

*Supplementary Information*

*for*

**A bench stable *N*-trifluoroacetylnitrene equivalent  
for a simple synthesis of 2-trifluoromethyloxazoles**

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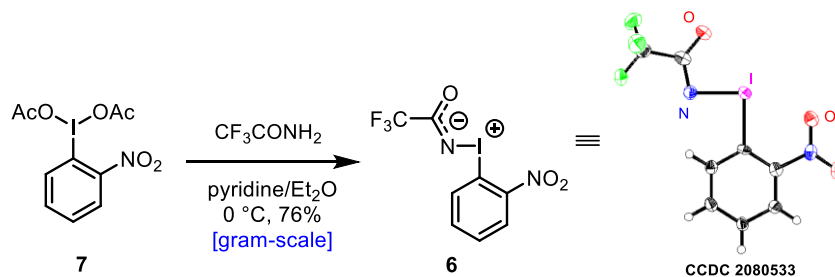
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## 1. General information

Solvents and materials were obtained from commercial suppliers and used without further purification. Analytical thin-layer chromatography was performed using Silica gel 60 plates (Merck, Darmstadt, Germany). Silica gel column chromatography was performed using Kanto silica gel 60 (particle size 63–210  $\mu\text{m}$ , Kanto, Tokyo, Japan) and Chromatorex BW-300 (Fuji silysia, Aichi, Japan). Proton nuclear magnetic resonance ( $^1\text{H}$  NMR) spectra were recorded on JNM-AL 400 (JEOL) at 400 MHz or Avance I 600 (Bruker Biospin AG, Switzerland) at 600 MHz. Chemical shifts were reported relative to  $\text{Me}_4\text{Si}$  ( $\delta$  0.00) in  $\text{CDCl}_3$ . Multiplicity was indicated by one or more of the following: s (singlet); d (doublet); t (triplet); q (quartet); m (multiplet); br (broad). Carbon nuclear magnetic resonance ( $^{13}\text{C}$  NMR) spectra were recorded on a JNM-AL 400 at 100 MHz or on an Avance I 600 at 150 MHz. Chemical shifts were reported relative to  $\text{CDCl}_3$  ( $\delta$  77.0). Fluorine nuclear magnetic resonance ( $^{19}\text{F}$  NMR) spectra were recorded on a JNM-AL 400 at 376 MHz. Infrared spectra were recorded on a FT/IR-4100 Fourier-transform infrared spectrometer (JASCO, Tokyo, Japan) ATR (attenuated total reflectance). High resolution mass spectra were recorded on a LCMS-IT-TOF (Shimadzu, Kyoto, Japan) for ESI-MS. All melting points were measured on BÜCHI M-565 melting point apparatus and are uncorrected.

## 2. Preparation of iminoiodinane 6



To a solution of trifluoroacetamide (1.1 g, 10 mmol) in pyridine/ether (13 mL, ca. 54v/v% pyridine in ether) was added 2-nitroiodobenzene diacetate **7**<sup>S1</sup> (1.8 g, 5.0 mmol) at  $0\text{ }^\circ\text{C}$ . After being stirred at the same temperature for 12 hours, the precipitate was collected by filtration and washed with ether several times to give desired iminoiodinane **6** (1.36 g, 76%).

Yellow solid; m.p.  $117\text{--}119\text{ }^\circ\text{C}$  ( $\text{CHCl}_3$ );  $^1\text{H}$ -NMR (300 MHz, DMSO)  $\delta$ : 8.54 (1H, dd,  $J = 8.2, 1.4$  Hz), 8.07 (1H, ddd,  $J = 8.4, 7.2, 1.5$  Hz), 7.96 – 7.81 (m, 2H);  $^{13}\text{C}$  NMR (75 MHz, DMSO)  $\delta$  165.70 (q,  $J = 32.0$  Hz), 145.81, 137.79, 132.13, 130.11, 127.84, 115.48 (q,  $J = 288.8$  Hz), 108.27;  $^{19}\text{F}$ -NMR (282 MHz, DMSO)  $\delta$ :  $-68.09$ ; FAB-HRMS Calcd. for  $\text{C}_8\text{H}_5\text{F}_3\text{IN}_2\text{O}_3$   $[\text{M}+\text{H}]^+$  360.9297; Found: 360.9301; IR (ATR) 1512, 1319, 1183, 1126  $\text{cm}^{-1}$ .

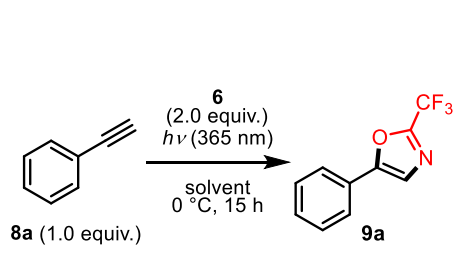
Single crystals of imoiniodinane **6** (CCDC 2080533) were obtained by recrystallization from CHCl<sub>3</sub>. A suitable crystal was selected and loop on a XtaLAB AFC11 (RCD3): quarter-chi single diffractometer. The crystal was kept at 93 K during data collection. Using Olex2,<sup>S2</sup> the structure was solved with the ShelXT<sup>S3</sup> structure solution program using Intrinsic Phasing and refined with the ShelXL<sup>S4</sup> refinement package using Least Squares minimization.

**Table S1.** Crystal data and structure refinement for imoiniodinane **6**

Empirical formula	C <sub>8</sub> H <sub>4</sub> F <sub>3</sub> IN <sub>2</sub> O <sub>3</sub>
Formula weight	360.03
Temperature/K	93
Crystal system	monoclinic
Space group	P2 <sub>1</sub> /c
a/Å	4.9637(2)
b/Å	20.0442(7)
c/Å	10.3335(4)
α/°	90
β/°	101.298(4)
γ/°	90
Volume/Å <sup>3</sup>	1008.19(7)
Z	4
ρ calcg/cm <sup>3</sup>	2.372
μ /mm <sup>-1</sup>	25.461
F(000)	680.0
Crystal size/mm <sup>3</sup>	0.3 × 0.1 × 0.1
Radiation	CuKα (λ = 1.54184)
2θ range for data collection/°	8.824 to 146.52
Index ranges	-4 ≤ h ≤ 5, -24 ≤ k ≤ 22, -12 ≤ l ≤ 12
Reflections collected	9201
Independent reflections	1959 [Rint = 0.0469, Rsigma = 0.0259]
Data/restraints/parameters	1959/0/154
Goodness-of-fit on F <sup>2</sup>	1.118
Final R indexes [I ≥ 2σ (I)]	R1 = 0.0641, wR2 = 0.1774
Final R indexes [all data]	R1 = 0.0650, wR2 = 0.1789
Largest diff. peak/hole / e Å <sup>-3</sup>	3.50/-3.62

### 3. Effect of solvent and equivalent of iodine

**Table S2.** Effect of solvent for the [3+2] cyclization of alkyne with iodine



entry	iminoiodinane	solvent	yield <sup>a</sup>
1	<b>5</b>	CH <sub>2</sub> Cl <sub>2</sub>	41%
2	<b>6</b>	CH <sub>2</sub> Cl <sub>2</sub>	56% <sup>b</sup>
3 <sup>c</sup>	<b>6</b>	CH <sub>2</sub> Cl <sub>2</sub>	28% <sup>b</sup>
4	<b>6</b>	MeCN	21%
5	<b>6</b>	THF	trace
6	<b>6</b>	MeNO <sub>2</sub>	0%

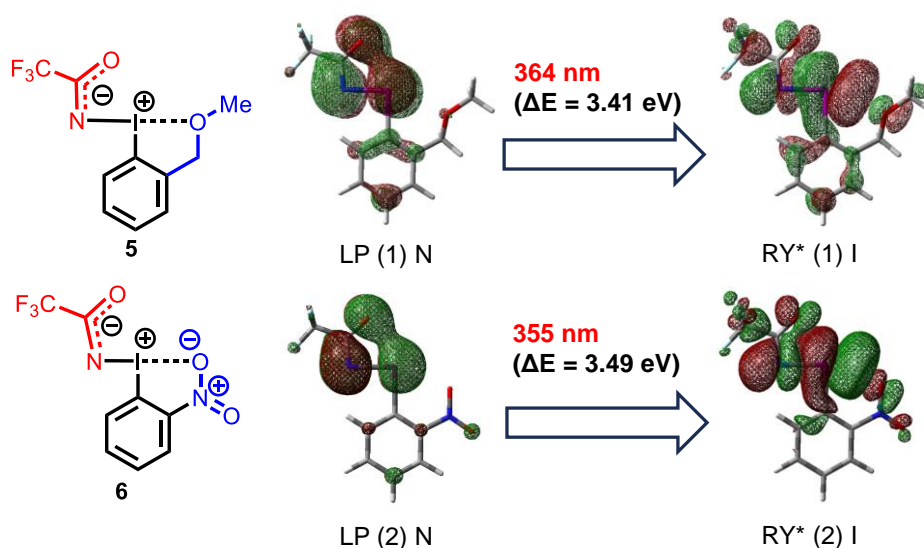
<sup>a</sup> Unless otherwise noted <sup>19</sup>F NMR yield was indicated using 3-(trifluoromethyl)benzoic acid as internal standard.

<sup>b</sup> Isolated yield. <sup>c</sup> 1.0 equiv of **6** was employed.

When one equivalent of iodine **6** was employed, the yield of **9a** decreased significantly (entry 3, Table S2), presumably due to the partial decomposition of iodine **6**. Among the solvents screened, the use of dichloromethane resulted in the best yield (entry 2 vs entries 4-6, Table S2).

### 4. DFT-TD experiments

As similarly as our previous report,<sup>S5</sup> we calculated the excitation energy of iodine **6** using a time-dependent density functional theory (DFT-TD)<sup>S6</sup> method at the B3LYP/6-31G(d,p) level, based on the optimized X-ray structure, using the Gaussian 09 program.<sup>S7</sup> The basis sets implemented in the program were used, and the DGDZVP basis set was used for iodine.<sup>S8</sup> As a result, the energy gap between the highest occupied molecular orbital (HOMO) and Rydberg orbital (RY\* (2) I) of **6** corresponded to the 355 nm wavelength (Figure S1).



**Figure S1.** DFT-TD experiments of iminoiodinane **5** and **6**

## 5. NBO analyses of iodine 5

The natural bond orbital (NBO) analyses of the intramolecular XB interaction were estimated to be 7.99 kcal/mol (the oxygen atom of the *N*-trifluoroacetyl group and the iodine atom, Figure S2A) and 8.50 kcal/mol (the oxygen atom of the nitro group and the iodine atom, Figure S2B). No intermolecular XB interaction was found in iminoiodine 5.

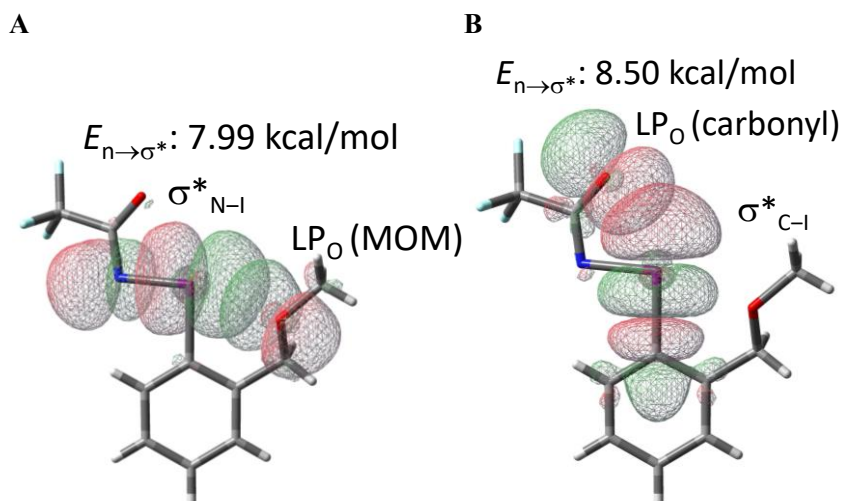
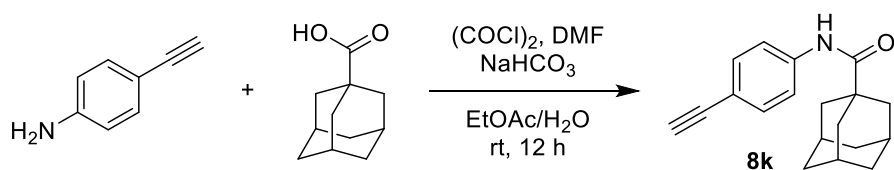


Figure S2. NBO analyses of iodine 5

## 6. Preparation of alkynes

Alkynes **8a–j** and *p*-ethynylaniline were purchased from Tokyo Chemical Industry Co., Ltd. Alkyne **8k** was prepared as described below.

