.

50. 5-(3-Chlorophenyl)-3-(p-tolyl)isoxazole (5y)



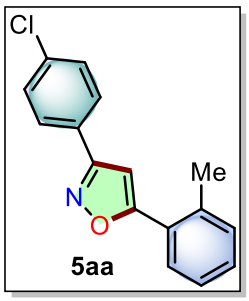
Compound **5y** was synthesized according to the general procedure through the treatment of 4-methylbenzaldehyde oxime (0.068 g, 0.5 mmol) and 1-ethynyl-3-chlorobenzene (0.102 g, 075 mmol) with Koser's reagent (0.275 g, 0.70 mmol) in 2 mL of THF at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **5y** (0.102 g, 76%) as a white solid. MP: 127.3–128.1 °C; **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 7.83–7.81 (m, 1H), 7.76–7.73 (m, 2H), 7.73–7.69 (m, 1H), 7.43–7.41 (m, 2H), 7.29 (d, *J* = 7.9 Hz, 2H), 6.82 (s, 1H), 2.41 (s, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 168.7, 163.0, 140.3, 135.0, 130.3, 129.6, 129.1, 126.7, 125.9, 125.8, 123.9, 98.2, 21.4; **HRMS (EI)**: m/z: calcd for $C_{16}H_{13}NOCl^+$ $[M+H]^+$ 270.0680, found 270.0685; **IR (cm^{-1})**: ν_{max} 3110, 2018, 2913, 2857, 1611, 1585, 1560, 1527, 1478, 1429, 1380, 1287, 1104, 1079, 1050, 793.

51. 5-(*o*-Tolyl)-3-(*p*-tolyl)isoxazole (5z)



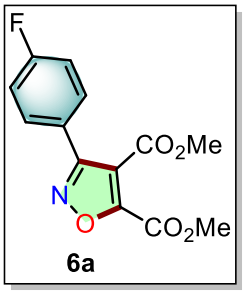
Compound **5z** was synthesized according to the general procedure through the treatment of 4-methylbenzaldehyde oxime (0.068 g, 0.5 mmol) and 1-ethynyl-2-methylbenzene (0.087 g, 0.75 mmol) with Koser's reagent (0.275 g, 0.70 mmol) in 2 mL of THF at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **5z** (0.0934 g, 75%) as a white solid. MP: 60.6–61.2 °C; **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 7.79–7.75 (m, 3H), 7.37–7.28 (m, 5H), 6.70 (s, 1H), 2.57 (s, 3H), 2.42 (s, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 170.4, 162.6, 140.1, 136.2, 131.3, 129.6, 128.5, 127.1, 126.7, 126.3, 126.2, 100.5, 21.5, 21.4. **HRMS (EI)**: m/z: calcd for $C_{17}H_{16}NO^+$ $[M+H]^+$ 250.1226, found 250.1231; **IR (cm^{-1})**: ν_{max} 3058, 3024, 2921, 2855, 1607, 1565, 1488, 1458, 1428, 1382, 1287, 119, 1039, 811.

52. 3-(4-Chlorophenyl)-5-(*o*-tolyl)isoxazole (5aa)



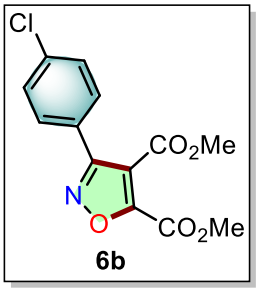
Compound **5aa** was synthesized according to the general procedure through the treatment of 4-chlorobenzaldehyde oxime (0.078 g, 0.5 mmol) and 1-ethynyl-2-methylbenzene (0.087 g, 0.75 mmol) with Koser's reagent (0.275 g, 0.70 mmol) in 2 mL of THF at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **5aa** (0.093 g, 69%) as a white solid. MP: 93.6–94.2 °C; **^{1}H NMR (500 MHz, CDCl$_3$)**: δ 7.82 (d, *J* = 8.7 Hz, 2H), 7.77–7.74 (m, 1H), 7.46 (d, *J* = 8.6 Hz, 2H), 7.40–7.35 (m, 1H), 7.35–7.30 (m, 2H), 6.70 (s, 1H), 2.57 (s, 3H); **^{13}C NMR (126 MHz, CDCl$_3$)**: δ 170.9, 161.6, 136.2, 136.0, 131.4, 130.2, 129.9, 129.6, 129.49, 129.2, 128.5, 128.1, 126.9, 126.3, 100.4, 21.5; **HRMS (EI)**: m/z: calcd for $C_{16}H_{13}NOCl^+$ $[M+H]^+$ 270.0680, found 270.0685; **IR (cm^{-1})**: ν_{max} 3129, 3063, 2969, 2926, 2853, 1598, 1564, 1492, 1423, 1374, 1284, 1236, 1086, 1047, 1008, 816.

53. Dimethyl 3-(4-fluorophenyl)isoxazole-4,5-dicarboxylate (6a)



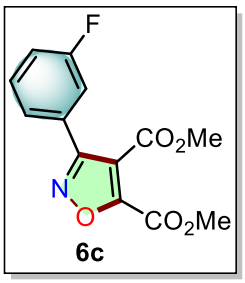
Compound **6a** was synthesized according to the general procedure through the treatment of 4-fluorobenzaldehyde oxime (0.069 g, 0.5 mmol) and dimethyl acetylenedicarboxylate (0.107 g, 0.75 mmol) with Koser's reagent (0.275 g, 0.70 mmol) in 2 mL of THF at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **6a** (0.104 g, 75%) as a white solid. MP: 108..4–109.2 °C; **^{1}H NMR (500 MHz, CDCl$_3$)**: δ 7.73–7.68 (m, 2H), 7.20–7.13 (m, 2H), 4.02 (s, 3H), 3.90 (s, 3H); **^{13}C NMR (126 MHz, CDCl$_3$)**: δ 165.2, 163.2, 160.7 (d, *J* = 253.0 Hz), 160.5, 156.4, 130.4 (d, *J* = 8.8 Hz), 123.0, 122.9, 116.1 (d, *J* = 22.1 Hz), 115., 53.5, 53.2; **HRMS (EI)**: m/z: calcd for $C_{13}H_{11}FNO_5^+$ $[M+H]^+$ 280.0616, found 280.0620 ; **IR (cm^{-1})**: ν_{max} 3066, 2967, 2923, 1721, 1603, 1520, 1448, 1312, 1267, 1207, 1142, 1064, 831.

54. Dimethyl 3-(4-chlorophenyl)isoxazole-4,5-dicarboxylate (6b)



Compound **6b** was synthesized according to the general procedure through the treatment of 4-chlorobenzaldehyde oxime (0.078 g, 0.5 mmol) and dimethyl acetylenedicarboxylate (0.107 g, 0.75 mmol) with Koser's reagent (0.275 g, 0.70 mmol) in 2 mL of THF at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **6b** (0.109 g, 74%) as a white solid. MP: 84.3–85.1 °C; **^{1}H NMR (500 MHz, CDCl$_3$)**: δ 7.66–7.63 (m, 2H), 7.47–7.44 (m, 2H), 4.02 (s, 3H), 3.90 (s, 3H); **^{13}C NMR (126 MHz, CDCl$_3$)**: δ 161.6, 160.4, 159.8, 156.4, 137.1, 129.6, 129.2, 125.3, 115.7, 53.5, 53.2; **HRMS (EI)**: m/z: calcd for $C_{13}H_{11}ClNO_5^+$ $[M+H]^+$ 296.0320, found 296.0325; **IR (cm^{-1})**: ν_{max} 2963, 2921, 1728, 1602, 1446, 1311, 1262, 1206, 1135, 1064, 820.

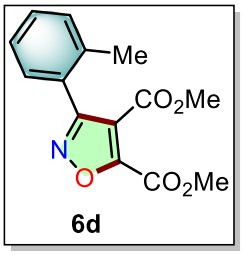
55. Dimethyl 3-(3-fluorophenyl)isoxazole-4,5-dicarboxylate (6c)



6c

Compound **6c** was synthesized according to the general procedure through the treatment of 3-fluorobenzaldehyde oxime (0.069 g, 0.5 mmol) and dimethyl acetylenedicarboxylate (0.107 g, 0.75 mmol) with Koser's reagent (0.275 g, 0.70 mmol) in 2 mL of THF at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **6c** (0.095 g, 68%) as a white solid. MP: 109.3-110.4 °C; **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 7.47–7.39 (m, 3H), 7.18 (s, 1H), 4.00 (s, 3H), 3.90 (s, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 163.5, 161.6, 160.6 (d, J = 246.2 Hz), 160.1, 156.2, 130.5 (d, J = 8.3 Hz), 128.7 (d, J = 8.5 Hz), 123.9, 123.9, 117.7 (d, J = 21.3 Hz), 115.3 (d, J = 23.6 Hz), 53.4, 53.2; **HRMS (EI)**: m/z: calcd for $C_{13}H_{11}FNO_5^+$ $[M+H]^+$ 280.0616, found 280.0619; **IR (cm^{-1})**: ν_{max} 2960, 1722, 1584, 1448, 1282, 1210, 1127, 1076, 780.

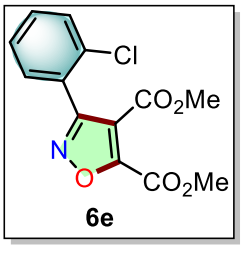
56. Dimethyl 3-(*o*-tolyl)isoxazole-4,5-dicarboxylate (6d)



6d

Compound **6d** was synthesized according to the general procedure through the treatment of 2-methylbenzaldehyde oxime (0.068 g, 0.5 mmol) and dimethyl acetylenedicarboxylate (0.107 g, 0.75 mmol) with Koser's reagent (0.275 g, 0.70 mmol) in 2 mL of THF at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **6d** (0.092 g, 67%) as a colourless oil. **^{1}H NMR (500 MHz, $CDCl_3$)**: 7.40–7.36 (m, 1H), 7.32–7.25 (m, 3H), 4.03 (s, 3H), 3.76 (s, 3H), 2.28 (s, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 162.3, 160.9, 159.9, 156.8, 137.4, 130.6, 130.3, 129.8, 126.5, 125.8, 116.5, 53.6, 52.9, 20.0; **HRMS (EI)**: m/z: calcd for $C_{14}H_{14}NO_5^+$ $[M+H]^+$ 276.0866, found 276.0868; **IR (cm^{-1})**: ν_{max} 3011, 2952, 2855, 1720, 1598, 1445, 1291, 1199, 1144, 1110, 1070, 765.

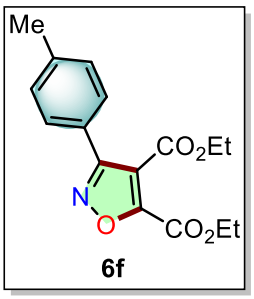
57. Dimethyl 3-(2-chlorophenyl)isoxazole-4,5-dicarboxylate (6e)



6e

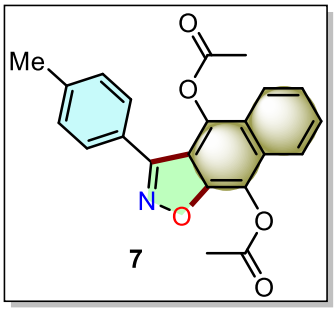
Compound **6e** was synthesized according to the general procedure through the treatment of 2-chlorobenzaldehyde oxime (0.078 g, 0.5 mmol) and dimethyl acetylenedicarboxylate (0.107 g, 0.75 mmol) with Koser's reagent (0.275 g, 0.70 mmol) in 2 mL of THF at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **6e** (0.089 g, 60%) as an off white viscous liquid; **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 7.52–7.42 (m, 3H), 7.41–7.36 (m, 1H), 4.03 (s, 3H), 3.77 (s, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 161.1, 160.5, 160.3, 156.7, 133.6, 131.7, 131.5, 129.8, 127.1, 126.7, 116.3, 53.6, 52.8; **HRMS (EI)**: m/z: calcd for $C_{13}H_{11}ClNO_5^+$ $[M+H]^+$ 296.0320, found 296.0317; **IR (cm^{-1})**: ν_{max} 3015, 2957, 1729, 1595, 1439, 1367, 1295, 1212, 1142, 1083, 765.

58. Diethyl 3-(*p*-tolyl)isoxazole-4,5-dicarboxylate (6f)



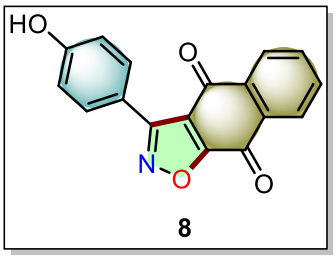
Compound **6f** was synthesized according to the general procedure through the treatment of 4-methylbenzaldehyde oxime (0.068 g, 0.5 mmol) and diethyl acetylenedicarboxylate (0.128 g, 0.75 mmol) with Koser's reagent (0.275 g, 0.70 mmol) in 2 mL of THF at ambient temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **6f** (0.112 g, 74%) as a white solid. MP: 46.6–47.4 °C; **^{1}H NMR (500 MHz, CDCl$_3$)**: δ 7.59 (d, *J* = 8.1 Hz, 2H), 7.28–7.27 (m, 1H), 7.26 (dd, *J* = 1.5, 0.9 Hz, 1H), 4.46 (q, *J* = 7.1 Hz, 2H), 4.37 (q, *J* = 7.1 Hz, 2H), 2.40 (s, 3H), 1.42 (t, *J* = 7.2 Hz, 3H), 1.32 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR (126 MHz, CDCl$_3$)**: δ 161.5, 161.1, 159.2, 156.1, 140.9, 129.5, 128.0, 124.0, 116.1, 62.8, 62.4, 21.4, 14.0, 13.8; **HRMS (EI)**: m/z: calcd for $C_{16}H_{18}NO_5^+$ $[M+H]^+$ 304.1179, found 304.1180; **IR (cm^{-1})**: ν_{max} 2984, 2916, 1729, 1609, 1444, 1269, 1209, 1136, 1063, 1006, 823.

59. 3-(*p*-Tolyl)-4,9-dihydronaphtho[2,3-*d*]isoxazole-4,9-diyl diacetate (7)



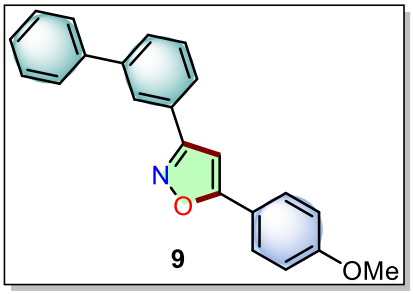
Compound **7** was synthesised according to the general procedure through the treatment of 3-(*p*-tolyl)naphtho[2,3-d]isoxazole-4,9-dione (0.115 g, 0.4 mmol) and Zn powder (0.026 g, 0.72 mmol) with 3 mL triethylamine in 4 mL of acetic acid at reflux temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **7** (0.102 g, 68%) as a viscous yellow. **^{1}H NMR (500 MHz, CDCl$_3$)**: δ 8.03 (d, *J* = 8.7 Hz, 1H), 7.98 (d, *J* = 8.7 Hz, 1H), 7.69 (d, *J* = 8.1 Hz, 2H), 7.64 (ddd, *J* = 8.6, 6.7, 1.1 Hz, 1H), 7.51 (ddd, *J* = 8.6, 6.7, 1.0 Hz, 1H), 7.37 (d, *J* = 7.8 Hz, 2H), 2.60 (s, 3H), 2.47 (s, 3H), 2.04 (s, 3H); **^{13}C NMR (126 MHz, CDCl$_3$)**: δ 168.5, 168.1, 157.8, 150.9, 140.4, 137.6, 129.3, 129.2, 128.4, 128.3, 125.5, 125.0, 124.8, 124.4, 122.2, 121.1, 115.9, 21.5, 20.6, 20.2. **HRMS (EI)**: m/z: calcd for $C_{22}H_{18}NO_5^+$ $[M+H]^+$ 376.1179, found 376.1199 ; **IR (cm^{-1})**: ν_{max} 3067, 3016, 2925, 2858, 1759, 1640, 1424, 1366, 1167, 1043, 886.

60. 3-(4-Hydroxyphenyl)naphtho[2,3-*d*]isoxazole-4,9-dione (8)



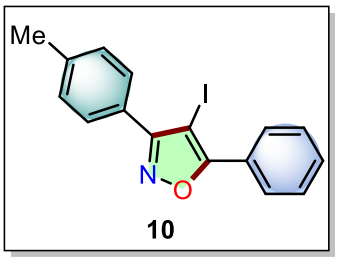
Compound **8** was synthesised according to the general procedure through the treatment of 3-(4-methoxyphenyl)naphtho[2,3-*d*]isoxazole-4,9-dione **3c** (0.071 g, 0.23 mmol) in 2 mL of 35% HBr in acetic acid at reflux temperature. Subsequent purification by column chromatography (EtOAc/hexane) furnished **8** (0.050 g, 74%) as a viscous yellow. **^{1}H NMR (500 MHz, DMSO-d6)**: δ 10.15 (s, 1H, 8.16 (d, *J* = 7.5 Hz, 2H), 7.99–7.93 (m, 4H), 6.95 (d, *J* = 8.7 Hz, 2H); **^{13}C NMR (126 MHz, DMSO-d6)**: δ 178.8, 173.4, 160.2, 160.1, 135.2, 134.4, 133.7, 131.9, 130.9, 127.1, 126.5, 118.7, 116.6, 115.5; **HRMS (EI)**: m/z: calcd for $C_{17}H_9NO_4^+$ $[M+H]^+$ 292,0604, found 292.0602 ; **IR (cm^{-1})**: ν_{max} 3486, 3078, 3017, 2921, 2921, 2853, 1738, 1681, 1585, 1432, 1372, 1252, 1211, 1165, 1096, 721.

61. 3-([1,1'-Biphenyl]-3-yl)-5-(4-methoxyphenyl)isoxazole (9)



Compound **9** was synthesised according to the general procedure through the treatment of **5s** (0.035 g, 0.106 mmol) phenylboronic acid (0.019 g, 0.16 mmol, 1.5 equiv), and K_2CO_3 (0.037 g, 0.265 mmol, 2.5 equiv) and $Pd(PPh_3)_4$ (0.005 g, 5 mol %) in a solvent mixture of H_2O:1,4-dioxane (1:3, 2 mL) . Subsequent purification by column chromatography (EtOAc/hexane) furnished **9** (0.0273 g, 79%) as a white solid. MP: 120.8–121.4 °C; **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 8.09 (t, *J* = 1.7 Hz, 1H), 7.84 (d, *J* = 7.7 Hz, 1H), 7.80 (d, *J* = 8.9 Hz, 2H), 7.70–7.64 (m, 3H), 7.55 (t, *J* = 7.7 Hz, 1H), 7.48 (t, *J* = 7.6 Hz, 2H), 7.41 – 7.36 (m, 1H), 7.01 (d, *J* = 8.9 Hz, 2H), 6.77 (s, 1H), 3.88 (s, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 170.6, 163.0, 161.3, 142.1, 140.6, 129.9, 129.4, 128.9, 128.8, 127.8, 127.6, 127.3, 125.7, 120.4, 114.5, 96.3, 55.5; **HRMS (EI)**: m/z: calcd for $C_{22}H_{18}NO_2^+$ $[M+H]^+$ 328.1332, found 328.1323; **IR (cm^{-1})**: ν_{max} 2962, 2920, 2851, 1610, 1512, 1487, 1459, 1433, 1372, 1305, 1254, 1175, 1157, 1027, 765.

62. 4-Iodo-5-phenyl-3-(*p*-tolyl)isoxazole (10)



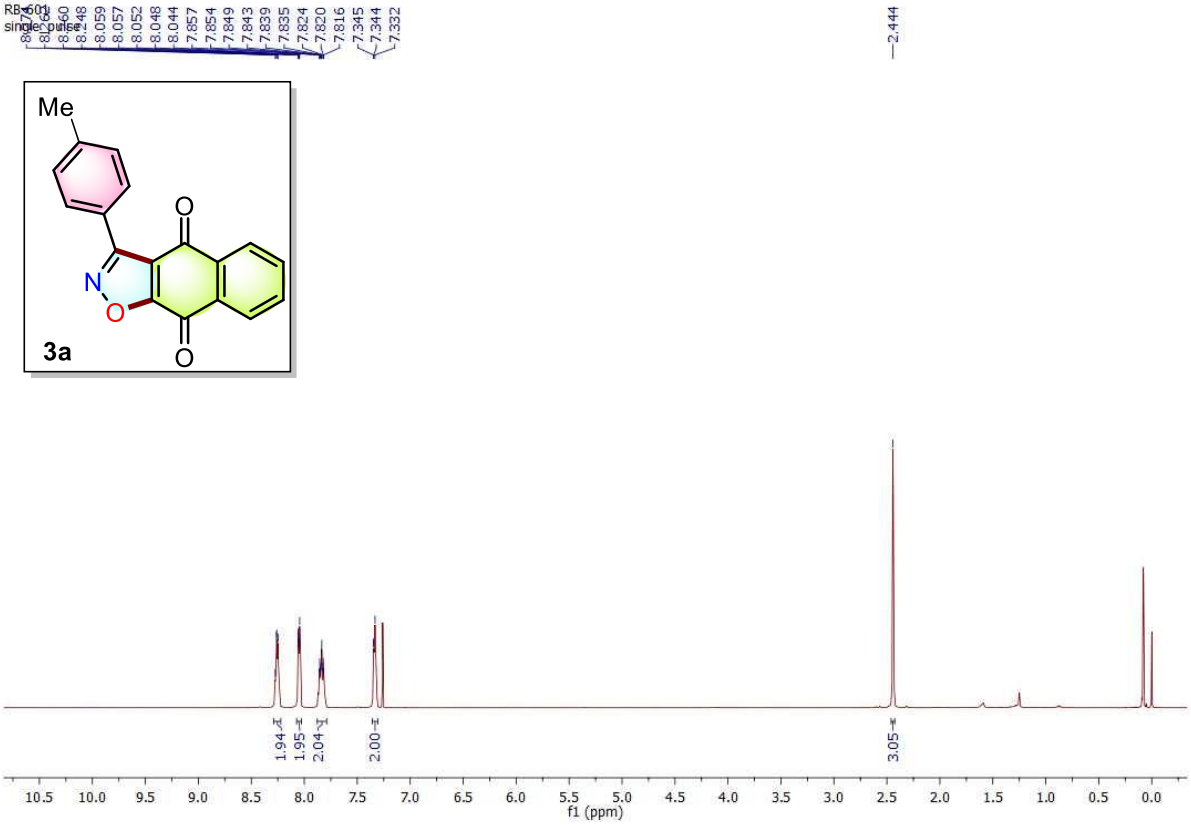
Compound **9** was synthesised according to the general procedure through the treatment of 5-phenyl-3-(*p*-tolyl)isoxazole **(5a)** (0.043 mmol, 0.100 g,) with *N*-iodosuccinimide (0.86 mmol), followed by the addition of 4 mL acetic acid. Subsequent purification by column chromatography (EtOAc/hexane) furnished **9** (0.163g, 96%) as a white sold. MP: 92.4–93.2 °C **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 8.10–8.05 (m, 2H), 7.69 (d, *J* = 8.1 Hz, 2H), 7.56–7.50 (m, 3H), 7.33 (d, *J* = 7.8 Hz, 2H), 2.44 (s, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 168.83, 164.65, 140.19, 130.64, 129.25, 128.85, 128.71, 127.77, 127.33, 125.79, 56.17, 21.46; **HRMS (EI)**: m/z: calcd for $C_{16}H_{13}INO^+$ $[M+H]^+$ 362.0036, found 362.0040; **IR (cm^{-1})**: ν_{max} 3031, 2915, 2856, 1609, 1557, 1485, 1443, 1410, 1372, 1181, 1100, 1070, 1021, 723.

References

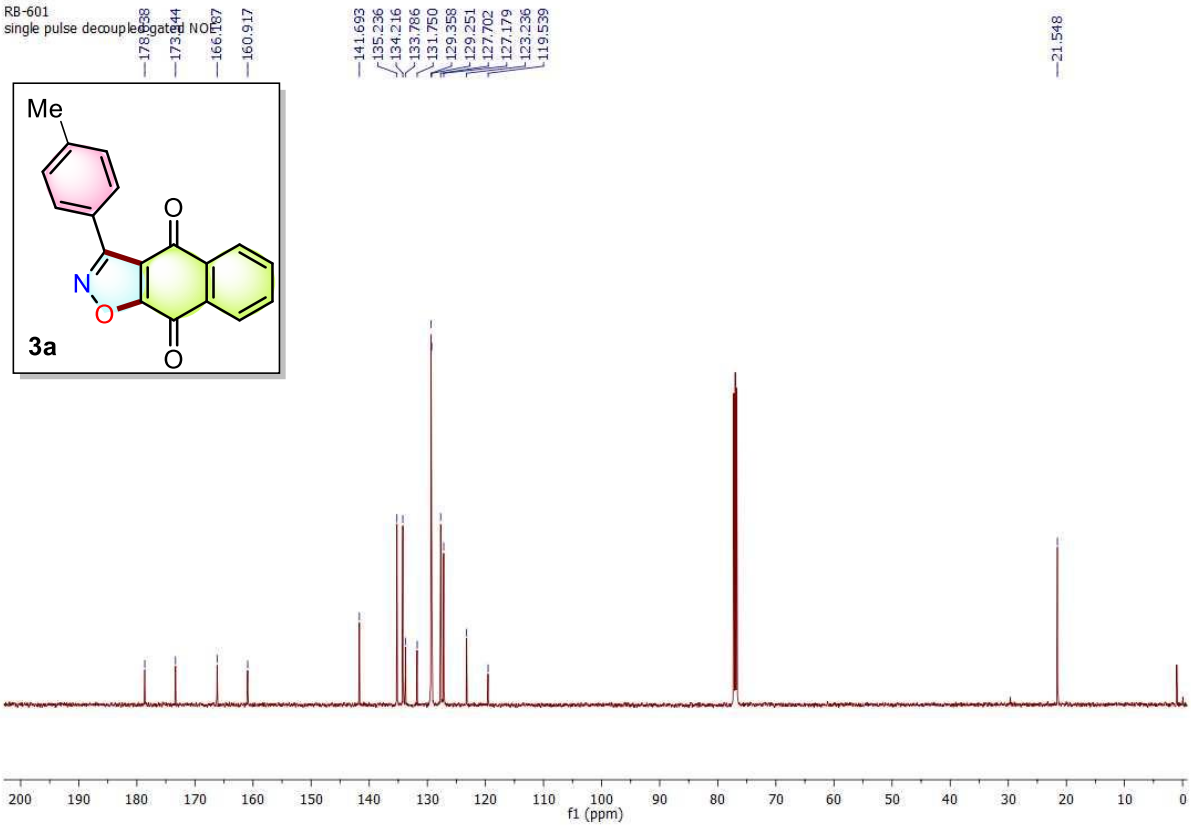
1. A. Dudek and J. Mlynarski, *J. Org. Chem.*, **2017**, *82*, 11218–11224.

2. E. A. Merritt, V. M. T. Carneiro, L. F. Silva J. and B. Olofsson, *J. Org. Chem.,* **2010**, *75*, 21, 7416–7419.

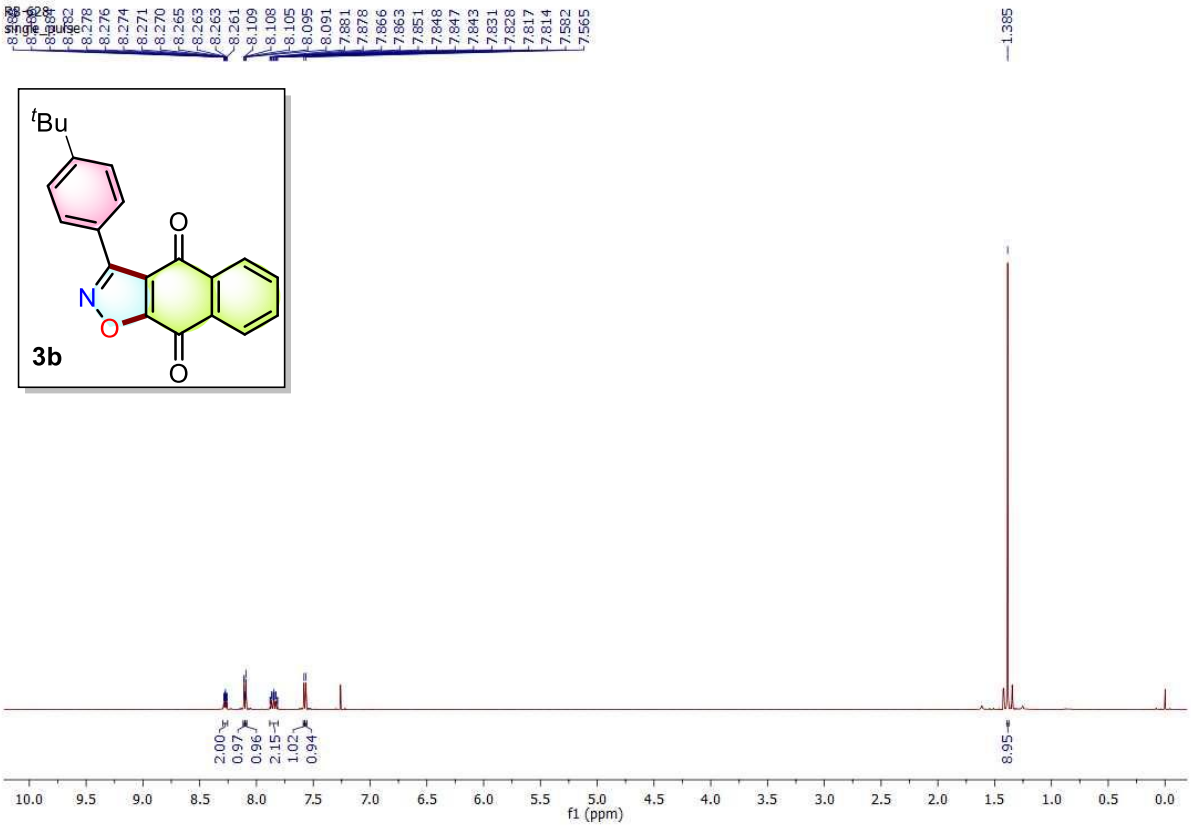
^{1}H NMR Spectrum of **3a** (500 MHz, Chloroform-*d*)



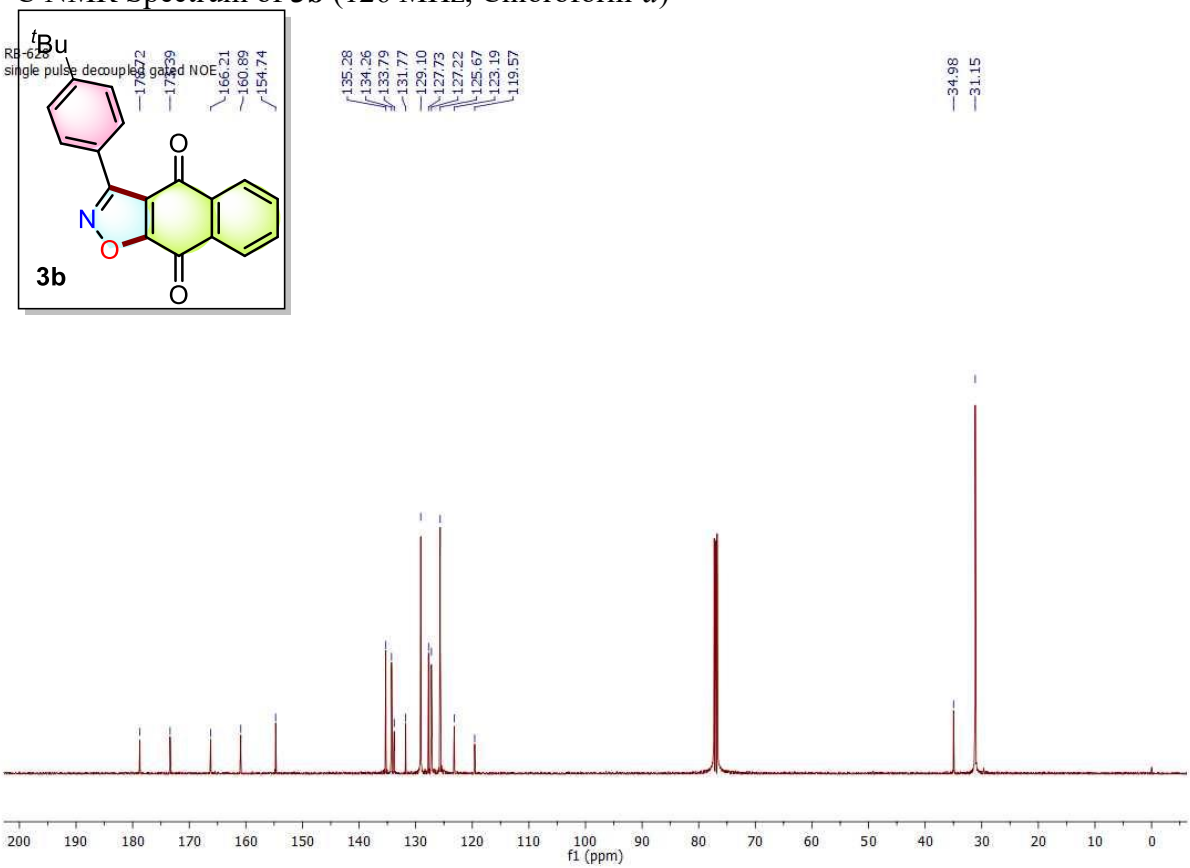
^{13}C NMR Spectrum of **3a** (126 MHz, Chloroform-*d*)



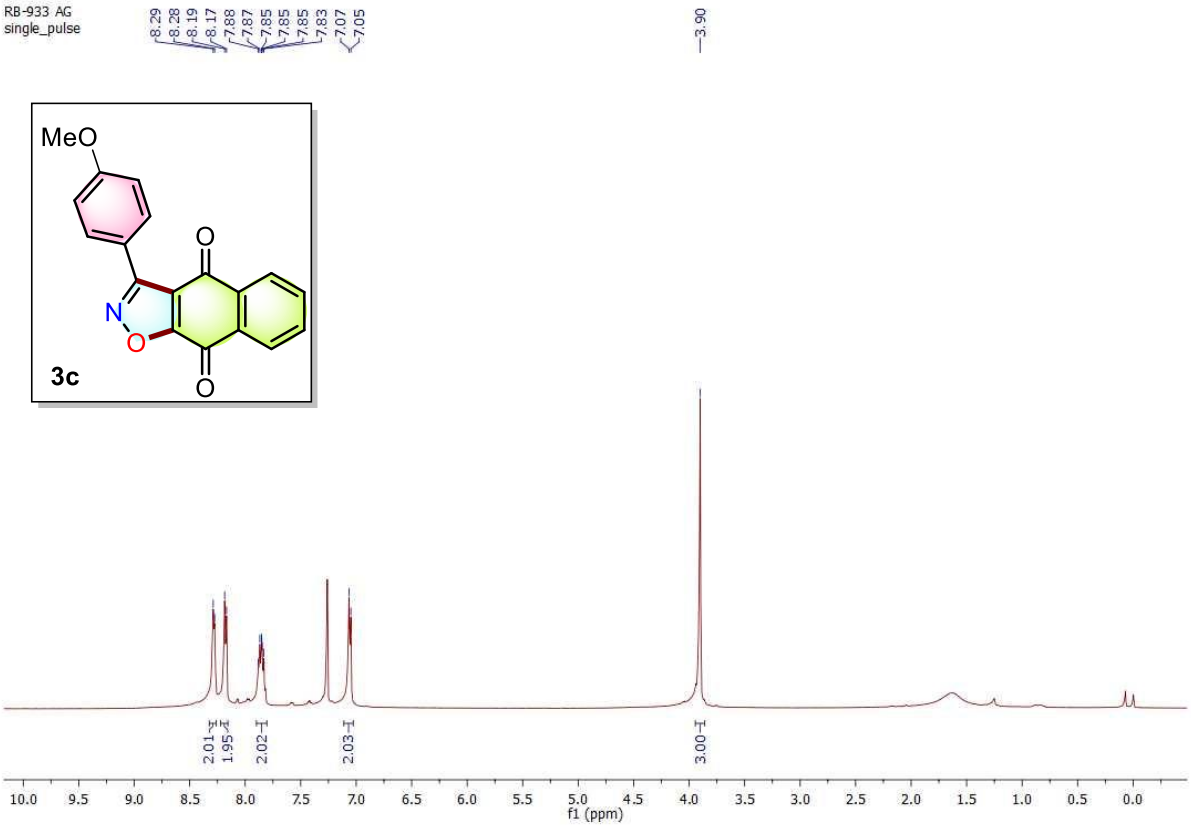
^{1}H NMR Spectrum of **3b** (500 MHz, Chloroform-*d*)



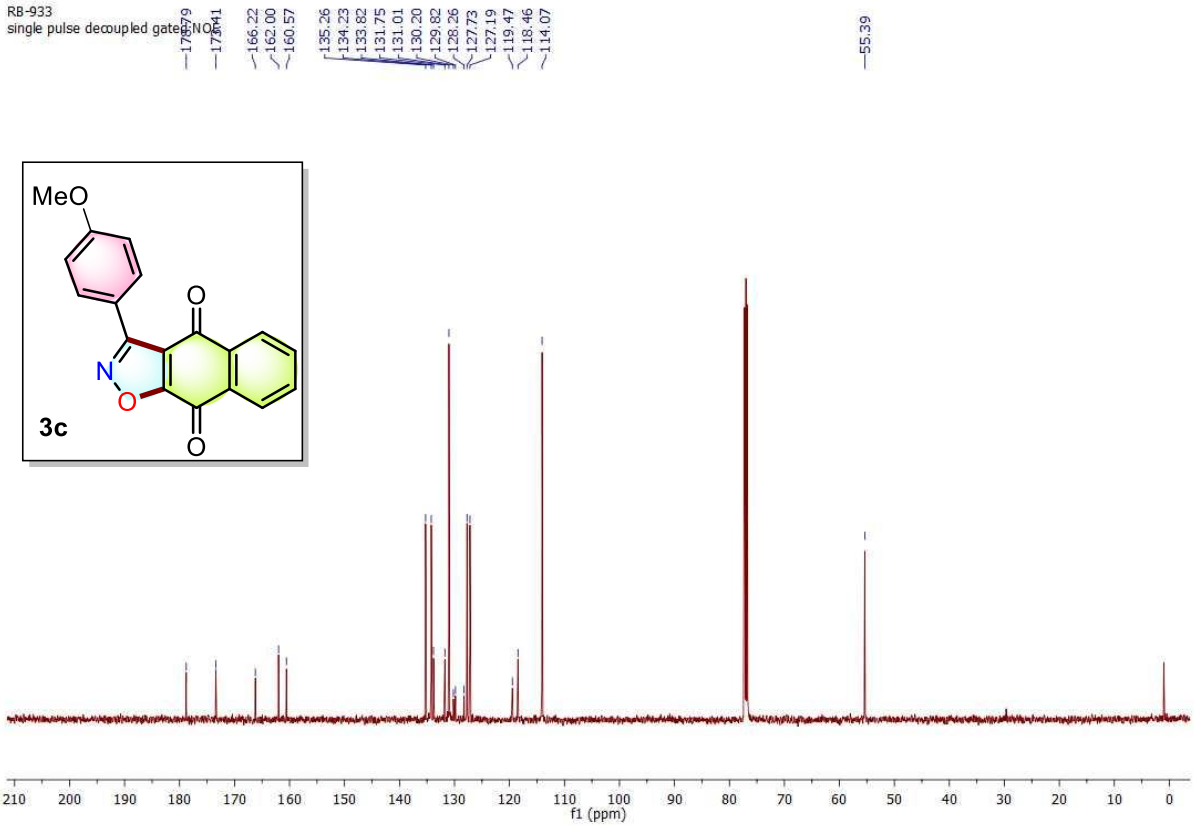
^{13}C NMR Spectrum of **3b** (126 MHz, Chloroform-*d*)



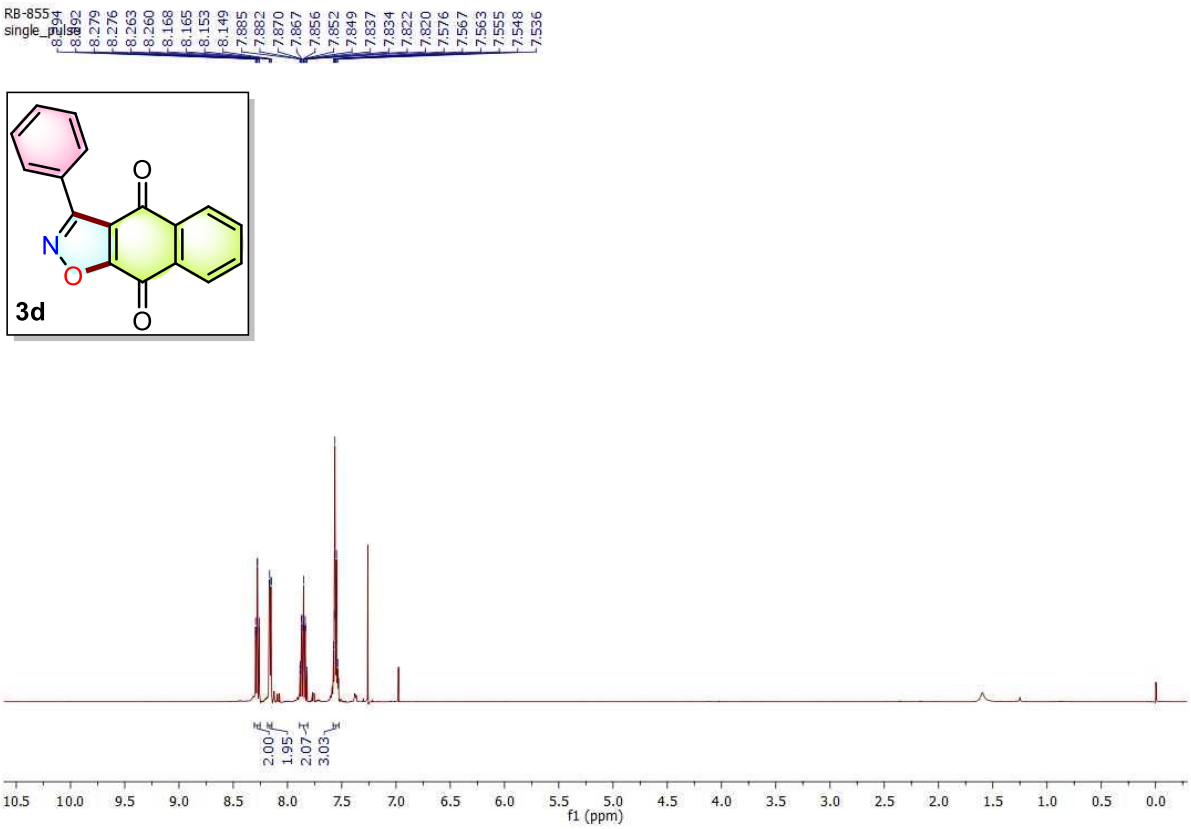
^{1}H NMR Spectrum of **3c** (500 MHz, Chloroform-*d*)



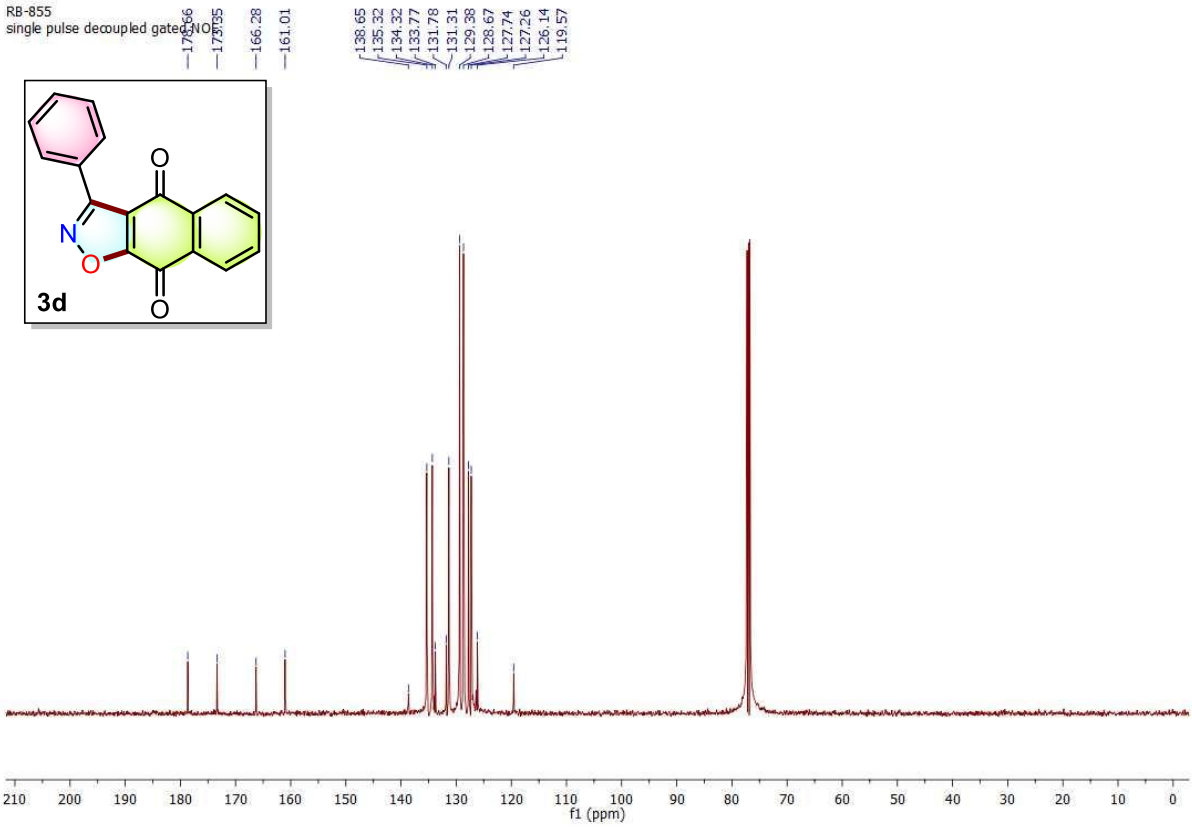
^{13}C NMR Spectrum of **3c** (126 MHz, Chloroform-*d*)



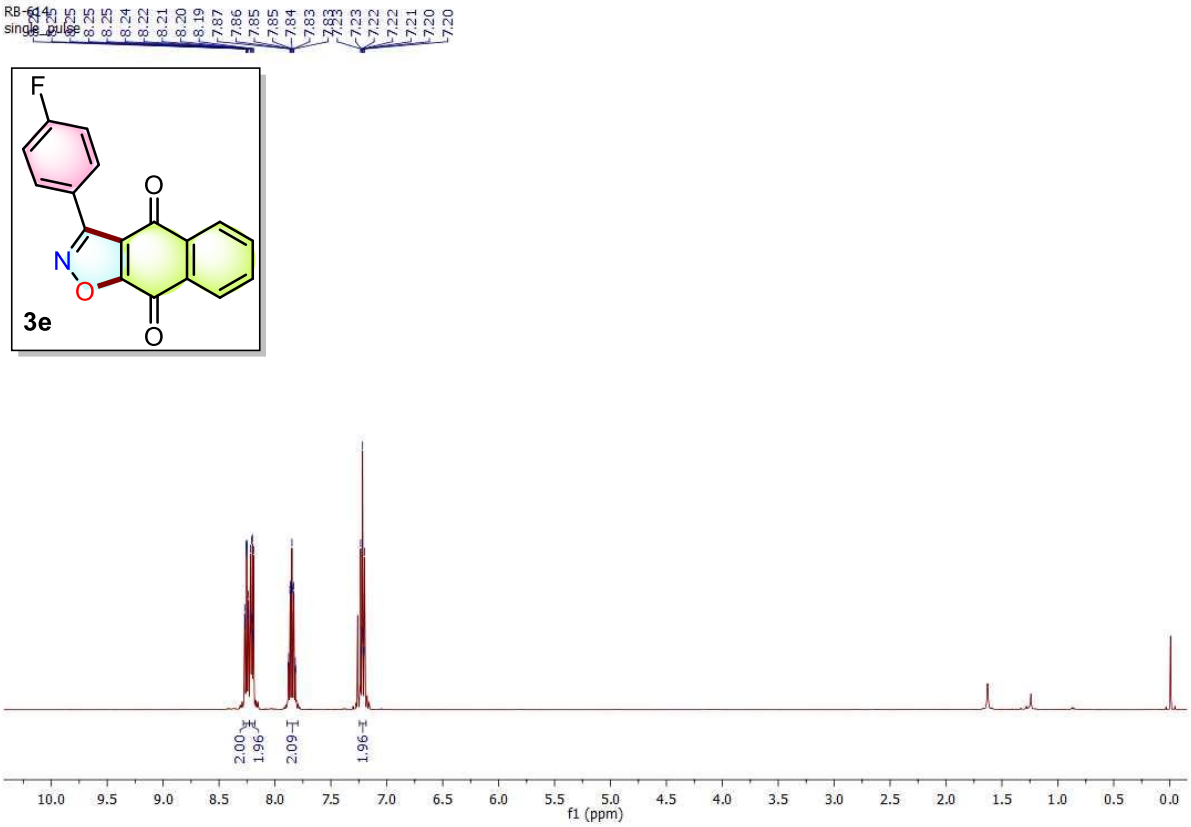
^{1}H NMR Spectrum of **3d** (500 MHz, Chloroform-*d*)



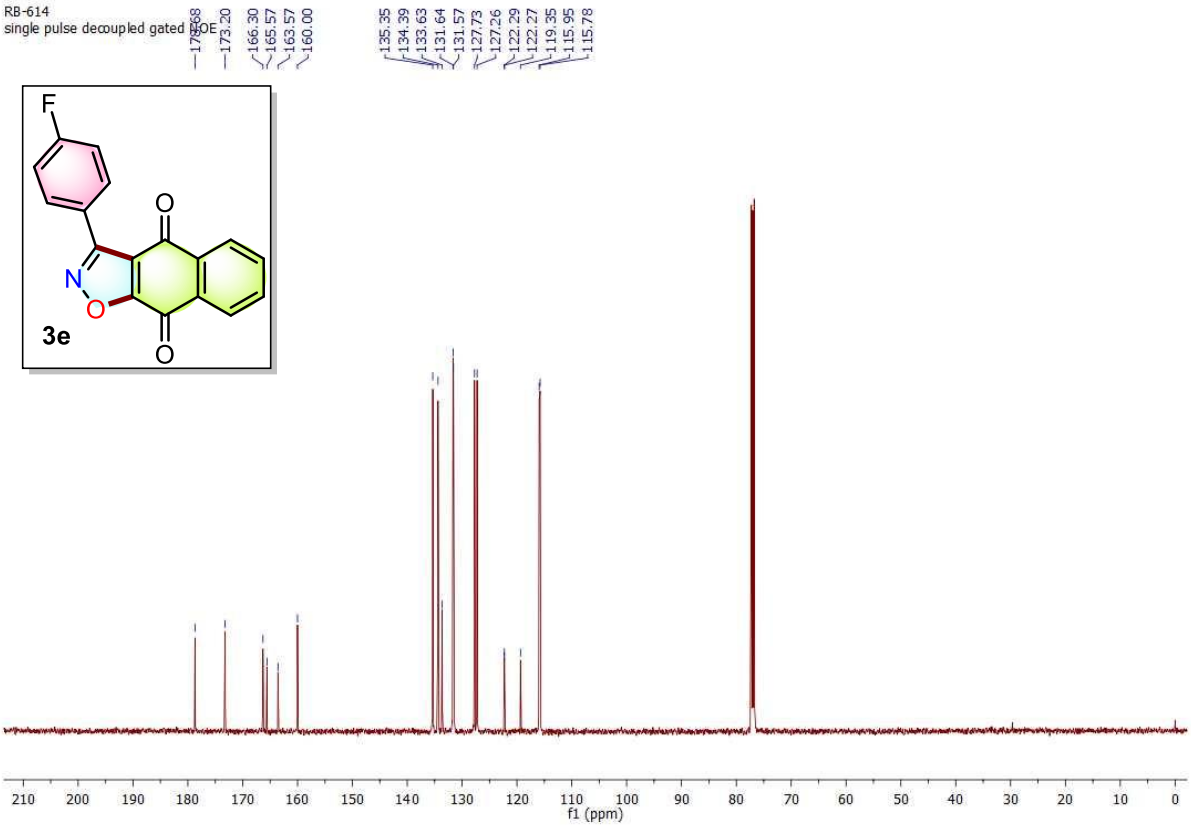
^{13}C NMR Spectrum of **3d** (126 MHz, Chloroform-*d*)



