Formal *meta*-Selective C–H Acylation of Pyridines *via* the Triplet State of Oxazinopyridine Intermediates

Fan Gao[a,‡], Yajing Bian[a, ‡], Shiqing Huang[a*] and Xiaoyu Yan[a*]

[a]Key Laboratory of Advanced Light Conversion Materials and Biophotonics, School of Chemistry and Life Resources, Renmin University of China, Beijing, 100872, China. E-mail: yanxy@ruc.edu.cn

[‡]F. G. and Y. B. contributed equally to this work.

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1. General information

All reagents were purchased and used directly without further purification. All reactions were monitored by thin-layer chromatography (TLC), and column chromatography was performed on 200–300 mesh of silica gel purchased from Qing Dao Hai Yang Chemical Industry. ^{1}H, ^{13}C and ^{19}F NMR spectra were recorded on a Bruker Ascend 600 MHz spectrometer operating at 600 MHz, 151 MHz and 564 MHz, respectively. All NMR spectra were recorded in $CDCl_3$ or CD_3CN at room temperature (20 ± 2 °C). Proton chemical shifts δ were given in ppm relative to tetramethylsilane (0.00 ppm) in $CDCl_3$. Spectra were calibrated relative to solvent's residual proton and carbon chemical shift: $CHCl_3$ (δ = 7.26 ppm for ^{1}H NMR and δ = 77.16 ppm for ^{13}C NMR), CH_3CN (δ = 1.94 ppm for ^{1}H NMR and δ = 118.26 ppm for ^{13}C NMR). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, brs = broad singlet, m = multiplet), coupling constants (Hz) and integration. All reactions have been studied in borosilicate glass vessels irradiated by white light from a photoreactor (RLH-18CU) manufactured by Beijing Roger Technology Co., Ltd. without using filters with magnetic stirring apparatus. High-resolution mass spectra (HRMS) were acquired on Thermo Q-Exactive instrument (quadrupole mass analyzer) using electrospray ionization mode (ESI). UV-vis absorption spectra were obtained with Agilent. Cary60 spectrophotometer. Fluorescence spectra were obtained with Edinburgh Instruments Ltd. FS5 spectrophotometer. Cyclic voltammetry of the compounds was carried out with Shanghai Zhenhua CHI 600D electrochemical workstation.

2. Emission spectrum of photoreactor lamp

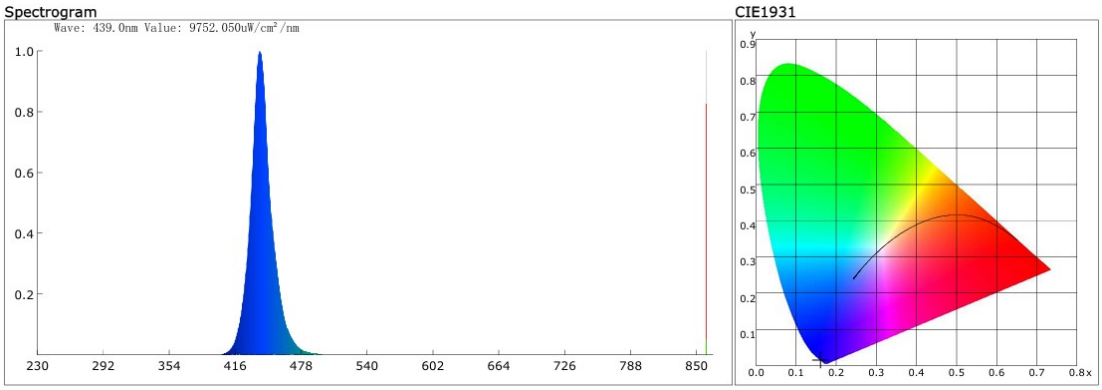


Figure S1. The emission spectrum of our lamp (blue LED 440 nm).

3. Synthesis and characterization data of substrates

Starting material oxazino pyridines **1** were synthesized according to the literature[1]. Starting material acyl azolium salts **2**[2-4]or sulfonyl azolium salts **4**[5] were synthesized according to the literature.

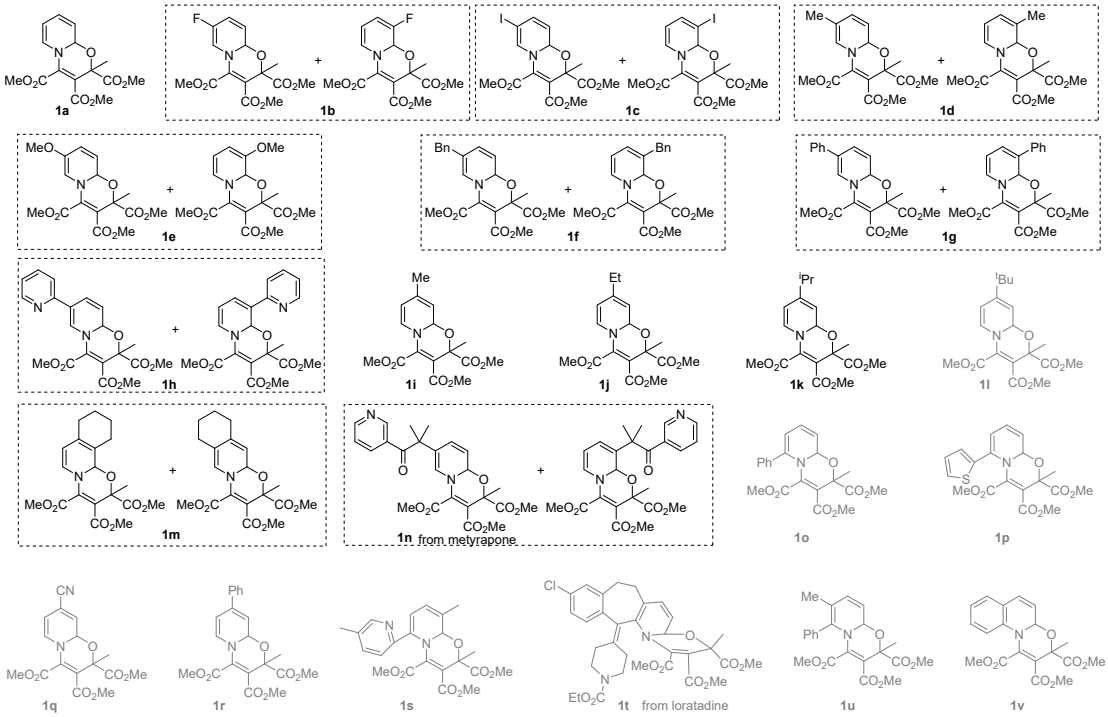


Figure S2. The synthesis of oxazine-pyridine **1**.

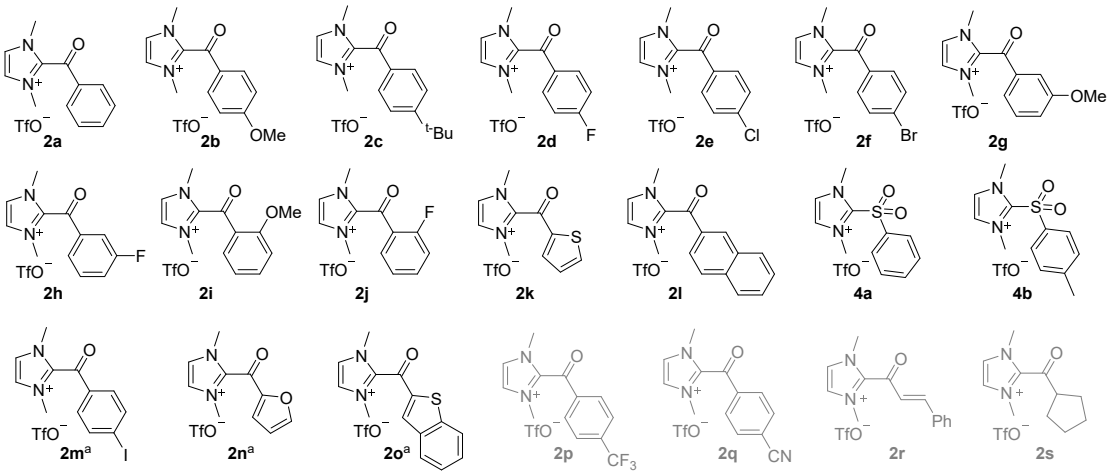
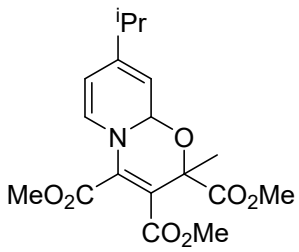


Figure S3. The synthesis of acyl azolium salts **2** or sulfonyl azolium salts **4**. [a] the yields of *meta*-acylated pyridines **3** determined by ^{1}H NMR were 10-15% under the standard reaction conditions.