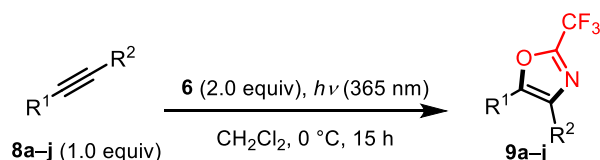


To a stirred solution of 1-adamantanecarboxylic acid (2.15 g, 11.95 mmol) in EtOAc (20 mL) was added oxalyl chloride (0.97 mL, 11.10 mmol) followed by a few drops of DMF (66  $\mu$ L, 0.85 mmol) at room temperature, and the reaction mixture was stirred at rt for 3 h (**solution A**). In another flask, *p*-ethynylaniline (1.00 g, 8.54 mmol) was dissolved in EtOAc (20 mL), and saturated aqueous bicarbonate solution (20 mL) was added. To a vigorously stirred bi-phase mixture, was added **solution A**, as described above, and the whole mixture was stirred for 12 hours. The organic phase was separated, washed with 1N HCl (20 mL) and saturated aqueous bicarbonate solution (20 mL). The

organic layer was dried over Na<sub>2</sub>SO<sub>4</sub> and evaporated to afford the crude solid, which was recrystallized from CH<sub>2</sub>Cl<sub>2</sub>/*n*-hexane to afford the pure anilides **8h** (1.46 g, 61%).

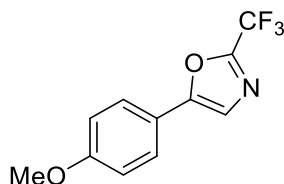
Colorless needles; m.p. 173–174°C (CH<sub>2</sub>Cl<sub>2</sub>/*n*-hexane); <sup>1</sup>H-NMR (500 MHz, CDCl<sub>3</sub>) δ: 7.52 (2H, d, *J* = 8.4 Hz), 7.44 (2H, d, *J* = 8.4 Hz, 2H), 7.33 (1H, brs), 3.04 (1H, s), 2.13–2.08 (3H, m), 1.96 (6H, m), 1.82–1.70 (6H, m); <sup>13</sup>C-NMR (126 MHz, CDCl<sub>3</sub>) δ: 176.2, 138.6, 132.9, 119.6, 117.4, 83.5, 76.7, 41.6, 39.2, 36.4, 28.1; EI-HRMS Calcd. for C<sub>19</sub>H<sub>21</sub>NO [M]<sup>+</sup> 279.1623; Found: 279.1623; IR (ATR) 3288, 2900, 1655 cm<sup>-1</sup>.

## 7. General procedure for photo-induced formal [3+2]-cyclization of alkynes with iminoiodinanes



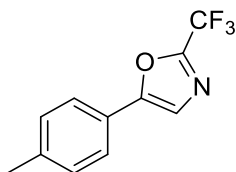
Alkyne **8b** (13.2 mg, 0.10 mmol) and iminoiodinane **6** (72.0 mg, 0.20 mmol) were dissolved in dichloromethane (1.0 mL) and the reaction mixture was stirred at 0 °C for 15 hours under UV light ( $\lambda = 365$  nm) irradiation. After concentration under reduced pressure, the reaction mixture was directly purified by flash column chromatography on silica gel (eluent: CHCl<sub>3</sub>) to give oxazole **9b** (17.4 mg, 71%).

### 5-(4-Methoxyphenyl)-2-(trifluoromethyl)oxazole (**9b**)



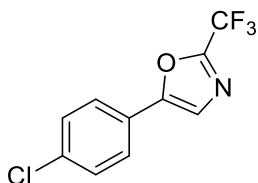
From 13.2 mg (0.10 mmol) of **8b**, 17.4 mg (71%) of **9b** was obtained as colorless oil; <sup>1</sup>H-NMR (600 MHz, CDCl<sub>3</sub>) δ: 7.63 (2H, d, *J* = 8.8 Hz), 7.32 (1H, s), 6.98 (2H, d, *J* = 8.8 Hz), 3.86 (3H, s); <sup>13</sup>C-NMR (150 MHz, CDCl<sub>3</sub>) δ: 160.9, 154.1, 149.2 (q, *J* = 43.9 Hz), 126.5, 120.9, 119.0, 116.6 (q, *J* = 270.0 Hz), 114.6; <sup>19</sup>F-NMR (376 MHz, CDCl<sub>3</sub>) δ: -65.49; ESI-HRMS Calcd. for C<sub>11</sub>H<sub>9</sub>F<sub>3</sub>NO<sub>2</sub> [M+H]<sup>+</sup> 244.0580; Found: 244.0585; IR (ATR) 1150 cm<sup>-1</sup>.

### 5-(*p*-Tolyl)-2-(trifluoromethyl)oxazole (**9c**)



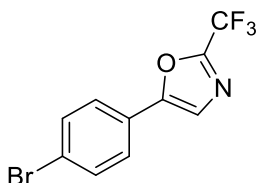
From 11.6 mg (0.10 mmol) of **8c**, 11.4 mg (50%) of **9c** was produced as Colorless oil;  $^1\text{H-NMR}$  (600 MHz,  $\text{CDCl}_3$ )  $\delta$ : 7.58 (2H, d,  $J = 7.7$  Hz), 7.39 (1H, s), 7.27 (2H, d,  $J = 8.2$  Hz), 2.40 (3H, s);  $^{13}\text{C-NMR}$  (150 MHz,  $\text{CDCl}_3$ )  $\delta$ : 154.2, 149.5 (q,  $J = 43.9$  Hz), 140.2, 129.8, 124.9, 123.5, 121.7, 116.6 (q,  $J = 270.4$  Hz), 21.4;  $^{19}\text{F-NMR}$  (376 MHz,  $\text{CDCl}_3$ )  $\delta$ : -65.55; ESI-HRMS Calcd. for  $\text{C}_{11}\text{H}_9\text{F}_3\text{NO}$   $[\text{M}+\text{H}]^+$  228.0631; Found: 228.0632; IR (ATR) 1149  $\text{cm}^{-1}$ .

#### 5-(4-Chlorophenyl)-2-(trifluoromethyl)oxazole (**9d**)



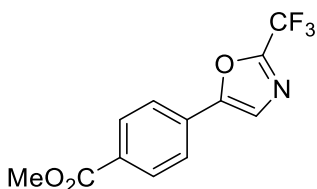
From 13.7 mg (0.10 mmol) of **8d**, 8.6 mg (35%) of **9d** was produced as white solid; m.p. 56.0–57.1  $^{\circ}\text{C}$  ( $\text{CHCl}_3$ );  $^1\text{H-NMR}$  (600 MHz,  $\text{CDCl}_3$ )  $\delta$ : 7.64 (2H, d,  $J = 8.8$  Hz), 7.46–7.45 (3H, m);  $^{13}\text{C-NMR}$  (150 MHz,  $\text{CDCl}_3$ )  $\delta$ : 152.9, 150.0 (q,  $J = 43.9$  Hz), 136.0, 129.5, 126.2, 124.7, 122.7, 116.5 (q,  $J = 270.4$  Hz);  $^{19}\text{F-NMR}$  (376 MHz,  $\text{CDCl}_3$ )  $\delta$ : -65.55; ESI-HRMS Calcd. for  $\text{C}_{10}\text{H}_6\text{ClF}_3\text{NO}$   $[\text{M}+\text{H}]^+$  248.0085; Found: 248.0088; IR (ATR) 1138  $\text{cm}^{-1}$ .

#### 5-(4-Bromophenyl)-2-(trifluoromethyl)oxazole (**9e**)



From 18.1 mg (0.10 mmol) of **8e**, 16.0 mg (55%) of **9e** was produced as white solid; m.p. 37.8–41.8  $^{\circ}\text{C}$  ( $\text{CHCl}_3$ );  $^1\text{H-NMR}$  (600 MHz,  $\text{CDCl}_3$ )  $\delta$ : 7.61 (2H, d,  $J = 8.8$  Hz), 7.57 (2H, d,  $J = 8.8$  Hz), 7.46 (1H, s);  $^{13}\text{C-NMR}$  (150 MHz,  $\text{CDCl}_3$ )  $\delta$ : 153.0, 150.0 (q,  $J = 43.9$  Hz), 132.5, 126.3, 125.2, 124.2, 122.8, 116.5 (q,  $J = 270.4$  Hz);  $^{19}\text{F-NMR}$  (376 MHz,  $\text{CDCl}_3$ )  $\delta$ : -65.55; ESI-HRMS Calcd. for  $\text{C}_{10}\text{H}_6\text{BrF}_3\text{NO}$   $[\text{M}+\text{H}]^+$  291.9579; Found: 291.9592; IR (ATR) 1139  $\text{cm}^{-1}$ .

#### Methyl 4-(2-(trifluoromethyl)oxazol-5-yl)benzoate (**9f**)

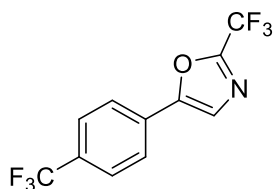


From 16.0 mg (0.10 mmol) of **8f**, 11.1 mg (41%) of **9f** was obtained as white solid; m.p. 95.9–97.2  $^{\circ}\text{C}$  ( $\text{CHCl}_3$ );  $^1\text{H-NMR}$  (600 MHz,  $\text{CDCl}_3$ )  $\delta$ : 8.14 (2H, d,  $J = 8.8$  Hz), 7.78 (2H, d,  $J = 8.2$  Hz), 7.57 (1H,



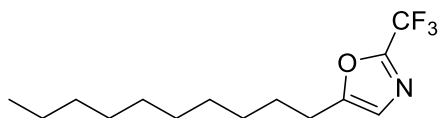
s), 3.96 (3H, s);  $^{13}\text{C}$ -NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$ : 166.2, 152.9, 150.5 (q,  $J = 44.3$  Hz), 131.2, 130.4, 130.1, 124.7, 124.0, 116.4 (q,  $J = 270.8$  Hz), 52.4;  $^{19}\text{F}$ -NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$ : -65.58; ESI-HRMS Calcd. for  $\text{C}_{12}\text{H}_9\text{F}_3\text{NO}_3$   $[\text{M}+\text{H}]^+$  272.0529; Found: 272.0516; IR (ATR) 1710, 1140  $\text{cm}^{-1}$ .

#### 2-(Trifluoromethyl)-5-(4-(trifluoromethyl)phenyl)oxazole (9g)



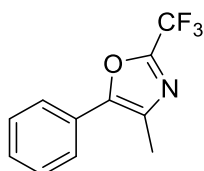
From 85.0 mg (0.50 mmol) of **8g** and 36.0 mg (0.10 mmol) of **6**, 17.4 mg (62% based on **6**) of **9g** was produced as white solid; m.p. 48.1–49.3 °C ( $\text{CHCl}_3$ );  $^1\text{H}$ -NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$ : 7.83 (2H, d,  $J = 8.2$  Hz), 7.74 (2H, d,  $J = 8.2$  Hz), 7.57 (1H, s);  $^{13}\text{C}$ -NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$ : 152.5, 150.6 (q,  $J = 44.3$  Hz), 131.7 (q,  $J = 33.3$  Hz), 129.5, 126.2 (q,  $J = 3.7$  Hz), 125.2, 124.0, 123.6 (q,  $J = 270.8$  Hz), 116.4 (q,  $J = 270.0$  Hz);  $^{19}\text{F}$ -NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$ : -62.87, -65.61; ESI-HRMS Calcd. for  $\text{C}_{11}\text{H}_4\text{F}_6\text{NO}$   $[\text{M}-\text{H}]^-$  280.0203; Found: 280.0201; IR (ATR) 1137  $\text{cm}^{-1}$ .