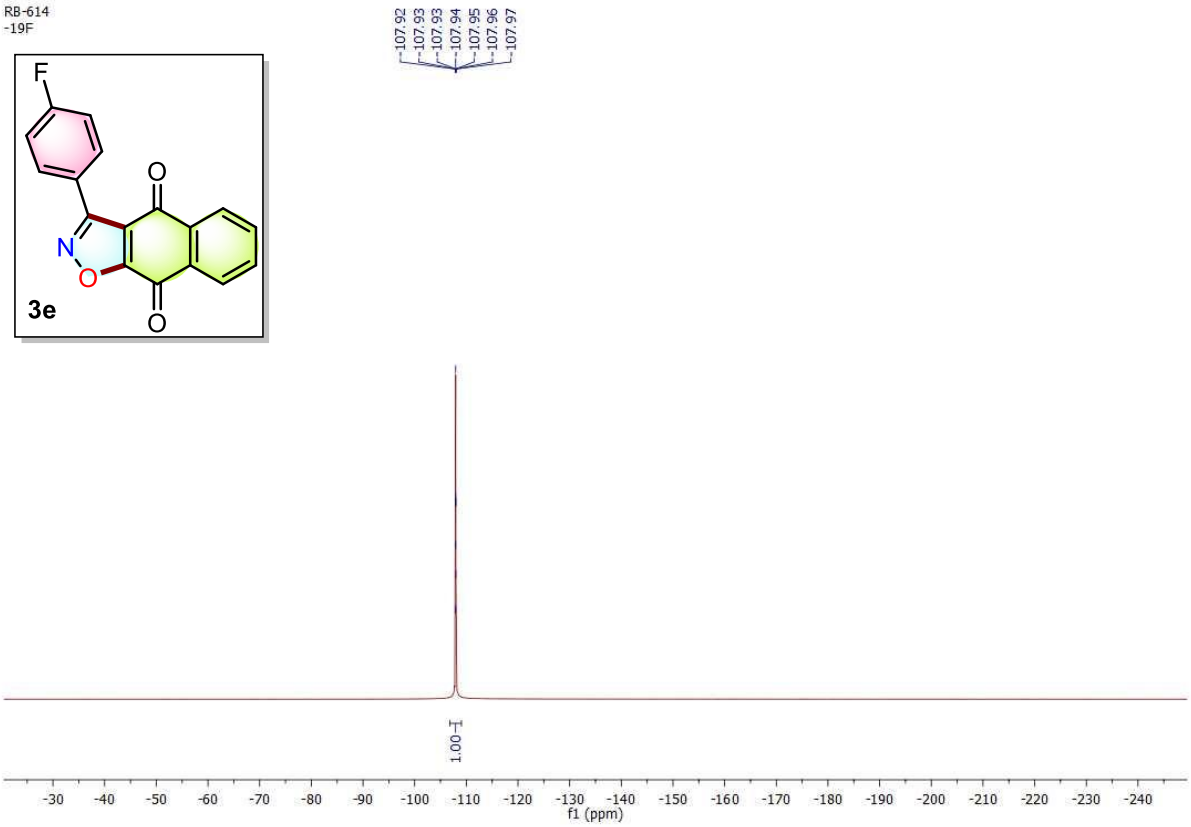
^{1}H NMR Spectrum of **3e** (500 MHz, Chloroform-*d*)



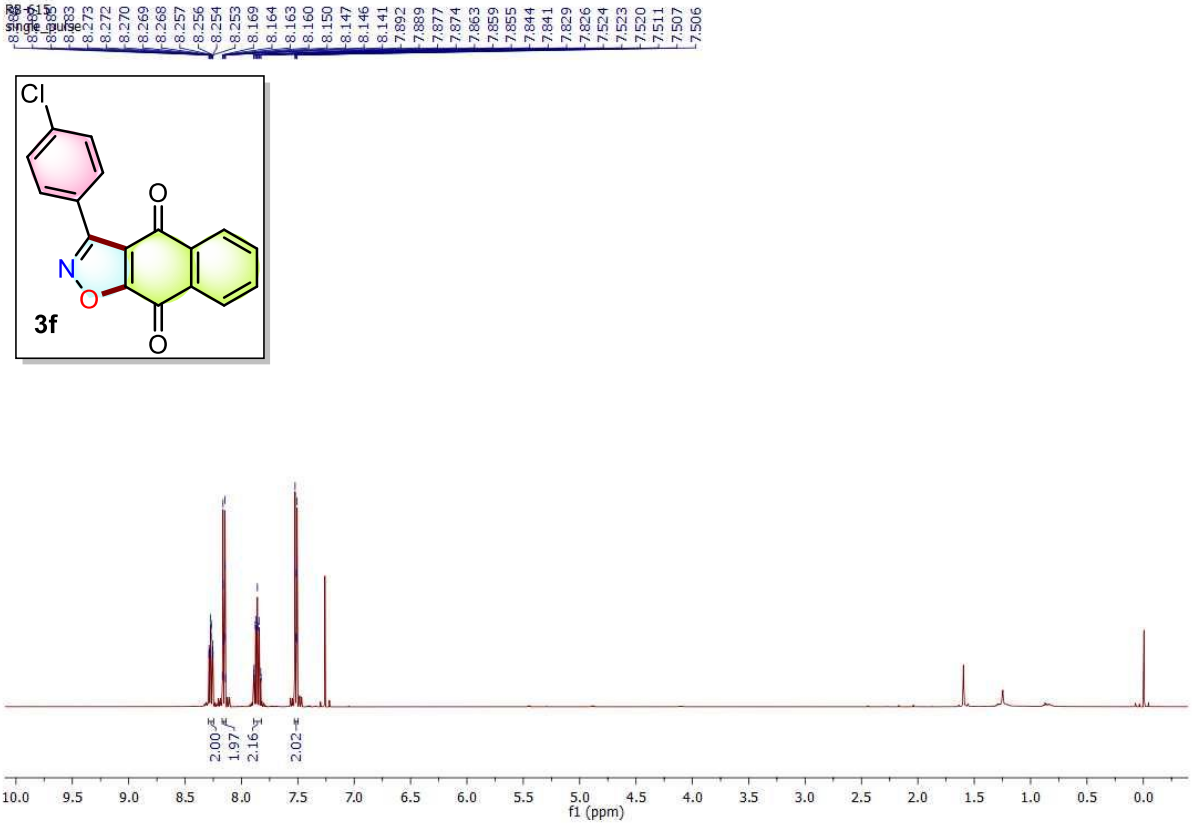
^{13}C NMR Spectrum of **3e** (126 MHz, Chloroform-*d*)



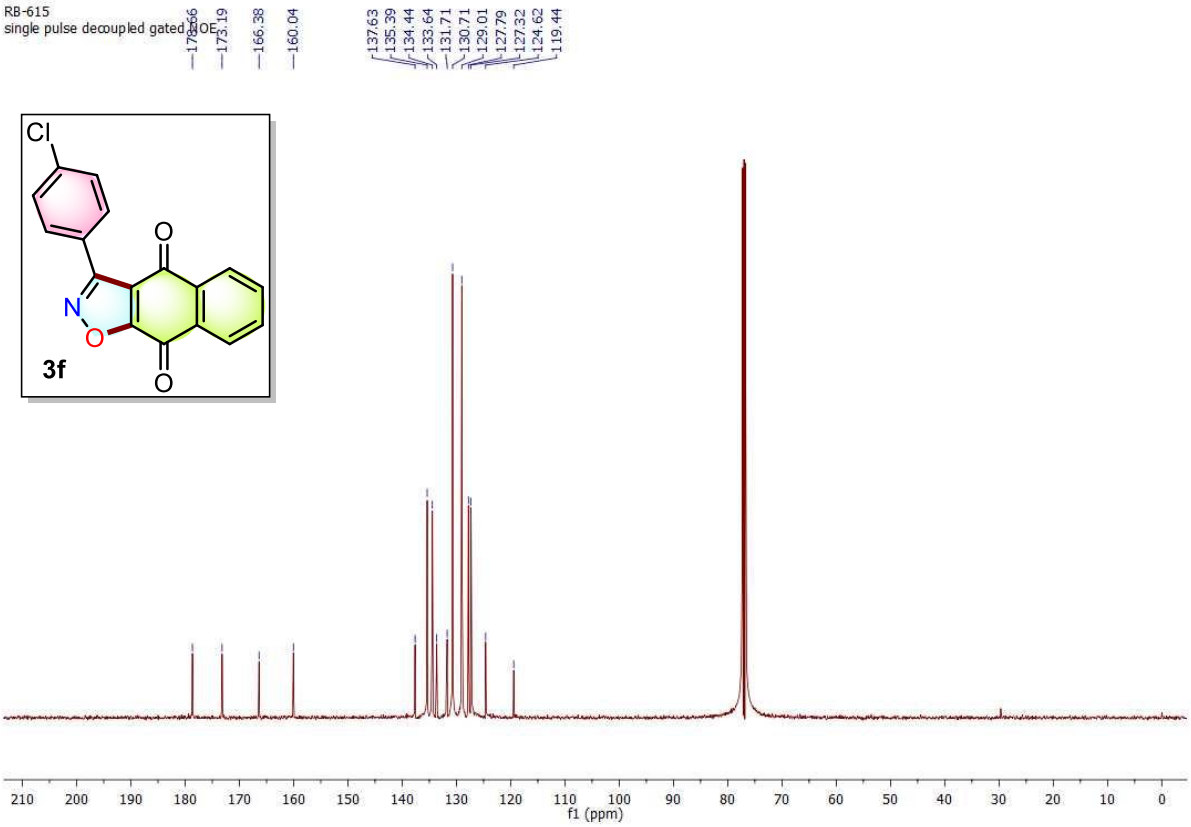
^{19}F NMR Spectrum of **3e** (471 MHz, Chloroform-*d*)



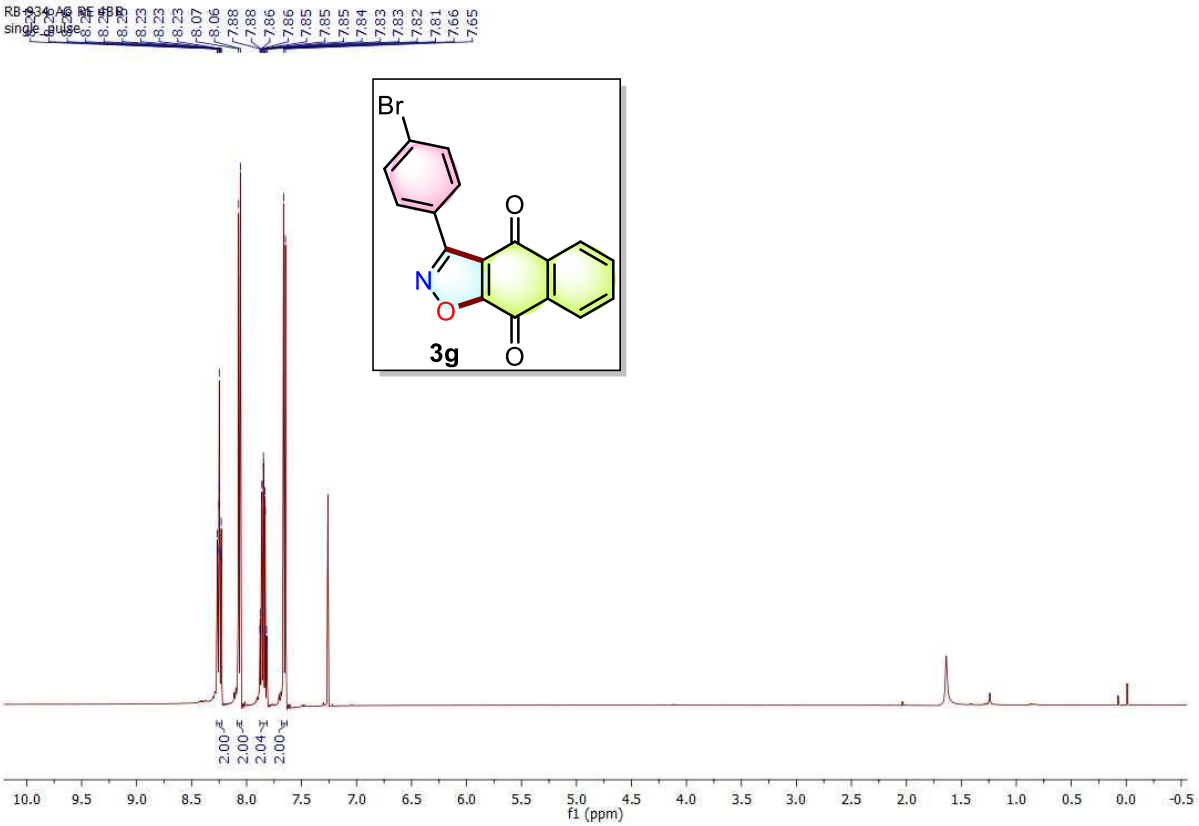
^{1}H NMR Spectrum of **3f** (500 MHz, Chloroform-*d*)



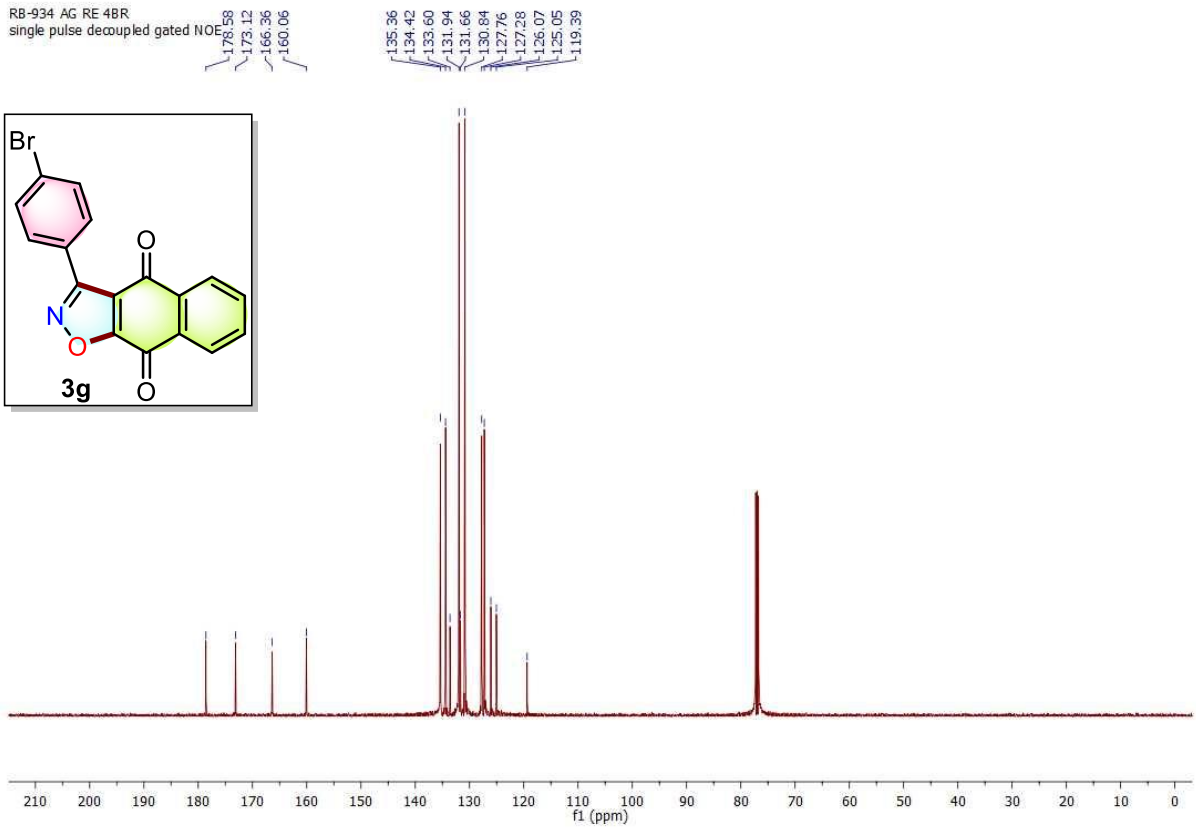
^{13}C NMR Spectrum of **3f** (126 MHz, Chloroform-*d*)



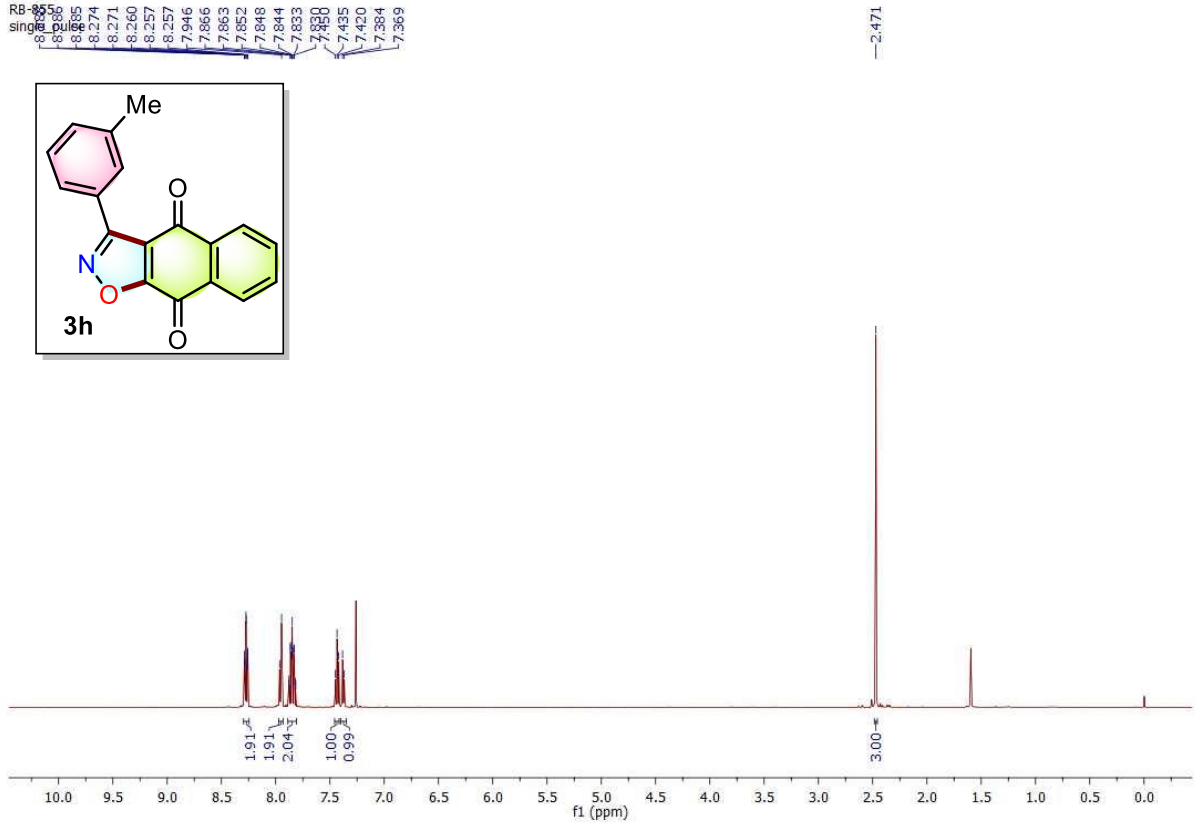
^{1}H NMR Spectrum of **3g** (500 MHz, Chloroform-*d*)



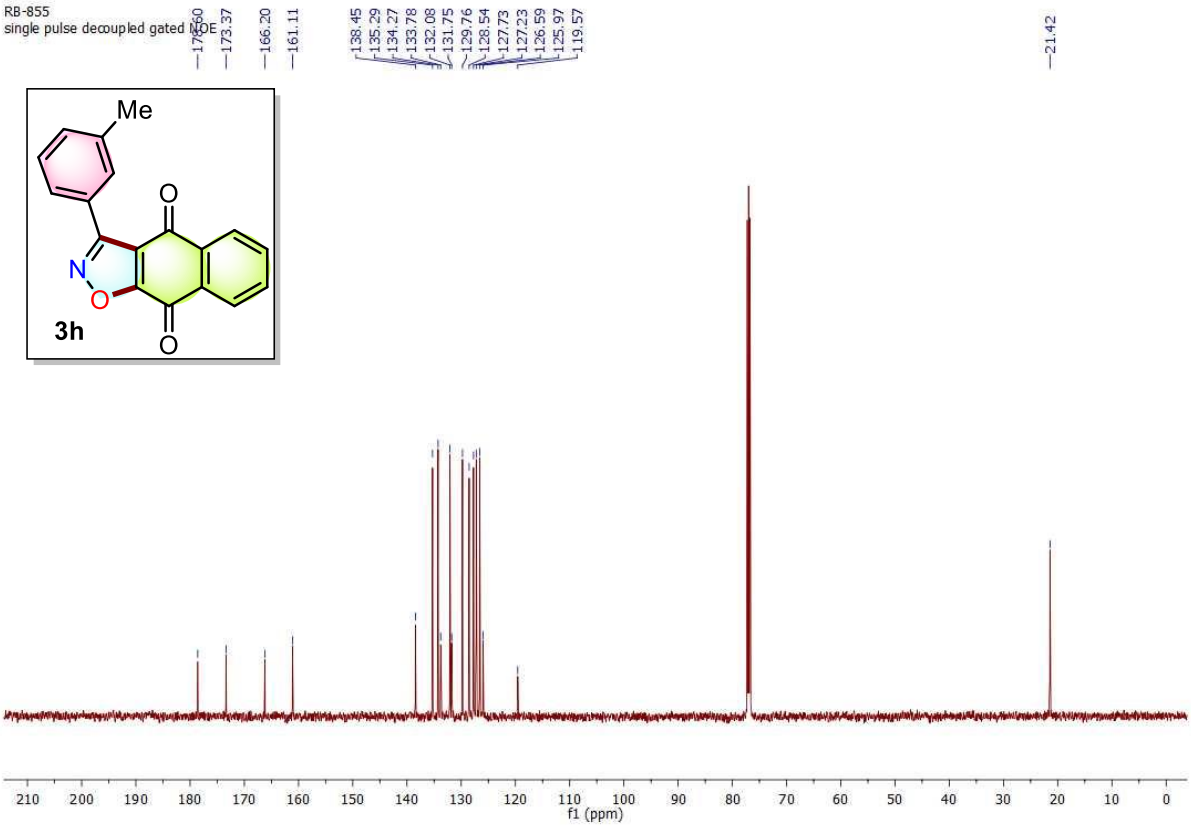
^{13}C NMR Spectrum of **3g** (126 MHz, Chloroform-*d*)



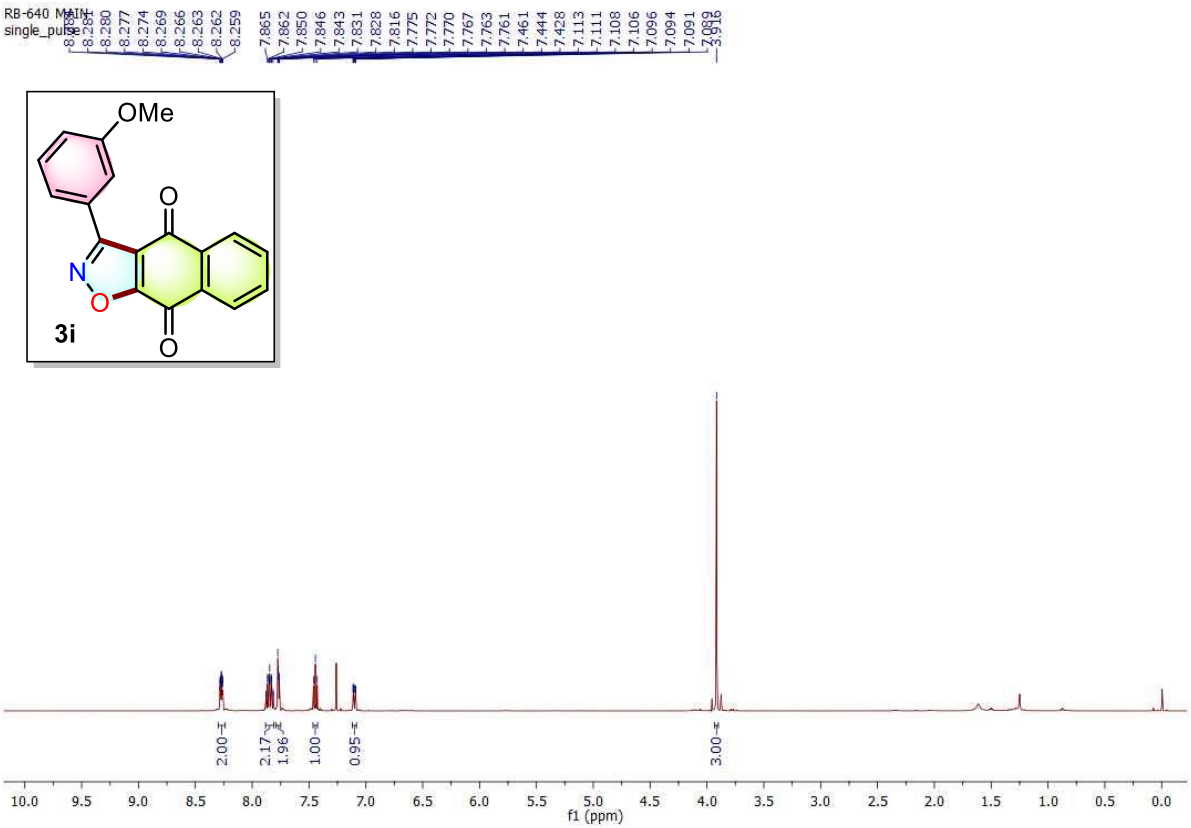
^{1}H NMR Spectrum of **3h** (500 MHz, Chloroform-*d*)



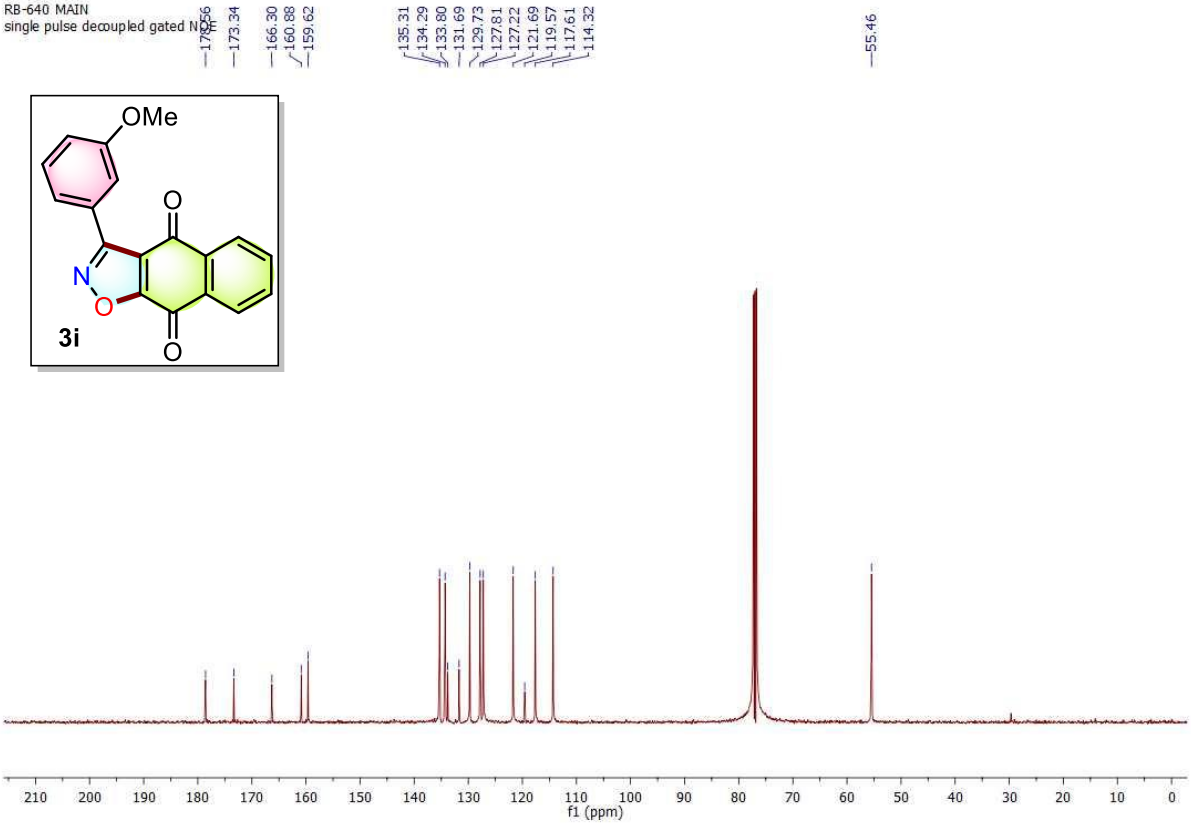
^{13}C NMR Spectrum of **3h** (126 MHz, Chloroform-*d*)



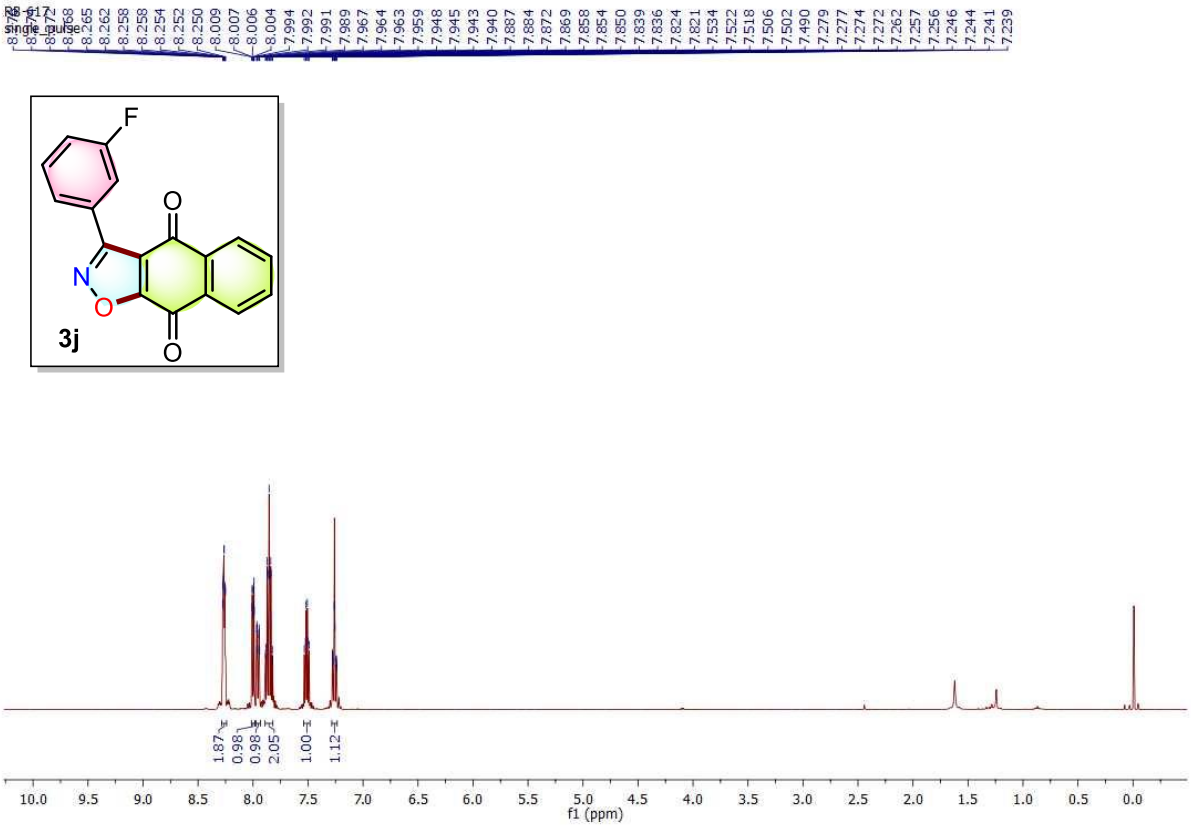
^{1}H NMR Spectrum of **3i** (500 MHz, Chloroform-*d*)



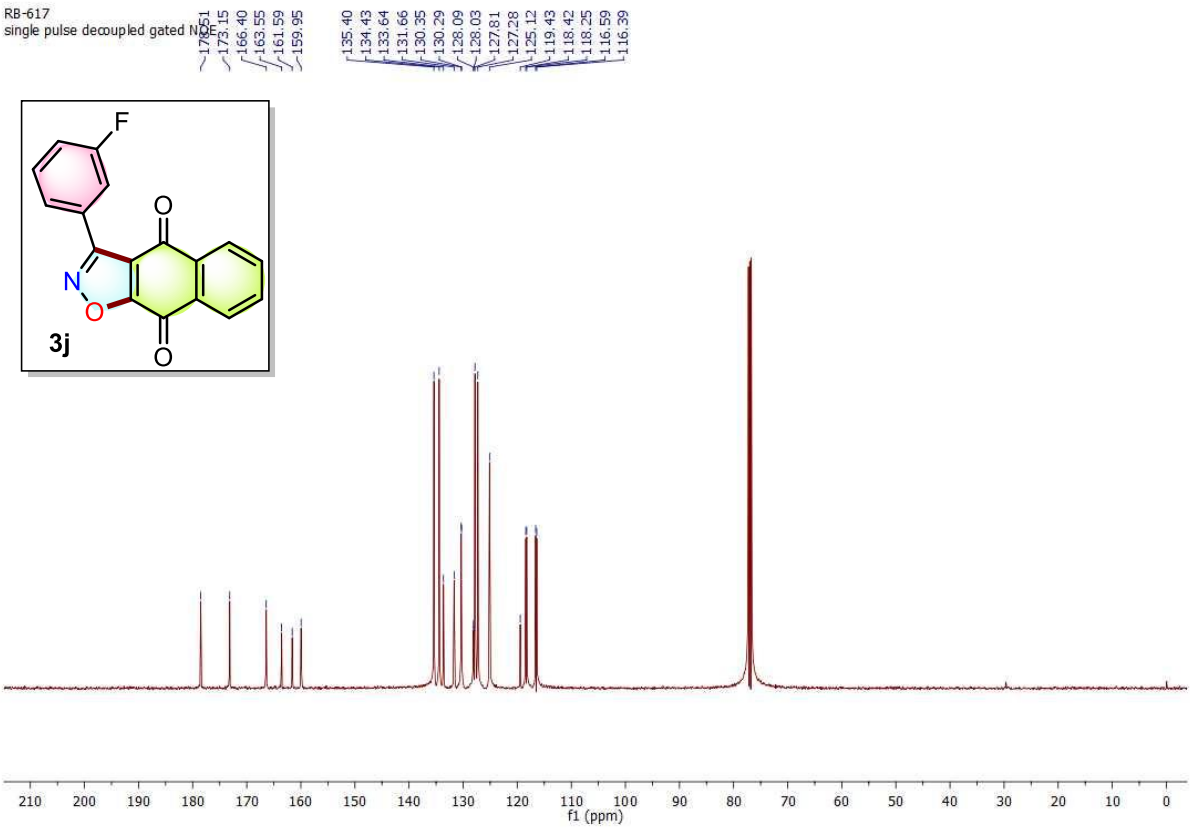
^{13}C NMR Spectrum of **3i** (126 MHz, Chloroform-*d*)



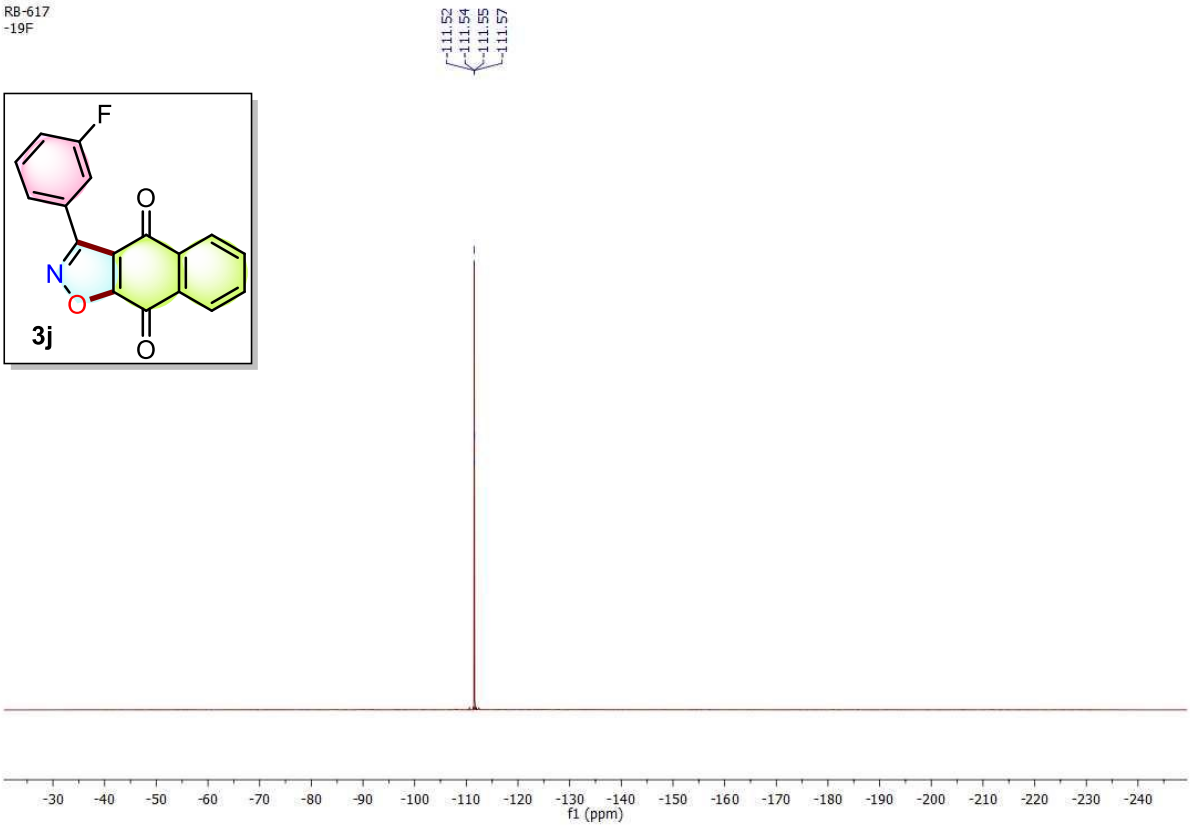
^{1}H NMR Spectrum of **3j** (500 MHz, Chloroform-*d*)



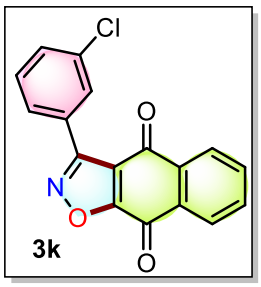
^{13}C NMR Spectrum of **3j** (126 MHz, Chloroform-*d*)

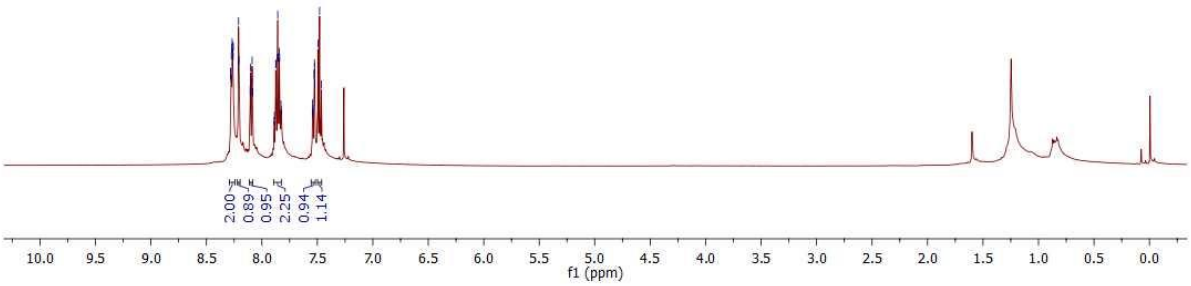


^{19}F NMR Spectrum of **3j** (471 MHz, Chloroform-*d*)

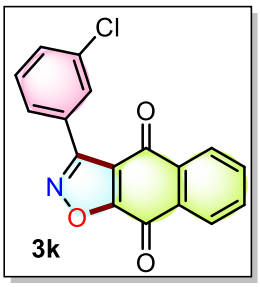


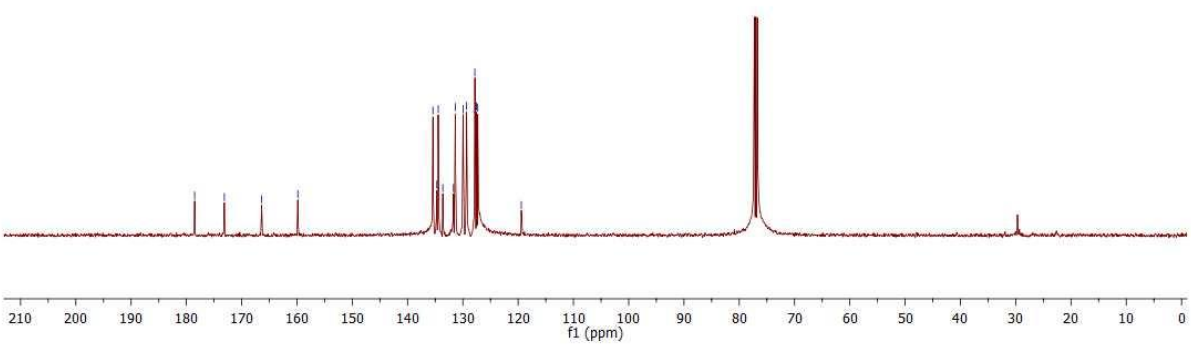
^{1}H NMR Spectrum of **3k** (500 MHz, Chloroform-*d*)



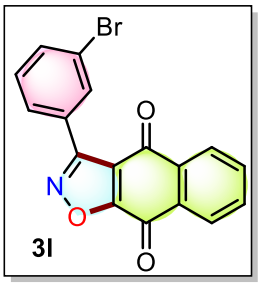


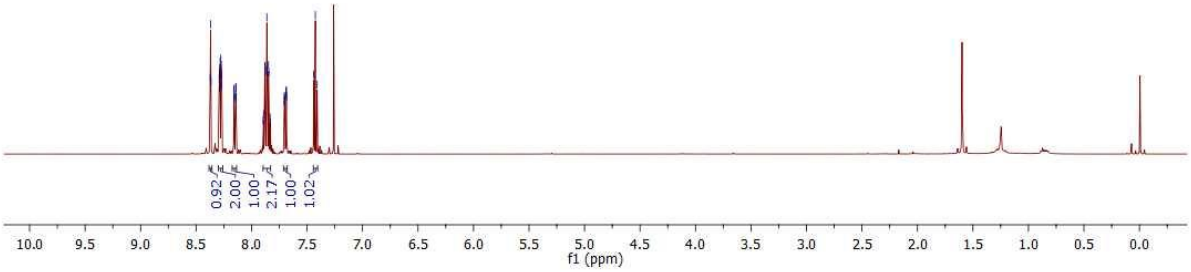
^{13}C NMR Spectrum of **3k** (126 MHz, Chloroform-*d*)



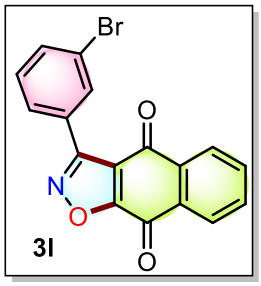


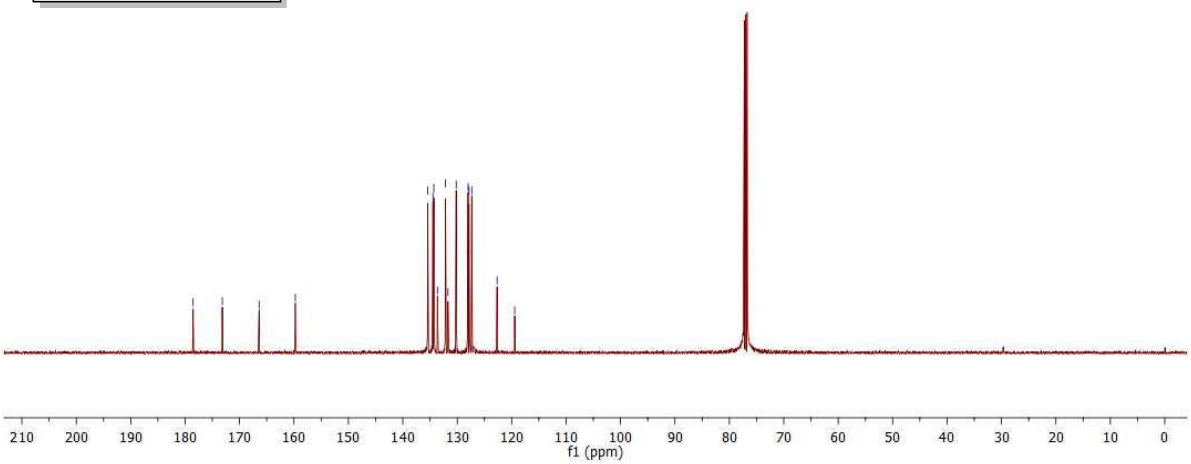
^{1}H NMR Spectrum of **3l** (500 MHz, Chloroform-*d*)



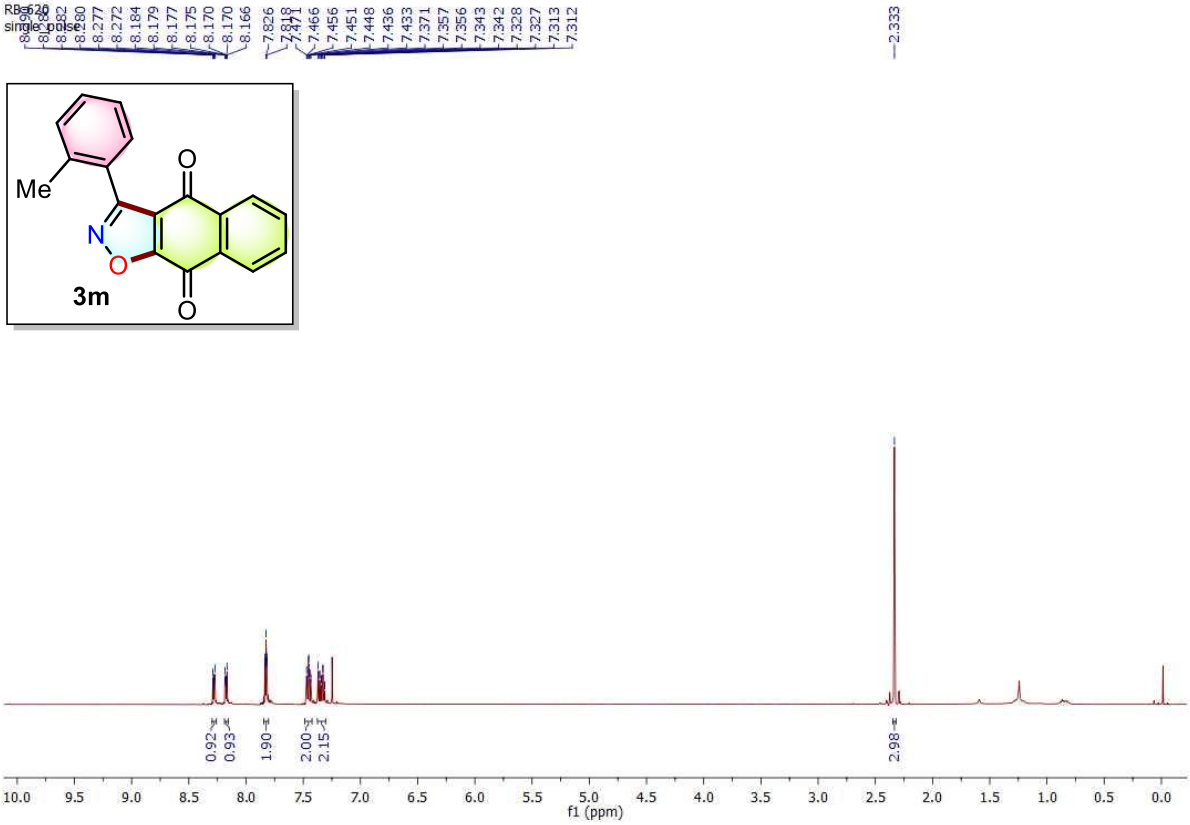


^{13}C NMR Spectrum of **3l** (126 MHz, Chloroform-*d*)

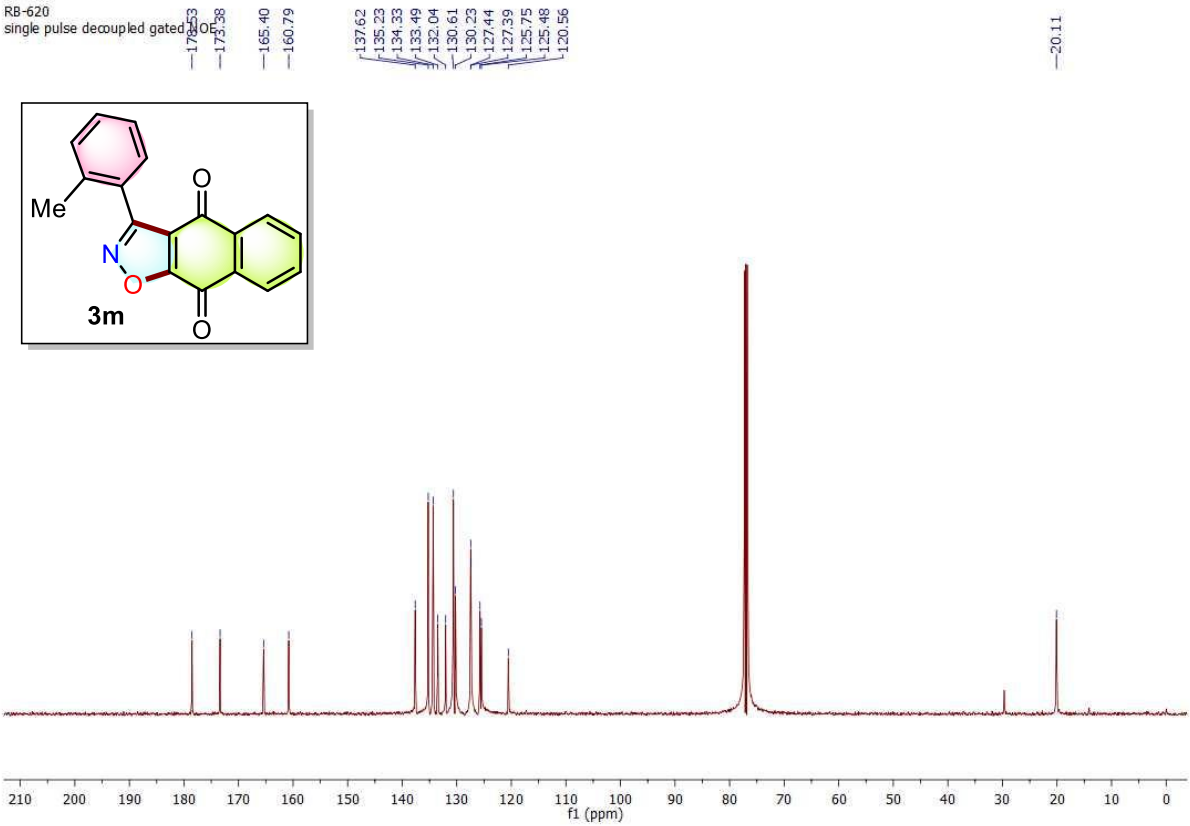




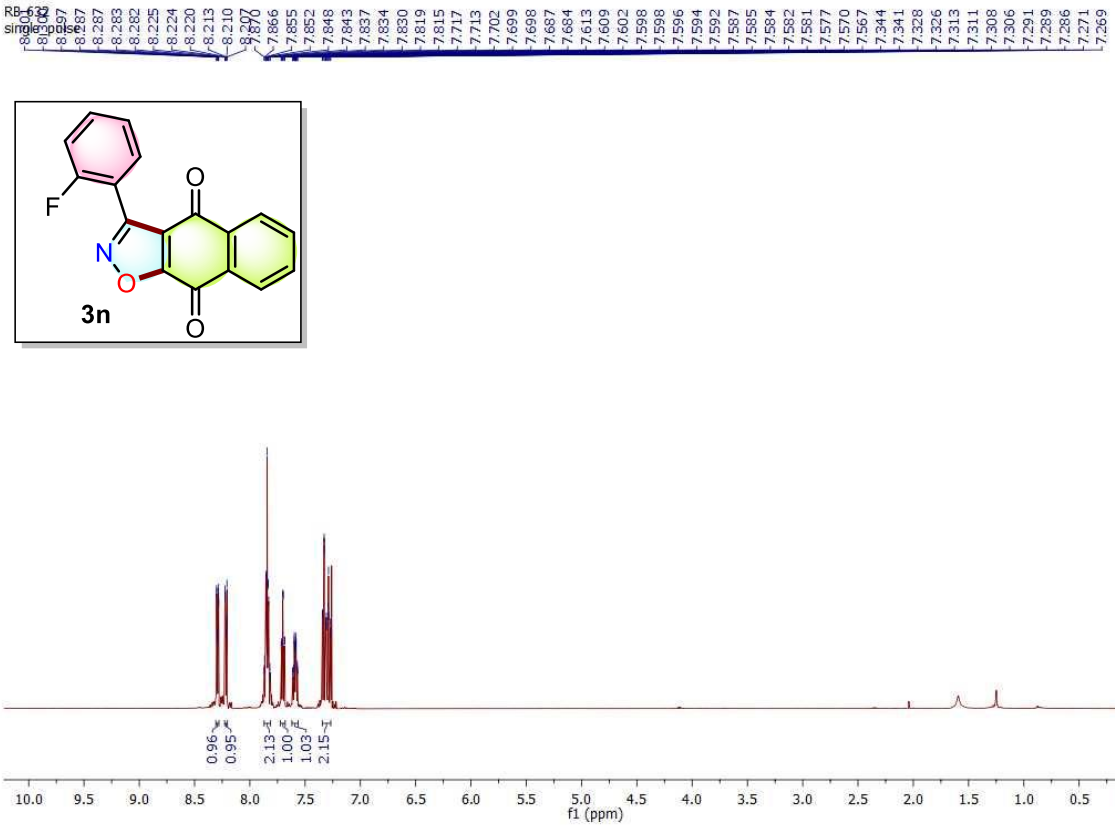
^{1}H NMR Spectrum of **3m** (500 MHz, Chloroform-*d*)



