Supporting Information

Cu-Catalyzed Tandem Cyclization and Coupling of Enynones with Enaminones for Multisubstituted Furans & Furano-pyrroles

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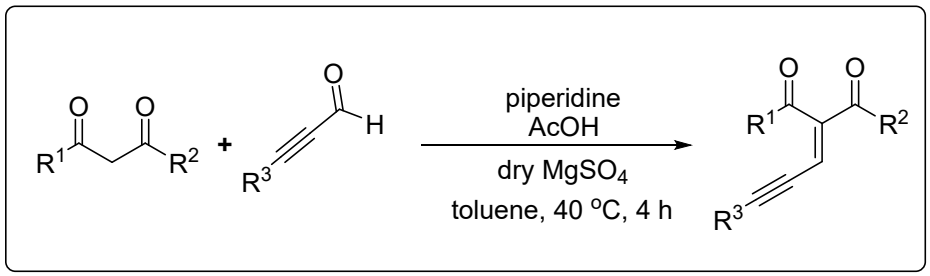
1. General Information and methods.

All reagents and solvents were purchased from commercial sources and used without purification. NMR spectra were recorded with a 300, 400 or 500 MHz spectrometer for ^{1}H NMR, 100 or 125 MHz for ^{13}C NMR spectroscopy. Chemical shifts are reported relative to the residual signals of tetramethylsilane in $CDCl_3$ or deuterated solvent $CDCl_3$ for ^{1}H and ^{13}C NMR spectroscopy. Multiplicities are reported as follows: singlet (s), doublet (d), doublet of doublets (dd), doublet of triplets (dt), triplet (t), quartet (q), multiplet (m). HRMS were recorded by using QT of mass spectrometer. Column chromatography was performed with silica gel (100–200 mesh) as the stationary phase. All reactions were monitored by using TLC.

2. Experimental Procedures

2.1. Preparation of Enynones General Procedure (GP-1):



General Procedure for the Synthesis of 2a-2k:[1]

To a 25 mL round bottom flask, the mixture of 1,3-diketones (5 mmol), AcOH (0.2 equiv), piperidine (0.1 equiv) and dry $MgSO_4$ (1 equiv) was added to a solution of propiolaldehyde (1.2 equiv) in toluene. The reaction was carried out at 40 °C stirring for 4 h while monitoring by TLC. After the completion of the reaction, the reaction mixture was filtered through *celite* and the resultant elute was concentrated to get the crude product. The enynone **2** was purified by chromatography on silica gel with the appropriate mixture of PE and EA in 60-90% yields (Z/E mixture, **1x** was isolated in 42% yield).

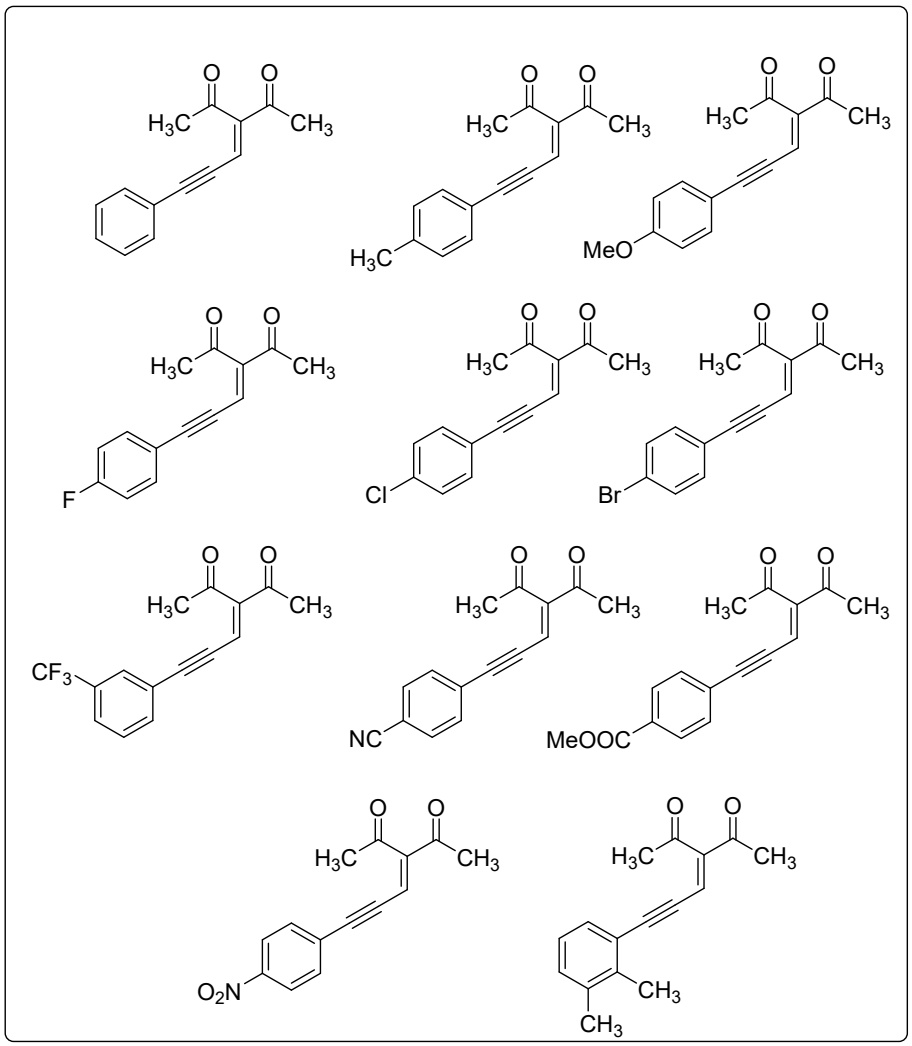
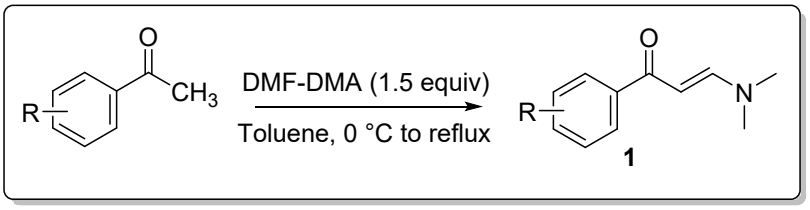


Table S1: List of Enynones

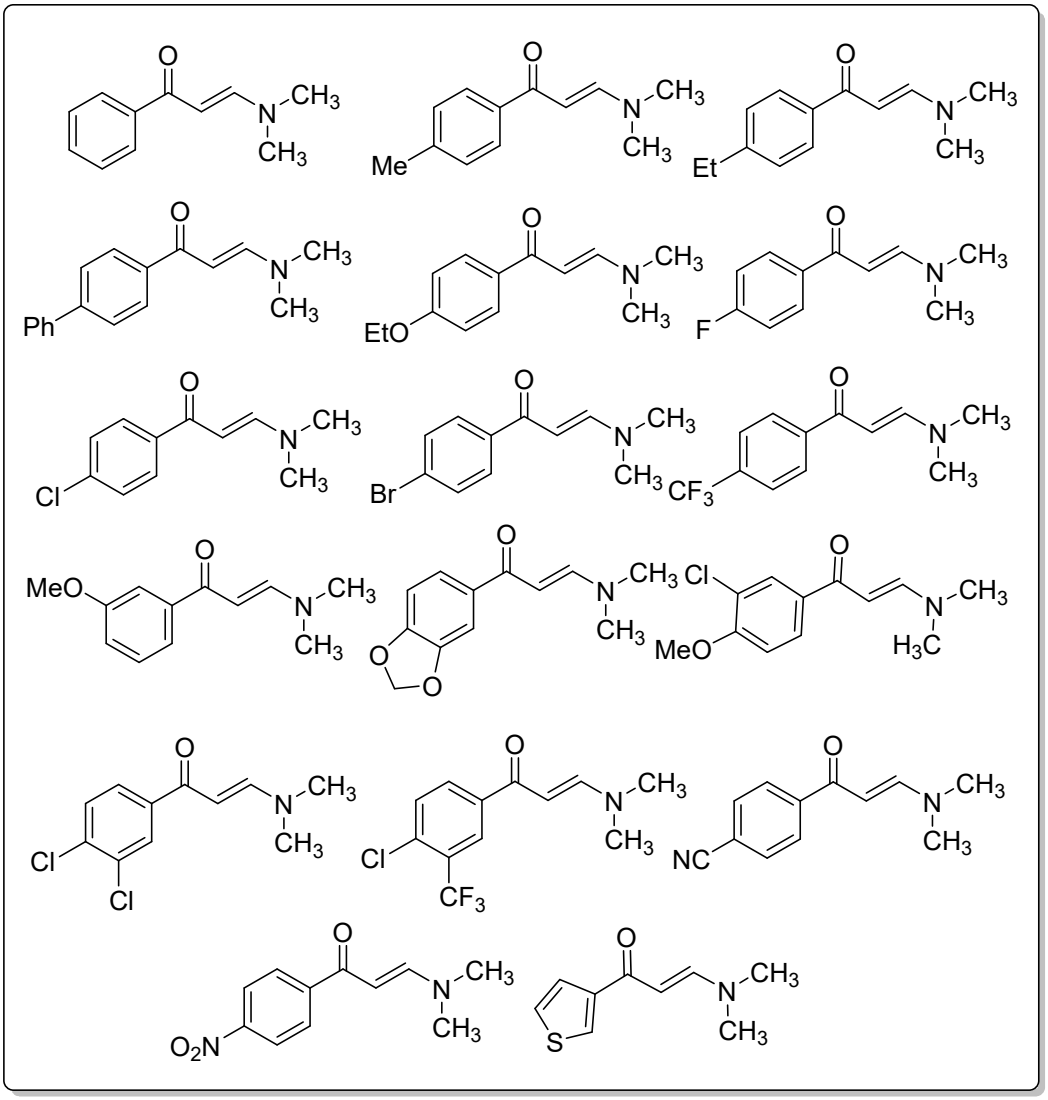
2.3. Preparation of Enaminones: General Procedure (GP-3):[2]



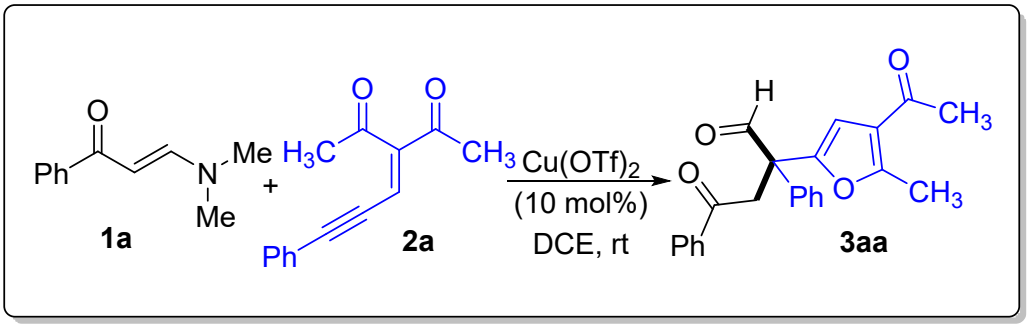
General Procedure for the Synthesis of 1a-1q:[2]

To a stirred solution of ketone 5 (5.0 mmol, 1.0 eq.) in 5.0 mL of toluene, 1,1-dimethoxy-N, N-dimethylmethanamine 6 (7.0 mmol, 1.4 eq.) was added and stirred at 110 ^{o}C. After completion of the reaction (monitored by TLC), it was quenched with water, extracted with ethyl acetate and dried with anhydrous Na_2SO_4. The reaction mixture was concentrated under reduced pressure and was purified by column chromatography (hexane:ethyl acetate = 1:1) to give the desired product **1**.

Table S2: List of Enaminones.



3. Optimization Studies

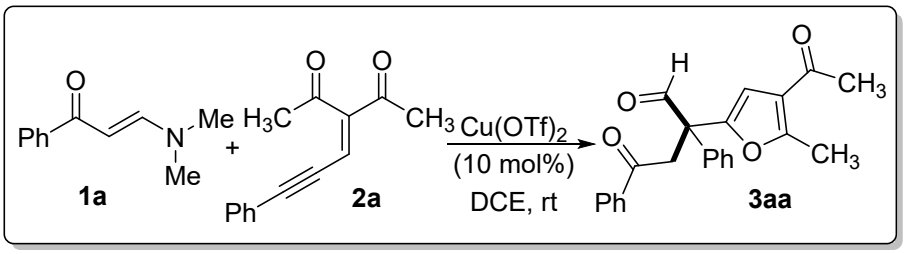


Entry	Variation from the standard conditions	Yield (%)[b]
1	None	80
2	$Cu(OAc)_2$ instead of $Cu(OTf)_2$	40
3	AgOTf instead of $Cu(OTf)_2$	60

4	CuI instead of $Cu(OTf)_2$	10
5	Cu(OTf) instead of $Cu(OTf)_2$	19
6	$Zn(OTf)_2$ instead of $Cu(OTf)_2$	2
7	DCM instead of DCE	60
8	THF instead of DCE	50
9	CH_3CN instead of DCE	48
10	60 °C instead of rt	55

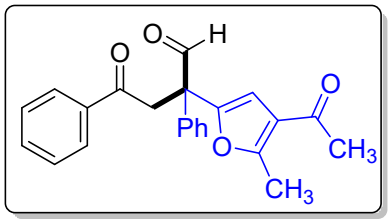
[a]Reaction conditions: **1** (1 equiv), **2** (1 equiv), $Cu(OTf)_2$ (10 mol%), DCE, rt for 15-30 min. [b] isolated yield.

4. General Procedure-A for Cu-Catalyzed Cyclizative Coupling of Enaminones (1a) with Enynones (2a) and Characteristic data:



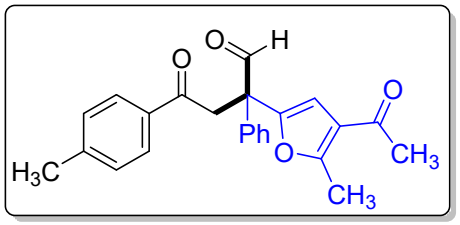
To a mixture of enaminone **1a** (52.5 mg, 0.3 mmol), enynone **2a** (63.6 mg, 0.3 mmol) in DCE was added $Cu(OTf)_2$ (10 mol%) into 10ml round-bottomed flask. The reaction mixture was stirred at rt in air for 15-30 min (monitored by TLC). After completion of reaction, the mixture was concentrated and was added with water and the aqueous layer was extracted with ethyl acetate (2×10 mL). The organic layer was evaporated and purified by column chromatography R_f= 0.50 (SiO_2, EtOAc:Hexane, 5:95) to get **3aa** as pale brown sticky solid in 80% (86.4 mg) yield.

2-(4-acetyl-5-methylfuran-2-yl)-4-oxo-2,4-diphenylbutanal (3aa):



The title compound was prepared from **1a** (52.5 mg, 0.3 mmol) and **2a** (63.6 mg, 0.3 mmol) according to general procedure **A**. Purification using column chromatography (R_f= 0.50, SiO_2, EtOAc:Hexane, 5:95) to give pure product as a pale yellow solid, (84.2 mg, 78 % yield). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 10.09 (s, 1H), 7.95 (dd, *J* = 8.4, 1.2 Hz, 2H), 7.62 – 7.55 (m, 1H), 7.49 – 7.44 (m, 2H), 7.39 – 7.34 (m, 2H), 7.31 (ddd, *J* = 8.5, 4.3, 1.3 Hz, 1H), 7.24 – 7.21 (m, 2H), 6.64 (s, 1H), 4.16 (d, *J* = 1.8 Hz, 2H), 2.50 (s, 3H), 2.40 (s, 3H) **^{13}C NMR (100 MHz, $CDCl_3$)** δ 196.5, 196.0, 194.1, 158.2, 150.7, 137.6, 136.2, 133.8, 129.1, 128.8, 128.3, 128.1, 127.8, 122.4, 109.3, 57.3, 45.3, 29.3, 14.6. **HRMS (ESI)** calcd for $C_{23}H_{21}O_4$ $[M+H]^+$ 361.1440, found 361.1429.

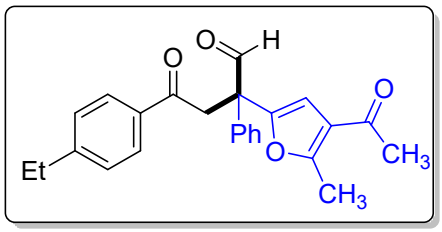
2-(4-acetyl-5-methylfuran-2-yl)-4-oxo-2-phenyl-4-(p-tolyl) butanal (3ba):



The title compound was prepared from **1b** (56.7 mg, 0.3 mmol) and **2a** (63.6 mg, 0.3 mmol) according to general procedure **A**. Purification using column chromatography (R_f = 0.50, SiO_2, EtOAc:Hexane, 5:95) gave pure product as a brown colour sticky

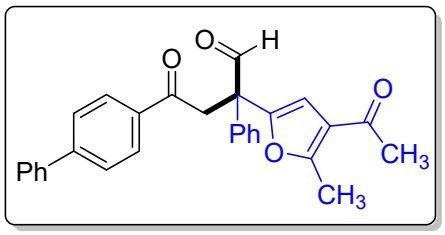
solid (87.5mg, 78% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 10.09 (s, 1H), 7.84 (d, *J* = 8.1 Hz, 2H), 7.37 (d, *J* = 6.9 Hz, 2H), 7.31 (d, *J* = 7.0 Hz, 1H), 7.26 (s, 2H), 7.22 (s, 1H), 7.14 (s, 1H), 6.64 (s, 1H), 4.14 (d, *J* = 2.9 Hz, 2H), 2.50 (s, 3H), 2.41 (s, 3H), 2.39 (s, 3H).**^{13}C NMR (125 MHz, $CDCl_3$)** δ 196.6, 195.7, 194.1, 158.1, 150.9, 144.7, 137.7, 133.8, 131.5, 129.5, 129.1, 128.4, 128.2, 128.1, 128.0, 127.8, 127.6, 122.4, 109.3, 57.3, 45.3, 29.3, 21.8, 14.5. **HRMS (ESI)** calcd for $C_{24}H_{23}O_4$ $[M+H]^+$ 375.1596, found 375.1584.

2-(4-acetyl-5-methylfuran-2-yl)-4-(4-ethylphenyl)-4-oxo-2-phenylbutanal (3ca):



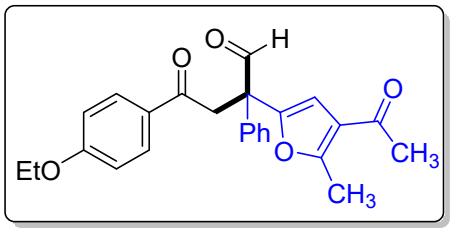
The title compound was prepared from **1c** (60.9 mg, 0.3 mmol) and **2a** (63.6 mg, 0.3 mmol) according to general procedure **A**. Purification using column chromatography (R_f = 0.5, SiO_2, EtOAc:Hexane, 05:95) gave pure product as a pale brown colour sticky solid (83.8 mg, 72% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 10.12 (s, 1H), 7.89 (d, *J* = 8.3 Hz, 2H), 7.39 (dd, *J* = 9.9, 4.6 Hz, 2H), 7.34 (dd, *J* = 5.3, 1.7 Hz, 1H), 7.32 – 7.27 (m, 3H), 7.24 (s, 1H), 6.66 (s, 1H), 4.17 (d, *J* = 2.0 Hz, 2H), 2.73 (q, *J* = 7.6 Hz, 2H), 2.52 (s, 3H), 2.41 (s, 3H), 1.28 (t, *J* = 7.6 Hz, 3H).). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 196.6, 195.7, 194.1, 158.1, 150.9, 150.8, 137.6, 133.9, 129.1, 128.5, 128.3, 128.1, 127.8, 122.4, 109.2, 57.2, 45.3, 29.3, 29.1, 15.3, 14.5. **HRMS (ESI)** calcd for $C_{25}H_{24}NaO_4$ $[M+Na]^+$ 411.1572, found 411.1564.

4-([1,1'-biphenyl]-4-yl)-2-(4-acetyl-5-methylfuran-2-yl)-4-oxo-2-phenylbutanal (3da):



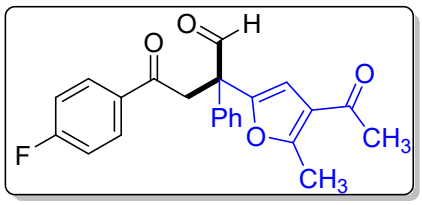
The title compound was prepared from **1d** (75.3 mg, 0.3 mmol) and **2a** (63.6 mg, 0.3 mmol) according to general procedure **A**. Purification using column chromatography (R_f = 0.5, SiO_2, EtOAc:Hexane, 5:95) gave pure product as a brown colour sticky solid (98.1 mg, 75% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 10.13 (s, 1H), 8.04 (d, *J* = 8.0 Hz, 2H), 7.70 (d, *J* = 8.0 Hz, 2H), 7.64 (d, *J* = 7.4 Hz, 2H), 7.49 (t, *J* = 7.3 Hz, 2H), 7.46 – 7.37 (m, 3H), 7.35 (d, *J* = 6.9 Hz, 1H), 7.28 (s, 2H), 6.69 (s, 1H), 4.21 (s, 2H), 2.54 (s, 3H), 2.42 (s, 3H). **^{13}C NMR (125 MHz, $CDCl_3$)** δ 196.46, 195.57, 194.07, 158.14, 150.76, 146.39, 139.72, 137.59, 134.86, 129.11, 129.08, 128.89, 128.47, 128.11, 127.77, 127.41, 127.36, 122.42, 109.32, 57.30, 45.33, 29.30, 14.53. **HRMS (ESI)** calcd for $C_{29}H_{23}O_4$ $[M+H]^+$ 437.1753, found 437.1746.

2-(4-acetyl-5-methylfuran-2-yl)-4-(4-ethoxyphenyl)-4-oxo-2-phenylbutanal (3ea):



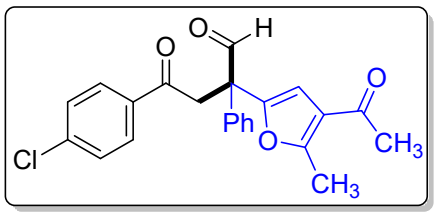
The title compound was prepared from **1e** (65.7 mg, 0.3 mmol) and **2a** (63.6 mg, 0.3 mmol) according to general procedure **A**. Purification using column chromatography (R_f = 0.4, SiO_2, EtOAc:Hexane, 7:93) gave pure product as a pale brown colour sticky solid (84.8 mg, 70% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 10.09 (s, 1H), 7.95 – 7.87 (m, 2H), 7.39 – 7.33 (m, 2H), 7.33 – 7.29 (m, 1H), 7.25 – 7.20 (m, 2H), 6.91 (d, *J* = 8.9 Hz, 2H), 6.64 (s, 1H), 4.11 (dd, *J* = 7.6, 6.0 Hz, 4H), 2.50 (s, 3H), 2.39 (s, 3H), 1.44 (t, *J* = 7.0 Hz, 3H). **^{13}C NMR (125 MHz, $CDCl_3$)** δ 196.7, 194.5, 194.2, 163.5, 158.1, 151.0, 137.7, 130.7, 129.1, 128.0, 127.8, 122.4, 114.4, 109.2, 63.9, 57.2, 45.1, 29.3, 14.7, 14.5. **HRMS (ESI)** calcd for $C_{25}H_{25}O_5$ $[M+H]^+$ 405.1702, found 405.1689.

2-(4-acetyl-5-methylfuran-2-yl)-4-(4-fluorophenyl)-4-oxo-2-phenylbutanal (3fa):



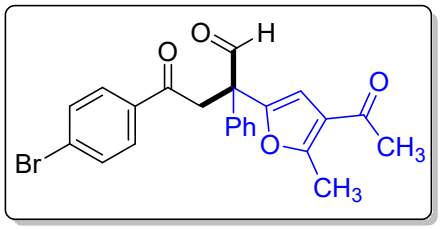
The title compound was prepared from **1f** (57.9 mg, 0.3 mmol) and **2a** (63.6 mg, 0.3 mmol) according to general procedure **A**. Purification using column chromatography (R_f = 0.5, SiO_2, EtOAc:Hexane, 5:95) gave pure product as a pale brown colour sticky solid (82.7 mg, 73% yield.**^{1}H NMR (400 MHz, $CDCl_3$)** δ 10.07 (s, 1H), 7.97 (dd, *J* = 8.7, 5.4 Hz, 2H), 7.39 – 7.30 (m, 3H), 7.21 (d, *J* = 7.2 Hz, 2H), 7.12 (t, *J* = 8.5 Hz, 2H), 6.65 (s, 1H), 4.11 (s, 2H), 2.50 (s, 3H), 2.40 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 196.3, 194.4, 194.1, 167.4, 164.8, 158.2, 150.6, 137.5, 132.7, 131.0, 130.9, 129.1, 128.9, 128.2, 127.7, 122.5, 116.1, 115.8, 109.3, 57.3, 45.1, 29.3, 14.5. **HRMS (ESI)** calcd for $C_{23}H_{20}FO_4$ $[M+H]^+$ 379.1346, found 379.1334.

2-(4-acetyl-5-methylfuran-2-yl)-4-(4-chlorophenyl)-4-oxo-2-phenylbutanal (3ga):



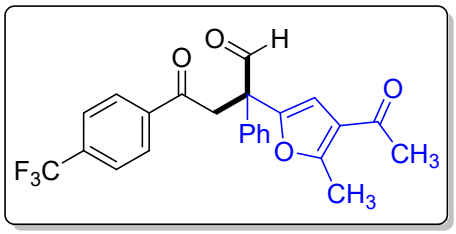
The title compound was prepared from **1g** (62.7 mg, 0.3 mmol) and **2a** (63.6 mg, 0.3 mmol) according to general procedure **A**. Purification using column chromatography (R_f = 0.50 SiO_2, EtOAc:Hexane, 4:96) gave pure product as a brown colour sticky solid (83.9 mg, 71% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 10.07 (s, 1H), 7.88 (d, *J* = 8.6 Hz, 2H), 7.43 (d, *J* = 8.5 Hz, 2H), 7.37 (t, *J* = 7.2 Hz, 2H), 7.34 – 7.31 (m, 1H), 7.23 – 7.19 (m, 2H), 6.64 (s, 1H), 4.10 (s, 2H), 2.51 (s, 3H), 2.40 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 196.2, 194.8, 194.0, 158.2, 150.5, 140.3, 137.4, 134.6, 129.7, 129.2, 129.2, 128.2, 127.7, 122.5, 109.4, 57.4, 45.1, 29.3, 14.6. **HRMS (ESI)** calcd for $C_{23}H_{20}ClO_4$ $[M+H]^+$ 395.1050, found 395.1037.

2-(4-acetyl-5-methylfuran-2-yl)-4-(4-bromophenyl)-4-oxo-2-phenylbutanal (3ha):



The title compound was prepared from **1h** (75.9 mg, 0.3 mmol) and **2a** ((63.6 mg, 0.3 mmol) according to general procedure **A**. Purification using column chromatography (R_f = 0.50, SiO_2, EtOAc:Hexane, 5:95) gave pure product as a brown solid (93.2 mg, 71% yield), mp 135-137 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 10.06 (s, 1H), 7.80 (d, *J* = 8.5 Hz, 2H), 7.60 (d, *J* = 8.5 Hz, 2H), 7.41 – 7.30 (m, 3H), 7.20 (d, *J* = 7.1 Hz, 2H), 6.63 (s, 1H), 4.09 (s, 2H), 2.51 (s, 3H), 2.40 (s, 3H).**^{13}C NMR (100 MHz, $CDCl_3$)** δ 196.2, 195.1, 194.0, 158.2, 150.5, 138.0, 137.5, 135.0, 132.2, 129.8, 129.2, 128.3, 127.8, 122.5, 109.4, 57.4, 45.0, 29.3, 14.6. **HRMS (ESI)** calcd for $C_{23}H_{19}BrO_4$ $[M+H]^+$ 439.0545, found 439.0541.

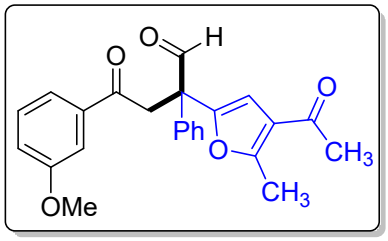
2-(4-acetyl-5-methylfuran-2-yl)-4-oxo-2-phenyl-4-(4-(trifluoromethyl) phenyl) butanal (3ia):



The title compound was prepared from **1i** (72.9 mg, 0.3 mmol) and **2a** (63.6 mg, 0.3 mmol) according to general procedure **A**. Purification using column chromatography (R_f = 0.5, SiO2, EtOAc:Hexane, 5:95) gave pure product as a brown colour sticky solid (78.3 mg, 61% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 10.06 (s, 1H), 8.04 (d, *J* = 8.1 Hz, 2H), 7.73 (d, *J* = 8.2 Hz, 2H), 7.40 –

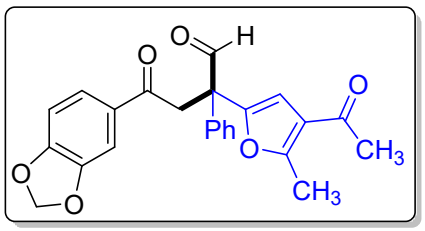
7.31 (m, 3H), 7.23 – 7.19 (m, 2H), 6.65 (s, 1H), 4.14 (s, 2H), 2.51 (s, 3H), 2.41 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 195.9, 195.1, 194.0, 158.3, 150.3, 139.0, 137.3, 129.3, 128.6, 128.3, 127.7, 125.9, 125.9, 122.6, 109.5, 57.5, 45.1, 29.3, 14.6.**HRMS (ESI)** calcd for $C_{24}H_{20}O_4$ $[M+H]^+$ 429.1314, found 429.1304.

2-(4-acetyl-5-methylfuran-2-yl)-4-(3-methoxyphenyl)-4-oxo-2-phenylbutanal (3ja):



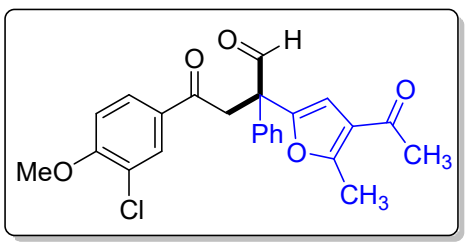
The title compound was prepared from **1j** (61.5 mg, 0.3 mmol) and **2a** (63.6 mg, 0.3 mmol) according to general procedure **A**. Purification using column chromatography (R_f = 0.4, SiO_2, EtOAc:Hexane, 8:92) gave pure product as a pale brown colour sticky solid (72.5 mg, 62% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 10.09 (s, 1H), 7.55 (d, *J* = 7.6 Hz, 1H), 7.44 (s, 1H), 7.37 (t, *J* = 7.5 Hz, 3H), 7.34 – 7.28 (m, 1H), 7.22 (d, *J* = 7.3 Hz, 2H), 7.13 (dd, *J* = 8.2, 2.4 Hz, 1H), 6.65 (s, 1H), 4.14 (s, 2H), 3.83 (s, 3H), 2.51 (s, 3H), 2.40 (s, 3H). **^{13}C NMR (125 MHz, $CDCl_3$)** δ 196.4, 195.9, 194.1, 159.9, 158.1, 150.7, 137.5, 137.5, 129.8, 129.1, 128.1, 127.7, 122.4, 120.9, 120.3, 112.4, 109.3, 57.3, 55.5, 45.3, 29.3, 14.5.**HRMS (ESI)** calcd for $C_{24}H_{23}O_5$ $[M+H]^+$ 391.1545, found 391.1534.

2-(4-acetyl-5-methylfuran-2-yl)-4-(benzo[d][1,3]dioxol-5-yl)-4-oxo-2-phenylbutanal (3ka):



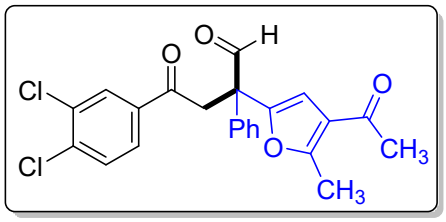
The title compound was prepared from **1k** (65.7 mg, 0.3 mmol) and **2a** (63.6 mg, 0.3 mmol) according to general procedure **A**. Purification using column chromatography (R_f = 0.30, SiO_2, EtOAc:Hexane, 8:92) gave pure product as a brown colour sticky solid (83.6 mg, 69% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 10.07 (s, 1H), 7.57 (dd, *J* = 8.2, 1.4 Hz, 1H), 7.36 (dd, *J* = 11.8, 4.5 Hz, 3H), 7.33 – 7.27 (m, 1H), 7.21 (d, *J* = 7.2 Hz, 2H), 6.84 (d, *J* = 8.2 Hz, 1H), 6.64 (s, 1H), 6.04 (s, 2H), 4.08 (d, *J* = 1.3 Hz, 2H), 2.50 (s, 3H), 2.39 (s, 3H). **^{13}C NMR (125 MHz, $CDCl_3$)** δ 196.5, 194.1, 194.1, 158.1, 152.3, 150.9, 148.4, 137.6, 131.0, 129.1, 128.1, 127.7, 124.7, 122.4, 109.2, 108.0, 102.1, 57.3, 45.2, 29.3, 14.5. **HRMS (ESI)** calcd for $C_{24}H_{21}O_6$ $[M+H]^+$ 405.1338, found 405.1330.

2-(4-acetyl-5-methylfuran-2-yl)-4-(3-chloro-4-methoxyphenyl)-4-oxo-2-phenylbutanal(3la):



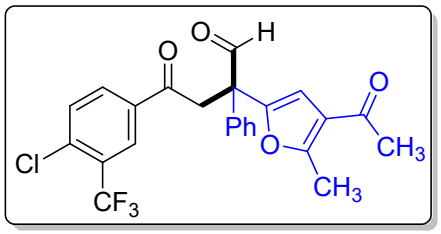
The title compound was prepared from **1l** (71.7 mg, 0.3 mmol) and **2a** (63.6 mg, 0.3 mmol) according to general procedure **A**. Purification using column chromatography (R_f = 0.40, SiO_2, EtOAc:Hexane, 8:92) gave pure product as a brown sticky solid (73.7 mg, 58% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 10.07 (s, 1H), 7.97 (d, *J* = 2.2 Hz, 1H), 7.86 (dd, *J* = 8.7, 2.2 Hz, 1H), 7.37 (dd, *J* = 8.1, 6.4 Hz, 2H), 7.32 (dd, *J* = 5.2, 1.8 Hz, 1H), 7.24 – 7.18 (m, 2H), 6.96 (d, *J* = 8.7 Hz, 1H), 6.64 (s, 1H), 4.07 (s, 2H), 3.97 (s, 3H), 2.51 (s, 3H), 2.40 (s, 3H).**^{13}C NMR (100 MHz, $CDCl_3$)** δ 196.3, 194.1, 193.7, 159.3, 158.2, 150.6, 137.5, 130.7, 129.8, 129.1, 128.8, 128.2, 127.8, 123.1, 122.4, 111.5, 109.3, 57.3, 56.6, 44.9, 29.3, 14.5. **HRMS (ESI)** calcd for $C_{20}H_{22}ClO_5$ $[M+H]^+$ 425.1156, found 425.1139.

2-(4-acetyl-5-methylfuran-2-yl)-4-(3,4-dichlorophenyl)-4-oxo-2-phenylbutanal(3ma):



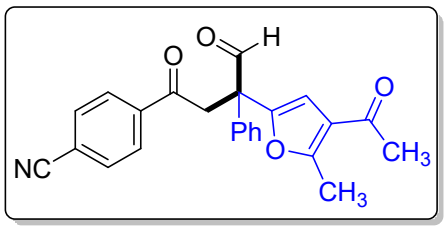
The title compound was prepared from **1m** (72.9 mg, 0.3 mmol) and **2a** (63.6 mg, 0.3 mmol) according to general procedure **A**. Purification using column chromatography (R_f = 0.50, SiO_2, EtOAc:Hexane, 4:96) gave pure product as a pale brown sticky solid (80.9 mg, 63% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 10.04 (s, 1H), 7.99 (d, *J* = 1.6 Hz, 1H), 7.75 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.53 (d, *J* = 8.3 Hz, 1H), 7.41 – 7.31 (m, 3H), 7.20 (d, *J* = 7.2 Hz, 2H), 6.65 (s, 1H), 4.06 (s, 2H), 2.52 (s, 3H), 2.40 (s, 3H).**^{13}C NMR (100 MHz, $CDCl_3$)** δ 195.8, 193.9, 193.8, 158.2, 150.2, 138.3, 137.2, 135.8, 133.5, 130.9, 130.3, 129.2, 129.0, 128.3, 127.7, 127.2, 122.5, 109.5, 57.5, 44.8, 29.3, 14.5. **HRMS (ESI)** calcd for $C_{23}H_{19}Cl_2O_4$ $[M+H]^+$ 429.0660, found 429.0653.

2-(4-acetyl-5-methylfuran-2-yl)-4-(4-chloro-3-(trifluoromethyl)phenyl)-4-oxo-2-phenylbutanal (3na):



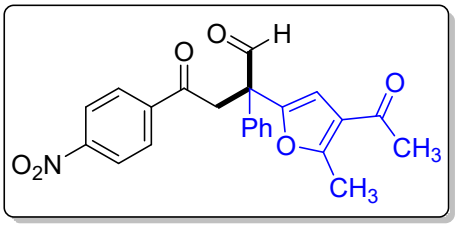
The title compound was prepared from **1n** (83.1 mg, 0.3 mmol) and **2a** (63.6 mg, 0.3 mmol) according to General procedure **A**. Purification using column chromatography (R_f = 0.50, SiO_2, EtOAc:Hexane, 5:95) gave pure product as a brown sticky solid (77.6 mg, 56% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 10.04 (s, 1H), 8.22 (d, *J* = 1.2 Hz, 1H), 8.03 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.61 (d, *J* = 8.3 Hz, 1H), 7.36 (dt, *J* = 14.2, 6.9 Hz, 3H), 7.20 (d, *J* = 7.1 Hz, 2H), 6.66 (s, 1H), 4.09 (s, 2H), 2.52 (s, 3H), 2.41 (s, 3H).**^{13}C NMR (125 MHz, $CDCl_3$)** δ 195.7, 193.9, 193.8, 158.3, 150.0, 138.0, 137.1, 134.7, 132.3, 132.2, 129.3, 128.4, 127.7, 127.5, 122.6, 109.6, 57.6, 44.6, 29.3, 14.5. **HRMS (ESI)** calcd for $C_{24}H_{19}ClF_3O_4$ $[M+H]^+$ 463.0924, found 463.0917.

4-(3-(4-acetyl-5-methylfuran-2-yl)-4-oxo-3-phenylbutanoyl) benzonitrile (3oa):



The title compound was prepared from **1o** (60 mg, 0.3 mmol) and **2a** (63.6 mg, 0.3 mmol) according to general procedure **A**. Purification using column chromatography (R_f = 0.40, SiO_2, EtOAc:Hexane, 7:93) gave pure product as a pale brown sticky solid (67 mg, 58% yield).**^{1}H NMR (500 MHz, $CDCl_3$)** δ 10.04 (s, 1H), 8.01 (d, *J* = 8.4 Hz, 2H), 7.76 (d, *J* = 8.4 Hz, 2H), 7.38 (t, *J* = 7.4 Hz, 2H), 7.33 (t, *J* = 7.2 Hz, 1H), 7.19 (d, *J* = 7.3 Hz, 2H), 6.64 (s, 1H), 4.10 (d, *J* = 2.6 Hz, 2H), 2.52 (s, 3H), 2.41 (s, 3H).**^{13}C NMR (100 MHz, $CDCl_3$)** δ 195.7, 194.7, 193.9, 158.3, 150.0, 139.2, 137.2, 132.7, 129.3, 128.7, 128.4, 127.7, 122.6, 117.8, 116.9, 109.5, 57.6, 44.9, 29.3, 14.5. **HRMS (ESI)** calcd for $C_{24}H_{20}NO_4$ $[M+H]^+$ 386.1392, found 386.1381.