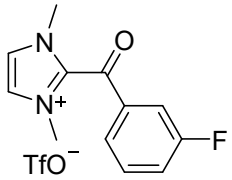
*Trimethyl 8-isopropyl-2-methyl-2H,9aH-pyrido[2,1-b][1,3]oxazine-2,3,4-tricarboxylate (**1k**)*



Purification by column chromatography on silica gel (eluting with pentane/ethyl acetate = 5/1, v/v)

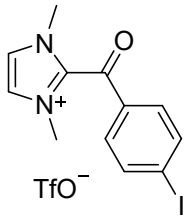
afforded the title compound as an yellow solid; ^{1}H NMR (600 MHz, $CDCl_3$) δ 6.26-6.24 (m, 1H), 5.75-5.59 (m, 1H), 5.33 – 5.19 (m, 2H), 3.91 (s, 3H), 3.77-3.74 (m, 3H), 3.71-3.70 (m, 3H), 2.37 (p, J = 6.8 Hz, 1H), 1.06 (dd, J = 6.9, 5.4 Hz, 6H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 171.4, 164.8, 163.8, 144.1, 142.5, 125.1, 109.1, 102.6, 79.9, 53.3, 52.8, 52.0, 33.1, 24.0, 21.4, 21.2.

*2-(3-fluorobenzoyl)-1,3-dimethyl-1H-imidazol-3-ium trifluoromethanesulfonate (**2h**)*



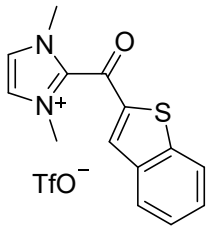
White solid; ^{1}H NMR (600 MHz, Acetonitrile-d3) δ 7.75 – 7.65 (m, 3H), 7.61 (m, 3H), 3.77 (s, 6H); ^{13}C{^{1}H} NMR (151 MHz, Acetonitrile-d3) δ 180.4, 163.9 (d, $J_{C\text{-}F}$ = 248.1 Hz), 137.7 (d, $J_{C\text{-}F}$ = 7.1 Hz), 132.9 (d, $J_{C\text{-}F}$ = 7.9 Hz), 127.48, 127.46, 126.5, 124.2 (d, $J_{C\text{-}F}$ = 21.3 Hz), 117.2 (d, $J_{C\text{-}F}$ = 23.2 Hz), 38.3; ^{19}F NMR (564 MHz, Acetonitrile-d3) δ -80.12, -112.83.

*2-(4-iodobenzoyl)-1,3-dimethyl-1H-imidazol-3-ium trifluoromethanesulfonate (**2m**)*



White solid; ^{1}H NMR (600 MHz, Acetonitrile-d3) δ 8.07 (dd, J = 8.7, 1.0 Hz, 2H), 7.63 – 7.60 (m, 2H), 7.58 (dd, J = 2.5, 1.3 Hz, 2H), 3.75 (s, 6H); ^{13}C{^{1}H} NMR (151 MHz, Acetonitrile-d3) δ 181.0, 140.0, 135.1, 132.2, 126.4, 105.9, 38.3; ^{19}F NMR (564 MHz, Acetonitrile-d3) δ -79.29.

*2-(benzo[b]thiophene-2-carbonyl)-1,3-dimethyl-1H-imidazol-3-ium trifluoromethanesulfonate (**2o**)*



Yellow solid; ^{1}H NMR (600 MHz, Acetonitrile-d3) δ 8.18 (d, J = 1.7 Hz, 1H), 8.09 – 8.05 (m, 2H), 7.69 – 7.66 (m, 1H), 7.62 – 7.60 (m, 2H), 7.57 (dt, J = 8.2, 0.9 Hz, 1H), 3.86 (s, 6H); ^{13}C{^{1}H} NMR (151 MHz, Acetonitrile-d3) δ 174.4, 145.2, 141.1, 139.8, 139.11, 139.13, 131.2, 128.6, 127.2, 126.1, 124.3, 38.0; ^{19}F NMR (564 MHz, Acetonitrile-d3) δ -79.32.

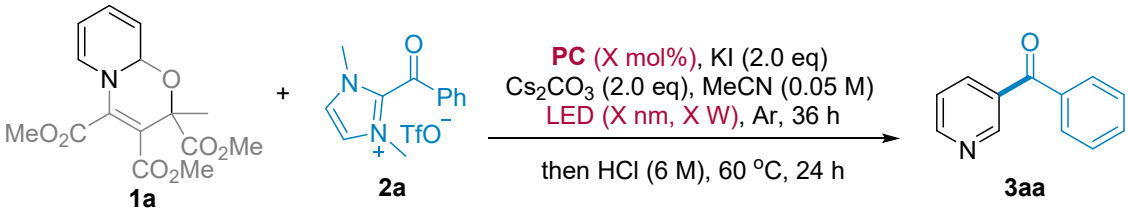
4. General Procedures

In an argon-filled glovebox, oxazino pyridines **1** (0.1 mmol), acyl azolium salts **2** or sulfonyl azolium salts **4** (2.0 equiv), [Ir(dF(CF_3)ppy(dtbpy)]PF_6 (2 mol%), Cs_2CO_3 (0.2 equiv), and KI (2.0

equiv) were sequentially added in a 25 mL reaction *vial*. The reaction *vial* was added MeCN (0.05 M). The *vial* was sealed and placed in a photoreactor (RLH-18CU). The reaction mixture was irradiated with blue LED (λ = 440 nm, 15 W) at room temperature for 24 h. After that, 6 M HCl (2 ml, equal to the volume of solvents) was added to the reaction mixture and the *vial* was heated at 60 °C for 36 h. then stirred at 60 °C and in air for 24 h. After completion, the reaction mixture was basified with saturated Na_2CO_3 and extracted by dichloromethane (3 x 5 mL). The combined organic phase was dried over Na_2SO_4 and filtered. The crude mixture was concentrated under reduced pressure. The resulting residue was purified by flash column chromatography to afford the desired product.