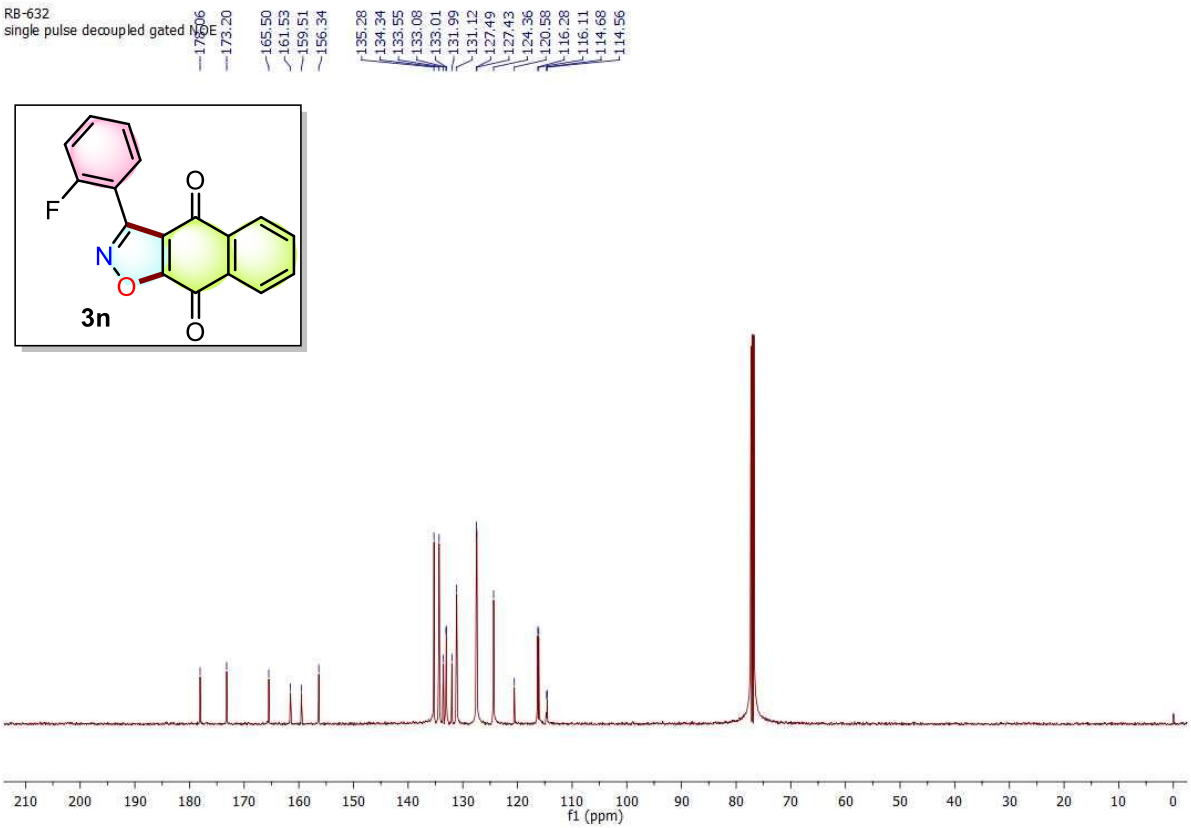
^{13}C NMR Spectrum of **3m** (126 MHz, Chloroform-*d*)



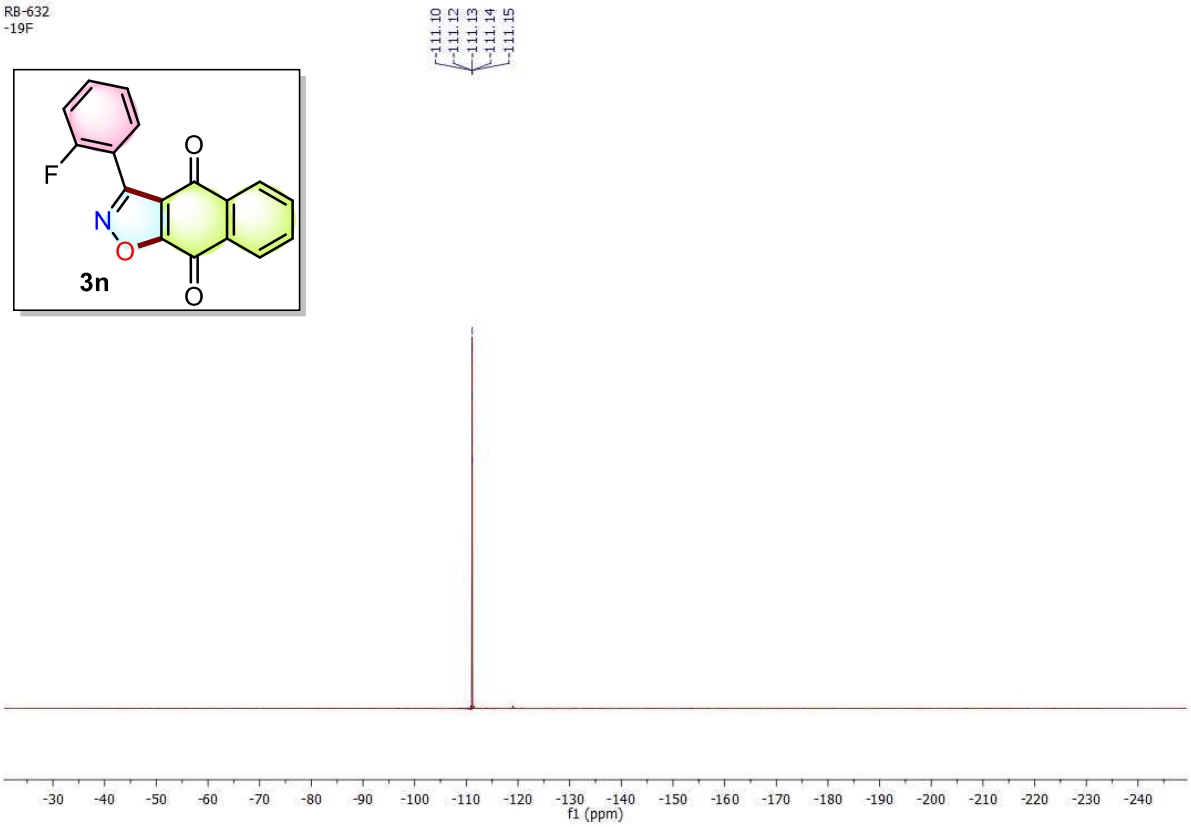
^{1}H NMR Spectrum of **3n** (500 MHz, Chloroform-*d*)



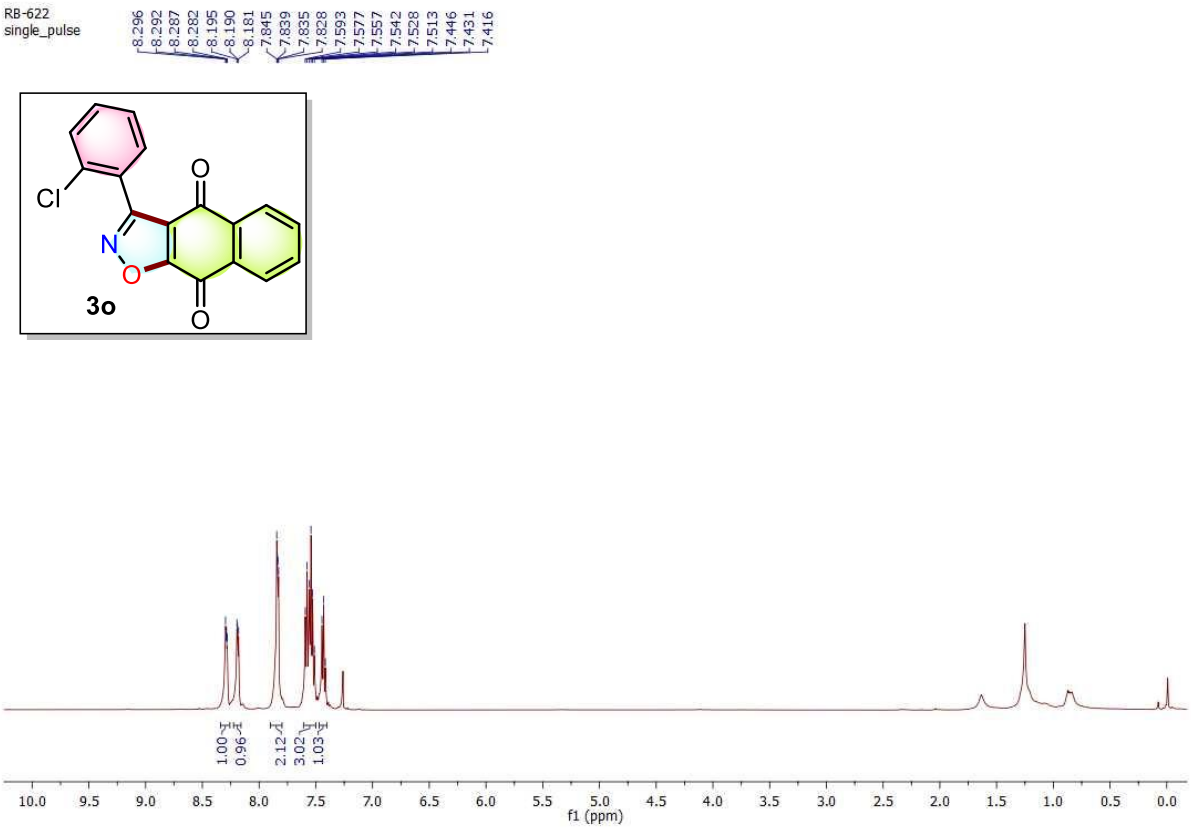
^{13}C NMR Spectrum of **3n** (126 MHz, Chloroform-*d*)



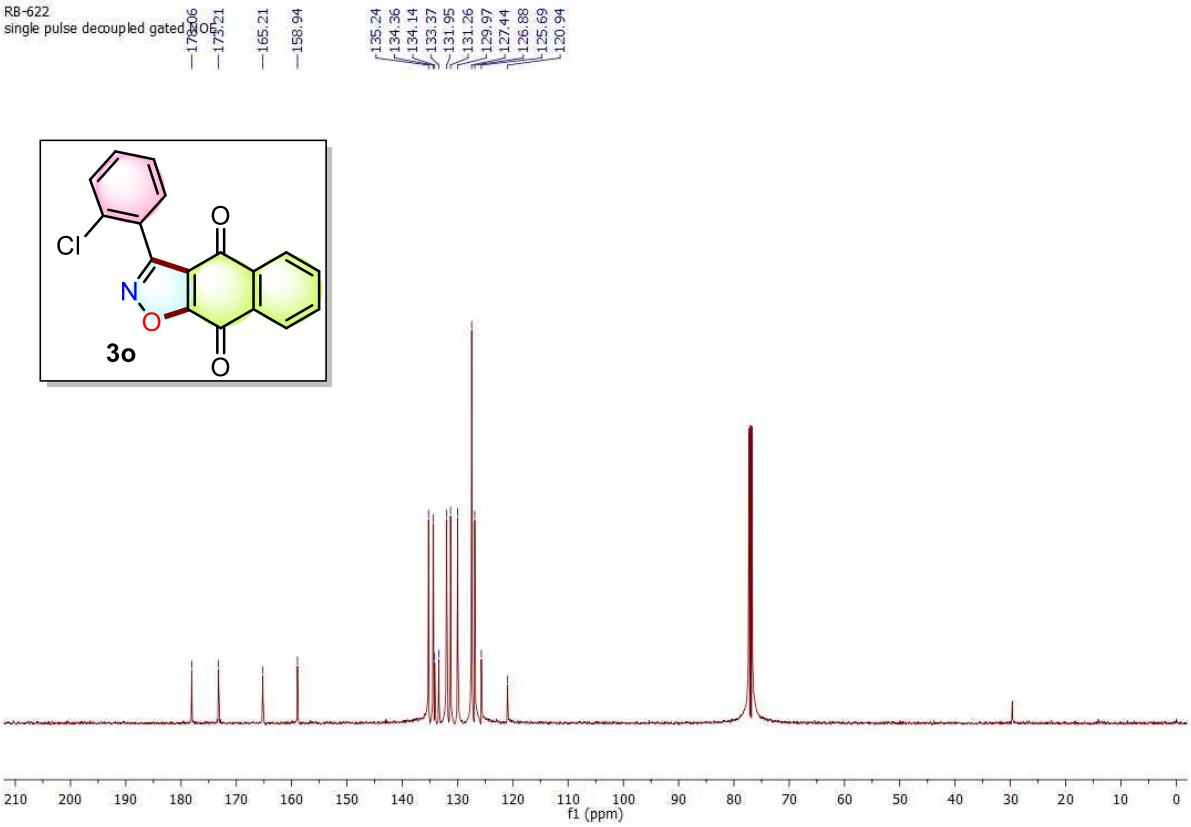
^{19}F NMR Spectrum of **3n** (471 MHz, Chloroform-*d*)



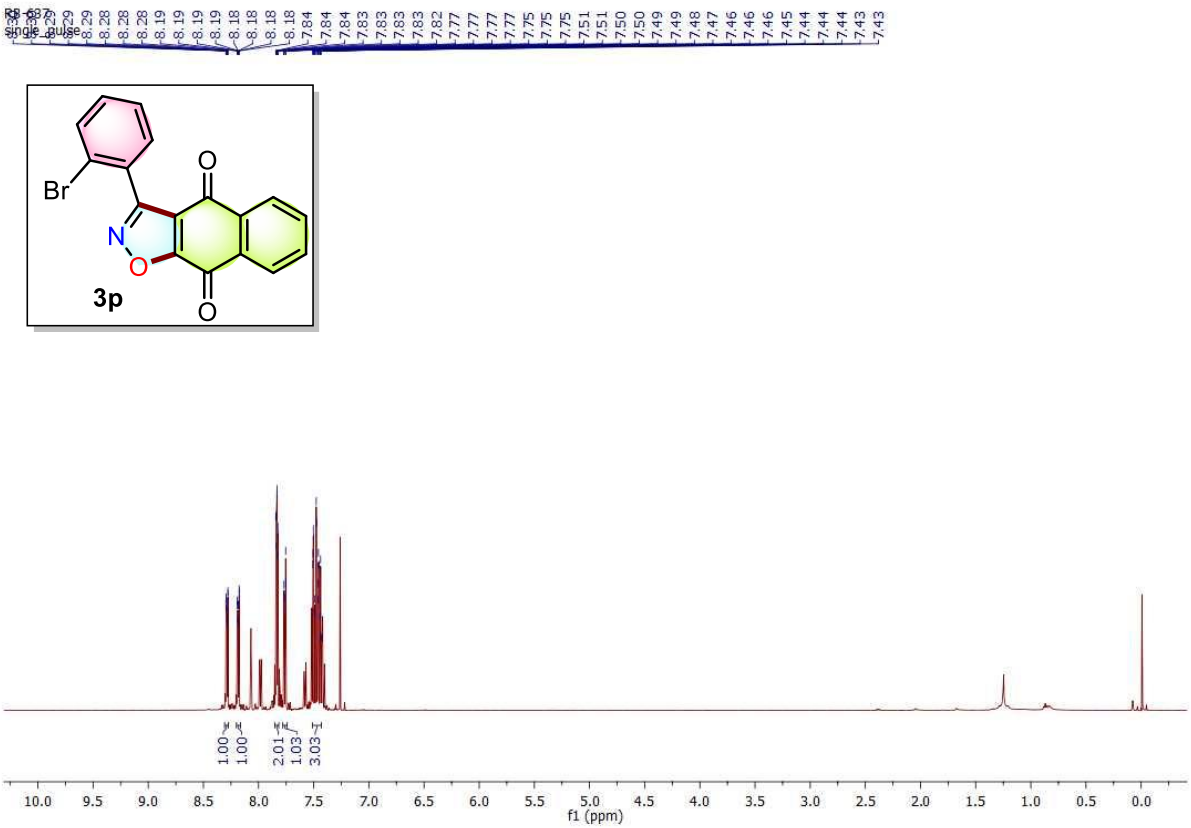
^{1}H NMR Spectrum of **3o** (500 MHz, Chloroform-*d*)



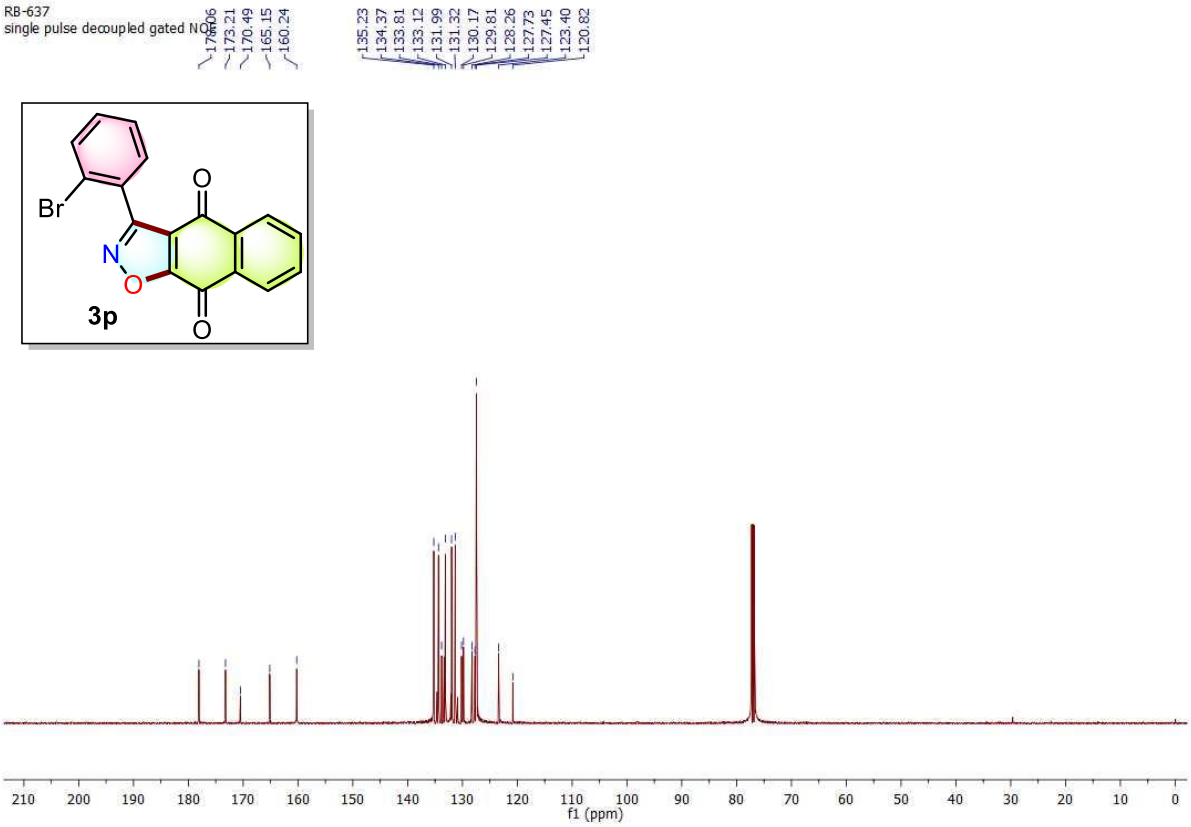
^{13}C NMR Spectrum of **3o** (126 MHz, Chloroform-*d*)



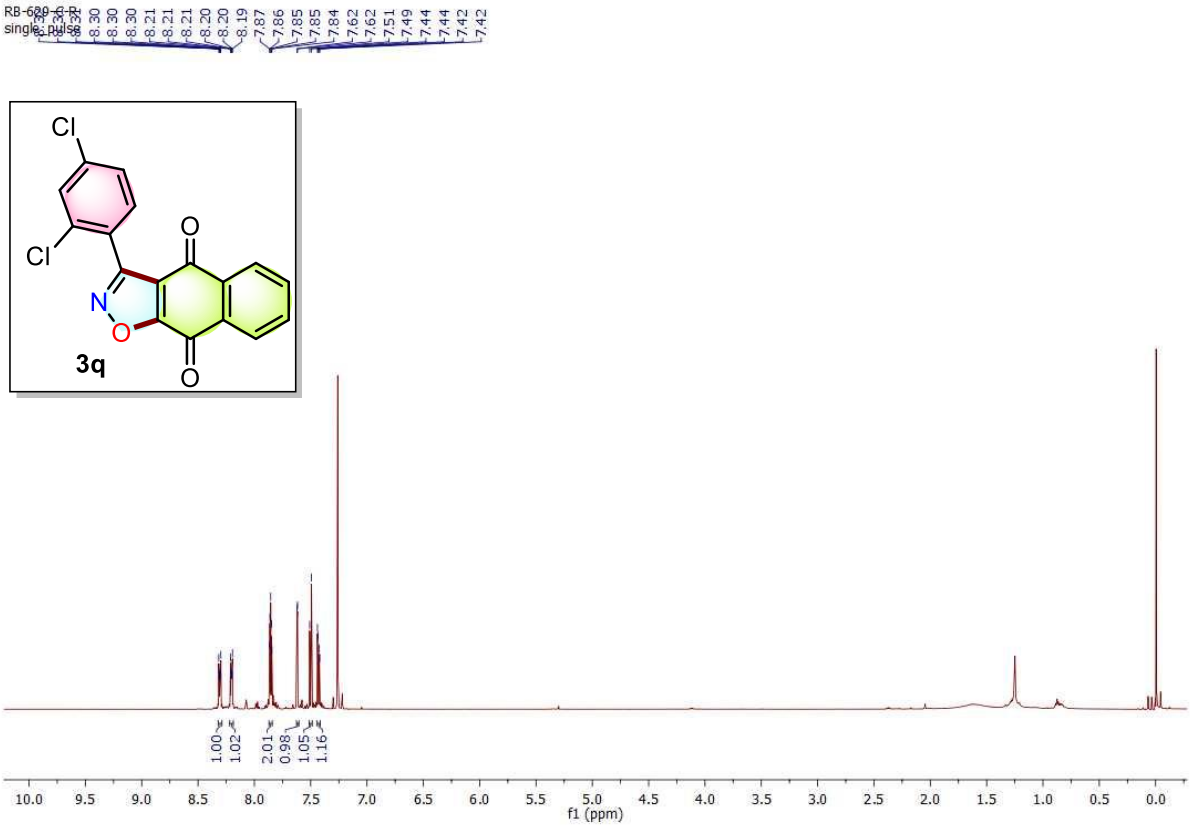
^{1}H NMR Spectrum of **3p** (500 MHz, Chloroform-*d*)



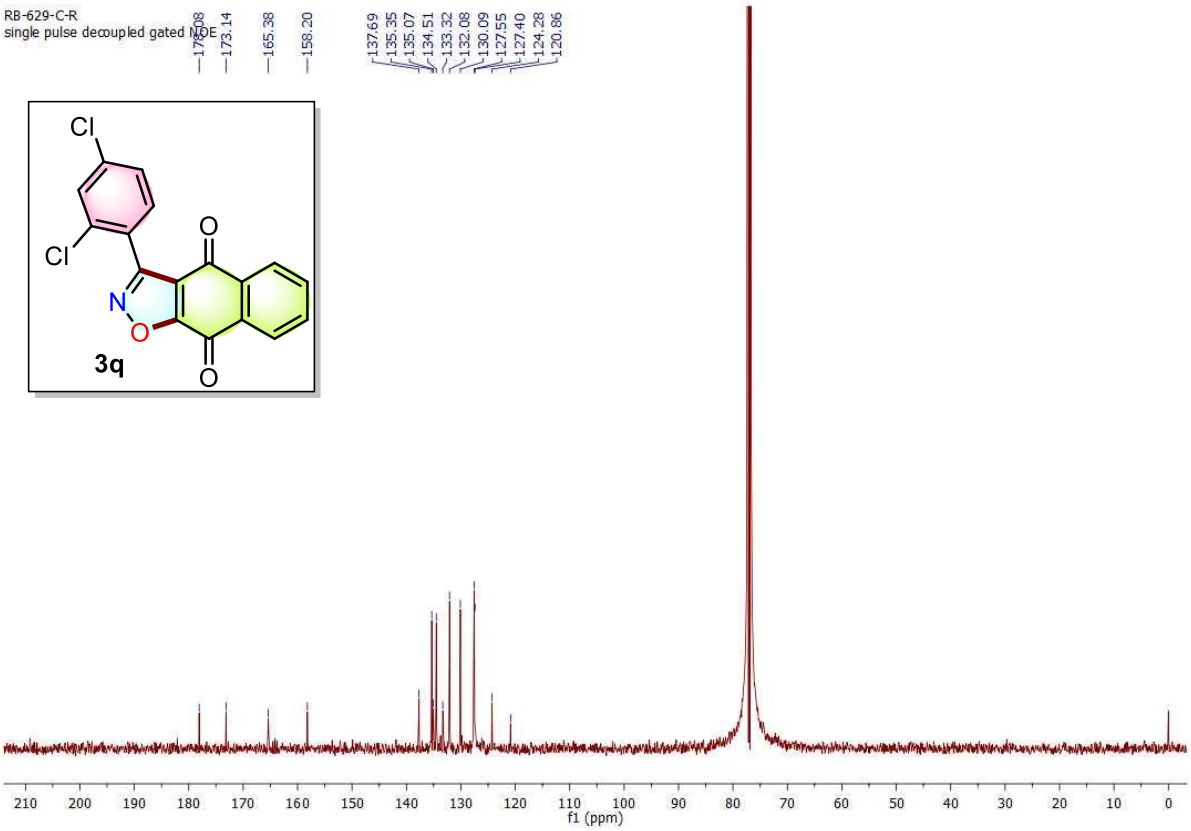
^{13}C NMR Spectrum of **3p** (126 MHz, Chloroform-*d*)



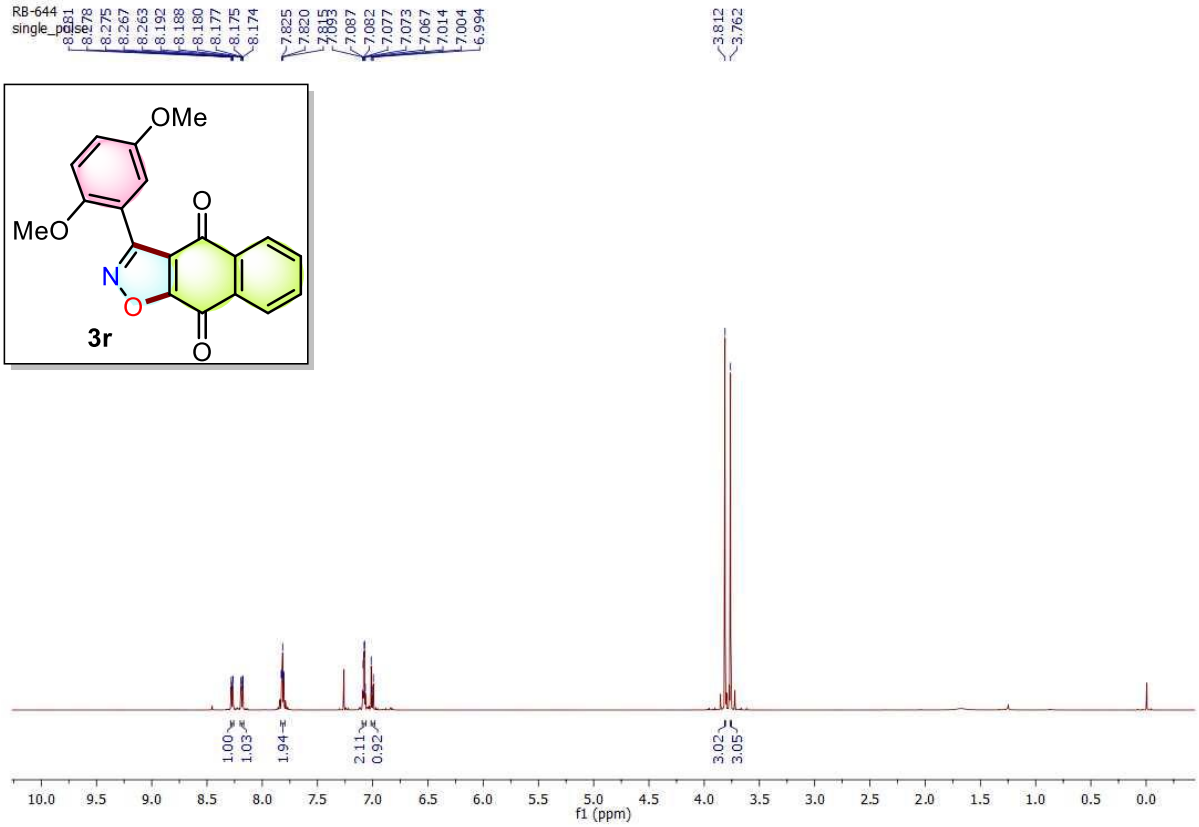
^{1}H NMR Spectrum of **3q** (500 MHz, Chloroform-*d*)



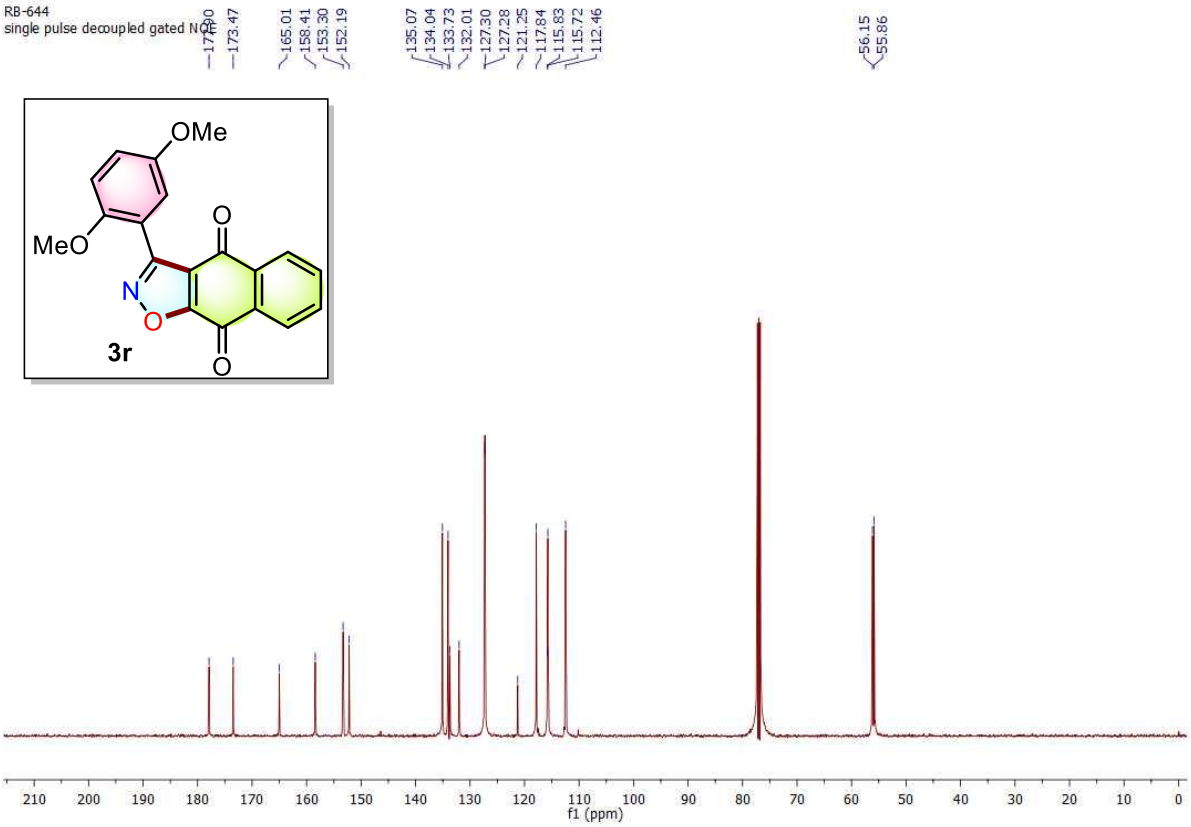
^{13}C NMR Spectrum of **3q** (126 MHz, Chloroform-*d*)



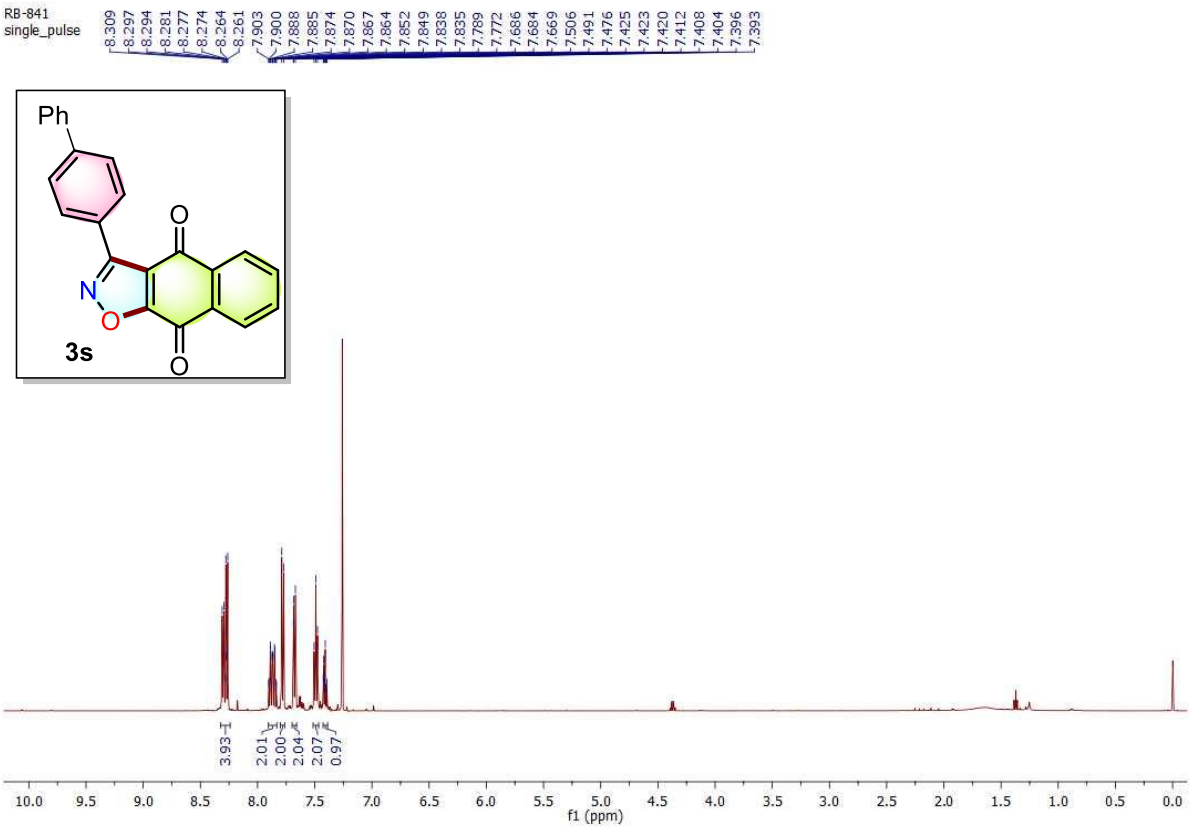
^{1}H NMR Spectrum of **3r** (500 MHz, Chloroform-*d*)



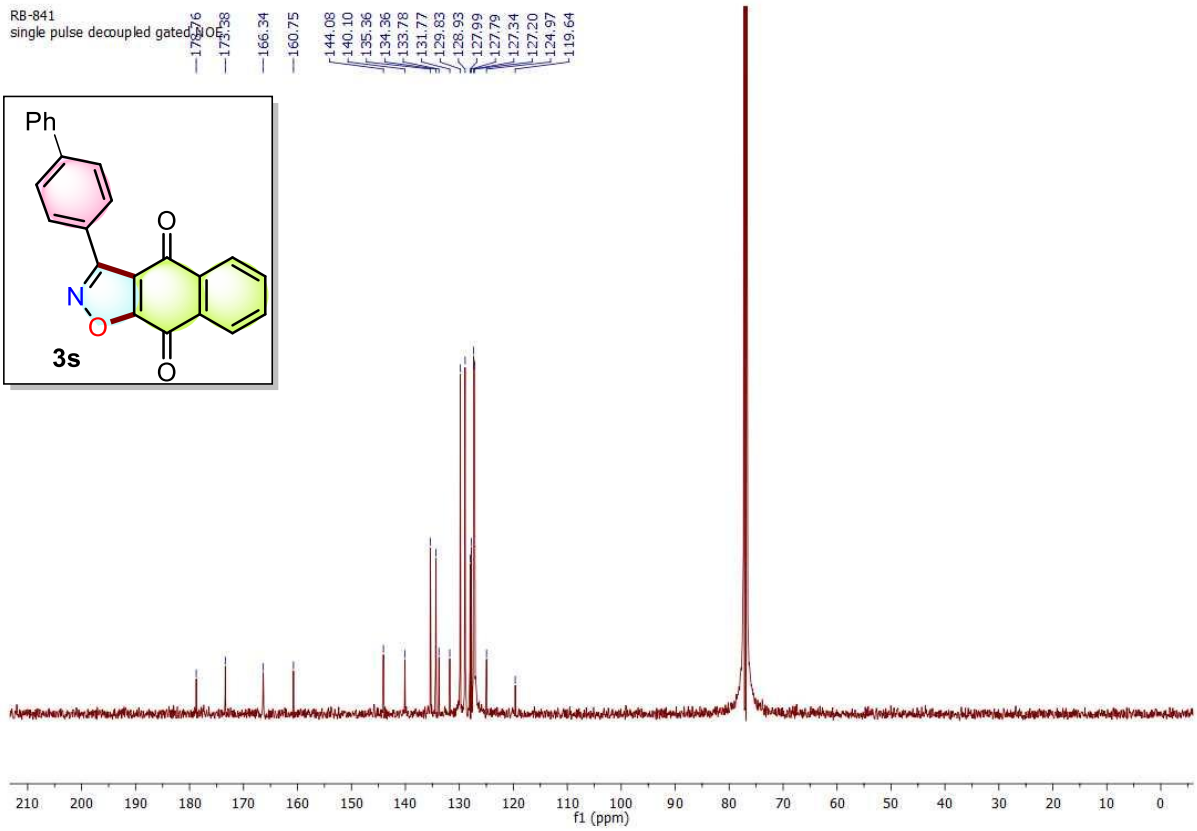
^{13}C NMR Spectrum of **3r** (126 MHz, Chloroform-*d*)



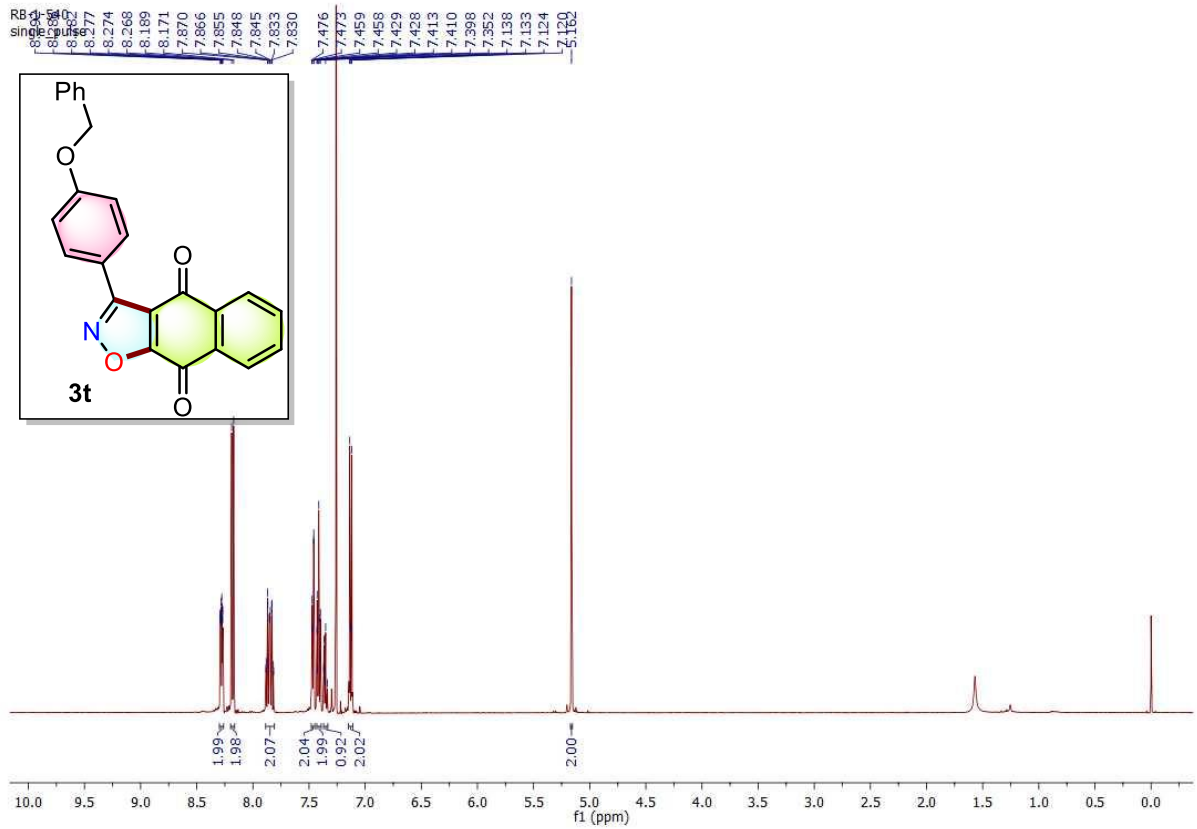
^{1}H NMR Spectrum of **3s** (500 MHz, Chloroform-*d*)



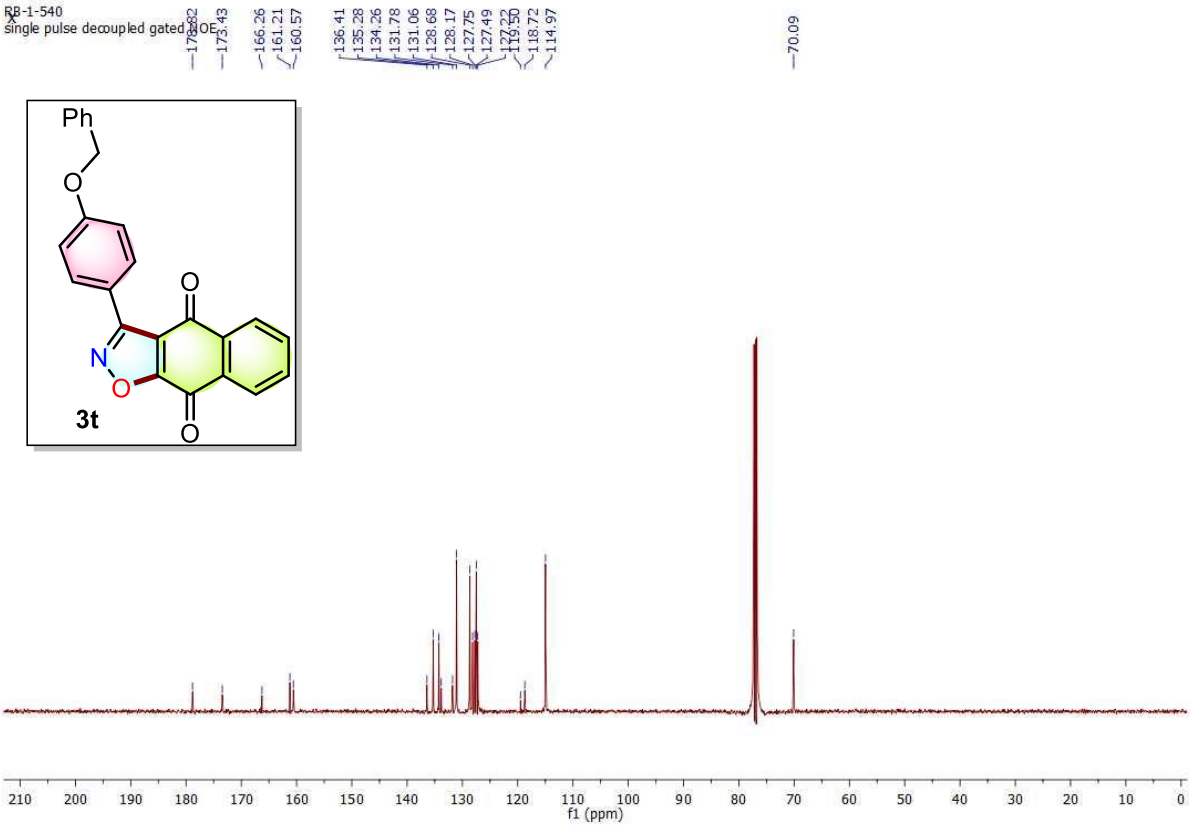
^{13}C NMR Spectrum of **3s** (126 MHz, Chloroform-*d*)



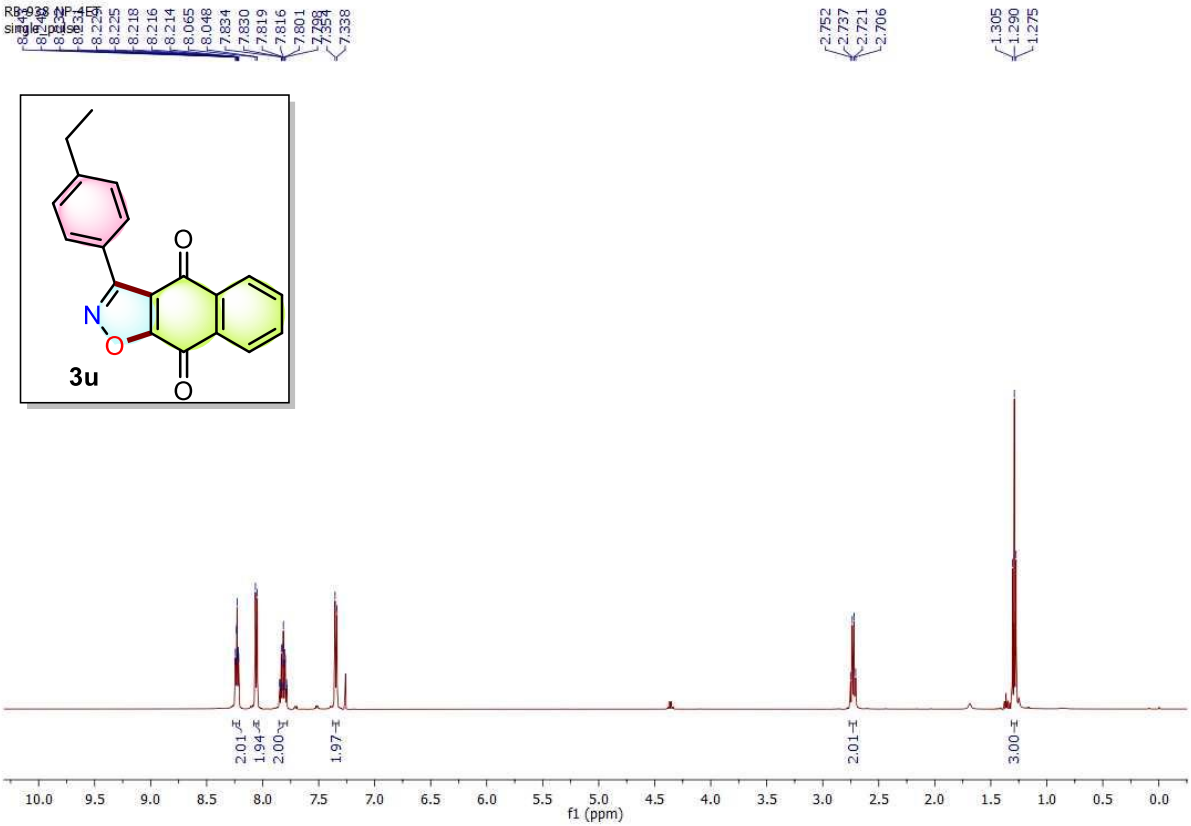
^{1}H NMR Spectrum of **3t** (500 MHz, Chloroform-*d*)



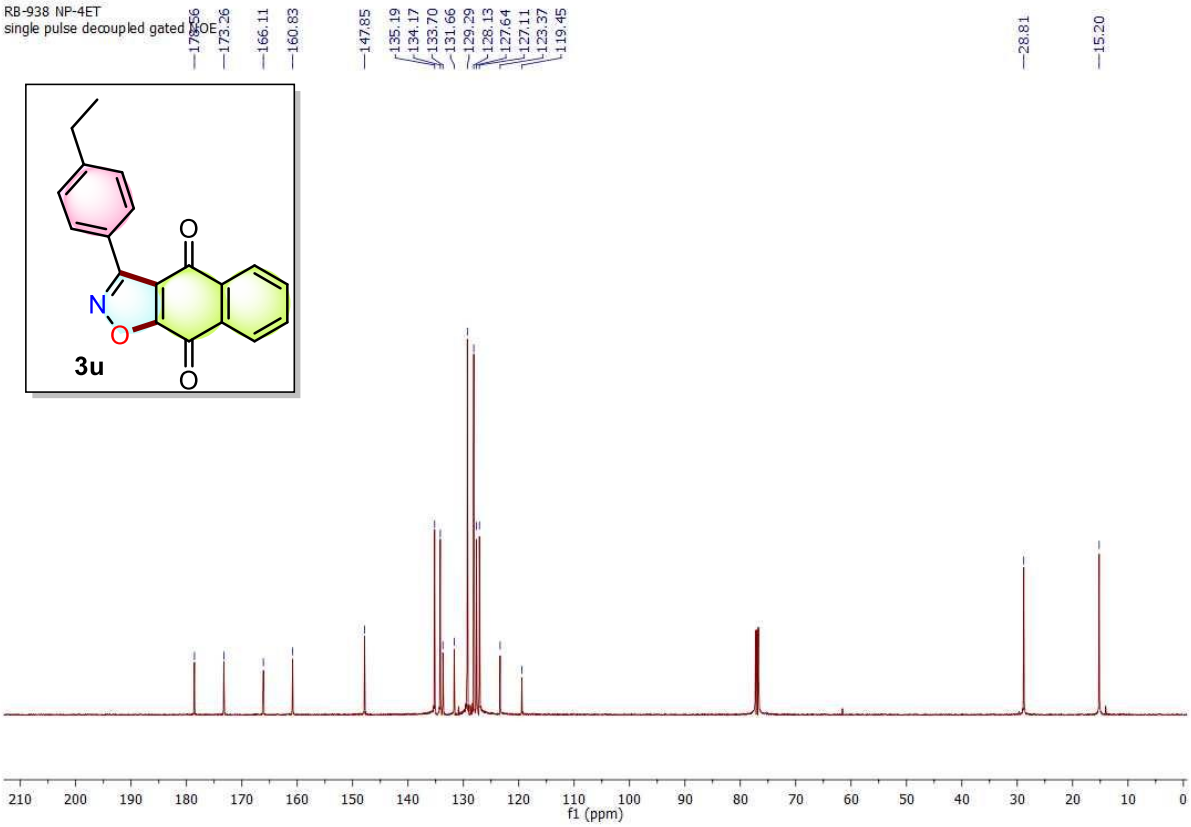
^{13}C NMR Spectrum of **3t** (126 MHz, Chloroform-*d*)



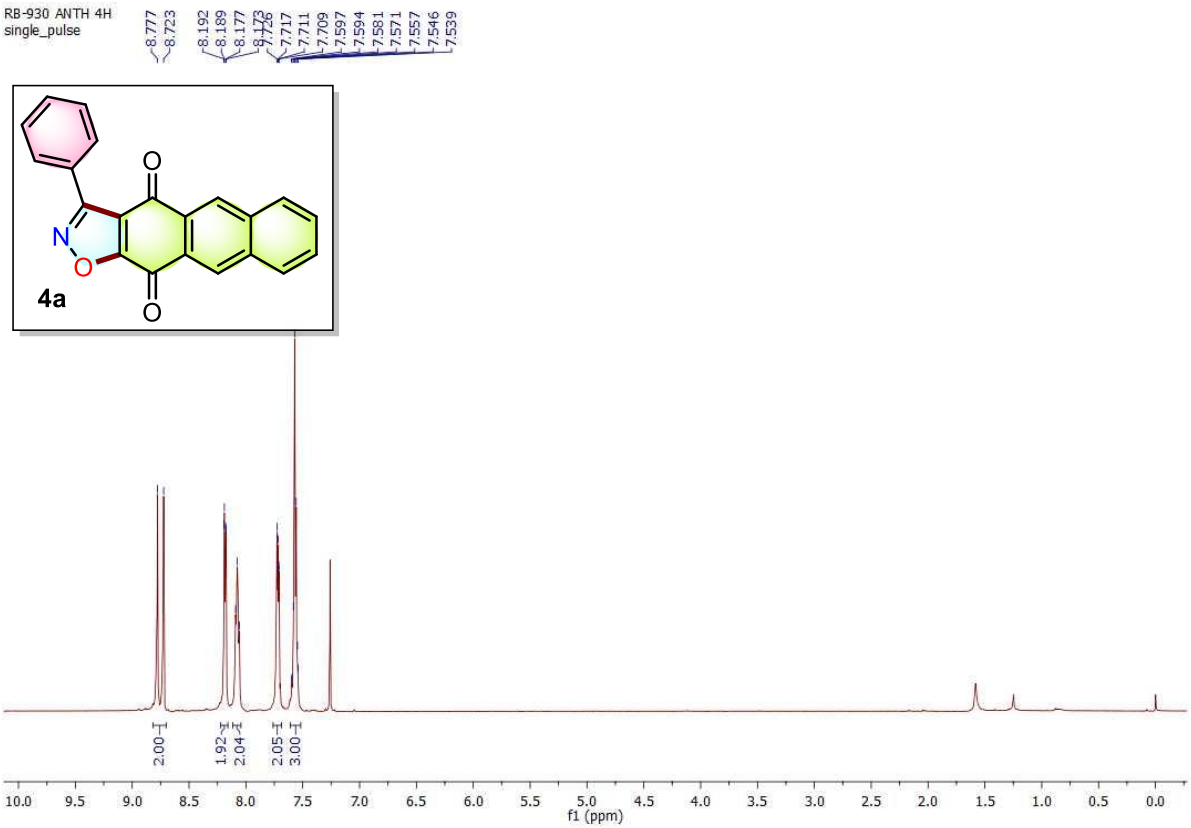
^{1}H NMR Spectrum of **3u** (500 MHz, Chloroform-*d*)