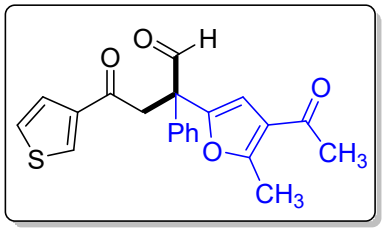
2-(4-acetyl-5-methylfuran-2-yl)-4-(4-nitrophenyl)-4-oxo-2-phenylbutanal (3pa):



The title compound was prepared from **1p** (66 mg, 0.3 mmol) and **2a** (63.6 mg, 0.3 mmol) according to general procedure **A**. Purification using column chromatography (R_f = 0.30, SiO_2, EtOAc:Hexane, 10:90) gave pure product as a brown sticky solid (72.9 mg, 60% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 10.05 (s, 1H),

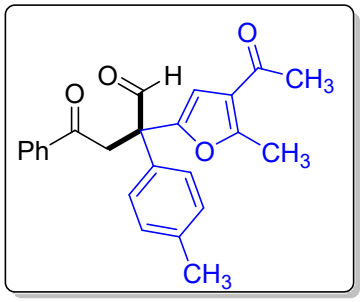
8.29 (d, J = 8.5 Hz, 2H), 8.08 (d, J = 8.6 Hz, 2H), 7.36 (dt, J = 14.0, 6.9 Hz, 3H), 7.20 (d, J = 7.2 Hz, 2H), 6.66 (s, 1H), 4.14 (s, 2H), 2.52 (s, 3H), 2.41 (s, 3H).**^{13}C NMR (100 MHz, $CDCl_3$)** δ 195.6, 194.6, 193.9, 158.3, 150.6, 149.9, 140.7, 137.1, 129.3, 128.4, 127.7, 124.0, 122.6, 109.6, 57.7, 45.1, 29.3, 14.6. **HRMS (ESI)** calcd for $C_{23}H_{20}NO_6$ $[M+H]^+$ 406.1291, found 406.1283.

2-(4-acetyl-5-methylfuran-2-yl)-4-oxo-2-phenyl-4-(thiophen-3-yl)butanal (3qa):



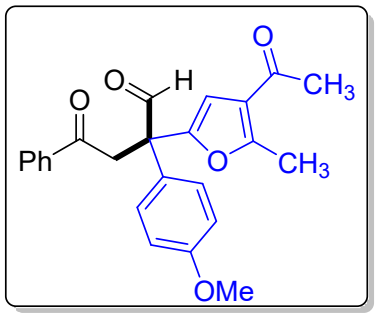
The title compound was prepared from **1q** (54.3 mg, 0.3 mmol) and **2a** (63.6 mg, 0.3 mmol) according to general procedure **A**. Purification using column chromatography (R_f = 0.50, SiO_2, EtOAc:Hexane, 5:95) gave pure product as a dark brown colour sticky solid (65.8 mg, 65% yield).**^{1}H NMR (400 MHz, $CDCl_3$)** δ 10.03 (s, 1H), 7.74 (dd, J = 3.8, 1.0 Hz, 1H), 7.65 (dd, J = 4.9, 1.0 Hz, 1H), 7.40 – 7.34 (m, 2H), 7.32 (dd, J = 5.3, 1.8 Hz, 1H), 7.24 – 7.20 (m, 2H), 7.12 (dd, J = 4.9, 3.9 Hz, 1H), 6.66 (s, 1H), 4.06 (s, 2H), 2.50 (s, 3H), 2.39 (s, 3H).**^{13}C NMR (100 MHz, $CDCl_3$)** δ 195.9, 194.1, 188.9, 158.3, 150.3, 143.4, 137.3, 134.5, 132.5, 129.2, 128.3, 128.2, 127.8, 122.4, 109.7, 57.5, 45.3, 29.3, 14.5. **HRMS (ESI)** calcd for $C_{21}H_{18}NaO_4S$ $[M+H]^+$ 389.0823, found 389.0829.

2-(4-acetyl-5-methylfuran-2-yl)-4-oxo-4-phenyl-2-(p-tolyl)butanal (3ab):



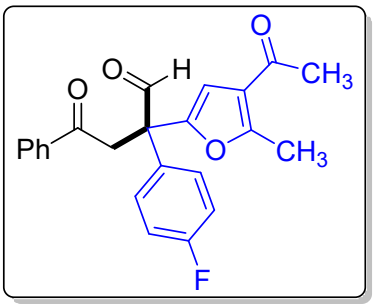
The title compound was prepared from **1a** (52.5 mg, 0.3 mmol) and **2b** (67.8 mg, 0.3 mmol) according to general procedure **A**. Purification using column chromatography (R_f = 0.50, SiO_2, EtOAc:Hexane, 5:95) gave pure product as a yellow colour sticky solid (78.5 mg, 70% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 10.05 (s, 1H), 7.94 (d, J = 7.3 Hz, 2H), 7.58 (t, J = 7.4 Hz, 1H), 7.46 (t, J = 7.7 Hz, 2H), 7.17 (d, J = 8.2 Hz, 2H), 7.11 (d, J = 8.3 Hz, 2H), 6.63 (s, 1H), 4.13 (d, J = 2.1 Hz, 2H), 2.49 (s, 3H), 2.39 (s, 3H), 2.34 (s, 3H).**^{13}C NMR (100 MHz, $CDCl_3$)** δ 196.4, 196.1, 194.1, 158.1, 150.9, 138.0, 136.3, 134.4, 133.7, 129.8, 128.8, 128.3, 127.6, 122.4, 109.2, 57.0, 45.1, 29.3, 21.1, 14.5. **HRMS (ESI)** calcd for $C_{24}H_{23}O_4$ $[M+H]^+$ 375.1596, found 375.1588.

2-(4-acetyl-5-methylfuran-2-yl)-2-(4-methoxyphenyl)-4-oxo-4-phenylbutanal (3ac):



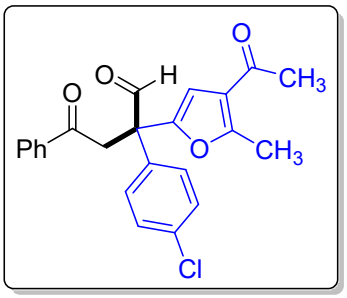
The title compound was prepared from **1a** (52.5 mg, 0.3 mmol) and **2c** (72.6 mg, 0.3 mmol) according to general procedure **A**. Purification using column chromatography (R_f = 0.4, SiO_2, EtOAc:Hexane, 8:92) gave pure product as a sticky solid (80.7 mg, 69% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 10.02 (s, 1H), 7.94 (dd, J = 8.3, 1.2 Hz, 2H), 7.61 – 7.54 (m, 1H), 7.45 (td, J = 7.6, 3.6 Hz, 2H), 7.16 – 7.12 (m, 2H), 6.91 – 6.87 (m, 2H), 6.63 (s, 1H), 4.11 (d, J = 3.7 Hz, 2H), 3.80 (s, 3H), 2.49 (s, 3H), 2.39 (s, 3H).**^{13}C NMR (100 MHz, $CDCl_3$)** δ 196.2, 196.2, 194.1, 159.4, 158.1, 150.9, 136.3, 133.7, 129.2, 129.0, 128.8, 128.3, 122.4, 114.5, 109.2, 56.7, 55.4, 45.1, 29.3, 14.5. **HRMS (ESI)** calcd for $C_{24}H_{23}O_5$ $[M+H]^+$ 391.1545, found 391.1537.

2-(4-acetyl-5-methylfuran-2-yl)-2-(4-fluorophenyl)-4-oxo-4-phenylbutanal (3ad):



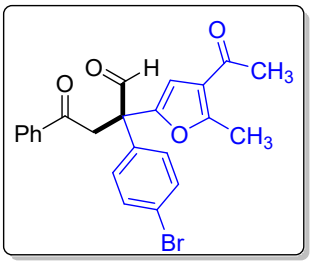
The title compound was prepared from **1a** (52.5 mg, 0.3 mmol) and **2d** (69 mg, 0.3 mmol) according to general procedure **A**. Purification using column chromatography (R_f = 0.50, SiO_2, EtOAc:Hexane, 5:95) gave pure product as a pale brown sticky solid(77 mg, 68% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 10.06 (s, 1H), 7.98 – 7.91 (m, 2H), 7.59 (ddd, *J* = 6.9, 2.4, 1.2 Hz, 1H), 7.46 (dd, *J* = 10.6, 4.8 Hz, 2H), 7.24 – 7.17 (m, 2H), 7.05 (ddd, *J* = 12.2, 6.2, 2.7 Hz, 2H), 6.63 (s, 1H), 4.13 (d, *J* = 3.0 Hz, 2H), 2.51 (s, 3H), 2.40 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 196.2, 195.9, 194.0, 163.6, 161.2, 158.4, 150.5, 136.1, 133.9, 133.4, 129.7, 129.6, 128.9, 128.3, 122.5, 116.1, 115.9, 109.5, 56.7, 45.5, 29.3, 14.5. **HRMS (ESI)** calcd for $C_{23}H_{20}FO_4$ $[M+H]^+$ 379.1346, found 379.1335.

2-(4-acetyl-5-methylfuran-2-yl)-2-(4-chlorophenyl)-4-oxo-4-phenylbutanal (3ae):



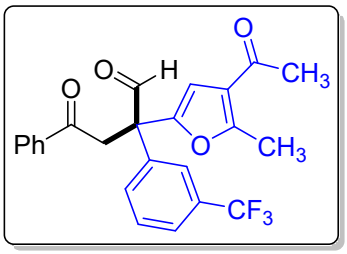
The title compound was prepared from **1a** (52.5 mg, 0.3 mmol) and **2e** (73.8 mg, 0.3 mmol) according to general procedure **A**. Purification using column chromatography (R_f = 0.50, SiO_2, EtOAc:Hexane, 5:95) gave pure product as a pale brown sticky solid(78 mg, 66% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 10.08 (s, 1H), 7.96 (dt, *J* = 8.5, 1.6 Hz, 2H), 7.64 – 7.59 (m, 1H), 7.52 – 7.46 (m, 2H), 7.37 – 7.33 (m, 2H), 7.22 – 7.18 (m, 2H), 6.65 (s, 1H), 4.15 (d, *J* = 3.7 Hz, 2H), 2.53 (s, 3H), 2.42 (s, 3H).**^{13}C NMR (125 MHz, $CDCl_3$)** δ 196.1, 195.8, 194.0, 158.5, 150.2, 136.2, 136.0, 134.2, 133.9, 129.3, 129.2, 128.9, 128.3, 122.5, 109.5, 56.8, 45.4, 29.3, 14.5. **HRMS (ESI)** calcd for $C_{23}H_{20}ClO_4$ $[M+H]^+$ 395.1050, found 395.1040.

2-(4-acetyl-5-methylfuran-2-yl)-2-(4-bromophenyl)-4-oxo-4-phenylbutanal (3af):



The title compound was prepared from **1a** (52.5 mg, 0.3 mmol) and **2f** (86.7 mg, 0.3 mmol) according to general procedure **A**. Purification using column chromatography (R_f = 0.50, SiO_2, EtOAc:Hexane, 5:95) gave pure product as a brown colour sticky solid (84 mg, 64% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 10.06 (s, 1H), 8.14 – 7.65 (m, 2H), 7.60 (dd, *J* = 10.5, 4.3 Hz, 1H), 7.53 – 7.42 (m, 5H), 7.15 – 7.07 (m, 2H), 6.62 (s, 1H), 4.13 (d, *J* = 3.8 Hz, 2H), 2.51 (s, 3H), 2.40 (s, 3H).**^{13}C NMR (100 MHz, $CDCl_3$)** δ 196.0, 195.8, 193.9, 158.5, 150.2, 136.8, 136.0, 133.9, 132.2, 129.6, 128.8, 128.3, 122.5, 122.4, 109.6, 56.8, 45.3, 29.3, 14.5. **HRMS (ESI)** calcd for $C_{23}H_{20}BrO_4$ $[M+H]^+$ 439.0545, found 439.0535.

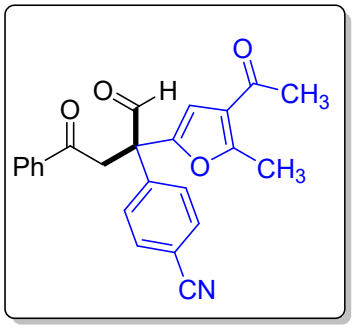
2-(4-acetyl-5-methylfuran-2-yl)-4-oxo-4-phenyl-2-(3-(trifluoromethyl) phenyl) butanal (3ag):



The title compound was prepared from **1a** (52.5 mg, 0.3 mmol) and **2g** (84 mg, 0.3 mmol) according to general procedure **A**. Purification using column chromatography (R_f = 0.5, SiO_2, EtOAc:Hexane, 5:95) gave pure product as a brown colour sticky solid (79.6 mg, 62% yield).**^{1}H NMR (500 MHz, $CDCl_3$)** δ 10.10 (s, 1H), 7.93 (dd, *J* = 8.3, 1.1 Hz, 2H), 7.59 (dt, *J* 15.4, 4.5 Hz, 2H), 7.46 (ddd, *J* = 22.8, 11.1, 5.3 Hz, 5H), 6.65 (s, 1H), 4.25 – 4.02 (m, 2H), 2.51 (s, 3H), 2.40 (s, 3H).**^{13}C NMR (100 MHz, $CDCl_3$)** δ 196.0, 195.7, 193.9, 158.7, 149.9, 139.0, 136.0,

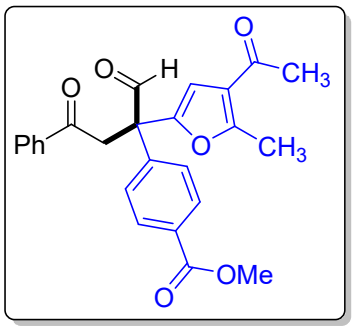
134.0, 131.5, 129.6, 128.9, 128.3, 125.1, 125.0, 124.6, 124.6, 122.6, 109.8, 57.1, 45.6, 29.3, 14.5. **HRMS (ESI)** calcd for $C_{24}H_{20}F_3O_4$ $[M+H]^+$ 429.1314, found 429.1313.

Methyl 4-(2-(4-acetyl-5-methylfuran-2-yl)-1,4-dioxo-4-phenylbutan-2-yl) benzoate (3ah):



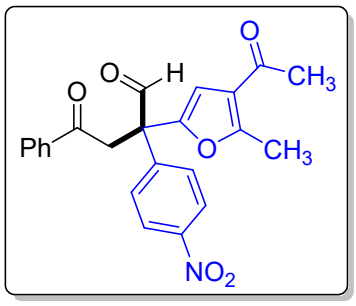
The title compound was prepared from **1a** (52.5 mg, 0.3 mmol) and **2h** (71.1 mg, 0.3 mmol) according to general procedure **A**. Purification using column chromatography (R_f = 0.3, SiO_2, EtOAc:Hexane, 12:88) gave pure product as a brown sticky solid (70.4 mg, 61% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 10.09 (s, 1H), 7.93 (dd, *J* = 8.3, 1.1 Hz, 2H), 7.67 – 7.63 (m, 2H), 7.60 (dd, *J* = 4.9, 3.7 Hz, 1H), 7.48 (dd, *J* = 10.7, 4.8 Hz, 2H), 7.40 – 7.36 (m, 2H), 6.64 (s, 1H), 4.17 (d, *J* = 2.3 Hz, 2H), 2.53 (s, 3H), 2.41 (s, 3H).**^{13}C NMR (125 MHz, $CDCl_3$)** δ 195.6, 195.5, 193.7, 158.9, 149.5, 143.8, 143.2, 142.3, 135.7, 134.1, 132.7, 129.0, 128.8, 128.3, 122.6, 118.4, 112.1, 109.9, 57.2, 45.6, 29.3, 14.6. **HRMS (ESI)** calcd for $C_{24}H_{20}NO_4$ $[M+H]^+$ 386.1392, found 386.1385.

2-(4-acetyl-5-methylfuran-2-yl)-2-(4-nitrophenyl)-4-oxo-4-phenylbutanal (3ai):



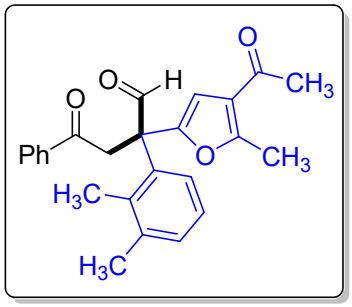
The title compound was prepared from **1a** (52.5 mg, 0.3 mmol) and **2i** (81 mg, 0.3 mmol) according to general procedure **A**. Purification using column chromatography (R_f = 0.30, SiO_2, EtOAc:Hexane, 10:90) gave pure product as a pale brown sticky solid (75.2 mg, 60% yield). **1H NMR (400 MHz, CDCl3)** δ 10.11 (s, 1H), 8.04 – 7.99 (m, 2H), 7.97 – 7.89 (m, 2H), 7.63 – 7.56 (m, 1H), 7.47 (dd, J = 10.7, 4.8 Hz, 2H), 7.36 – 7.30 (m, 2H), 6.63 (s, 1H), 4.18 (d, J = 1.8 Hz, 2H), 3.91 (s, 3H), 2.51 (s, 3H), 2.40 (s, 3H). **^{13}C NMR (125 MHz, $CDCl_3$)** δ 196.1, 195.7, 193.9, 166.6, 158.5, 150.2, 142.8, 136.0, 133.9, 130.2, 129.9, 128.9, 128.3, 127.9, 122.5, 109.6, 52.4, 45.4, 29.3, 14.5.**HRMS (ESI)** calcd for $C_{25}H_{23}O_6$ $[M+H]^+$ 419.1495, found 419.1479.

2-(4-acetyl-5-methylfuran-2-yl)-2-(4-nitrophenyl)-4-oxo-4-phenylbutanal (3aj):



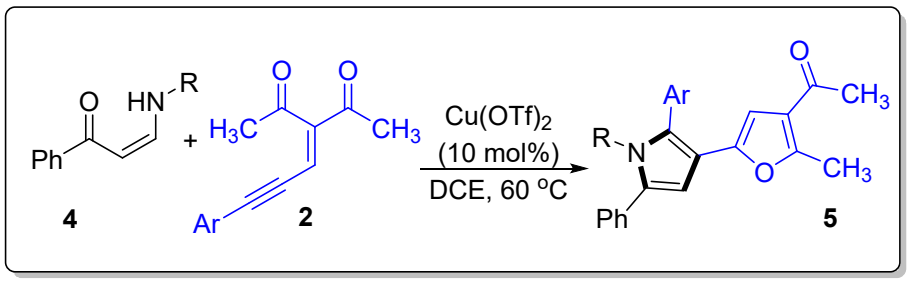
The title compound was prepared from **1a** (52.5 mg, 0.3 mmol) and **2j** (77.1 mg, 0.3 mmol) according to general procedure **A**. Purification using column chromatography (R_f = 0.3, SiO_2, EtOAc:Hexane, 15:85) gave pure product as a yellow colour sticky solid (72.9 mg, 60% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 10.11 (s, 1H), 8.20 (d, *J* = 8.9 Hz, 2H), 7.98 – 7.89 (m, 2H), 7.61 (d, *J* = 7.4 Hz, 1H), 7.47 (dd, *J* = 15.0, 8.3 Hz, 4H), 6.65 (s, 1H), 4.20 (d, *J* = 1.9 Hz, 2H), 2.53 (s, 3H), 2.41 (s, 3H).**^{13}C NMR (100 MHz, $CDCl_3$)** δ 195.5, 195.4, 193.7, 159.0, 149.5, 147.5, 145.2, 135.7, 134.2, 129.1, 129.0, 128.4, 124.0, 122.7, 110.0, 57.2, 45.7, 29.3, 14.6. **HRMS (ESI)** calcd for $C_{23}H_{20}NO_6$ $[M+H]^+$ 406.1291, found 406.1282.

2-(4-acetyl-5-methylfuran-2-yl)-2-(2,3-dimethylphenyl)-4-oxo-4-phenylbutanal(3ak):



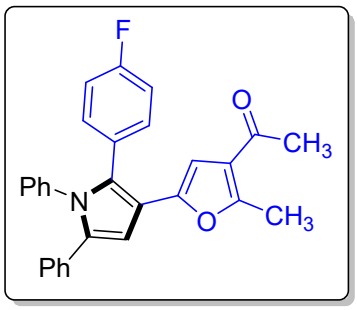
The title compound mixture was prepared from **1a** (52.5 mg, 0.3 mmol) and **2k** (72 mg, 0.3 mmol) according to general procedure **A**. Purification using column chromatography (R_f = 0.50, SiO_2, EtOAc:Hexane, 5:95) gave pure product as a sticky pale yellow sticky solid (80.3 mg, 69% yield**. ^{1}H NMR (500 MHz, $CDCl_3$)** δ 10.04 (s, 1H), 7.99 – 7.90 (m, 2H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.7 Hz, 2H), 7.12 (d, *J* = 7.9 Hz, 1H), 6.98 (d, *J* = 1.6 Hz, 1H), 6.93 (dd, *J* = 7.9, 1.9 Hz, 1H), 6.64 (s, 1H), 4.12 (d, *J* = 6.3 Hz, 2H), 2.49 (s, 3H), 2.39 (s, 3H), 2.24 (s, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 196.4, 196.2, 194.2, 158.0, 151.0, 137.5, 136.8, 136.4, 134.8, 133.7, 130.4, 128.8, 128.3, 125.1, 122.4, 109.2, 57.0, 45.0, 29.3, 20.2, 19.5, 14.5. **HRMS (ESI)** calcd for $C_{25}H_{25}O_4$ $[M+H]^+$ 389.1753, found 389.1741.

General procedure-B for the synthesis of 2-ester polysubstituted 1*H*-pyrrole (5)



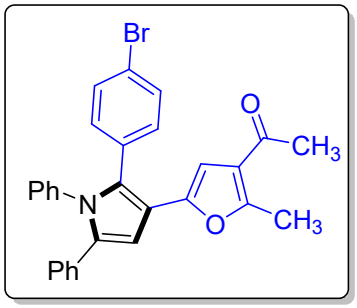
A mixture of enynone **2** (69 mg, 0.3 mmol) and $Cu(OTf)_2$ (10.8 mg, 0.1 mmol) in DCE (5 mL) was stirred at 60 °C for 1 min, and enaminone **4** (66.9 , 0.3 mmol) was added slowly at 60 °C. The reaction was monitored by TLC to ensure its completion. The reaction mixture was cooled to ambient temperature and evaporated all the volatiles under reduced pressure. The resultant residue was purified by silica gel column chromatography (eluent: EtOAc:Hexane = 5:95, v/v), affording **5** (78.3 mg, 60%) as a pale yellow solid.

1-(5-(2-(4-fluorophenyl)-1,5-diphenyl-1H-pyrrol-3-yl)-2-methylfuran-3-yl)ethan-1-one (5a):



The title compound was prepared from **4** (66.9 mg, 0.3 mmol) and **2d** (69 mg, 0.3 mmol) according to general procedure **B**. Purification using column chromatography (R_f = 0.50, SiO_2, EtOAc:Hexane, 5:95) gave pure product as a pale yellow solid (78.3 mg, 60% yield), mp 136-138 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.31 (dd, *J* = 8.9, 5.4 Hz, 2H), 7.26 – 7.24 (m, 2H), 7.23 (s, 2H), 7.16 (dd, *J* = 3.4, 1.4 Hz, 2H), 7.13 – 7.12 (m, 2H), 7.11 (dd, *J* = 3.4, 1.3 Hz, 2H), 6.98 (t, *J* = 8.8 Hz, 2H), 6.59 (s, 1H), 6.09 (s, 1H), 2.40 (s, 3H), 2.20 (s, 3H). **^{13}C NMR (125 MHz, $CDCl_3$)** δ 194.2, 162.8, 160.8, 158.2, 143.7, 138.8, 136.7, 132.3, 131.6, 129.5, 129.5, 128.8, 128.7, 128.6, 128.2, 128.0, 127.0, 126.3, 122.5, 121.4, 29.2, 14.4. **HRMS (ESI)** calcd for $C_{29}H_{23}FNO_2$ $[M+H]^+$ 436.1713, found 436.1741.

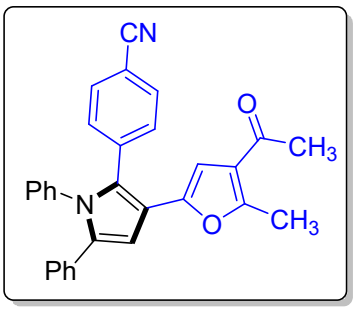
1-(5-(2-(4-bromophenyl)-1,5-diphenyl-1H-pyrrol-3-yl)-2-methylfuran-3-yl)ethan-1-one (5b):



The title compound was prepared from **4** (66.9 mg, 0.3 mmol) and **2f** (86.7 mg, 0.3 mmol) according to general procedure **B**. Purification using column chromatography (R_f = 0.50, SiO_2, EtOAc:Hexane, 5:95) gave pure product as a pale yellow solid (90.5 mg, 61% yield), mp 142-144 °C. **^{1}H NMR (400**

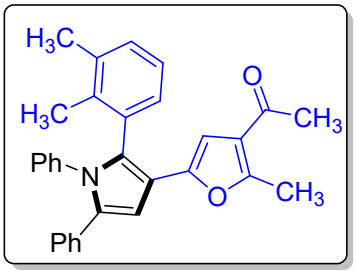
MHz, $CDCl_3$) δ 7.45 – 7.43 (m, 1H), 7.43 – 7.41 (m, 1H), 7.28 (dd, *J* = 5.0, 1.9 Hz, 3H), 7.26 – 7.23 (m, 2H), 7.21 – 7.17 (m, 3H), 7.16 – 7.12 (m, 4H), 6.63 (s, 1H), 6.14 (s, 1H), 2.44 (s, 3H), 2.24 (s, 3H).**^{13}C NMR (100 MHz, $CDCl_3$)** δ 194.1, 158.3, 143.5, 138.7, 136.9, 134.5, 132.2, 131.5, 129.5, 128.8, 128.7, 128.6, 128.2, 128.0, 127.1, 126.0, 122.5, 121.5, 120.3, 112.2, 109.7, 29.2, 14.4. **HRMS (ESI)** calcd for $C_{29}H_{23}BrNO_2$ $[M+H]^+$ 496.0912, found 496.0915.

4-(3-(4-acetyl-5-methylfuran-2-yl)-1,5-diphenyl-1H-pyrrol-2-yl) benzonitrile (5c):



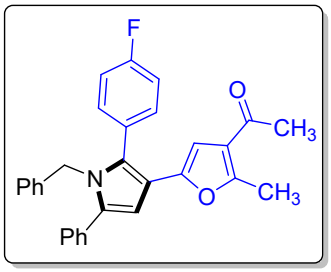
The title compound was prepared from **4** (66.9 mg, 0.3 mmol) and **2h** (132.6 mg, 0.3 mmol) according to general procedure **B**. Purification using column chromatography (R_f = 0.50, SiO_2, EtOAc:Hexane, 5:95) gave pure product as a pale yellow solid (79.5 mg, 60% yield), mp 150-152 °C. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.58 – 7.53 (m, 2H), 7.43 – 7.38 (m, 2H), 7.26 – 7.24 (m, 2H), 7.22 (s, 1H), 7.18 – 7.14 (m, 3H), 7.12 – 7.07 (m, 4H), 6.63 (s, 1H), 6.11 (s, 1H), 2.41 (s, 3H), 2.20 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 193.9, 158.5, 143.0, 140.4, 138.3, 137.4, 132.2, 131.9, 128.9, 128.6, 128.3, 128.2, 127.3, 125.2, 122.6, 122.3, 119.4, 112.5, 109.6, 109.5, 29.1, 14.4. **HRMS (ESI)** calcd for $C_{30}H_{23}N_2O_2$ $[M+H]^+$ 443.1760, found 443.1748.

1-(5-(2-(2,3-dimethylphenyl)-1,5-diphenyl-1H-pyrrol-3-yl)-2-methylfuran-3-yl)ethan-1-one (5d):

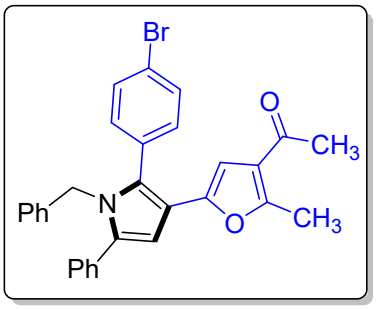


The title compound was prepared from **4** (66.9 mg, 0.3 mmol) and **2j** (72 mg, 0.3 mmol) according to general procedure **B**. Purification using column chromatography (R_f = 0.50, SiO_2, EtOAc:Hexane, 5:95) gave pure product as a pale yellow solid (89.4 mg, 67% yield), mp 140-142 °C. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.26 (s, 1H), 7.19 – 7.14 (m, 6H), 7.11 (dd, *J* = 7.9, 1.6 Hz, 2H), 6.97 (dd, *J* = 7.1, 5.2 Hz, 4H), 6.88 (dd, *J* = 6.4, 5.0 Hz, 1H), 6.76 (s, 1H), 6.07 (s, 1H), 2.57 (s, 3H), 2.27 (s, 3H), 2.22 (s, 3H), 2.14 (s, 3H).**^{13}C NMR (100 MHz, $CDCl_3$)** δ 208.2, 136.0, 134.9, 132.5, 129.3, 129.0, 128.6, 128.1, 127.3, 126.6, 122.8, 113.5, 107.8, 103.8, 29.2, 19.7, 14.5. **HRMS (ESI)** calcd for $C_{31}H_{28}NO_2$ $[M+H]^+$ 446.2120, found 446.2102.

1-(5-(1-benzyl-2-(4-fluorophenyl)-5-phenyl-1H-pyrrol-3-yl)-2-methylfuran-3-yl)ethan-1-one (5e): The title compound was prepared from **4** (71.1 mg, 0.3 mmol) and **2d** (69 mg, 0.5 mmol) according to general procedure **B**. Purification using column chromatography (R_f = 0.50, SiO_2, EtOAc:Hexane, 5:95) gave pure product as a white colour solid (78.1 mg, 58% yield), mp 145-147 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.36 – 7.31 (m, 3H), 7.30 (d, *J* = 1.8 Hz, 1H), 7.28 (dd, *J* = 3.5, 1.7 Hz, 1H), 7.22 (dddd, *J* = 7.7, 4.3, 2.4, 1.8 Hz, 3H), 7.18 – 7.14 (m, 2H), 6.94 – 6.88 (m, 2H), 6.83 – 6.79 (m, 2H), 6.44 (s, 1H), 6.18 (s, 1H), 5.09 (s, 2H), 2.42 (s, 3H), 2.18 (s, 3H). **^{13}C NMR (125 MHz, $CDCl_3$)** δ 194.2, 162.6, 160.7, 158.5, 143.8, 139.0, 137.5, 132.7, 131.7, 129.2, 129.1, 128.7, 128.6, 127.9, 127.2, 126.3, 126.0, 122.5, 120.1, 115.3, 115.2, 112.2, 109.5, 49.2, 29.2, 14.5. **HRMS (ESI)** calcd for $C_{30}H_{25}FNO_2$ $[M+H]^+$ 450.1869, found 450.1860.

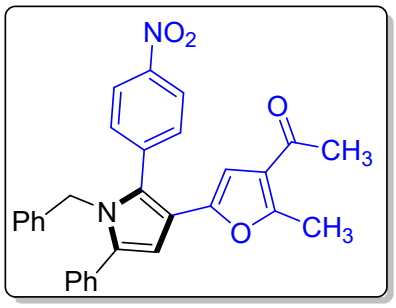


1-(5-(1-benzyl-2-(4-bromophenyl)-5-phenyl-1H-pyrrol-3-yl)-2-methylfuran-3-yl)ethan-1-one (5f):



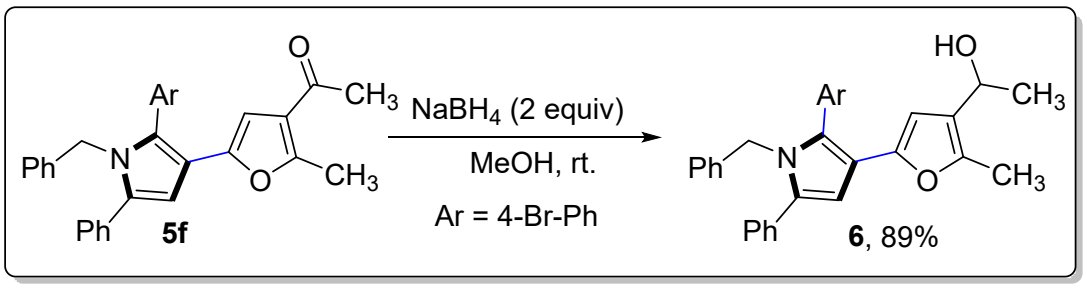
The title compound was prepared from **4** (71.1 mg, 0.3 mmol) and **2f** (86.7 mg, 0.3 mmol) according to general procedure **B**. Purification using column chromatography (R_f = 0.50, SiO_2, EtOAc:Hexane, 5:95) gave pure product as a white colour solid (91.6 mg, 60% yield), mp 148-150 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.41 – 7.37 (m, 4H), 7.34 (dt, *J* = 6.6, 4.2 Hz, 3H), 7.23 (s, 1H), 7.20 (dt, *J* = 4.6, 3.2 Hz, 4H), 6.86 (d, *J* = 6.7 Hz, 2H), 6.51 (s, 1H), 6.26 (s, 1H), 5.14 (s, 2H), 2.48 (s, 3H), 2.25 (s, 3H). **^{13}C NMR (75 MHz, $CDCl_3$)** δ 194.1, 158.7, 143.6, 138.9, 137.6, 134.6, 132.6, 131.5, 129.1, 128.7, 128.6, 127.9, 127.2, 126.0, 122.5, 120.2, 120.0, 112.4, 109.3, 49.2, 29.2, 14.5. **HRMS (ESI)** calcd for $C_{30}H_{25}BrNO_2$ $[M+H]^+$ 510.1069, found 510.1093.

1-(5-(1-benzyl-2-(4-nitrophenyl)-5-phenyl-1H-pyrrol-3-yl)-2-methylfuran-3-yl)ethan-1-one (5g):



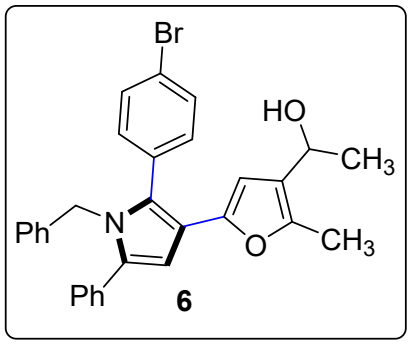
The title compound was prepared from **4** (71.1 mg, 0.3 mmol) and **2j** (77.1 mg, 0.3 mmol) according to general procedure **B**. Purification using column chromatography (R_f = 0.50, SiO_2, EtOAc:Hexane, 5:95) gave pure product as a white colour solid (78.5 mg, 55% yield), mp 155-157 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.17 – 8.04 (m, 2H), 7.46 – 7.43 (m, 1H), 7.42 (t, *J* = 2.2 Hz, 1H), 7.38 (qd, *J* = 6.4, 2.9 Hz, 5H), 7.25 (s, 1H), 7.24 – 7.19 (m, 2H), 6.90 – 6.81 (m, 2H), 6.60 (s, 1H), 6.31 (s, 1H), 5.15 (s, 2H), 2.50 (s, 3H), 2.26 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 193.9, 159.0, 145.9, 145.1, 143.0, 142.6, 138.5, 138.2, 132.2, 129.2, 128.8, 128.7, 128.3, 127.6, 127.4, 126.0, 124.9, 123.9, 122.7, 121.5, 112.9, 109.4, 49.3, 29.2, 14.5. **HRMS (ESI)** calcd for $C_{30}H_{25}N_2O_4$ $[M+H]^+$ 477.1814, found 477.1861.

General procedure for the synthesis of 6:

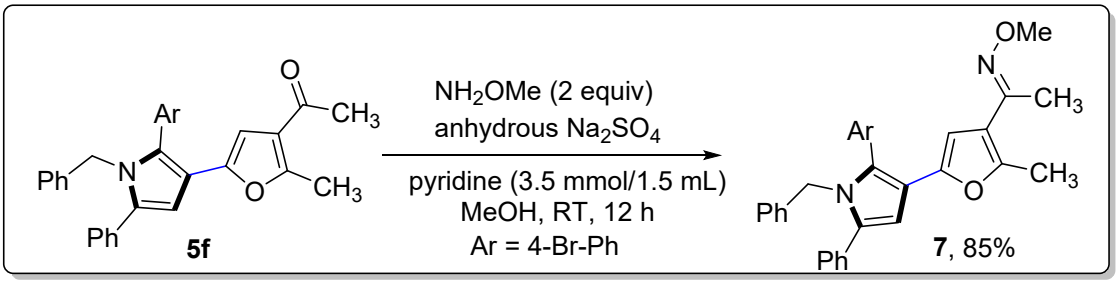


To a solution of **5f** (0.20 mmol, 102 mg) in MeOH (2 mL) was added $NaBH_4$ (0.40 mmol, 15.12 mg) at room temperature and the reaction mixture was stirred at the same temperature for 30 min under nitrogen atmosphere. The mixture was poured into H_2O (5 mL) and extracted with EtOAc (10 mL). The organic layer was washed with brine (10 mL) and dried with Na_2SO_4. After removal of the solvent, the residue was subjected to column chromatography to get **6** as brown color sticky solid (56.3 mg, 55% yield), (R_f = 0.4, SiO_2 EtOAc:Hexane, 10:90).

1-(5-(1-benzyl-2-(4-bromophenyl)-5-phenyl-1H-pyrrol-3-yl)-2-methylfuran-3-yl)ethan-1-ol (6): ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38 (t, *J* = 2.0 Hz, 2H), 7.36 (dd, *J* = 4.0, 1.5 Hz, 3H), 7.34 (d, *J* = 1.7 Hz, 1H), 7.33 – 7.31 (m, 1H), 7.26 (s, 1H), 7.22 (d, *J* = 1.9 Hz, 1H), 7.20 (d, *J* = 1.8 Hz, 2H), 7.19 (t, *J* = 1.9 Hz, 1H), 6.85 (d, *J* = 6.7 Hz, 2H), 6.49 (s, 1H), 6.04 (s, 1H), 5.14 (s, 2H), 4.74 (q, *J* = 6.4 Hz, 1H), 2.21 (s, 3H), 1.32 (d, *J* = 6.4 Hz, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 148.0, 143.4, 139.1, 137.1, 135.0, 132.9, 131.3, 129.2, 128.6, 128.5, 128.4, 127.7, 127.0, 126.9, 126.2, 125.1, 121.8, 119.7, 110.9, 109.2, 62.8, 49.2,24.0, 12.0. **HRMS (ESI)** calcd for $C_{30}H_{25}BrNO$ [M-OH] 494.1120, found 494.1109.

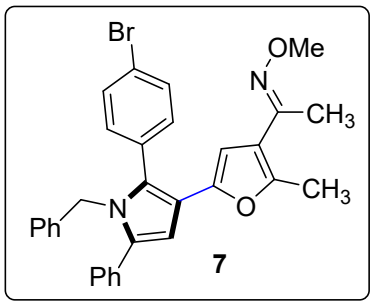


General Procedure for the Preparation of Oxime Ether 7:

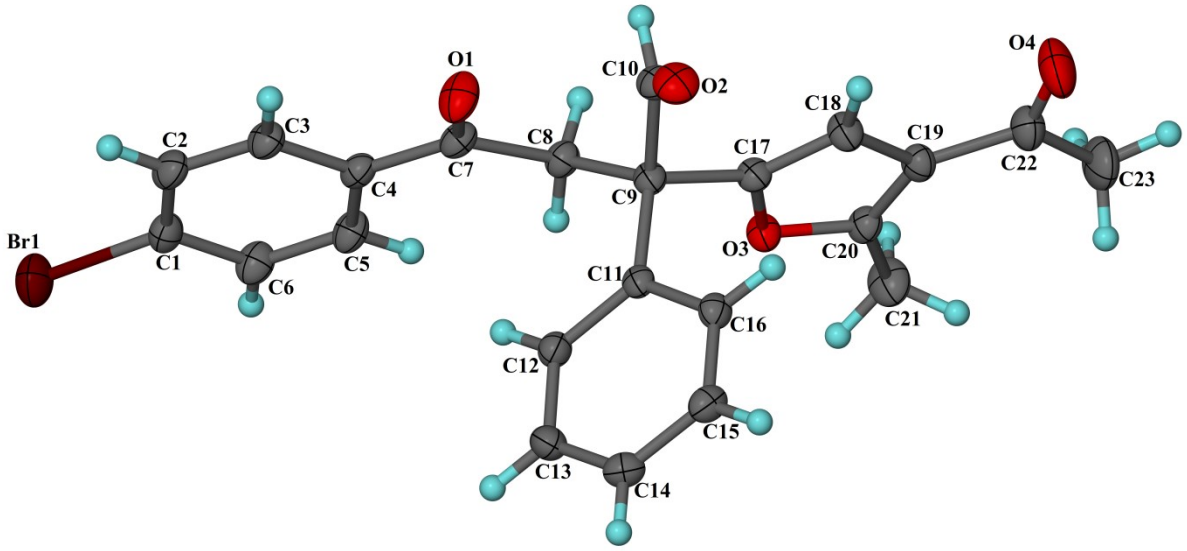


Compound **5f** (0.2 mmol, 102 mg), methoxylamine hydrochloride (0.4 mmol, 2.0 equiv, 33.2 mg), anhydrous Na_2SO_4 (.4 mmol, 2.0 equiv, 56.8 mg), pyridine (.2 mmol, 1.0 equiv, .016 ml), and methanol (2 ml) were added to a 10 ml round-bottom flask. The reaction mixture was stirred at room temperature overnight. The mixture was diluted with saturated NH_4Cl solution (25 mL) and extracted with EtOAc (3 × 25 mL). The organic layers were combined, washed with brine, and dried over anhydrous $MgSO_4$. The solvent was removed under vacuum, and the residue was purified by flash column chromatography (R_f = 0.8, SiO_2 EtOAc:Hexane, 2:98) as the eluent to give the desired product **7** (51.8 mg, 85% yield).