5. Conditions Optimization

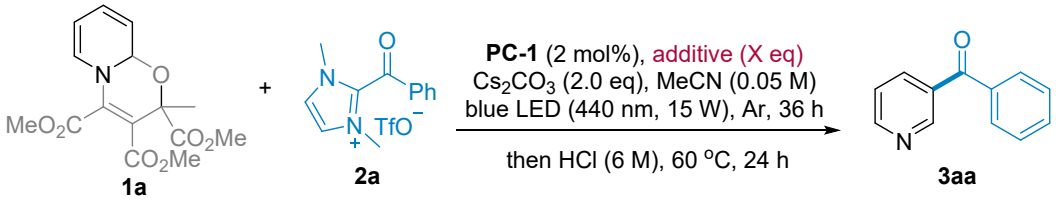
Table S1. Optimization of the photocatalysts and wavelength [a]



Entry	**PC** (X mol%)	Wavelength (nm, W)	Yield **3aa** [%]
1	[Ir(dF(CF$_3$)ppy(dtbpy)]PF$_6$ (2 mol%)	440, 15	74
2	Ir(ppy)$_3$ (2 mol%)	440, 15	38
3	Ir(dFppy)$_3$ (2 mol%)	440, 15	63
4	[Ru(bpy)$_3$](PF$_6$)$_2$ (2 mol%)	440, 15	53
5	Esoin Y-Na$_2$ (5 mol%)	440, 15	25
6	[Ir(dF(CF$_3$)ppy(dtbpy)]PF$_6$ (1 mol%)	440, 15	52
7	[Ir(dF(CF$_3$)ppy(dtbpy)]PF$_6$ (0 mol%)	440, 15	0
8	[Ir(dF(CF$_3$)ppy(dtbpy)]PF$_6$ (2 mol%)	410, 15	40
9	[Ir(dF(CF$_3$)ppy(dtbpy)]PF$_6$ (2 mol%)	455, 15	32
10	[Ir(dF(CF$_3$)ppy(dtbpy)]PF$_6$ (2 mol%)	In dark	0

[a] All reactions were performed by using **1a** (0.1 mmol), **2a** (2.0 equiv), **PC** (X mol%), KI (2.0 equiv), Cs_2CO_3 (2.0 equiv), MeCN (0.05 M) under light (X nm, X W), stirred at room temperature and in Ar for 36 h; then added 6 M HCl, equal to the volume of solvents, stirred at 60 °C and in air for 24 h. [a] yield was determined by ^{1}H NMR.

Table S2. Optimization of the additives [a]



Entry	Additives (X equiv)	Yield **3aa** [%]	Entry	Additives (X equiv)	Yield **3aa** [%]

1	CsF (2.0)	46	9	KBr (2.0)	36
2	NaF (2.0)	22	10	NaI (2.0)	68
3	KF (2.0)	38	11	KI (2.0)	74
4	NaCl (2.0)	26	12	4-$ClC_6H_4SO_2Na$ (2.0)	48
5	KCl (2.0)	32	13	KI (4.0)	67
6	LiCl (2.0)	6	14	KI (1.0)	34
7	CsBr (2.0)	24	15	KI (0.5)	31
8	NaBr (2.0)	26	16	KI (0)	24

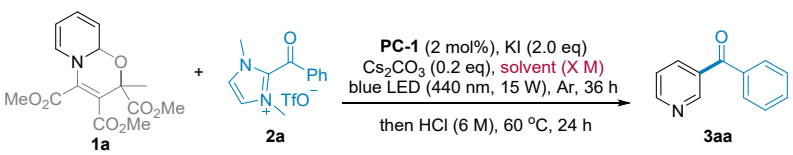
[a] All reactions were performed by using **1a** (0.1 mmol), **2a** (2.0 equiv), **PC-1** (2 mol%), additives (X equiv), Cs_2CO_3 (2.0 equiv), MeCN (0.05 M) under blue LED (440 nm, 15 W), stirred at room temperature and in Ar for 36 h; then added 6 M HCl, equal to the volume of solvents, stirred at 60 °C and in air for 24 h. [a] yield was determined by ^{1}H NMR.

Table S3. Optimization of the bases [a]

Entry	Base (X equiv)	Yield **3aa** [%]
1	Cs_2CO_3 (2.0)	74
2	K_2CO_3 (2.0)	53
3	Na_2CO_3 (2.0)	64
4	K_3PO_4 (2.0)	62
5	^{t}-BuOK (2.0)	0
6	DBU (2.0)	2
7	Cs_2CO_3 (4.0)	33
8	Cs_2CO_3 (1.0)	64
9	Cs_2CO_3 (0.5)	63
10	Cs_2CO_3 (0.2)	74
11	Cs_2CO_3 (0)	52

[a] All reactions were performed by using **1a** (0.1 mmol), **2a** (2.0 equiv), **PC-1** (2 mol%), KI (2.0 equiv), bases (X equiv), MeCN (0.05 M) under blue LED (440 nm, 15 W), stirred at room temperature and in Ar for 36 h; then added 6 M HCl, equal to the volume of solvents, stirred at 60 °C and in air for 24 h. [a] yield was determined by ^{1}H NMR.

Table S4. Optimization of the solvents [a]

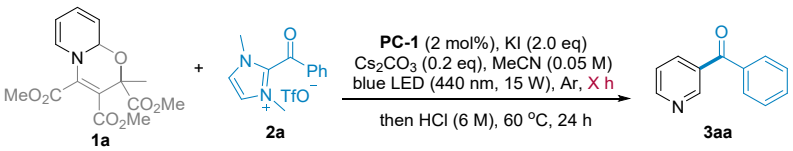


Entry	Solvents (X M)	Yield **3aa** [%]
1	MeCN (0.05 M)	74

2	EA (0.05 M)	33
3	DCM (0.05 M)	15
4	DCE (0.05 M)	36
5	DMSO (0.05 M)	39
6	THF (0.05 M)	37
7	DMF (0.05 M)	44
8	PhCl (0.05 M)	6
9	MTBE (0.05 M)	3
10	MeCN (0.025 M)	35
11	MeCN (0.1 M)	46

[a] All reactions were performed by using **1a** (0.1 mmol), **2a** (2.0 equiv), **PC-1** (2 mol%), KI (2.0 equiv), Cs_2CO_3 (0.2 equiv), solvents (X M) under blue LED (440 nm, 15 W), stirred at room temperature and in Ar for 36 h; then added 6 M HCl, equal to the volume of solvents, stirred at 60 °C and in air for 24 h. [a] yield was determined by ^{1}H NMR.

Table S5. Optimization of time [a]



Entry	Time (X h)	Yield **3aa** [%]
1	6	43
2	12	44
3	18	52
4	24	57
5	30	65
6	36	74

[a] All reactions were performed by using **1a** (0.1 mmol), **2a** (2.0 equiv), **PC-1** (2 mol%), KI (2.0 equiv), Cs_2CO_3 (0.2 equiv),), MeCN (0.05 M) under blue LED (440 nm, 15 W), stirred at room temperature and in Ar for X h; then added 6 M HCl, equal to the volume of solvents, stirred at 60 °C and in air for 24 h. [a] yield was determined by ^{1}H NMR.

6. Control experiments

1a (0.1 mmol), **2a** (2.0 equiv), **PC-1** (2 mol%), Cs_2CO_3 (0.2 equiv), KI (2.0 equiv) and additives (4.0 equiv) including TEMPO and BHT were sequentially added in a 25 mL reaction vial. The reaction system added MeCN (0.05 M) was sealed under Ar and stirred under the irradiation of blue LED (440 nm, 15 W) at room temperature for 36 h, then added 6 M HCl, equal to the volume of solvents, stirred at 60 °C and in air for 24 h. After reaction, corresponding yields were determined by ^{1}H NMR of the reaction solution. Additionally, before adding 6 M HCl, equal to the volume of solvents, we successfully detected the adduct **A**, **B** and **C** by high-resolution mass spectrometry (HRMS)