#### 5-Decyl-2-(trifluoromethyl)oxazole (9h)



From 83.2 mg (0.50 mmol) of **8h** and 36.0 mg (0.10 mmol) of **6**, 7.0 mg (25% based on **6**) of **9h** was produced as colorless oil;  $^1\text{H}$ -NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$ : 6.89 (1H, s), 2.71 (2H, t,  $J = 7.7$  Hz), 1.70–1.65 (2H, m), 1.35–1.28 (14H, m), 0.88 (3H, t,  $J = 7.1$  Hz);  $^{13}\text{C}$ -NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$ : 156.3, 149.6 (q,  $J = 42.8$  Hz), 123.4, 116.5 (q,  $J = 270.0$  Hz), 31.9, 29.5, 29.4, 29.3, 29.1, 29.0, 27.2, 25.4, 22.7, 14.1;  $^{19}\text{F}$ -NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$ : -65.79; ESI-HRMS Calcd. for  $\text{C}_{14}\text{H}_{23}\text{F}_3\text{NO}$   $[\text{M}+\text{H}]^+$  278.1726; Found: 278.1734; IR (ATR) 1137  $\text{cm}^{-1}$ .

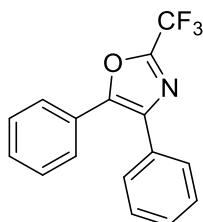
#### 4-Methyl-5-phenyl-2-(trifluoromethyl)oxazole (9i)



From 11.6 mg (0.10 mmol) of **8i**, 10.8 mg (48%) of **9i** was produced as colorless oil;  $^1\text{H}$ -NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$ : 7.65 (2H, d,  $J = 7.7$  Hz), 7.49 (2H, t,  $J = 8.0$  Hz), 7.41 (1H, t,  $J = 7.4$  Hz), 2.49 (3H, s);  $^{13}\text{C}$ -NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$ : 148.2 (q,  $J = 43.9$  Hz), 148.2, 132.7, 129.0, 129.0, 127.4, 126.0,

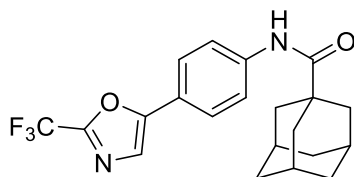
116.6 (q,  $J = 270.4$  Hz), 13.1;  $^{19}\text{F}$ -NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$ : -65.67; ESI-HRMS Calcd. for  $\text{C}_{11}\text{H}_9\text{F}_3\text{NO}$   $[\text{M}+\text{H}]^+$  228.0631; Found: 228.0633; IR (ATR)  $1154\text{ cm}^{-1}$ .

#### 4,5-Diphenyl-2-(trifluoromethyl)oxazole (9j)



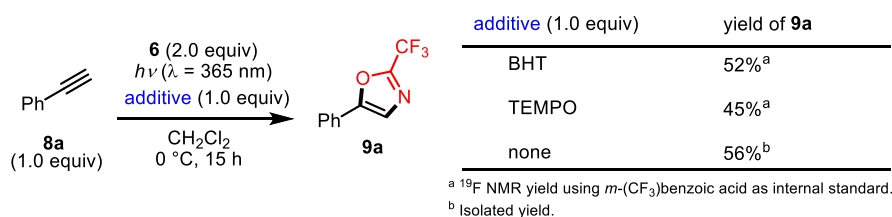
From 17.8 mg (0.10 mmol) of **8j** 12.1 mg (42%) of **9j** was produced as colorless oil;  $^1\text{H}$ -NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$ : 7.66–7.64 (4H, m), 7.42–7.39 (6H, m);  $^{13}\text{C}$ -NMR (150 MHz,  $\text{CDCl}_3$ )  $\delta$ : 149.2 (q,  $J = 42.8$  Hz), 148.0, 136.0, 130.7, 129.9, 128.9, 128.9, 128.8, 128.0, 127.3, 127.1, 116.6 (q,  $J = 271.1$  Hz);  $^{19}\text{F}$ -NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$ : -65.67; ESI-HRMS Calcd. for  $\text{C}_{16}\text{H}_{12}\text{F}_3\text{NO}$   $[\text{M}+\text{H}]^+$  290.0787; Found: 290.0788; IR (ATR)  $1169\text{ cm}^{-1}$ .

#### *N*-(4-(2-(Trifluoromethyl)oxazol-5-yl)phenyl)adamantane-1-carboxamide (9k)



From 27.9 mg (0.1 mmol) of **8k**, 12.9 mg (33%) of **9k** was obtained as off-white solid; m.p. 136–138 °C ( $\text{CHCl}_3$ )  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$ : 7.68 (2H, d,  $J = 8.8$  Hz), 7.65 (2H, d,  $J = 8.8$  Hz), 7.42 (1H, brs), 7.39 (1H, s), 2.17–2.09 (3H, m), 1.98 (6H, m), 1.80–1.71 (6H, m);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  176.3, 153.7, 149.5 (q,  $J = 44.1$  Hz), 139.6, 125.8, 121.9, 121.7, 120.1, 116.6 (q,  $J = 269.6$  Hz), 41.7, 39.3, 36.4, 28.1;  $^{19}\text{F}$ -NMR (470 MHz,  $\text{CDCl}_3$ )  $\delta$ : -65.58; EI-HRMS Calcd. for  $\text{C}_{21}\text{H}_{21}\text{F}_3\text{N}_2\text{O}_2$   $[\text{M}]^+$  390.1555; Found: 390.1558; IR (ATR) 3319, 2905,  $1655\text{ cm}^{-1}$ .

### 8. Effect of radical scavengers



To a mixture of phenylacetylene **8a** (10.2 mg, 0.10 mmol) and iminoiodinane **6** (72.0 mg, 0.20 mmol) in dichloromethane (1.0 mL) was added 2,6-di-*tert*-butyl-*p*-cresol (BHT, 22.0 mg, 0.10 mmol) or

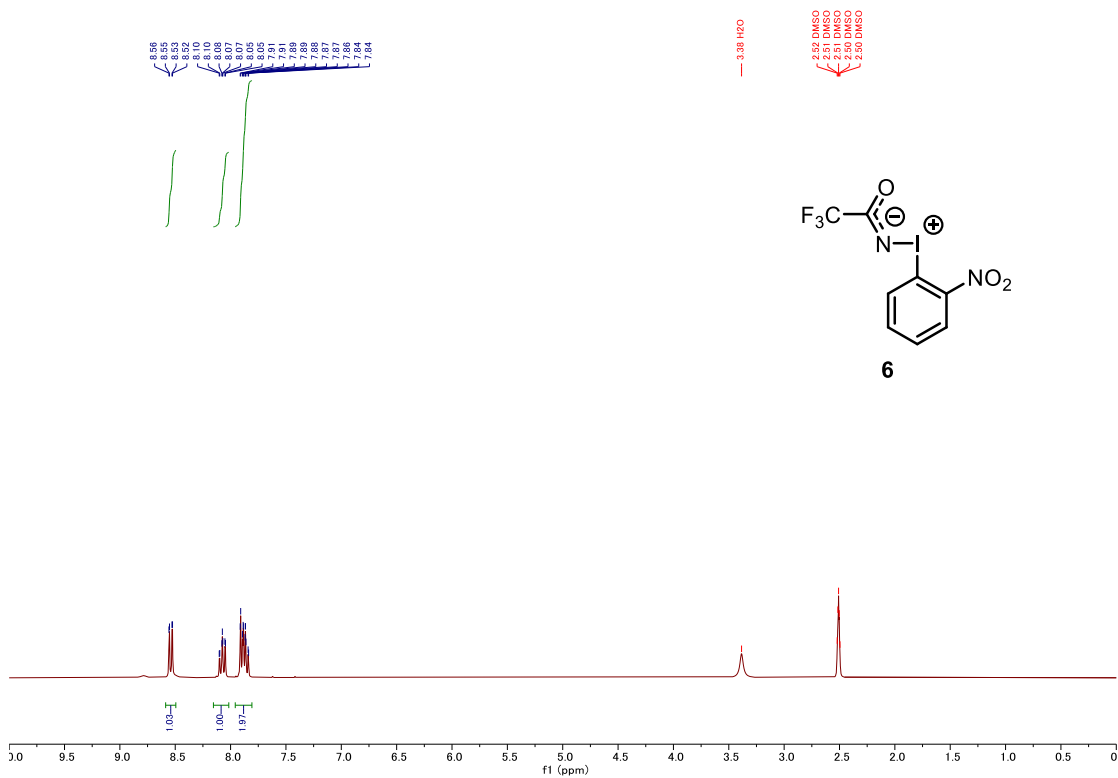
2,2,6,6-tetramethylpiperidine 1-oxyl (TEMPO, 15.6 mg, 0.10 mmol) at the ambient temperature, and the reaction mixture was stirred at 0 °C for 15 hours under UV light ( $\lambda = 365$  nm) irradiation. After concentration of volatiles under reduced pressure,  $^{19}\text{F}$  NMR yields of **9a** were calculated using 3-(trifluoromethyl)benzoic acid as an internal standard.

## 9. References

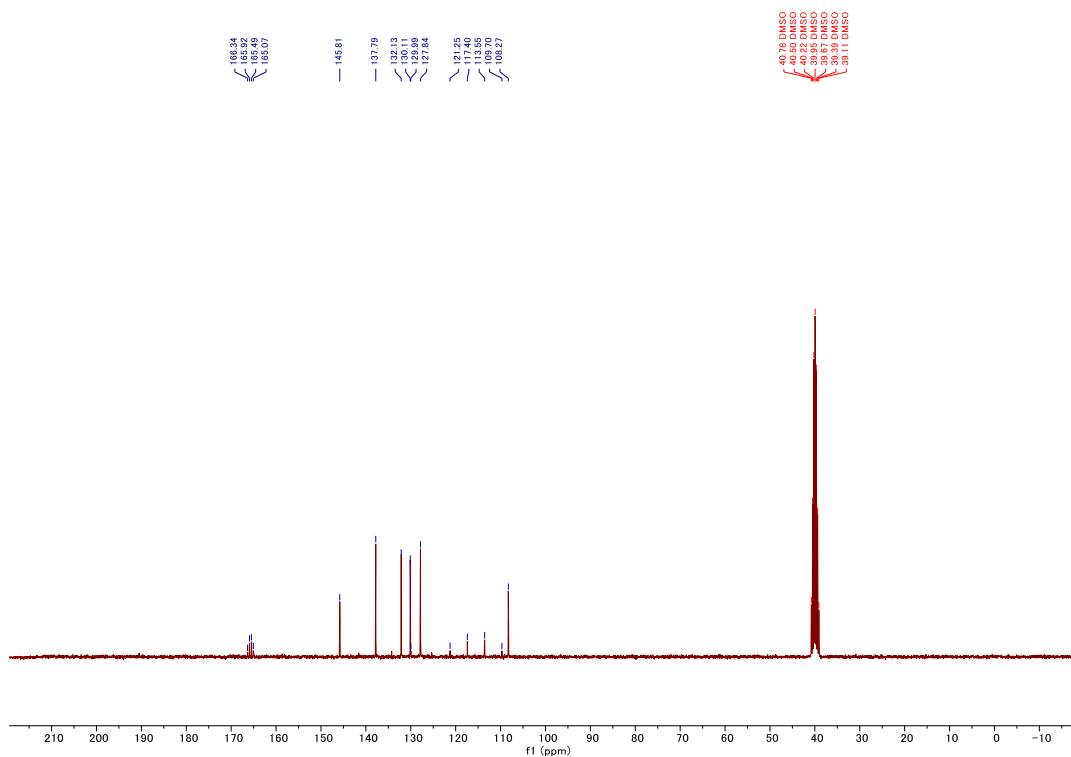
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## 10. Copies of <sup>1</sup>H and <sup>13</sup>C NMR charts