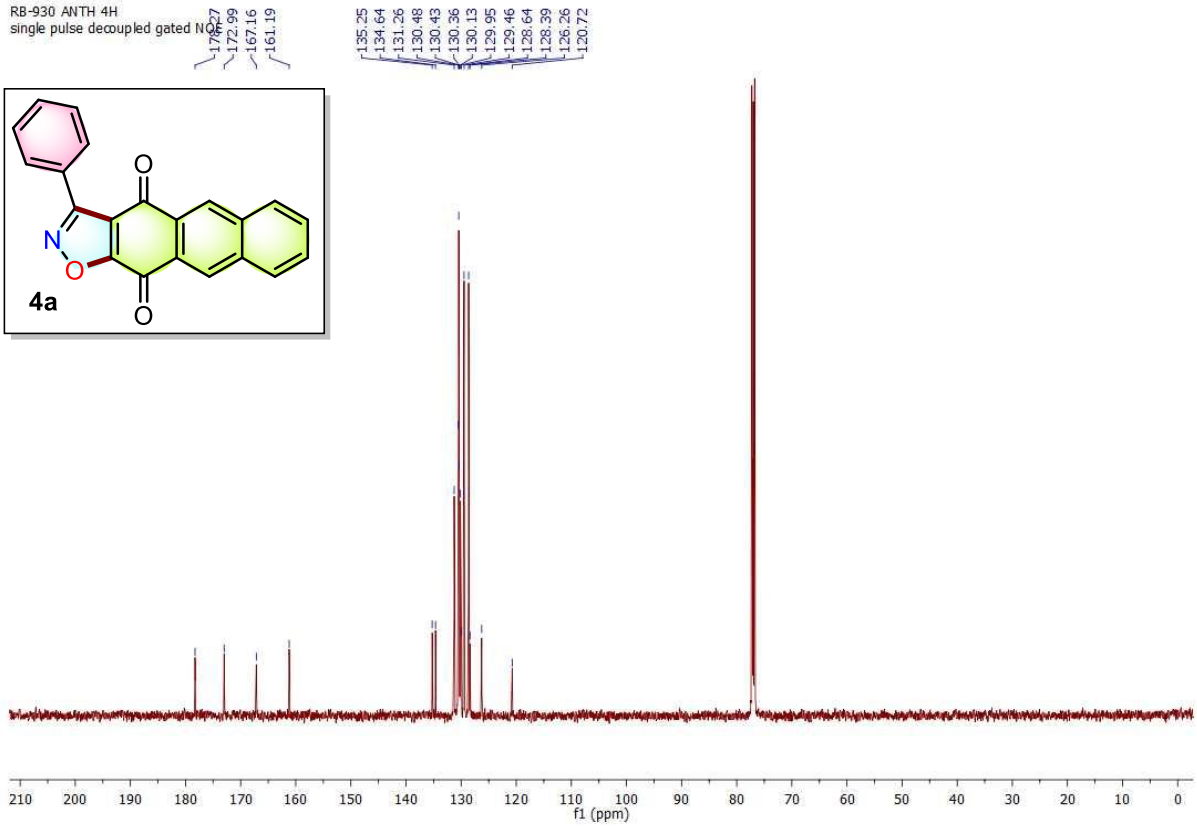
^{13}C NMR Spectrum of **3u** (126 MHz, Chloroform-*d*)



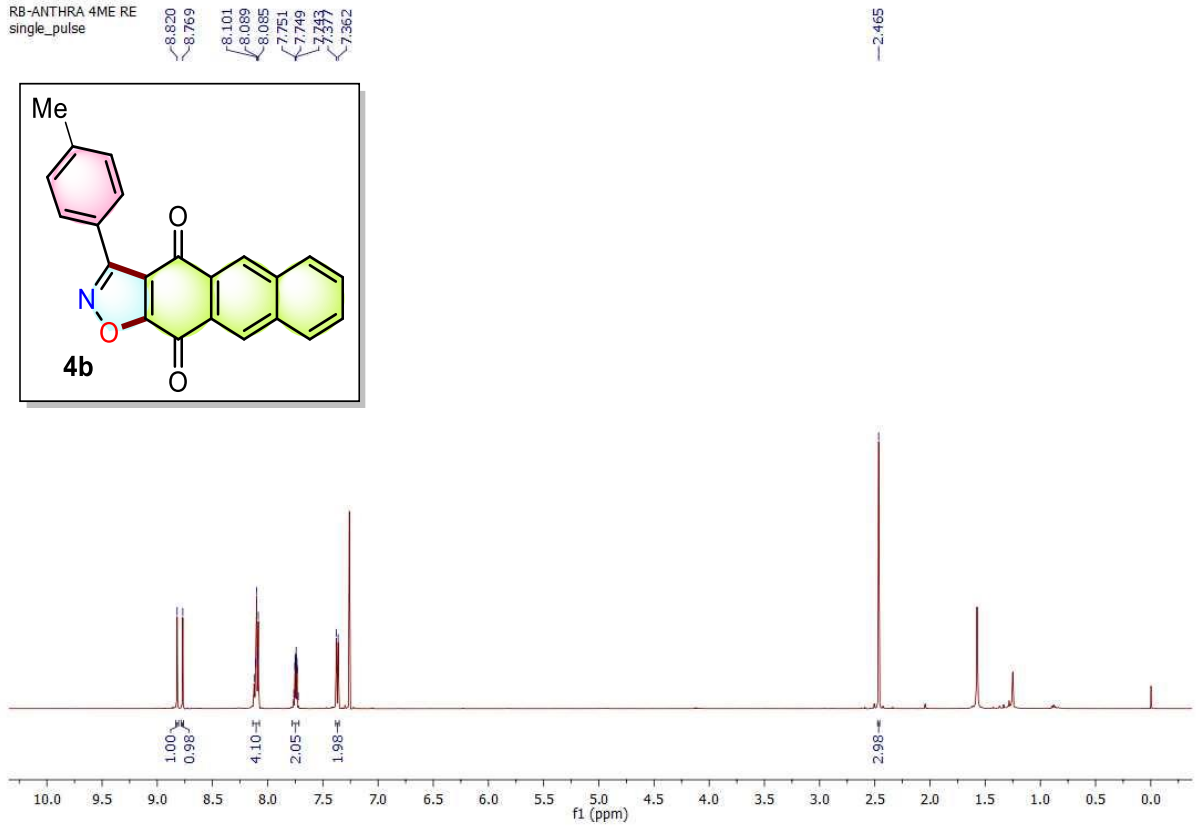
^{1}H NMR Spectrum of **4a** (500 MHz, Chloroform-*d*)



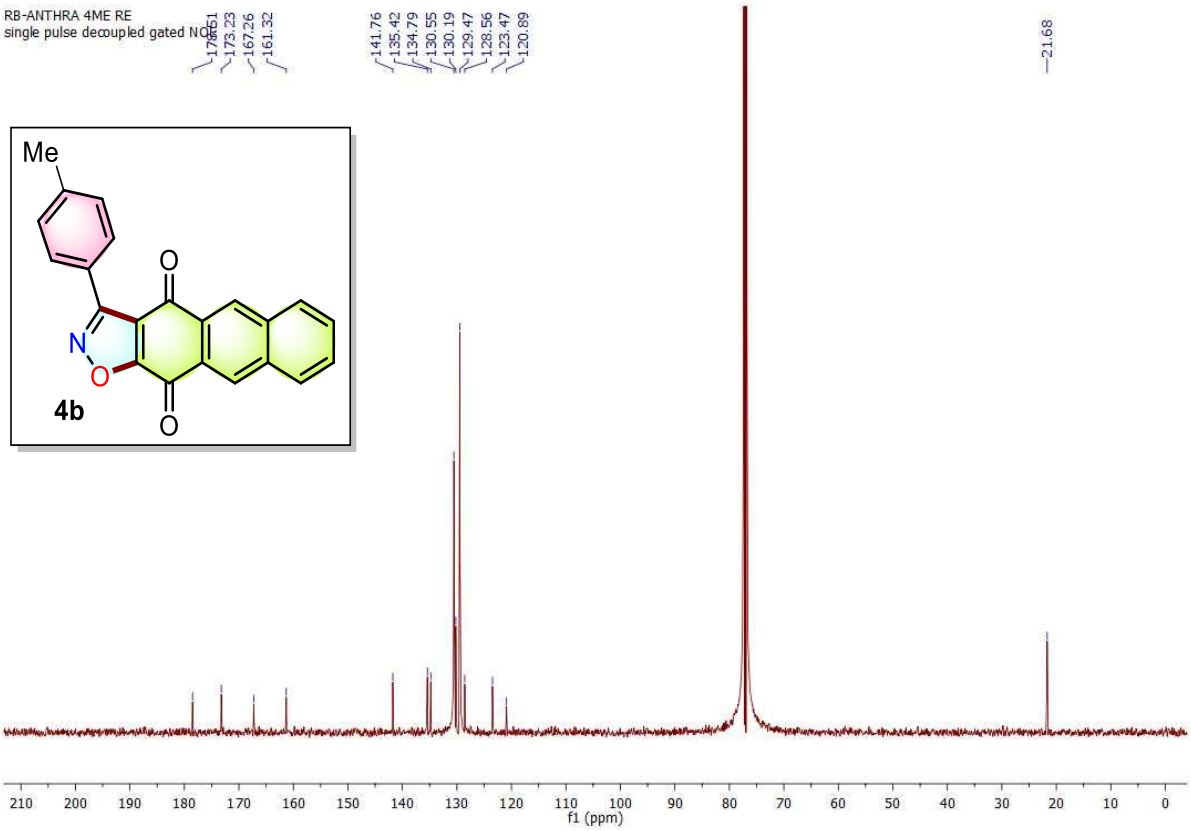
^{13}C NMR Spectrum of **4a** (126 MHz, Chloroform-*d*)



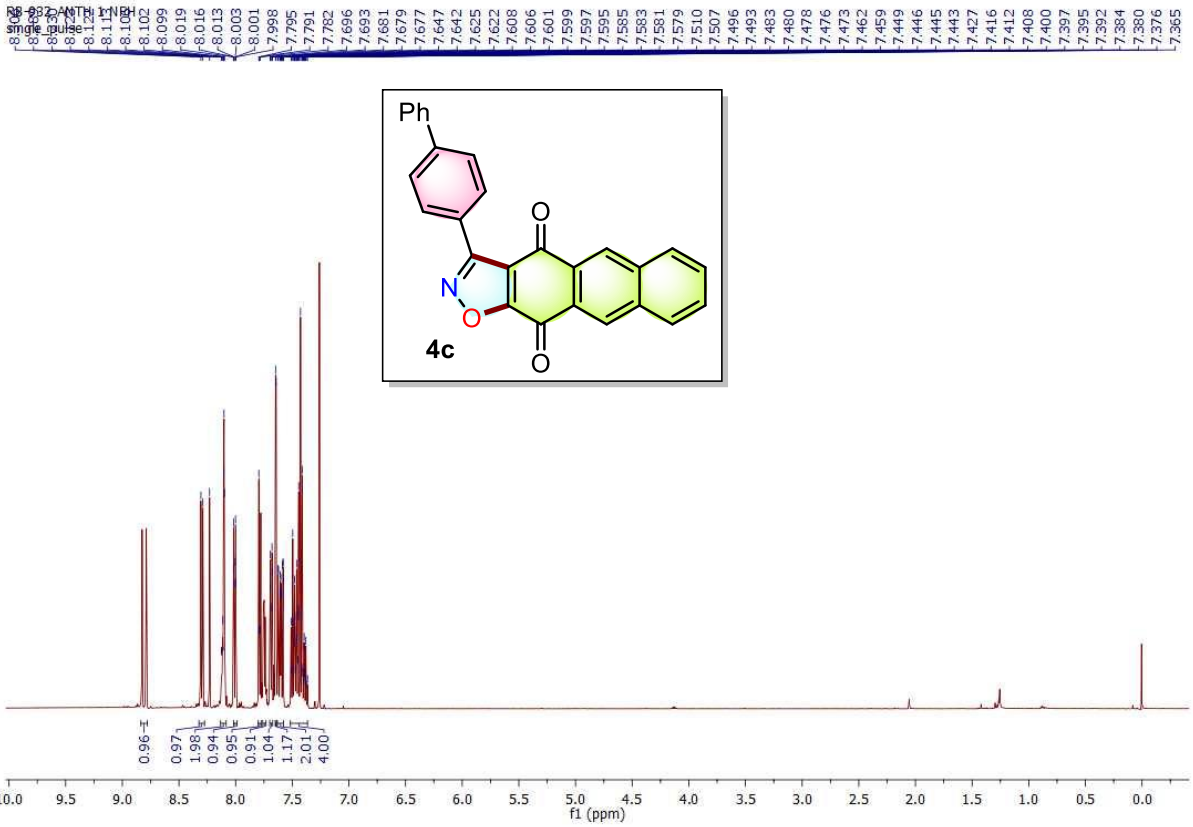
^{1}H NMR Spectrum of **4b** (500 MHz, Chloroform-*d*)



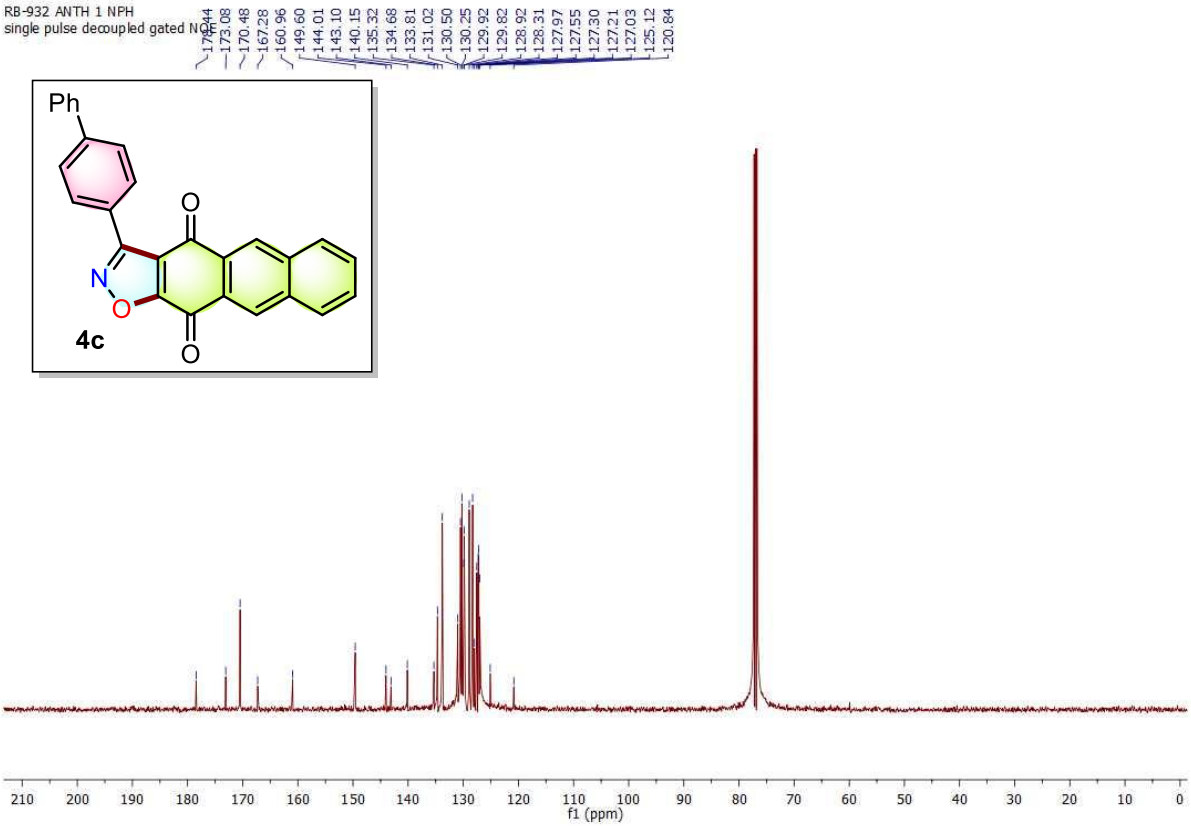
^{13}C NMR Spectrum of **4b** (126 MHz, Chloroform-*d*)



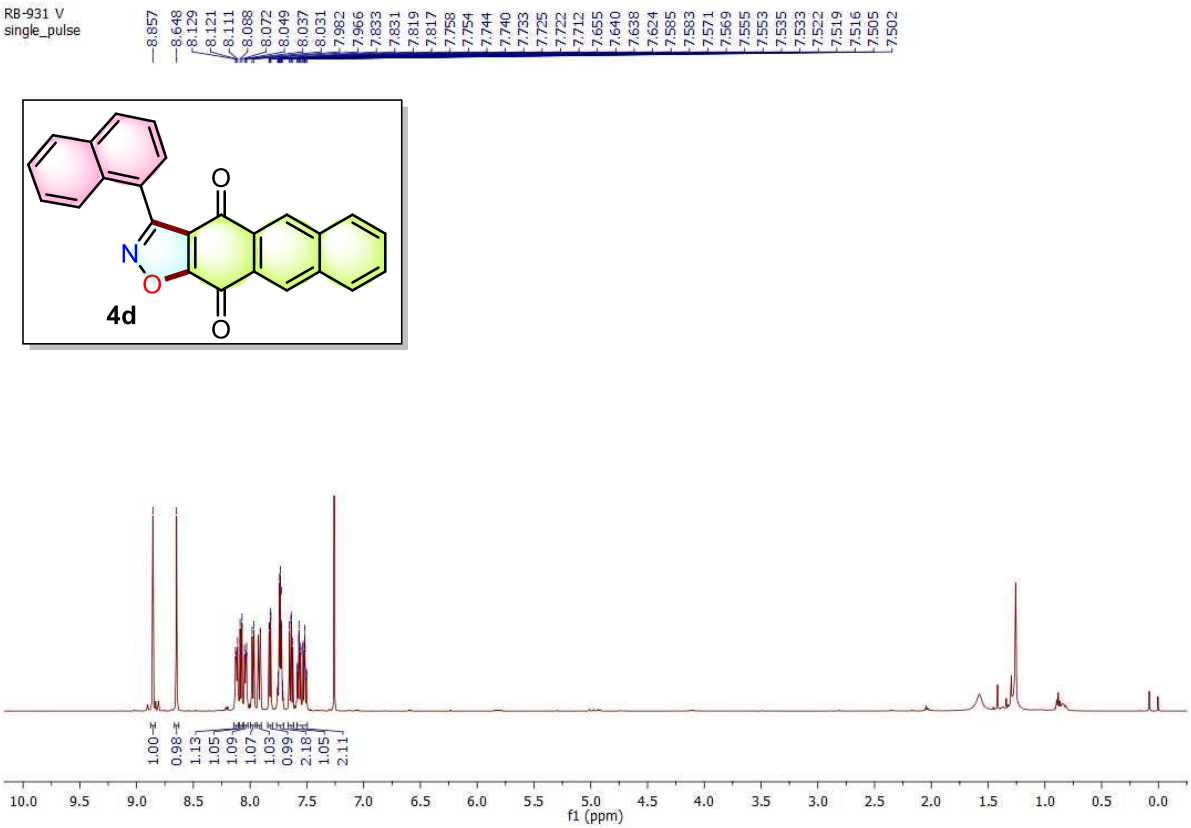
^{1}H NMR Spectrum of **4c** (500 MHz, Chloroform-*d*)



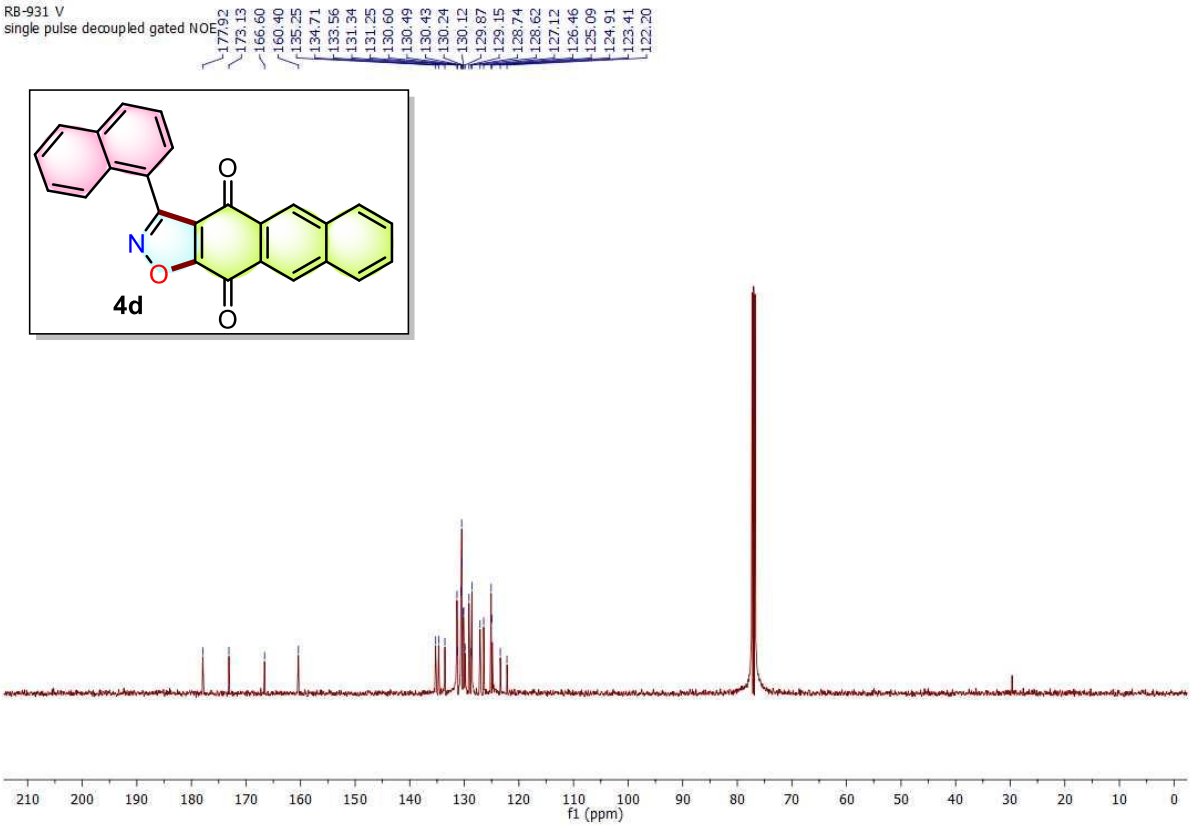
^{13}C NMR Spectrum of **4c** (126 MHz, Chloroform-*d*)



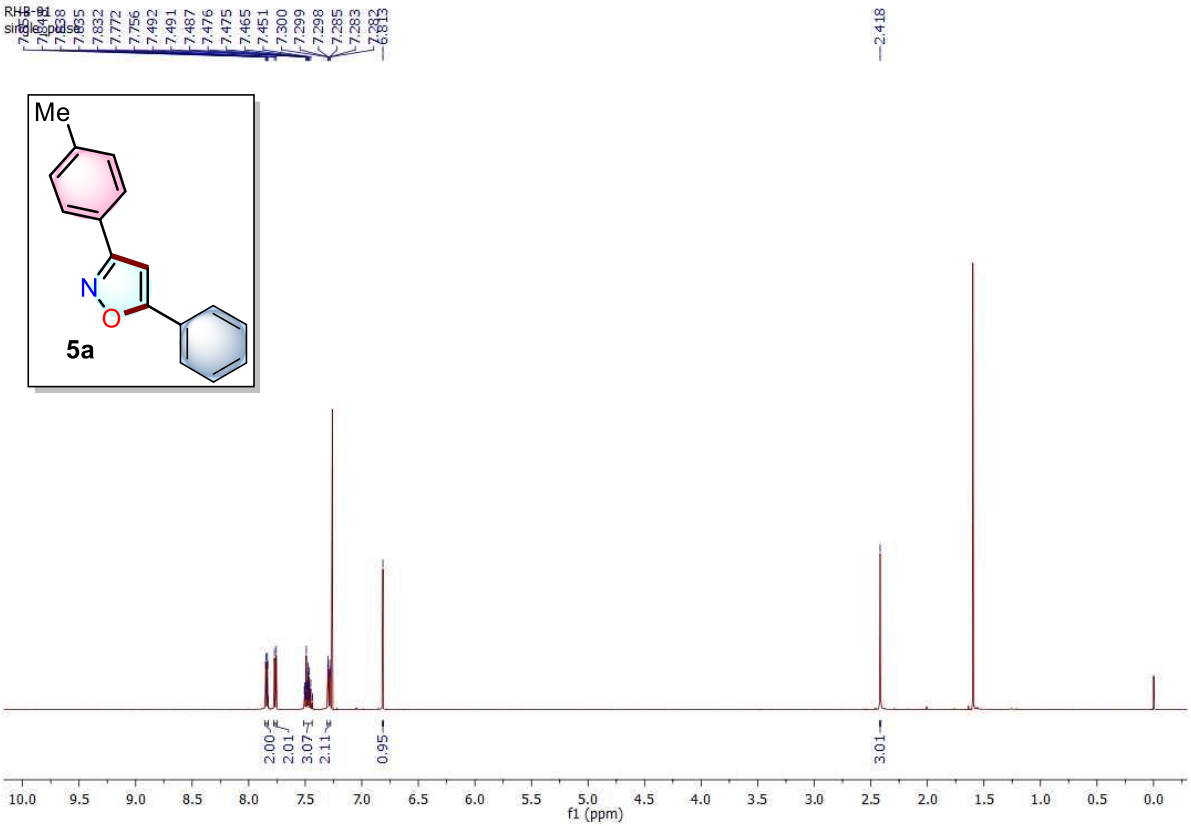
^{1}H NMR Spectrum of **4d** (500 MHz, Chloroform-*d*)



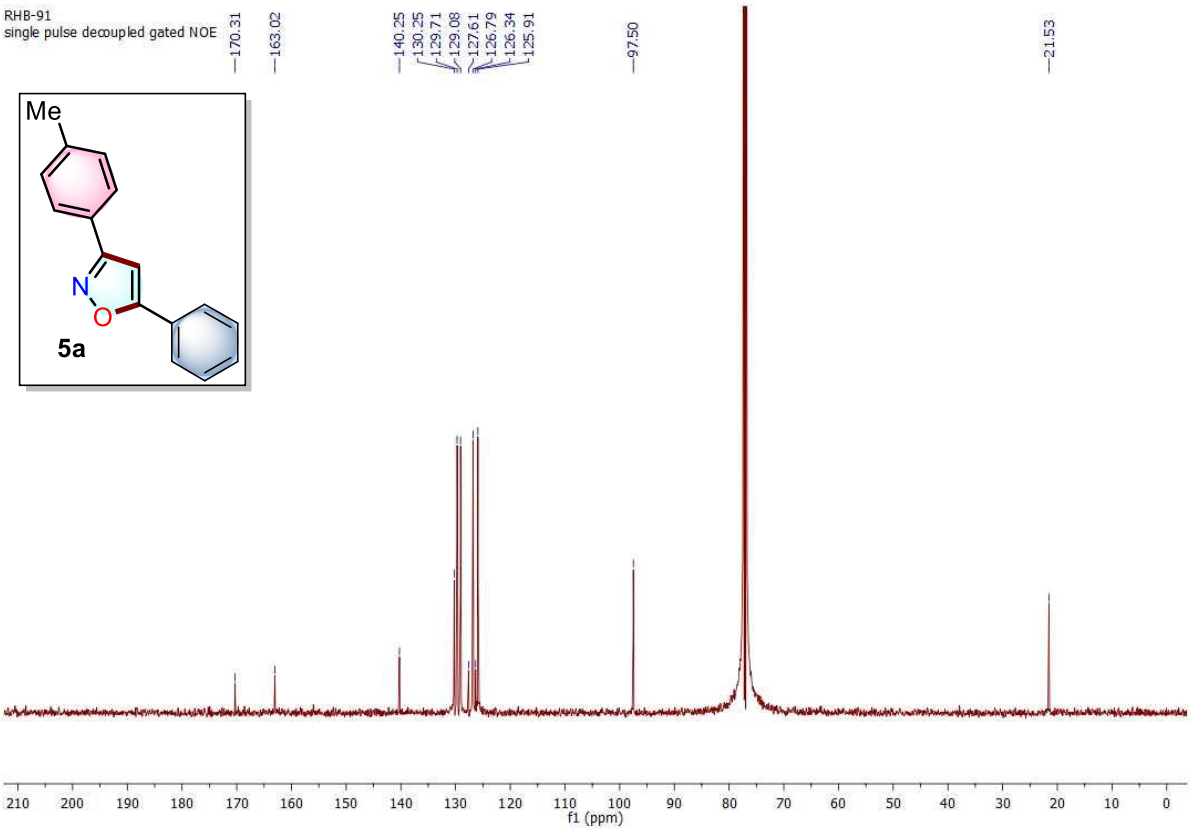
^{13}C NMR Spectrum of **4d** (126 MHz, Chloroform-*d*)



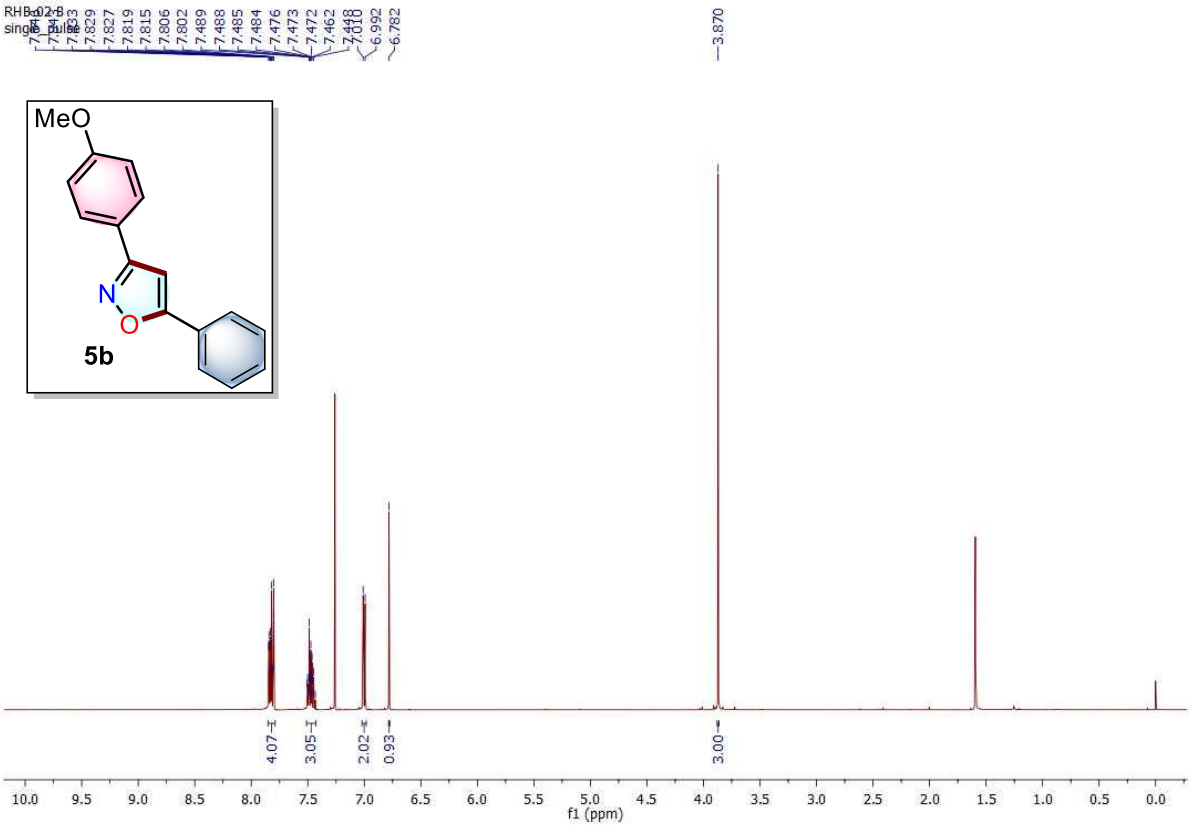
^{1}H NMR Spectrum of **5a** (500 MHz, Chloroform-*d*)



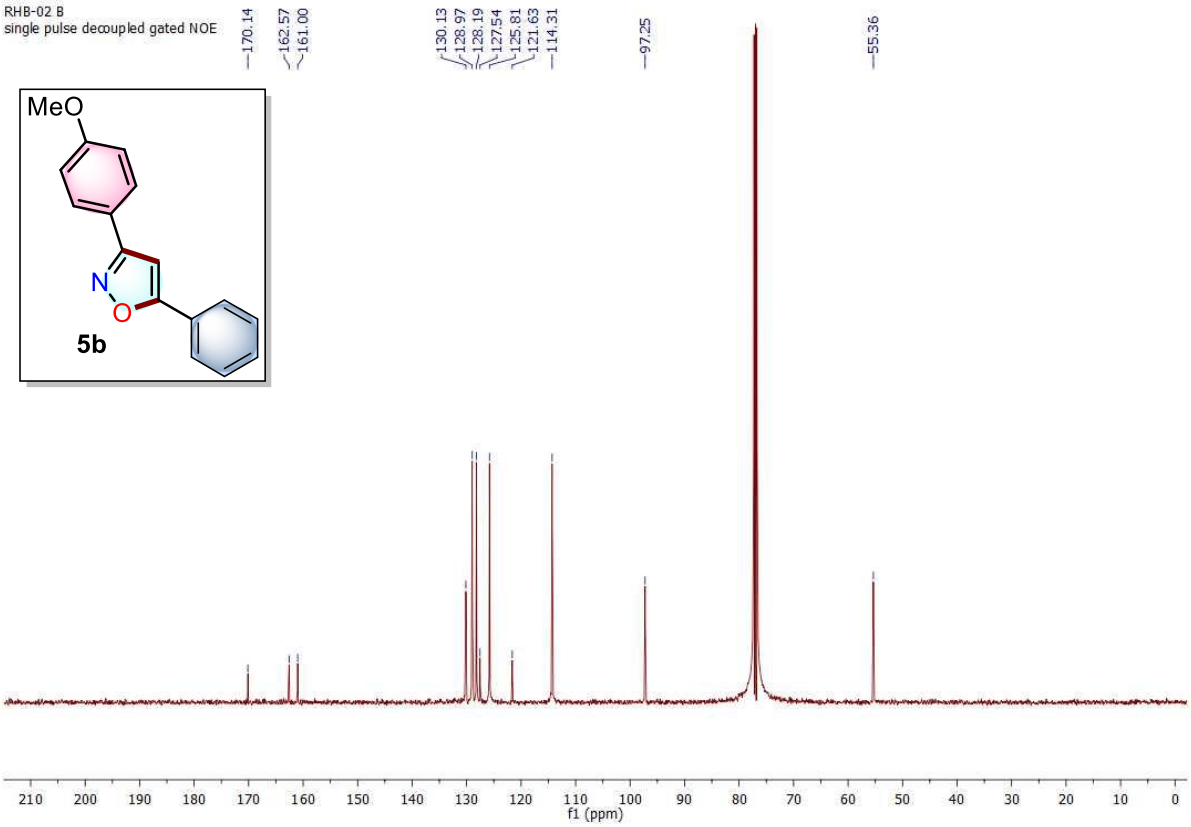
^{13}C NMR Spectrum of **5a** (126 MHz, Chloroform-*d*)



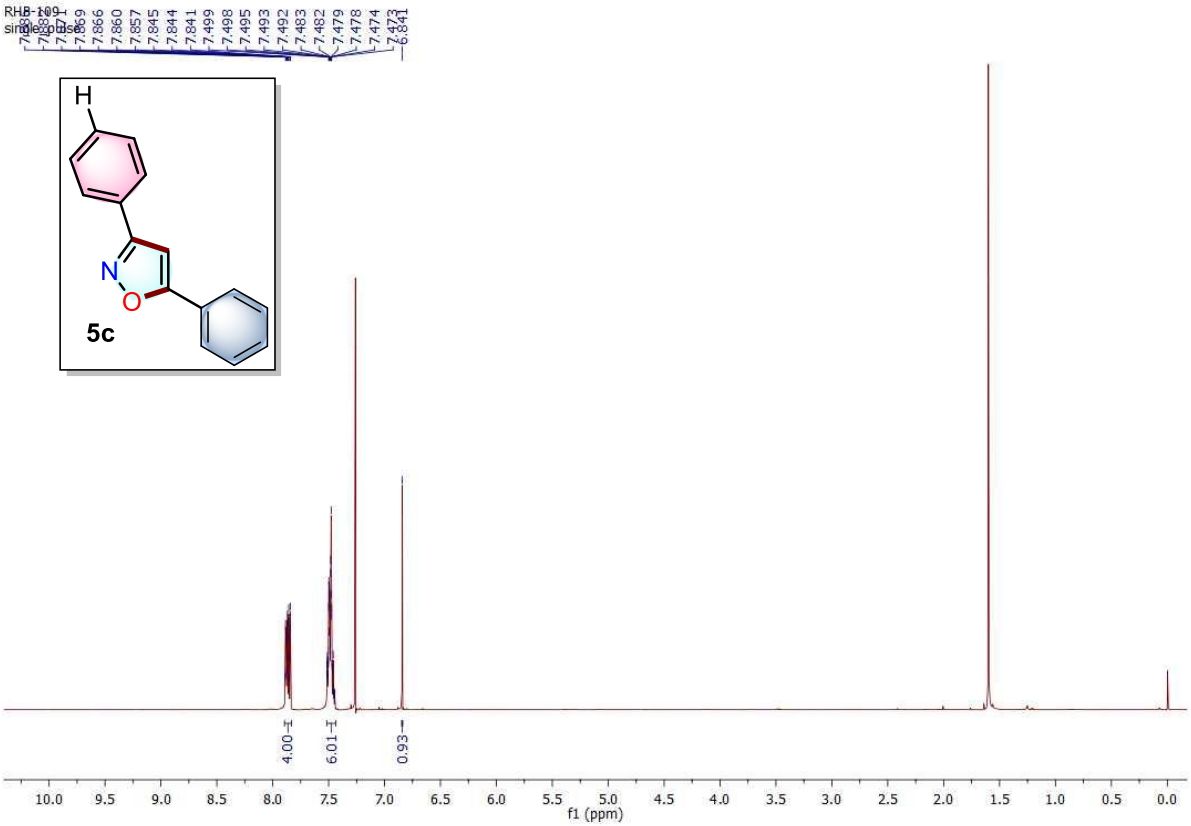
^{1}H NMR Spectrum of **5b** (500 MHz, Chloroform-*d*)



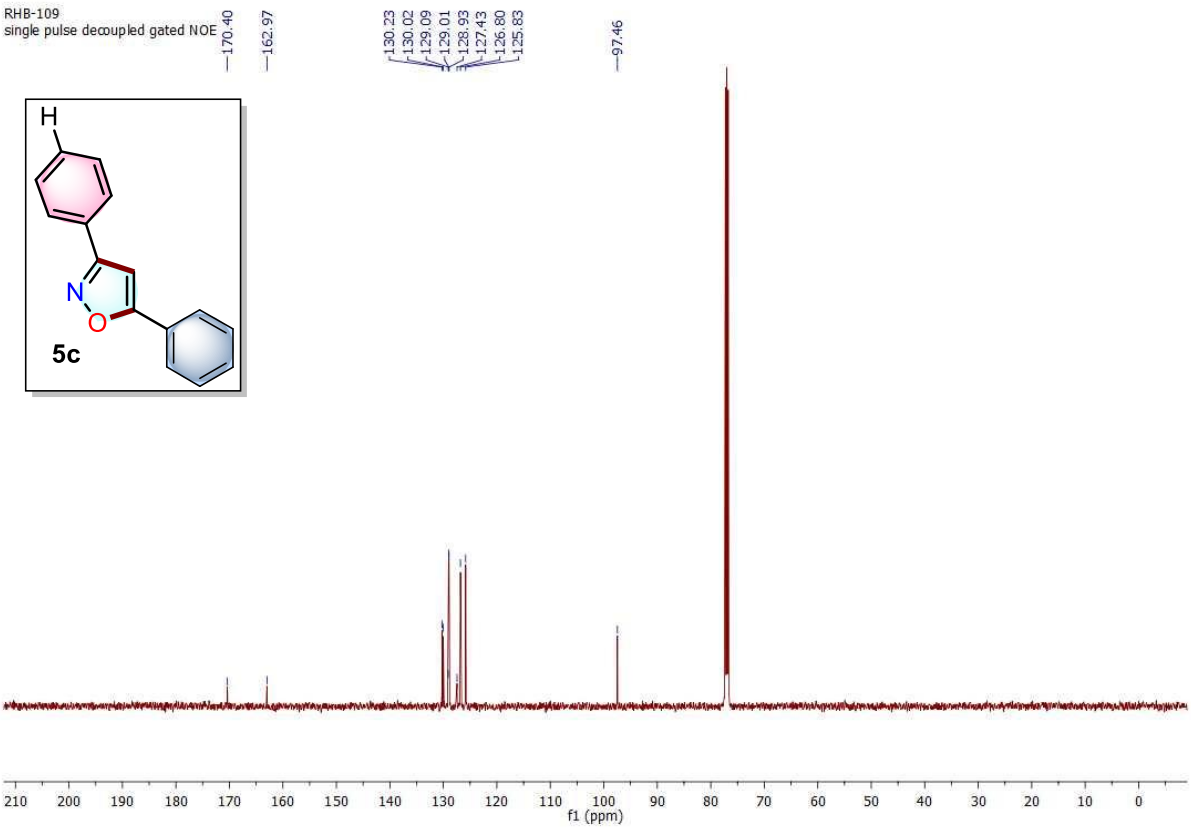
^{13}C NMR Spectrum of **5b** (126 MHz, Chloroform-*d*)



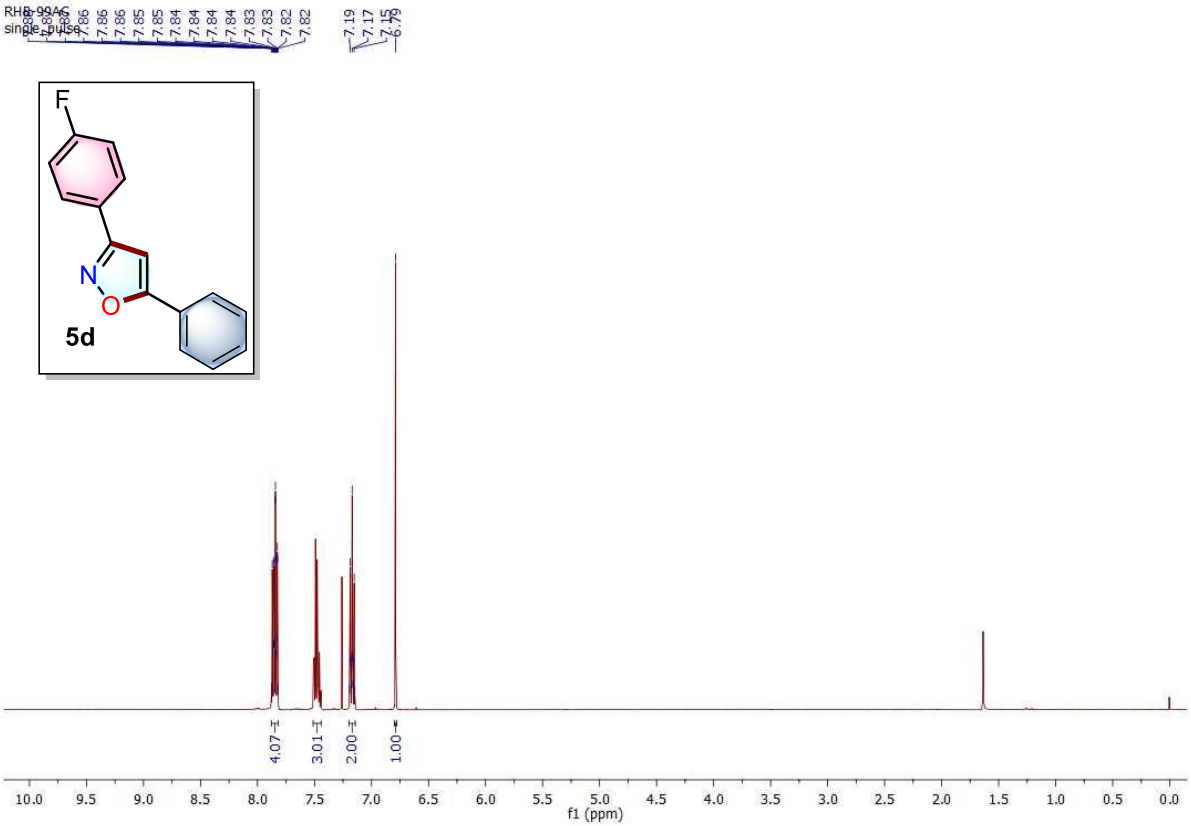
^{1}H NMR Spectrum of **5c** (500 MHz, Chloroform-*d*)



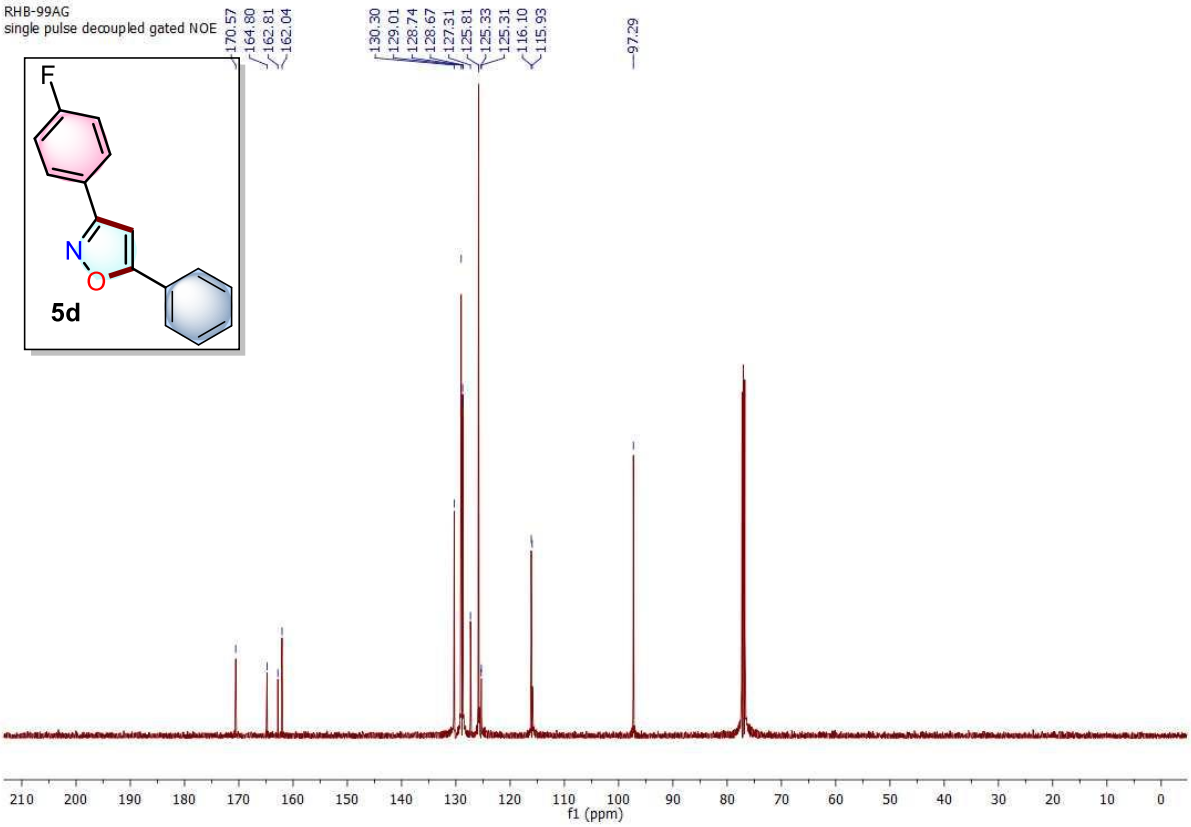
^{13}C NMR Spectrum of **5c** (126 MHz, Chloroform-*d*)



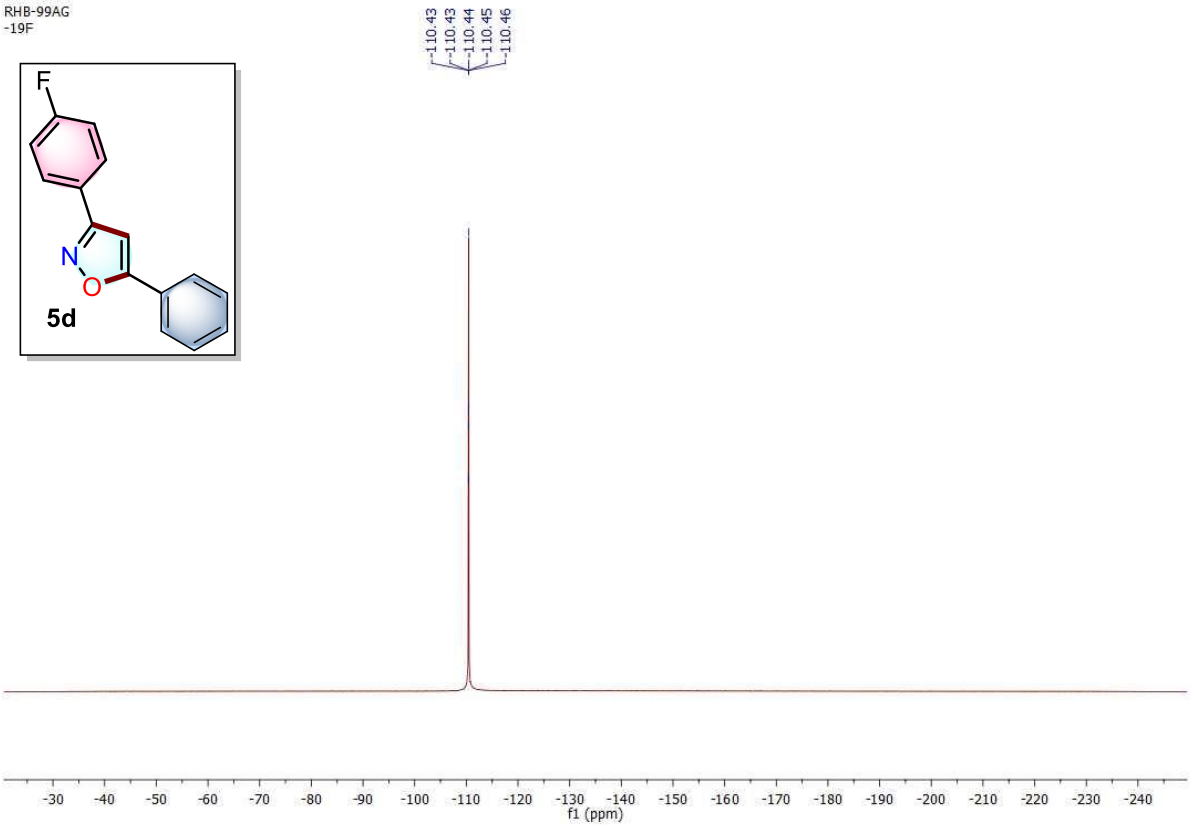
^{1}H NMR Spectrum of **5d** (500 MHz, Chloroform-*d*)



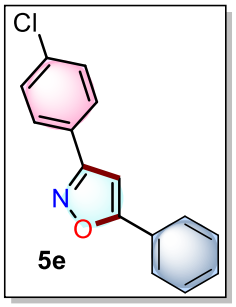
^{13}C NMR Spectrum of **5d** (126 MHz, Chloroform-*d*)

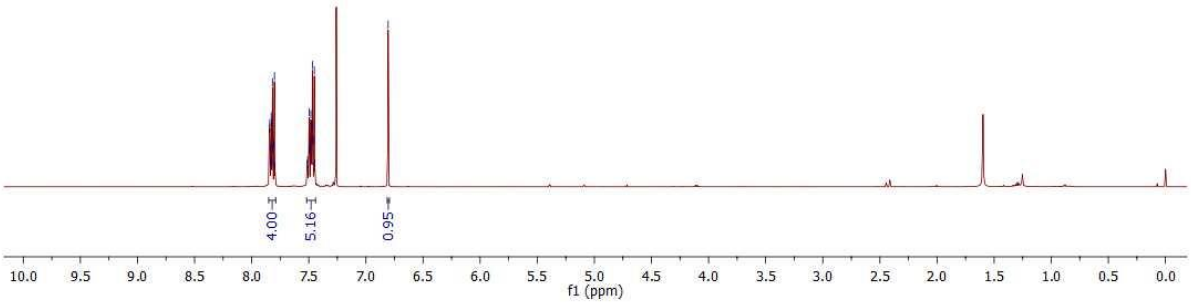


^{19}F NMR Spectrum of **5d** (571 MHz, Chloroform-*d*)

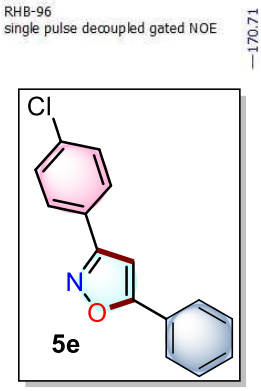


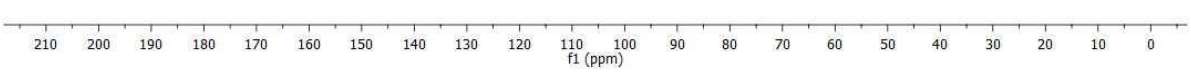
^{1}H NMR Spectrum of **5e** (500 MHz, Chloroform-*d*)