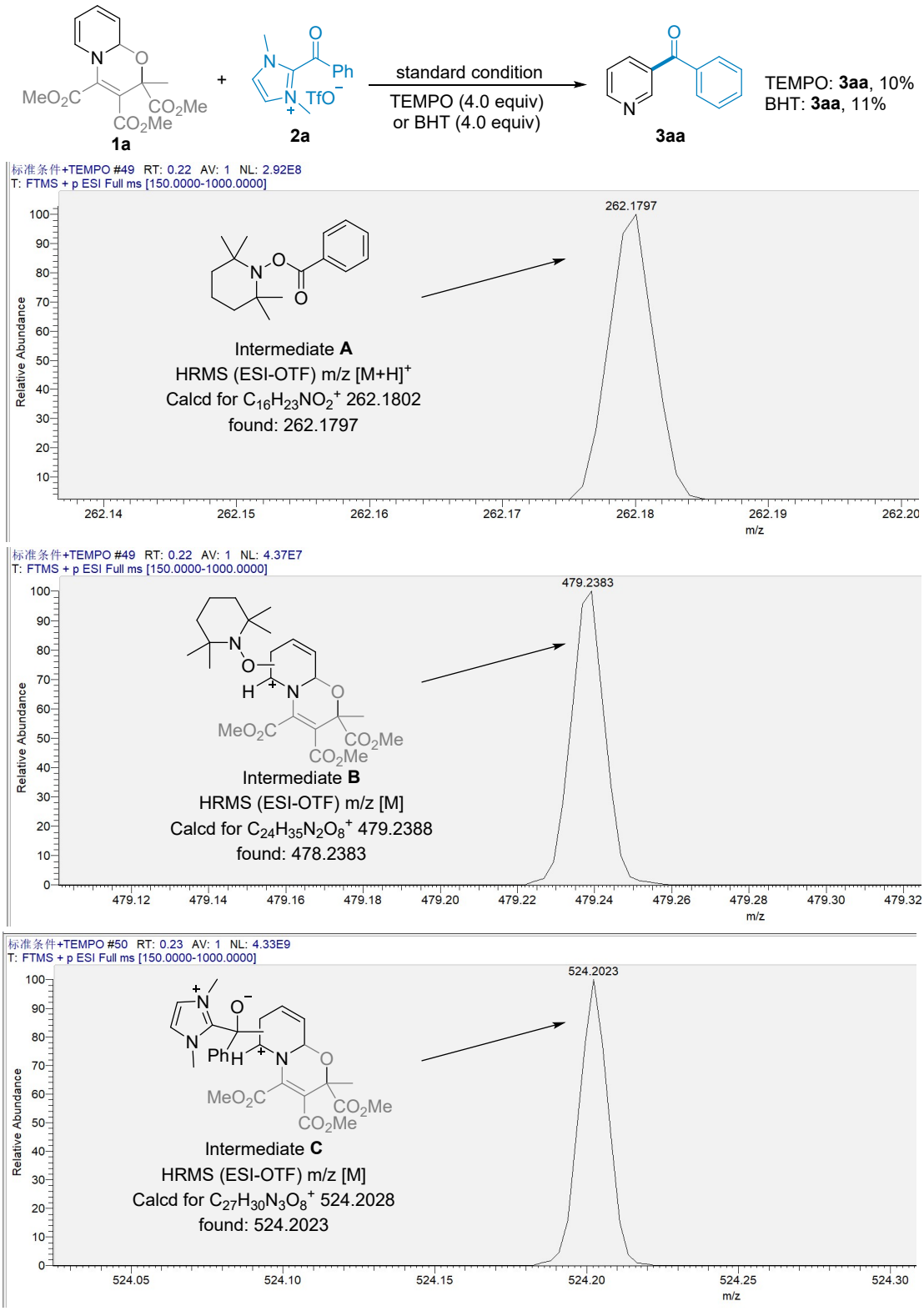


Figure S4. The mixture of reaction with TEMPO were detected by HRMS

7. Cyclic voltammetry studies

Cyclic voltammetry of the compounds was carried out with Shanghai Zhenhua CHI

600D electrochemical workstation. Samples **1a** (1×10^{-3} M) were measured under inert atmosphere in an Ar atmosphere glovebox at room temperature in dry MeCN solution containing tetrabutylammonium hexafluorophosphate (0.1 M). The measurement was operated with a three-electrode setup containing a glassy carbon as working electrode, a platinum wire as a counter electrode, and an organic silver electrode as reference electrode. Unless otherwise stated, all CVs were run at a scan rate of 100 mV/s. Potentials were measured in MeCN with respect to Fc/Fc^{+} ion pair (as external standard).

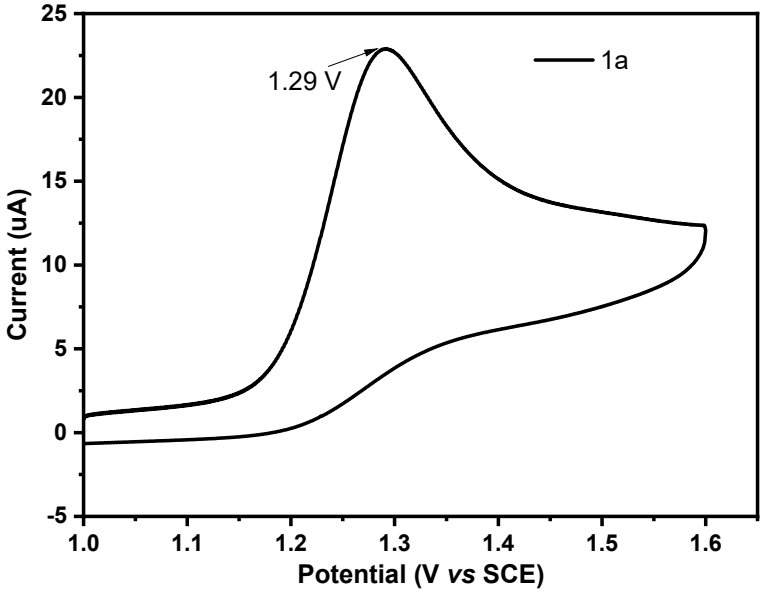


Figure S5. The cyclic voltammetry of **1a**

8. UV-vis Absorption Spectra

The UV-vis absorption spectra of sulfonium salts **1a** (2×10^{-5} M), **2a** (2×10^{-5} M), and **1a** + **2a** (2×10^{-5} M) in MeCN were recorded in 1 cm path quartz cuvettes, respectively.

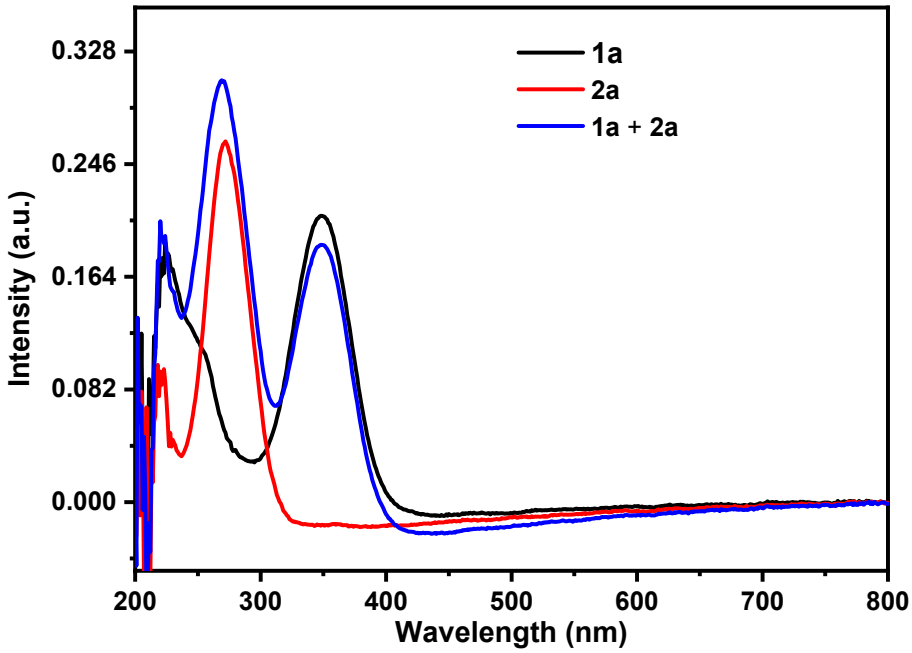


Figure S6. UV-vis absorption spectra

9. Stern-Volmer fluorescence quenching experiments

Emission intensities were recorded using Edinburgh Instruments Ltd. FS5 spectrophotometer. All Stern-Volmer fluorescence quenching experiments were excited at 375 nm and the emission intensity was collected at 450 nm. The fluorescence emission spectrum was measured from 400 nm to 650 nm. A freshly prepared solution of 5×10^{-5} M solution of **PC-1** in dry and degassed MeCN was added the appropriate amount of a quencher (**1a** and **2a**) in a screw-top quartz cuvette at room temperature.