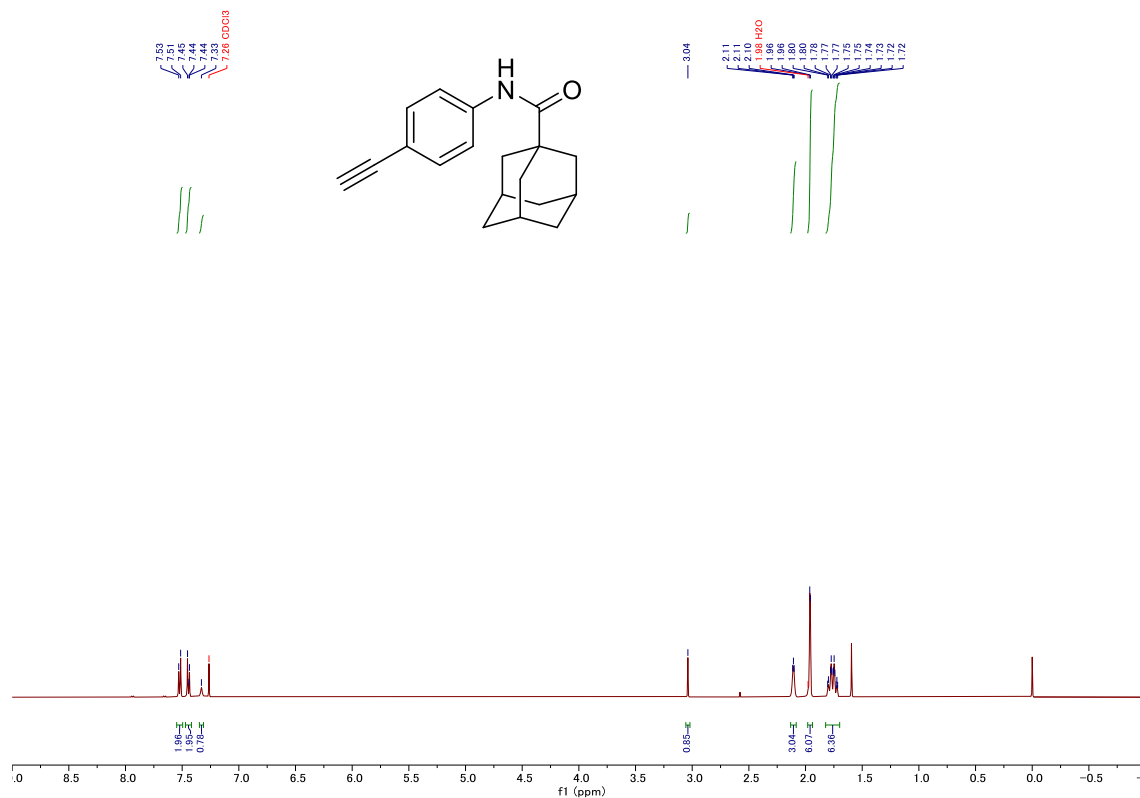
### 6 <sup>1</sup>H-NMR (300 MHz, DMSO)



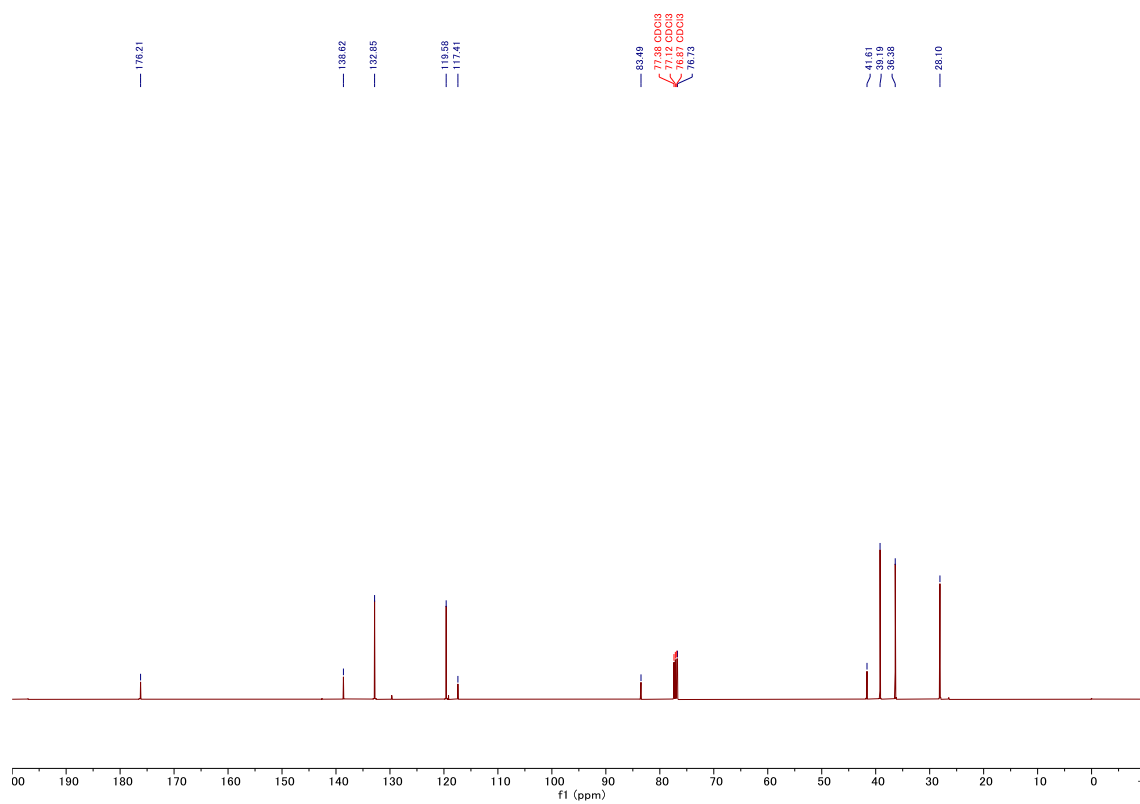
### 6 <sup>13</sup>C-NMR (75 MHz, DMSO)



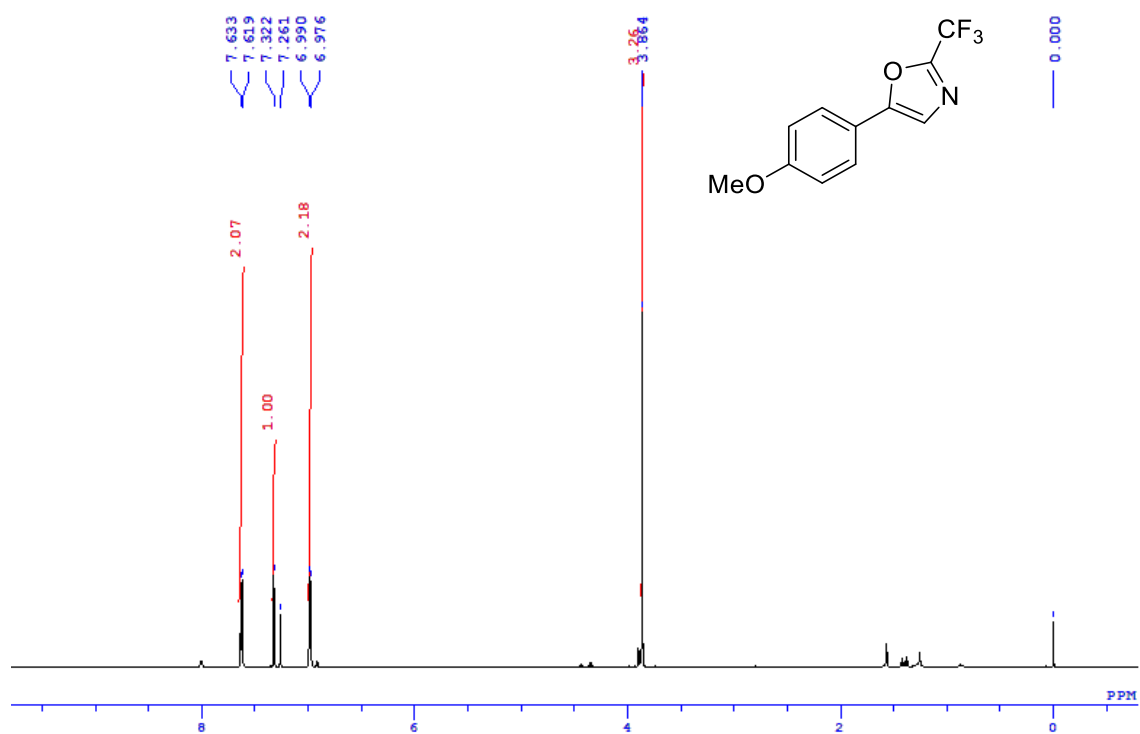
**8k**  $^1\text{H-NMR}$  (500 MHz,  $\text{CDCl}_3$ )



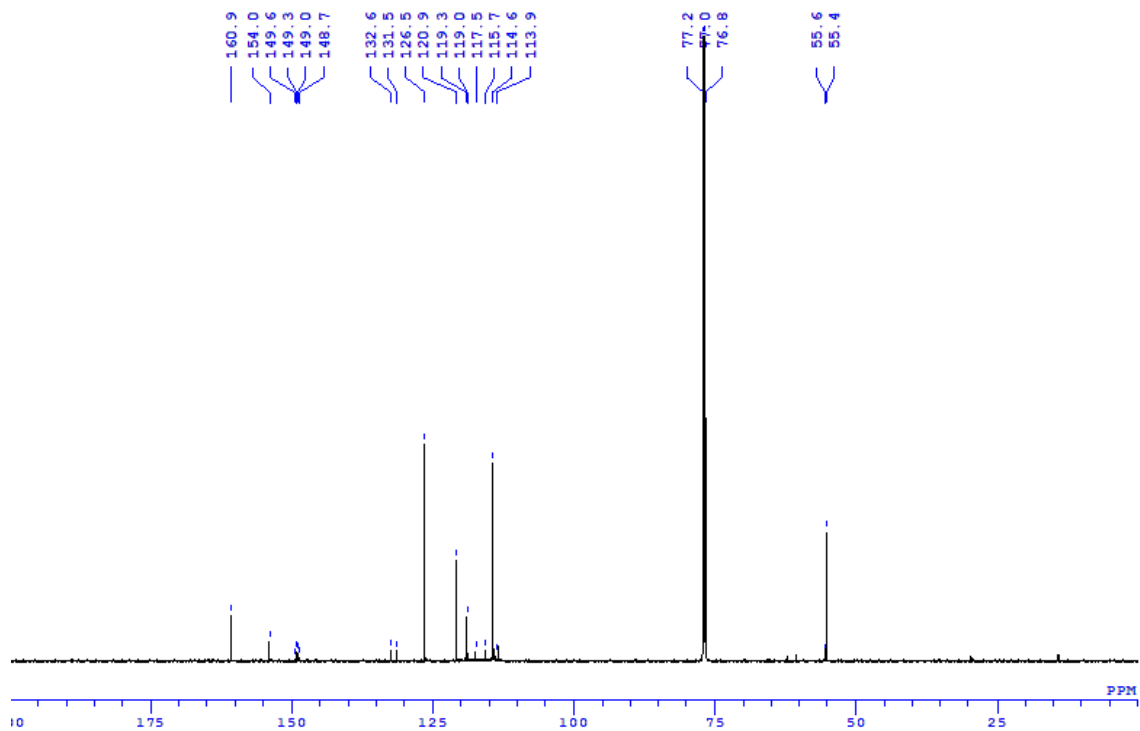
**8k**  $^{13}\text{C-NMR}$  (126 MHz,  $\text{CDCl}_3$ )