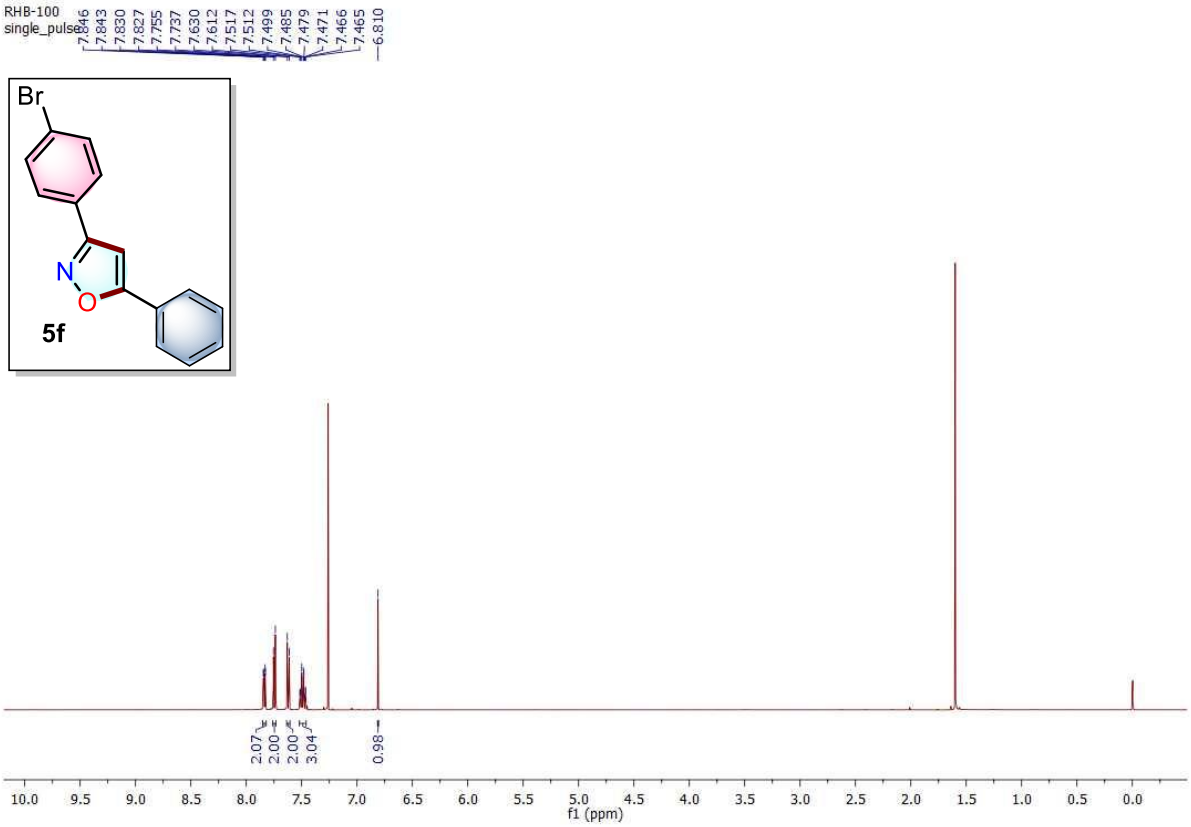


^{13}C NMR Spectrum of **5e** (126 MHz, Chloroform-*d*)

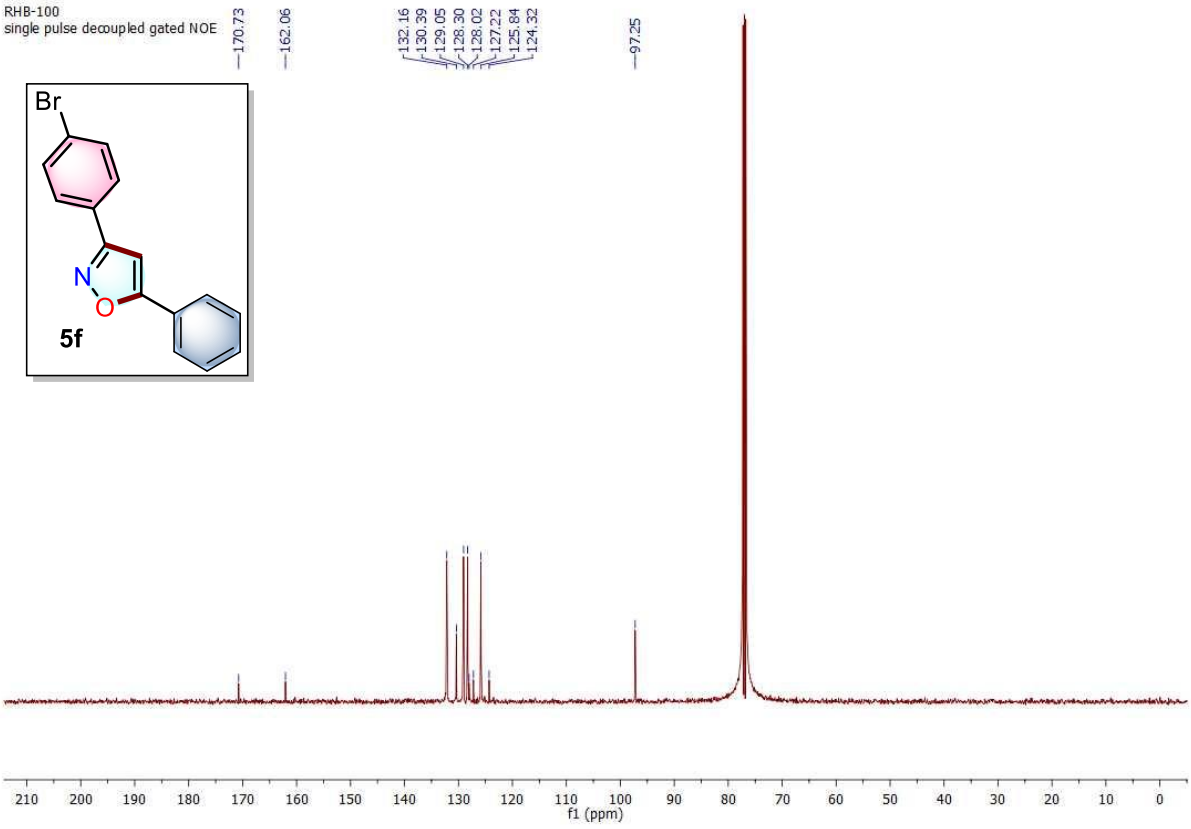




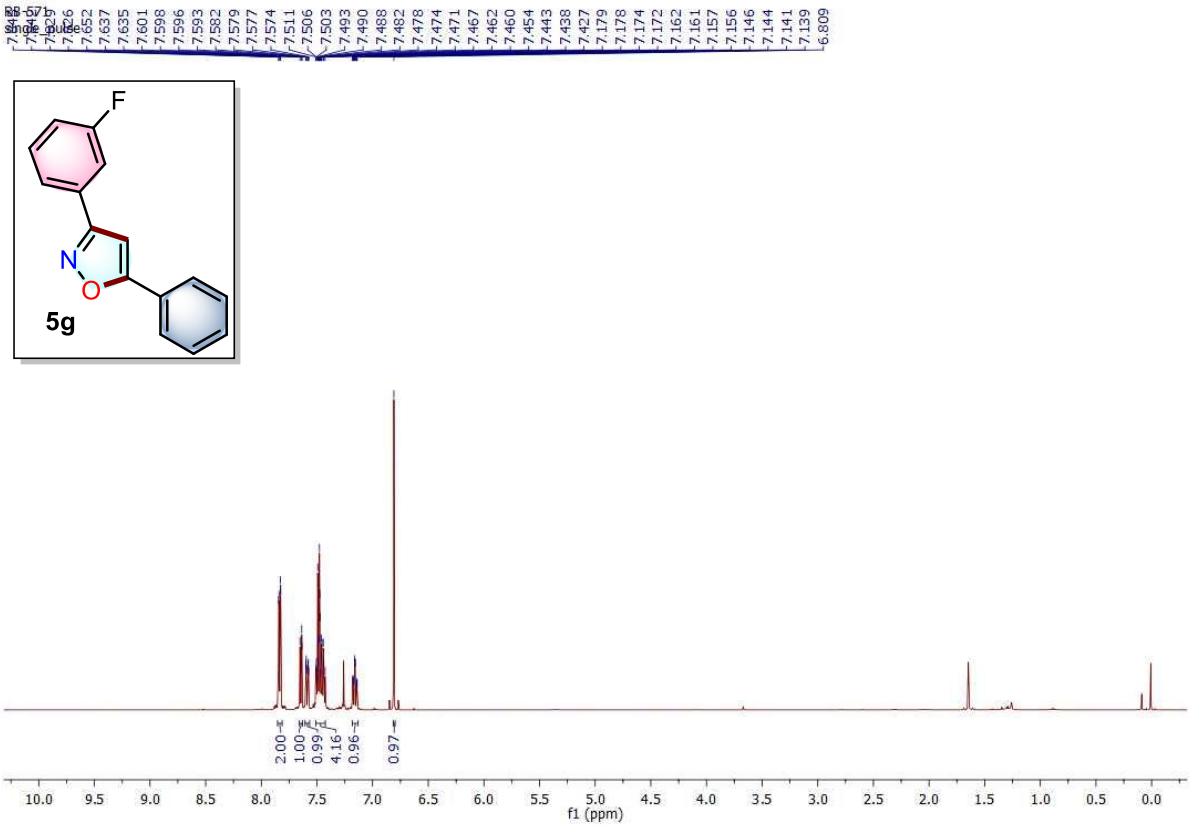
^{1}H NMR Spectrum of **5f** (500 MHz, Chloroform-*d*)



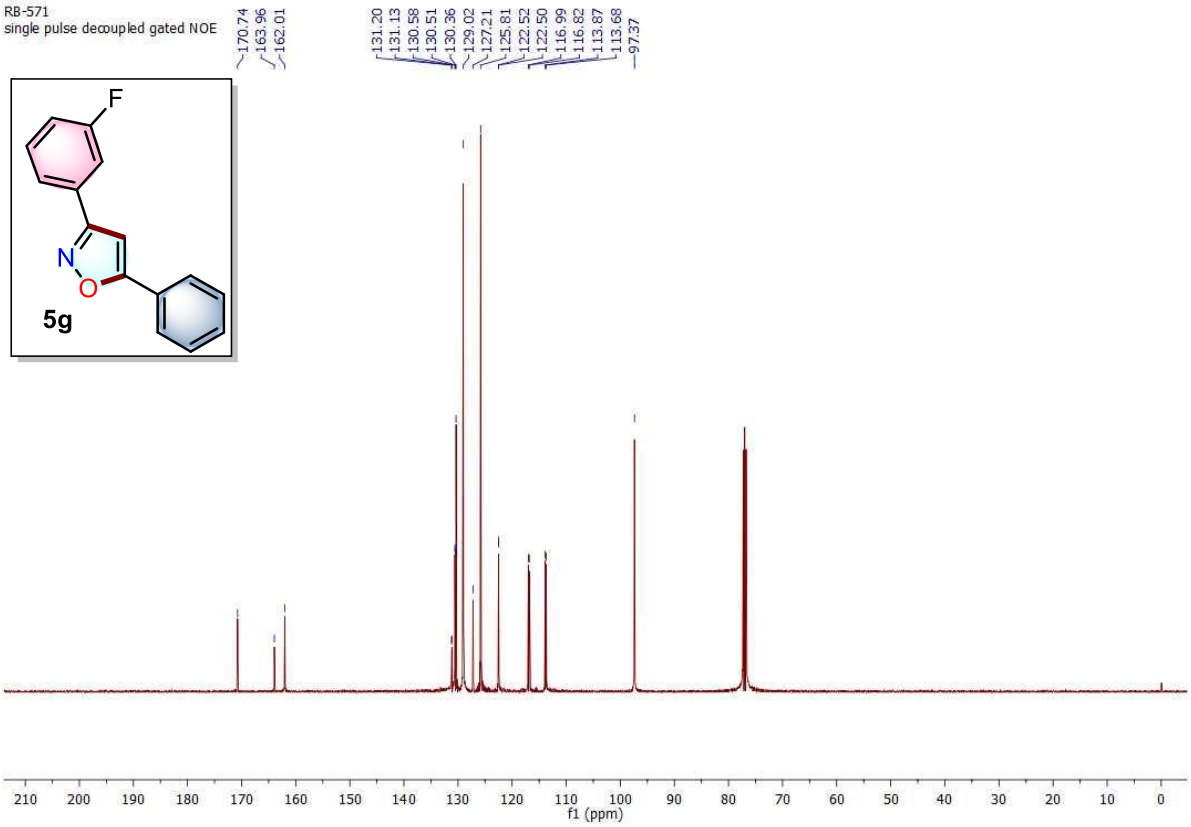
^{13}C NMR Spectrum of **5f** (126 MHz, Chloroform-*d*)



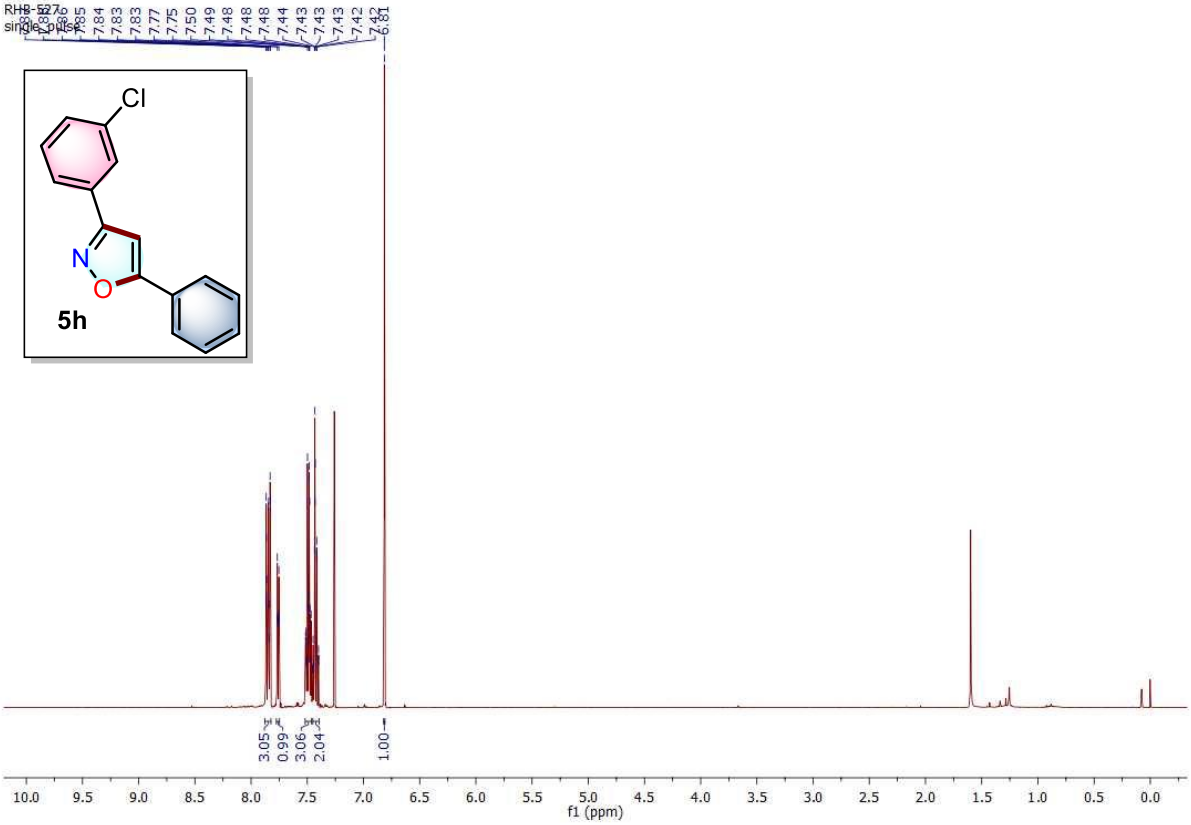
^{1}H NMR Spectrum of **5g** (500 MHz, Chloroform-*d*)



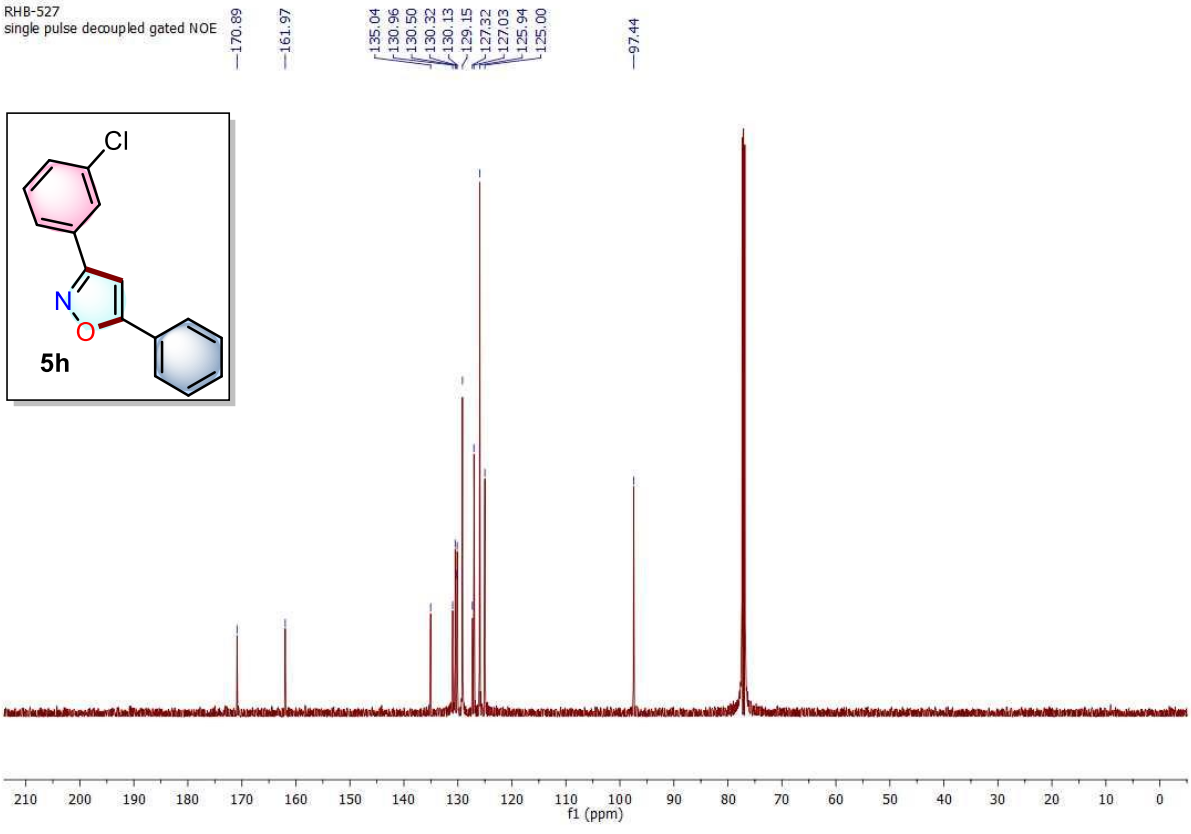
^{13}C NMR Spectrum of **5g** (126 MHz, Chloroform-*d*)



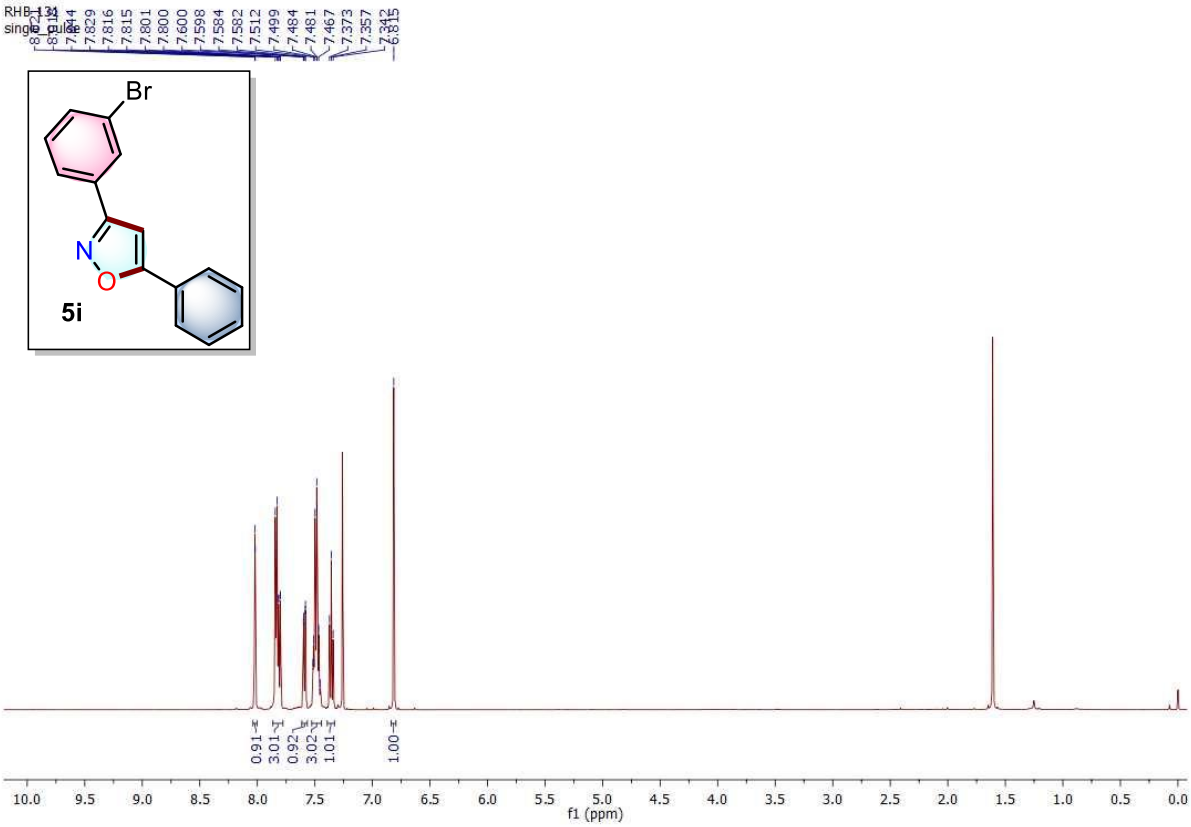
^{1}H NMR Spectrum of **5h** (500 MHz, Chloroform-*d*)



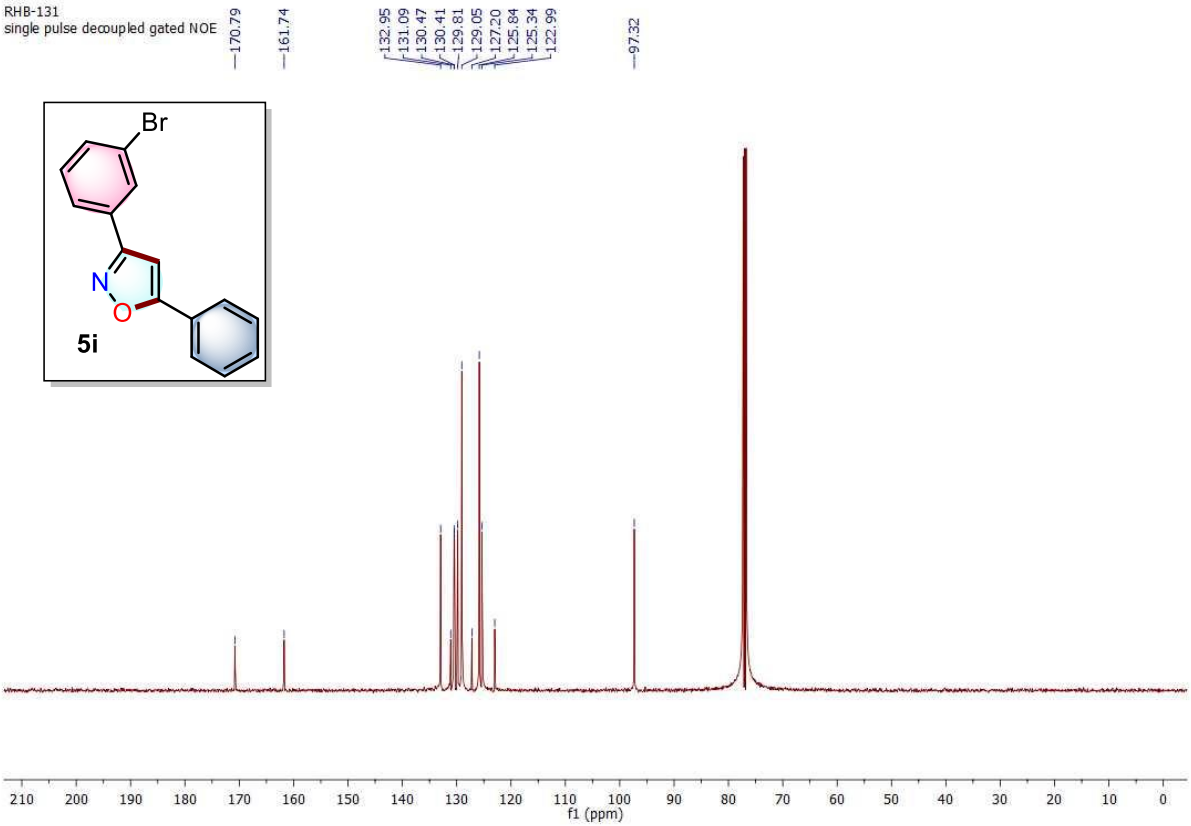
^{13}C NMR Spectrum of **5h** (126 MHz, Chloroform-*d*)



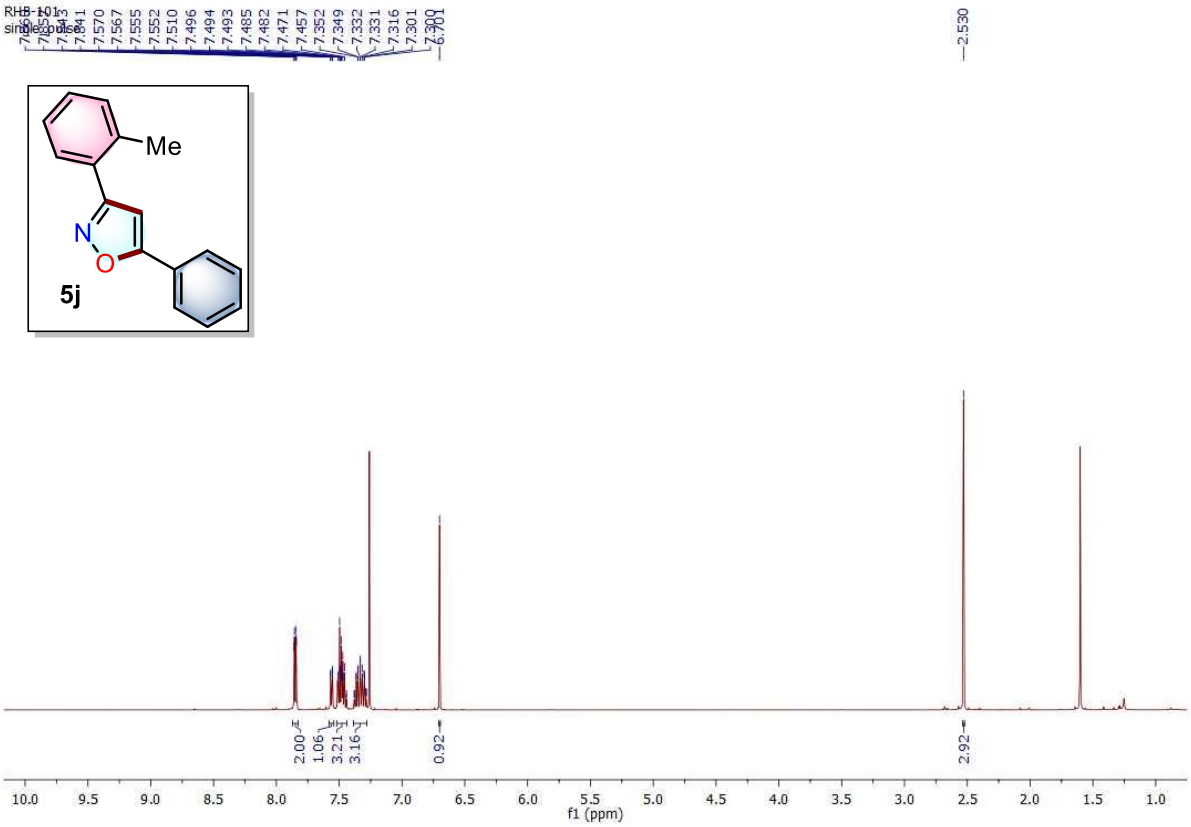
^{1}H NMR Spectrum of **5i** (500 MHz, Chloroform-*d*)



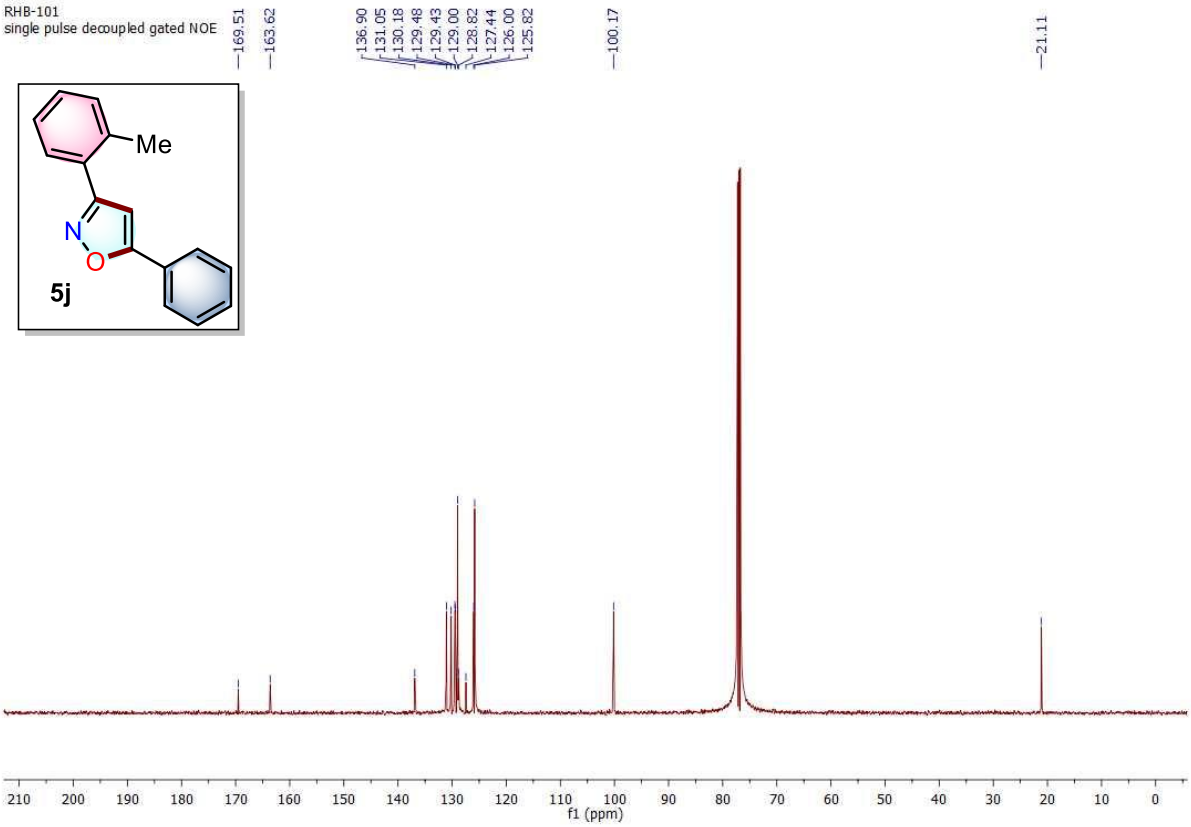
^{13}C NMR Spectrum of **5i** (126 MHz, Chloroform-*d*)



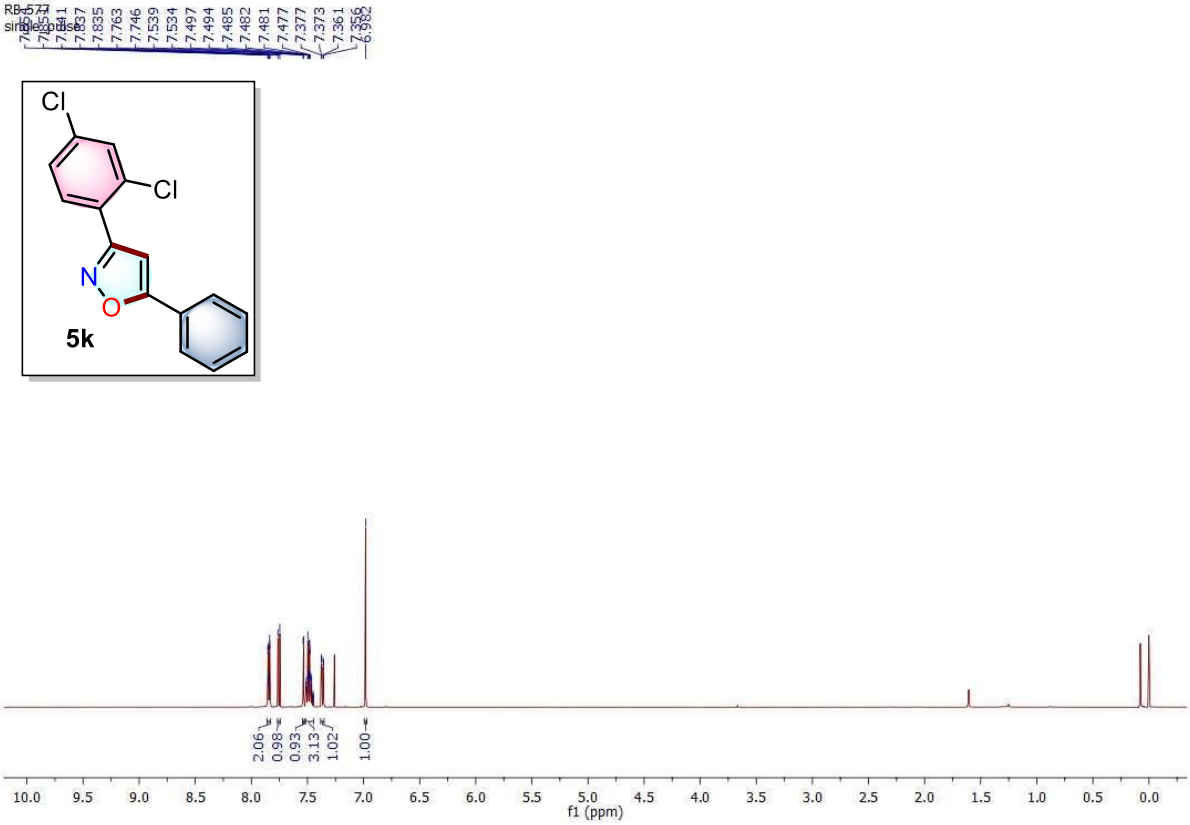
^{1}H NMR Spectrum of **5j** (500 MHz, Chloroform-*d*)



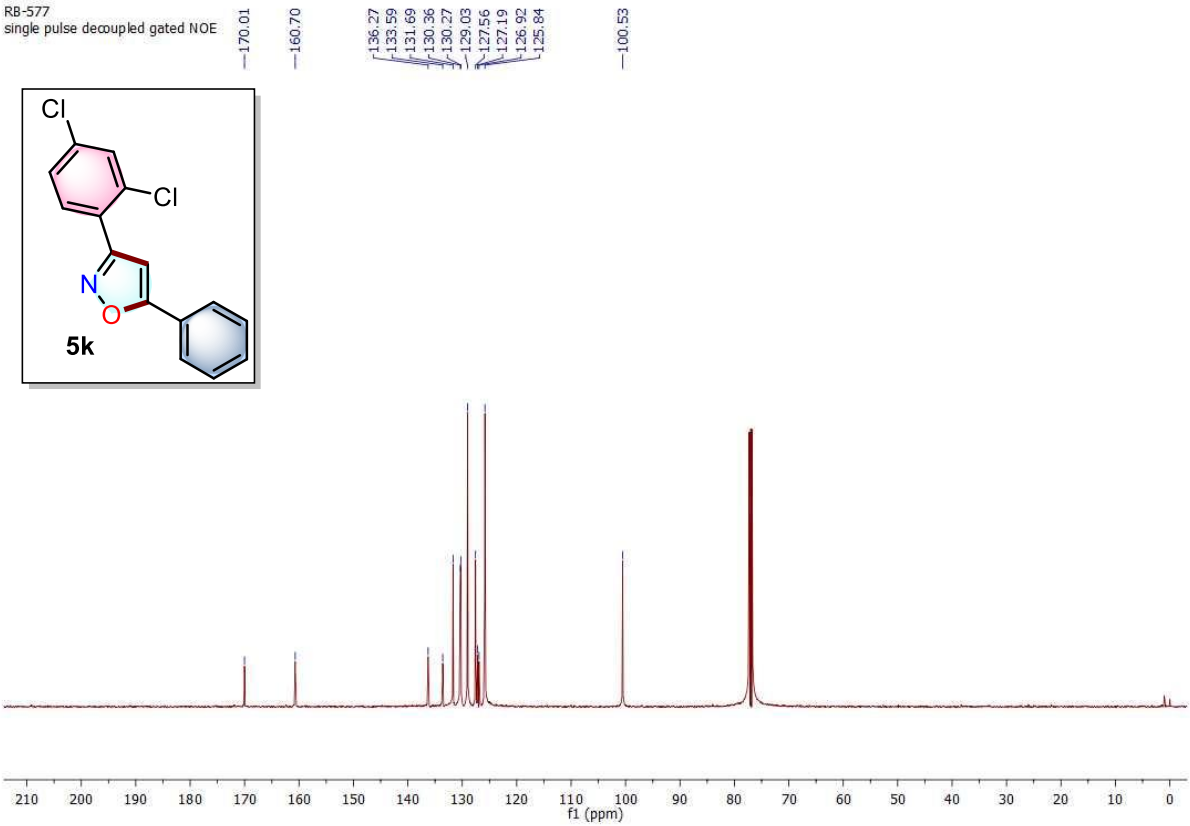
^{13}C NMR Spectrum of **5j** (126 MHz, Chloroform-*d*)



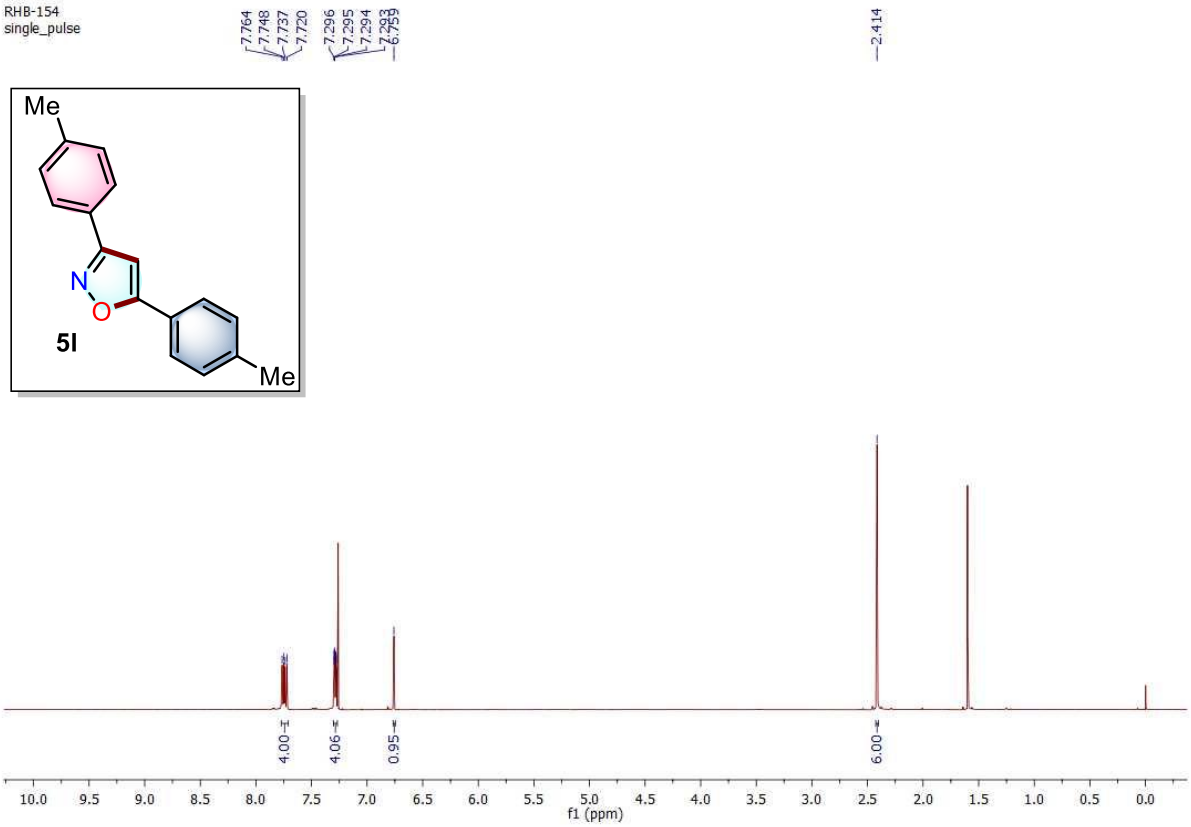
^{1}H NMR Spectrum of **5k** (500 MHz, Chloroform-*d*)



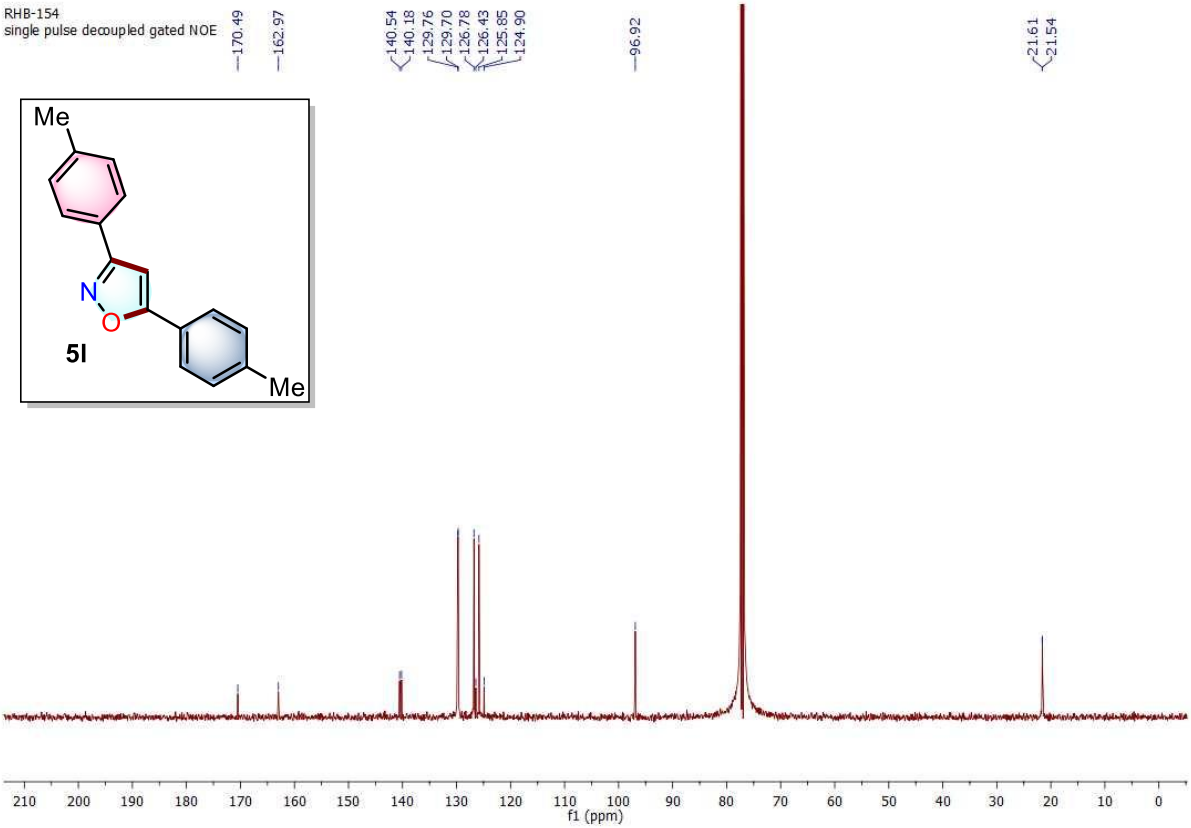
^{13}C NMR Spectrum of **5k** (126 MHz, Chloroform-*d*)



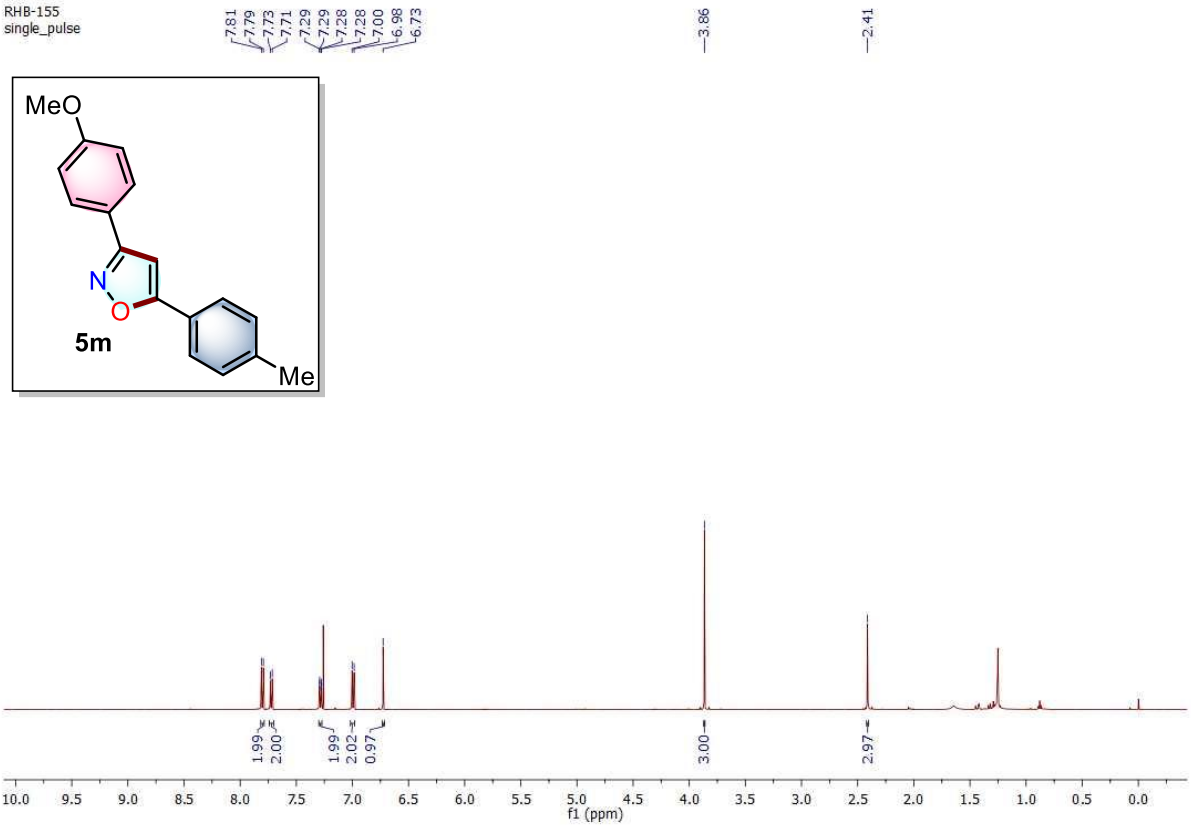
^{1}H NMR Spectrum of **5l** (500 MHz, Chloroform-*d*)



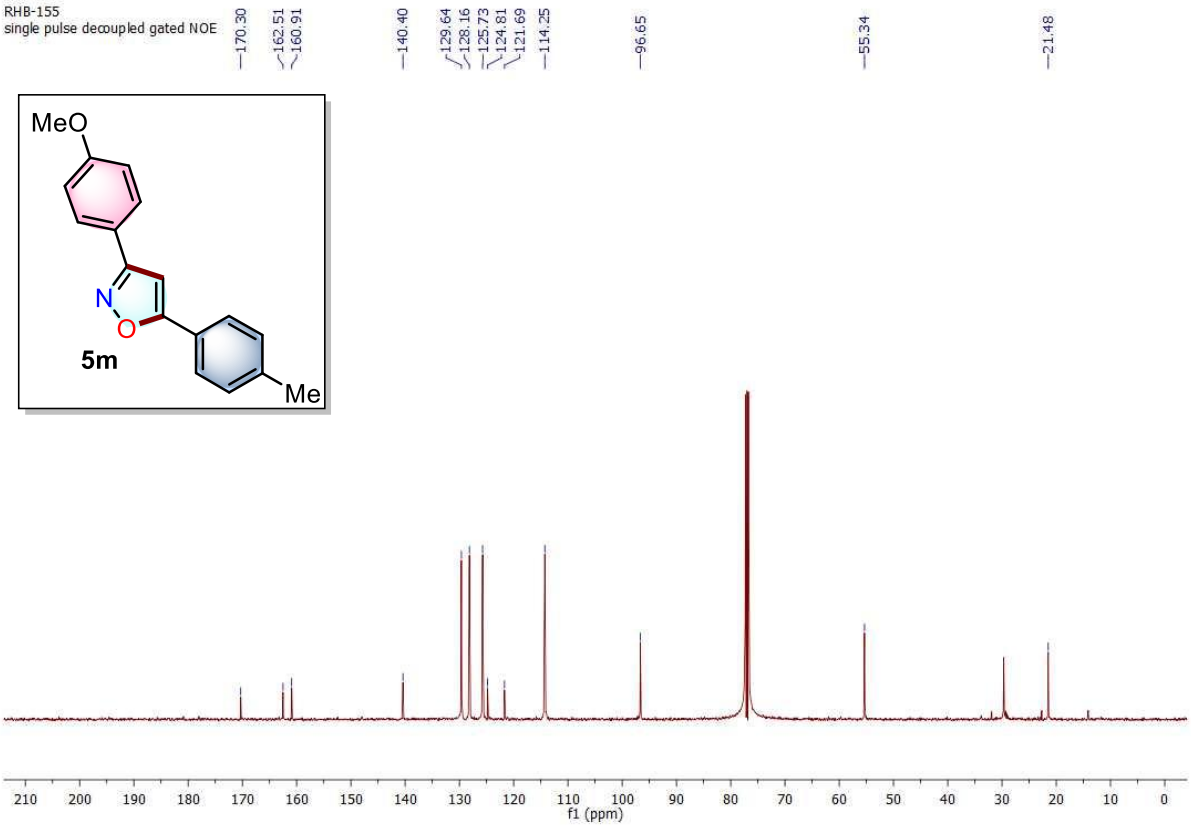
^{13}C NMR Spectrum of **5l** (126 MHz, Chloroform-*d*)



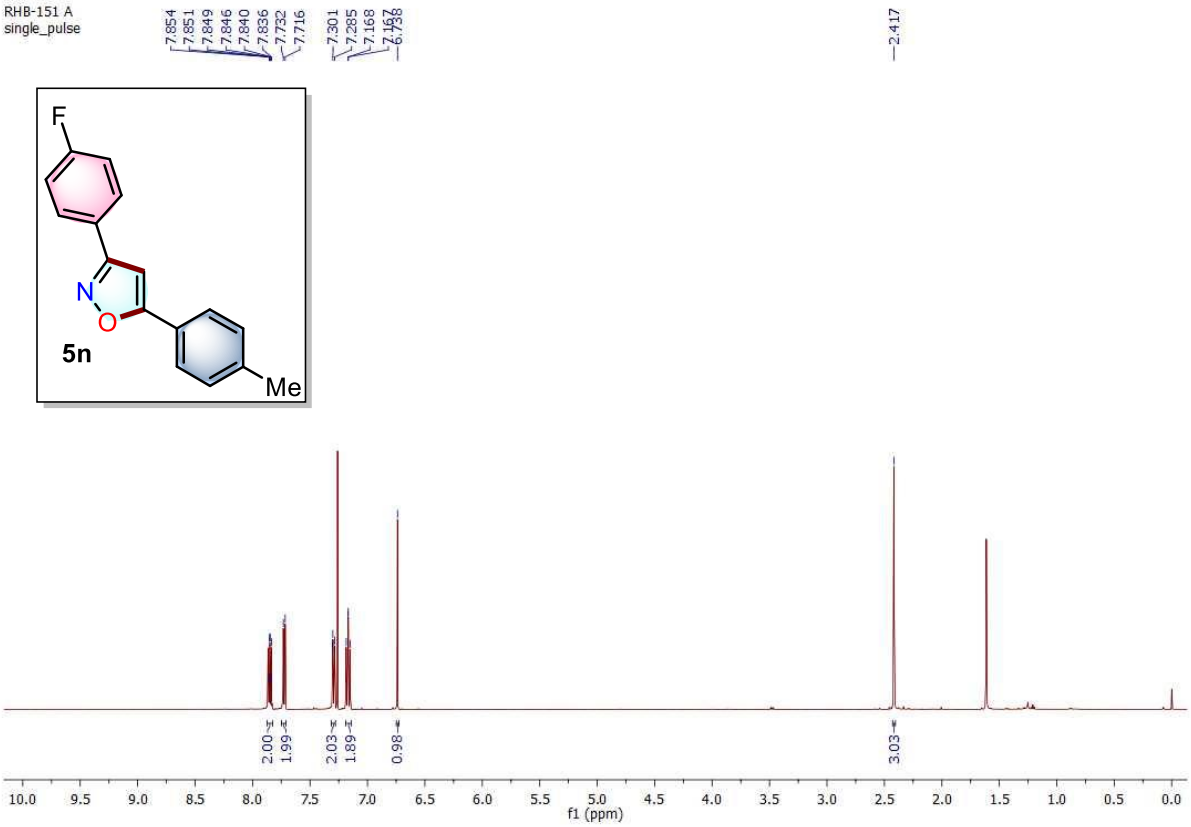
^{1}H NMR Spectrum of **5m** (500 MHz, Chloroform-*d*)