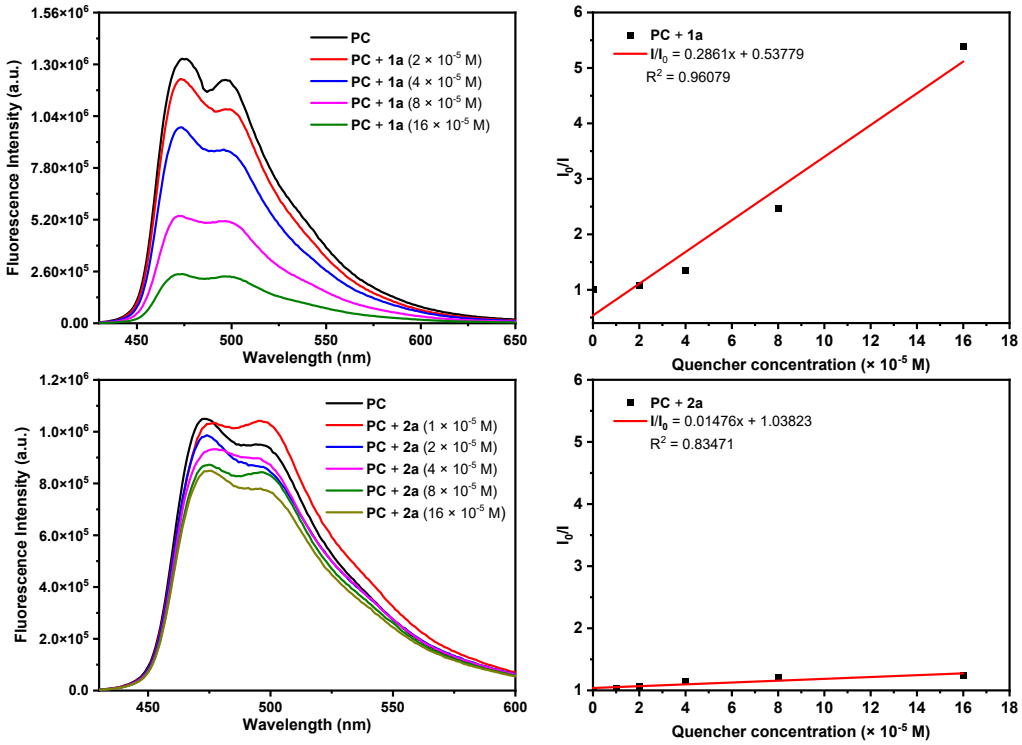


Figure S7. Fluorescence quenching experiments.

10. On/off experiments

The reactions were conducted under the standard conditions at sequential periods of visible light irradiation (15 W blue LED). After reaction, adding 6 M HCl, equal to the volume of solvents, corresponding yields of **3aa** were determined by ^{1}H NMR.

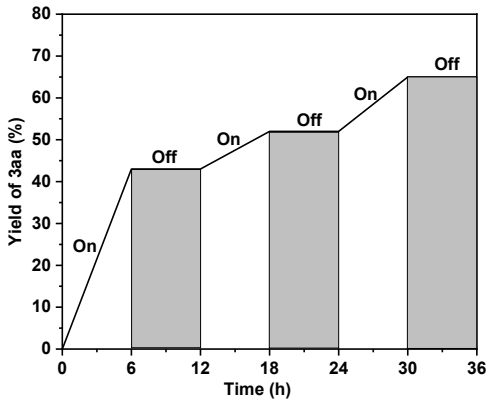


Figure S8. Visible light irradiation on/off experiments

11. Proposed mechanism

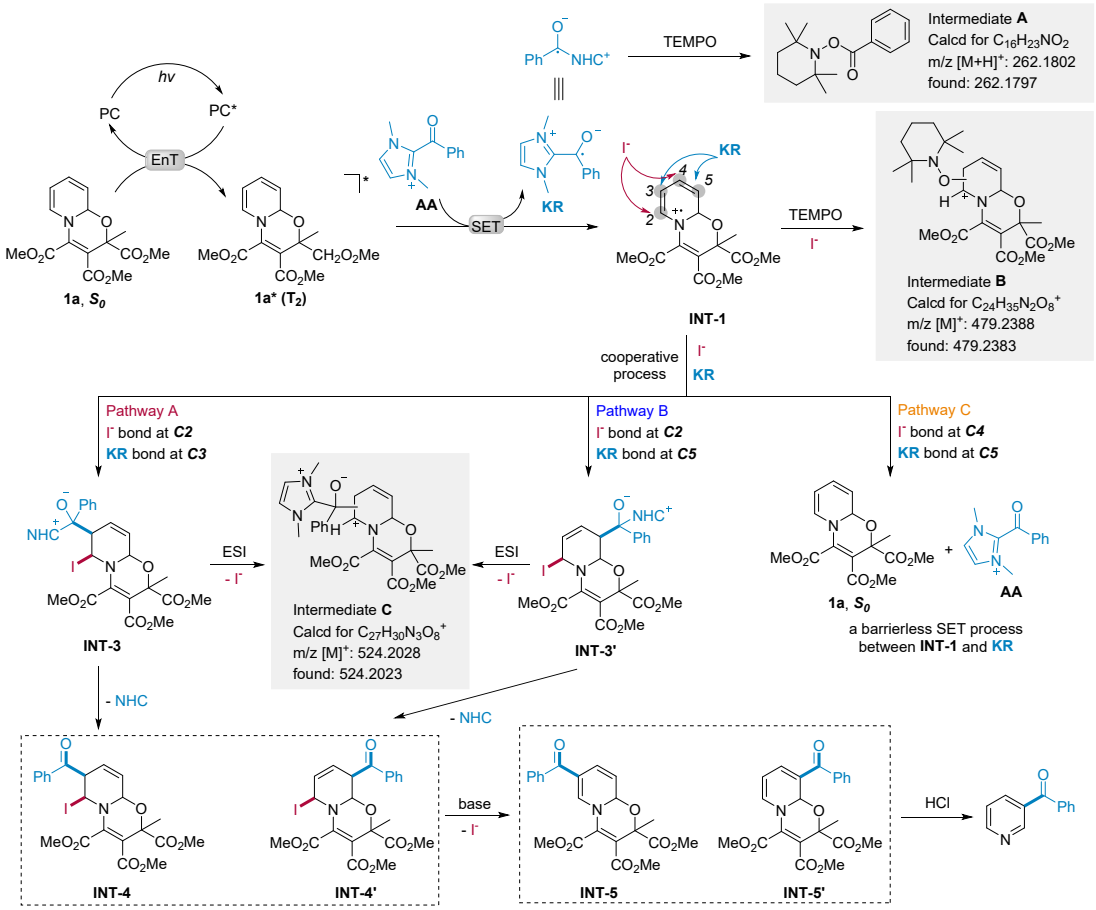
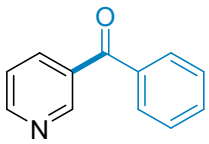


Figure S9. Proposed mechanism for *meta*-selective C–H acylation of pyridines

12. Characterization data of products

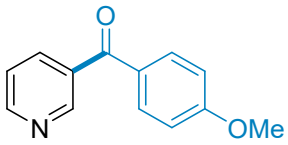
*phenyl(pyridin-3-yl)methanone (**3aa**)*[6]



Purification by column chromatography on silica gel (eluting with pentane/ethyl acetate = 5/1, v/v)

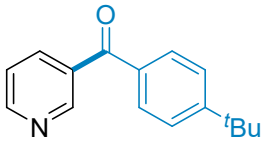
afforded the title compound as a pale yellow solid (12.6 mg, 69% yield); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.92 (s, 1H), 8.74 (d, *J* = 4.1 Hz, 1H), 8.14 – 7.94 (m, 2H), 7.74 (d, *J* = 7.7 Hz, 2H), 7.56 (t, *J* = 7.4 Hz, 1H), 7.45 (t, *J* = 7.7 Hz, 2H), 7.38 (dd, *J* = 7.8, 4.9 Hz, 1H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 195.0, 152.9, 151.0, 137.3, 136.8, 133.3, 130.1, 128.7, 123.5.