(E)-1-(5-(1-benzyl-2-(4-bromophenyl)-5-phenyl-1H-pyrrol-3-yl)-2-methylfuran-3-yl)ethan-1-one O-methyl oxime (7): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 – 7.38 (m, 5H), 7.38 – 7.31 (m, 3H), 7.28 – 7.19 (m, 4H), 6.93 – 6.78 (m, 2H), 6.53 (s, 1H), 6.16 (s, 1H), 5.17 (s, 2H), 3.94 (s, 3H), 2.42 (s, 3H), 2.00 (s, 3H).**^{13}C NMR (100 MHz, $CDCl_3$)** δ 150.8, 150.3, 143.3, 139.1, 137.2, 134.8, 132.9, 131.4, 129.1, 128.6, 128.5, 127.8, 127.1, 126.1, 125.3, 112.0, 109.3, 61.8, 49.1, 14.2, 14.1. **HRMS (ESI)** calcd for $C_{31}H_{28}BrN_2O_2$ $[M+H]^+$ 539.1334, found 539.1326.



5. X-ray crystallography data



Sample Preparation for Crystal Growth: The compound **3ha** was dissolved in $CDCl_3$ in beaker and kept for slow evaporation at room temperature. Formation of needle shape crystals was observed after seven days. The single crystals were then subjected to X-ray diffraction analysis.

Figure caption: ORTEP diagram of KB187 compound with the atom-numbering. Displacement ellipsoids are drawn at the 35% probability level and H atoms are shown as small spheres of arbitrary radius. **CCDC deposition number 2164031** contains the supplementary crystallographic data for this paper which can be obtained free of charge at https://www.ccdc.cam.ac.uk/structures/

Crystal data for KB187: $C_{23}H_{19}O_2Br_1$, M = 439.29, Monoclinic, Space group $P2_1/n$ (No. 14), a = 11.9543(16)Å, b = 13.1009(16)Å, c = 12.3965(14)Å, α = 90°, β = 98.422(3)°, γ = 90°, V = 1920.5(4)Å^3, Z = 4, D_c = 1.519 g/cm^3, F_{000} = 896, Bruker D8 QUEST PHOTON-III-C7 detector, Mo-Kα radiation, λ = 0.71073 Å, T = 293(2)K, $2\theta_{max}$ = 56º, μ= 2.167 mm^{-1}, 29016 reflections collected, 4708 unique (R_{int} = 0.0521), 255 parameters, *R1* = 0.0389, *wR2* =0.0939, *R* indices based on 3349 reflections with I > 2σ(I) (refinement on F^2), Final *GooF* = 1.026, largest difference hole and peak = -0.530 and 0.382 e.Å^{-3}.

Data collection and Structure solution details:

X-ray data for the compound were collected at room temperature on a Bruker D8 QUEST instrument with an IμS Mo microsource (λ = 0.7107 A) and a PHOTON-100 detector. The raw data frames were reduced and corrected for absorption effects using the Bruker Apex 3 software suite programs [1]. The structure was solved using intrinsic phasing method [2] and further refined with the SHELXL [2-3] program and expanded using Fourier techniques. Anisotropic displacement parameters were included for all non-hydrogen atoms. All C bound H atoms were positioned geometrically and treated as riding on their parent C atoms [C-H =

0.93-0.97 Å, and Uiso(H) = 1.5Ueq(C) for methyl H or 1.2Ueq(C) for other H atoms]. **CCDC deposition number 2164031** contains the supplementary crystallographic data for this paper which can be obtained free of charge at https://www.ccdc.cam.ac.uk/structures/

1. Bruker (2016). APEX3, SAINT and SADABS. Bruker AXS, Inc., Madison, Wisconsin, USA.
2. Sheldrick G. M. (2015).ActaCrystallogr C71: 3-8.
3. Muller, P, Herbst-Imer, R, Spek, A. L, Schneider, T. R, and Sawaya, M. R. Crystal Structure Refinement: A Crystallographer's Guide to SHELXL. Muller, P. Ed. 2006 Oxford University Press: Oxford, New York, pp. 57–91.

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) KB187_0m

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: KB187_0m

```
Bond precision:   C-C = 0.0030 A          Wavelength=0.71073

Cell:             a=11.9543(16)     b=13.1009(16)      c=12.3965(14)
                  alpha=90          beta=98.422(3)     gamma=90
Temperature:      293 K

                  Calculated                Reported
Volume            1920.5(4)                 1920.5(4)
Space group       P 21/n                    P 21/n
Hall group        -P 2yn                    -P 2yn
Moiety formula    C23 H19 Br O4             C23 H19 Br O4
Sum formula       C23 H19 Br O4             C23 H19 Br O4
Mr                439.28                    439.29
Dx,g cm-3         1.519                     1.519
Z                 4                         4
Mu (mm-1)         2.167                     2.167
F000              896.0                     896.0
F000'             895.26
h,k,lmax          15,17,16                  15,17,16
Nref              4784                      4708
Tmin,Tmax         0.551,0.634               0.612,0.746
Tmin'             0.540

Correction method= # Reported T Limits: Tmin=0.612 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.984           Theta(max)= 28.317

R(reflections)= 0.0389( 3349)                wR2(reflections)=
                                             0.1072( 4708)
S = 1.026                Npar= 255
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...     -0.879 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        74 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....        19 Note
```

Alert level G

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PLAT019_ALERT_1_G _diffrn_measured_fraction_theta_full/*_max < 1.0      0.994 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C23 Check
PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O3       .      107.3 Degree
PLAT793_ALERT_4_G Model has Chirality at C9          (Centro SPGR)          R Verify
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          1 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          7 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         12 Info
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   3 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  11 ALERT level G = General information/check it is not something unexpected

   4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   3 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
   3 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

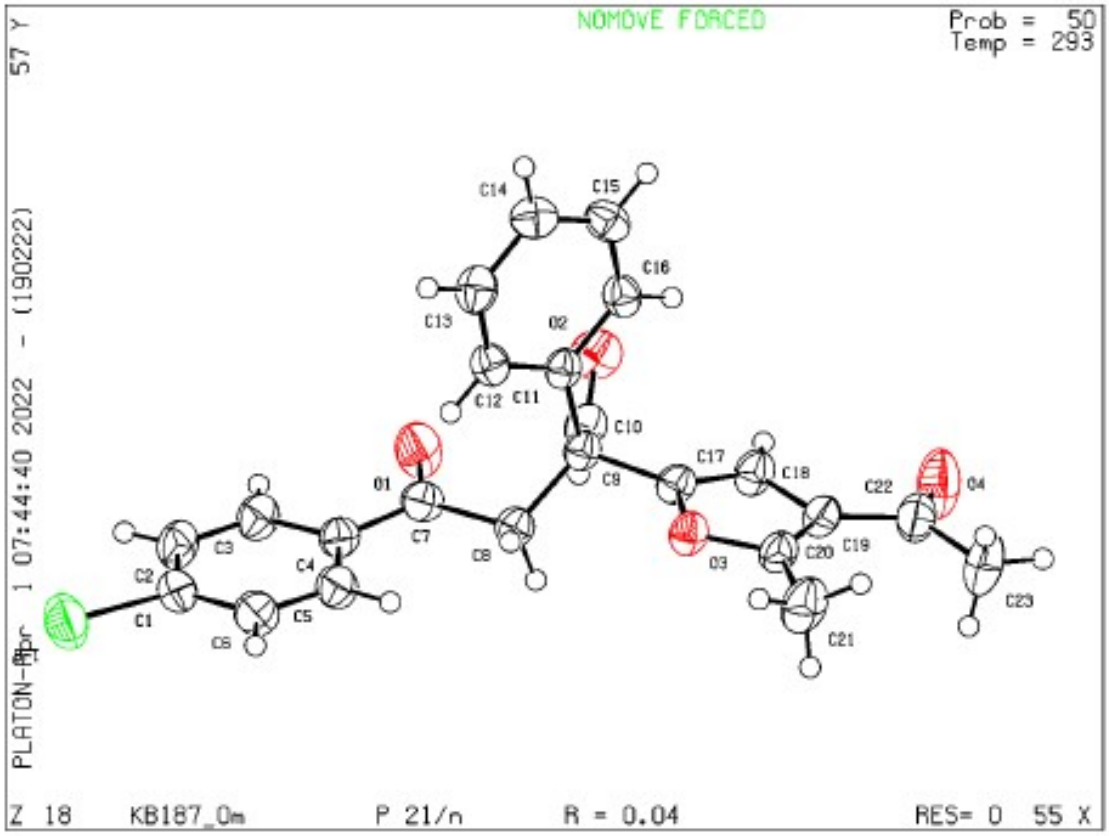
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

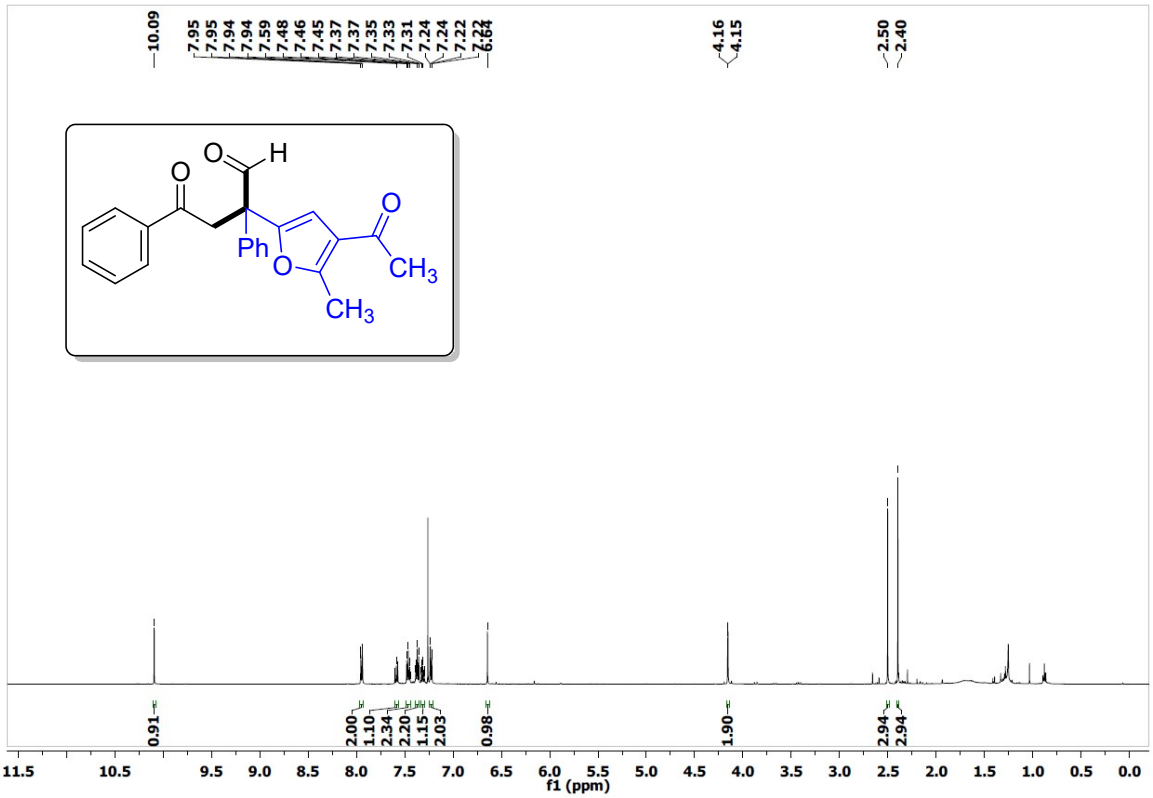
PLATON version of 19/02/2022; check.def file version of 19/02/2022

Datablock KB187_0m - ellipsoid plot



6. References

1) M. Ni, J. Zhang, X. Liang, Y. Jiang,T-P. Loh, *Chem. Commun*., 2017, **53**, 12286.
2) Y. Yu, Y. Chen, W. Wu, H. Jiang., *Chem. Commun*., 2017, **53**, 640.
3) Li, C.; Li, J.; Zhou, F.; Li, C.; Wu, W. *J. Org. Chem*., 2019, **84**, 11958.
4) H. Suzuki, S. Yoshioka, A. Igesaka, H. Nishioka, Y. Takeuchi, *Tetrahedron*., 2013, **69**, 6399.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7.33
7.31
7.24
7.24
7.22
7.22
6.64
4.16
4.15
2.50
2.40
O
H
O
Ph
O
O
CH3
CH3
0.91
2.00
1.10
2.34
2.20
1.15
2.03
0.98
1.90
2.94
2.94
11.5
10.5
9.5
9.0
8.5
8.0
7.5
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6.0
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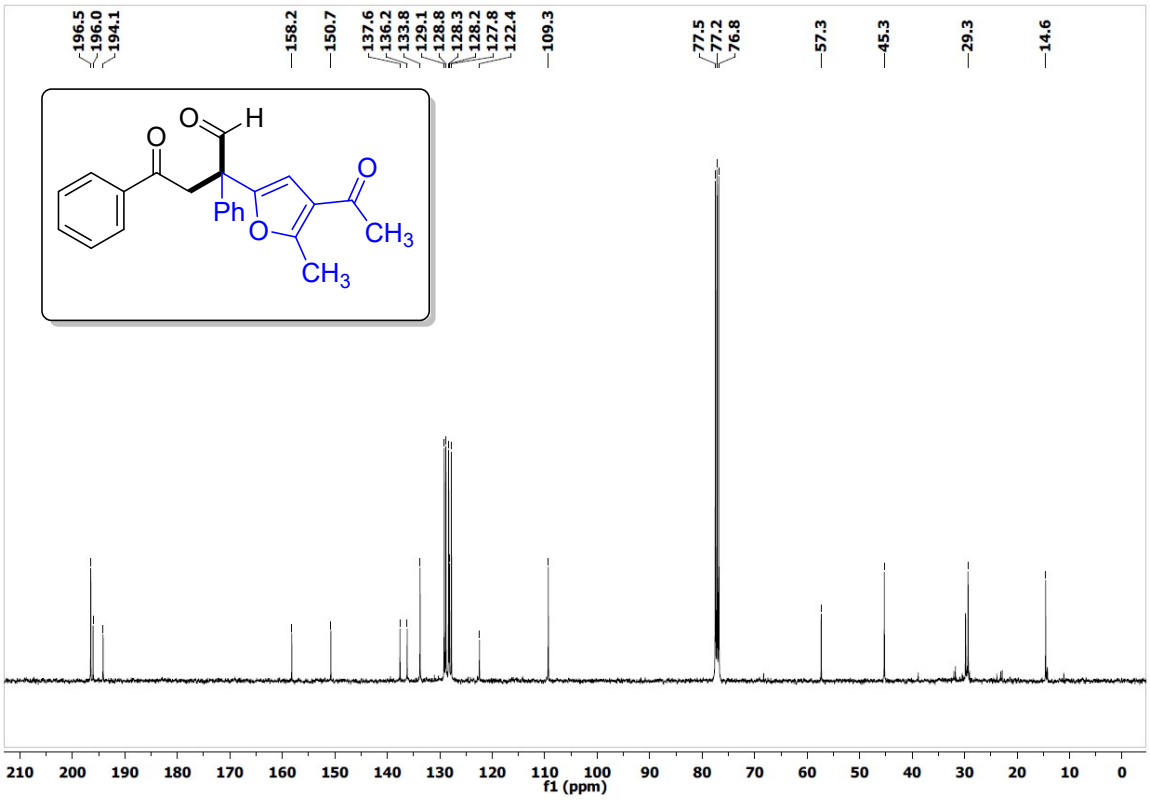
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137.6
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128.8
128.3
128.2
127.8
122.4
109.3
77.5
77.2
76.8
57.3
45.3
29.3
14.6
O
H
O
Ph
O
O
CH3
CH3
210
200
190
180
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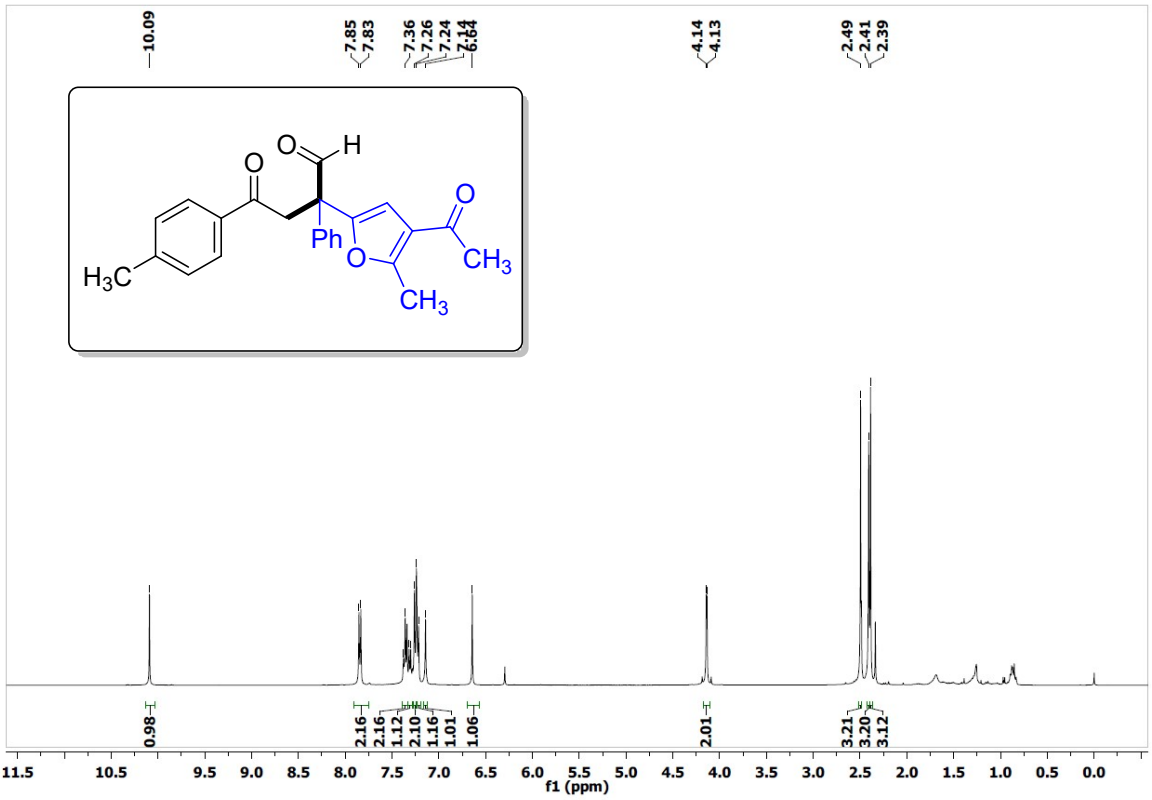
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O
Ph
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H3C
CH3
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2.16
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2.10
1.16
1.01
1.06
2.01
3.21
3.20
3.12
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10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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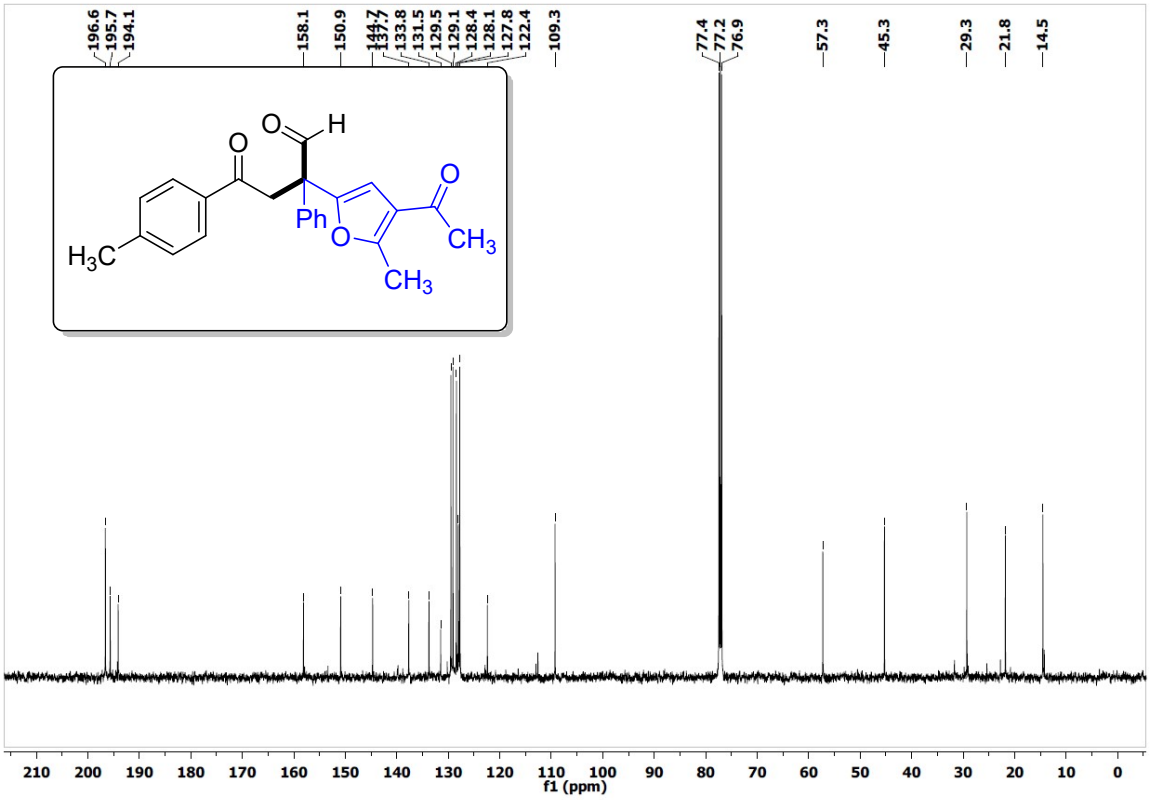
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77.2
76.9
57.3
45.3
29.3
21.8
14.5
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H
O
Ph
O
O
CH3
H3C
CH3
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180
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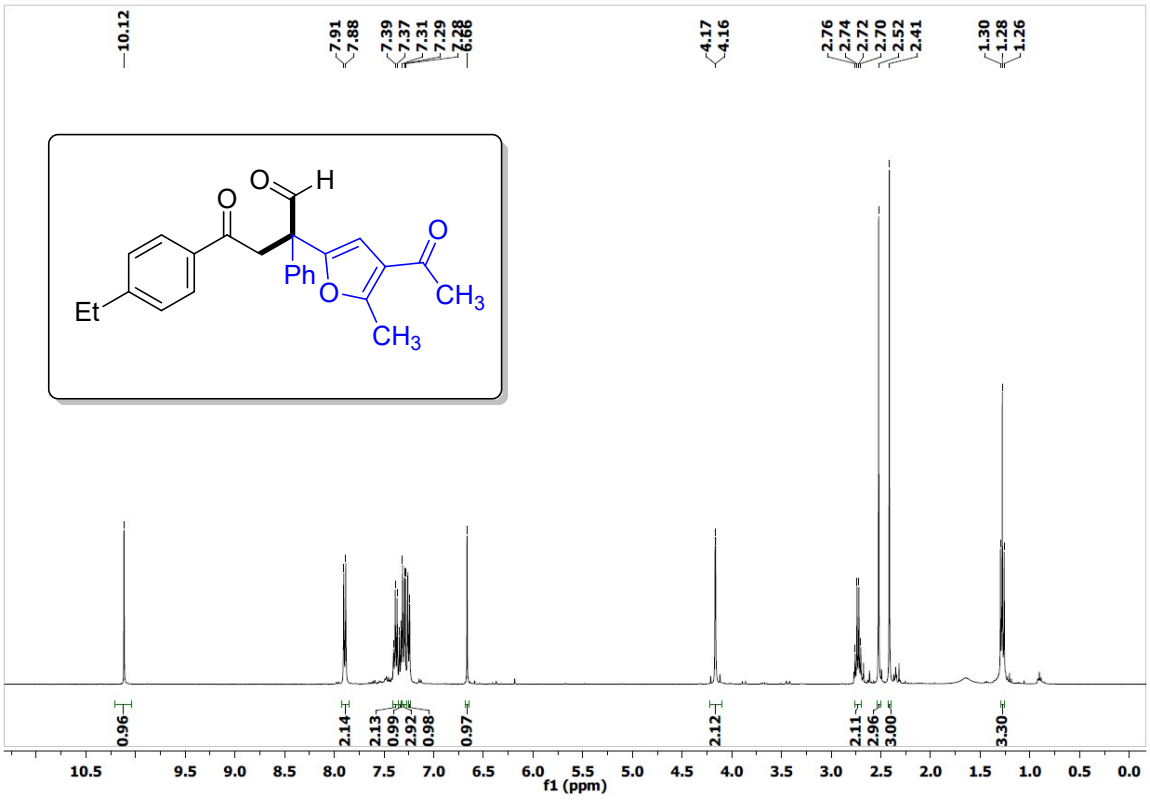
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1.26
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0.98
0.97
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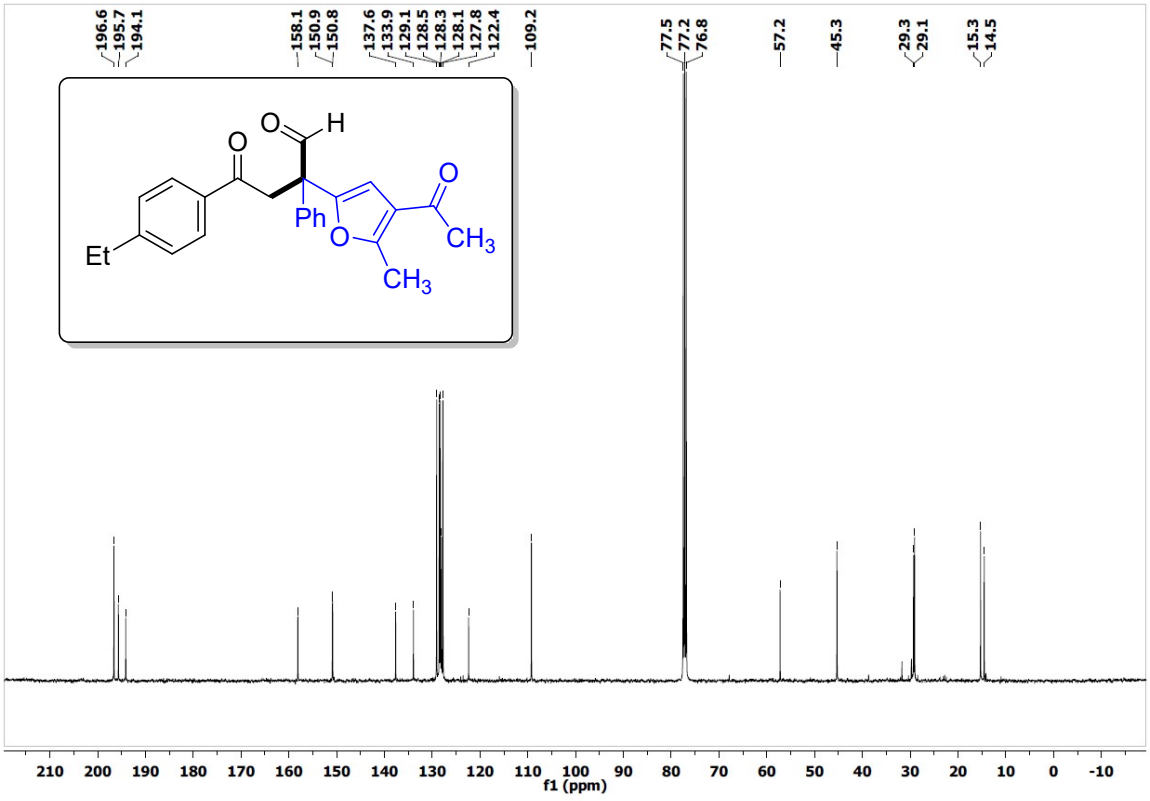
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76.8
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45.3
29.3
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H
O
Ph
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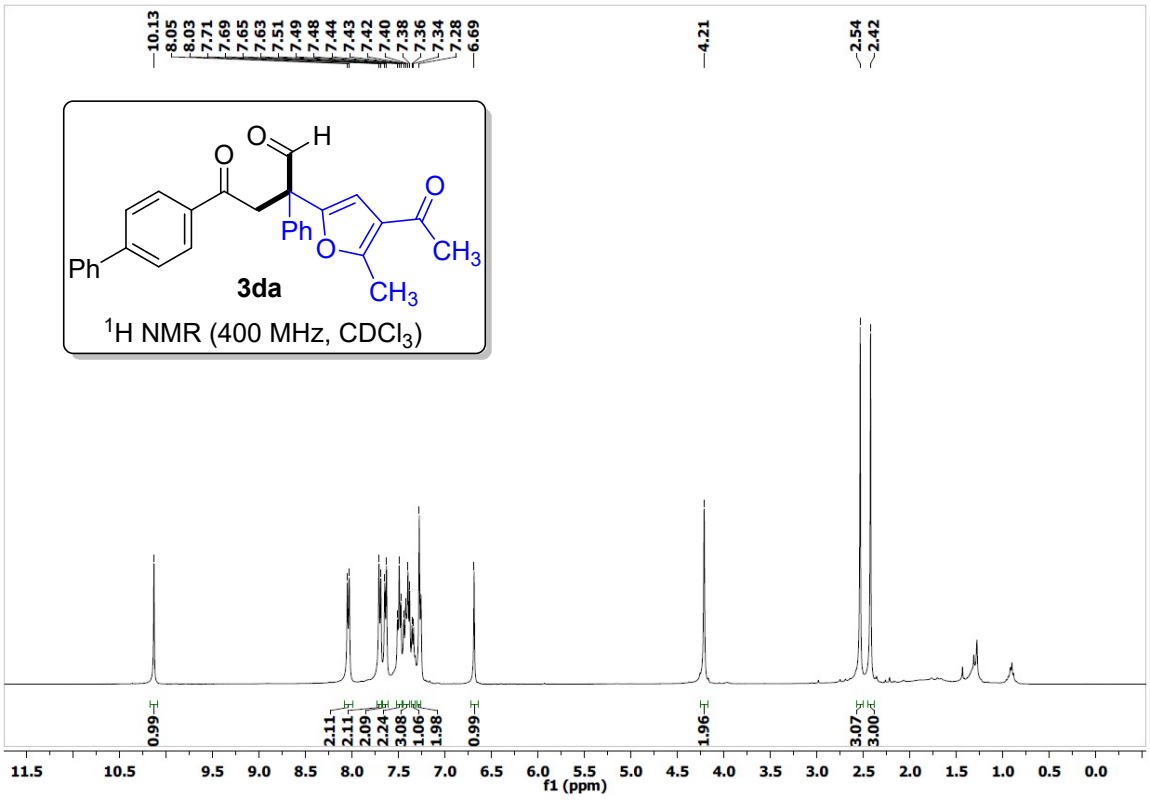
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Ph
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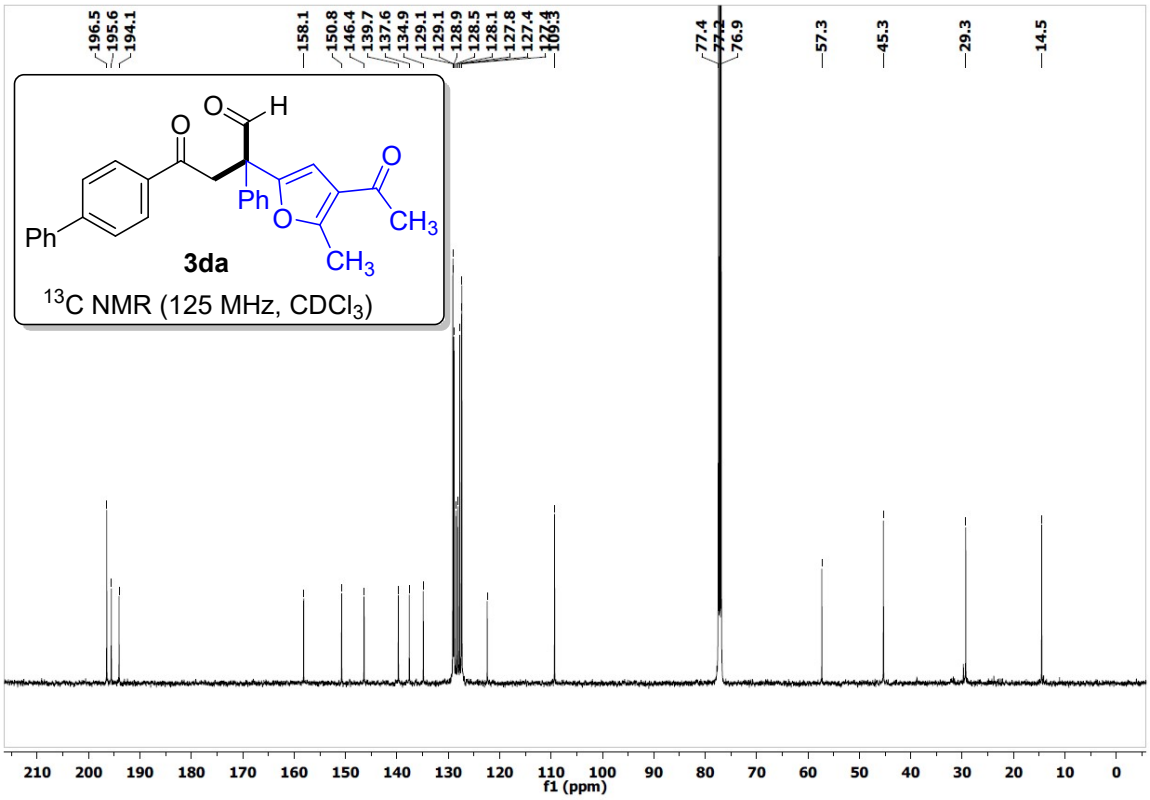
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76.9
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45.3
29.3
14.5
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H
O
O
Ph
O
CH3
Ph
CH3
3da
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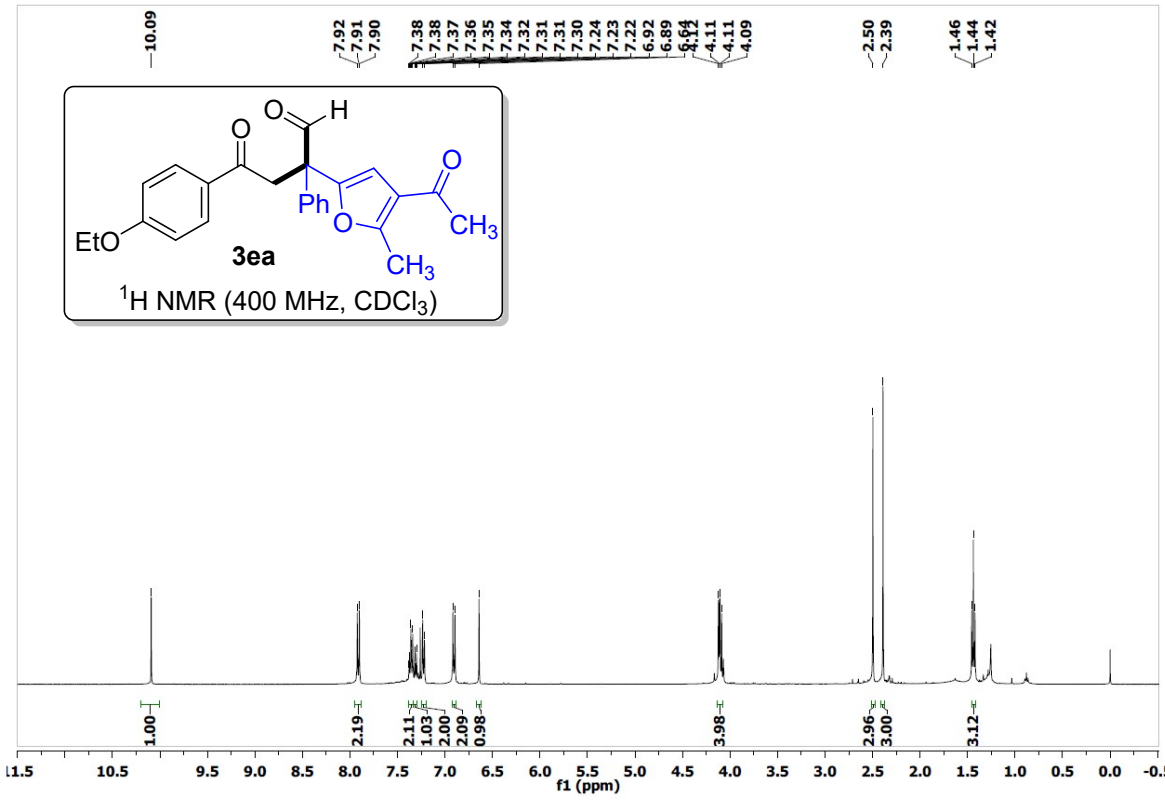
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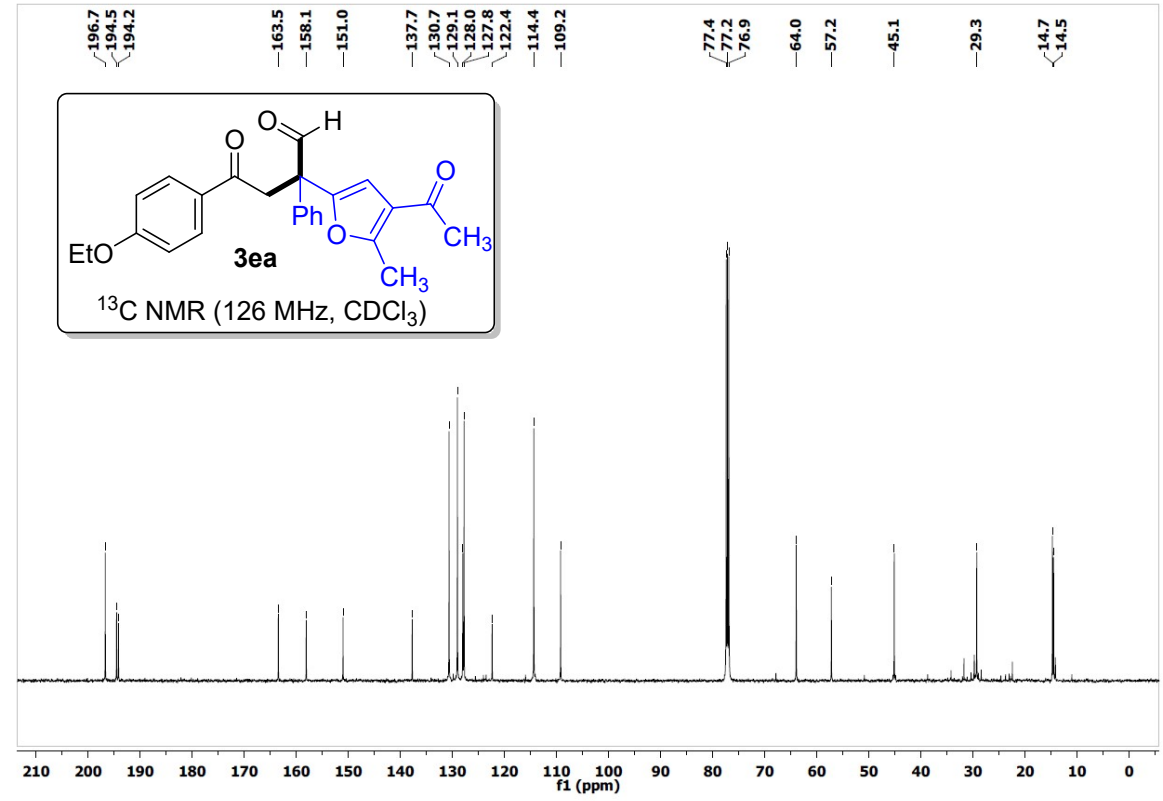
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76.9
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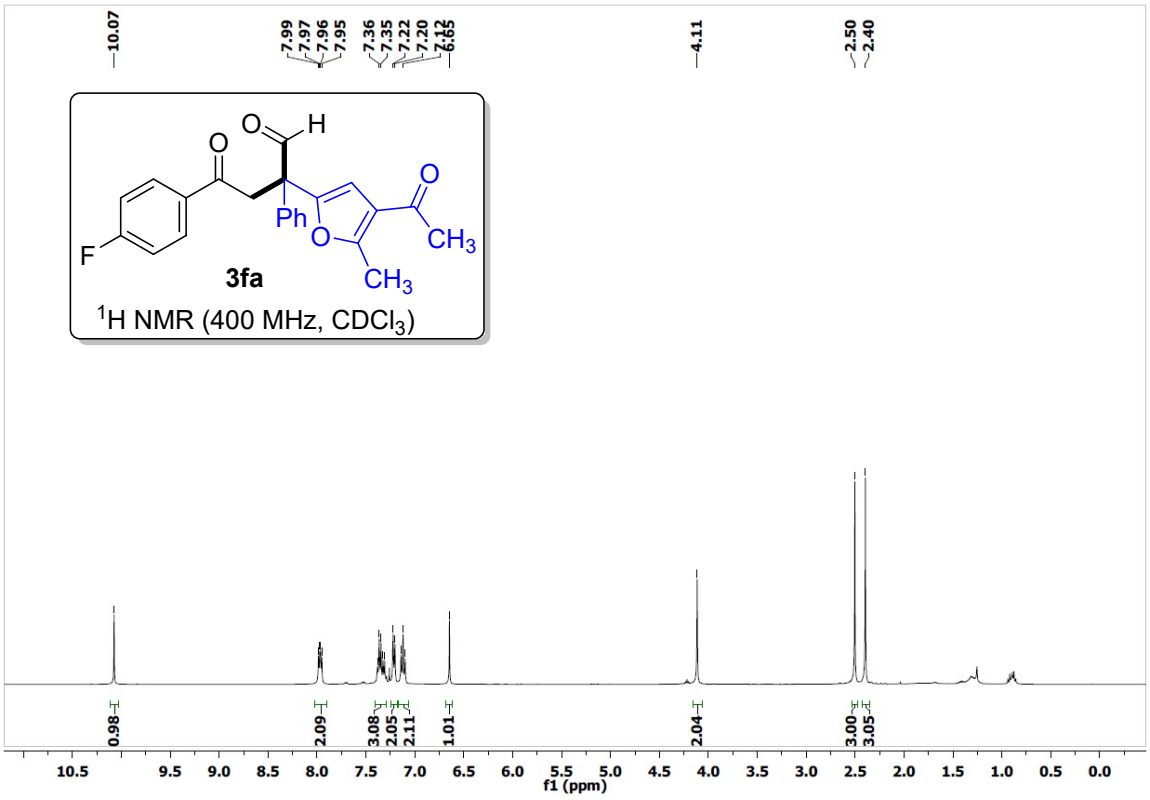
f1 (ppm)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Ph
O
CH3
F
O
CH3
3fa
1H NMR (400 MHz, CDCl3)
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3.08
2.05
2.11
1.01
2.04
3.00
3.05
10.5
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9.0
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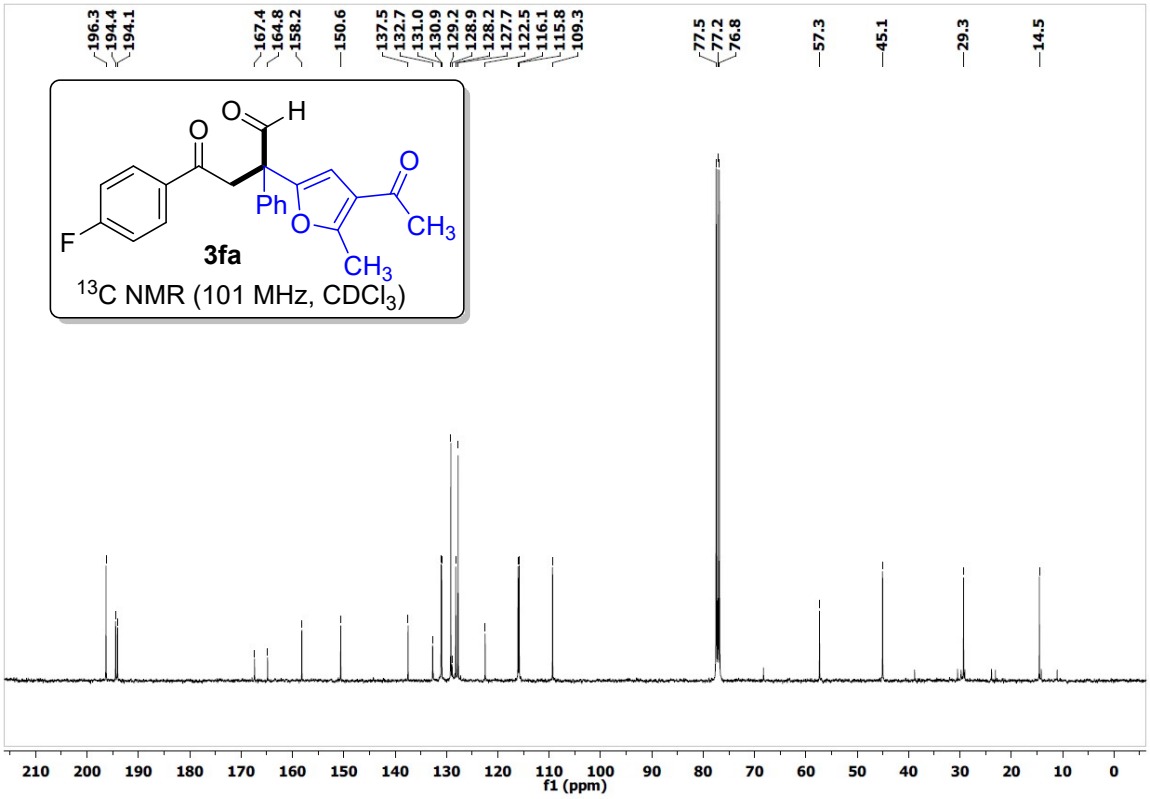
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127.7
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116.1
115.8
109.3
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77.2
76.8
57.3
45.1
29.3
14.5
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O
Ph
O
CH3
F
O
CH3
3fa
13C NMR (101 MHz, CDCl3)
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180
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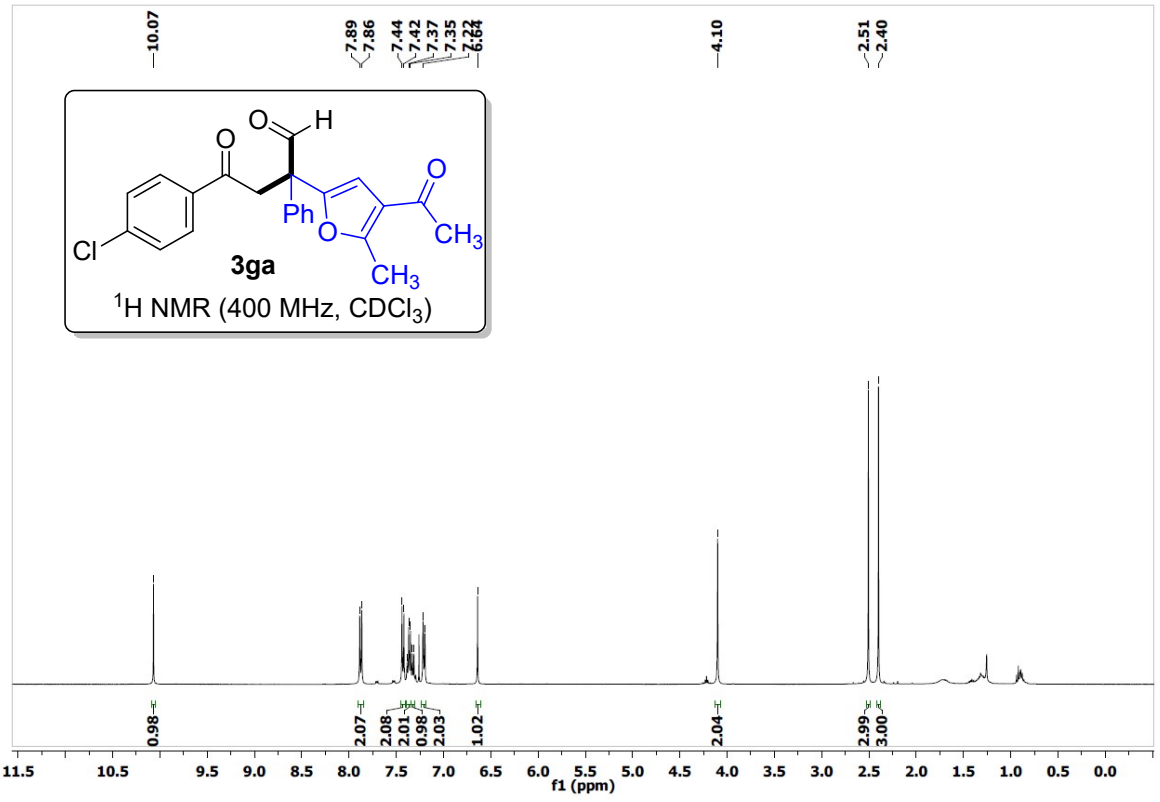
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O
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Cl
CH3
3ga
1H NMR (400 MHz, CDCl3)
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2.08
2.01
0.98
2.03
1.02
2.04
2.99
3.00
11.5
10.5
9.5
9.0
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6.5
6.0
5.5
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2.0
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1.0
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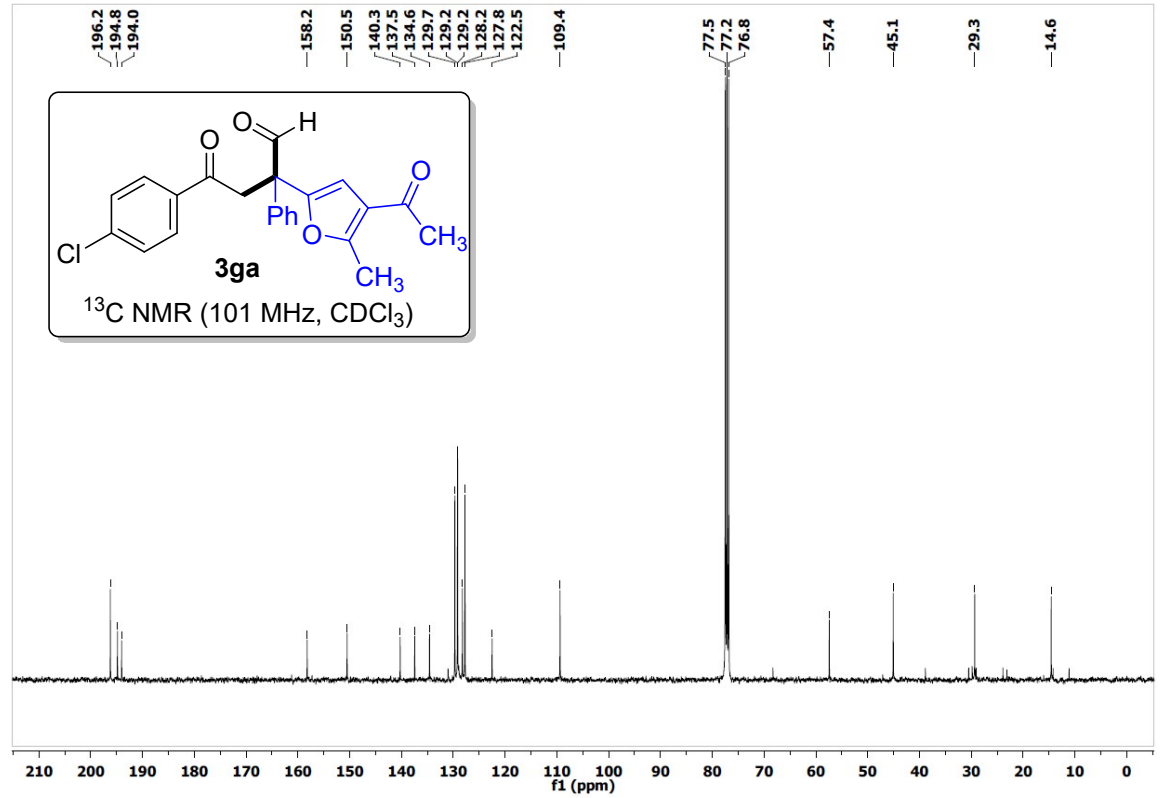
f1 (ppm)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128.2
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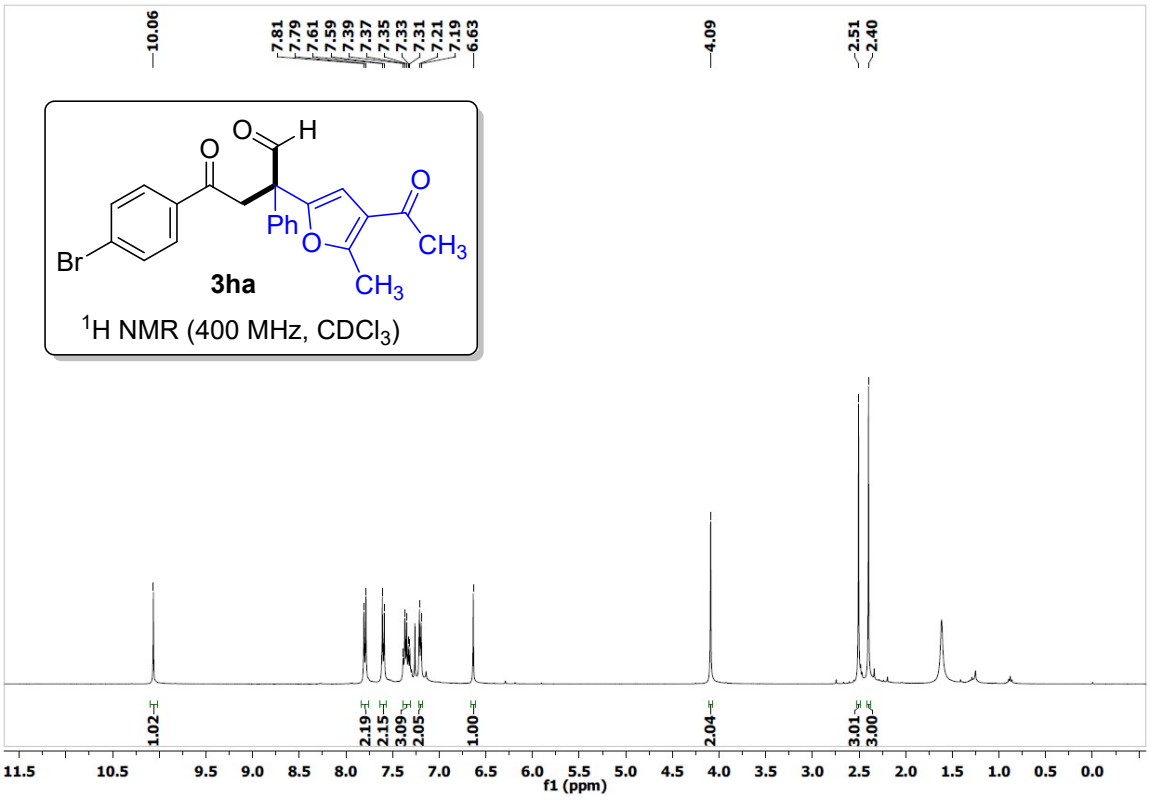
109.4
77.5
77.2
76.8
57.4
45.1
29.3
14.6
O
H
O
Ph
O
O
CH3
Cl
CH3
3ga
13C NMR (101 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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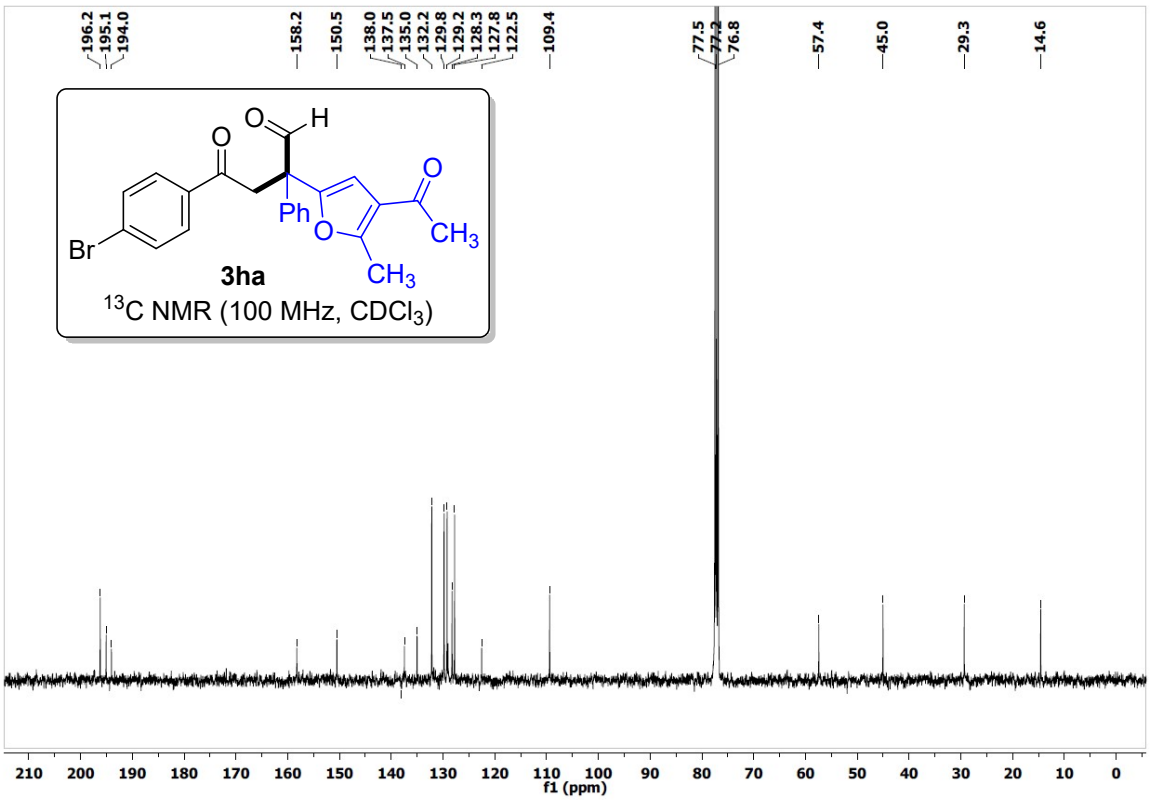
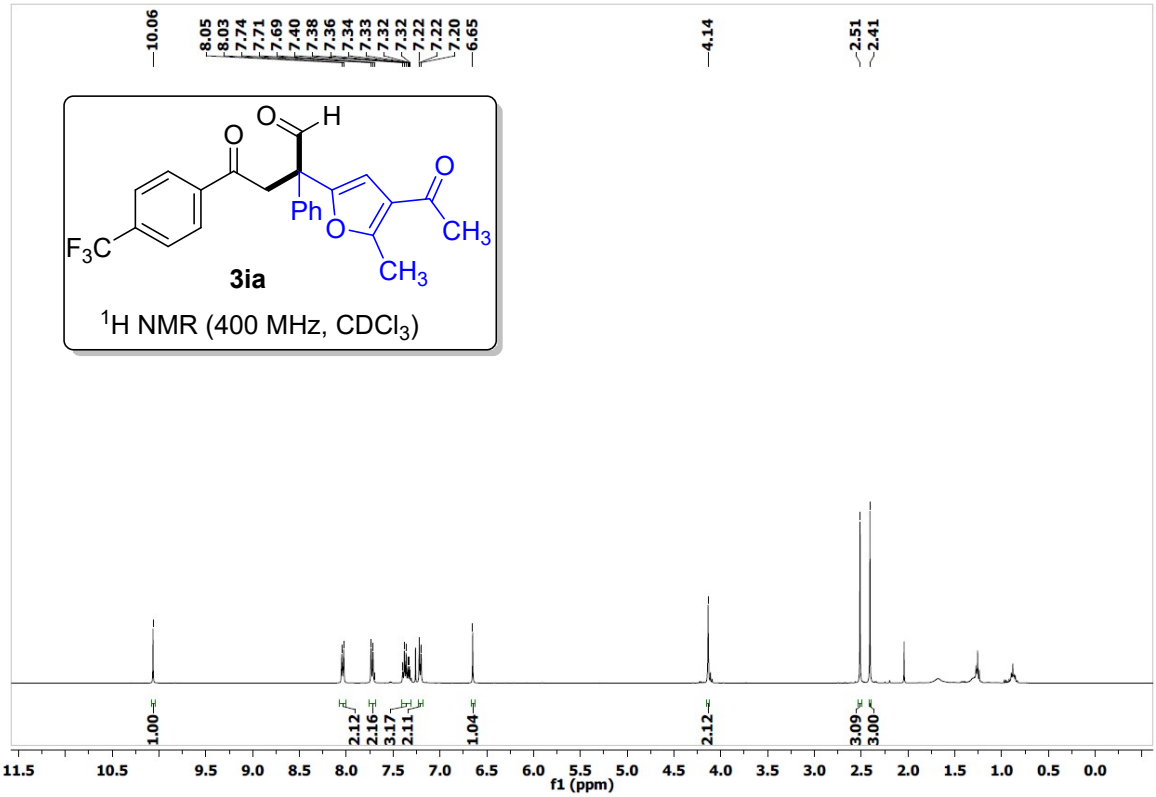
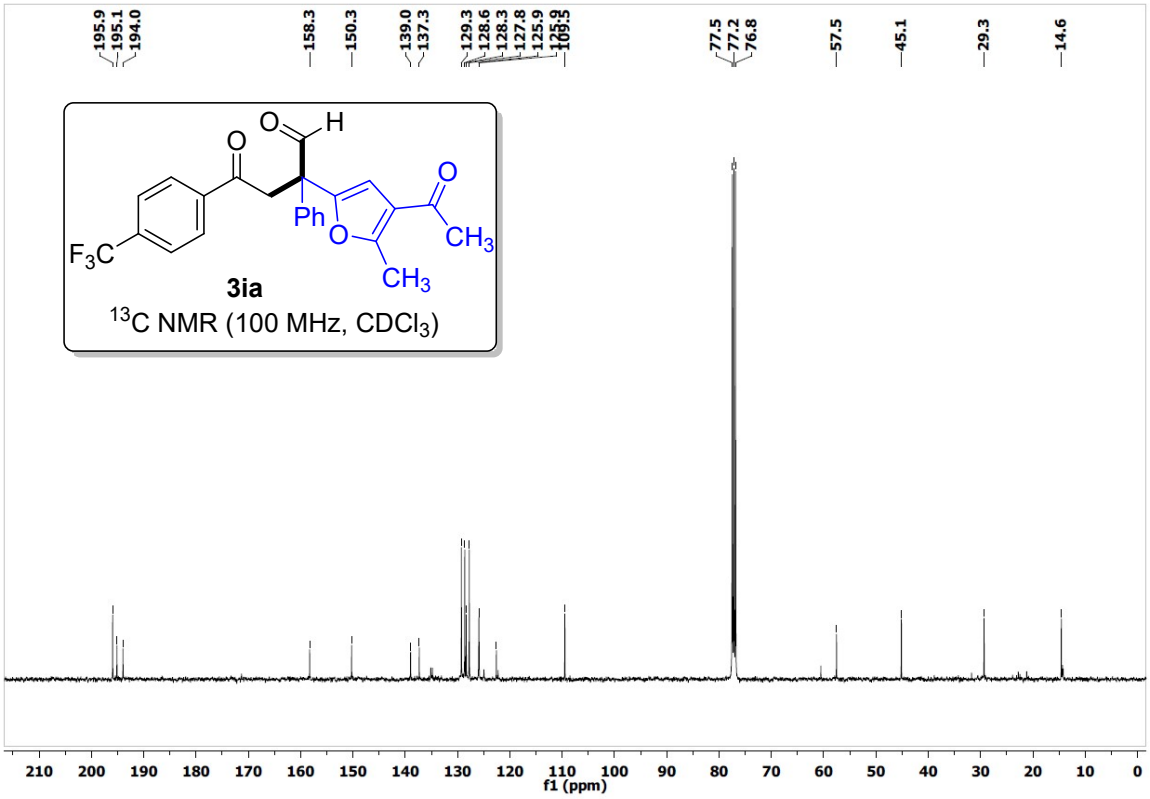
7.81
7.79
7.61
7.59
7.39
7.37
7.35
7.33
7.31
7.21
7.19
6.63
4.09
2.51
2.40
O
H
O
Ph
O
O
CH3
Br
CH3
3ha
1H NMR (400 MHz, CDCl3)
1.02
2.19
2.15
3.09
2.05
1.00
2.04
3.01
3.00
f1 (ppm)