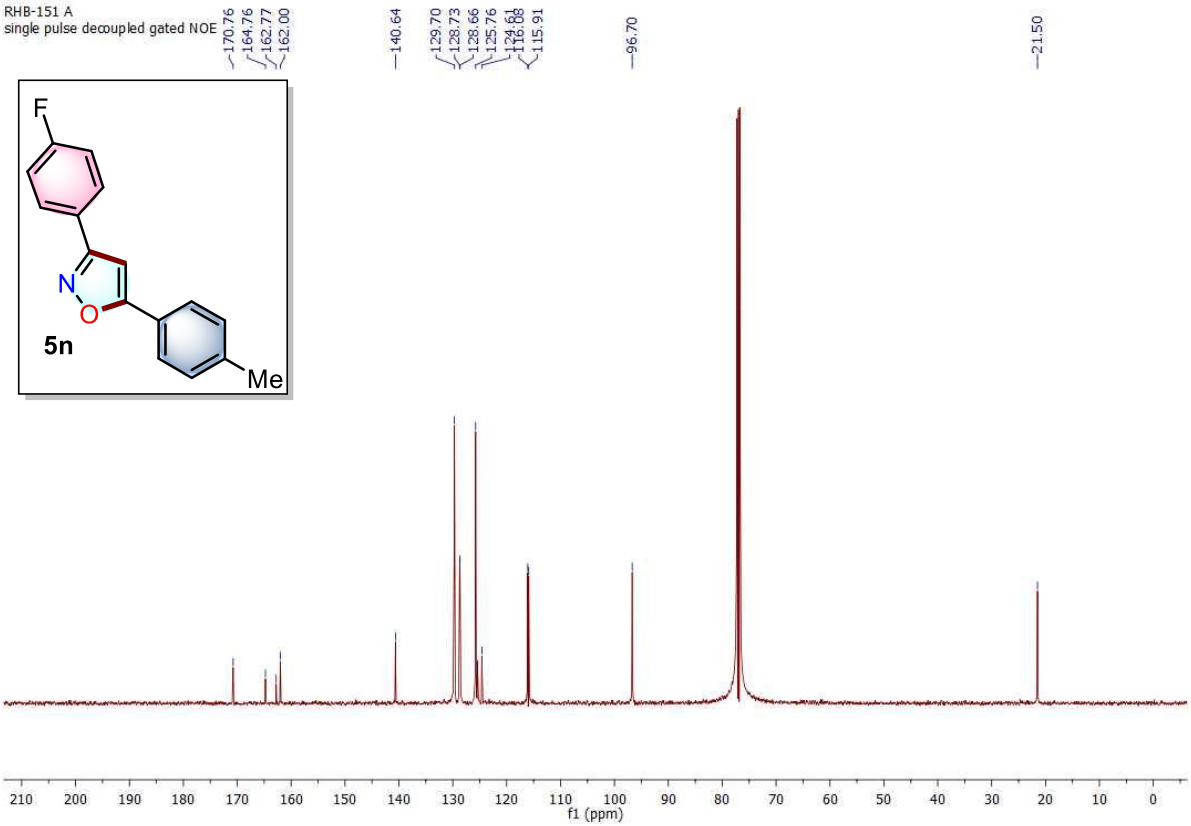
^{13}C NMR Spectrum of **5m** (126 MHz, Chloroform-*d*)



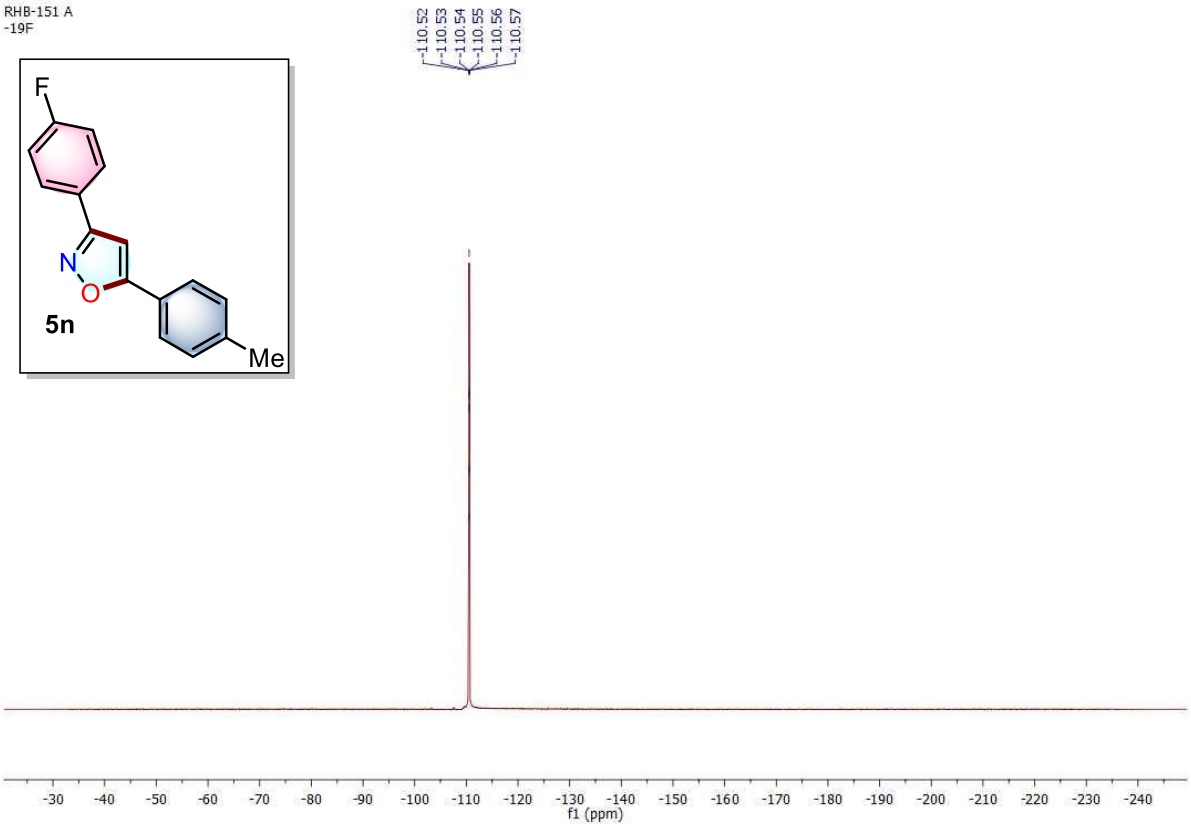
^{1}H NMR Spectrum of **5n** (500 MHz, Chloroform-*d*)



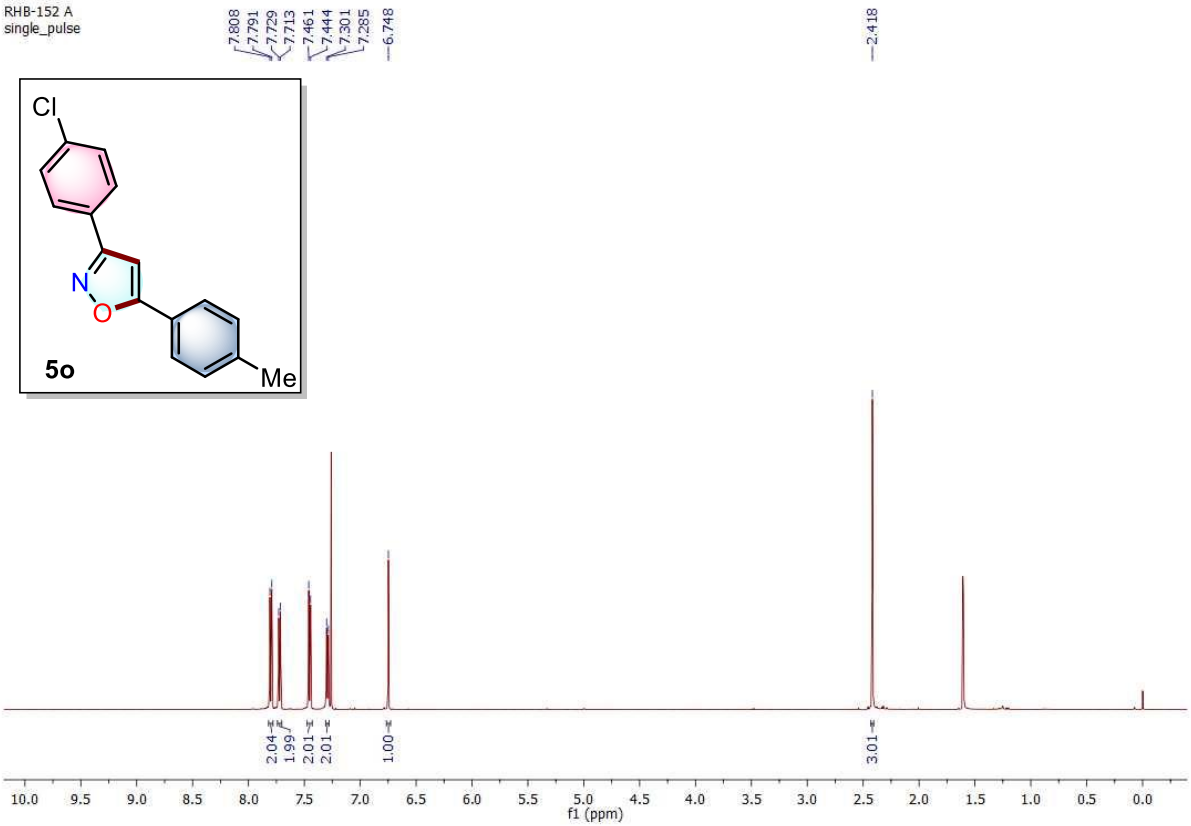
^{13}C NMR Spectrum of **5n** (126 MHz, Chloroform-*d*)



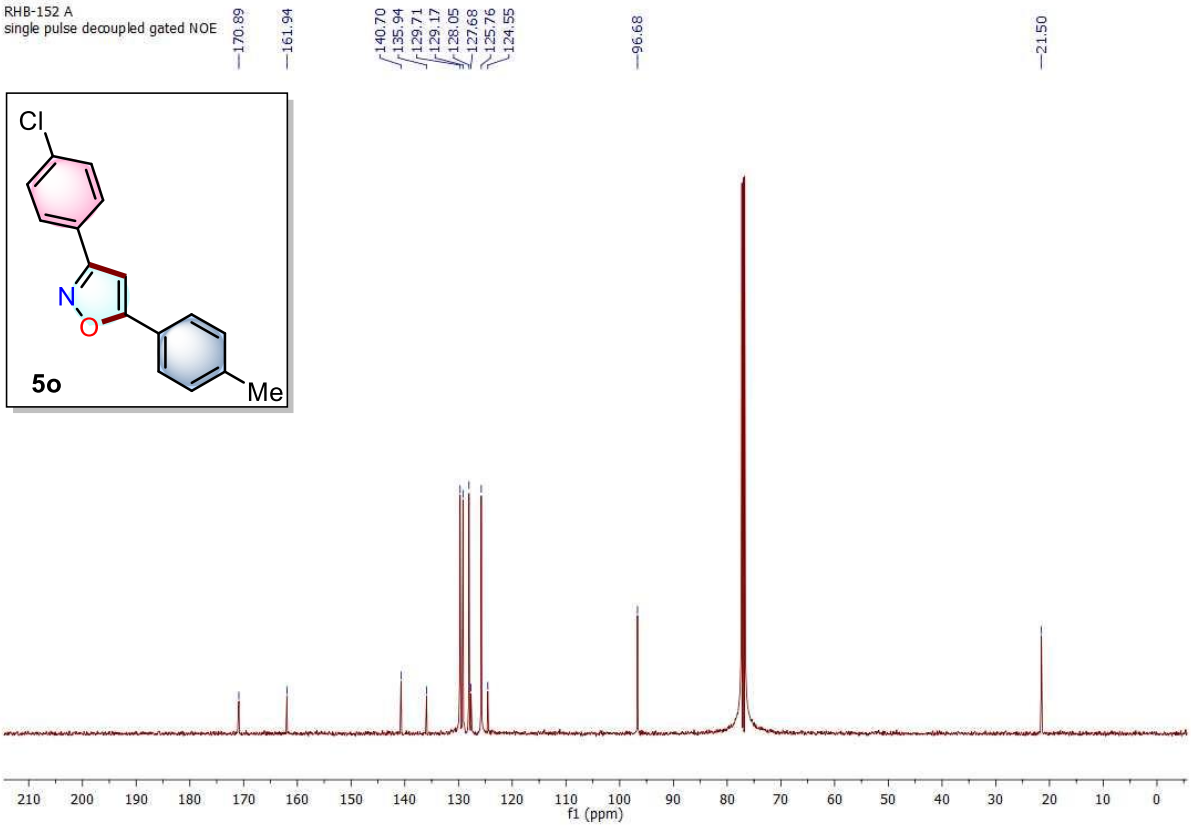
^{19}F NMR Spectrum of **5n** (471 MHz, Chloroform-*d*)



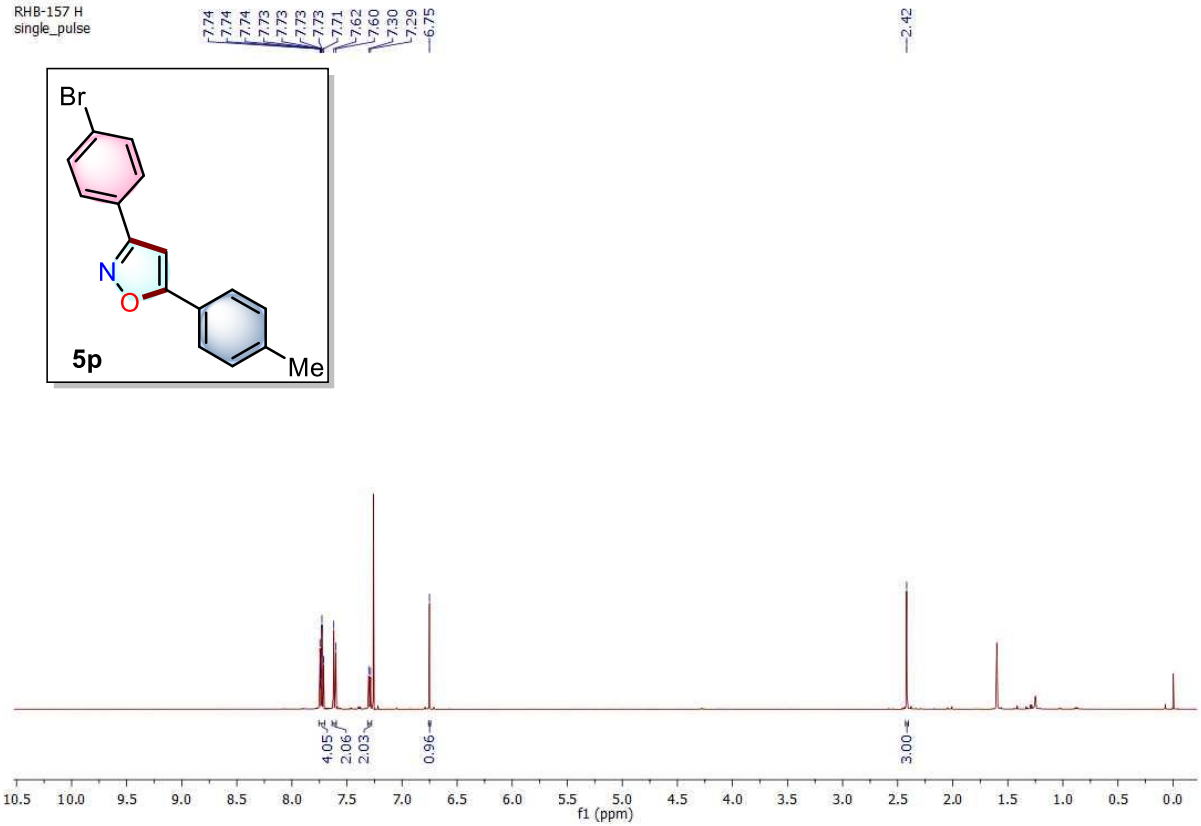
^{1}H NMR Spectrum of **5o** (500 MHz, Chloroform-*d*)



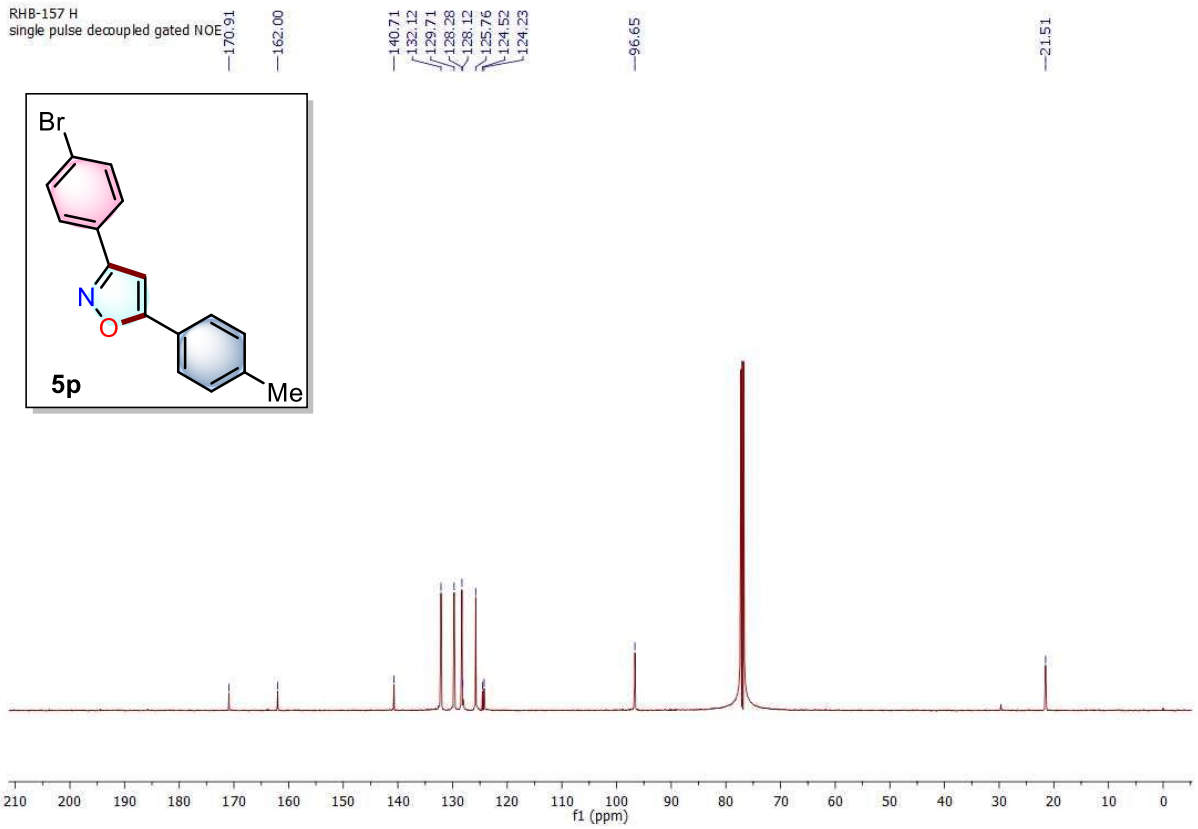
^{13}C NMR Spectrum of **5o** (126 MHz, Chloroform-*d*)



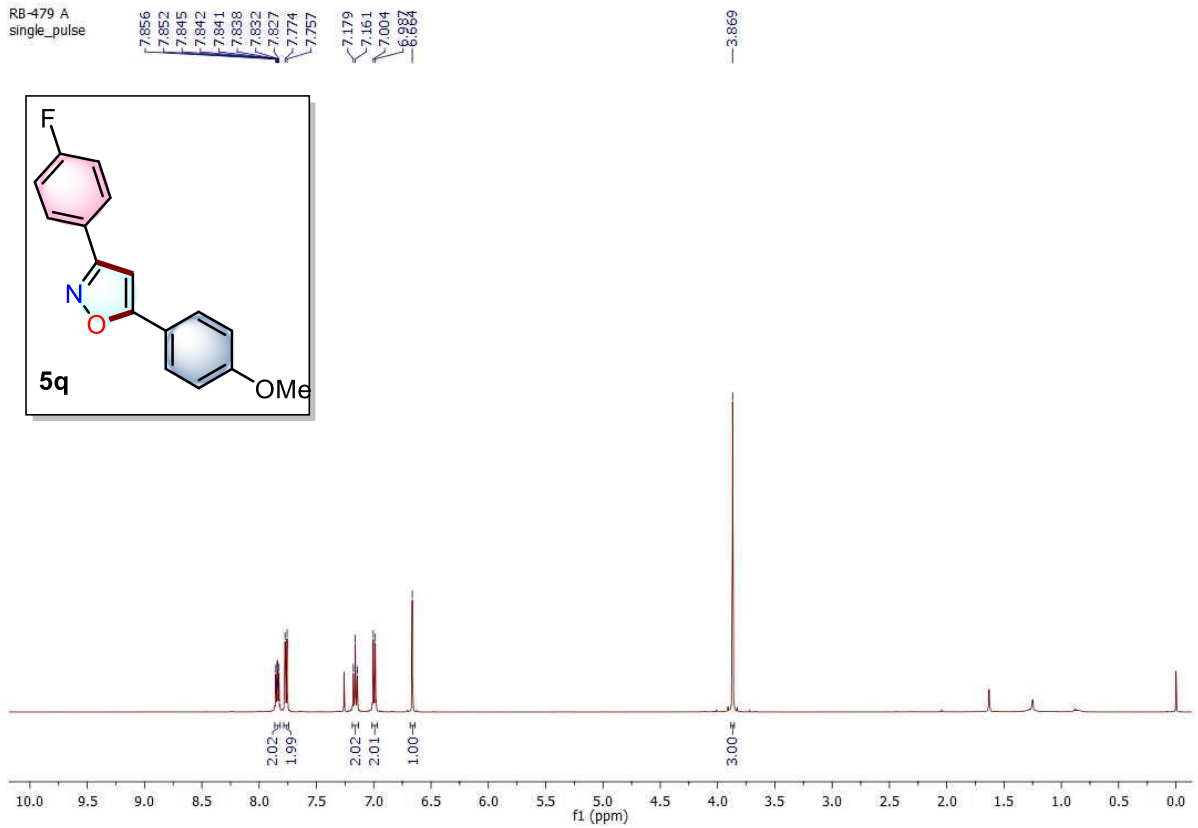
^{1}H NMR Spectrum of **5p** (500 MHz, Chloroform-*d*)



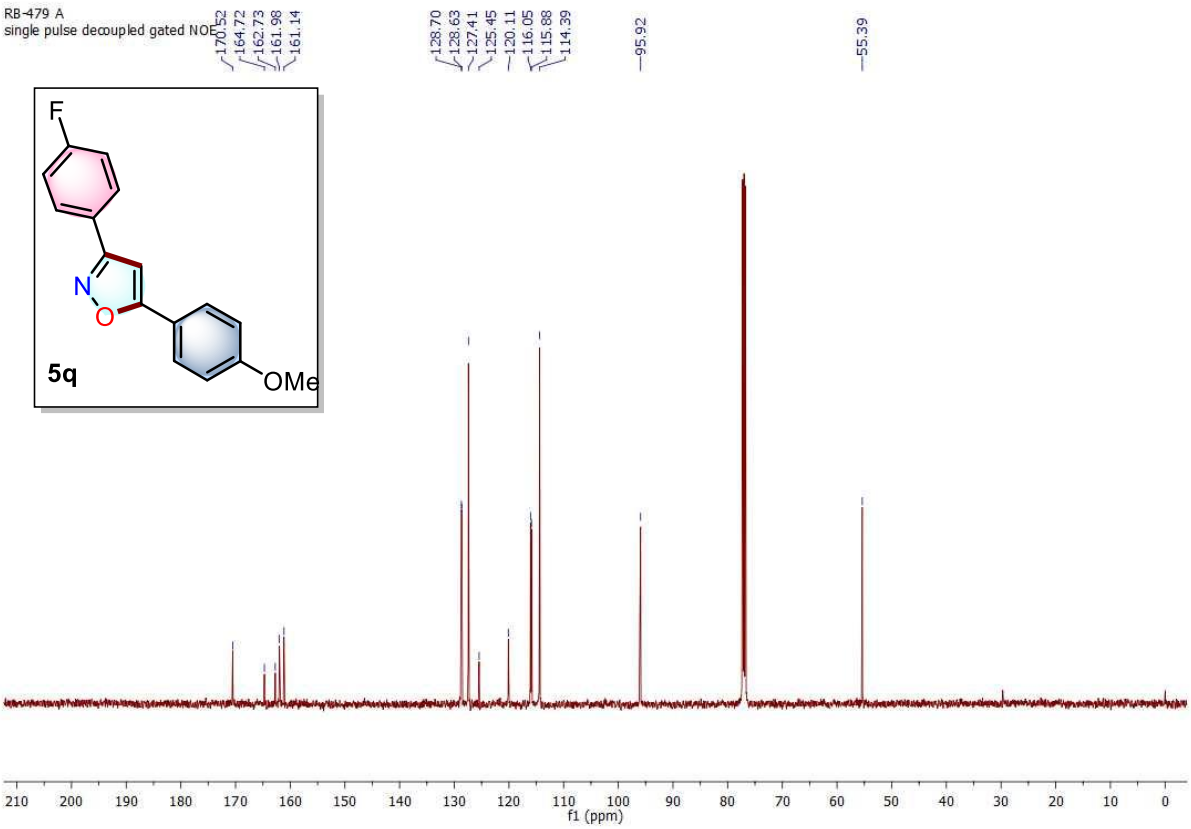
^{13}C NMR Spectrum of **5p** (126 MHz, Chloroform-*d*)



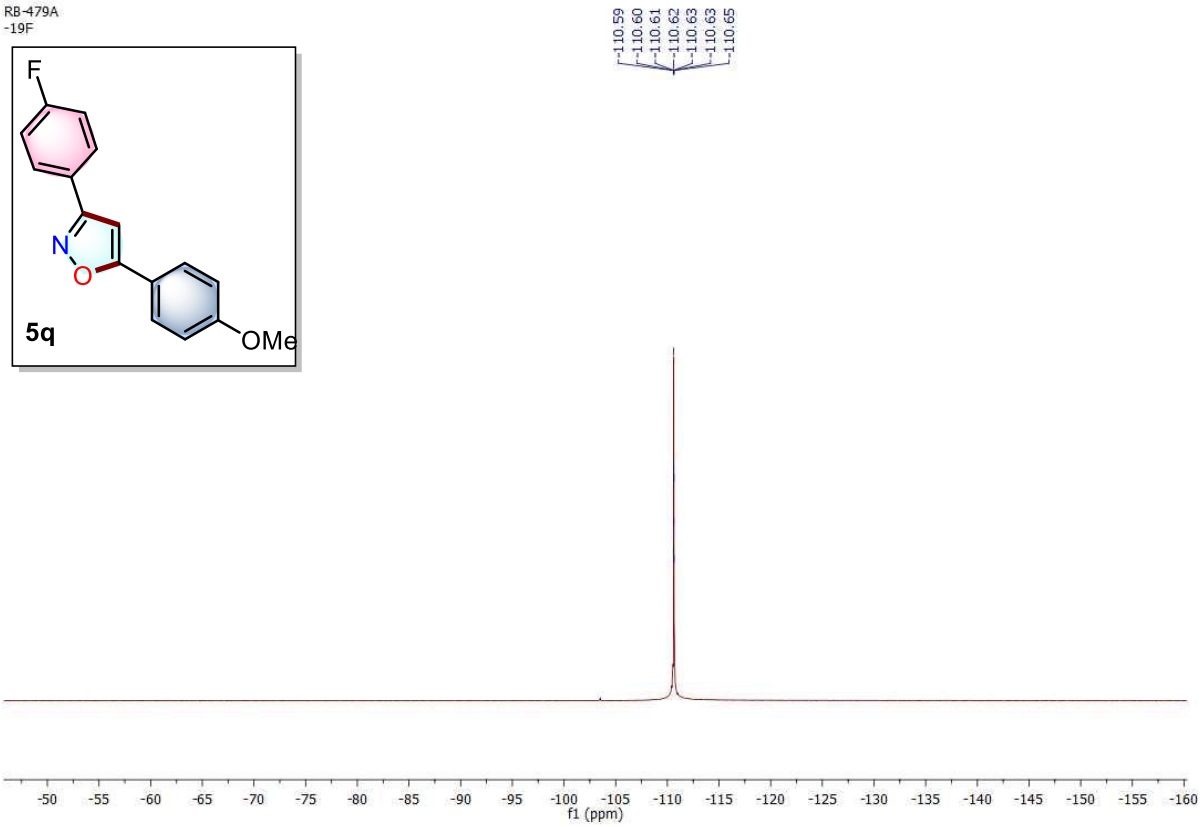
^{1}H NMR Spectrum of **5q** (500 MHz, Chloroform-*d*)



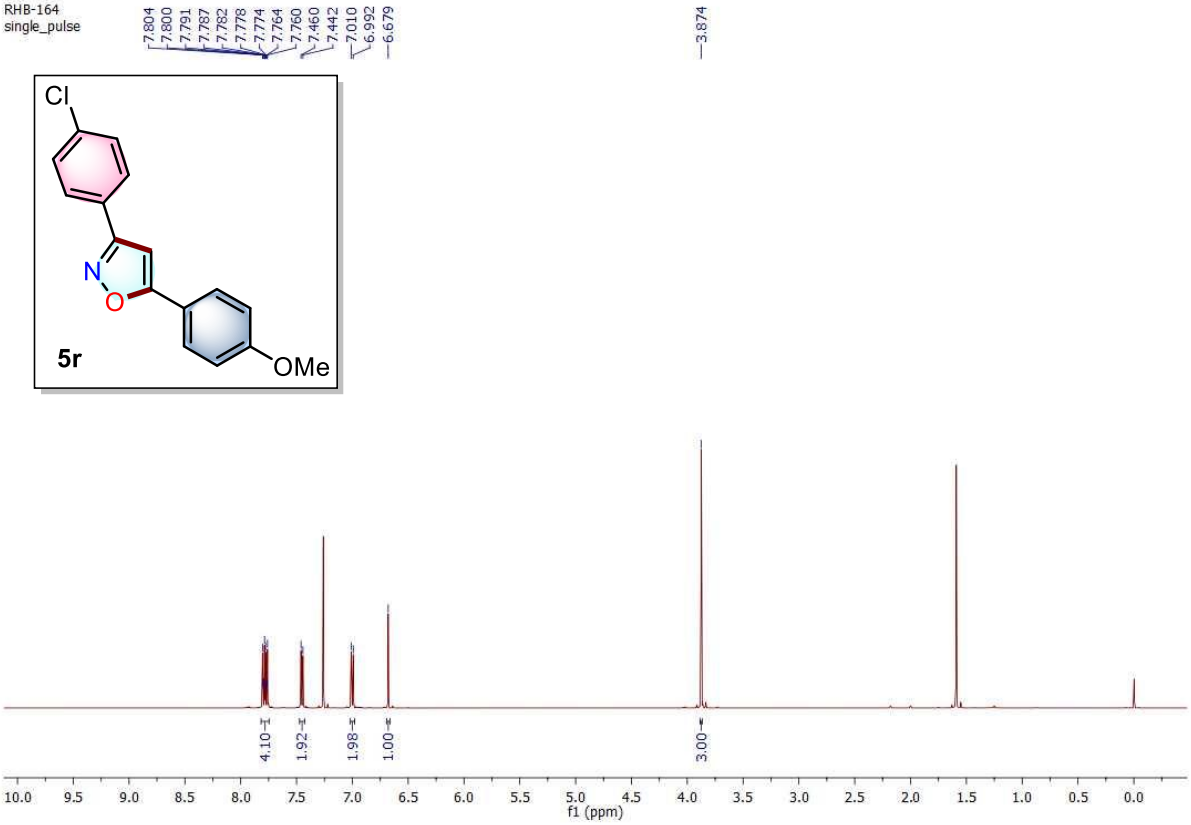
^{13}C NMR Spectrum of **5q** (126 MHz, Chloroform-*d*)



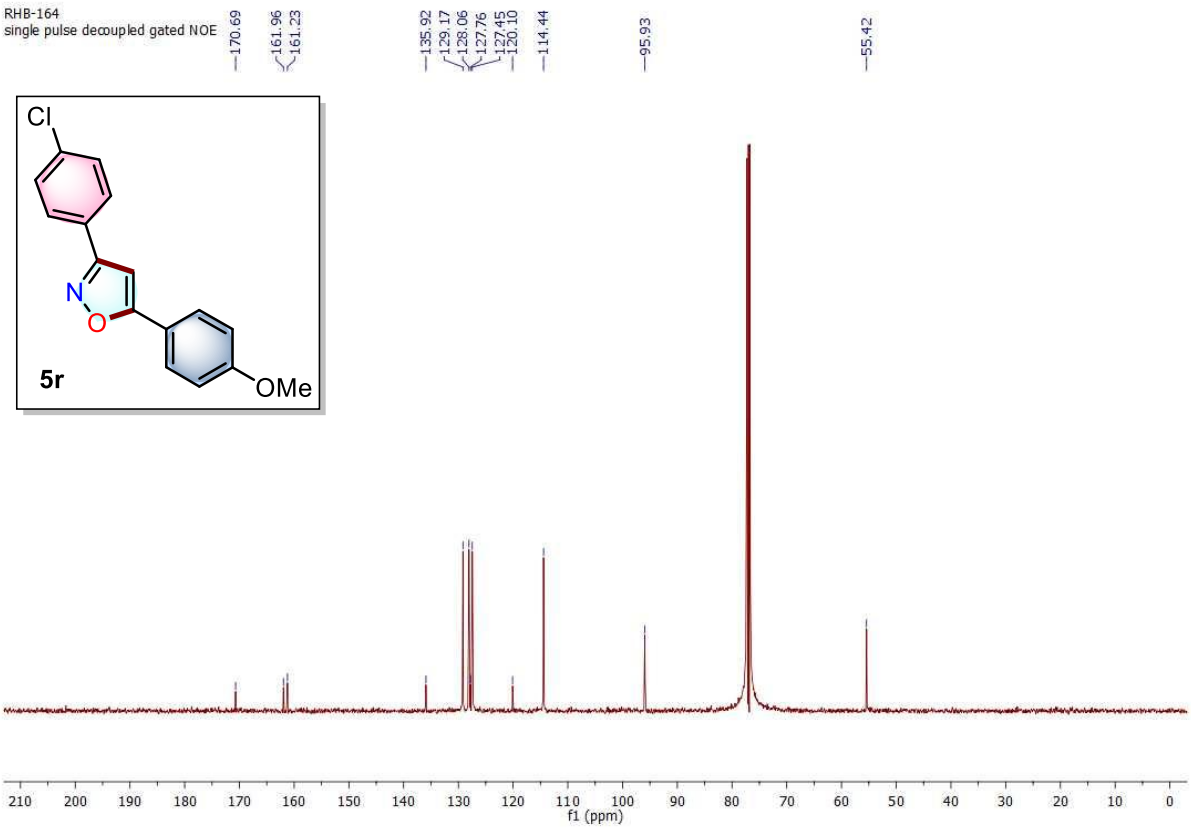
^{19}F NMR Spectrum of **5q** (471 MHz, Chloroform-*d*)



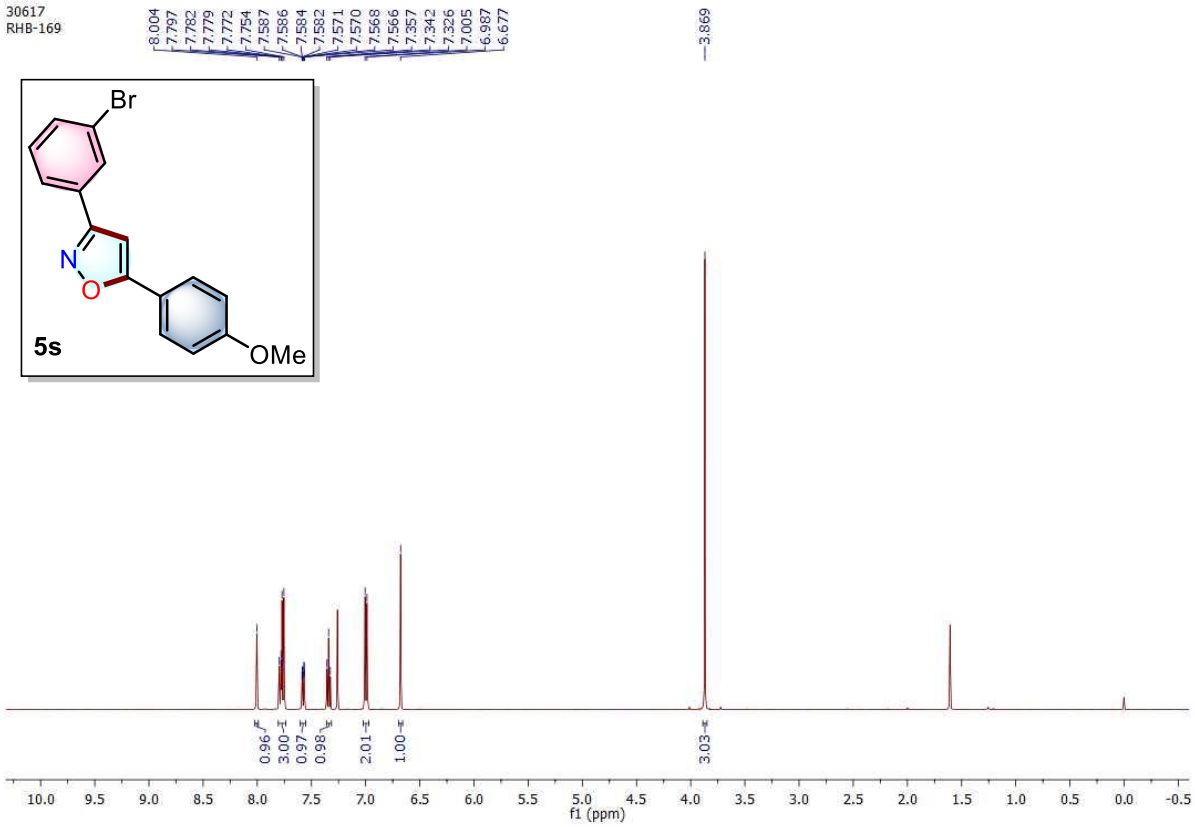
^{1}H NMR Spectrum of **5r** (500 MHz, Chloroform-*d*)



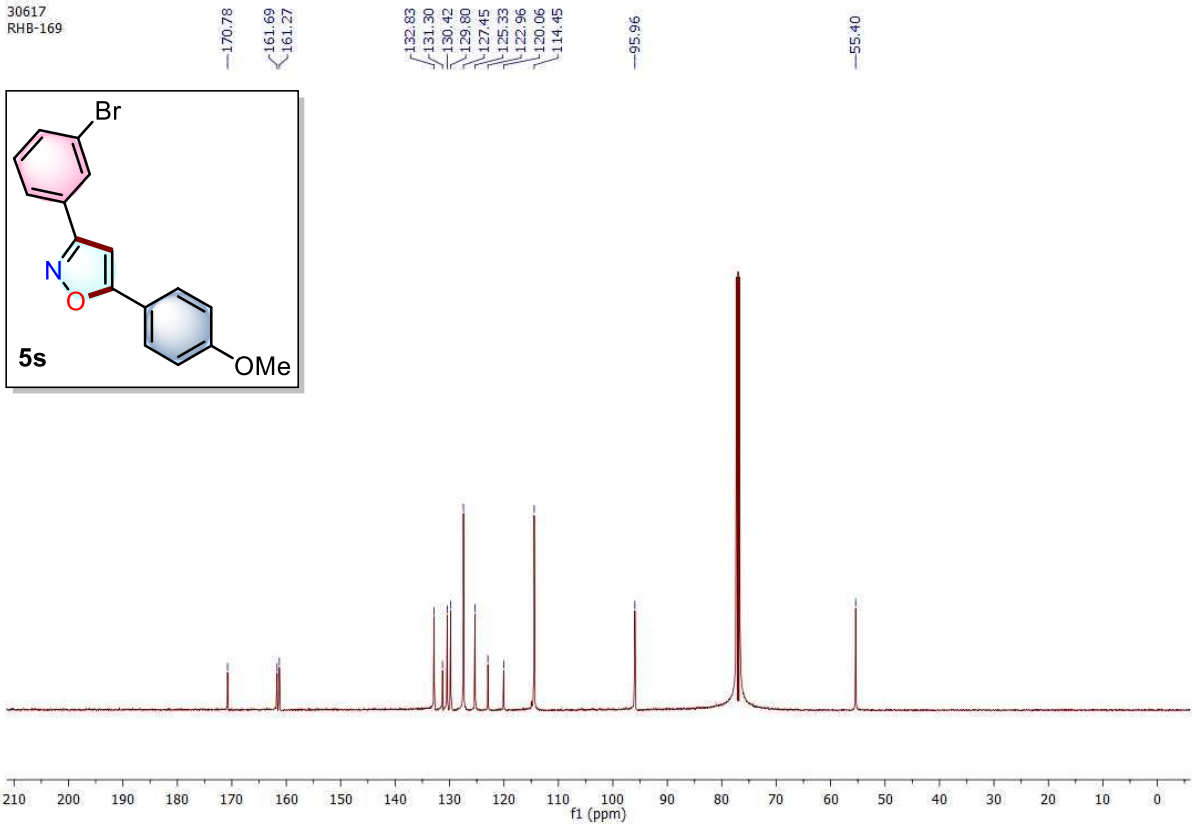
^{13}C NMR Spectrum of **5r** (126 MHz, Chloroform-*d*)



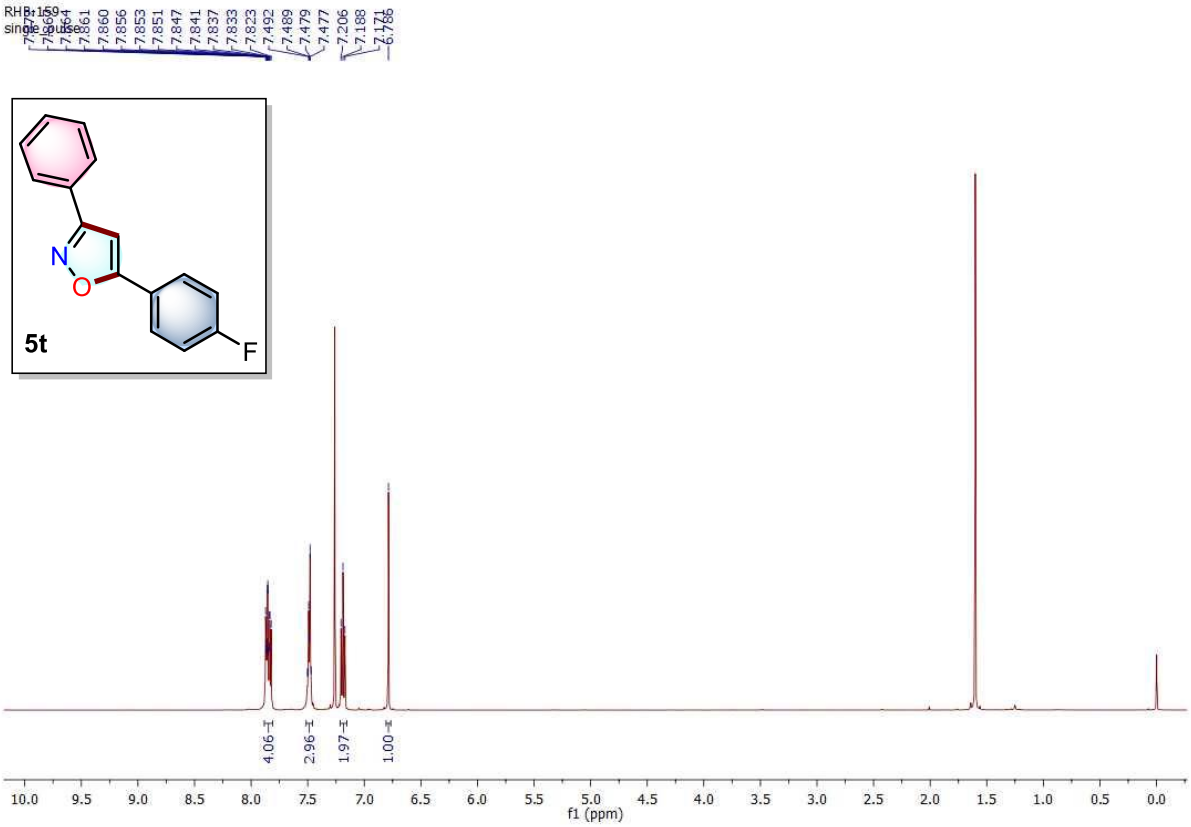
^{1}H NMR Spectrum of **5s** (500 MHz, Chloroform-*d*)



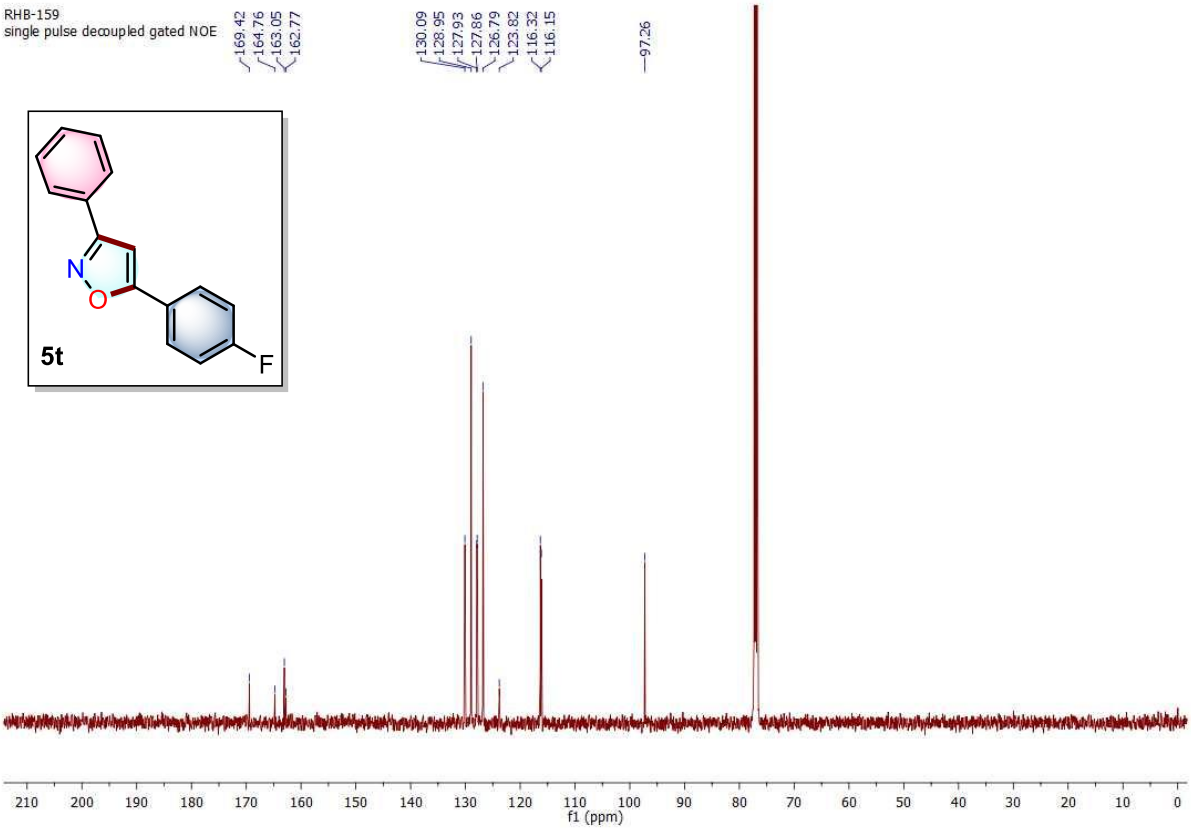
^{13}C NMR Spectrum of **5s** (126 MHz, Chloroform-*d*)



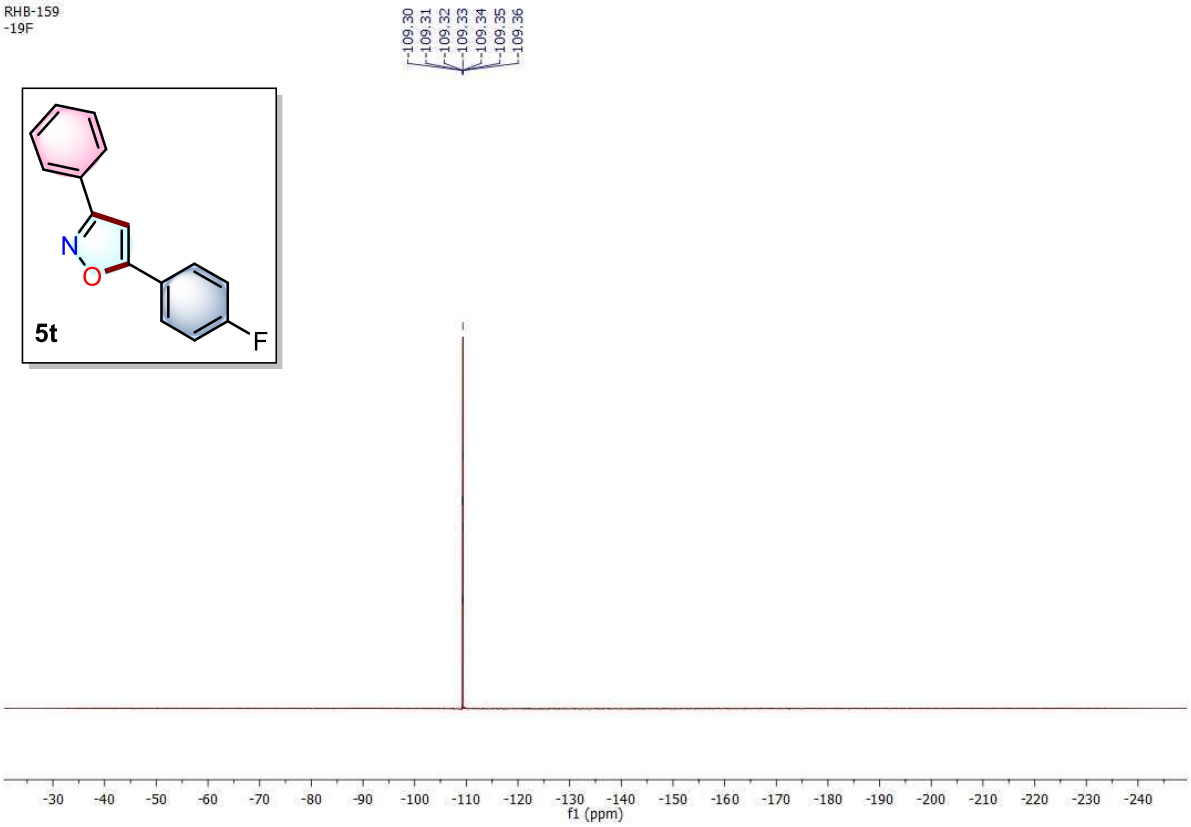
^{1}H NMR Spectrum of **5t** (500 MHz, Chloroform-*d*)



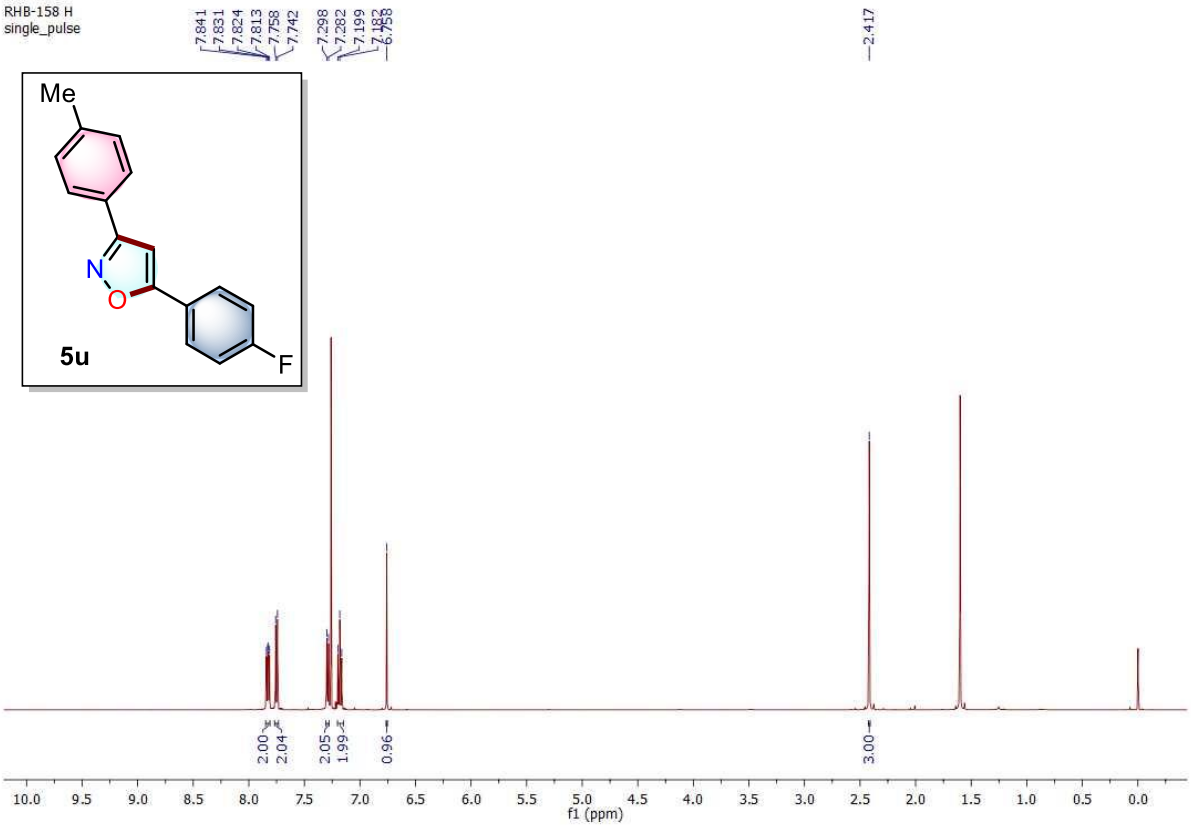
^{13}C NMR Spectrum of **5t** (126 MHz, Chloroform-*d*)