*(4-methoxyphenyl)(pyridin-3-yl)methanone (**3ab**)*[7]



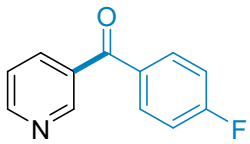
Purification by column chromatography on silica gel (eluting with pentane/ethyl acetate = 4/1, v/v) afforded the title compound as a pale yellow solid (11.3 mg, 53% yield); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.88 (s, 1H), 8.72 (d, J = 4.1 Hz, 1H), 8.03 – 7.95 (m, 2H), 7.76 (d, J = 8.8 Hz, 2H), 7.37 (dd, J = 7.7, 4.9 Hz, 1H), 6.92 (d, J = 8.8 Hz, 2H), 3.83 (s, 3H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 193.6, 163.9, 152.5, 150.6, 137.1, 134.0, 132.7, 129.5, 123.5, 114.0, 55.7.

*(4-(tert-butyl)phenyl)(pyridin-3-yl)methanone (**3ac**)*



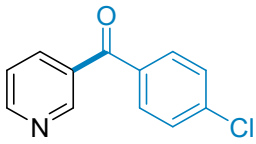
Purification by column chromatography on silica gel (eluting with pentane/ethyl acetate = 5/1, v/v) afforded the title compound as a pale yellow solid (12.9 mg, 54% yield); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.93 – 8.91 (m, 1H), 8.73 (d, *J* = 3.7 Hz, 1H), 8.08 – 8.00 (m, 1H), 7.70 (d, *J* = 8.4 Hz, 2H), 7.45 (d, *J* = 8.4 Hz, 2H), 7.37 (dd, *J* = 7.7, 4.9 Hz, 1H), 1.30 (s, 9H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 194.6, 157.2, 152.7, 150.9, 137.2, 134.1, 133.6, 130.2, 125.7, 123.4, 35.3, 31.2. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{16}H_{18}NO$ 240.1383, found 240.131.

*(4-fluorophenyl)(pyridin-3-yl)methanone (**3ad**)*[8]



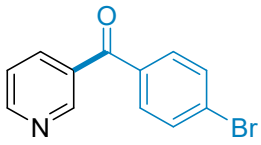
Purification by column chromatography on silica gel (eluting with pentane/ethyl acetate = 5/1, v/v) afforded the title compound as an orange solid (13.1 mg, 65% yield); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.91 (s, 1H), 8.77 (s, 1H), 8.04 (d, J = 7.6 Hz, 1H), 7.80 (dd, J = 8.7, 5.4 Hz, 3H), 7.41 (s, 1H), 7.13 (t, J = 8.5 Hz, 2H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 193.5, 165.9 (d, $J_{C\text{-}F}$ = 255.6 Hz), 153.0, 150.7, 137.2, 133.3, 133.1 (d, $J_{C\text{-}F}$ = 2.8 Hz), 132.8 (d, $J_{C\text{-}F}$ = 9.3 Hz), 123.7, 116.0 (d, $J_{C\text{-}F}$ = 22.0 Hz); ^{19}F NMR (564 MHz, $CDCl_3$) δ -104.39.

*(4-chlorophenyl)(pyridin-3-yl)methanone (**3ae**)*[6]



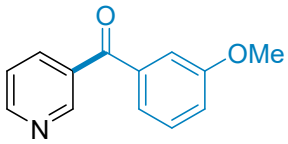
Purification by column chromatography on silica gel (eluting with pentane/ethyl acetate = 5/1, v/v) afforded the title compound as a pale white solid (5.2 mg, 24% yield); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.91 (s, 1H), 8.77 (s, 1H), 8.05 (d, *J* = 7.2 Hz, 1H), 7.71 (d, *J* = 8.2 Hz, 2H), 7.44 – 7.43 (m, 3H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 193.6, 153.0, 150.7, 140.0, 137.5, 135.1, 133.2, 131.6, 129.2, 123.8.

*(4-bromophenyl)(pyridin-3-yl)methanone (**3af**)*[9]



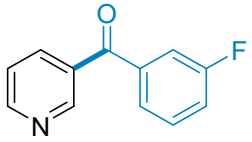
Purification by column chromatography on silica gel (eluting with pentane/ethyl acetate = 5/1, v/v) afforded the title compound as an orange solid (9.4 mg, 36% yield); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.93 – 8.87 (m, 1H), 8.82 – 8.71 (m, 1H), 8.03 (dt, *J* = 7.9, 1.9 Hz, 1H), 7.71 – 7.51 (m, 4H), 7.40 (dd, *J* = 7.8, 4.9 Hz, 1H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 193.9, 153.2, 150.9, 137.2, 135.5, 132.9, 132.1, 131.6, 128.6, 123.6.

*(3-methoxyphenyl)(pyridin-3-yl)methanone (**3ag**)*[8]



Purification by column chromatography on silica gel (eluting with pentane/ethyl acetate = 3/1, v/v) afforded the title compound as an orange oil (10.2 mg, 48% yield); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.93 (s, 1H), 8.81 – 8.71 (m, 1H), 8.06 (dt, J = 7.8, 1.8 Hz, 1H), 7.39 (dd, J = 7.7, 4.9 Hz, 1H), 7.34 (t, J = 7.9 Hz, 1H), 7.31 – 7.29 (m, 1H), 7.27 (d, J = 7.6 Hz, 1H), 7.13 – 7.09 (m, 1H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 194.8, 160.0, 152.9, 151.0, 138.1, 137.4, 133.4, 129.7, 123.5, 123.0, 119.8, 114.3, 55.7.

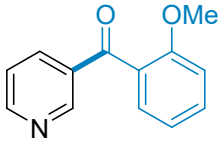
*(3-fluorophenyl)(pyridin-3-yl)methanone (**3ah**)*



Purification by column chromatography on silica gel (eluting with pentane/ethyl acetate = 5/1, v/v) afforded the title compound as an orange solid (8.2 mg, 41% yield); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.93 (s, 1H), 8.79 – 8.69 (m, 1H), 8.06 (d, *J* = 7.8 Hz, 1H), 7.51 (d, *J* = 7.6 Hz, 1H), 7.48 – 7.40 (m, 3H), 7.28 (td, *J* = 8.2, 2.2 Hz, 1H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 193.6, 162.8 (d, $J_{C\text{-}F}$ = 248.8 Hz), 153.2, 150.9, 138.8 (d, $J_{C\text{-}F}$ = 6.4 Hz), 137.4, 132.9, 130.5 (d, $J_{C\text{-}F}$ = 7.7 Hz), 126.0 (d, $J_{C\text{-}F}$ = 3.3 Hz), 123.7, 120.4 (d, $J_{C\text{-}F}$ = 21.5 Hz), 116.8 (d, $J_{C\text{-}F}$ = 22.6 Hz); ^{19}F NMR (564 MHz, $CDCl_3$) δ -

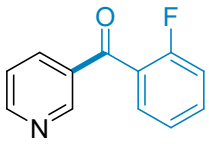
111.18. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{12}H_9FNO$ 202.0663, found 202.0662.