196.2
195.1
194.0
158.2
150.5
138.0
137.5
135.0
132.2
129.8
129.2
128.3
127.8
122.5
109.4
77.5
77.2
76.8
57.4
45.0
29.3
14.6
O
H
O
Ph
O
O
CH3
Br
CH3
3ha
13C NMR (100 MHz, CDCl3)
f1 (ppm)


10.06
8.05
8.03
7.74
7.71
7.69
7.40
7.38
7.36
7.34
7.33
7.32
7.32
7.22
7.22
7.20
6.65
4.14
2.51
2.41
O
H
O
Ph
O
O
CH3
F3C
CH3
3ia
1H NMR (400 MHz, CDCl3)
1.00
2.12
2.16
3.17
2.11
1.04
2.12
3.09
3.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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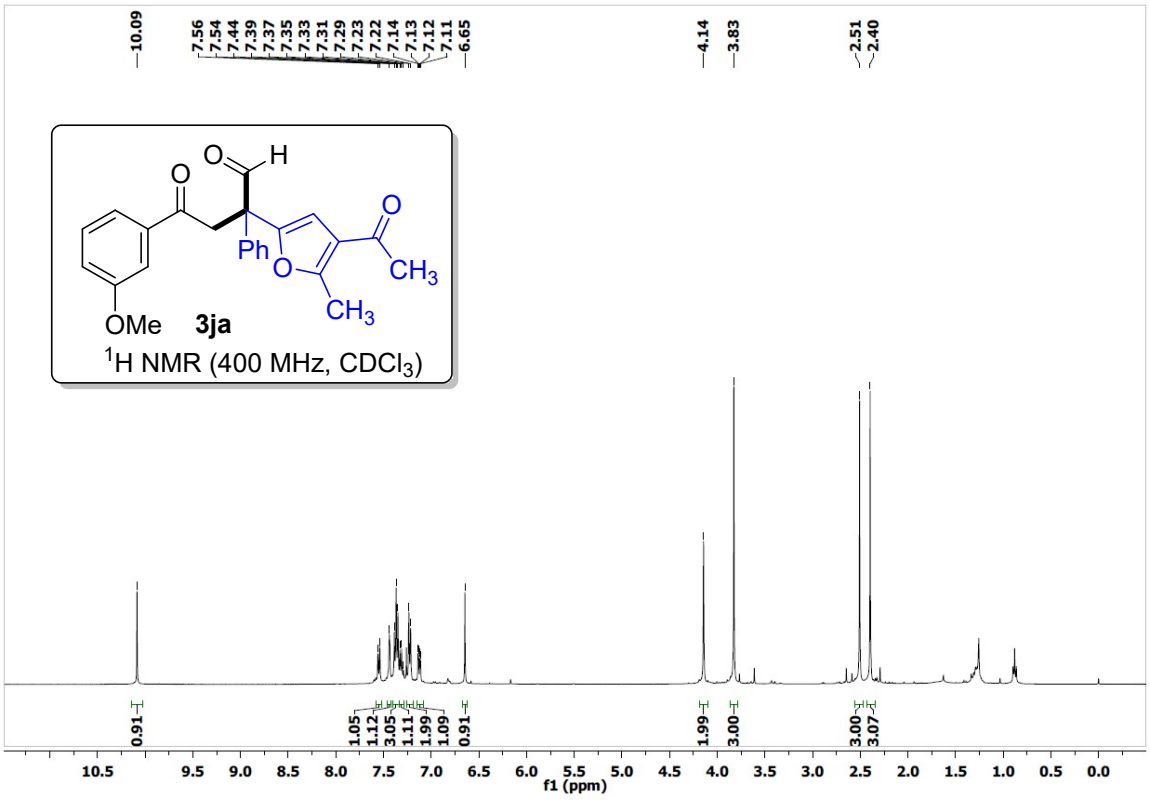
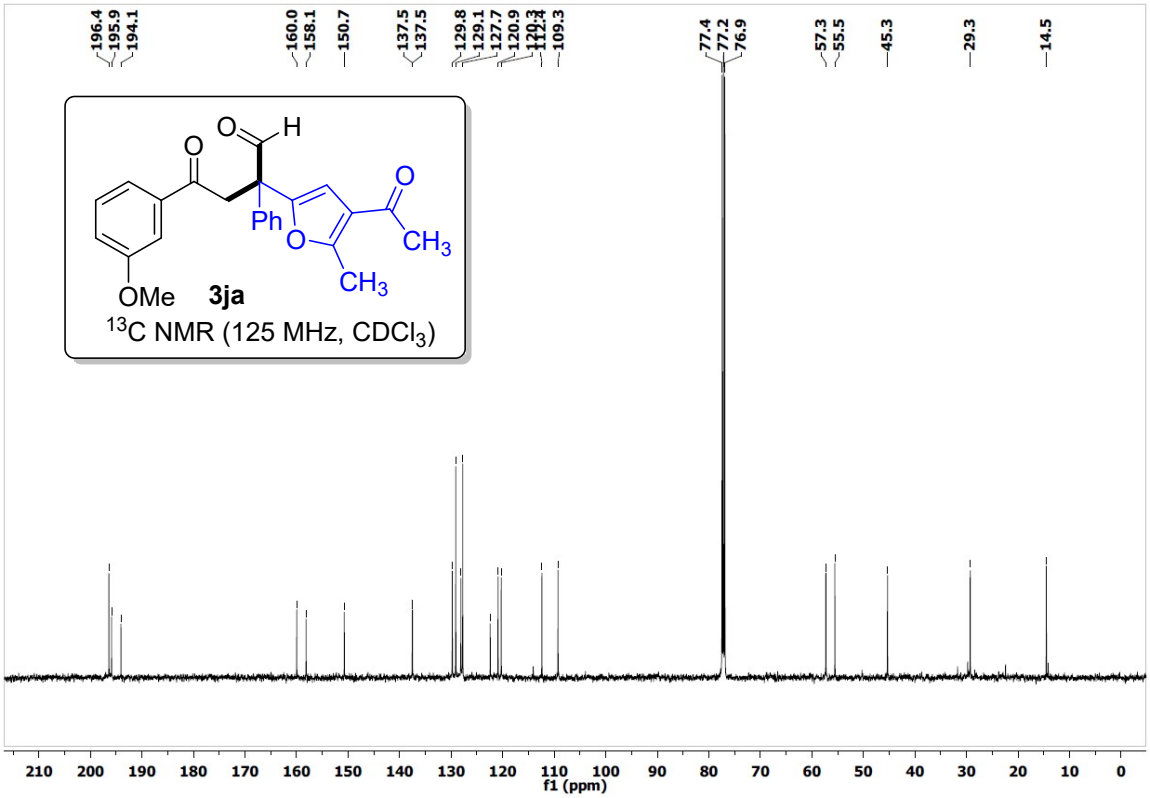
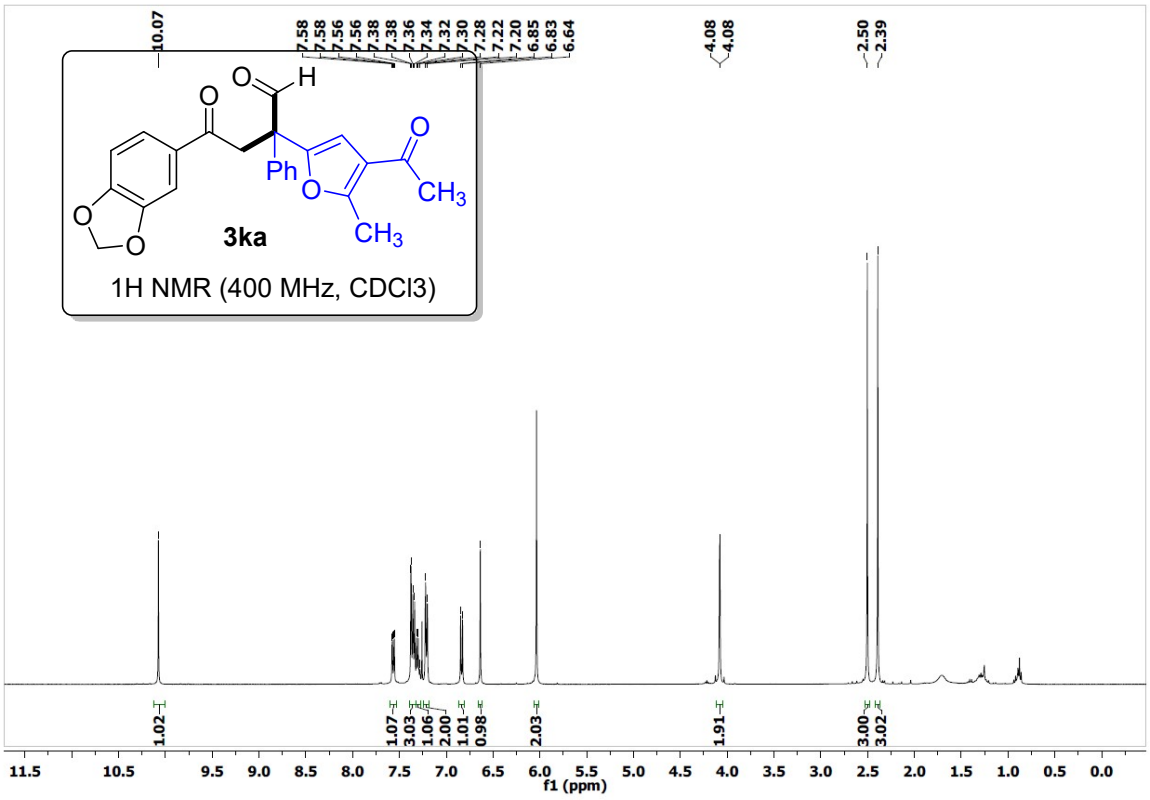
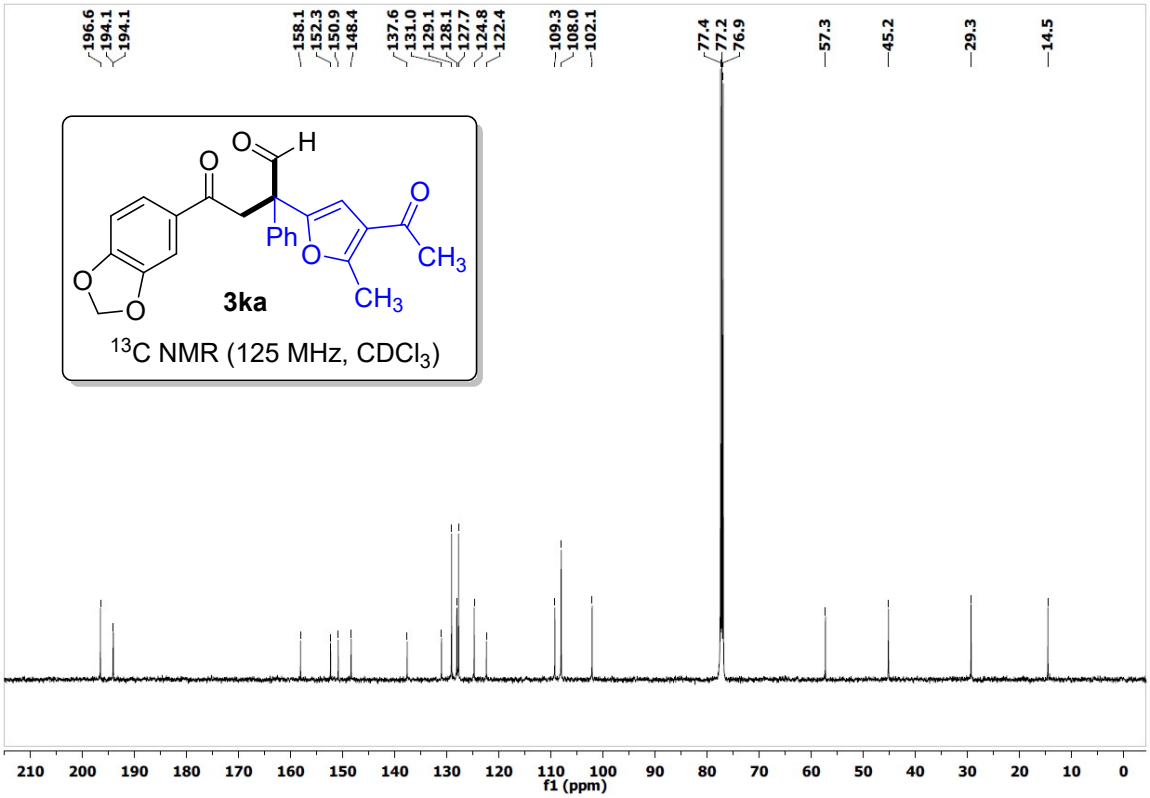
195.1
194.0
158.3
150.3
139.0
137.3
129.3
128.6
128.3
127.8
125.9
77.5
77.2
76.8
57.5
45.1
29.3
14.6
O
H
O
Ph
O
O
CH3
F3C
CH3
3ia
13C NMR (100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


10.09
7.56
7.54
7.44
7.39
7.37
7.35
7.33
7.31
7.29
7.23
7.22
7.14
7.13
7.12
7.11
6.65
4.14
3.83
2.51
2.40
O
H
O
Ph
O
O
CH3
CH3
OMe
3ja
1H NMR (400 MHz, CDCl3)
0.91
1.05
1.12
3.05
1.11
1.99
1.09
0.91
1.99
3.00
3.00
3.07
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


196.4
195.9
194.1
160.0
158.1
150.7
137.5
137.5
129.8
129.1
127.7
120.9
120.3
112.4
109.3
77.4
77.2
76.9
57.3
55.5
45.3
29.3
14.5
O
H
O
Ph
O
O
CH3
CH3
OMe
3ja
13C NMR (125 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