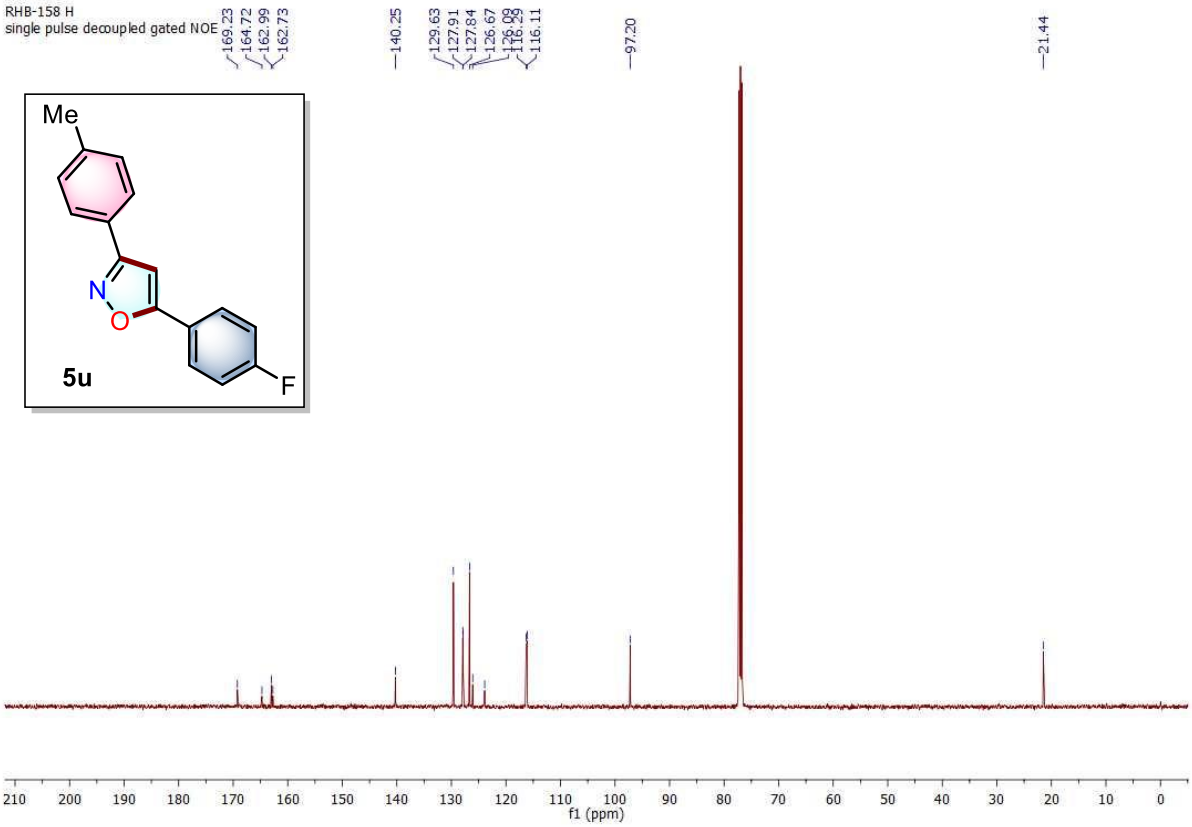
^{19}F NMR Spectrum of **5t** (471 MHz, Chloroform-*d*)



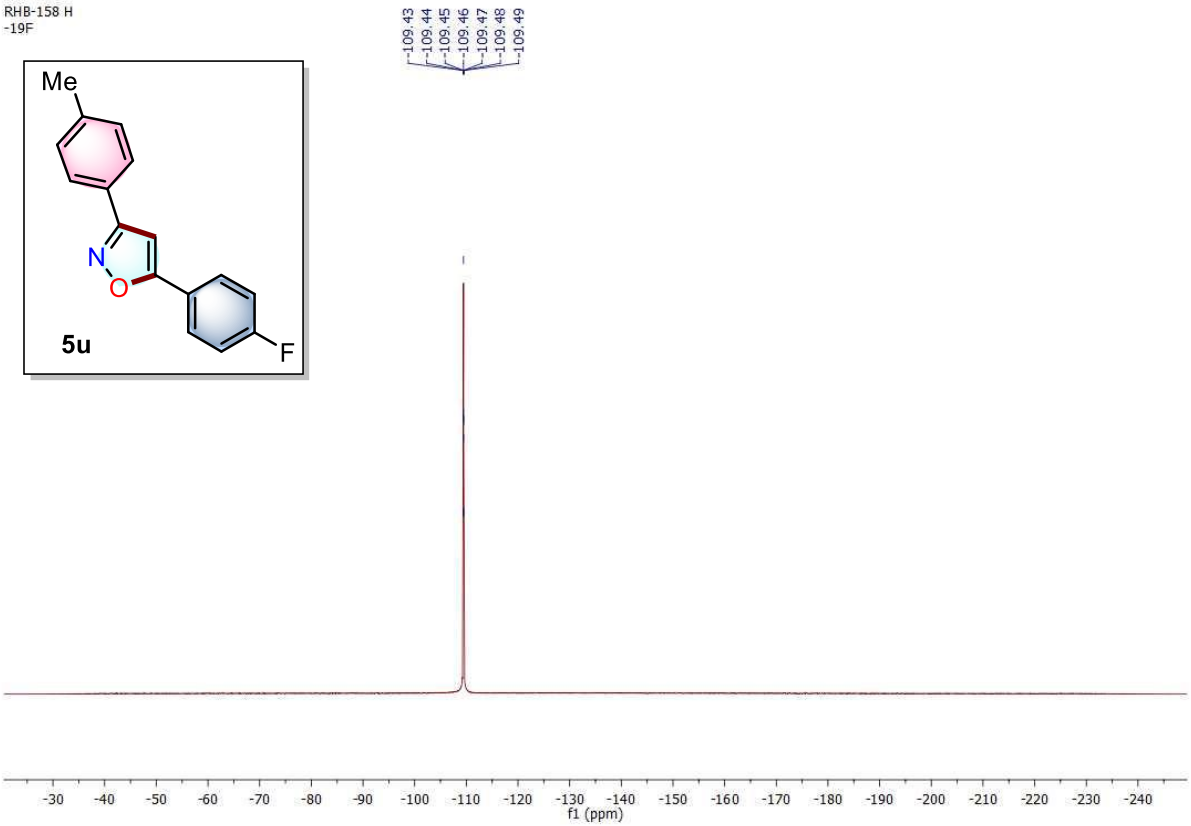
^{1}H NMR Spectrum of **5u** (500 MHz, Chloroform-*d*)



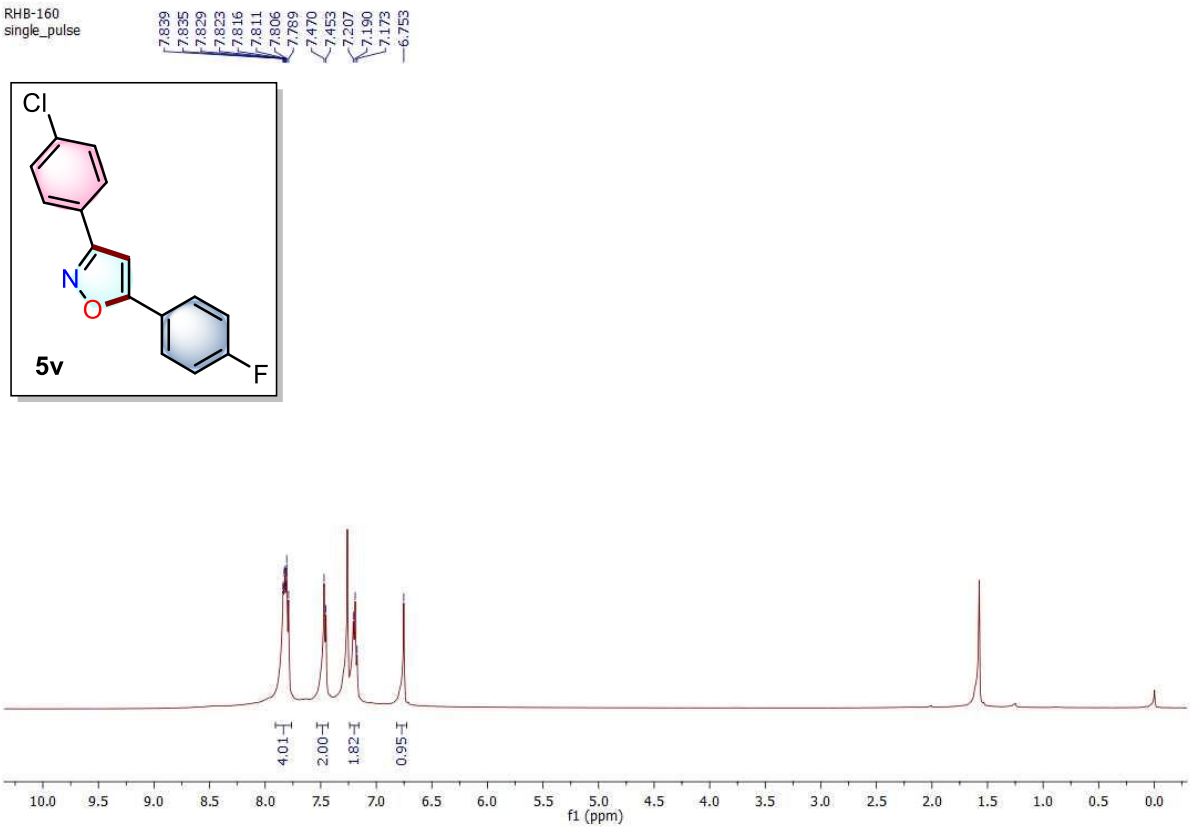
^{13}C NMR Spectrum of **5u** (126 MHz, Chloroform-*d*)



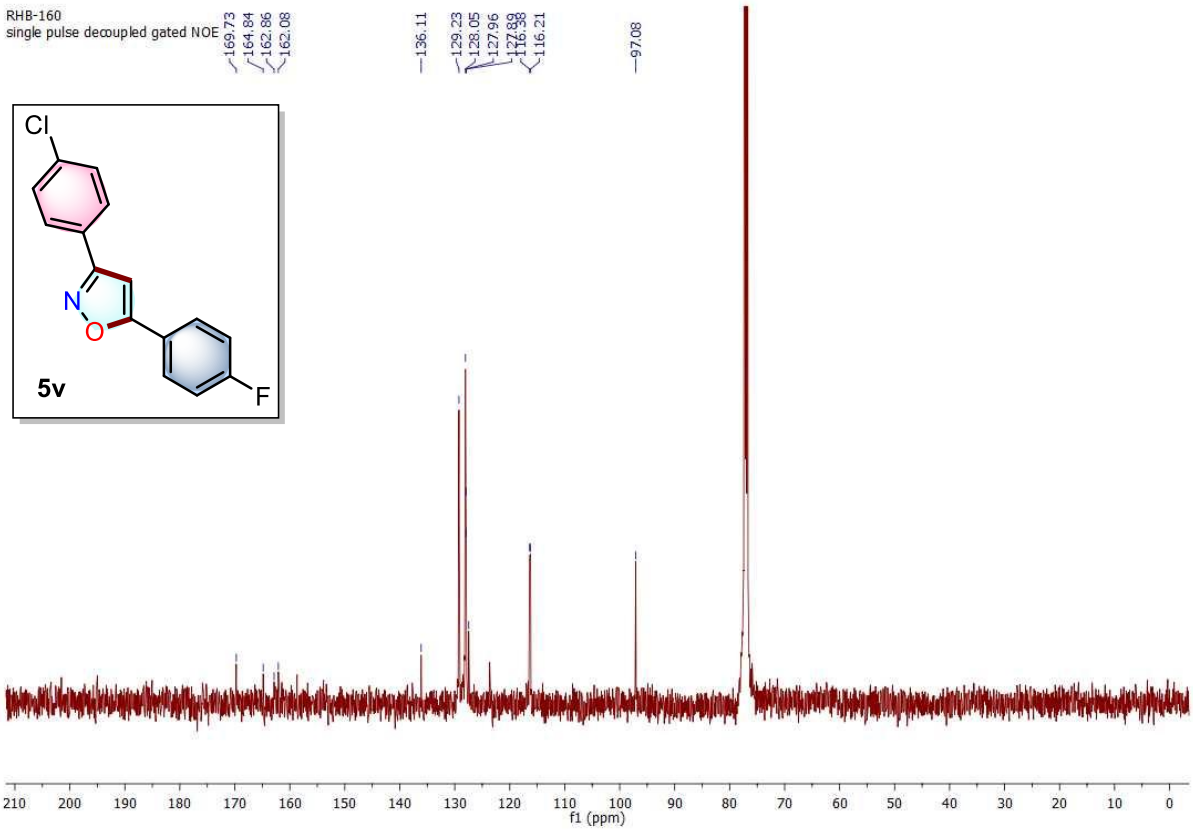
^{19}F NMR Spectrum of **5u** (471 MHz, Chloroform-*d*)



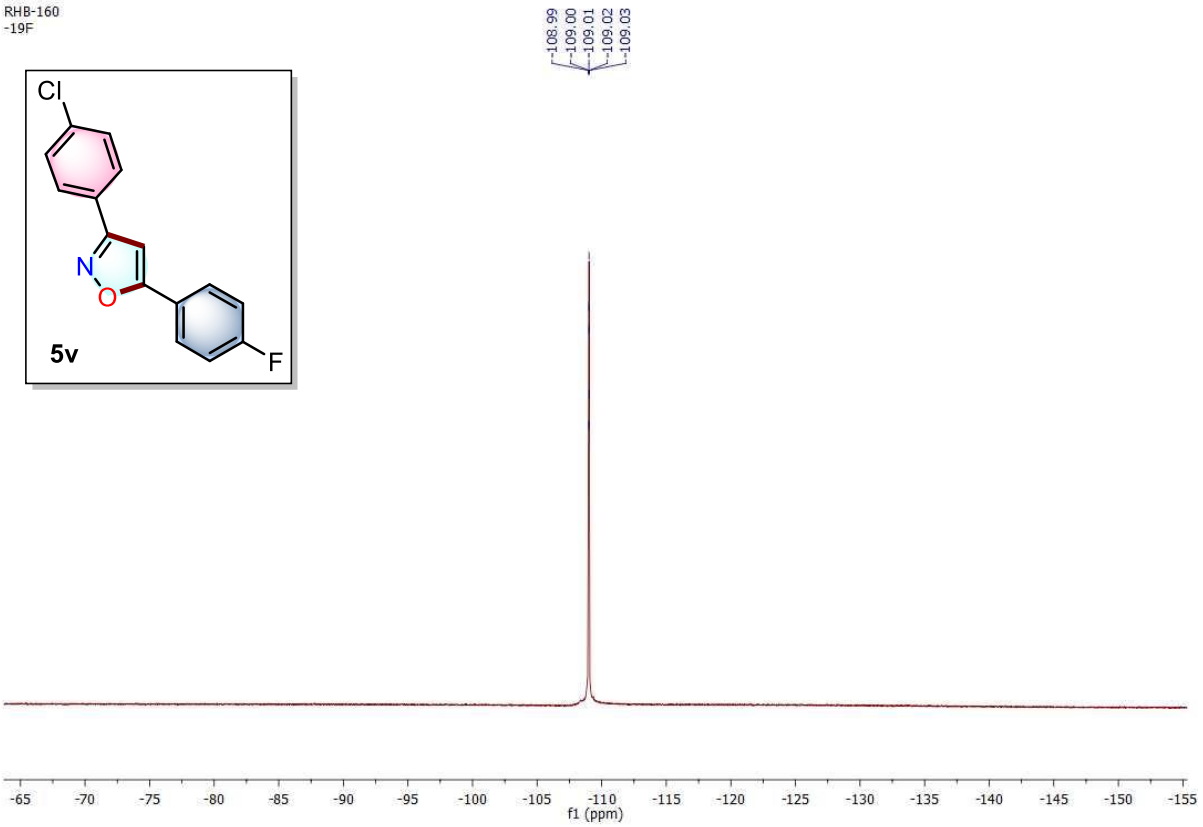
^{1}H NMR Spectrum of **5v** (500 MHz, Chloroform-*d*)



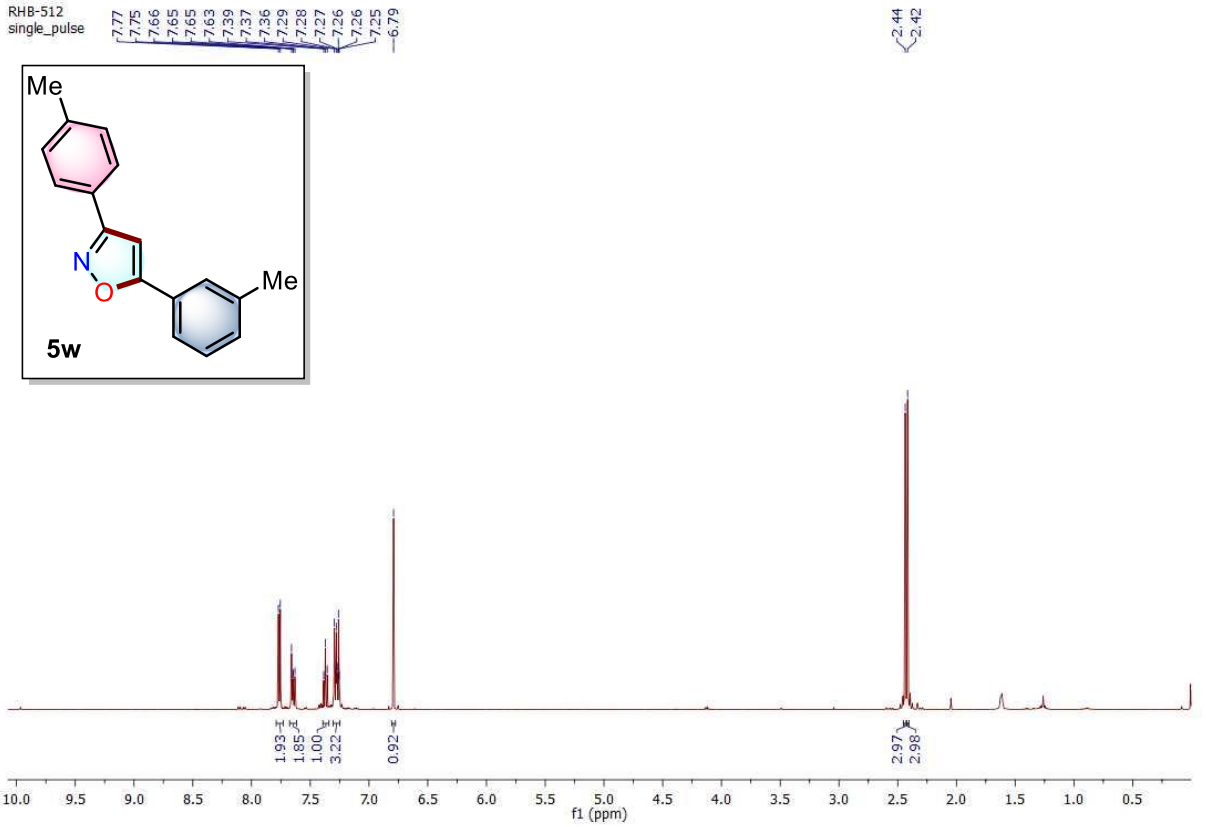
^{13}C NMR Spectrum of **5v** (126 MHz, Chloroform-*d*)



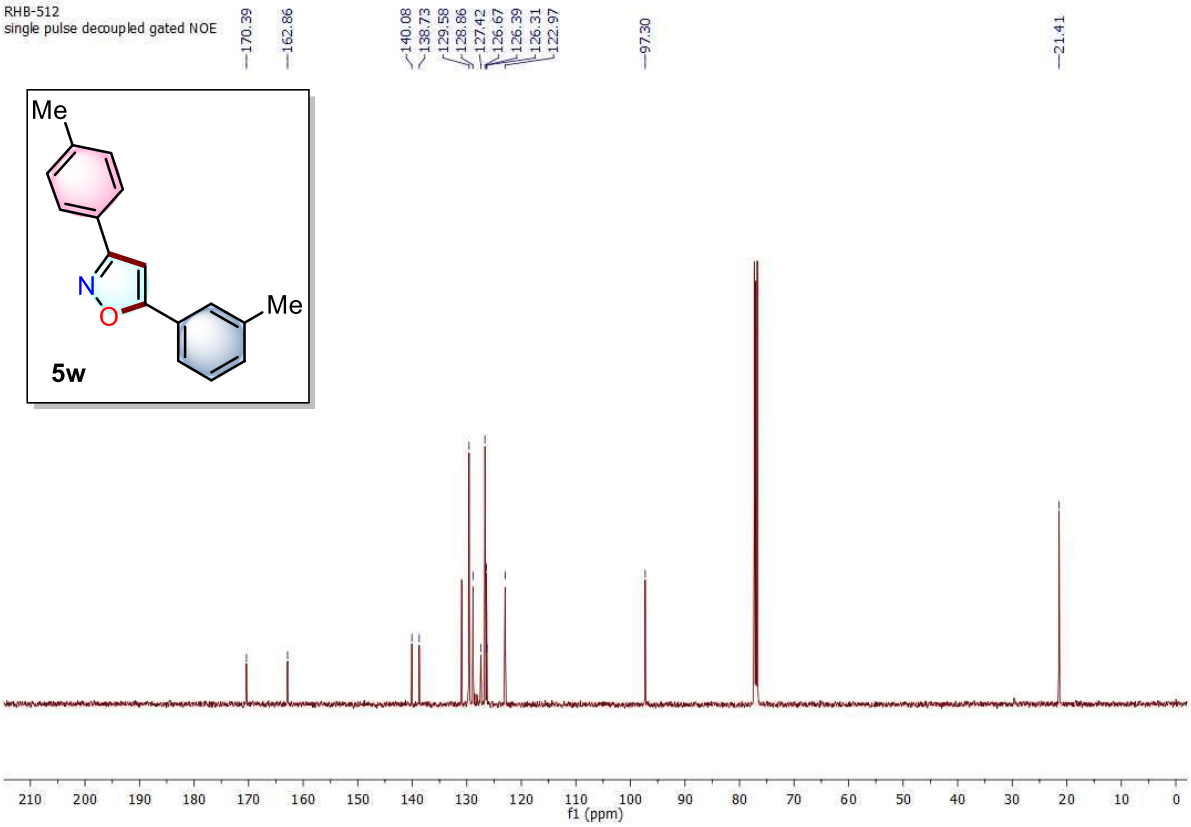
^{19}F NMR Spectrum of **5v** (471 MHz, Chloroform-*d*)



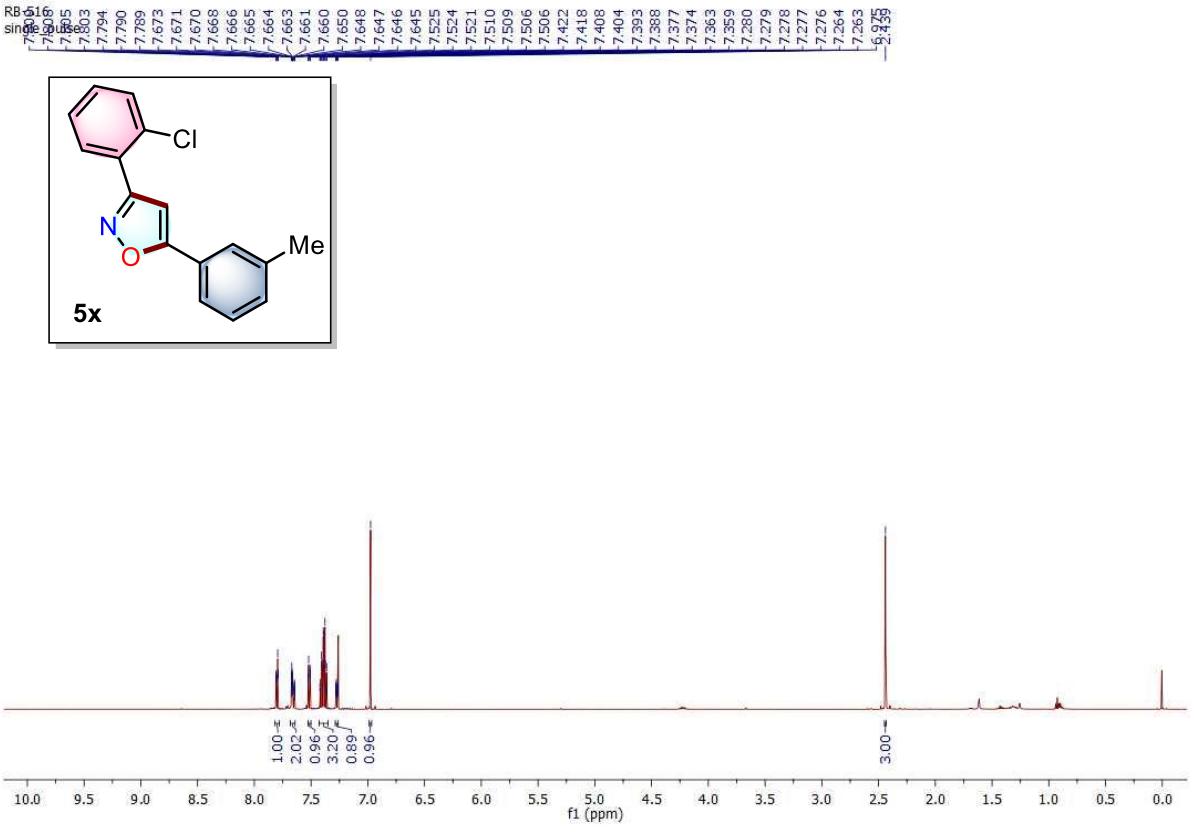
^{1}H NMR Spectrum of **5w** (500 MHz, Chloroform-*d*)



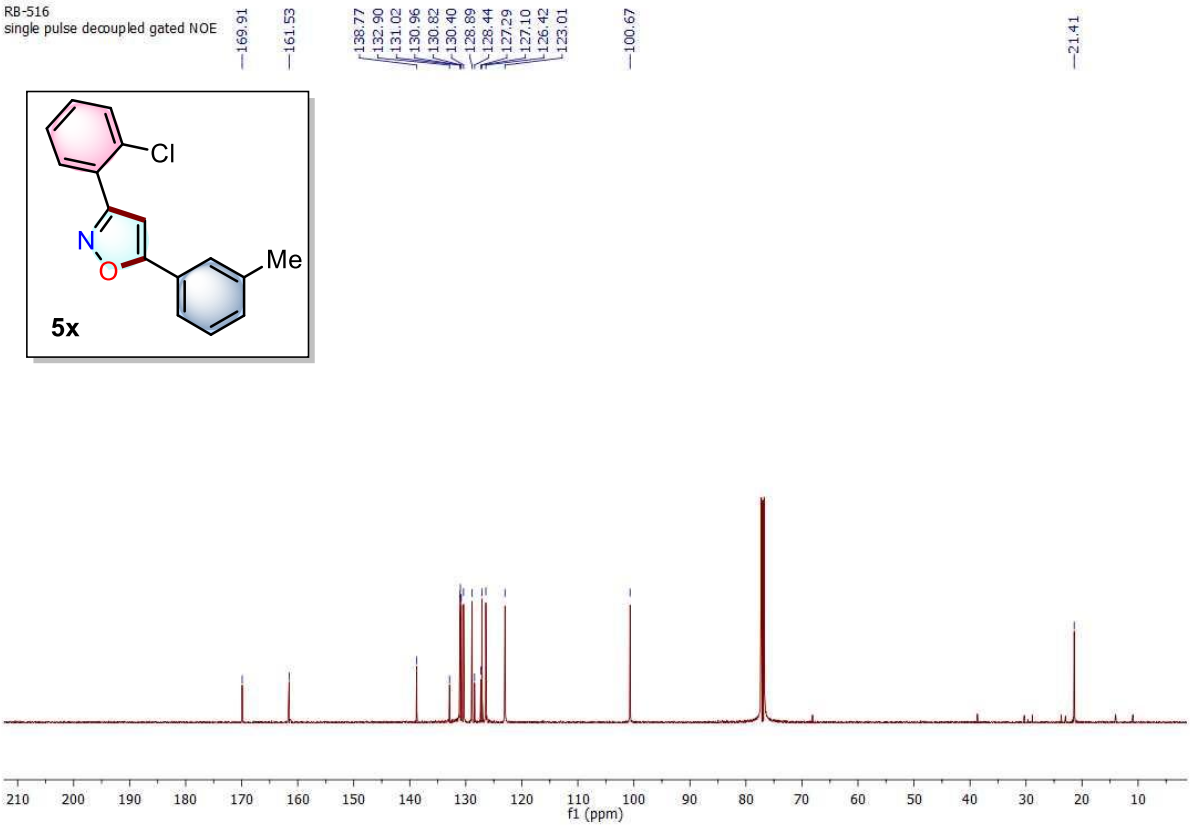
^{13}C NMR Spectrum of **5w** (126 MHz, Chloroform-*d*)



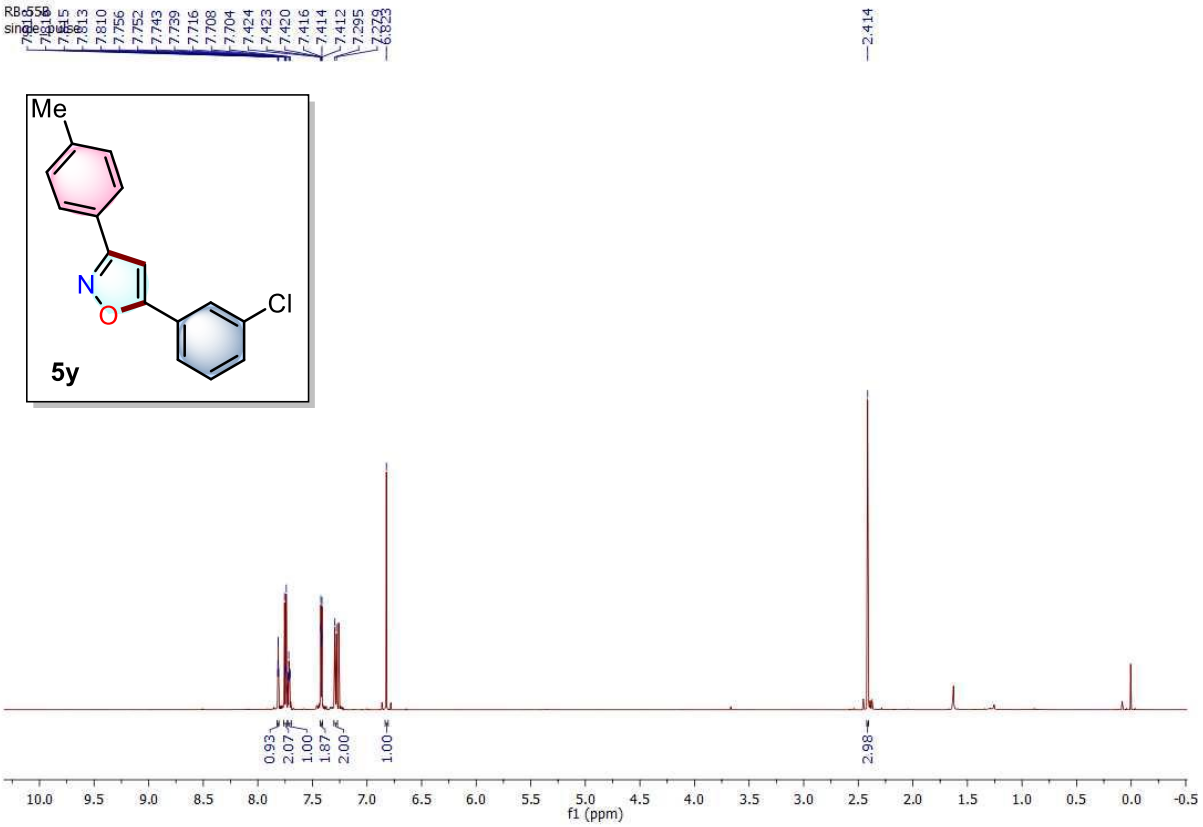
^{1}H NMR Spectrum of **5x** (500 MHz, Chloroform-*d*)



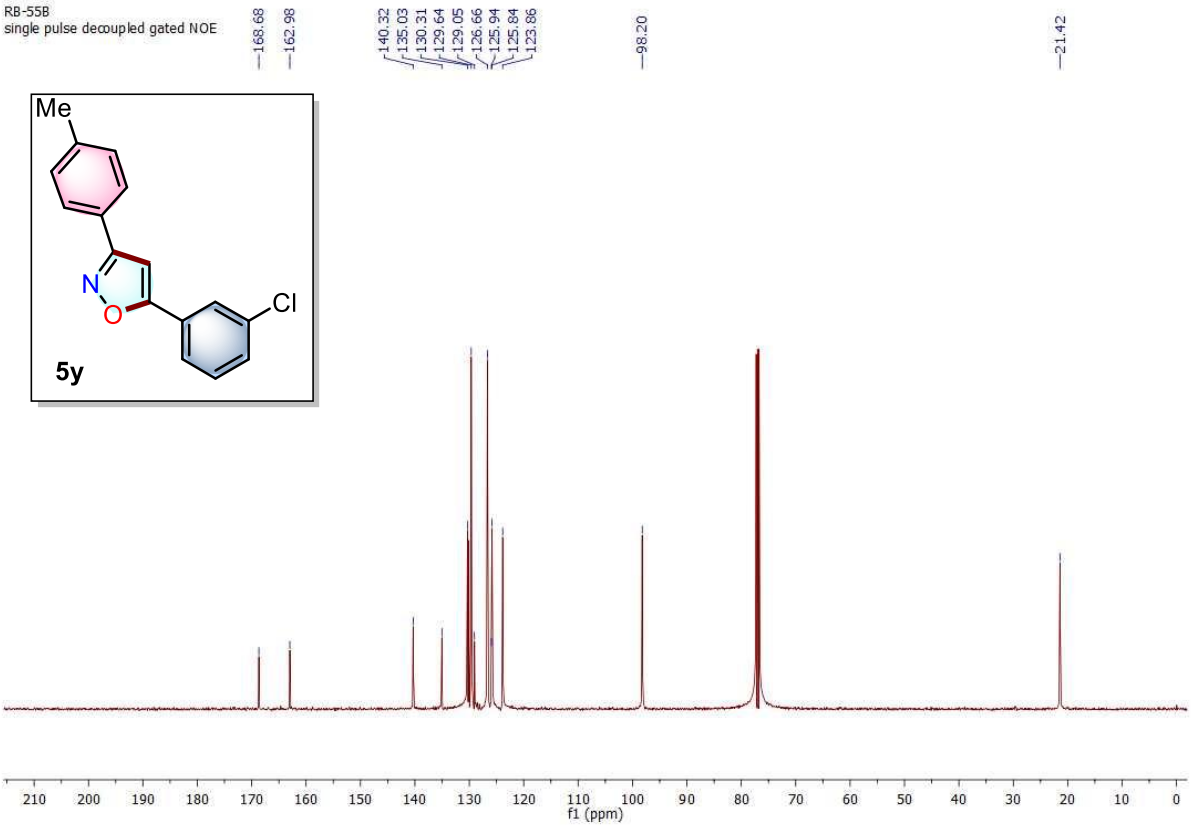
^{13}C NMR Spectrum of **5x** (126 MHz, Chloroform-*d*)



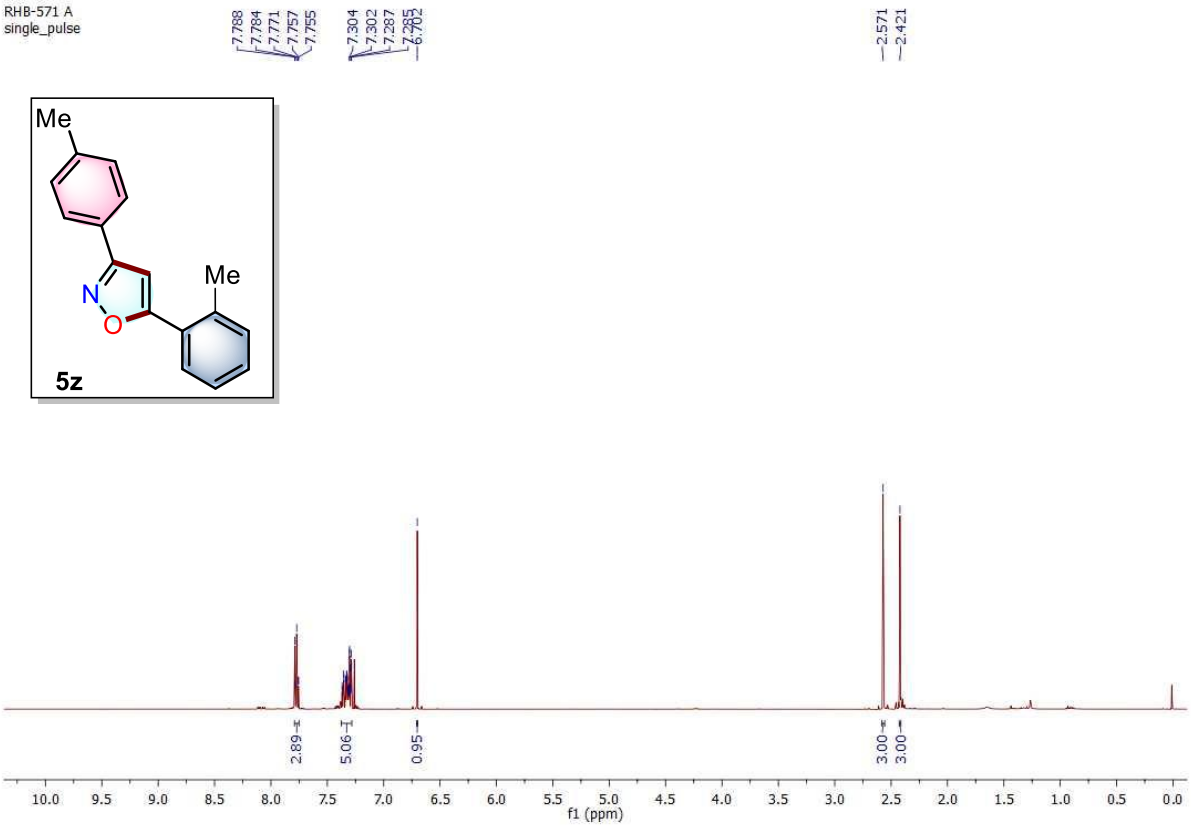
^{1}H NMR Spectrum of **5y** (500 MHz, Chloroform-*d*)



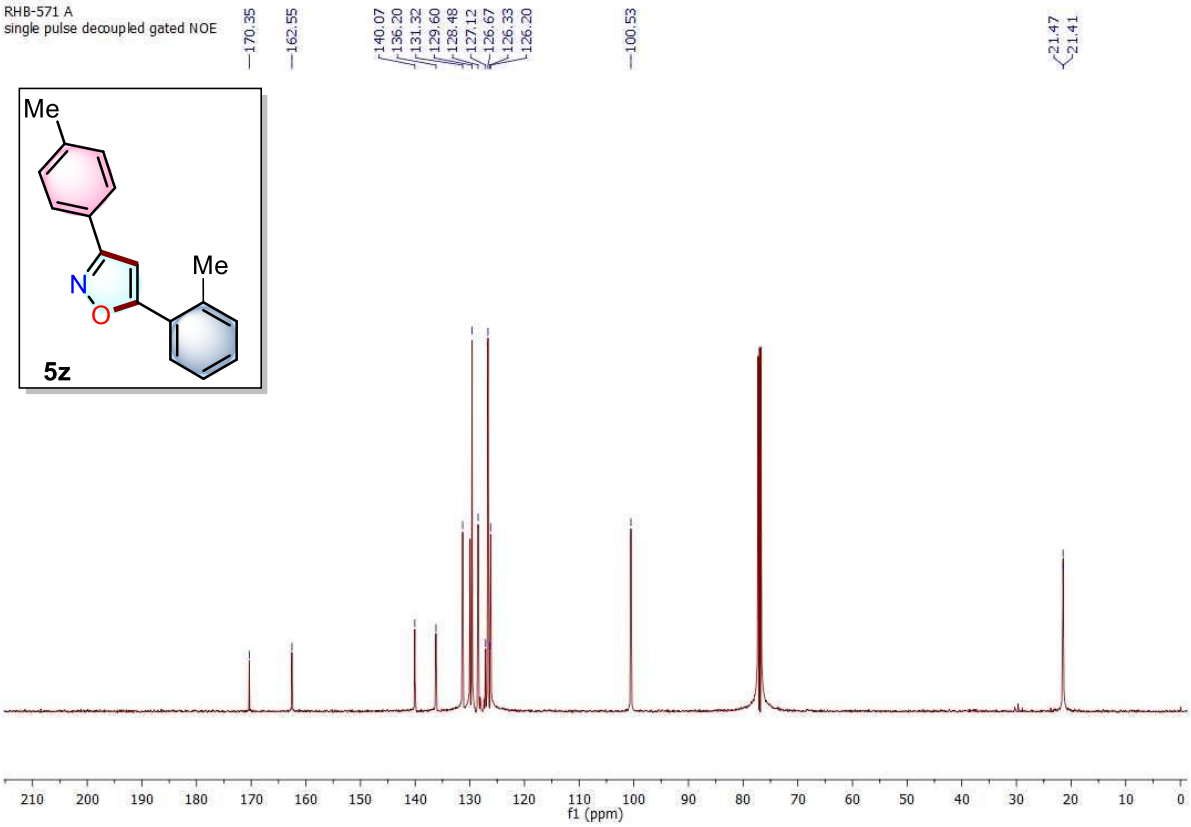
^{13}C NMR Spectrum of **5y** (126 MHz, Chloroform-*d*)



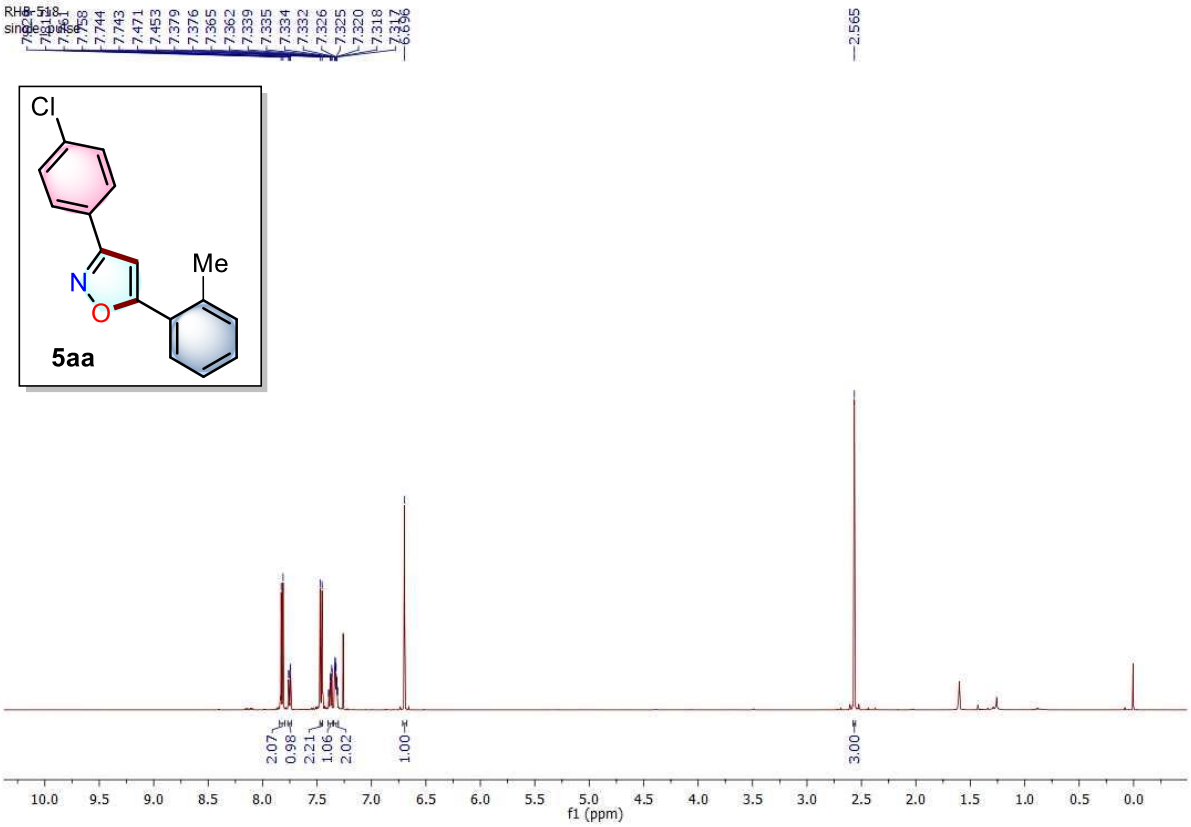
^{1}H NMR Spectrum of **5z** (500 MHz, Chloroform-*d*)



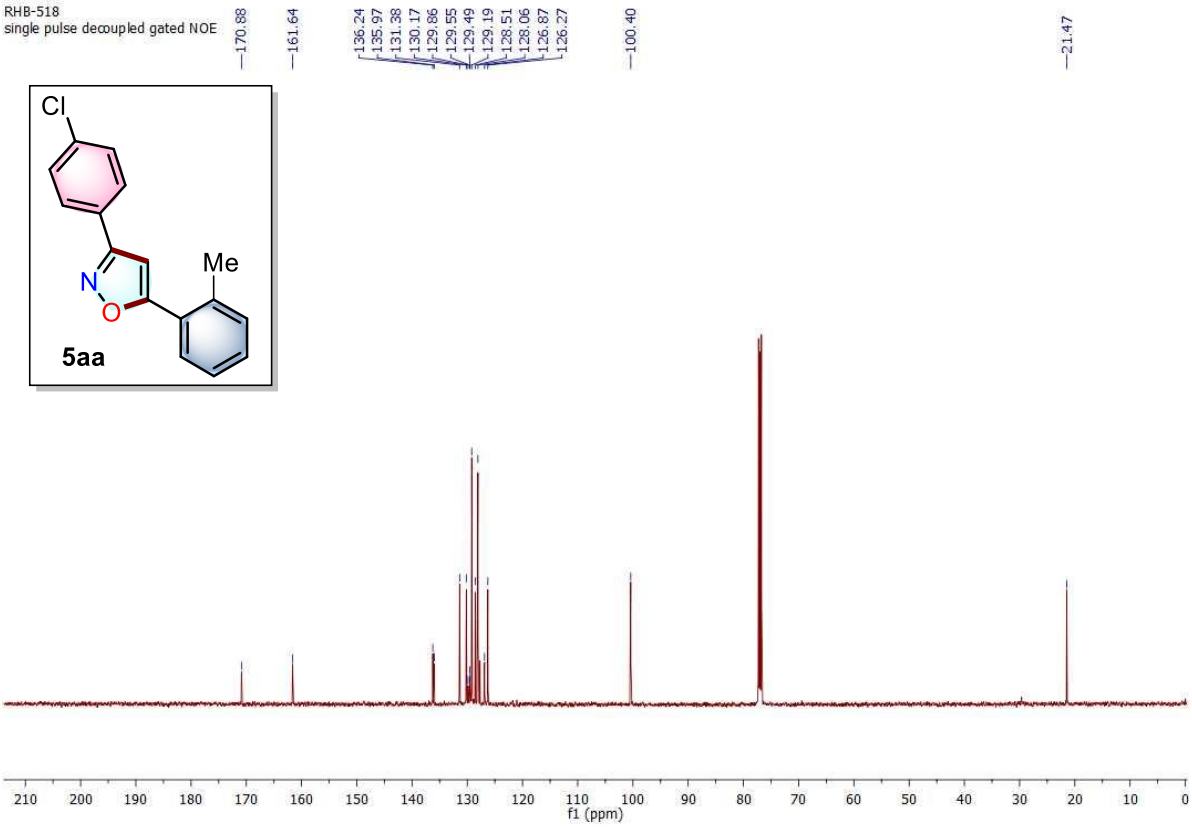
^{13}C NMR Spectrum of **5z** (126 MHz, Chloroform-*d*)



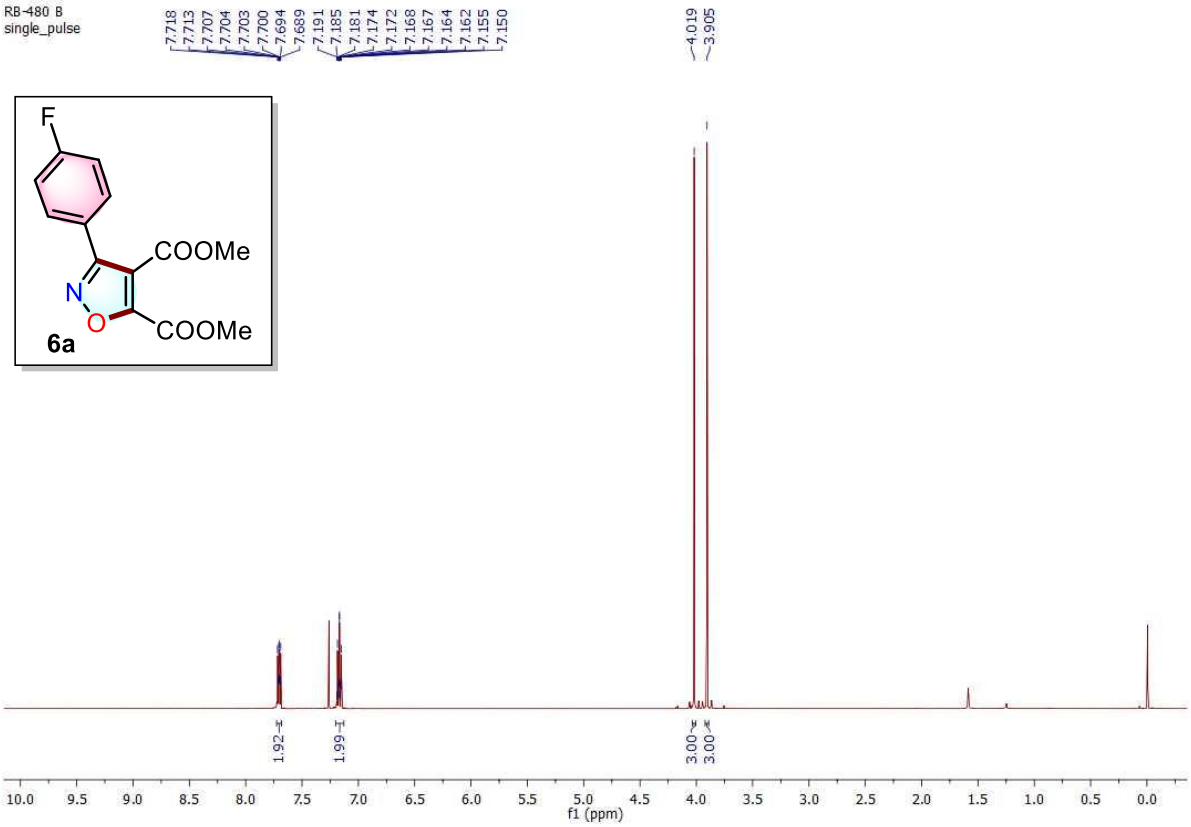
^{1}H NMR Spectrum of **5aa** (500 MHz, Chloroform-*d*)



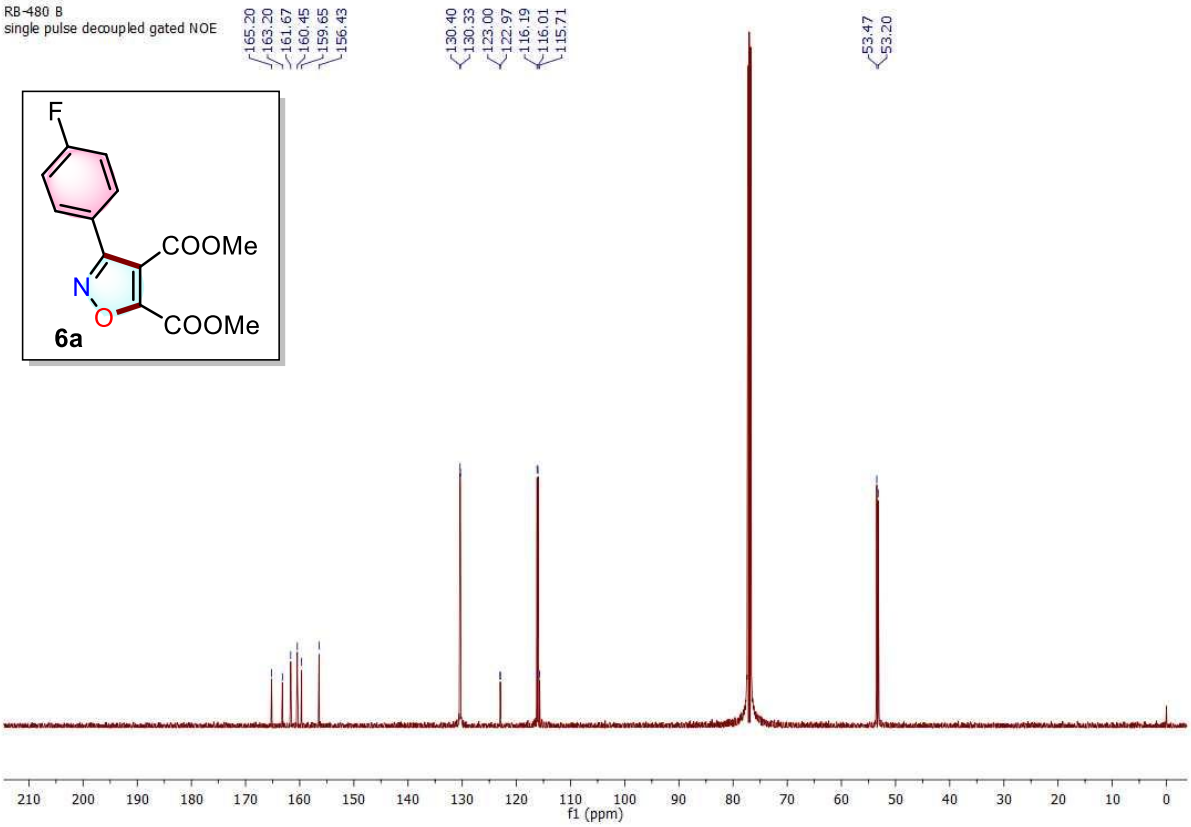
^{13}C NMR Spectrum of **5aa** (126 MHz, Chloroform-*d*)