*(2-methoxyphenyl)(pyridin-3-yl)methanone (**3ai**)*[10]



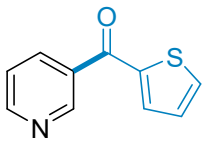
Purification by column chromatography on silica gel (eluting with pentane/ethyl acetate = 4/1, v/v) afforded the title compound as an orange solid (4.9 mg, 23% yield); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.94 – 8.81 (m, 1H), 8.78 – 8.62 (m, 1H), 8.09 (d, *J* = 7.6 Hz, 1H), 7.50 – 7.44 (m, 1H), 7.41 – 7.33 (m, 1H), 7.02 (t, *J* = 7.4 Hz, 2H), 6.94 (d, *J* = 8.4 Hz, 1H), 3.64 (s, 1H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 194.9, 157.7, 152.7, 151.0, 137.0, 133.2, 130.3, 130.2, 128.8, 127.7, 121.1, 111.6, 55.7.

*(2-fluorophenyl)(pyridin-3-yl)methanone (**3aj**)*



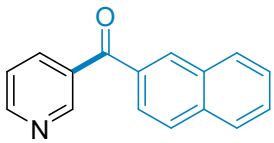
Purification by column chromatography on silica gel (eluting with pentane/ethyl acetate = 5/1, v/v) afforded the title compound as an orange oil (7.2 mg, 36% yield); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.92 (s, 1H), 8.74 (d, *J* = 3.8 Hz, 1H), 8.12 – 8.01 (m, 1H), 7.59 – 7.47 (m, 2H), 7.38 (dd, *J* = 7.9, 4.9 Hz, 1H), 7.25 (td, *J* = 7.6, 0.8 Hz, 1H), 7.15 – 7.06 (m, 1H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 192.1, 160.4 (d, $J_{C\text{-}F}$ = 253.3 Hz), 153.7, 151.1, 136.8, 134.2 (d, $J_{C\text{-}F}$ = 8.3 Hz), 133.2, 131.1 (d, $J_{C\text{-}F}$ = 2.6 Hz), 126.1 (d, $J_{C\text{-}F}$ = 14.1 Hz), 124.8 (d, $J_{C\text{-}F}$ = 3.9 Hz), 123.6, 116.7 (d, $J_{C\text{-}F}$ = 21.9 Hz); ^{19}F NMR (564 MHz, $CDCl_3$) δ -109.78. $[M + H]^+$ calcd for $C_{12}H_9FNO$ 202.0663, found 202.0661.

*pyridin-3-yl(thiophen-2-yl)methanone (**3ak**)*[7]



Purification by column chromatography on silica gel (eluting with pentane/ethyl acetate = 5/1, v/v) afforded the title compound as a pale yellow solid (7.6 mg, 40% yield); ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.06 – 8.95 (m, 1H), 8.85 – 8.70 (m, 1H), 8.09 (dt, *J* = 7.9, 1.9 Hz, 1H), 7.72 (dd, *J* = 4.9, 0.9 Hz, 1H), 7.59 (dd, *J* = 3.8, 0.9 Hz, 1H), 7.40 (dd, *J* = 7.8, 4.9 Hz, 1H), 7.14 (dd, *J* = 4.8, 3.9 Hz, 1H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 186.3, 152.9, 150.0, 143.2, 136.7, 135.4, 135.3, 133.94, 128.5, 123.6.

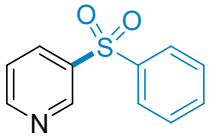
*naphthalen-2-yl(pyridin-3-yl)methanone (**3al**)*



Purification by column chromatography on silica gel (eluting with pentane/ethyl acetate = 5/1, v/v)

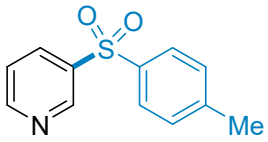
afforded the title compound as an orange solid (9.1 mg, 39% yield); ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.00 (s, 1H), 8.86 – 8.68 (m, 1H), 8.20 (s, 1H), 8.11 (d, *J* = 7.8 Hz, 1H), 7.94 – 7.77 (m, 4H), 7.63 – 7.54 (m, 1H), 7.51 (t, *J* = 7.6 Hz, 1H), 7.43 (dd, *J* = 7.6, 5.0 Hz, 1H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 194.9, 152.9, 151.0, 137.5, 135.7, 134.1, 133.7, 132.4, 132.4, 129.7, 129.0, 128.9, 128.0, 127.2, 125.4, 123.6. $[M + H]^+$ calcd for $C_{16}H_{12}NO$ 234.0914, found 234.0911.

*3-(phenylsulfonyl)pyridine (**5aa**)*[11]



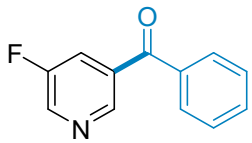
Purification by column chromatography on silica gel (eluting with pentane/ethyl acetate = 5/1, v/v) afforded the title compound as a pale yellow solid (13.6 mg, 62% yield); ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.07 (d, *J* = 1.9 Hz, 1H), 8.76 – 8.61 (m, 1H), 8.15 (dt, *J* = 8.1, 2.0 Hz, 1H), 7.99 – 7.82 (m, 2H), 7.63 – 7.51 (m, 1H), 7.48 (t, *J* = 7.7 Hz, 2H), 7.38 (dd, *J* = 8.0, 4.8 Hz, 1H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 153.8, 148.8, 140.9, 138.4, 135.4, 134.0, 129.7, 127.9, 124.0.

*3-tosylpyridine (**5ab**)*[11]



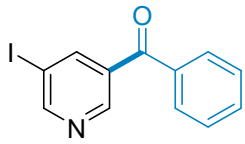
Purification by column chromatography on silica gel (eluting with pentane/ethyl acetate = 5/1, v/v) afforded the title compound as a pale yellow solid (14.9 mg, 67% yield); ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.05 (d, *J* = 2.1 Hz, 1H), 8.69 (dd, *J* = 4.8, 1.4 Hz, 1H), 8.13 (dt, *J* = 8.1, 1.9 Hz, 1H), 7.78 (d, *J* = 8.3 Hz, 2H), 7.37 (dd, *J* = 8.0, 4.8 Hz, 1H), 7.26 (d, *J* = 8.1 Hz, 2H), 2.34 (s, 3H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 153.6, 148.7, 145.1, 138.8, 137.9, 135.2, 130.3, 128.0, 123.9, 21.8.

*(5-fluoropyridin-3-yl)(phenyl)methanone (**3ba**)*



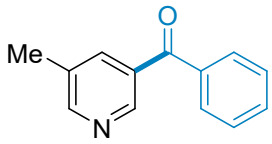
Purification by column chromatography on silica gel (eluting with pentane/ethyl acetate = 5/1, v/v) afforded the title compound as an orange oil (7.0 mg, 35% yield); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.79 – 8.70 (m, 1H), 8.61 (d, *J* = 2.8 Hz, 1H), 7.89 – 7.67 (m, 3H), 7.64 – 7.56 (m, 1H), 7.47 (t, *J* = 7.8 Hz, 1H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 193.5, 159.3 (d, $J_{C\text{-}F}$ = 259.5 Hz), 146.8 (d, $J_{C\text{-}F}$ = 4.3 Hz), 141.7 (d, $J_{C\text{-}F}$ = 23.4 Hz), 136.5, 134.6 (d, $J_{C\text{-}F}$ = 2.7 Hz), 133.6, 130.1, 128.9, 123.7 (d, $J_{C\text{-}F}$ = 18.8 Hz); ^{19}F NMR (564 MHz, $CDCl_3$) δ -120.37. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{12}H_9FNO^+$ 202.0663, found 202.0661.

*(5-iodopyridin-3-yl)(phenyl)methanone (**3ca**)*



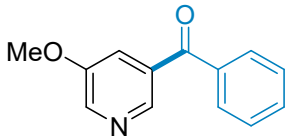
Purification by column chromatography on silica gel (eluting with pentane/ethyl acetate = 5/1, v/v) afforded the title compound as an orange oil (6.8 mg, 22% yield); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.95 (d, *J* = 2.1 Hz, 1H), 8.83 (d, *J* = 1.8 Hz, 1H), 8.36 (t, *J* = 2.0 Hz, 1H), 7.73 (dd, *J* = 8.3, 1.2 Hz, 2H), 7.65 – 7.54 (m, 1H), 7.47 (t, *J* = 7.8 Hz, 2H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 193.4, 158.8, 149.2, 145.3, 136.4, 134.9, 133.7, 130.1, 128.9, 93.3. HRMS (ESI-TOF) *m/z* [M + H]$^+$ calcd for $C_{12}H_9{}^{129}INO$ 309.9724, found 309.9721.