10.07
7.58
7.58
7.56
7.56
7.38
7.38
7.36
7.34
7.32
7.30
7.28
7.22
7.20
6.85
6.83
6.64
4.08
4.08
2.50
2.39
O
H
O
Ph
O
O
CH3
O
O
CH3
3ka
1H NMR (400 MHz, CDCl3)
1.02
1.07
3.03
1.06
2.00
1.01
0.98
2.03
1.91
3.00
3.02
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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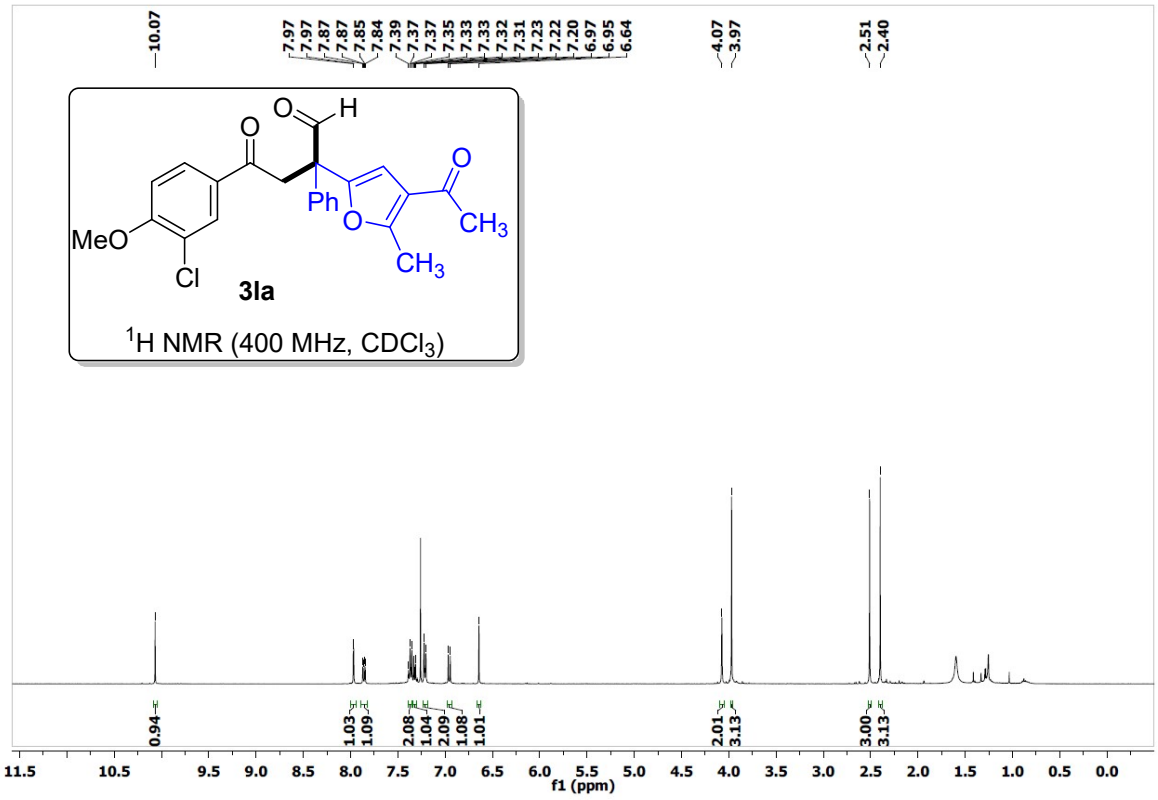
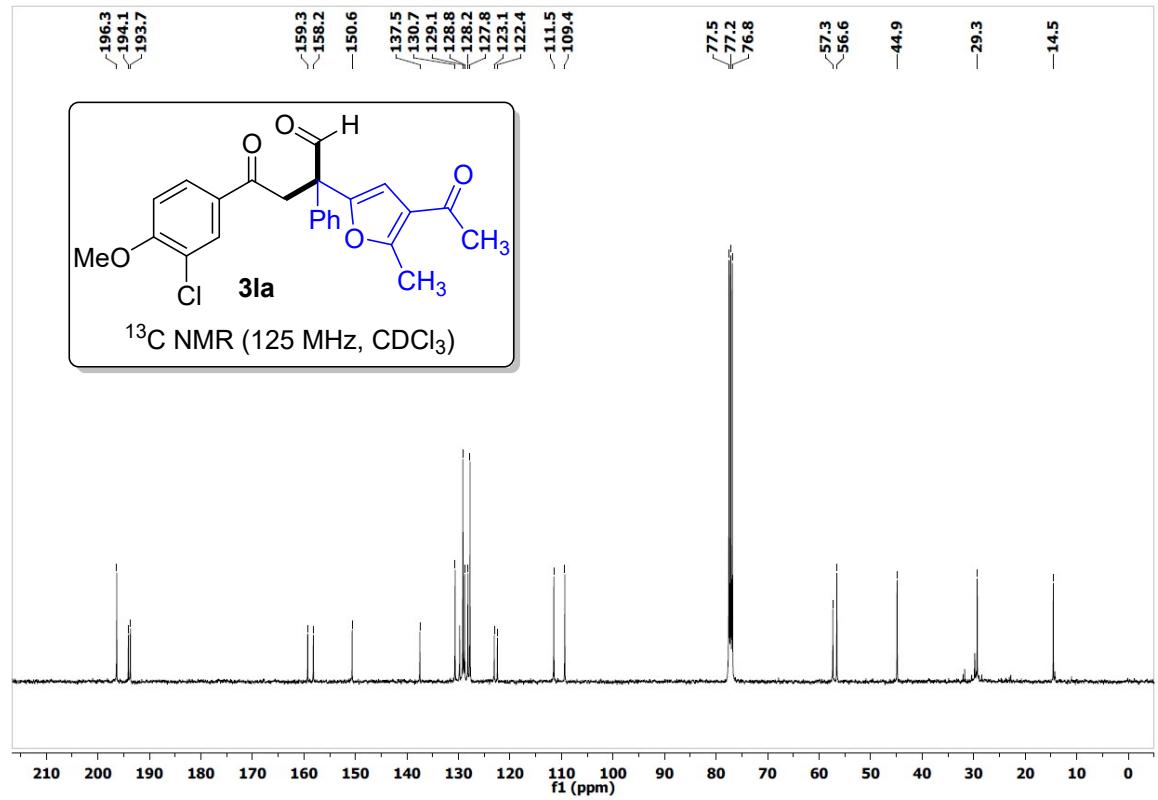
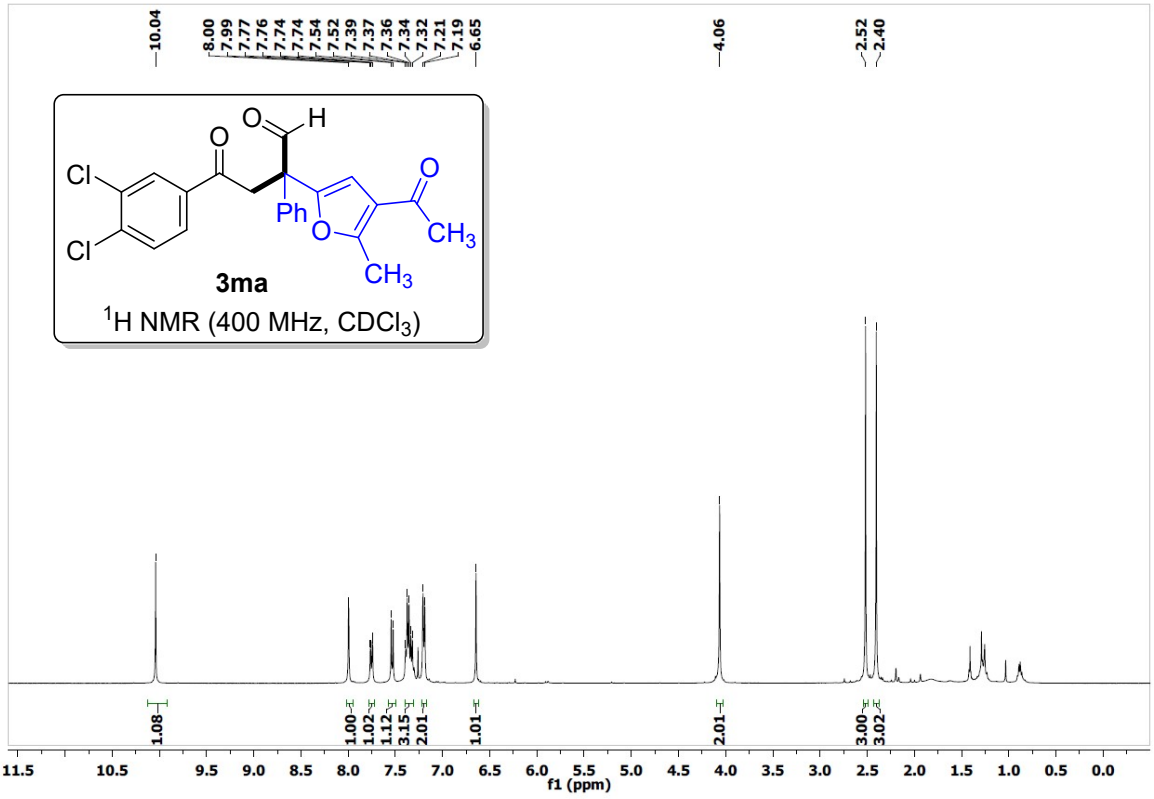
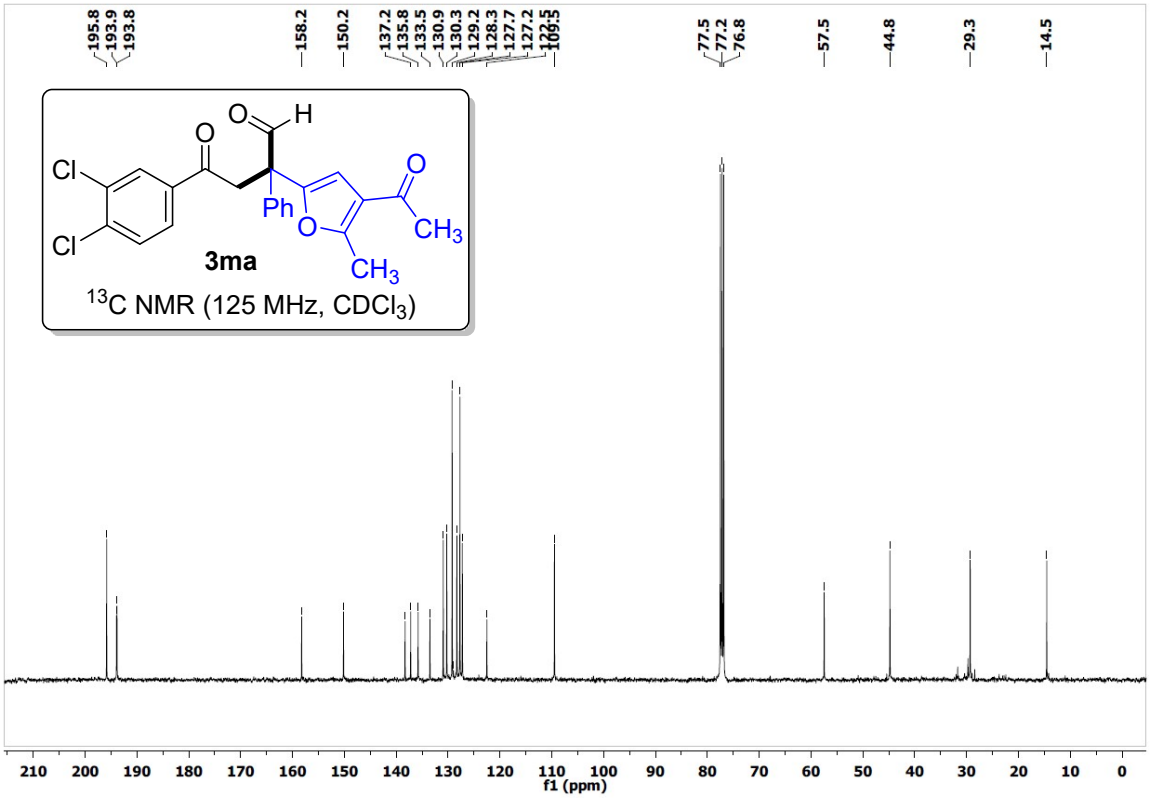
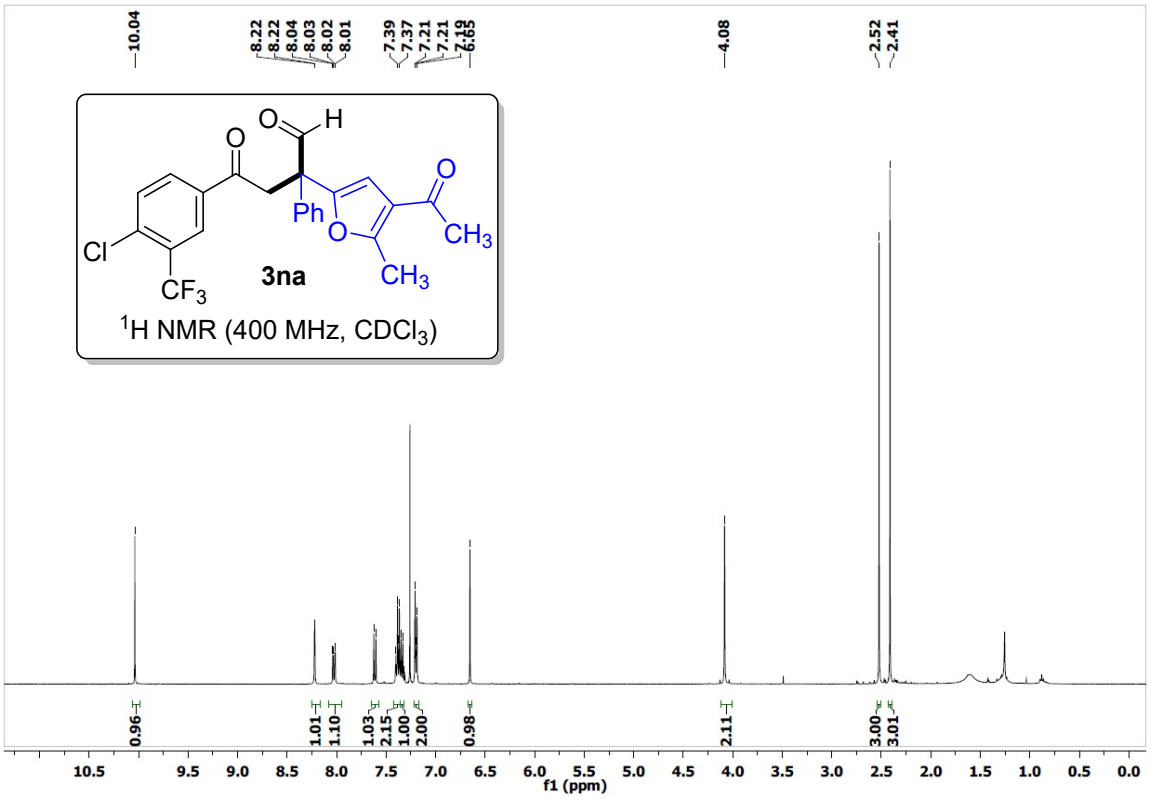
194.1
194.1
158.1
152.3
150.9
148.4
137.6
131.0
129.1
128.1
127.7
124.8
122.4
109.3
108.0
102.1
77.4
77.2
76.9
57.3
45.2
29.3
14.5
O
H
O
Ph
O
O
CH3
O
O
CH3
3ka
13C NMR (125 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

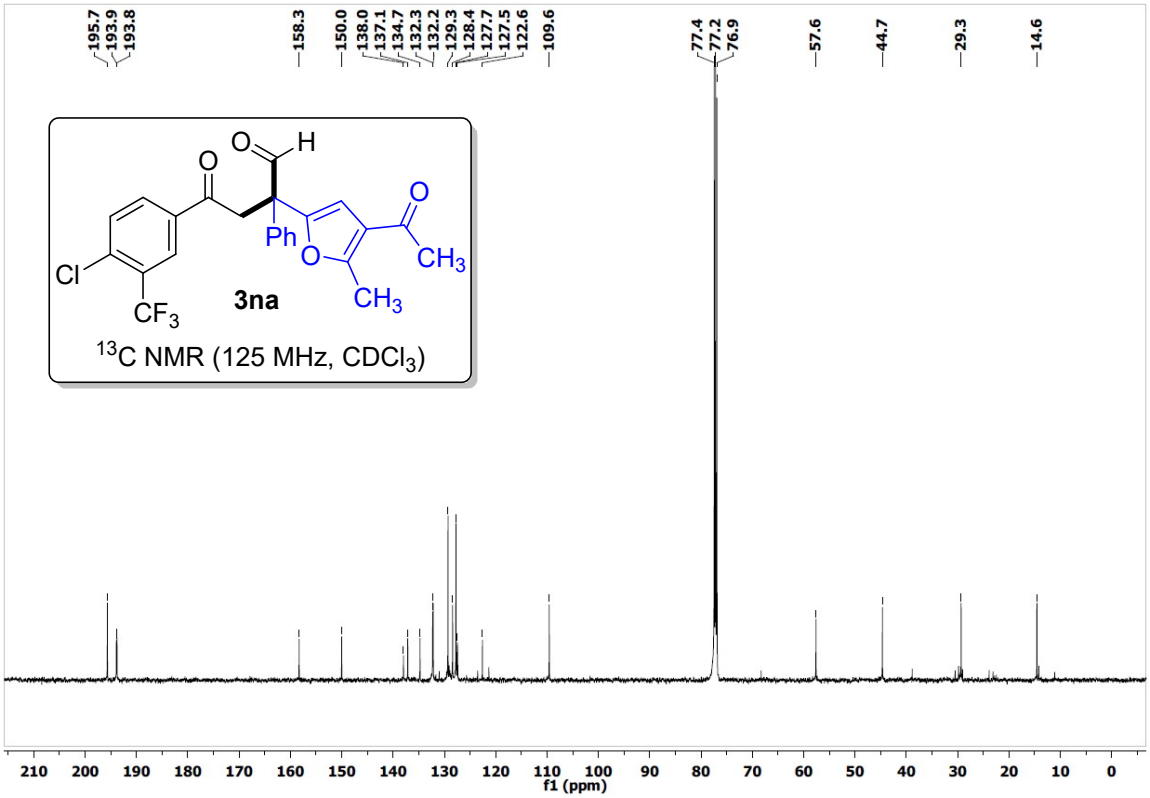

10.07
7.97
7.97
7.87
7.87
7.85
7.84
7.39
7.37
7.37
7.35
7.33
7.33
7.32
7.31
7.23
7.22
7.20
6.97
6.95
6.64
4.07
3.97
2.51
2.40
O
H
O
Ph
O
O
CH3
CH3
MeO
Cl
3la
1H NMR (400 MHz, CDCl3)
0.94
1.03
1.09
2.08
1.04
2.09
1.08
1.01
2.01
3.13
3.00
3.13
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

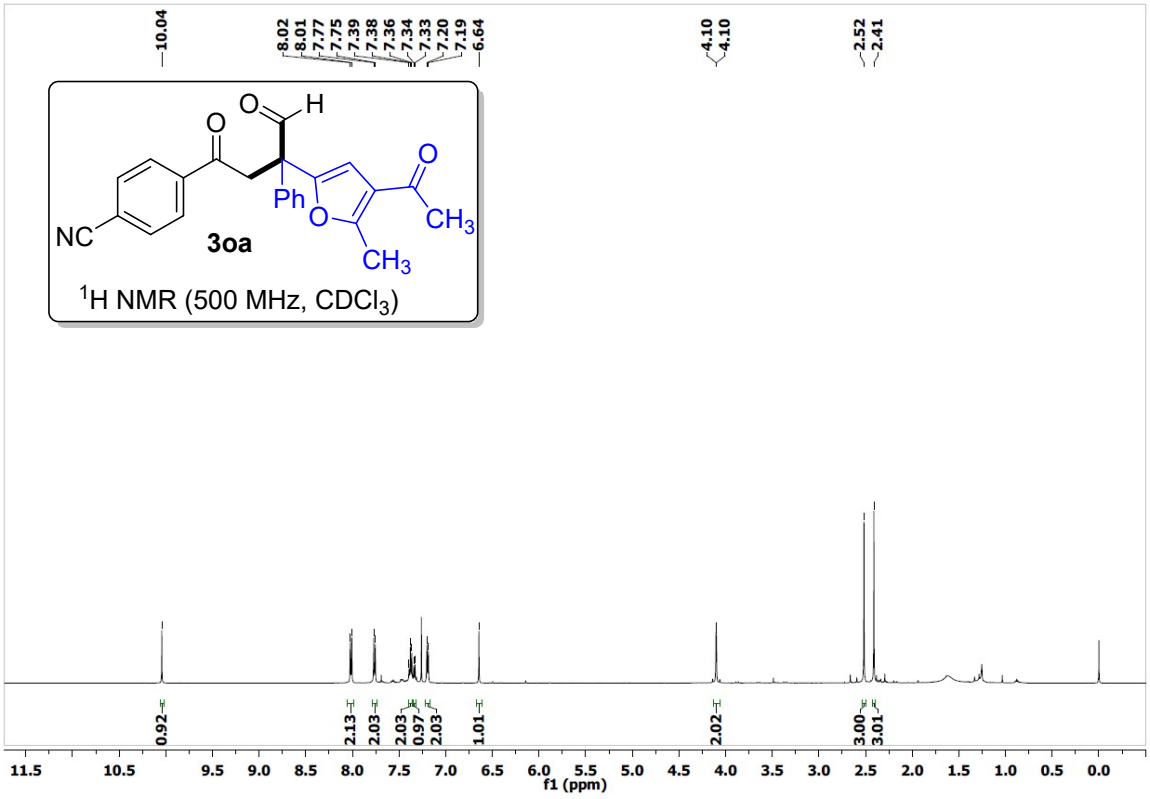

196.3
194.1
193.7
159.3
158.2
150.6
137.5
130.7
129.1
128.8
128.2
127.8
123.1
122.4
111.5
109.4
77.5
77.2
76.8
57.3
56.6
44.9
29.3
14.5
O
H
O
Ph
O
O
CH3
CH3
MeO
Cl
3la
13C NMR (125 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

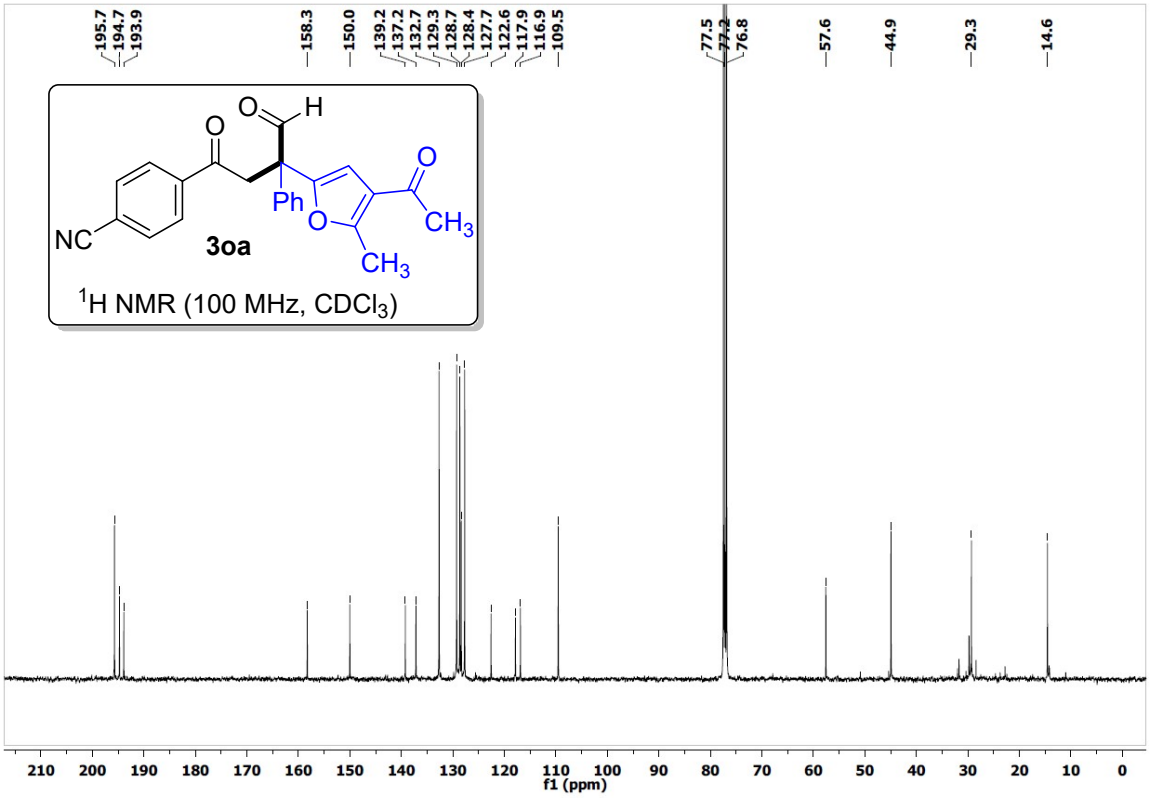

10.04
8.00
7.99
7.77
7.76
7.74
7.74
7.54
7.52
7.39
7.37
7.36
7.34
7.32
7.21
7.19
6.65
4.06
2.52
2.40
O
H
O
Cl
Cl
Ph
O
O
CH3
CH3
3ma
1H NMR (400 MHz, CDCl3)
1.08
1.00
1.02
1.12
3.15
2.01
1.01
2.01
3.00
3.02
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

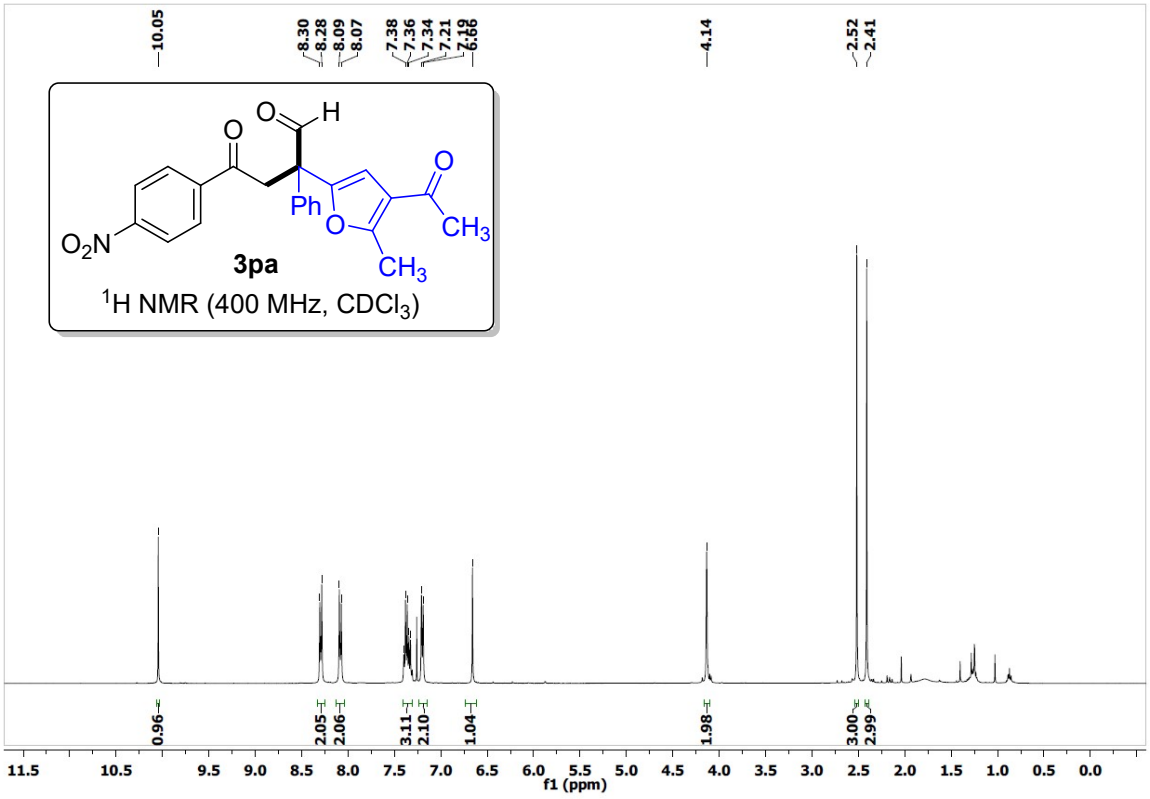

195.8
193.9
193.8
158.2
150.2
137.2
135.8
133.5
130.9
130.3
129.2
128.3
127.7
127.2
122.5
109.5
77.5
77.2
76.8
57.5
44.8
29.3
14.5
O
H
O
Cl
Cl
Ph
O
O
CH3
CH3
3ma
13C NMR (125 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

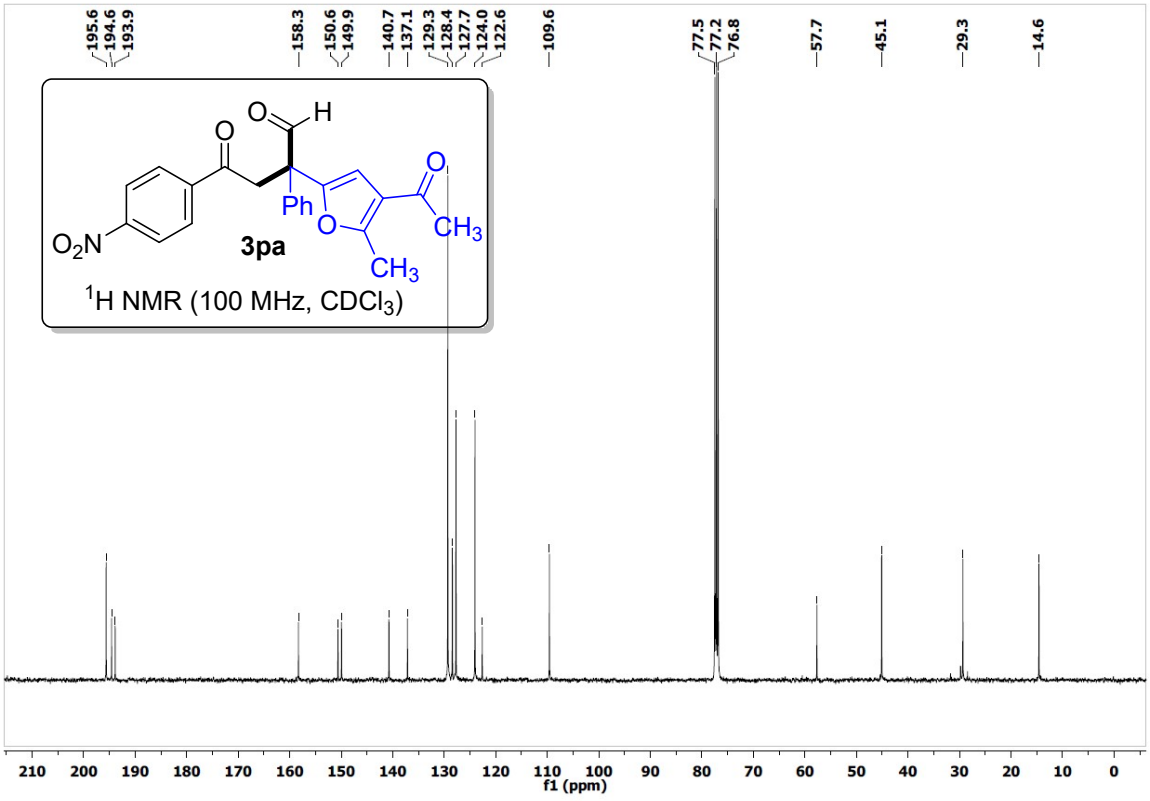

10.04
8.22
8.22
8.04
8.03
8.02
8.01
7.39
7.37
7.21
7.21
7.19
6.65
4.08
2.52
2.41
O
H
O
Ph
O
O
CH3
Cl
CF3
CH3
3na
1H NMR (400 MHz, CDCl3)
0.96
1.01
1.10
1.03
2.15
1.00
2.00
0.98
2.11
3.00
3.01
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

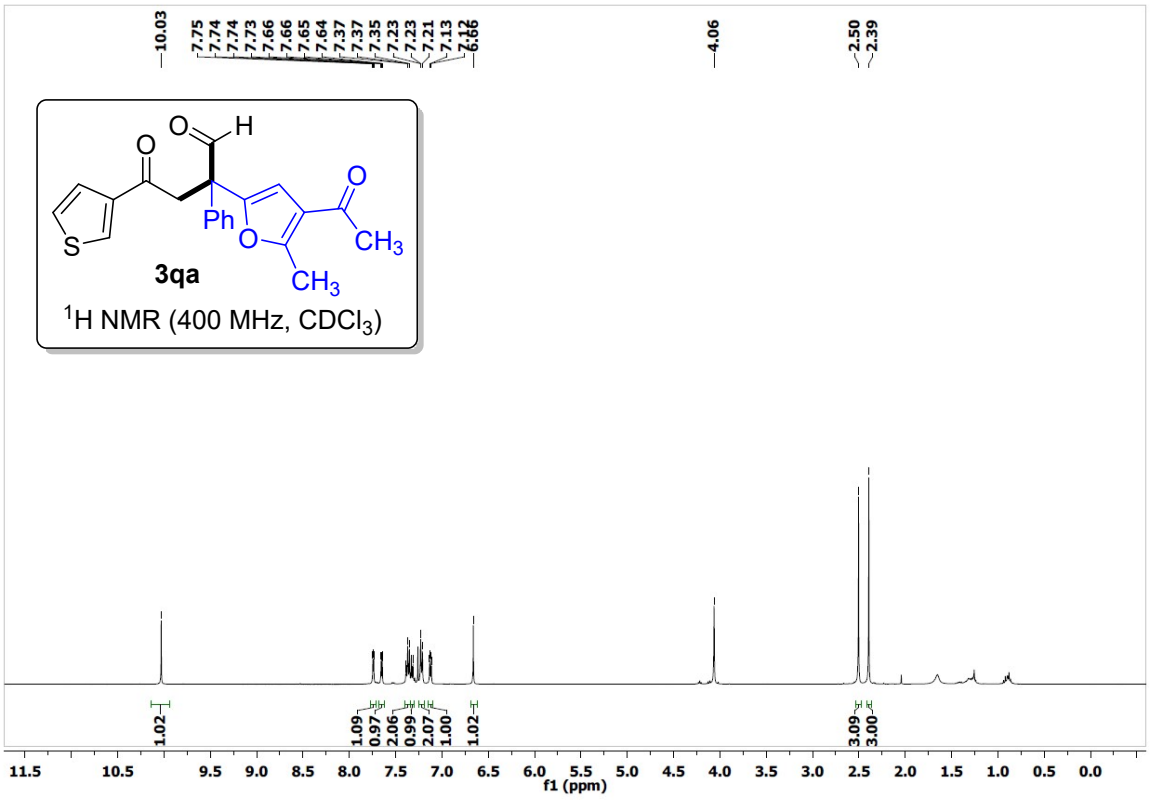

195.7
193.9
193.8
158.3
150.0
138.0
137.1
134.7
132.3
132.2
129.3
128.4
127.7
127.5
122.6
109.6
77.4
77.2
76.9
57.6
44.7
29.3
14.6
O
H
O
Ph
O
O
CH3
Cl
CF3
CH3
3na
13C NMR (125 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

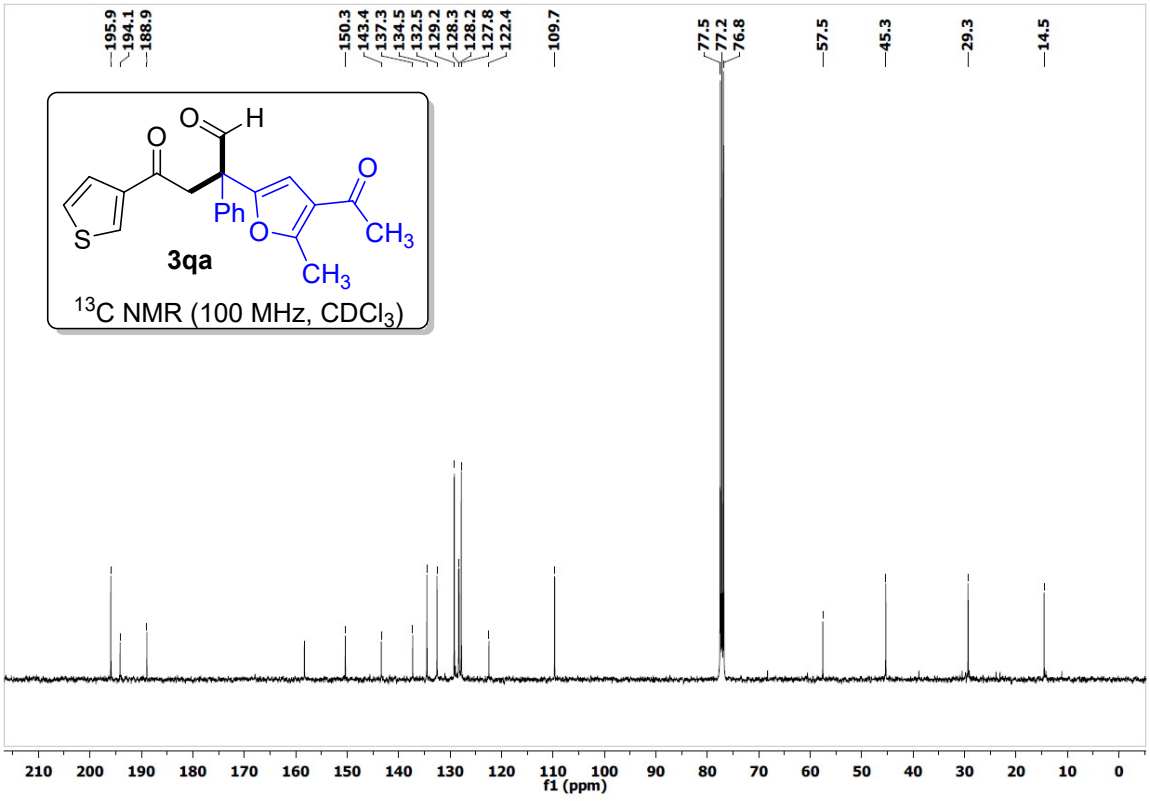

10.04
8.02
8.01
7.77
7.75
7.39
7.38
7.36
7.34
7.33
7.20
7.19
6.64
4.10
4.10
2.52
2.41
O
H
O
Ph
O
O
CH3
NC
CH3
3oa
1H NMR (500 MHz, CDCl3)
0.92
2.13
2.03
2.03
0.97
2.03
1.01
2.02
3.00
3.01
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

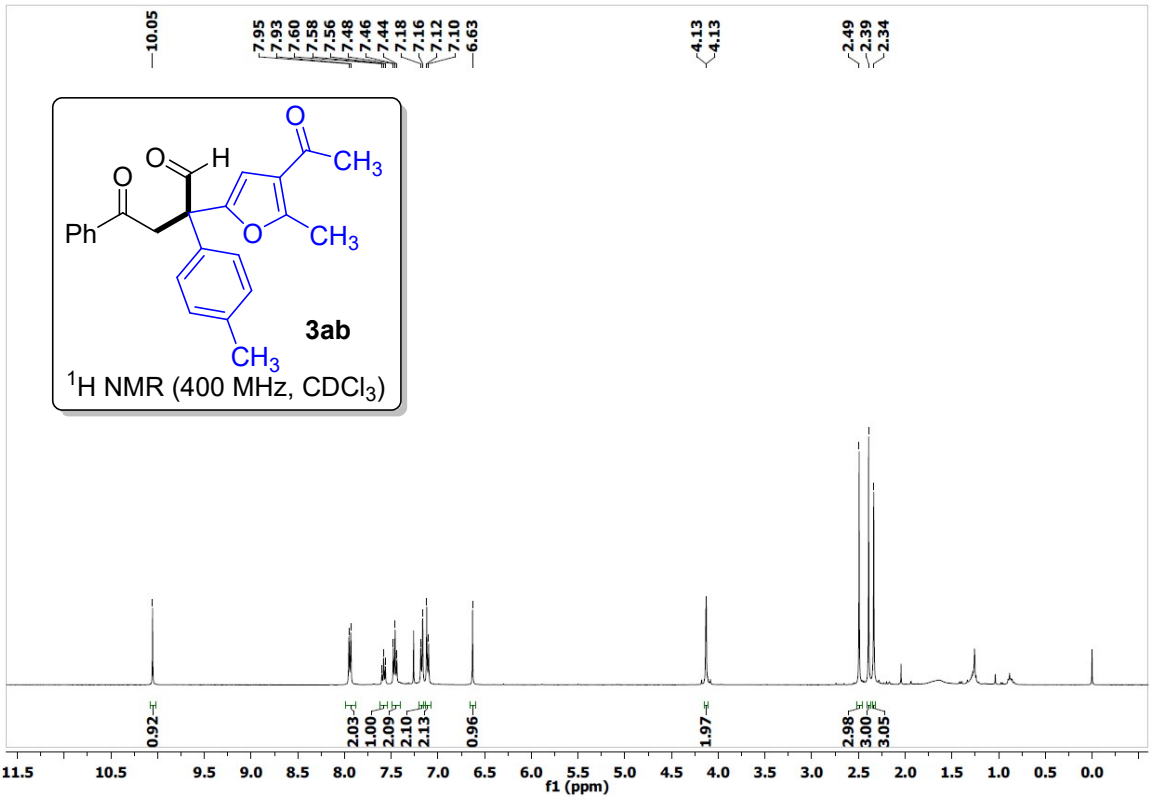

195.7
194.7
193.9
158.3
150.0
139.2
137.2
132.7
129.3
128.7
128.4
127.7
122.6
117.9
116.9
109.5
77.5
77.2
76.8
57.6
44.9
29.3
14.6
O
H
O
Ph
O
O
CH3
NC
CH3
3oa
1H NMR (100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