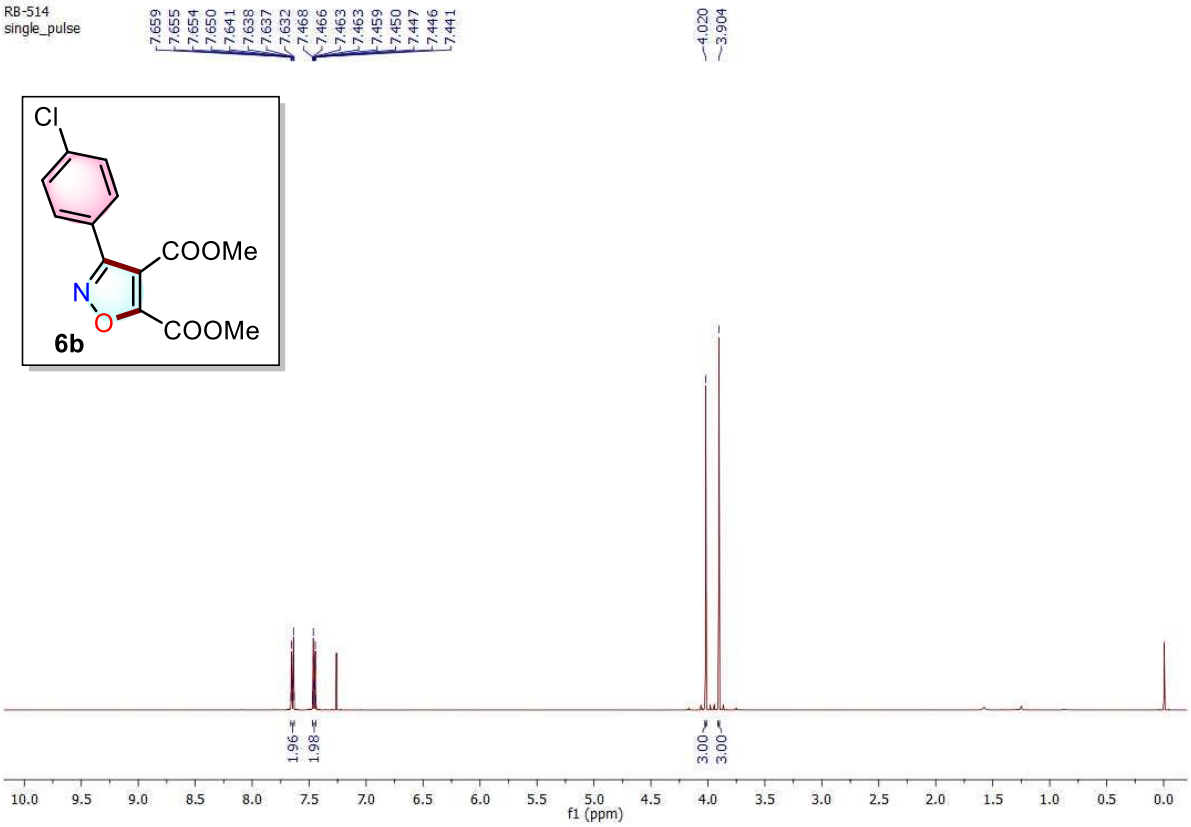
^{1}H NMR Spectrum of **6a** (500 MHz, Chloroform-*d*)



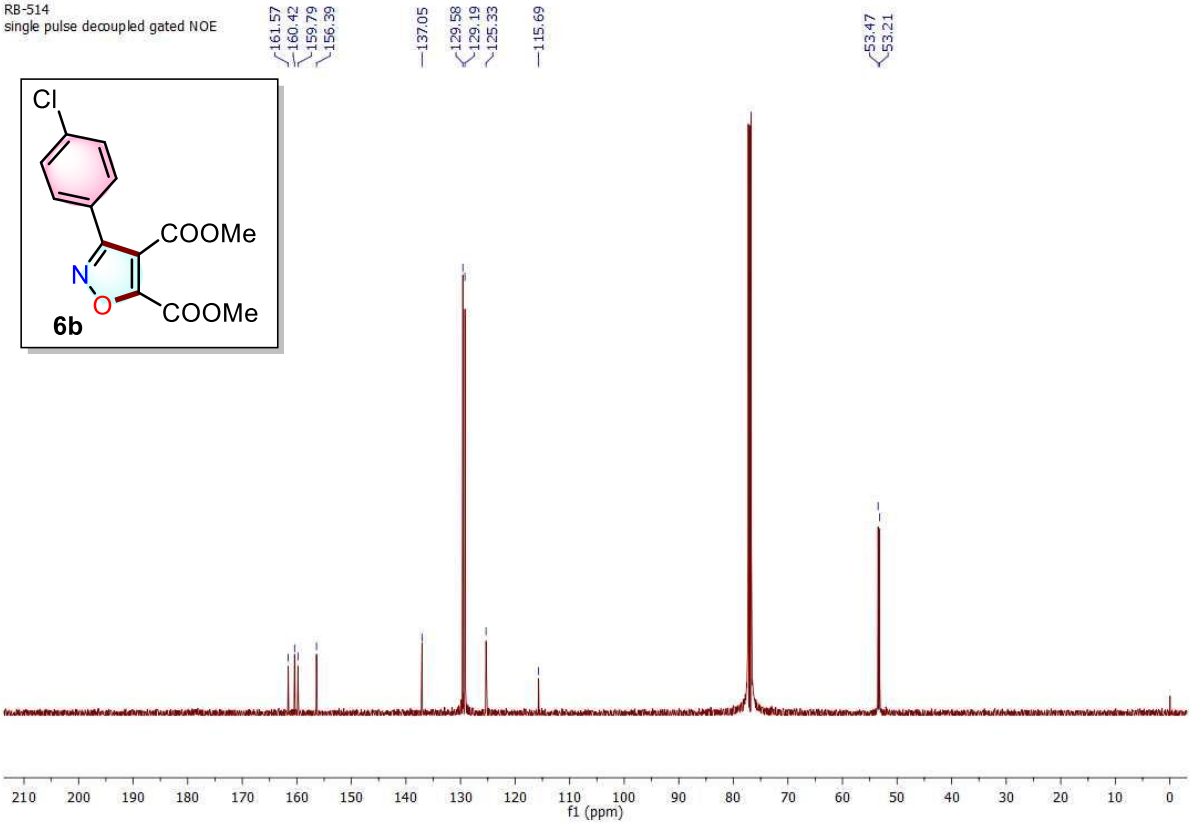
^{13}C NMR Spectrum of **6a** (126 MHz, Chloroform-*d*)



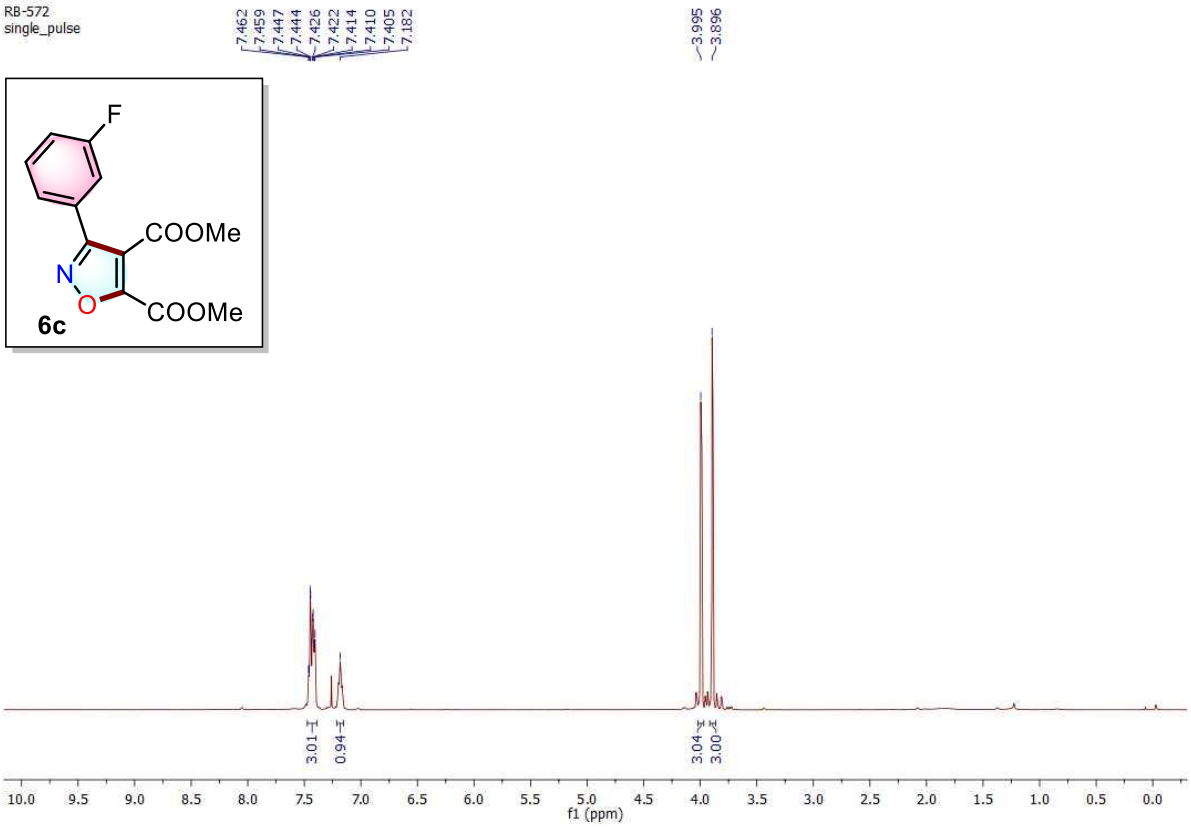
^{1}H NMR Spectrum of **6b** (500 MHz, Chloroform-*d*)



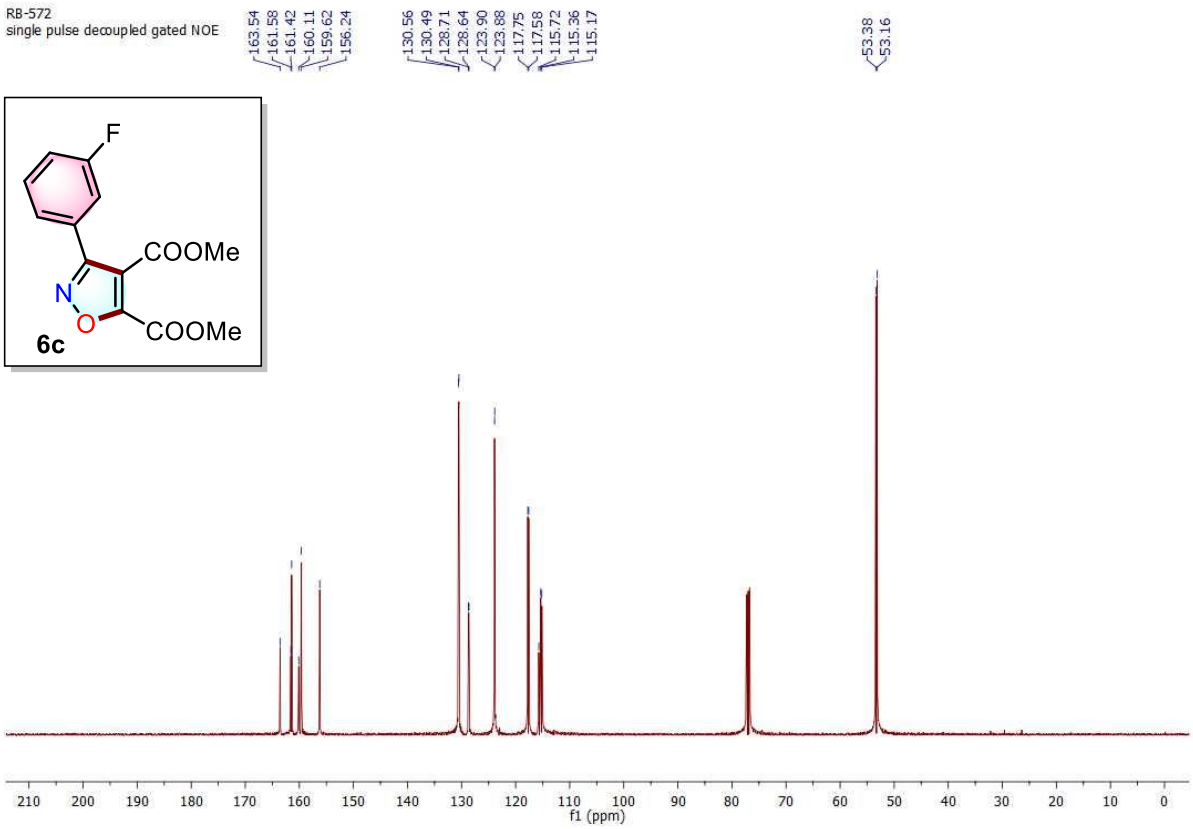
^{13}C NMR Spectrum of **6b** (126 MHz, Chloroform-*d*)



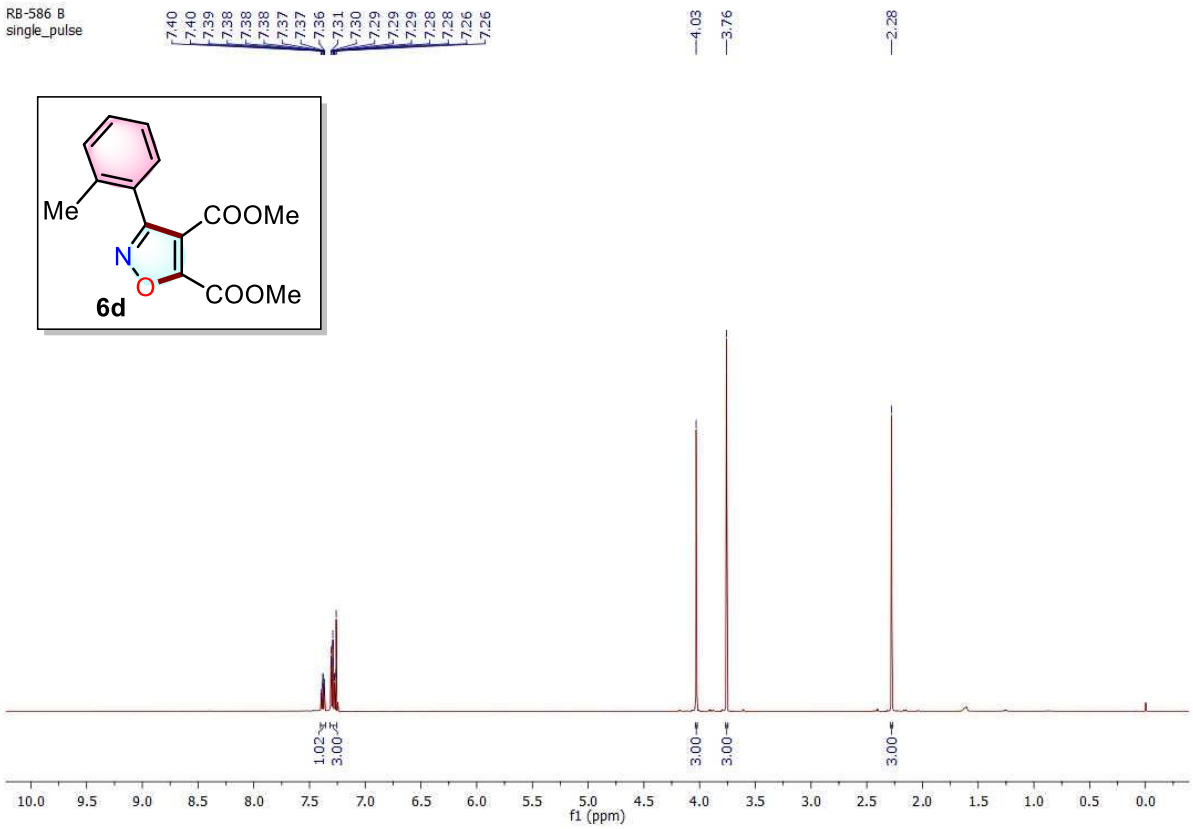
^{1}H NMR Spectrum of **6c** (500 MHz, Chloroform-*d*)



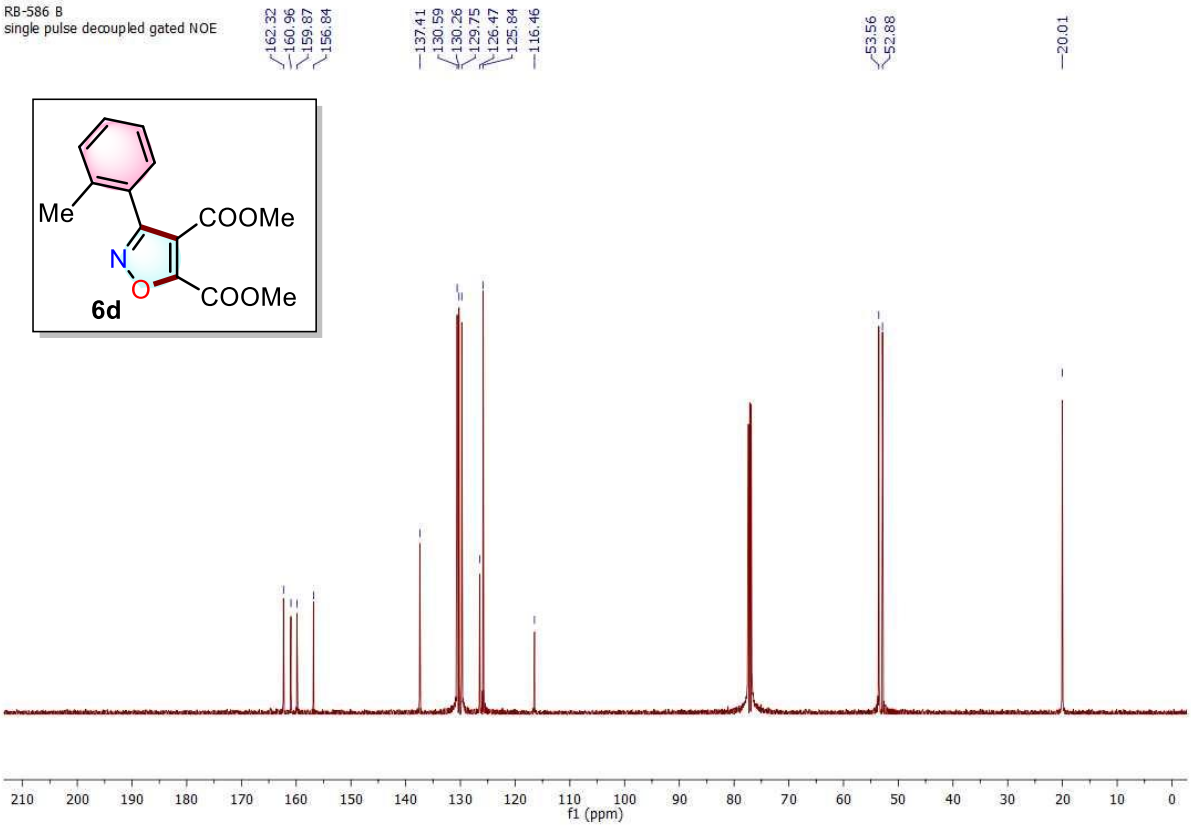
^{13}C NMR Spectrum of **6c** (126 MHz, Chloroform-*d*)



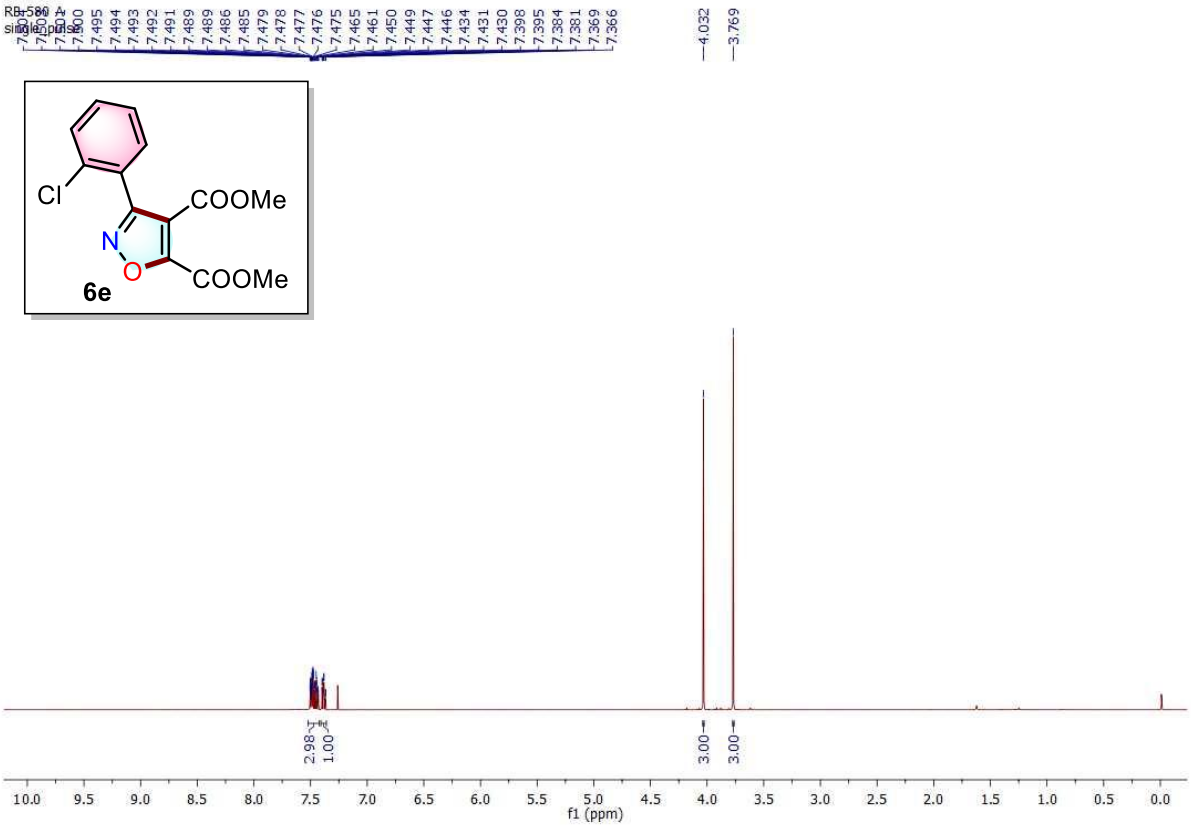
^{1}H NMR Spectrum of **6d** (500 MHz, Chloroform-*d*)



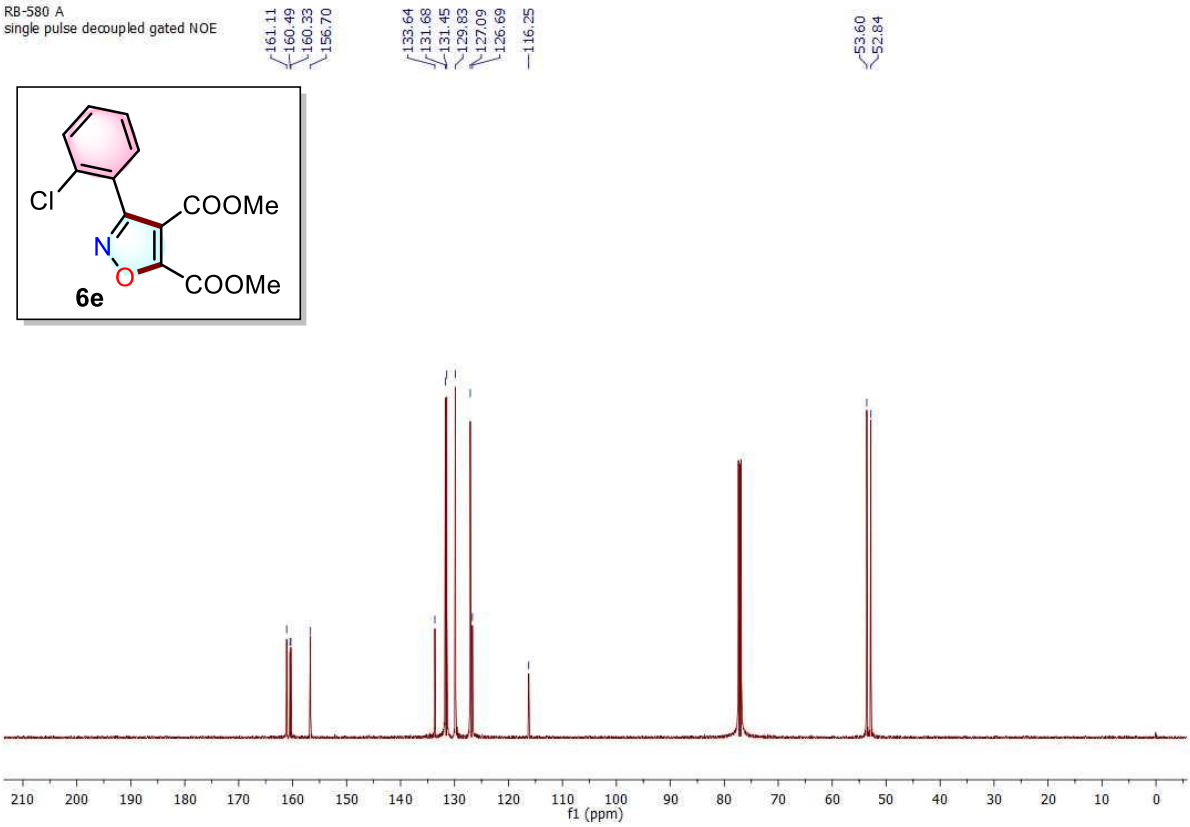
^{13}C NMR Spectrum of **6d** (126 MHz, Chloroform-*d*)



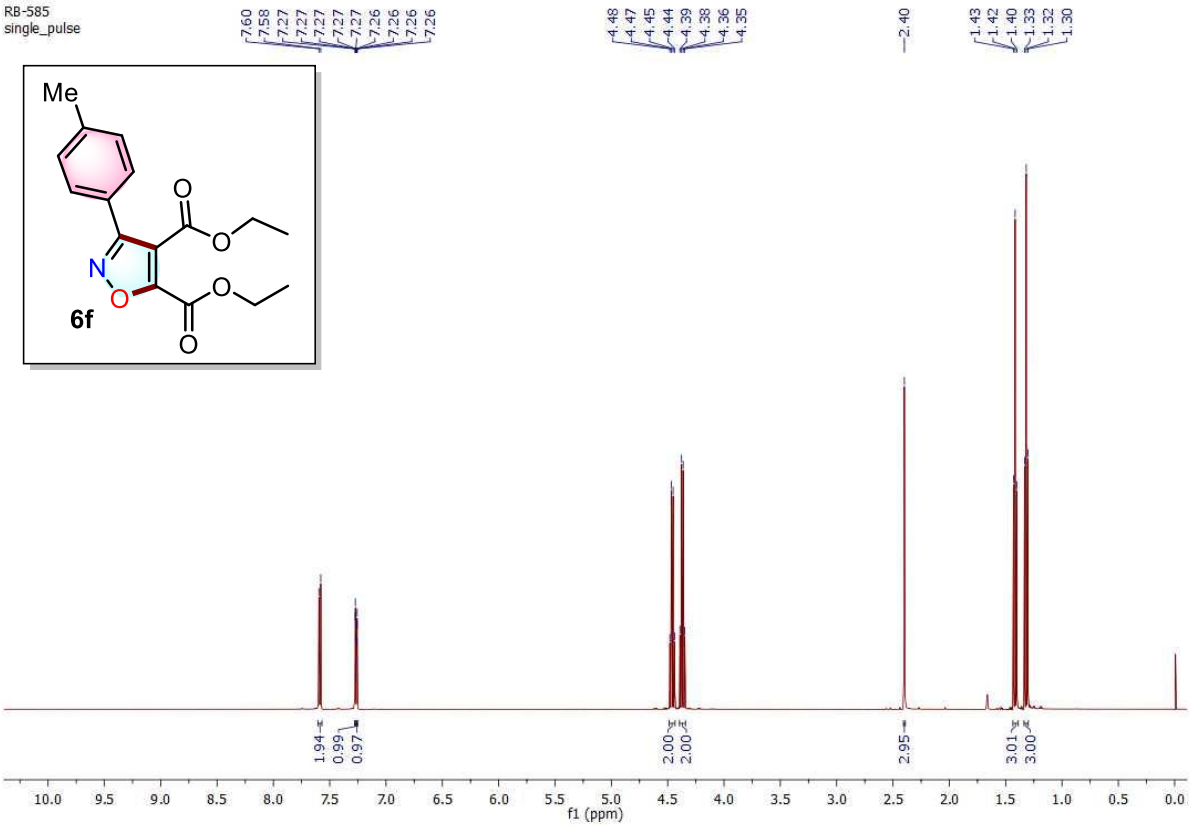
^{1}H NMR Spectrum of **6e** (500 MHz, Chloroform-*d*)



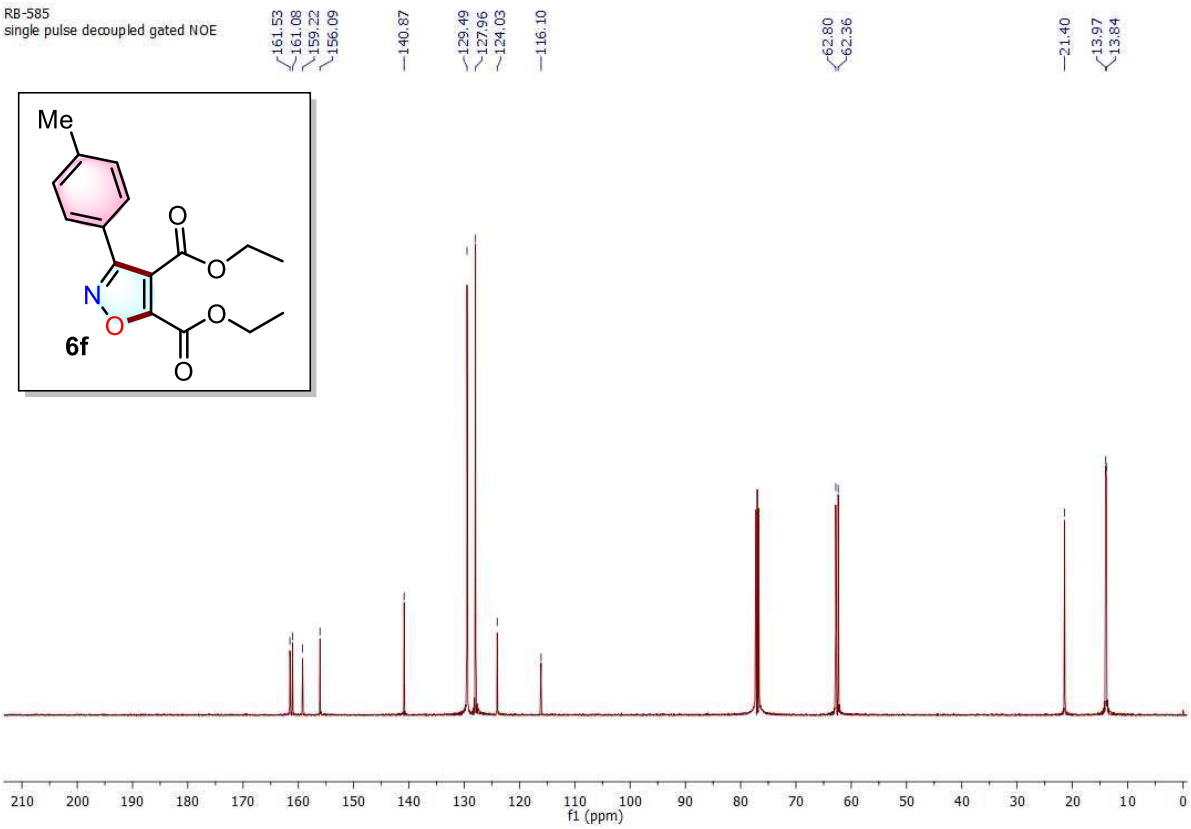
^{13}C NMR Spectrum of **6e** (126 MHz, Chloroform-*d*)



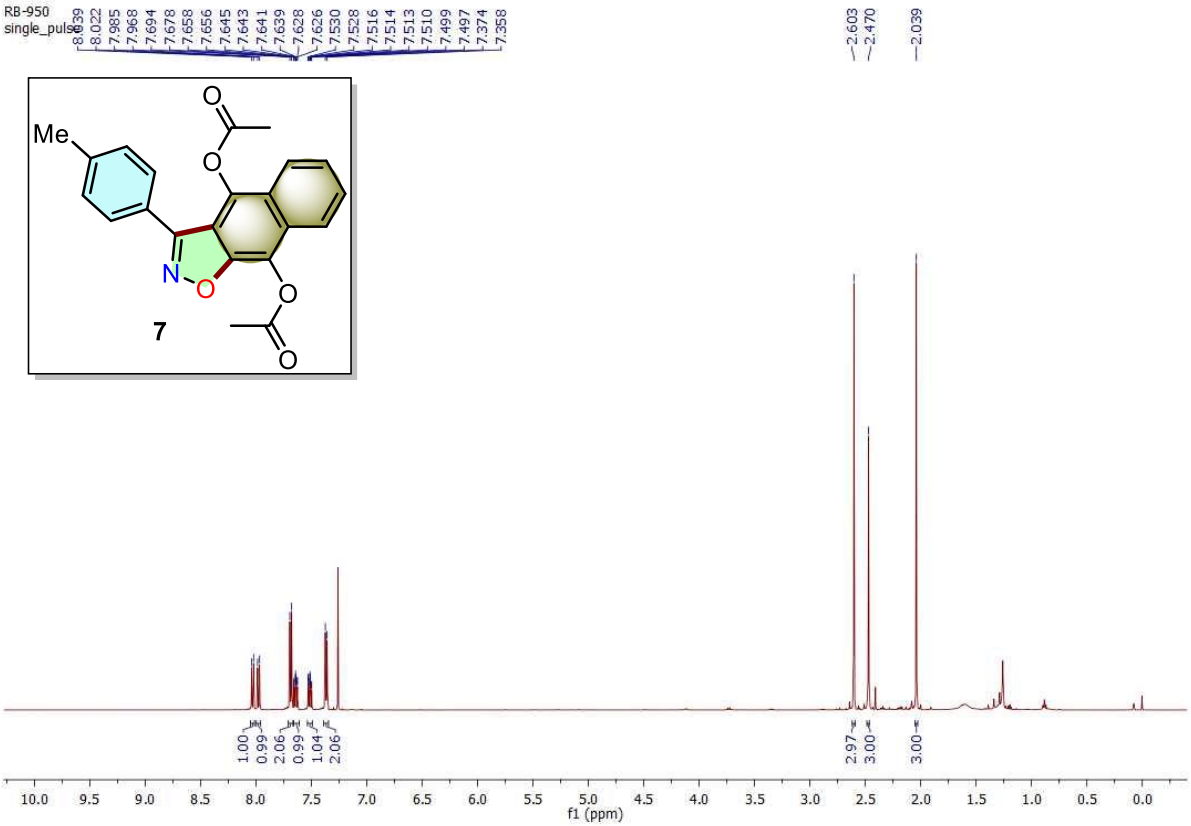
^{1}H NMR Spectrum of **6f** (500 MHz, Chloroform-*d*)



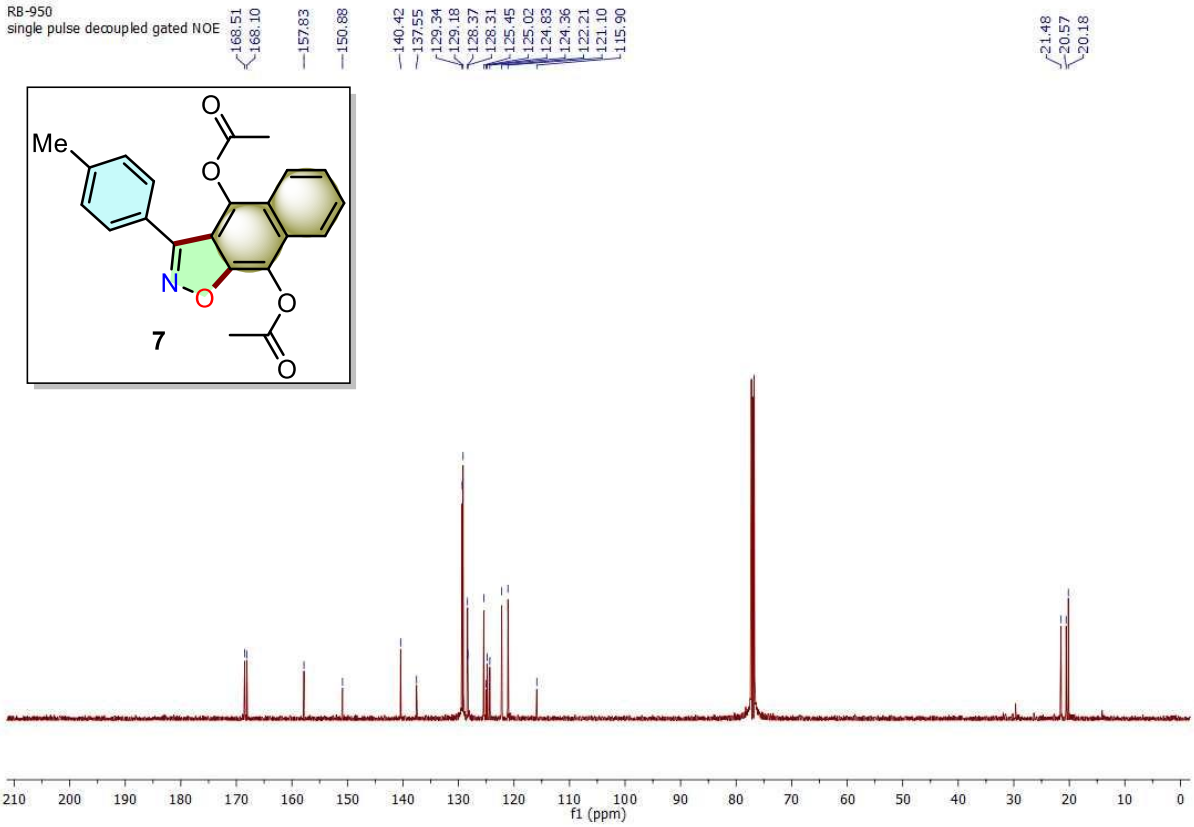
^{13}C NMR Spectrum of **6f** (126 MHz, Chloroform-*d*)



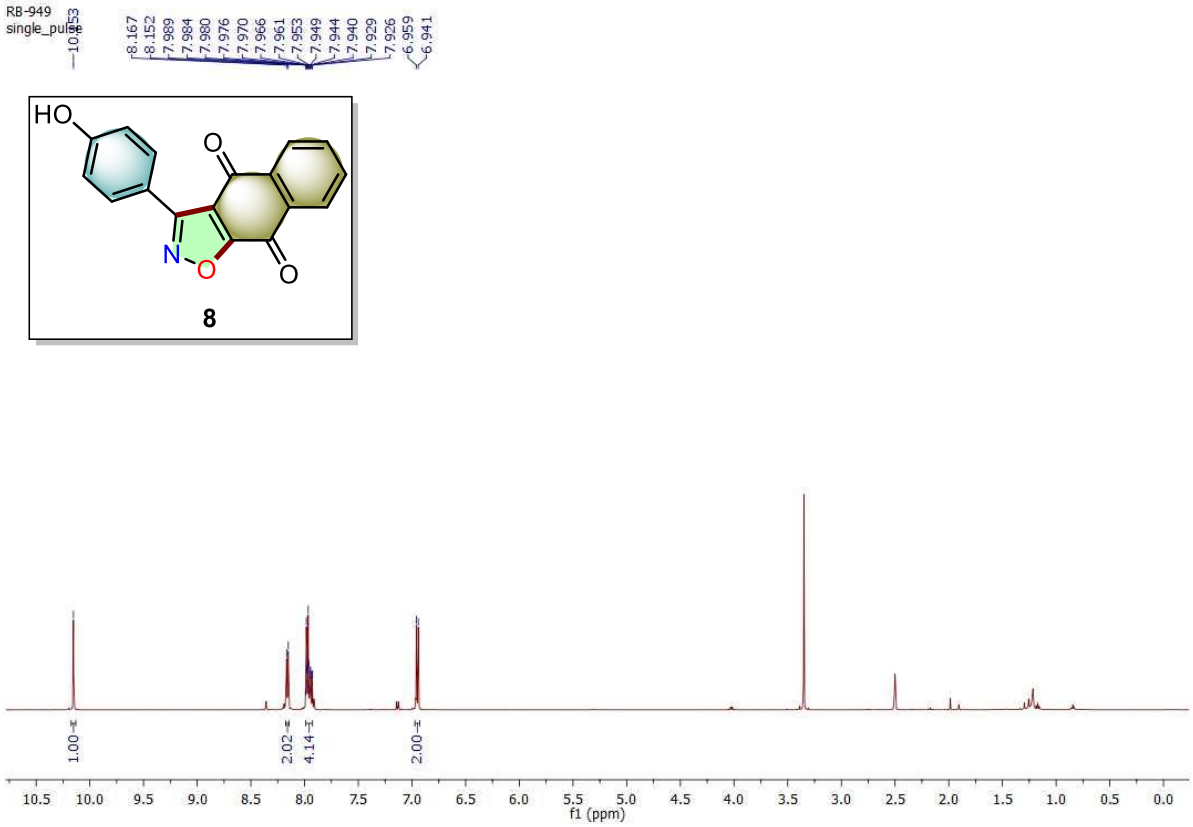
^{1}H NMR Spectrum of **7** (500 MHz, Chloroform-*d*)



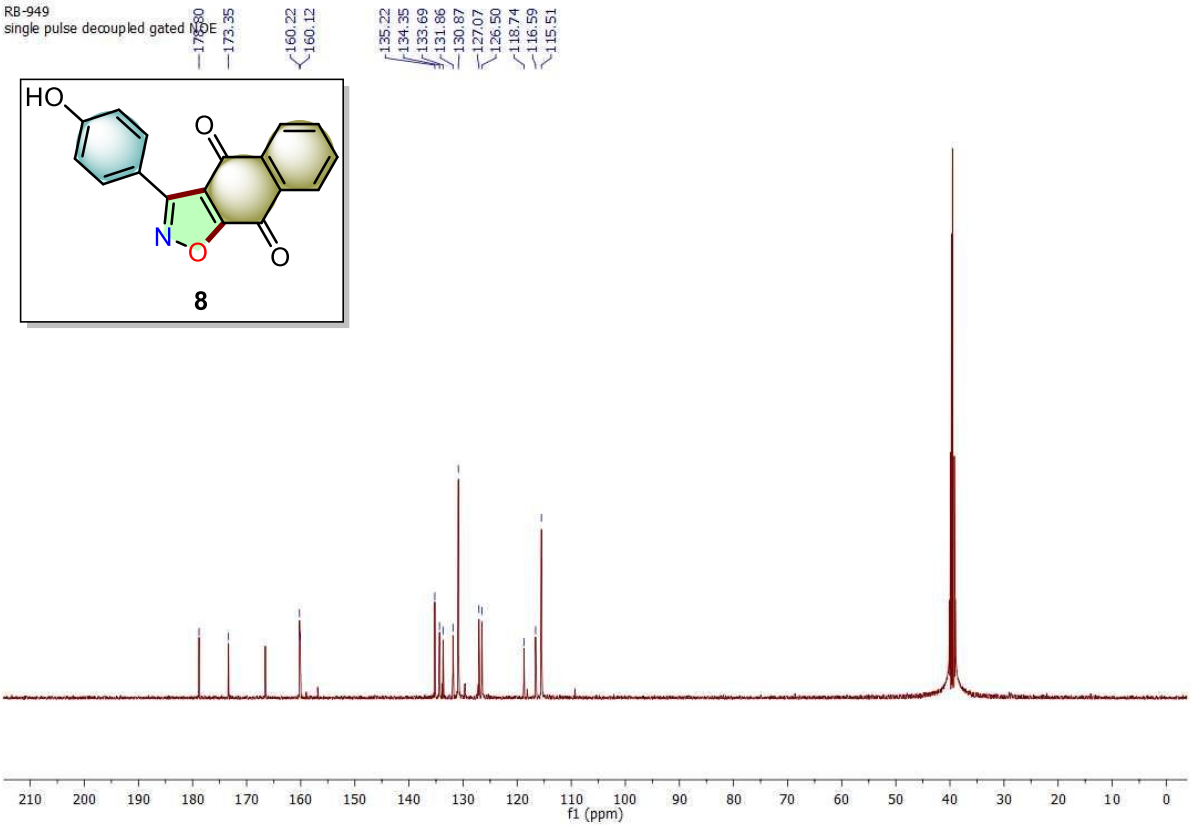
^{13}C NMR Spectrum of **7** (126 MHz, Chloroform-*d*)



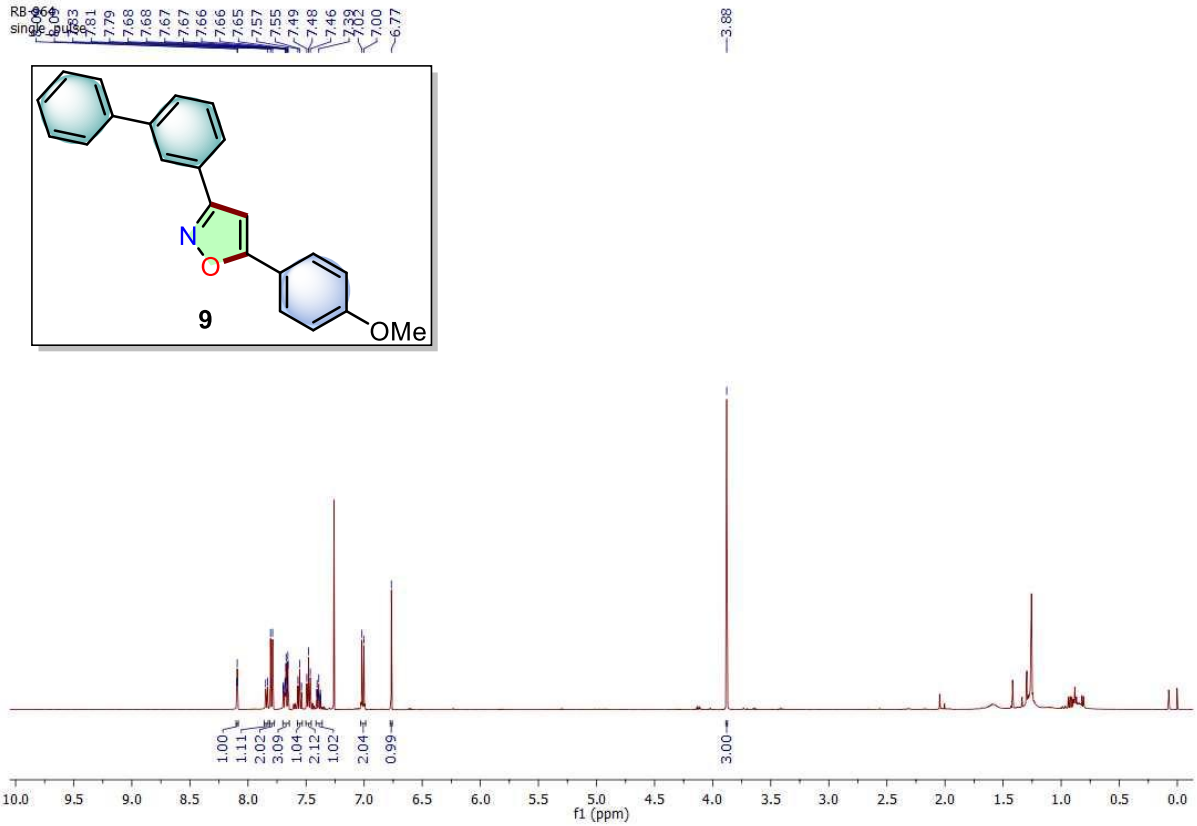
^{1}H NMR Spectrum of **8** (500 MHz, DMSO-d_6)



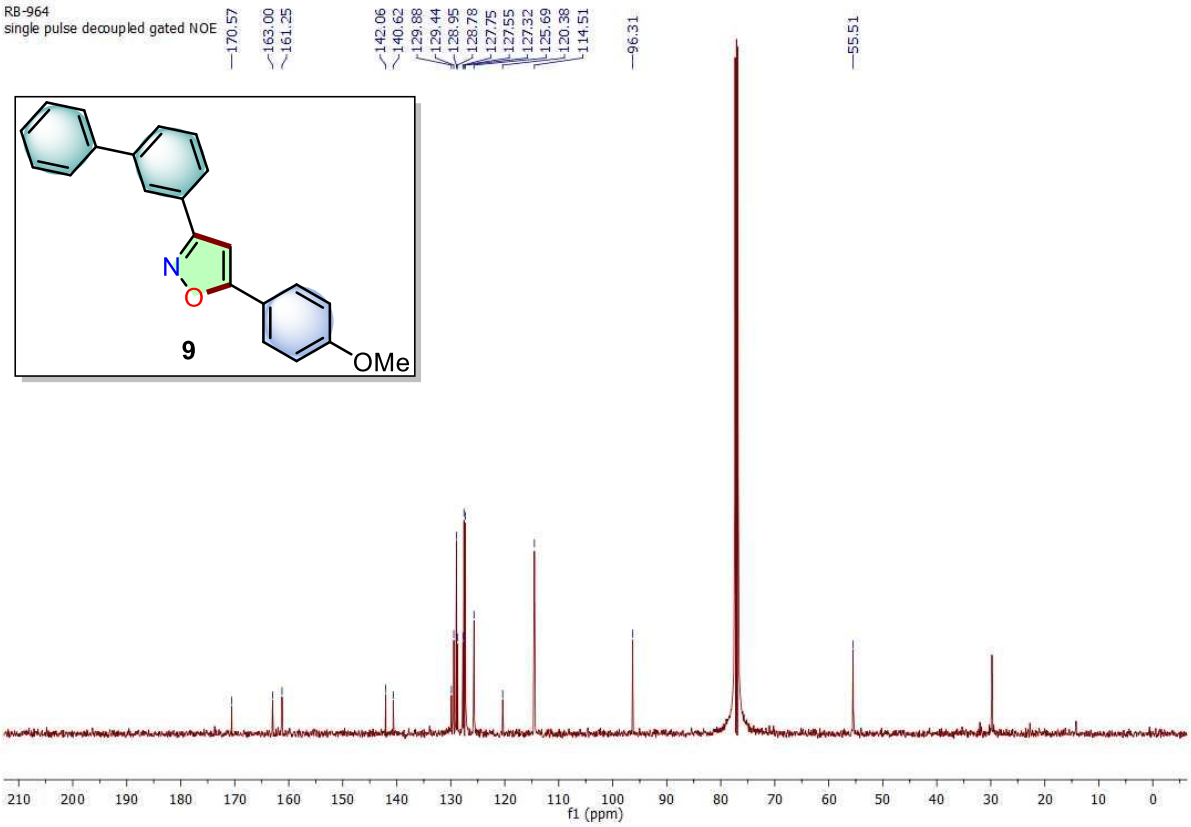
^{13}C NMR Spectrum of **8** (126 MHz, DMSO-d_6)



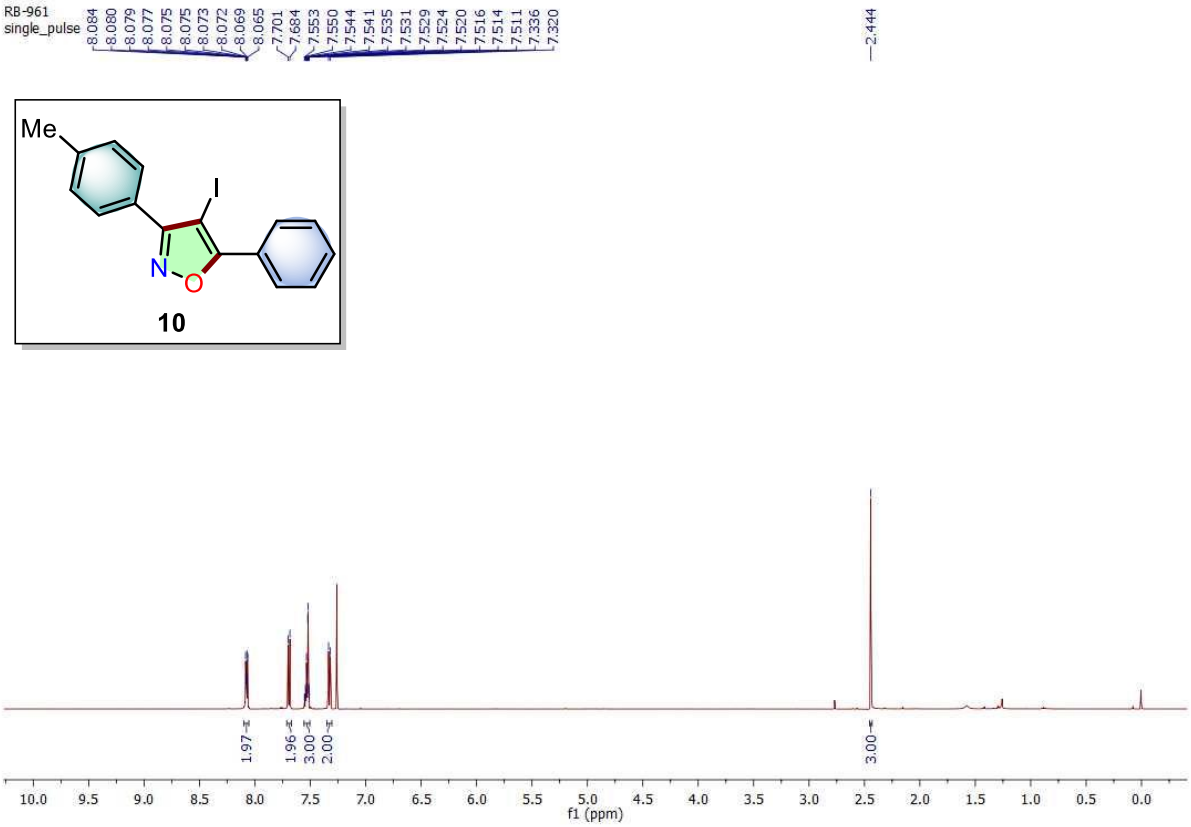
^{1}H NMR Spectrum of **9** (500 MHz, Chloroform-*d*)



^{13}C NMR Spectrum of **9** (126 MHz, Chloroform-*d*)



^{1}H NMR Spectrum of **10** (500 MHz, Chloroform-*d*)



^{13}C NMR Spectrum of **10** (126 MHz, Chloroform-*d*)