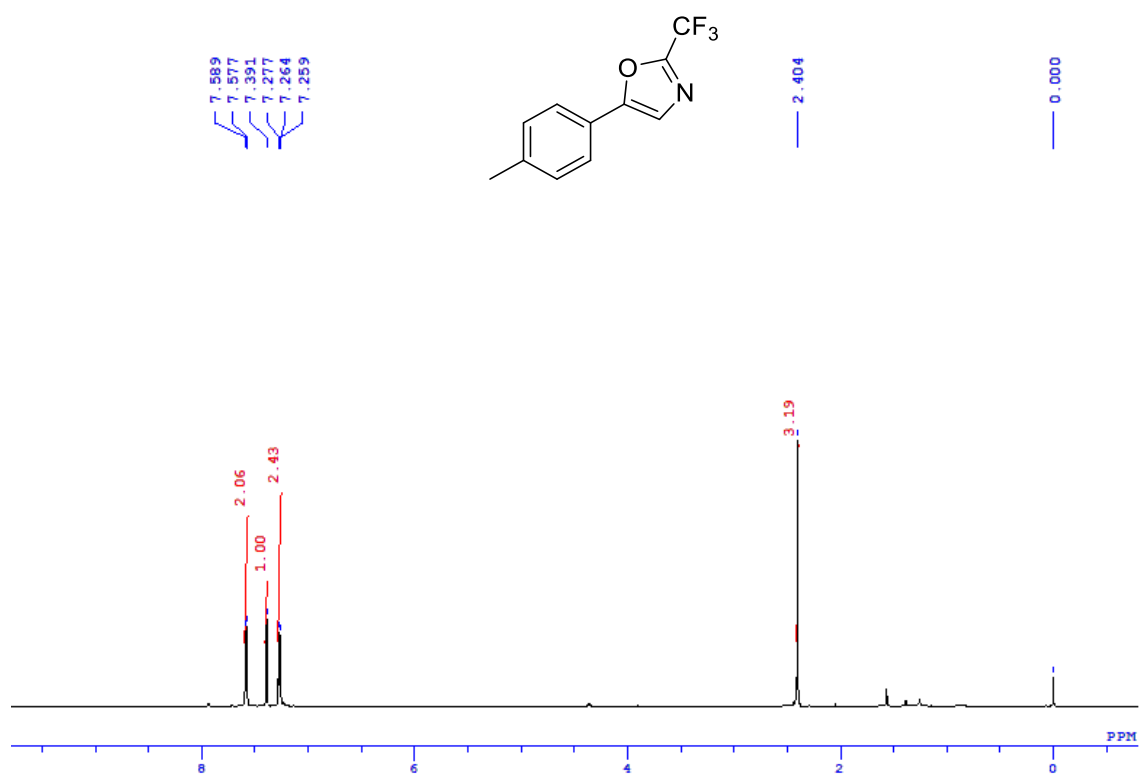
9b <sup>1</sup>H-NMR (600 MHz, CDCl<sub>3</sub>)



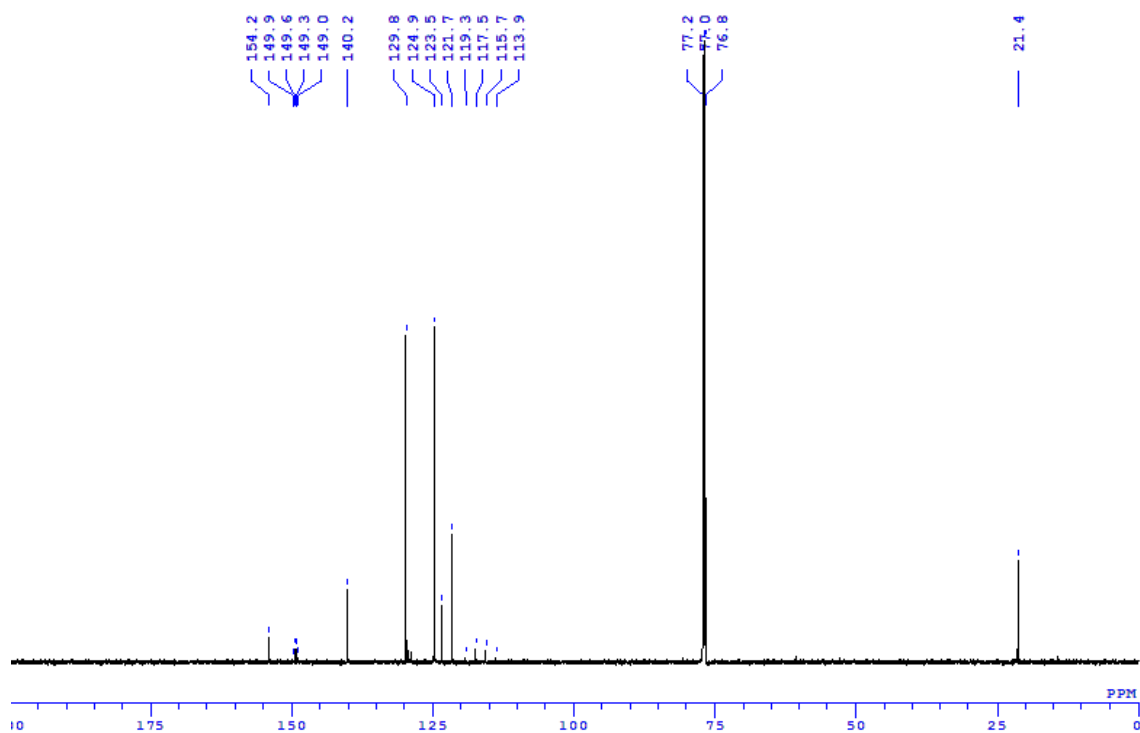
9b <sup>13</sup>C-NMR (150 MHz, CDCl<sub>3</sub>)



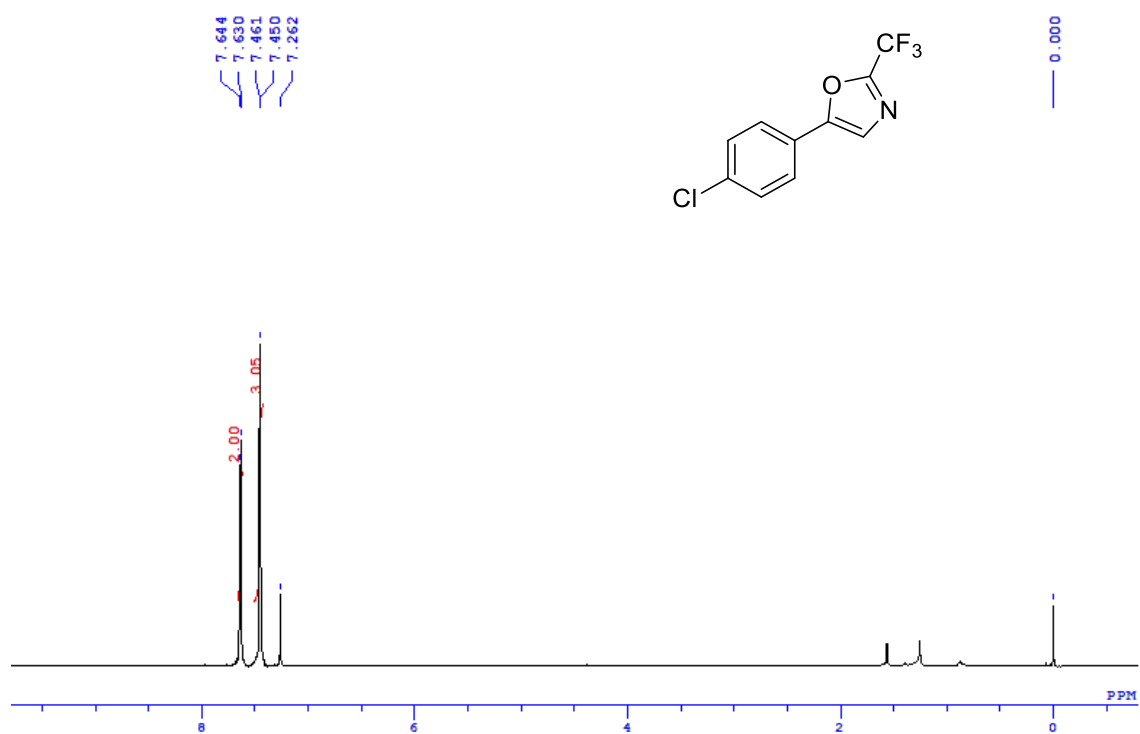
9c <sup>1</sup>H-NMR (600 MHz, CDCl<sub>3</sub>)



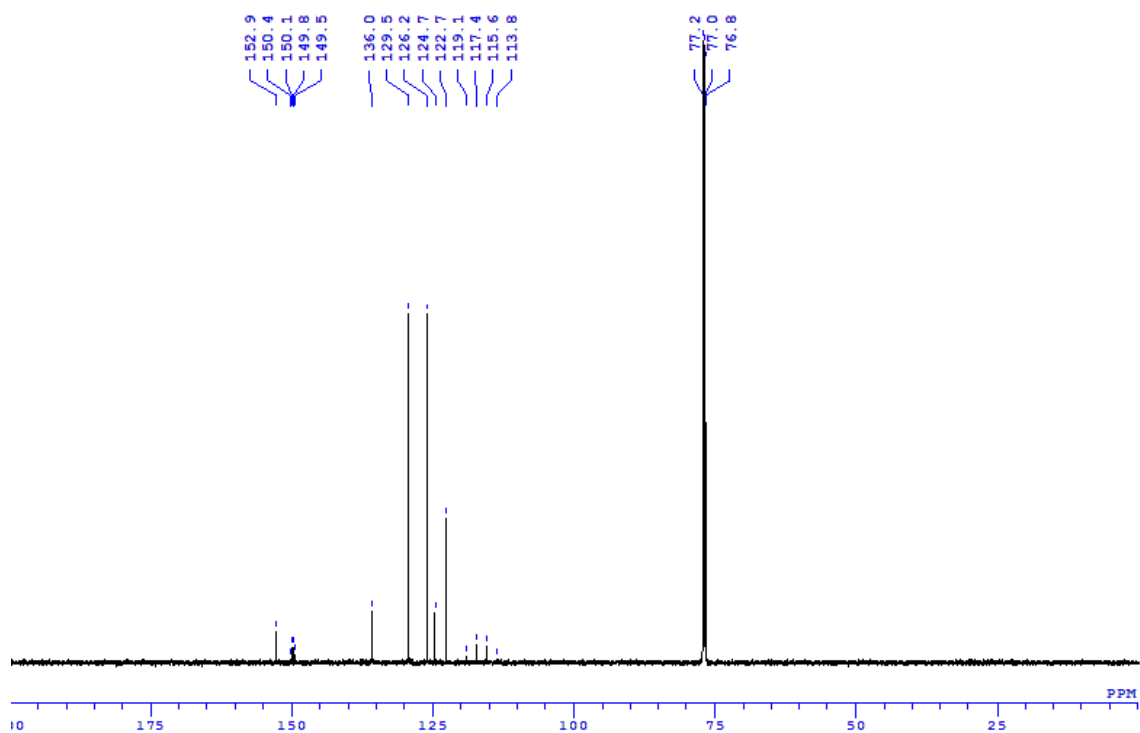
9c <sup>13</sup>C-NMR (150 MHz, CDCl<sub>3</sub>)