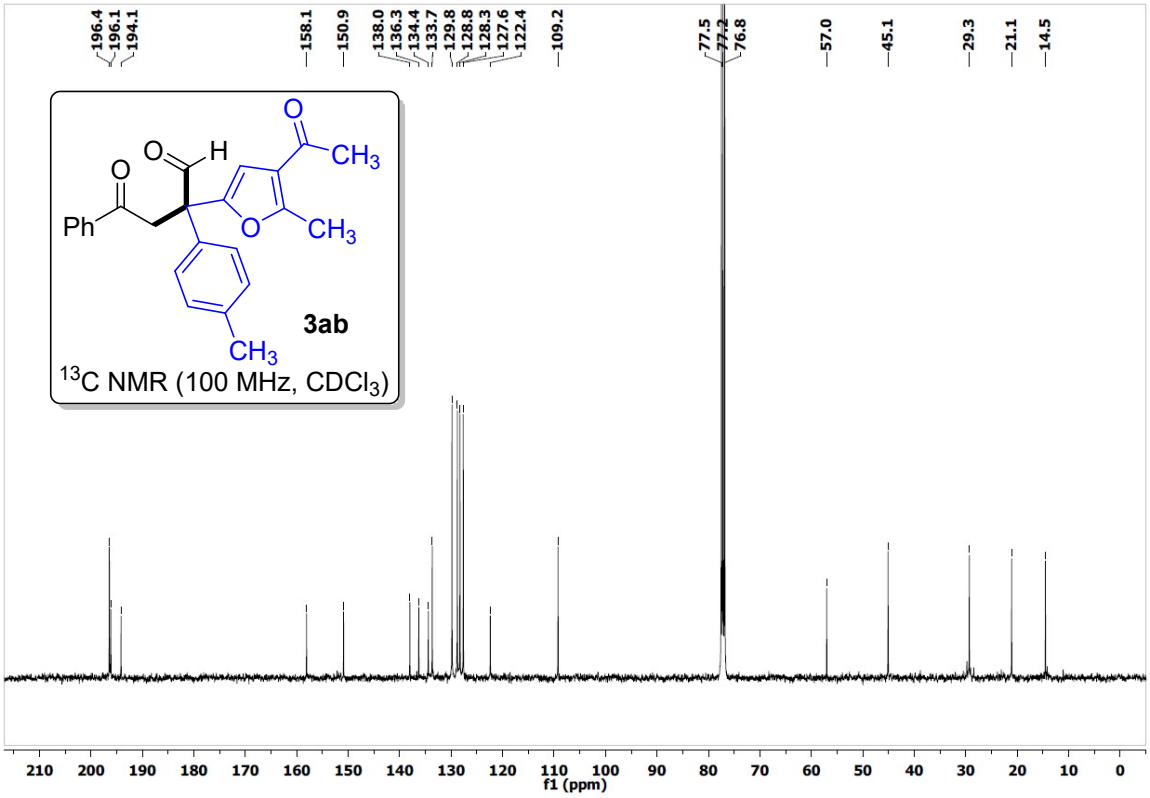

10.05
8.30
8.28
8.09
8.07
7.38
7.36
7.34
7.21
7.19
6.68
4.14
2.52
2.41
O
H
O
Ph
O
CH3
O2N
CH3
3pa
1H NMR (400 MHz, CDCl3)
0.96
2.05
2.06
3.11
2.10
1.04
1.98
3.00
2.99
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

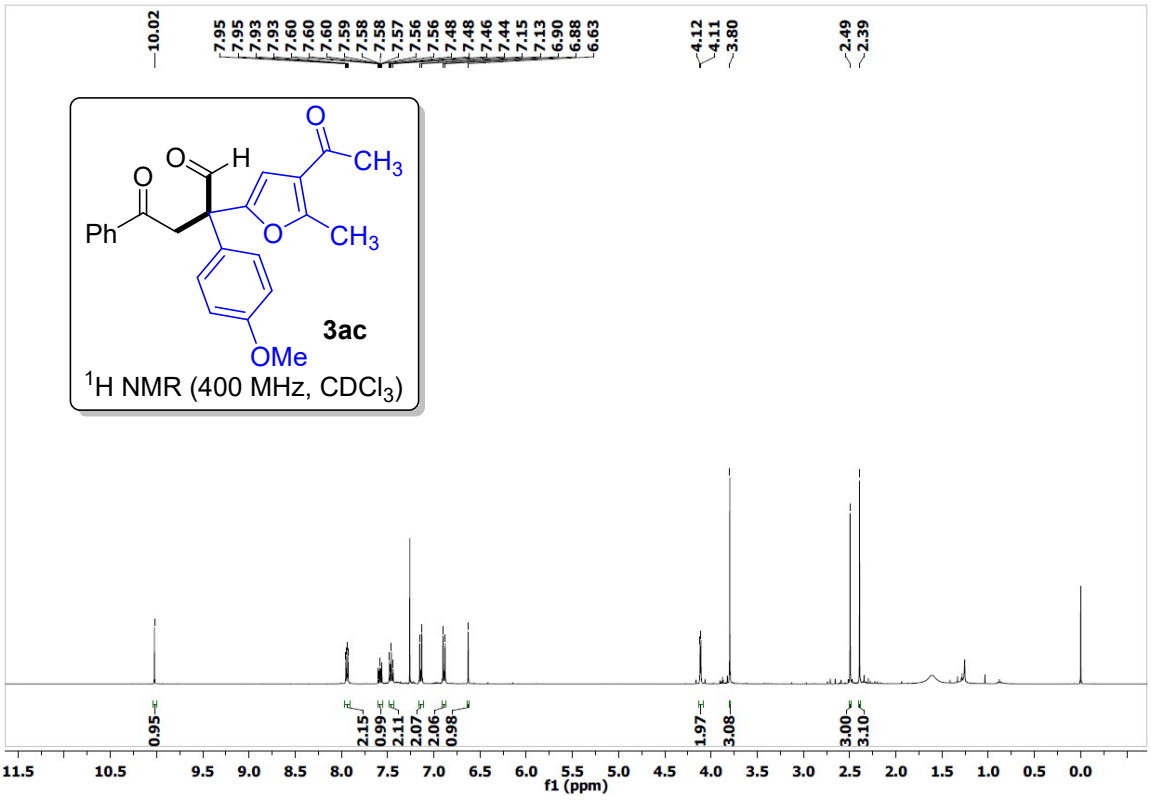

195.6
194.6
193.9
158.3
150.6
149.9
140.7
137.1
129.3
128.4
127.7
124.0
122.6
109.6
77.5
77.2
76.8
57.7
45.1
29.3
14.6
O
H
O
Ph
O
CH3
O2N
CH3
3pa
1H NMR (100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

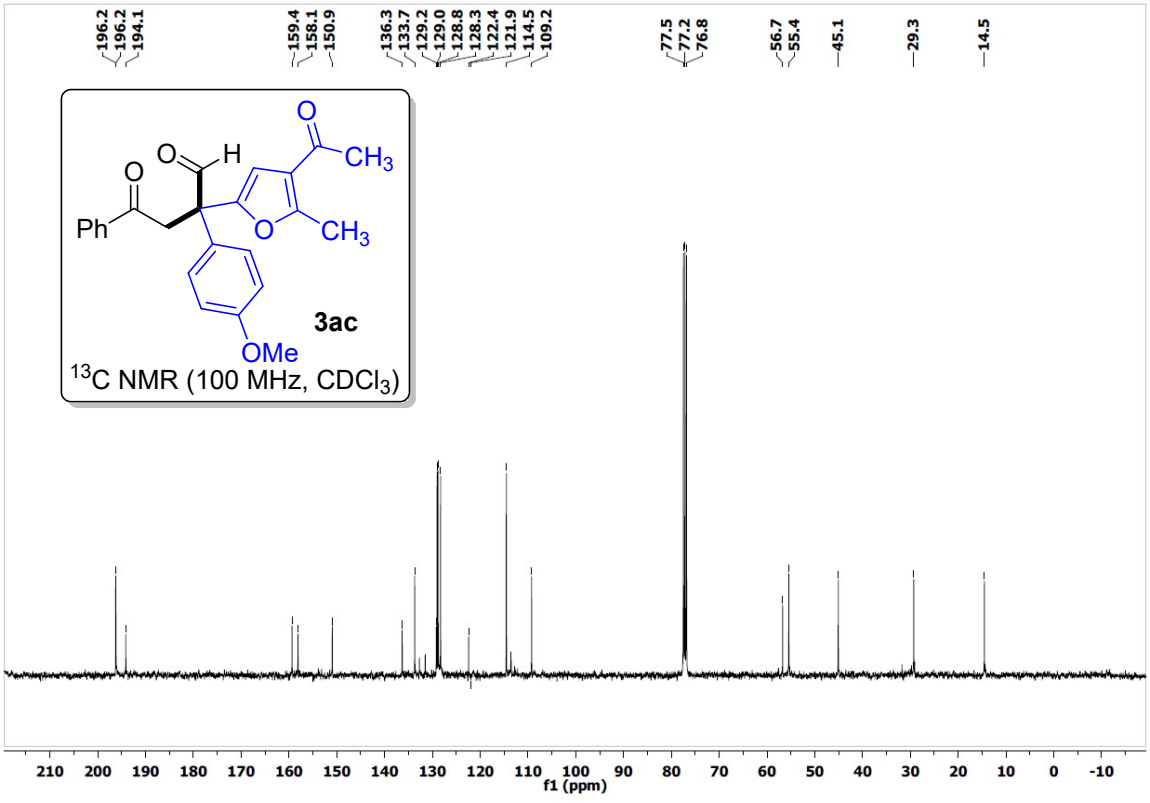

10.03
7.75
7.74
7.74
7.73
7.66
7.66
7.65
7.64
7.37
7.37
7.35
7.23
7.23
7.21
7.13
6.66
4.06
2.50
2.39
O
H
O
Ph
O
O
CH3
S
CH3
3qa
1H NMR (400 MHz, CDCl3)
1.02
1.09
0.97
2.06
0.99
2.07
1.00
1.02
3.09
3.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

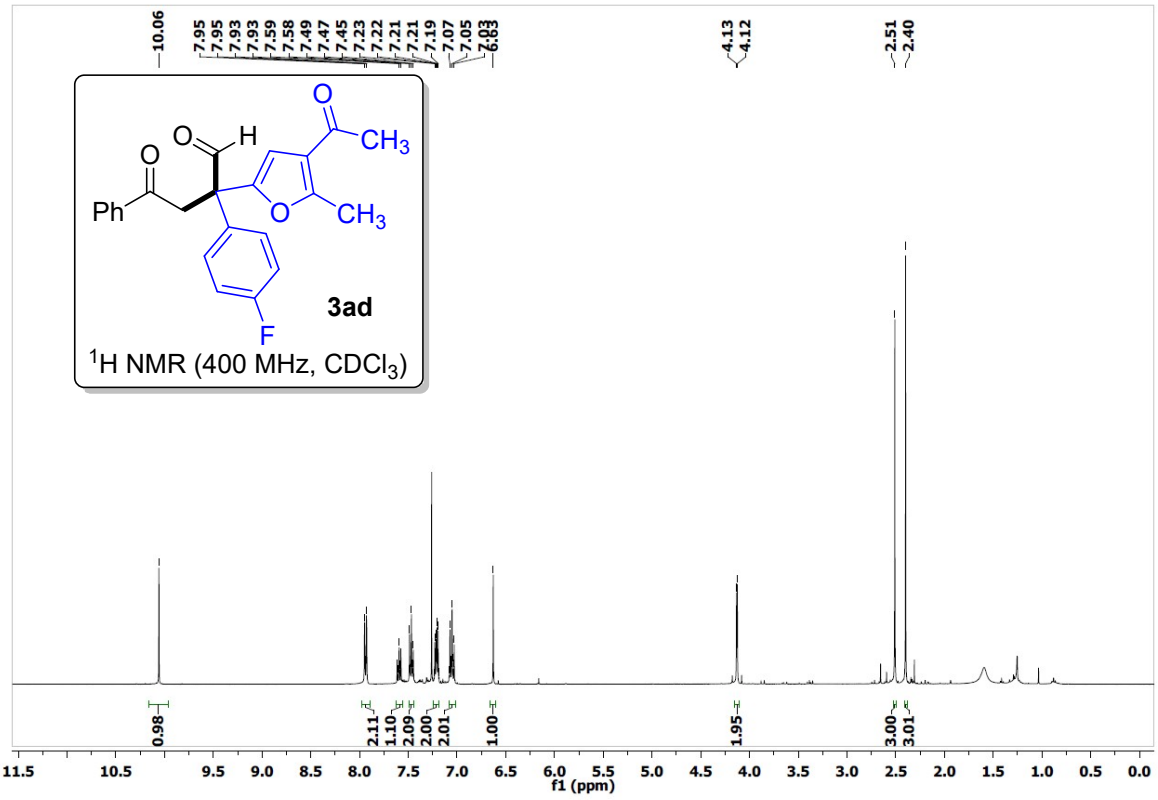

195.9
194.1
188.9
150.3
143.4
137.3
134.5
132.5
129.2
128.3
128.2
127.8
122.4
109.7
77.5
77.2
76.8
57.5
45.3
29.3
14.5
O
H
O
Ph
O
O
CH3
S
CH3
3qa
13C NMR (100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

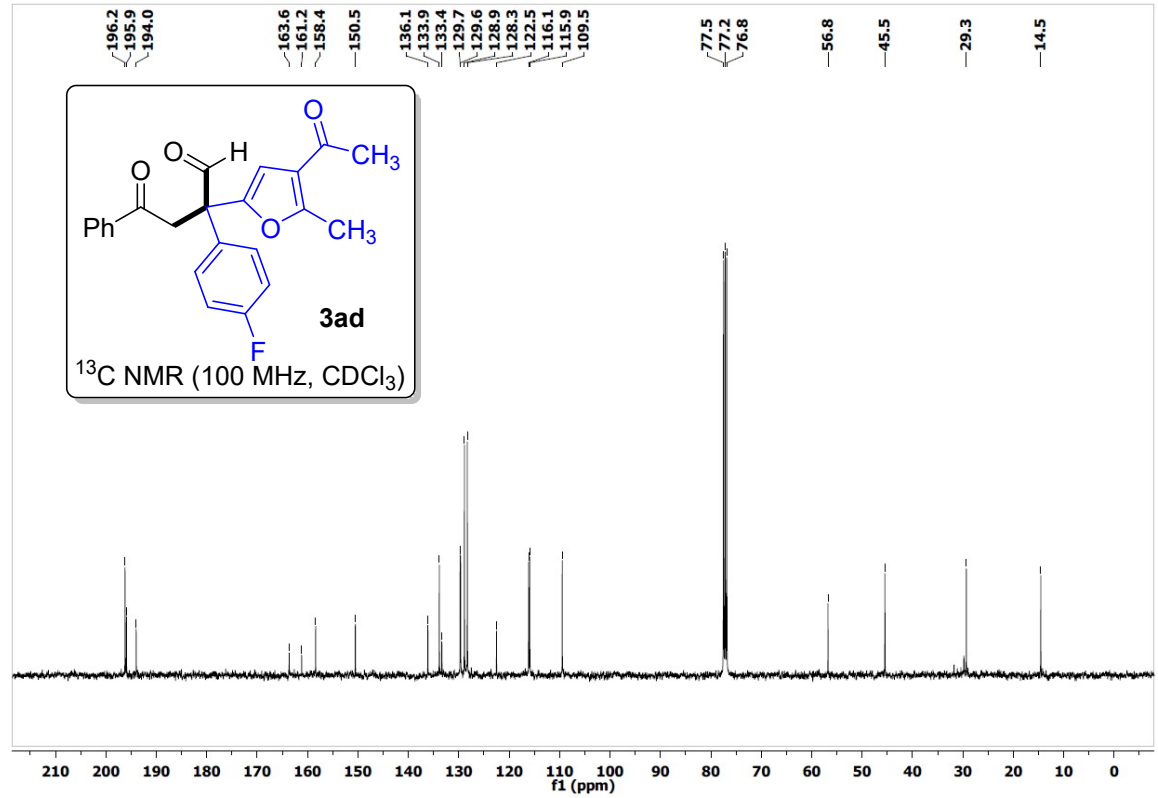

10.05
7.95
7.93
7.60
7.58
7.56
7.48
7.46
7.44
7.18
7.16
7.12
7.10
6.63
4.13
4.13
2.49
2.39
2.34
O
O
H
CH3
O
Ph
O
CH3
CH3
3ab
1H NMR (400 MHz, CDCl3)
0.92
2.03
1.00
2.09
2.10
2.13
0.96
1.97
2.98
3.00
3.05
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

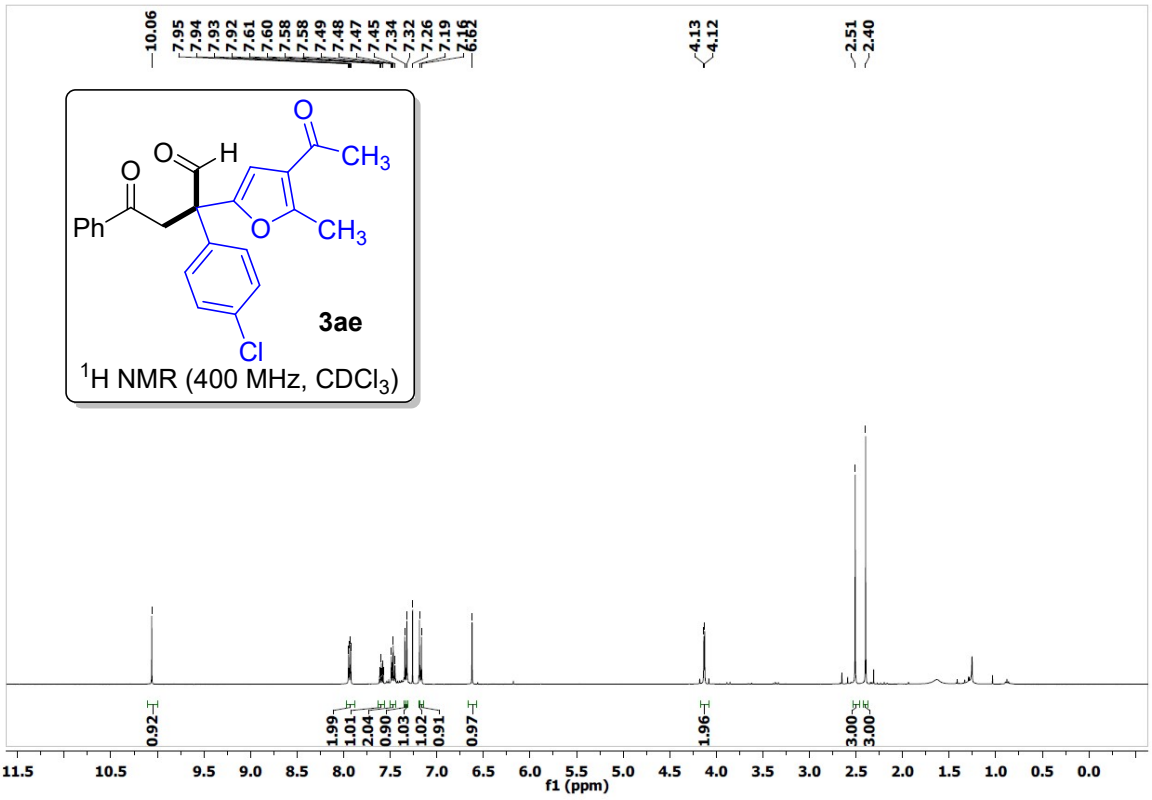

196.4
196.1
194.1
158.1
150.9
138.0
136.3
134.4
133.7
129.8
128.8
128.3
127.6
122.4
109.2
77.5
77.2
76.8
57.0
45.1
29.3
21.1
14.5
O
O
H
CH3
O
Ph
O
CH3
CH3
3ab
13C NMR (100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

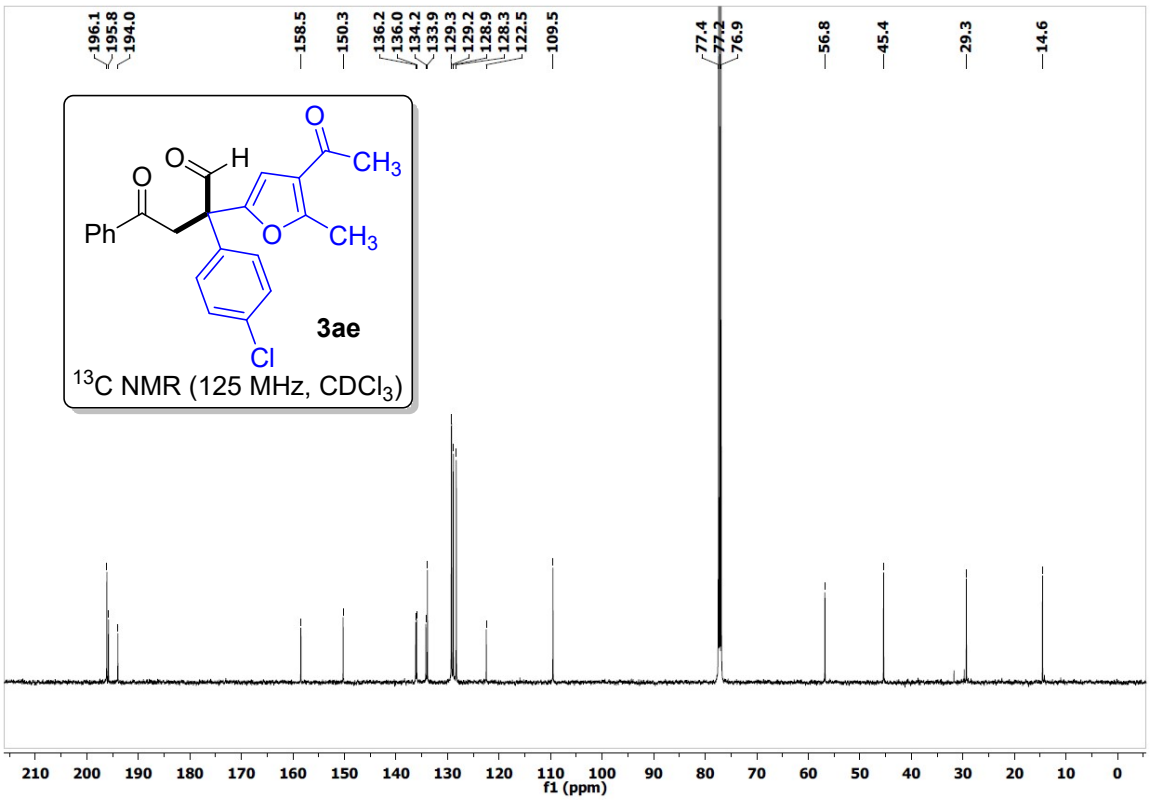

10.02
7.95
7.95
7.93
7.93
7.60
7.60
7.60
7.59
7.58
7.58
7.57
7.56
7.56
7.48
7.48
7.46
7.44
7.15
7.13
6.90
6.88
6.63
4.12
4.11
3.80
2.49
2.39
O
CH3
O
H
O
Ph
O
CH3
OMe
3ac
1H NMR (400 MHz, CDCl3)
0.95
2.15
0.99
2.11
2.07
2.06
0.98
1.97
3.08
3.00
3.10
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

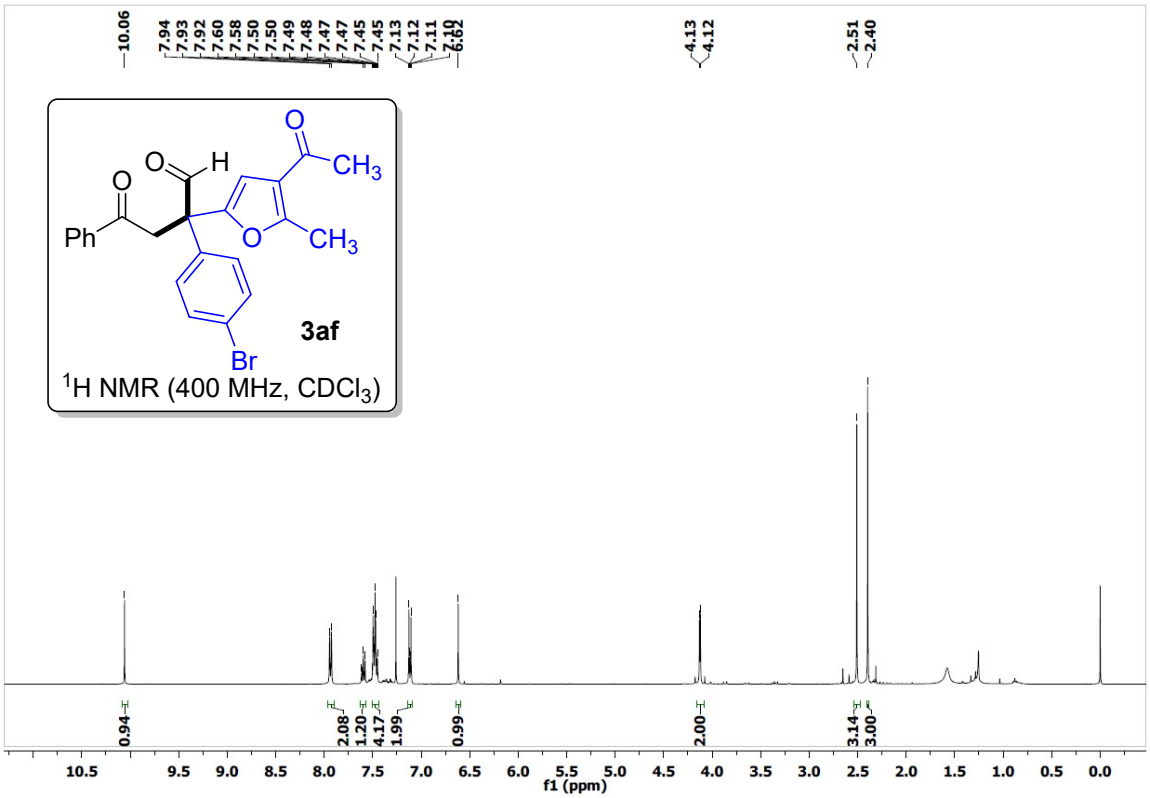

196.2
196.2
194.1
159.4
158.1
150.9
136.3
133.7
129.2
129.0
128.8
128.3
122.4
121.9
114.5
109.2
77.5
77.2
76.8
56.7
55.4
45.1
29.3
14.5
O
CH3
O
H
O
Ph
O
CH3
OMe
3ac
13C NMR (100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

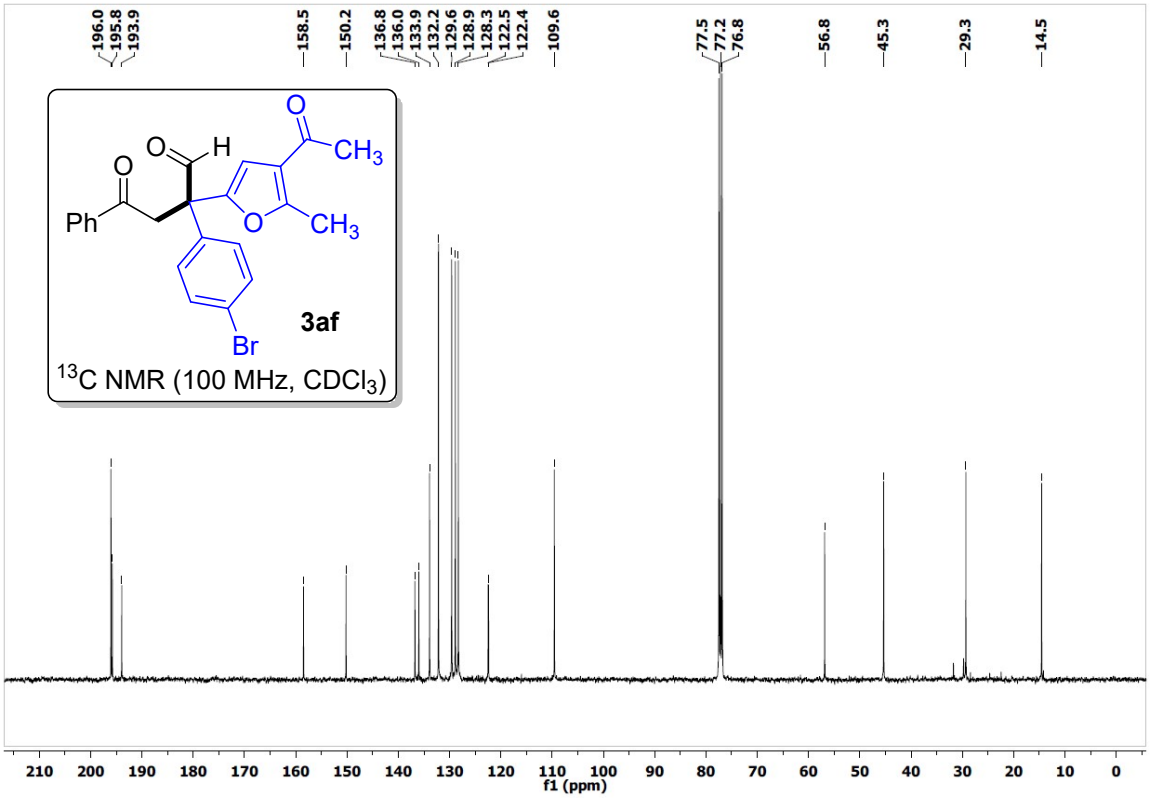

10.06
7.95
7.95
7.93
7.93
7.59
7.58
7.49
7.47
7.45
7.23
7.22
7.21
7.21
7.19
7.07
7.05
7.03
6.83
4.13
4.12
2.51
2.40
O
O
H
CH3
Ph
O
CH3
F
3ad
1H NMR (400 MHz, CDCl3)
0.98
2.11
1.10
2.09
2.00
2.01
1.00
1.95
3.00
3.01
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

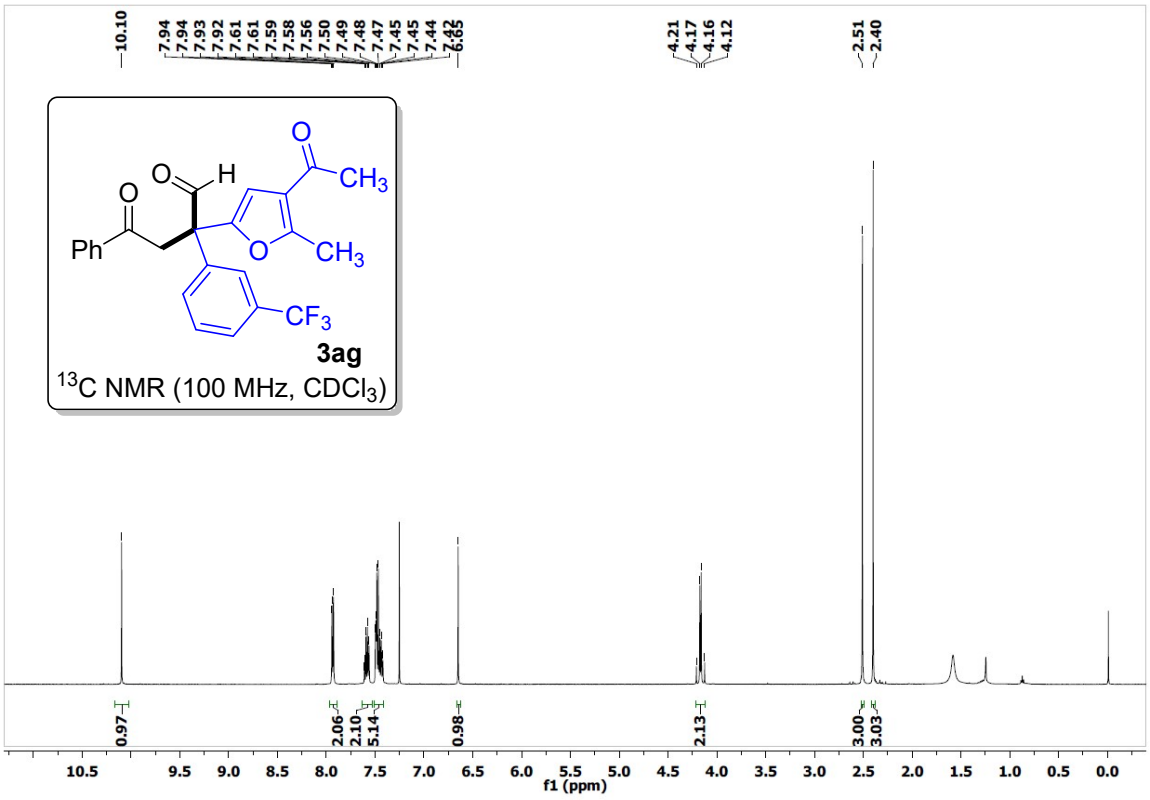

196.2
195.9
194.0
163.6
161.2
158.4
150.5
136.1
133.9
133.4
129.7
129.6
128.9
128.3
122.5
116.1
115.9
109.5
77.5
77.2
76.8
56.8
45.5
29.3
14.5
O
O
H
CH3
Ph
O
CH3
F
3ad
13C NMR (100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

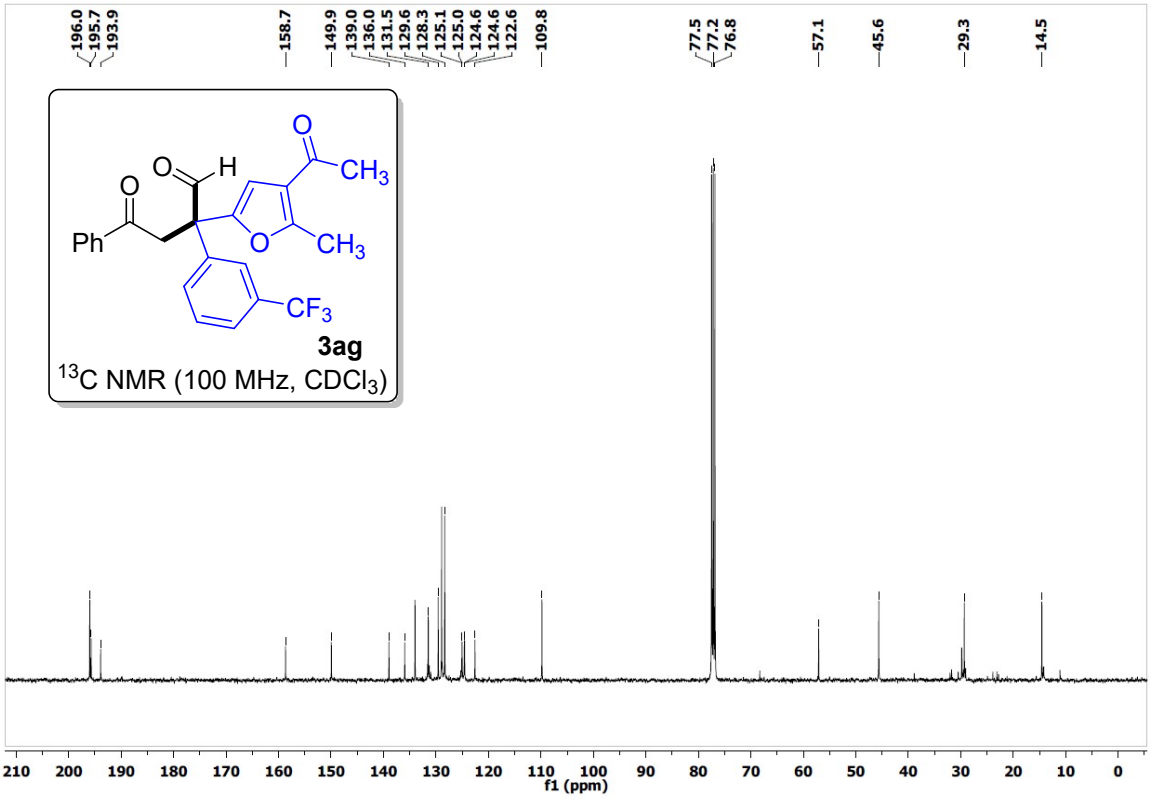

10.06
7.95
7.94
7.93
7.92
7.61
7.60
7.58
7.58
7.49
7.48
7.47
7.45
7.34
7.32
7.26
7.19
7.16
6.82
4.13
4.12
2.51
2.40
O
CH3
O
H
O
Ph
O
CH3
Cl
3ae
1H NMR (400 MHz, CDCl3)
0.92
1.99
1.01
2.04
0.90
1.03
1.02
0.91
0.97
1.96
3.00
3.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

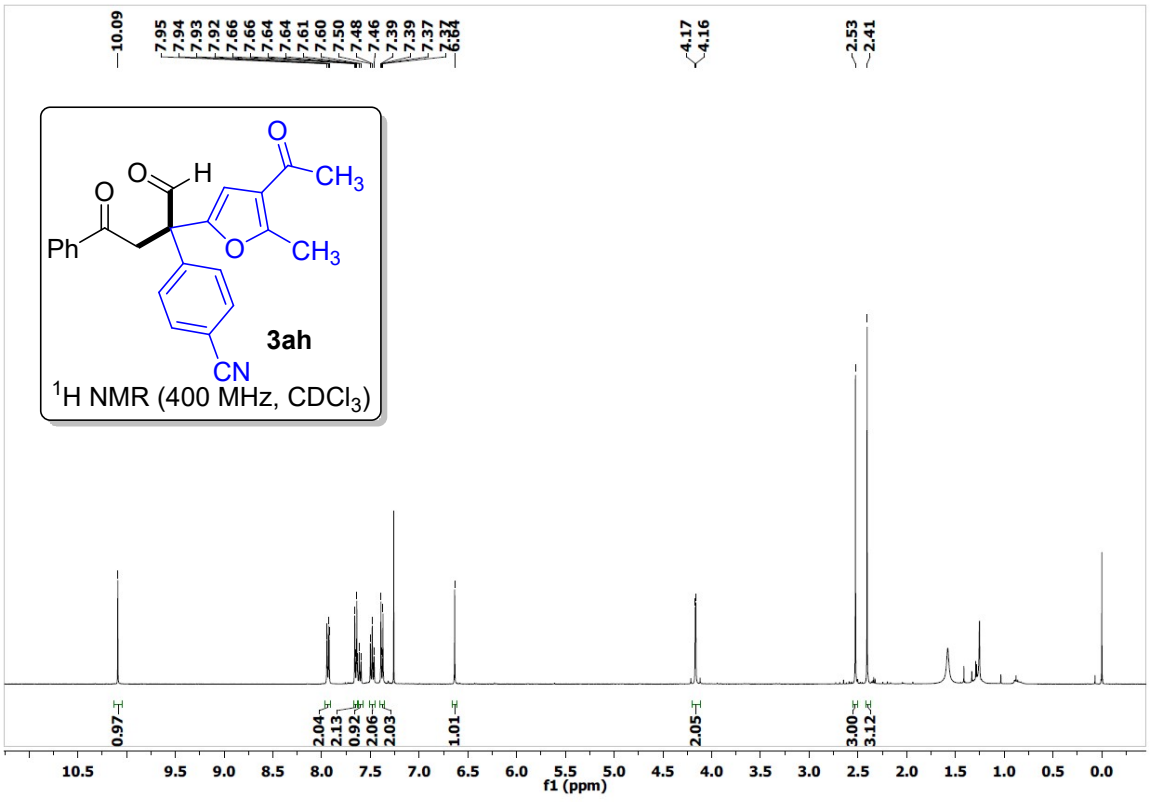

196.1
195.8
194.0
158.5
150.3
136.2
136.0
134.2
133.9
129.3
129.2
128.9
128.3
122.5
109.5
77.4
77.2
76.9
56.8
45.4
29.3
14.6
O
CH3
O
H
O
Ph
O
CH3
Cl
3ae
13C NMR (125 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

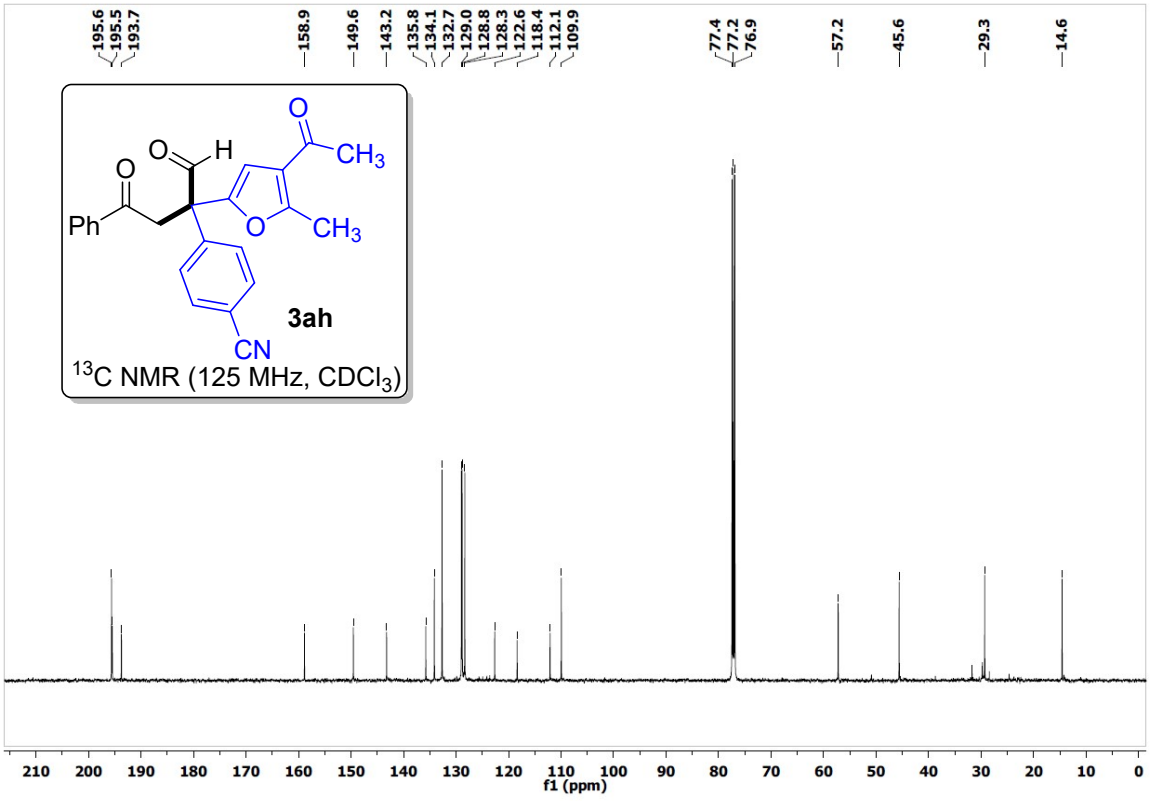

10.06
7.94
7.93
7.92
7.60
7.58
7.50
7.50
7.49
7.48
7.47
7.47
7.45
7.45
7.13
7.12
7.11
7.10
6.62
4.13
4.12
2.51
2.40
O
O
H
CH3
O
Ph
O
CH3
Br
3af
1H NMR (400 MHz, CDCl3)
0.94
2.08
1.20
4.17
1.99
0.99
2.00
3.14
3.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

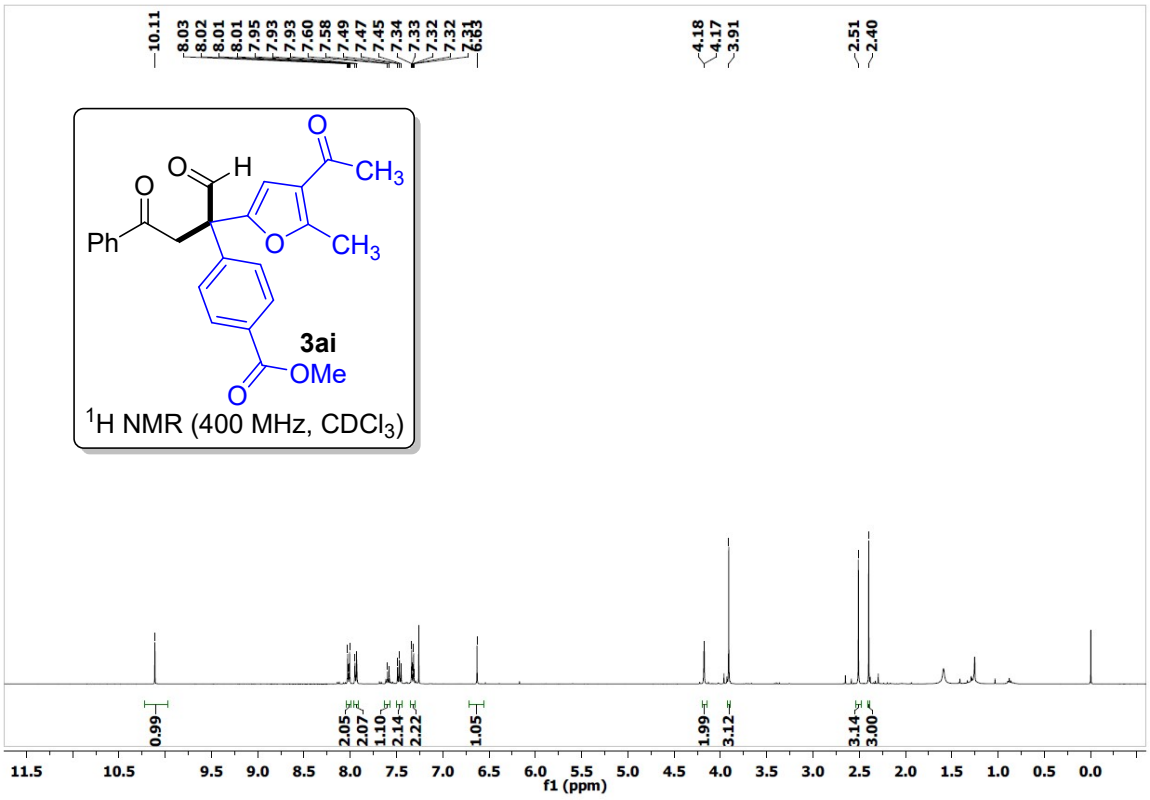

196.0
195.8
193.9
158.5
150.2
136.8
136.0
133.9
132.2
129.6
128.9
128.3
122.5
122.4
109.6
77.5
77.2
76.8
56.8
45.3
29.3
14.5
O
O
H
CH3
O
Ph
O
CH3
Br
3af
13C NMR (100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

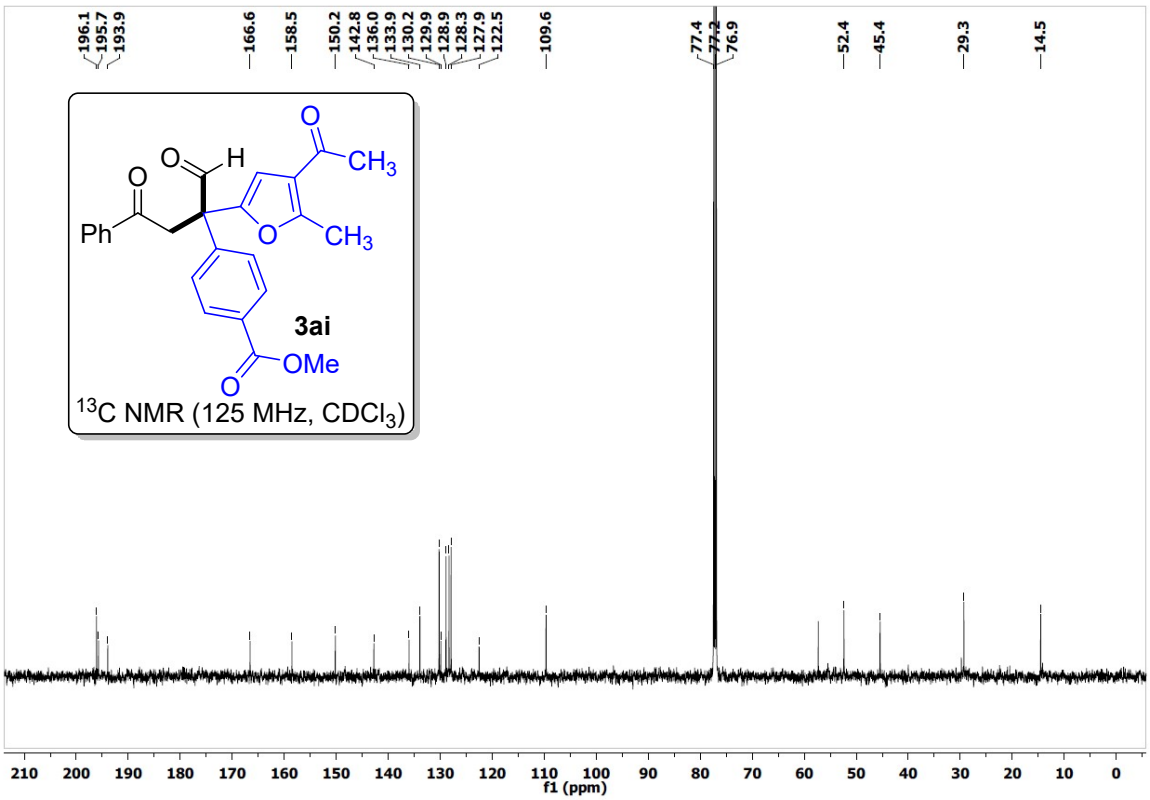

10.10
7.94
7.94
7.93
7.92
7.61
7.61
7.59
7.58
7.56
7.50
7.49
7.48
7.47
7.45
7.45
7.44
7.42
6.65
4.21
4.17
4.16
4.12
2.51
2.40
O
O
H
CH3
O
Ph
O
CH3
CF3
3ag
13C NMR (100 MHz, CDCl3)
0.97
2.06
2.10
5.14
0.98
2.13
3.00
3.03
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

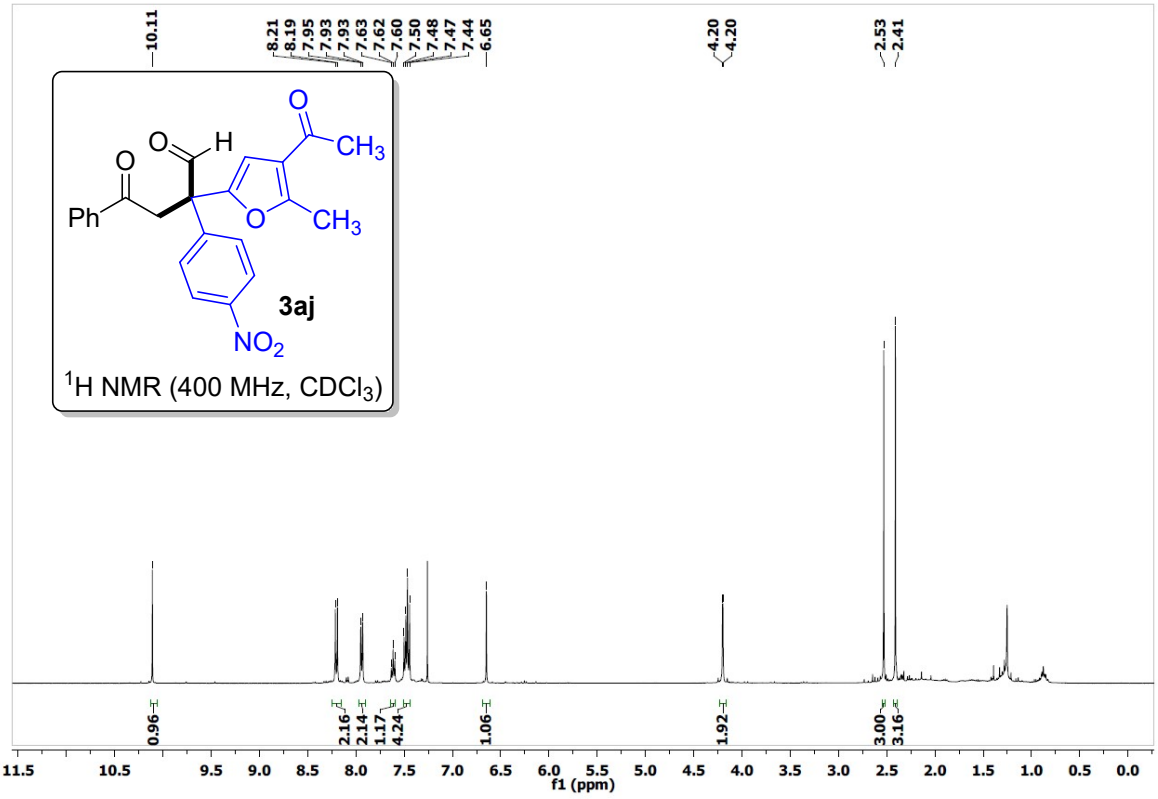

196.0
195.7
193.9
158.7
149.9
139.0
136.0
131.5
129.6
128.3
125.1
125.0
124.6
124.6
122.6
109.8
77.5
77.2
76.8
57.1
45.6
29.3
14.5
O
O
H
CH3
O
Ph
O
CH3
CF3
3ag
13C NMR (100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

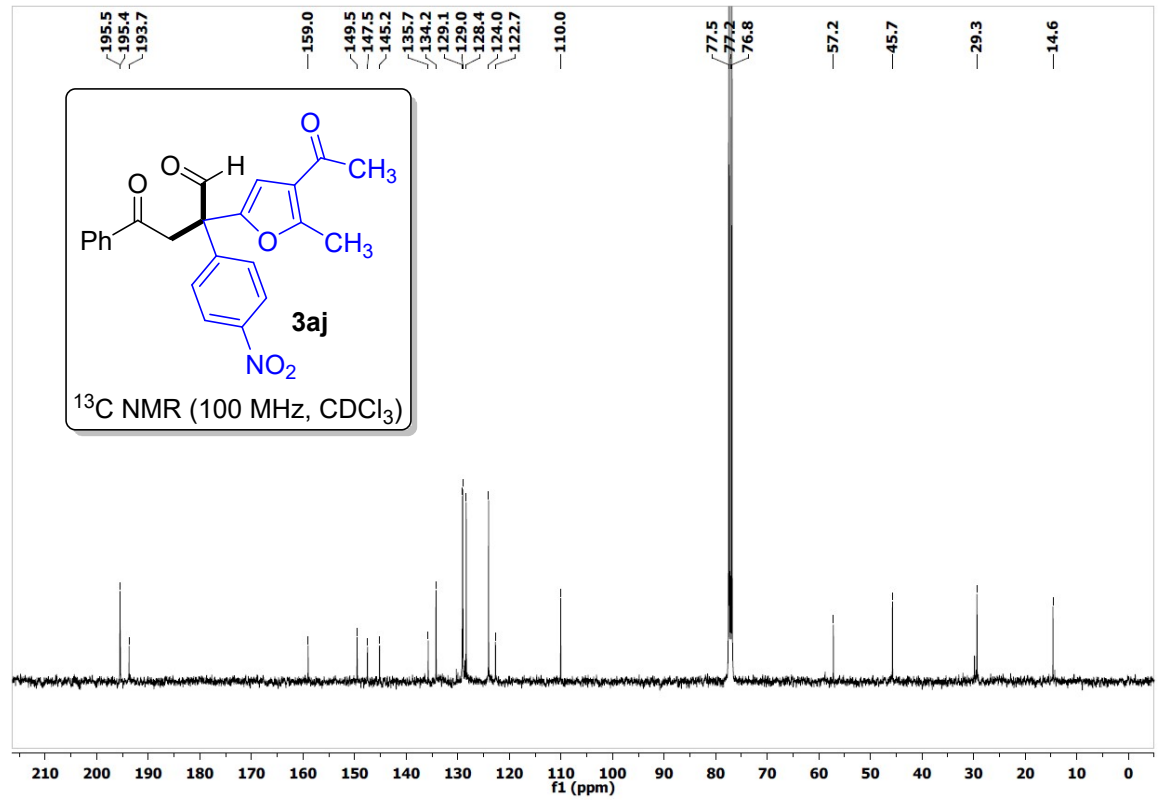

10.09
7.95
7.94
7.93
7.92
7.66
7.66
7.64
7.64
7.61
7.60
7.50
7.48
7.46
7.39
7.39
7.37
7.37
6.84
4.17
4.16
2.53
2.41
O
O
H
CH3
Ph
O
CH3
3ah
CN
1H NMR (400 MHz, CDCl3)
0.97
2.04
2.13
0.92
2.06
2.03
1.01
2.05
3.00
3.12
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

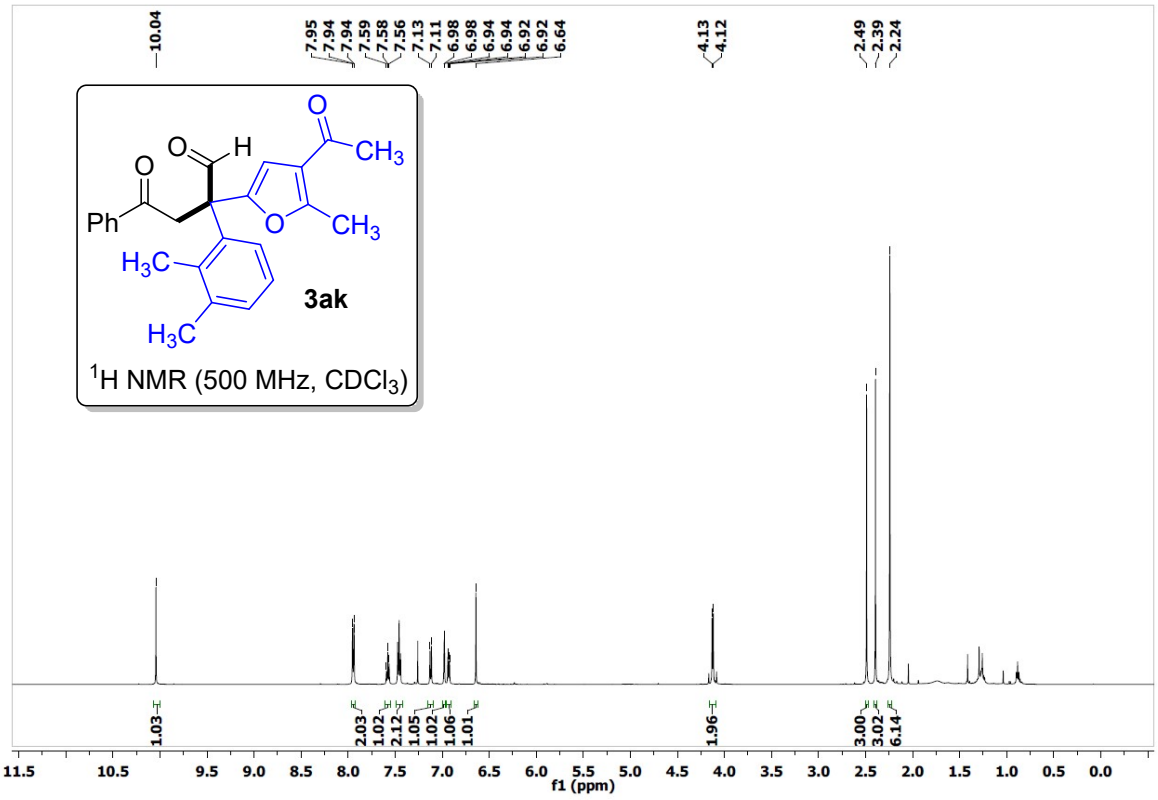

195.6
195.5
193.7
158.9
149.6
143.2
135.8
134.1
132.7
129.0
128.8
128.3
122.6
118.4
112.1
109.9
77.4
77.2
76.9
57.2
45.6
29.3
14.6
O
O
H
CH3
Ph
O
CH3
3ah
CN
13C NMR (125 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

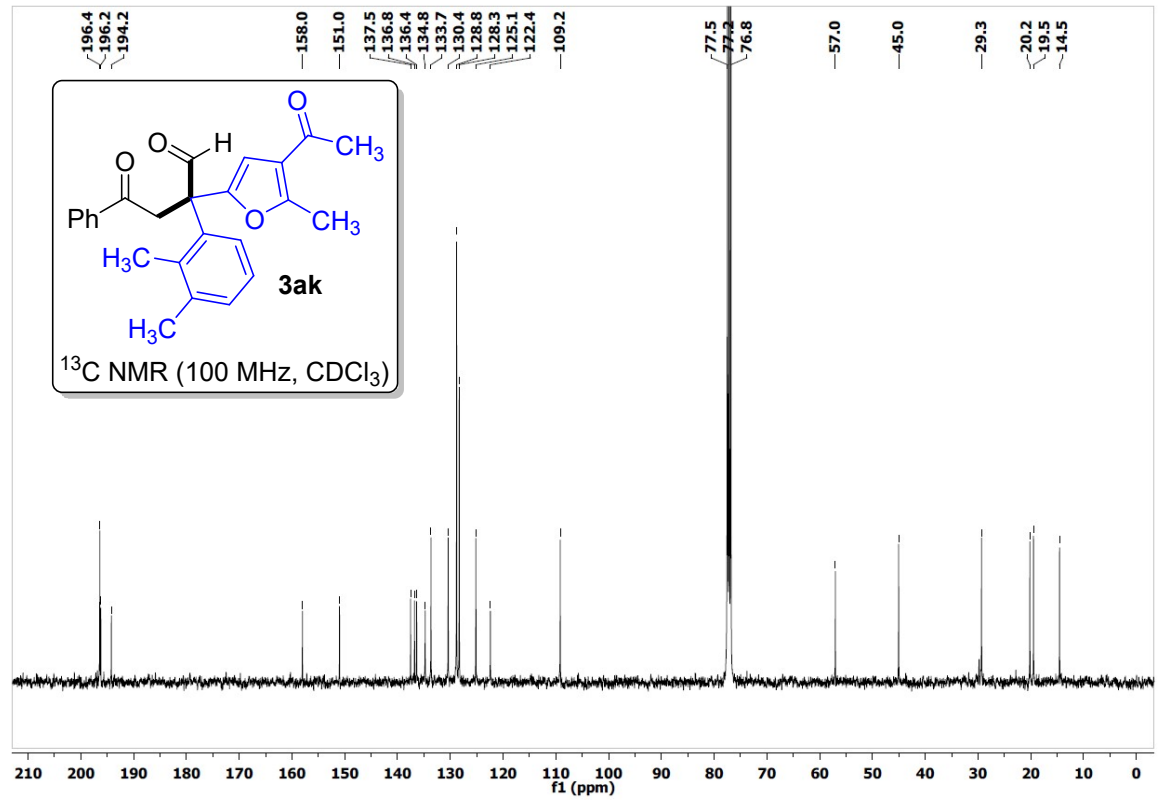

10.11
8.03
8.02
8.01
8.01
7.95
7.93
7.93
7.60
7.58
7.49
7.47
7.45
7.34
7.33
7.32
7.32
7.31
6.83
4.18
4.17
3.91
2.51
2.40
O
O
H
O
CH3
Ph
O
CH3
3ai
OMe
O
1H NMR (400 MHz, CDCl3)
0.99
2.05
2.07
1.10
2.14
2.22
1.05
1.99
3.12
3.14
3.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

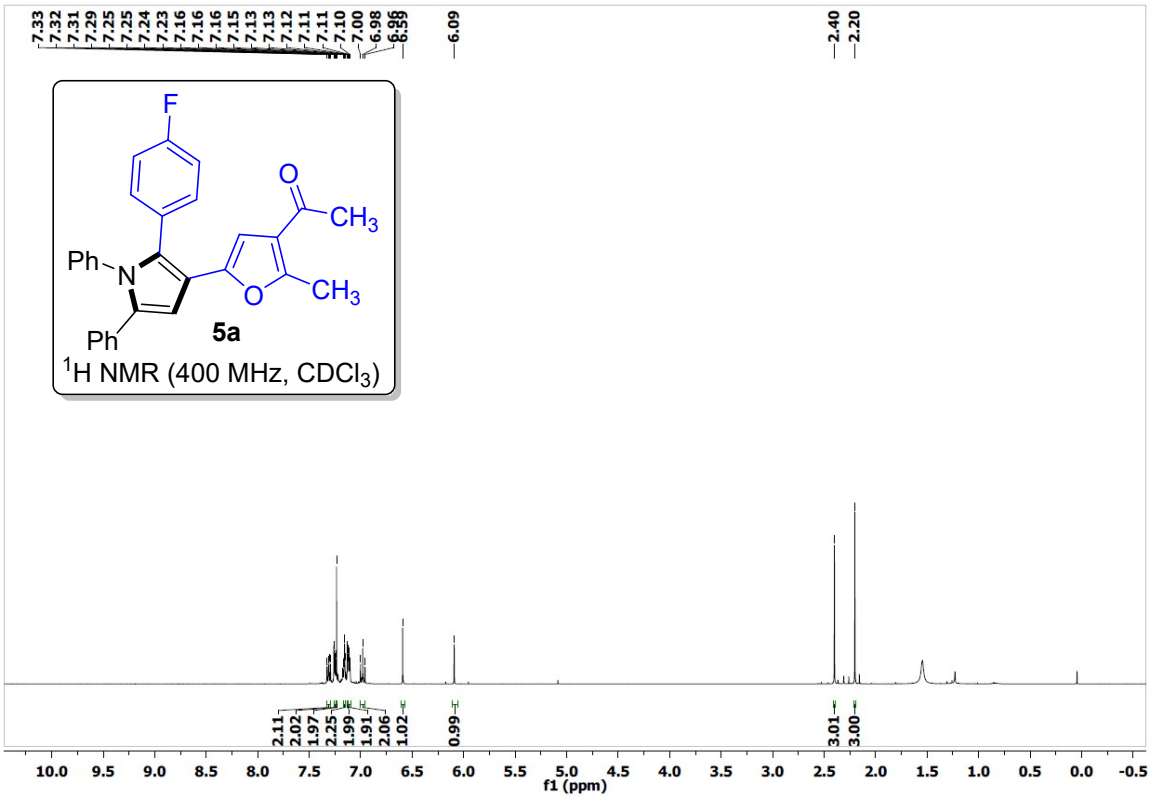

196.1
195.7
193.9
166.6
158.5
150.2
142.8
136.0
133.9
130.2
129.9
128.9
128.3
127.9
122.5
109.6
77.4
77.2
76.9
52.4
45.4
29.3
14.5
O
O
H
O
CH3
Ph
O
CH3
3ai
OMe
O
13C NMR (125 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

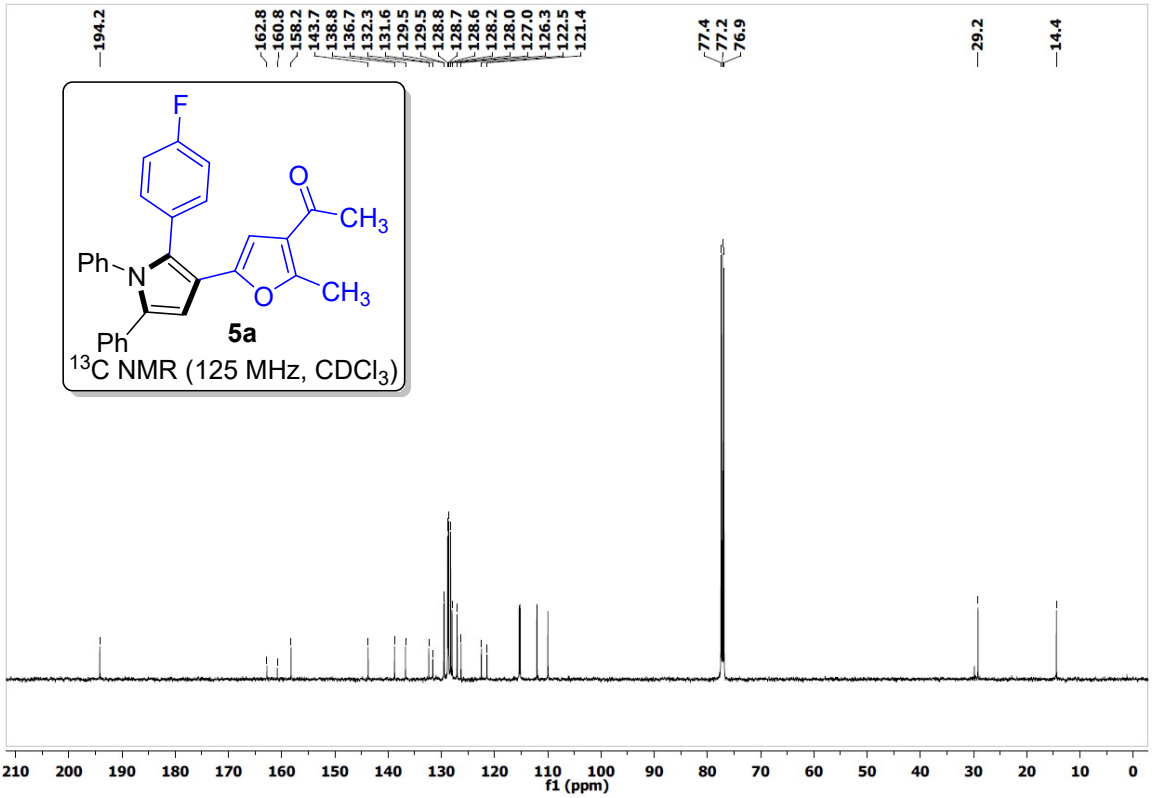

10.11
8.21
8.19
7.95
7.93
7.93
7.63
7.62
7.60
7.50
7.48
7.47
7.44
6.65
4.20
4.20
2.53
2.41
O
O
H
CH3
Ph
O
CH3
3aj
NO2
1H NMR (400 MHz, CDCl3)
0.96
2.16
2.14
1.17
4.24
1.06
1.92
3.00
3.16
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

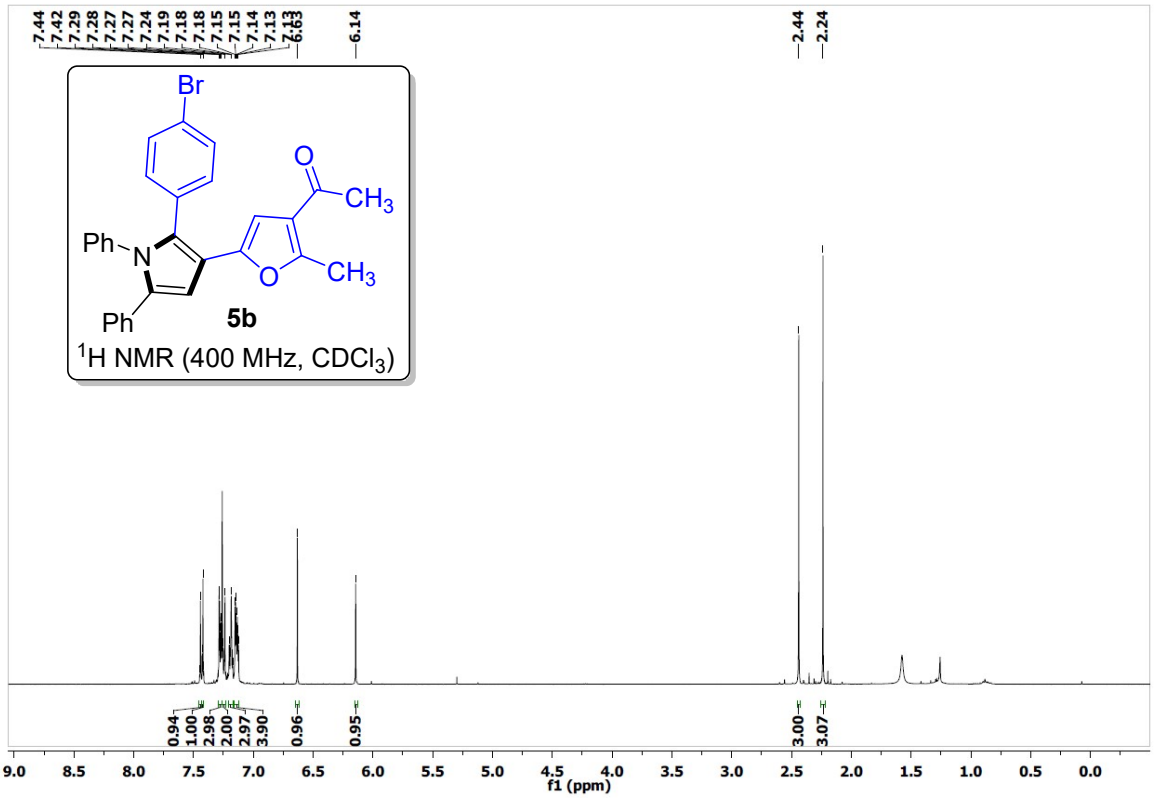

195.5
195.4
193.7
159.0
149.5
147.5
145.2
135.7
134.2
129.1
129.0
128.4
124.0
122.7
110.0
77.5
77.2
76.8
57.2
45.7
29.3
14.6
O
O
H
CH3
Ph
O
CH3
3aj
NO2
13C NMR (100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

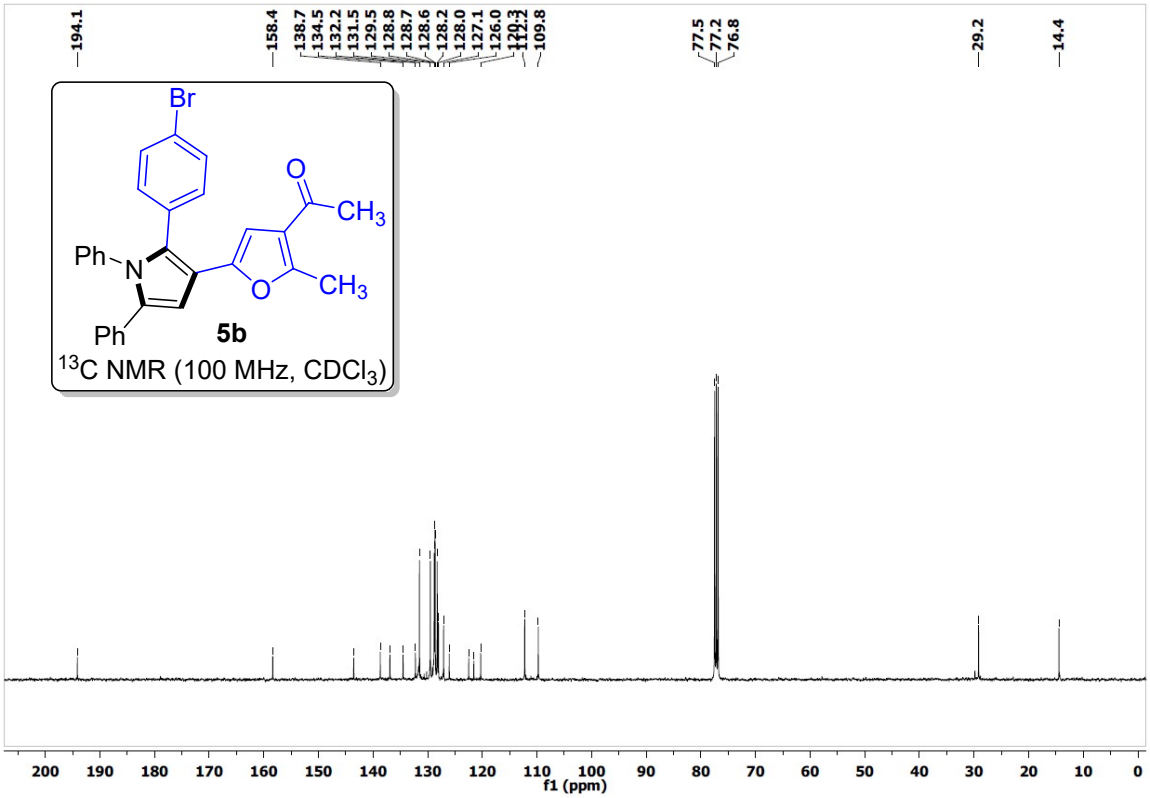

3ak
^{1}H NMR (500 MHz, $CDCl_3$)
f1 (ppm)

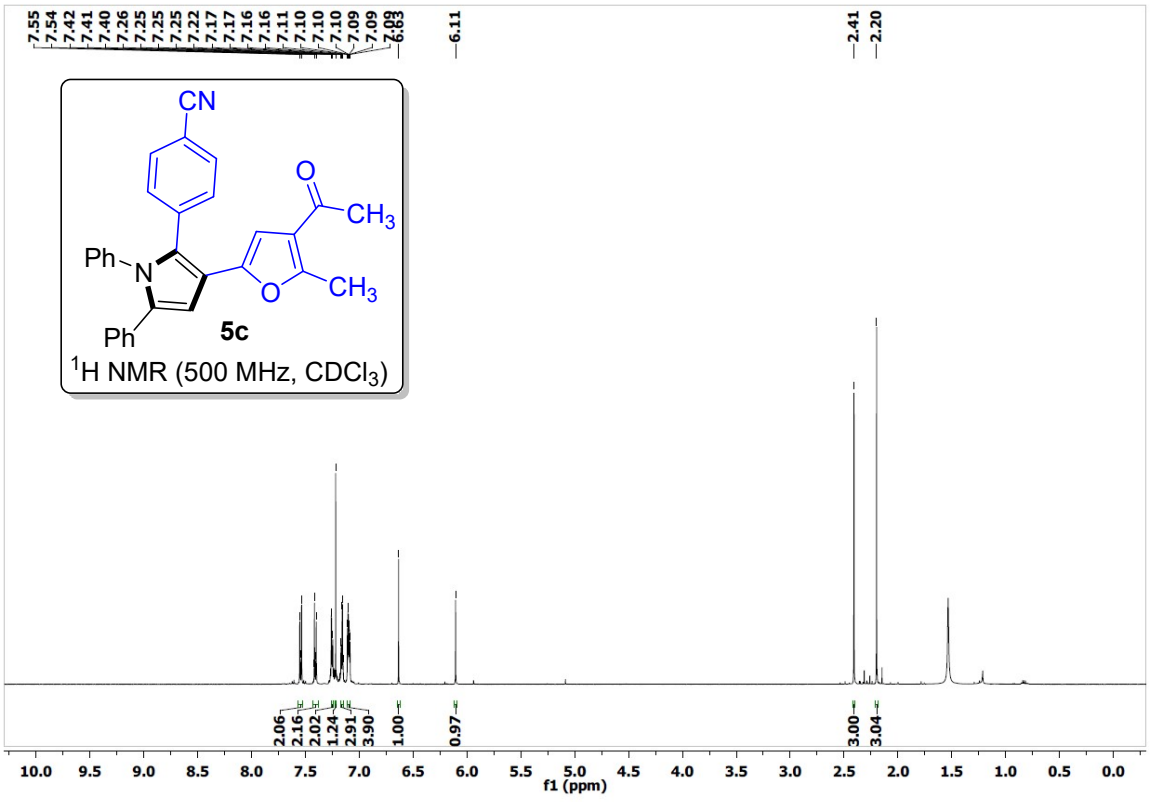

3ak
^{13}C NMR (100 MHz, $CDCl_3$)
f1 (ppm)

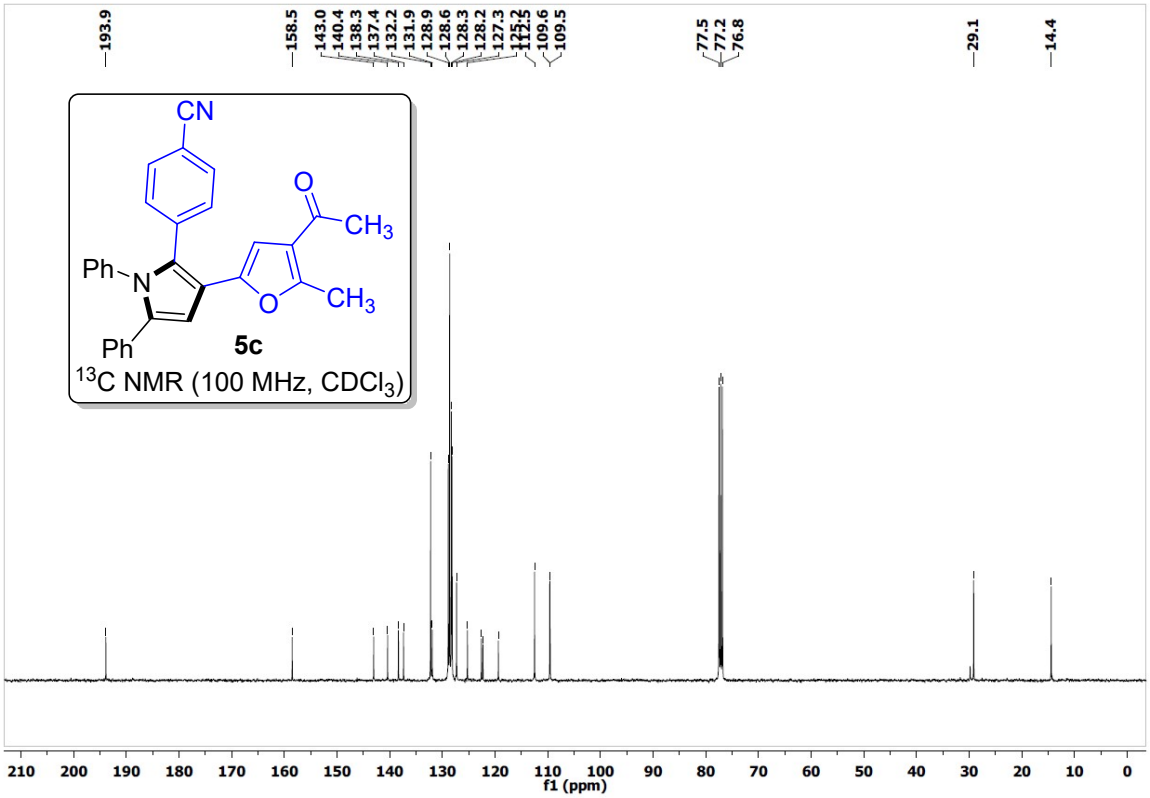

F
O
CH3
Ph
N
O
CH3
Ph
5a
1H NMR (400 MHz, CDCl3)
f1 (ppm)