**9d**  $^1\text{H-NMR}$  (600 MHz,  $\text{CDCl}_3$ )

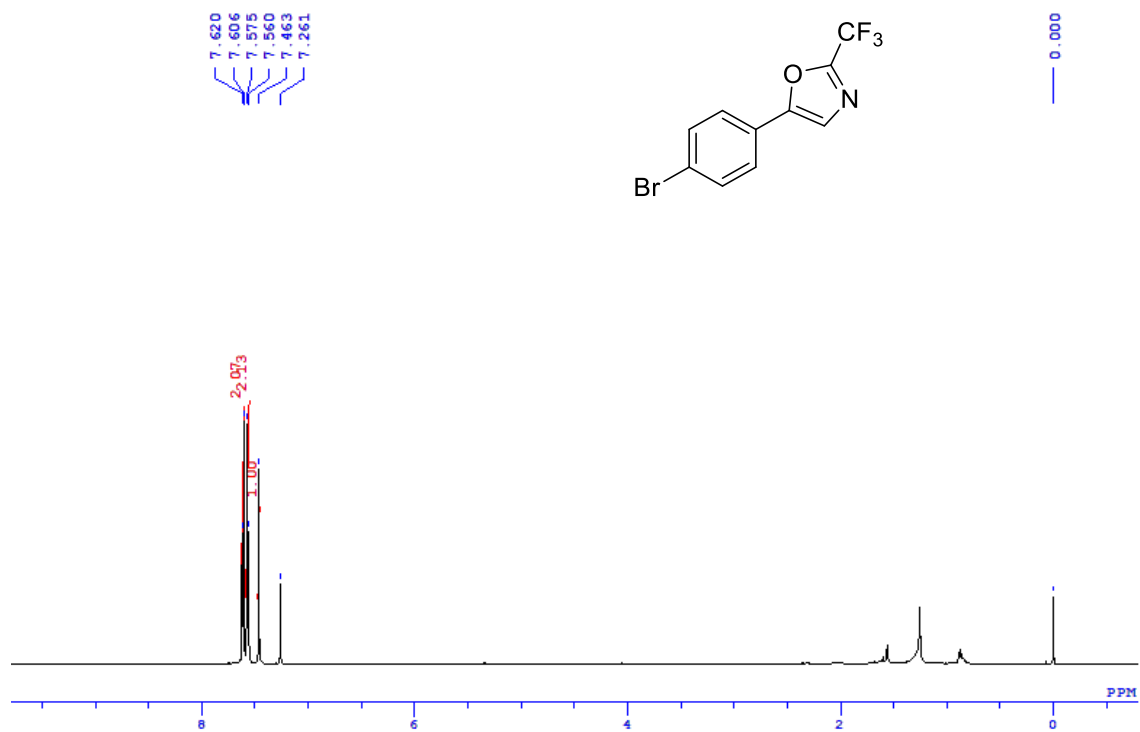


**9d**  $^{13}\text{C-NMR}$  (150 MHz,  $\text{CDCl}_3$ )

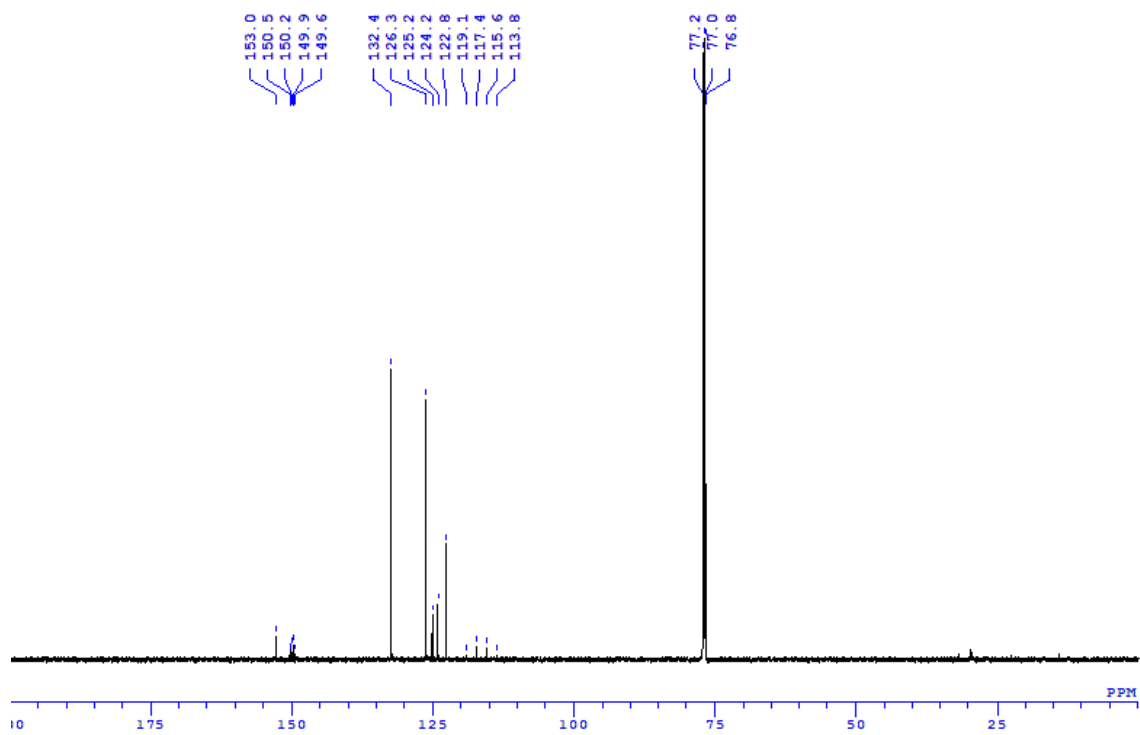




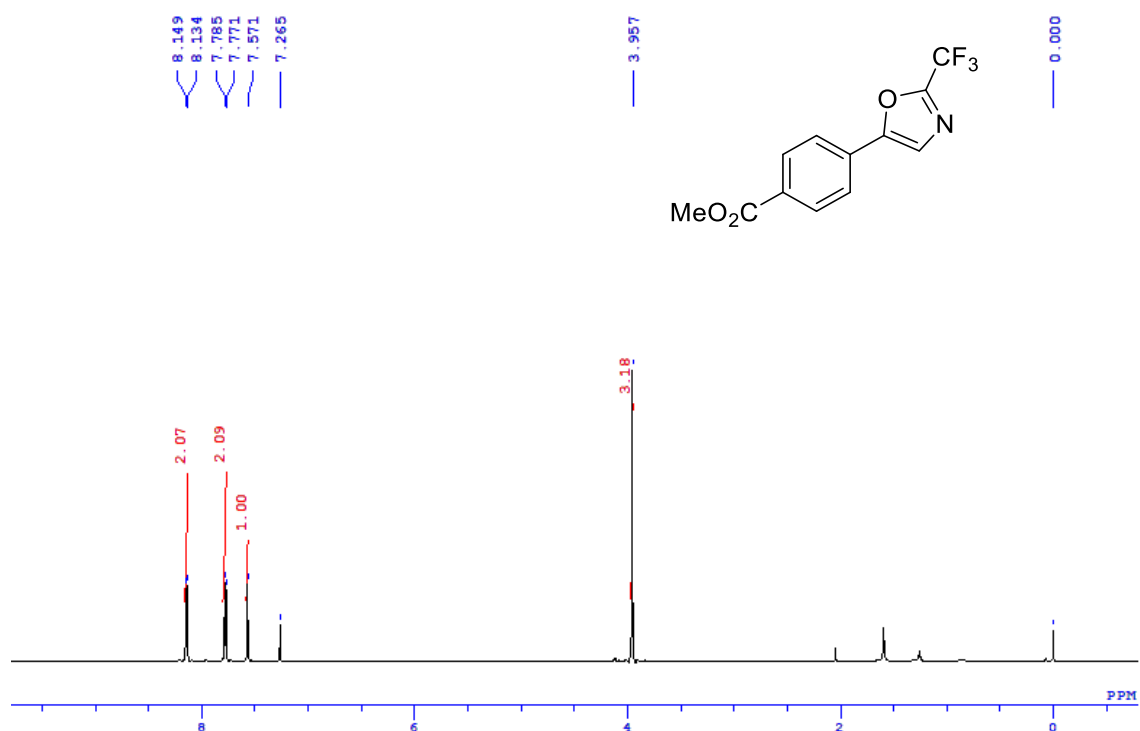
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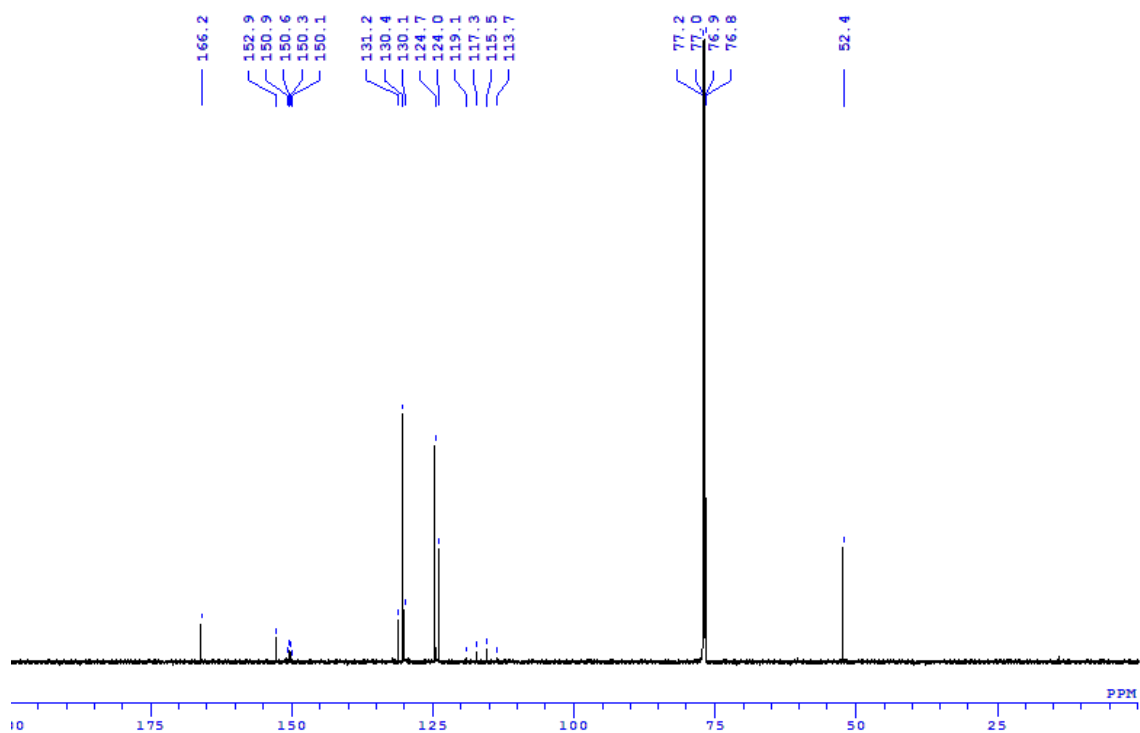
9e <sup>13</sup>C-NMR (150 MHz, CDCl<sub>3</sub>)



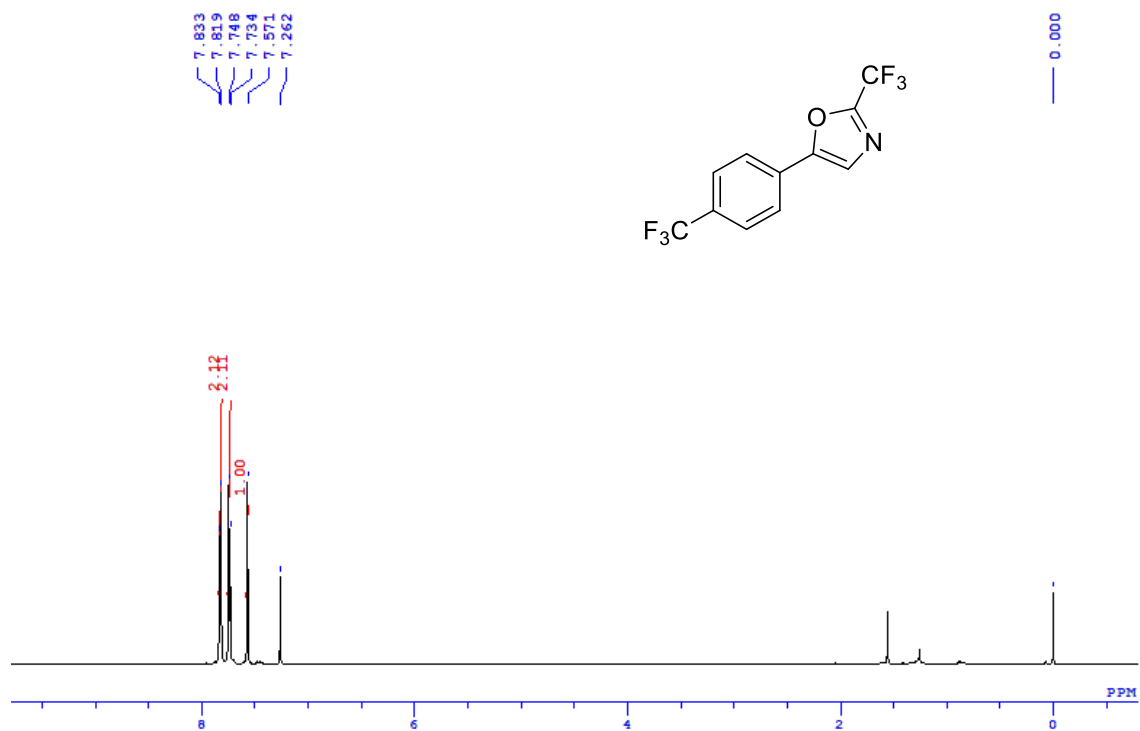
**9f** <sup>1</sup>H-NMR (600 MHz, CDCl<sub>3</sub>)



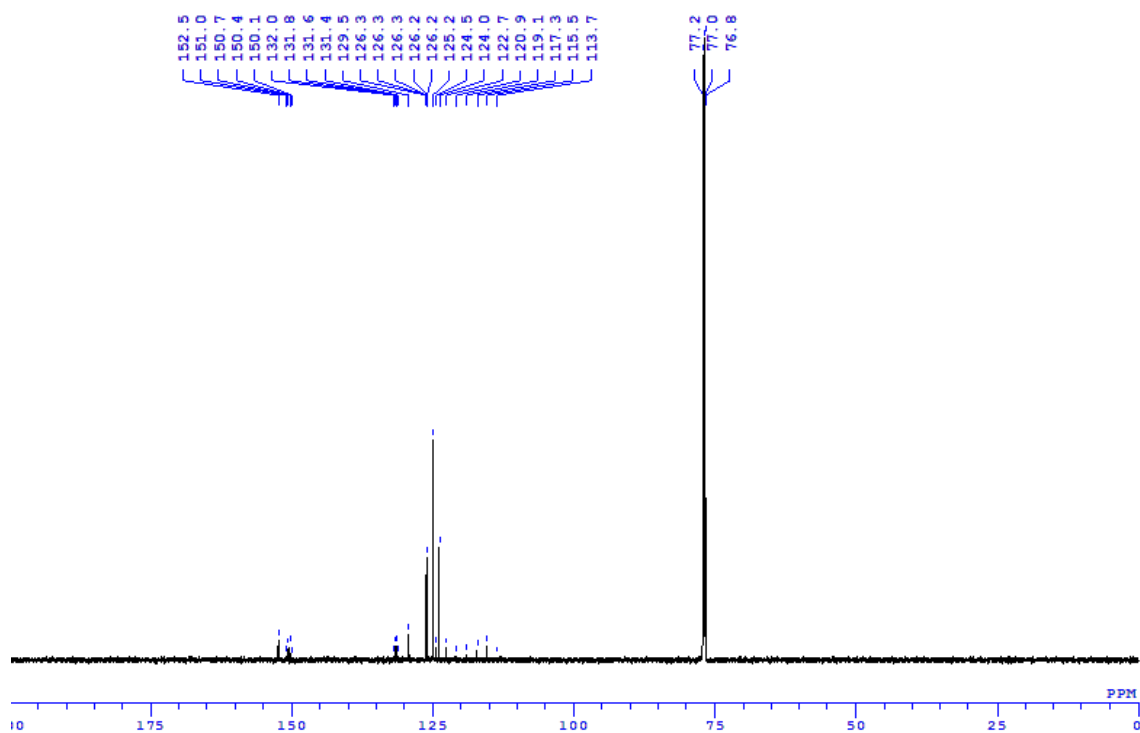
**9f** <sup>13</sup>C-NMR (150 MHz, CDCl<sub>3</sub>)



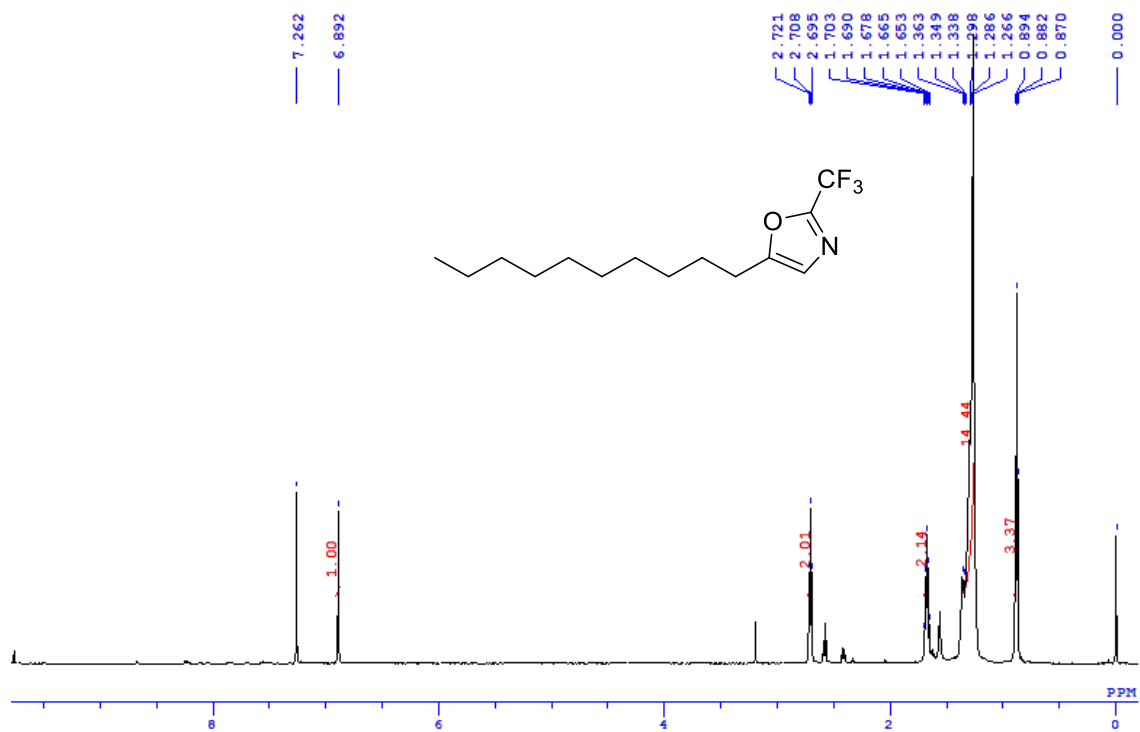
9g <sup>1</sup>H-NMR (600 MHz, CDCl<sub>3</sub>)



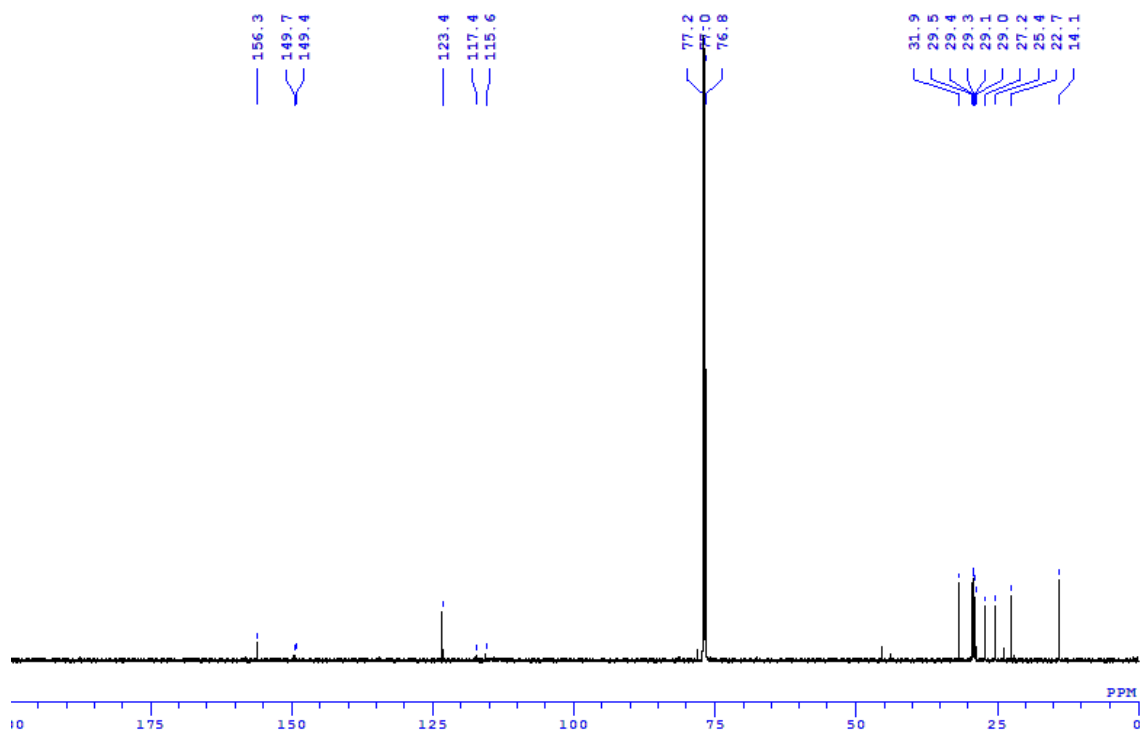
9g <sup>13</sup>C-NMR (150 MHz, CDCl<sub>3</sub>)



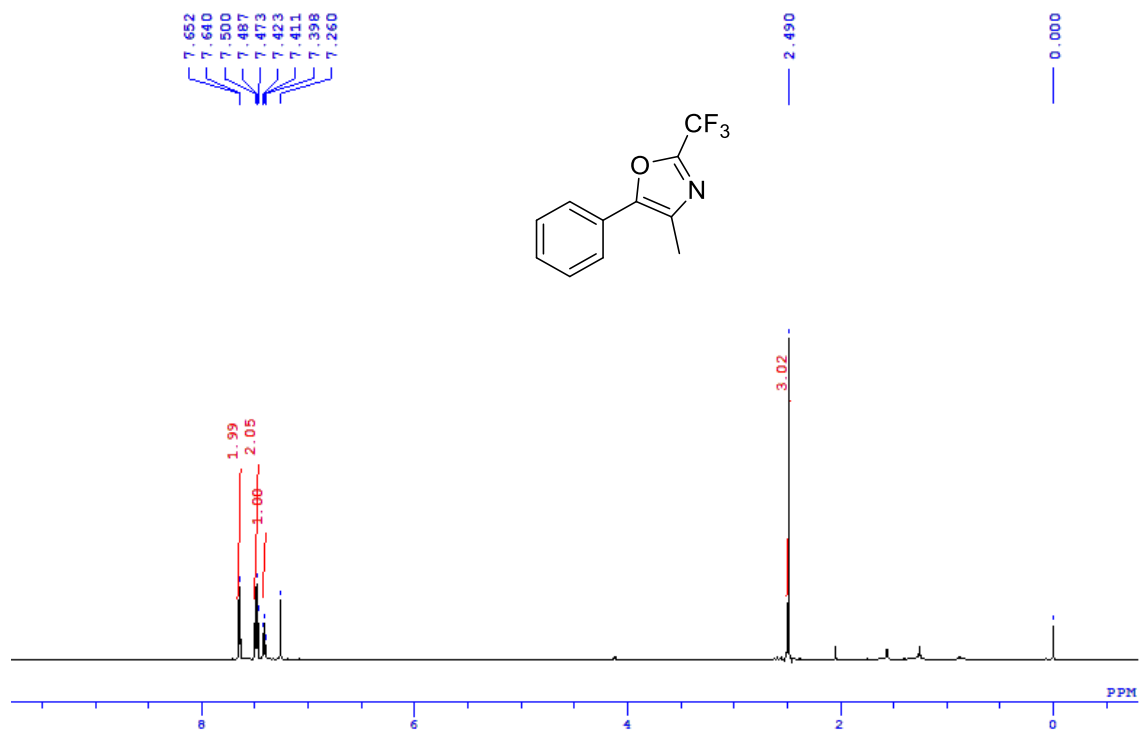
9h <sup>1</sup>H-NMR (600 MHz, CDCl<sub>3</sub>)