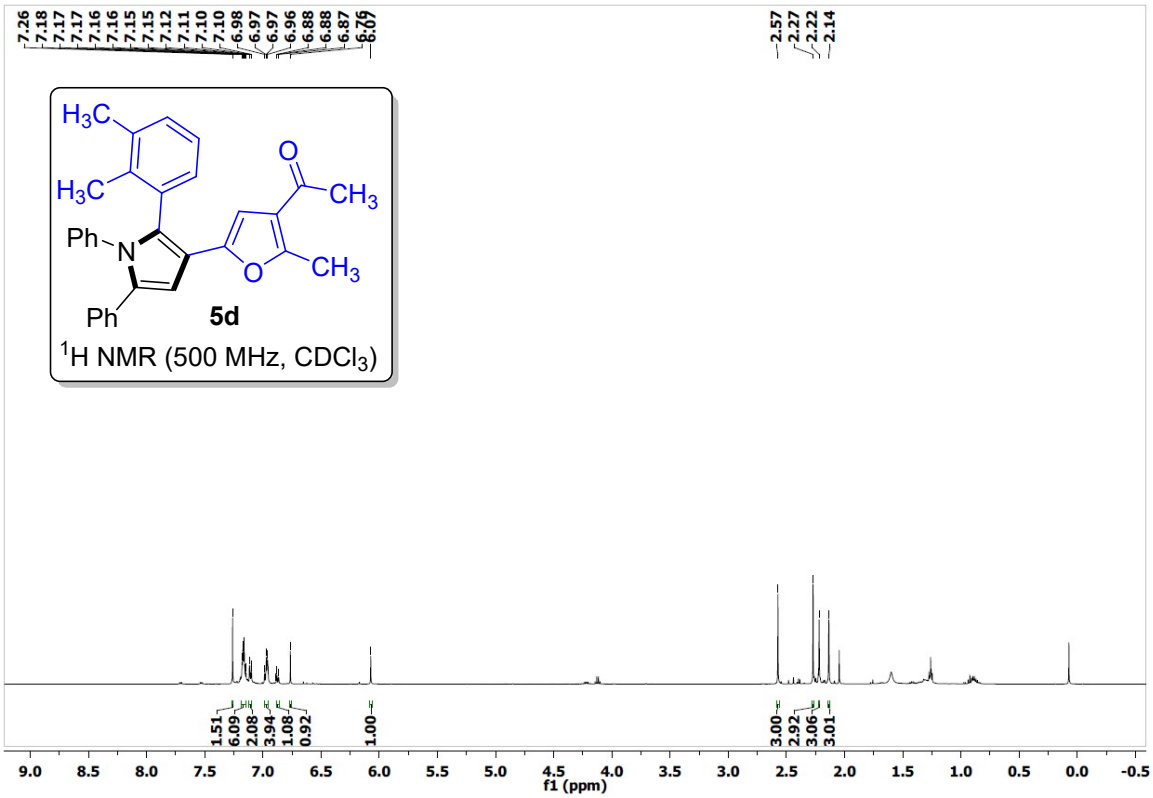

F
O
CH3
Ph
N
O
CH3
Ph
5a
13C NMR (125 MHz, CDCl3)
f1 (ppm)

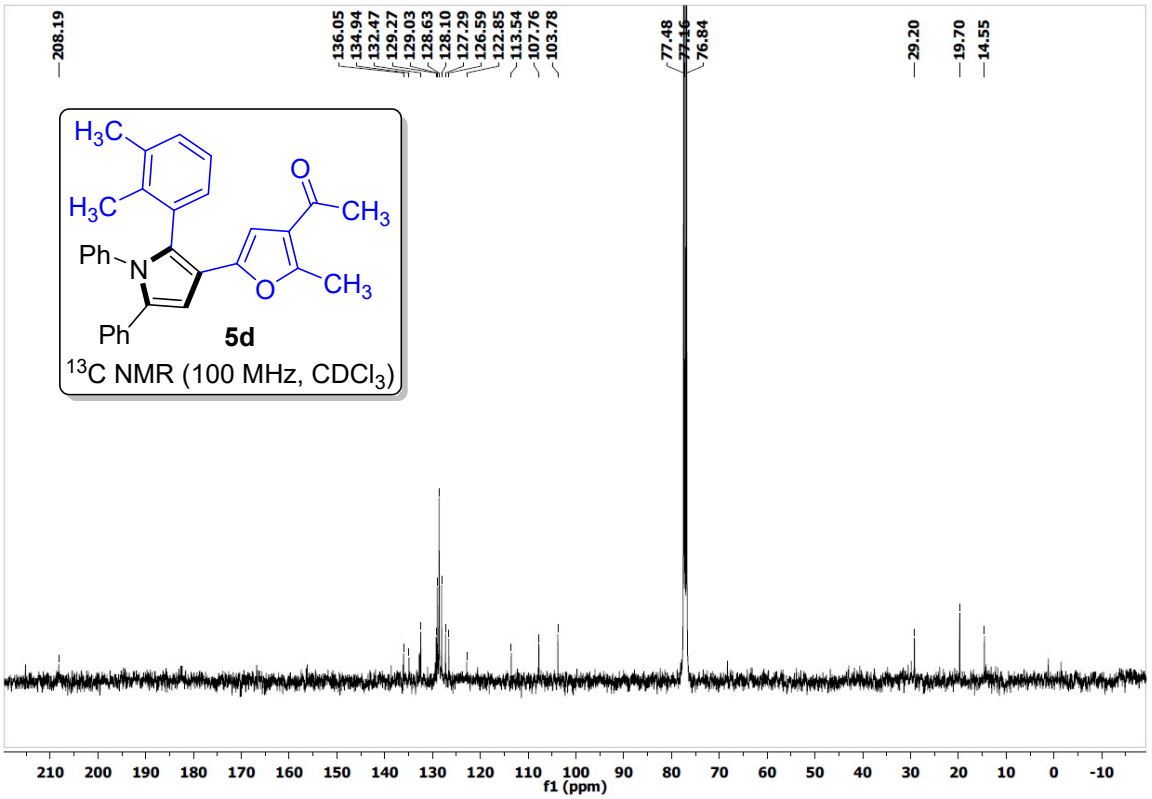

Br
O
CH3
Ph
N
O
CH3
Ph
5b
1H NMR (400 MHz, CDCl3)
f1 (ppm)

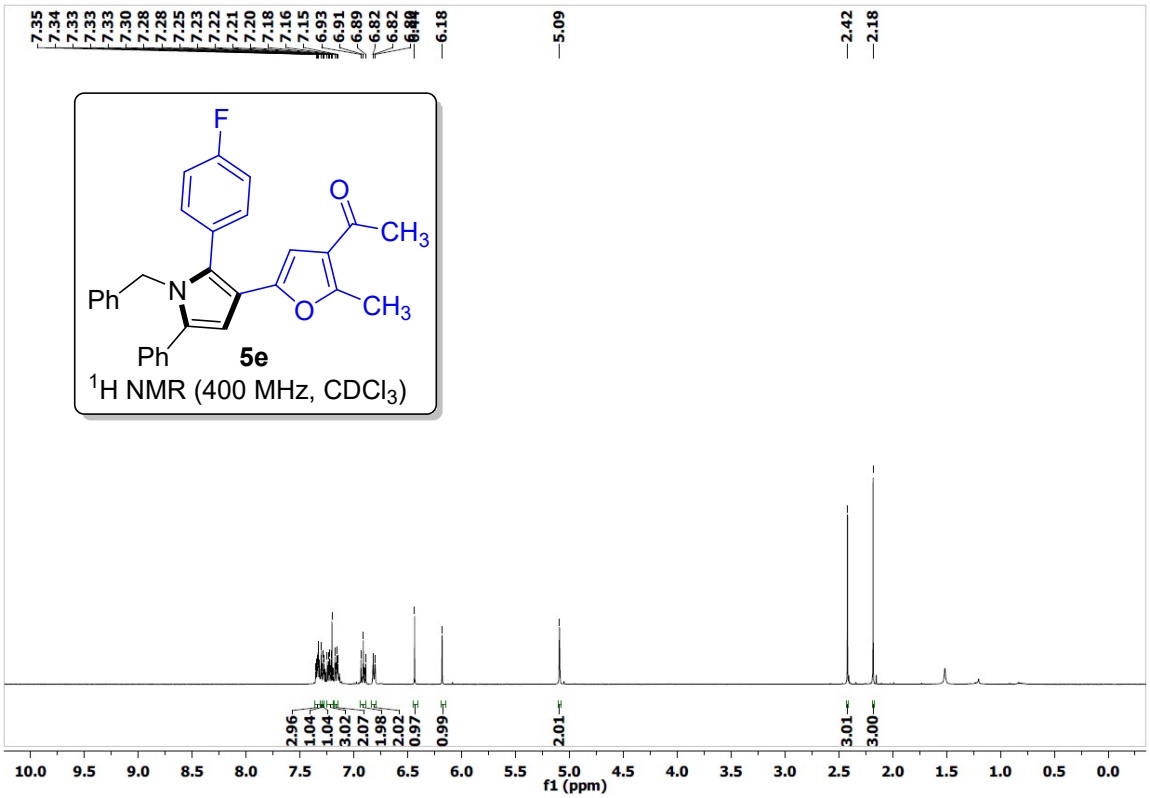

Br
O
CH3
Ph
N
O
CH3
Ph
5b
13C NMR (100 MHz, CDCl3)
f1 (ppm)

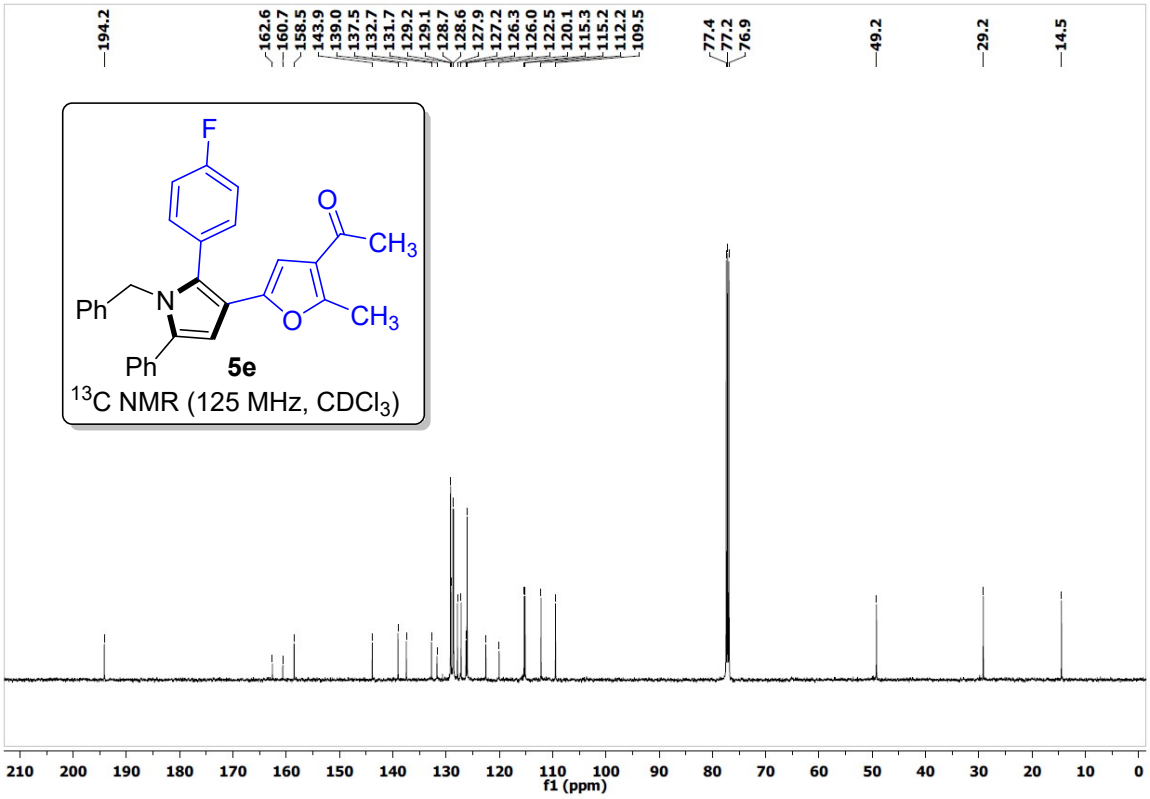

CN
O
CH3
Ph
N
O
CH3
Ph
5c
1H NMR (500 MHz, CDCl3)
f1 (ppm)

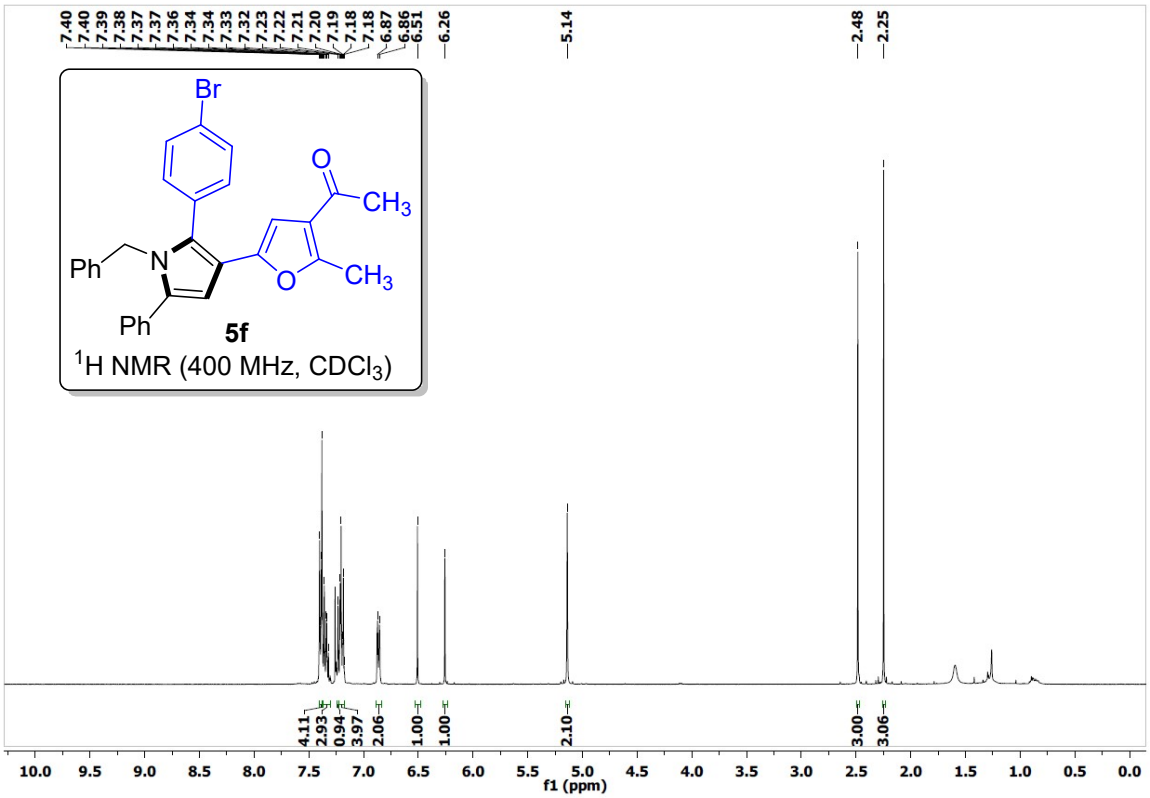

CN
O
CH3
Ph
N
O
CH3
Ph
5c
13C NMR (100 MHz, CDCl3)
f1 (ppm)

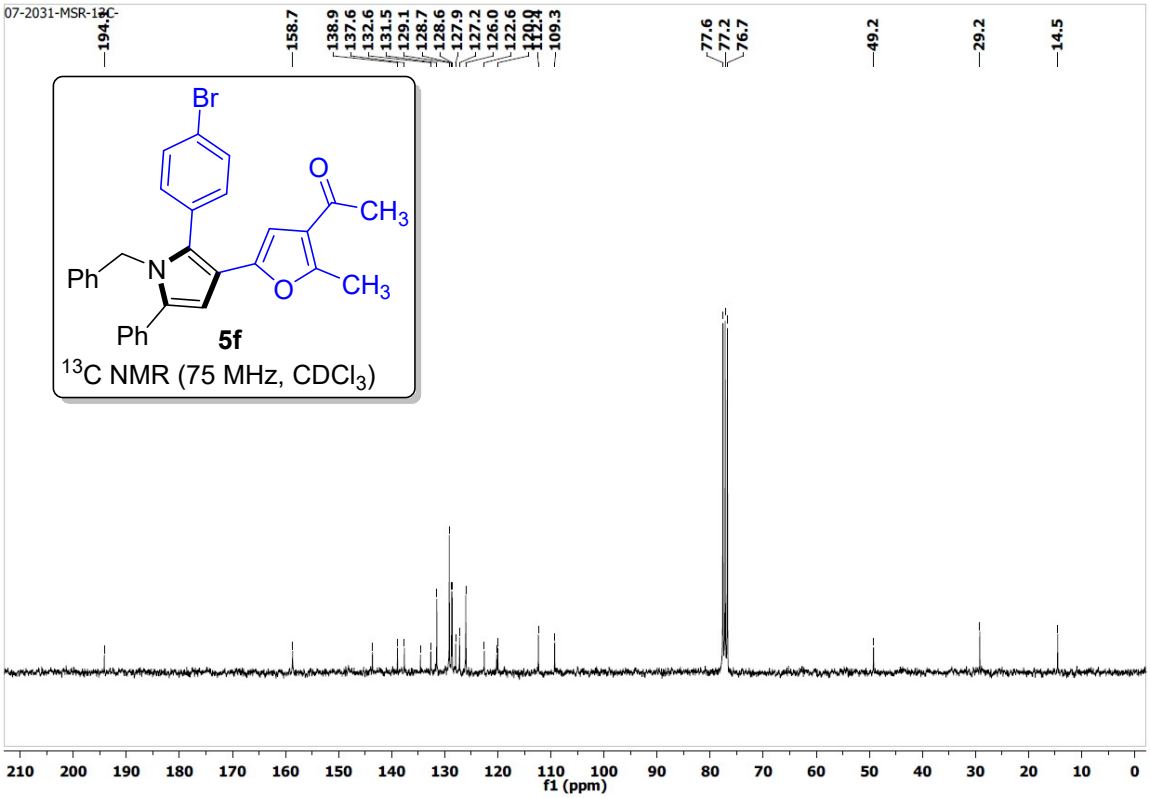

7.26
7.18
7.17
7.17
7.16
7.16
7.15
7.15
7.12
7.11
7.10
7.10
6.98
6.97
6.97
6.96
6.88
6.88
6.87
6.76
6.76
2.57
2.27
2.22
2.14
H3C
H3C
O
CH3
Ph
N
O
CH3
Ph
5d
1H NMR (500 MHz, CDCl3)
1.51
6.09
2.08
3.94
1.08
0.92
1.00
3.00
2.92
3.06
3.01
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

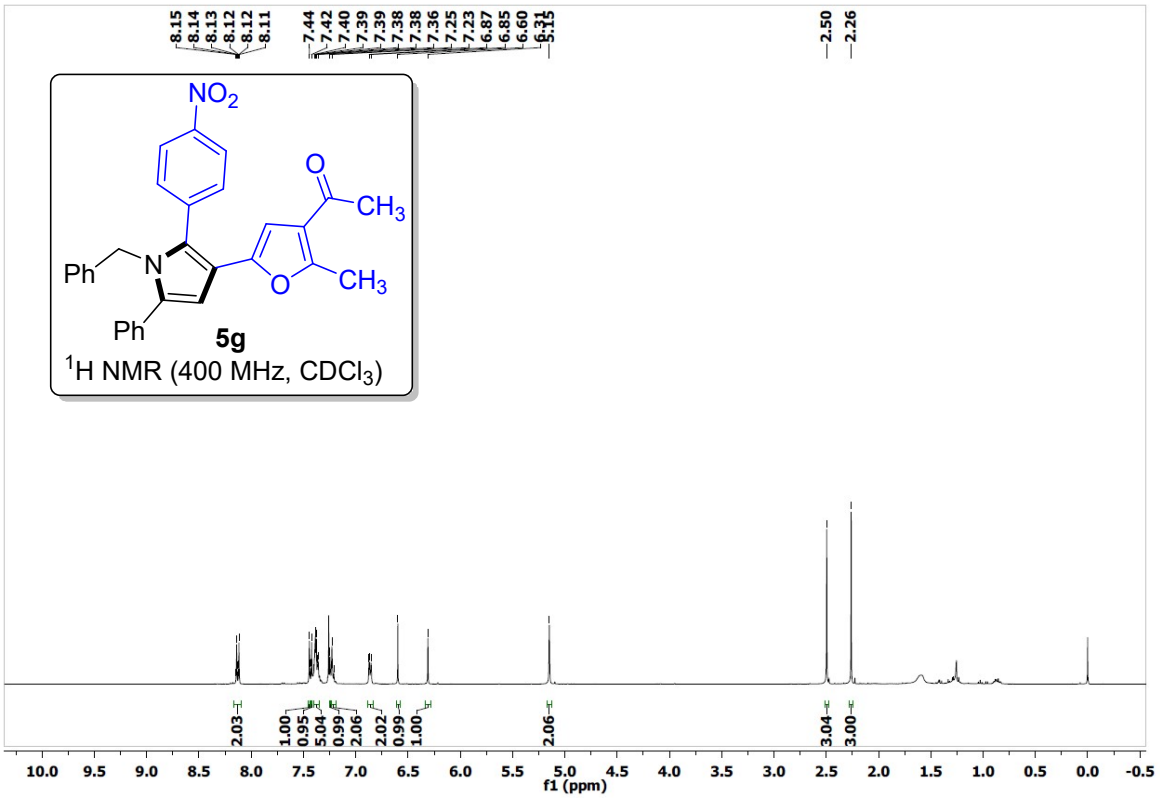

208.19
136.05
134.94
132.47
129.27
129.03
128.63
128.10
127.29
126.59
122.85
113.54
107.76
103.78
77.48
77.16
76.84
29.20
19.70
14.55
H3C
H3C
O
CH3
Ph
N
O
CH3
Ph
5d
13C NMR (100 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

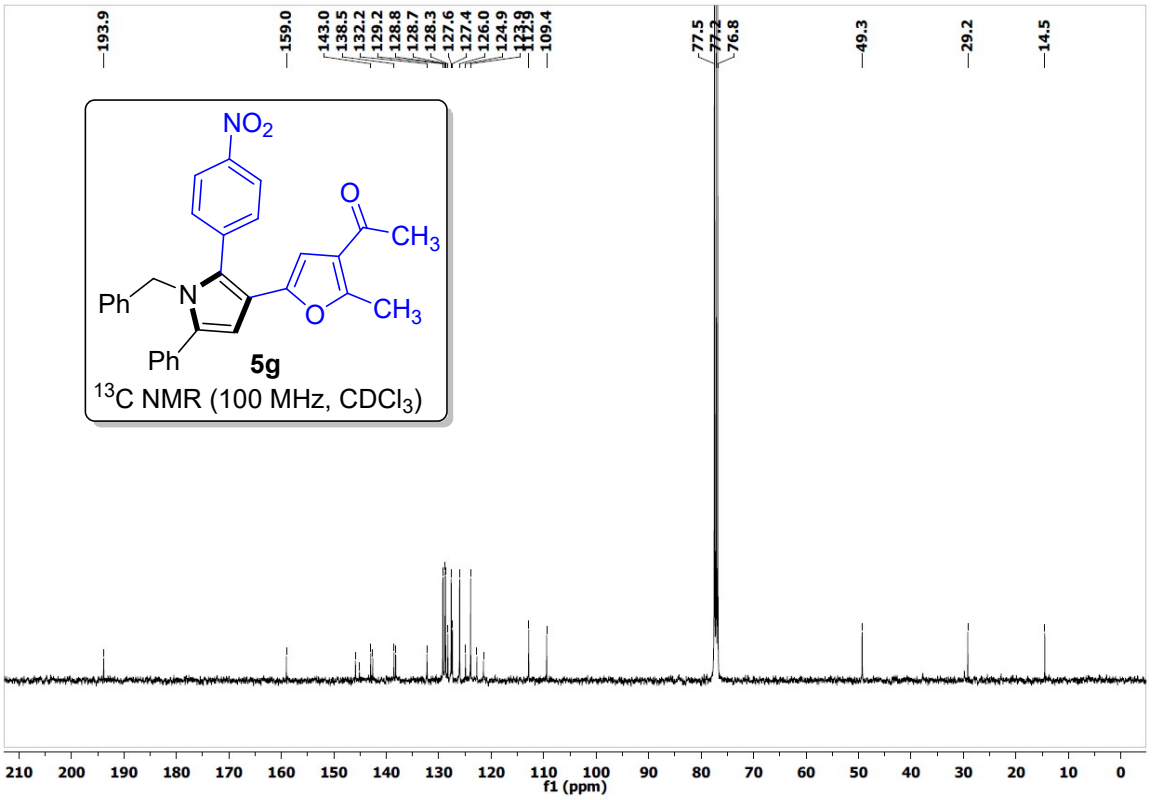

F
O
CH3
Ph
N
O
CH3
Ph
5e
1H NMR (400 MHz, CDCl3)
f1 (ppm)

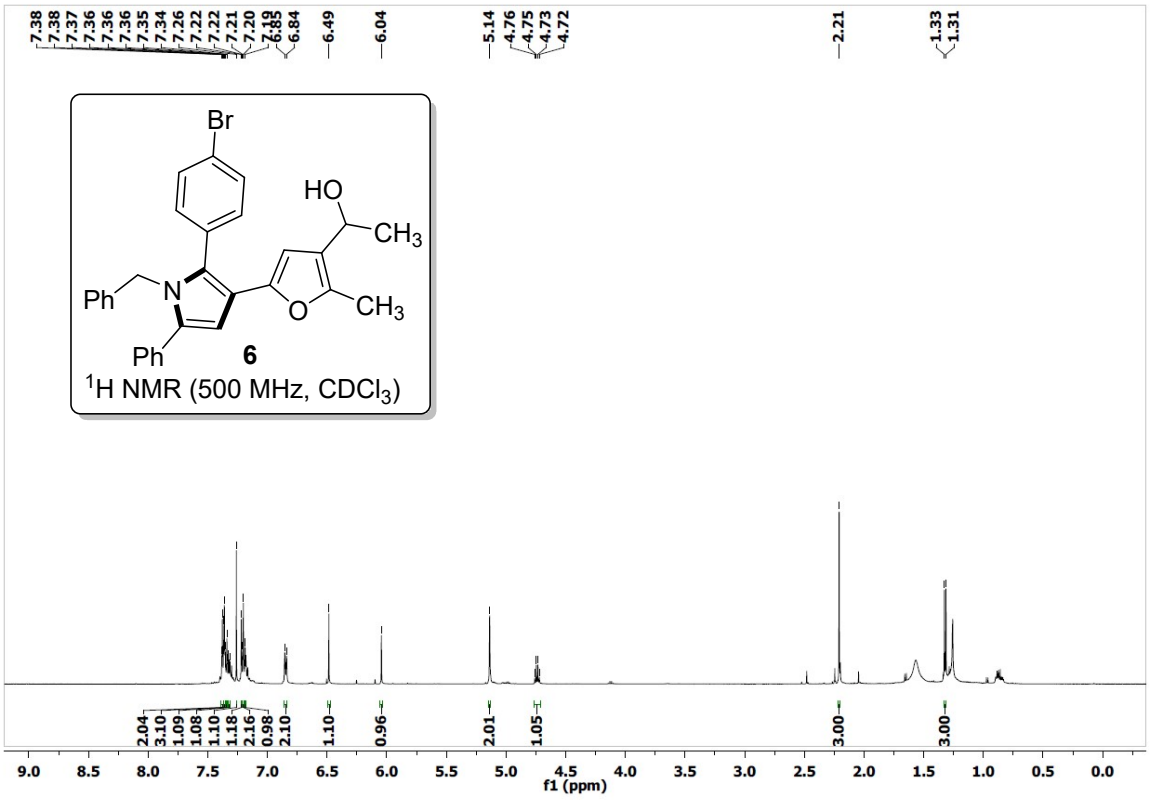

F
O
CH3
Ph
N
O
CH3
Ph
5e
13C NMR (125 MHz, CDCl3)
f1 (ppm)

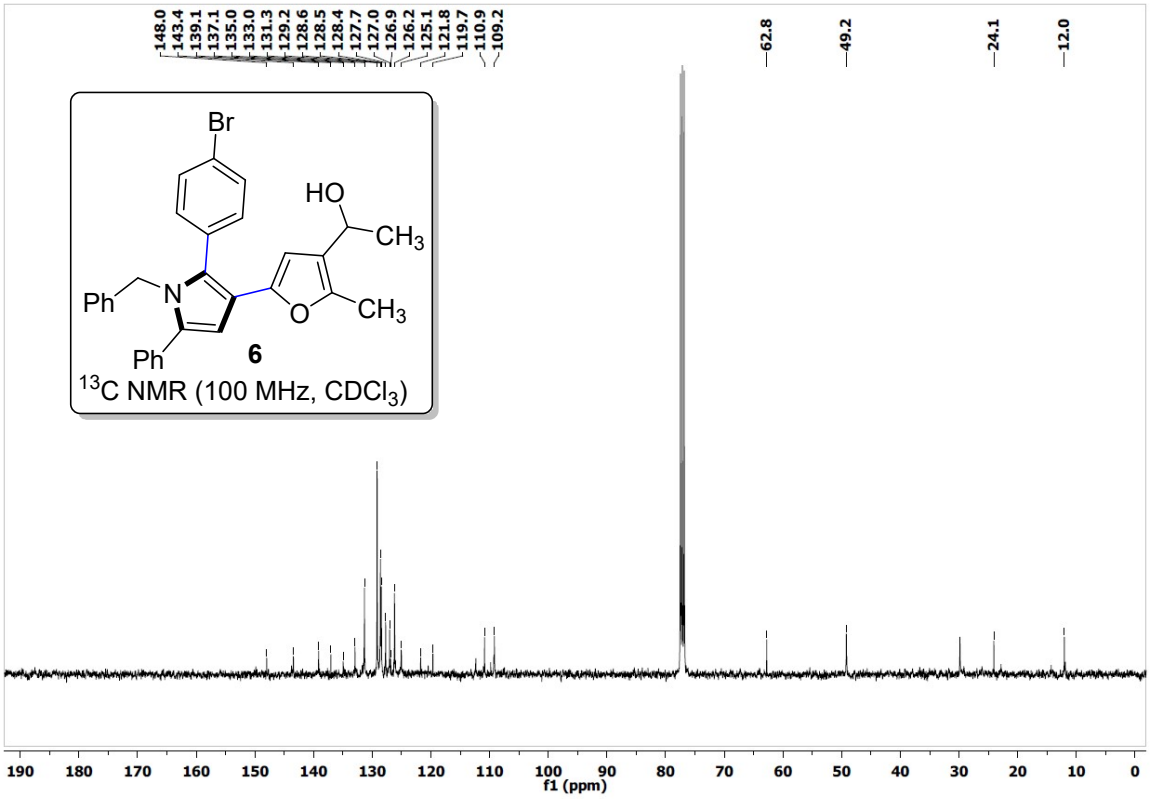

Br
O
CH3
Ph
N
O
CH3
Ph
5f
1H NMR (400 MHz, CDCl3)
7.40
7.40
7.39
7.38
7.37
7.37
7.36
7.34
7.34
7.33
7.32
7.23
7.22
7.21
7.20
7.19
7.18
6.87
6.86
6.51
6.26
5.14
2.48
2.25
4.11
2.93
0.94
3.97
2.06
1.00
1.00
2.10
3.00
3.06
f1 (ppm)

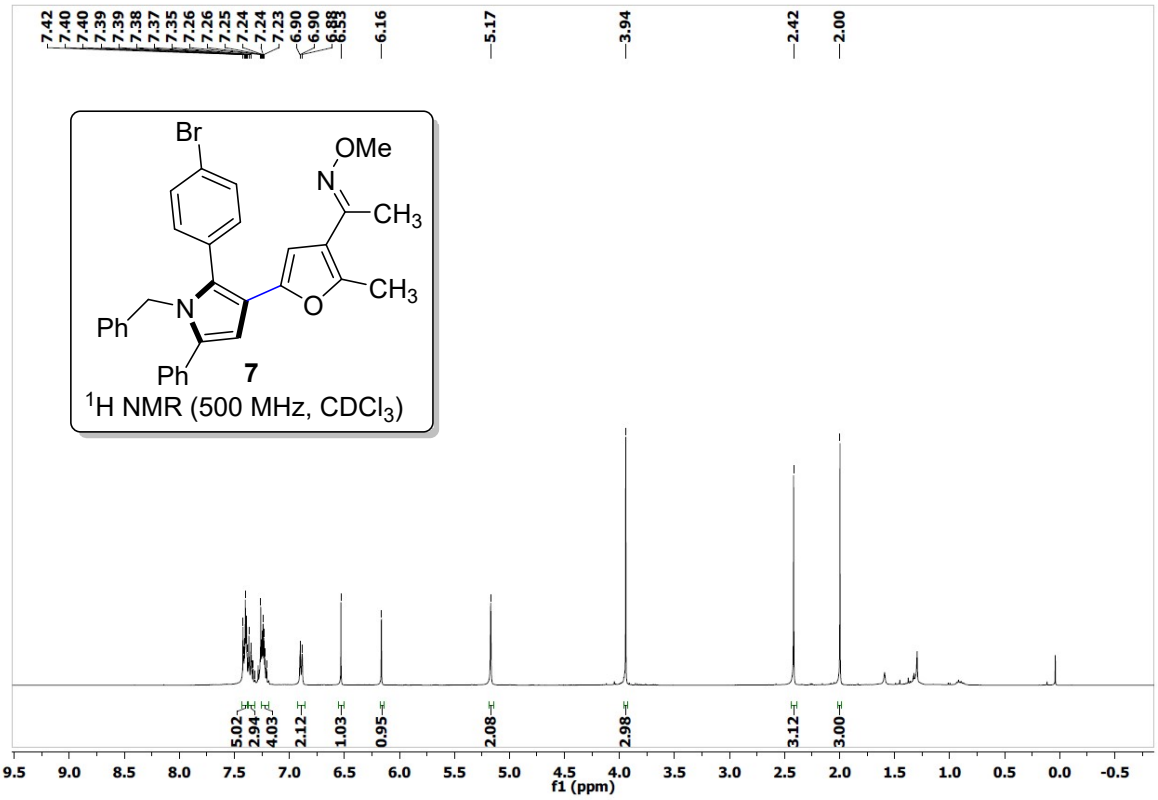

Br
O
CH3
Ph
N
O
CH3
Ph
5f
13C NMR (75 MHz, CDCl3)
194.2
158.7
138.9
137.6
132.6
131.5
129.1
128.7
128.6
127.9
127.2
126.0
122.6
120.9
112.4
109.3
77.6
77.2
76.7
49.2
29.2
14.5
f1 (ppm)

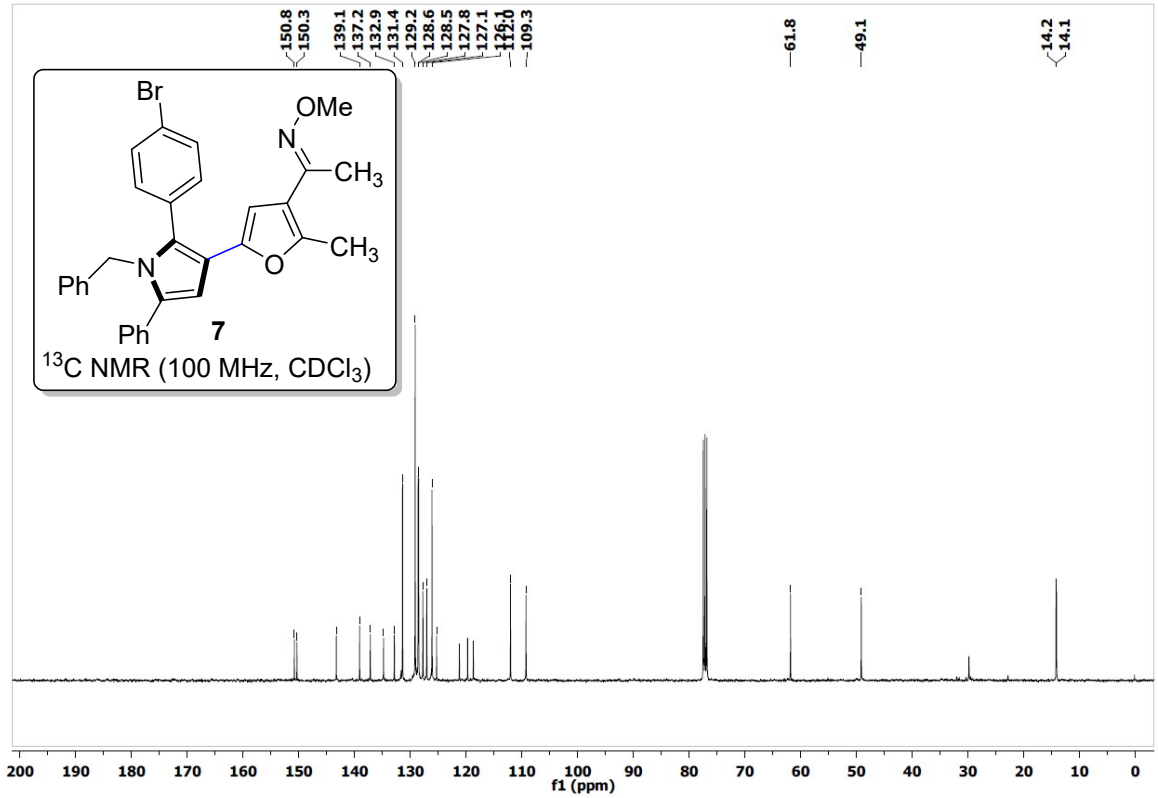

8.15
8.14
8.13
8.12
8.12
8.11
7.44
7.42
7.40
7.39
7.39
7.38
7.38
7.36
7.25
7.23
6.87
6.85
6.60
6.31
5.15
2.50
2.26
NO2
O
CH3
Ph
N
O
CH3
Ph
5g
1H NMR (400 MHz, CDCl3)
2.03
1.00
0.95
5.04
0.99
2.06
2.02
0.99
1.00
2.06
3.04
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


193.9
159.0
143.0
138.5
132.2
129.2
128.8
128.7
128.3
127.6
127.4
126.0
124.9
123.9
123.3
109.4
77.5
77.2
76.8
49.3
29.2
14.5
NO2
O
CH3
Ph
N
O
CH3
Ph
5g
13C NMR (100 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


Br
HO
CH3
Ph
N
O
CH3
Ph
6
1H NMR (500 MHz, CDCl3)
f1 (ppm)


Br
HO
CH3
Ph
N
O
CH3
Ph
6
13C NMR (100 MHz, CDCl3)
f1 (ppm)


Br
OMe
N
CH3
CH3
O
N
Ph
Ph
7
1H NMR (500 MHz, CDCl3)
7.42
7.40
7.40
7.39
7.39
7.38
7.37
7.35
7.26
7.26
7.25
7.24
7.24
7.23
6.90
6.90
6.88
6.88
6.16
5.17
3.94
2.42
2.00
5.02
2.94
4.03
2.12
1.03
0.95
2.08
2.98
3.12
3.00
f1 (ppm)


Br
OMe
N
CH3
CH3
O
N
Ph
Ph
7
13C NMR (100 MHz, CDCl3)
150.8
150.3
139.1
137.2
132.9
131.4
129.2
128.6
128.5
127.8
127.1
109.3
61.8
49.1
14.2
14.1
f1 (ppm)