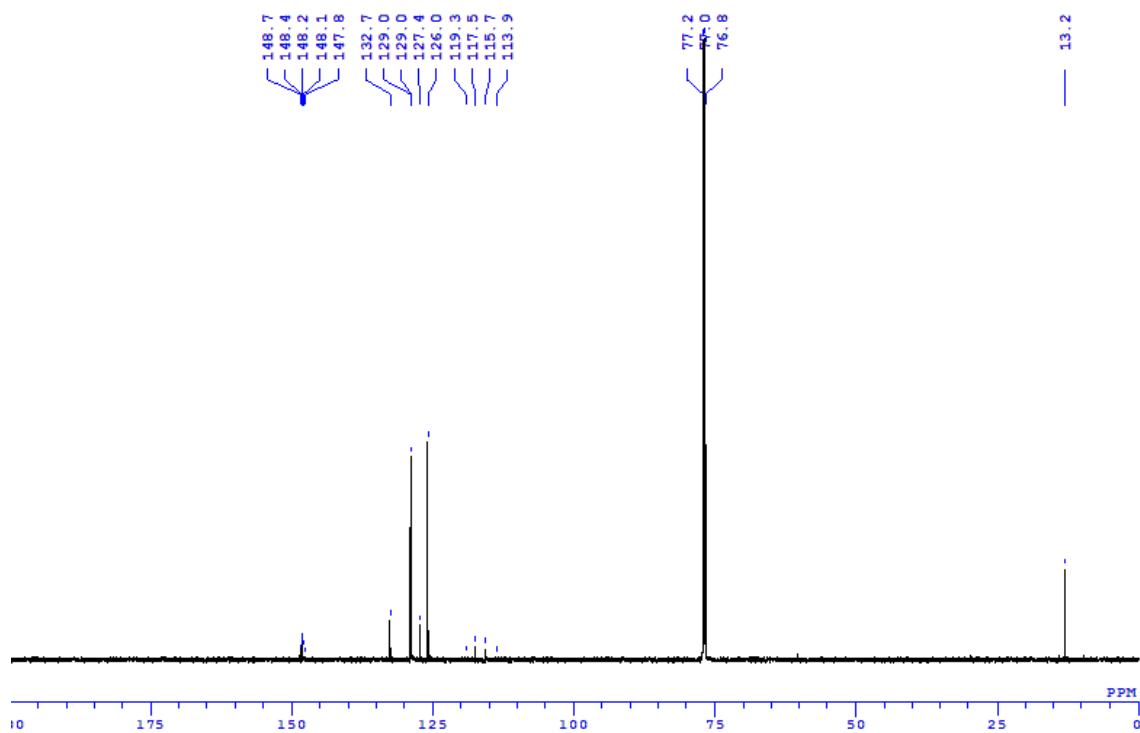
9h <sup>13</sup>C-NMR (150 MHz, CDCl<sub>3</sub>)



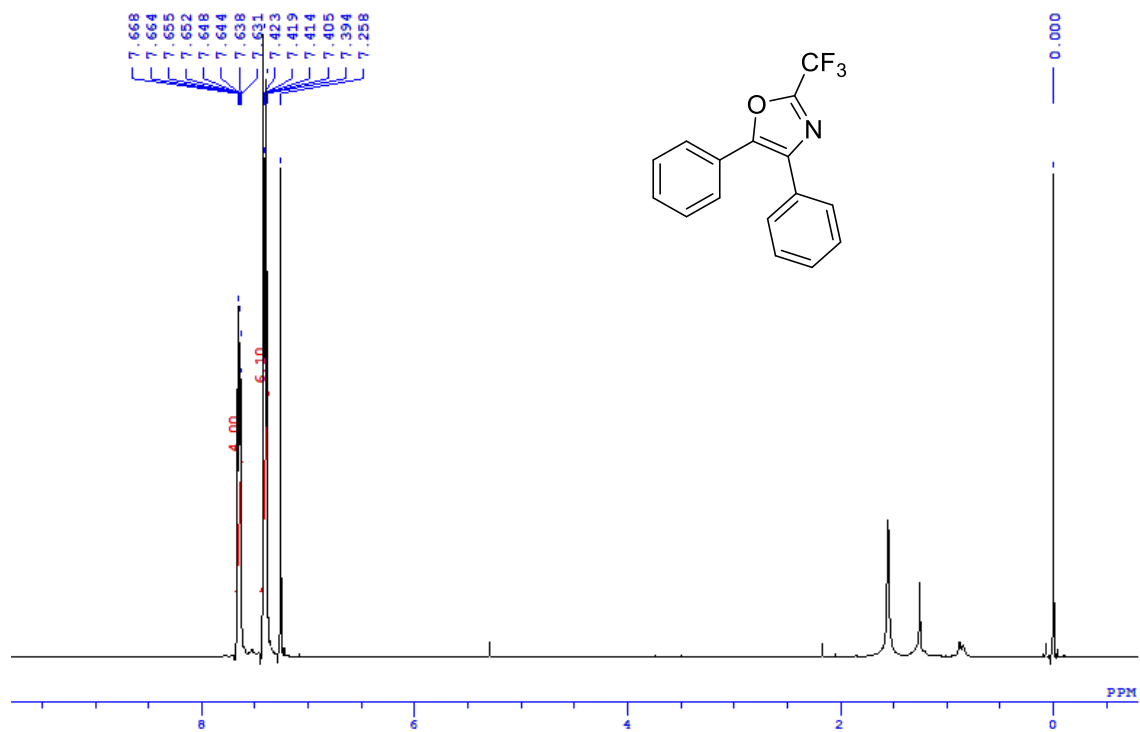
**9i** <sup>1</sup>H-NMR (600 MHz, CDCl<sub>3</sub>)



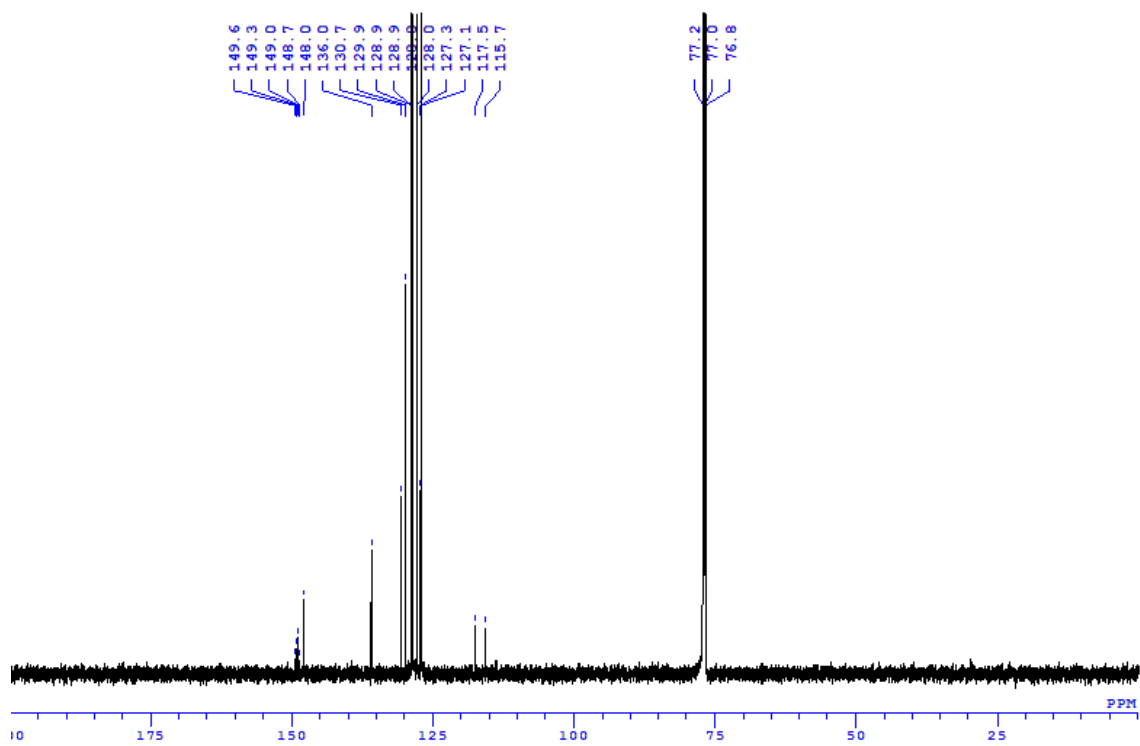
**9i** <sup>13</sup>C-NMR (150 MHz, CDCl<sub>3</sub>)



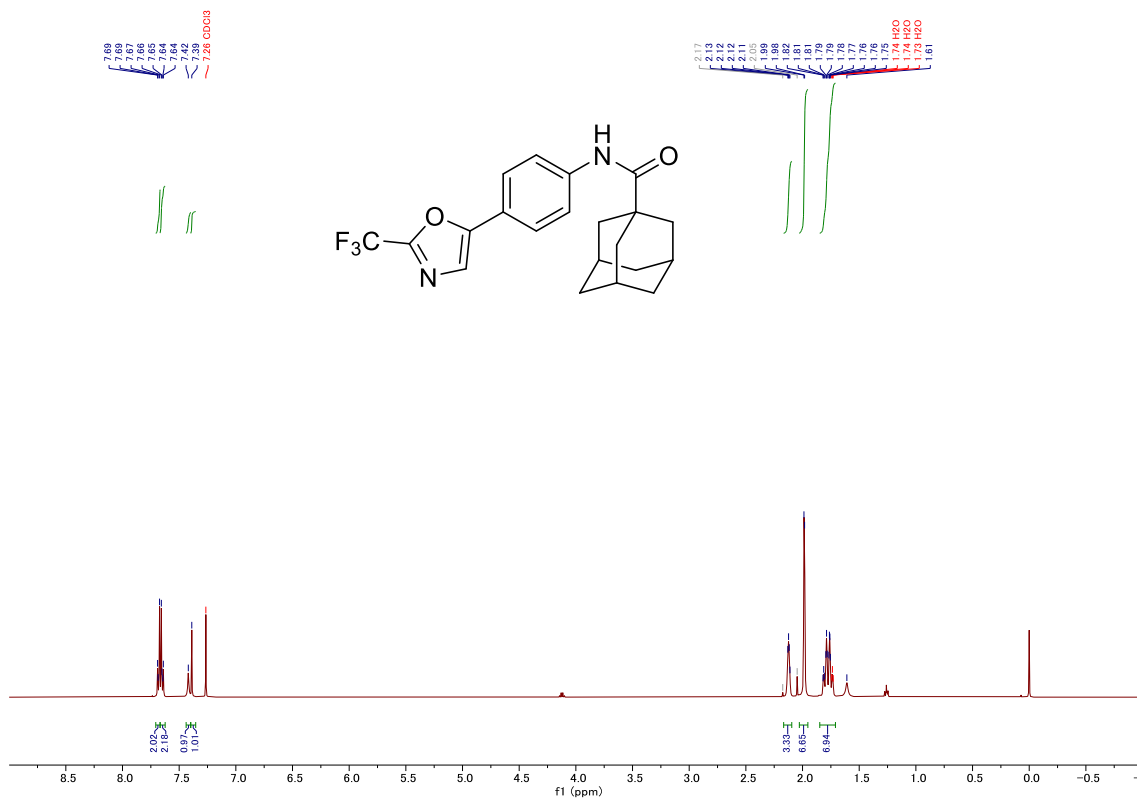
9j <sup>1</sup>H-NMR (600 MHz, CDCl<sub>3</sub>)



9j <sup>13</sup>C-NMR (150 MHz, CDCl<sub>3</sub>)



9k <sup>1</sup>H-NMR (500 MHz, CDCl<sub>3</sub>)



9k <sup>13</sup>C-NMR (126 MHz, CDCl<sub>3</sub>)