*(5-methylpyridin-3-yl)(phenyl)methanone (**3da**)*



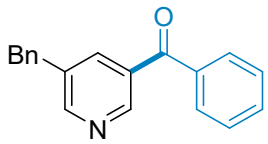
Purification by column chromatography on silica gel (eluting with pentane/ethyl acetate = 5/1, v/v) afforded the title compound as an orange oil (8.1 mg, 41% yield); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.75 (s, 1H), 8.62 (s, 1H), 7.94 (s, 1H), 7.75 (d, *J* = 7.3 Hz, 2H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 2.40 (s, 3H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 195.2, 153.3, 148.1, 137.8, 137.0, 133.3, 130.9, 130.1, 128.7, 128.2, 18.6. HRMS (ESI-TOF) *m/z* [M + H]$^+$ calcd for $C_{12}H_{13}NO$ 198.0914, found 198.0913.

*(5-methoxypyridin-3-yl)(phenyl)methanone (**3ea**)*



Purification by column chromatography on silica gel (eluting with pentane/ethyl acetate = 4/1, v/v) afforded the mixture compound of **3ea** and (1-methyl-1H-imidazol-2-yl)(phenyl)methanone as an orange oil (2.3 mg, 11% yield, [**3ea** : (1-methyl-1H-imidazol-2-yl)(phenyl)methanone = 34 : 1, determined by ^{1}H NMR]; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.48 (s, 1H), 8.45 (d, J = 2.4 Hz, 1H), 7.78 – 7.71 (m, 2H), 7.59 – 7.54 (m, 3H), 7.45 (t, J = 7.8 Hz, 2H), 3.86 (s, 3H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 194.9, 143.3, 141.9, 137.0, 133.3, 130.9, 130.2, 128.7, 128.2, 120.2, 56.0. ^{1}H NMR data for (1-methyl-1H-imidazol-2-yl)(phenyl)methanone: ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.22 – 8.13 (m, 2H), 7.53 – 7.48 (m, 1H), 7.42 (t, J = 7.7 Hz, 2H), 7.17 (s, 1H), 7.05 (s, 1H), 4.02 (s, 3H). HRMS (ESI-TOF) *m/z* [M + H]$^+$ calcd for $C_{13}H_{12}NO_2$ 214.0863, found 214.0860.

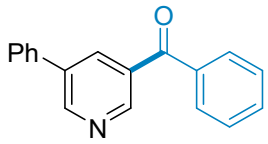
*(5-benzylpyridin-3-yl)(phenyl)methanone (**3fa**)*



Purification by column chromatography on silica gel (eluting with pentane/ethyl acetate = 5/1, v/v)

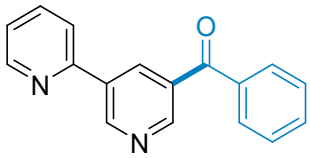
afforded the title compound as an orange oil (10.9 mg, 40% yield); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.76 (s, 1H), 8.63 (s, 1H), 7.87 (s, 1H), 7.70 (d, *J* = 7.3 Hz, 2H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.41 (t, *J* = 7.7 Hz, 2H), 7.24 (t, *J* = 7.5 Hz, 2H), 7.16 (t, *J* = 7.4 Hz, 1H), 7.12 (d, *J* = 7.3 Hz, 2H), 4.00 (s, 2H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 195.0, 153.2, 148.9, 139.2, 137.5, 136.9, 133.3, 130.1, 129.00, 128.97, 128.7, 126.9, 39.1. HRMS (ESI-TOF) *m/z* [M + H]$^+$ calcd for $C_{19}H_{16}NO$ 274.1227, found 274.1225.

*phenyl(5-phenylpyridin-3-yl)methanone (**3ga**)*



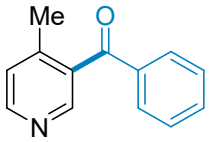
Purification by column chromatography on silica gel (eluting with pentane/ethyl acetate = 5/1, v/v) afforded the title compound as an orange oil (8.5 mg, 33% yield); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.89 (s, 1H), 8.24 (s, 1H), 7.84 – 7.70 (m, 2H), 7.62 – 7.53 (m, 3H), 7.46 (dt, *J* = 15.3, 7.8 Hz, 4H), 7.38 (t, *J* = 7.4 Hz, 1H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 195.0, 151.2, 149.4, 136.9, 136.8, 135.6, 133.4, 130.2, 129.4, 128.8, 128.8, 127.4. HRMS (ESI-TOF) *m/z* [M + H]$^+$ calcd for $C_{18}H_{14}N_2O$ 260.1070, found 260.1066.

*[2,3'-bipyridin]-5'-yl(phenyl)methanone (**3ha**)*



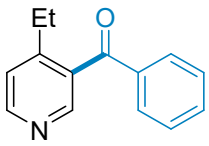
Purification by column chromatography on silica gel (eluting with pentane/ethyl acetate = 3/1, v/v) afforded the title compound as an orange oil (11.2 mg, 43% yield); ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.36 (s, 1H), 8.96 (s, 1H), 8.77 – 8.55 (m, 2H), 7.82 – 7.74 (m, 4H), 7.63 – 7.57 (m, 1H), 7.47 (t, *J* = 7.8 Hz, 2H), 7.27 (ddd, *J* = 6.7, 4.8, 2.0 Hz, 1H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 194.9, 153.9, 151.2, 150.8, 150.4, 137.3, 136.9, 135.5, 133.4, 130.2, 128.8, 123.5, 121.0. HRMS (ESI-TOF) *m/z* [M + H]$^+$ calcd for $C_{17}H_{13}N_2O$ 261.1023, found 261.1019.

*(4-methylpyridin-3-yl)(phenyl)methanone (**3ia**)*[12]



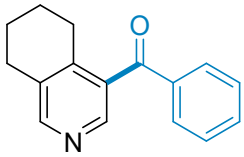
Purification by column chromatography on silica gel (eluting with pentane/ethyl acetate = 5/1, v/v) afforded the title compound as a deep red oil (7.7 mg, 39% yield); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.53 (d, *J* = 4.3 Hz, 1H), 8.50 (s, 1H), 7.73 (d, *J* = 8.3 Hz, 2H), 7.56 (t, *J* = 7.4 Hz, 1H), 7.42 (t, *J* = 7.8 Hz, 2H), 7.19 (d, *J* = 5.1 Hz, 1H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 196.4, 151.0, 149.2, 146.8, 137.4, 133.9, 130.2, 128.7, 126.2, 19.8.

*(4-ethylpyridin-3-yl)(phenyl)methanone (**3ja**)*



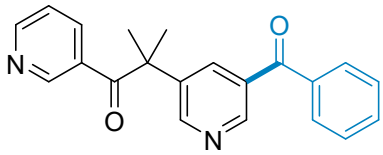
Purification by column chromatography on silica gel (eluting with pentane/ethyl acetate = 5/1, v/v) afforded the title compound as a deep red oil (6.5 mg, 31% yield); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.68 – 8.54 (m, 1H), 8.51 – 8.35 (m, 1H), 7.74 (d, *J* = 7.3 Hz, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.43 (t, *J* = 7.7 Hz, 2H), 7.31 – 7.25 (m, 1H), 2.66 (q, *J* = 7.4 Hz, 2H), 1.14 (t, *J* = 7.6 Hz, 3H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 196.2, 153.5, 150.5, 148.3, 137.3, 134.1, 130.3, 129.1, 128.9, 124.6, 26.2, 14.8. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{14}H_{14}NO$ 212.1070, found 212.1067.

*phenyl(5,6,7,8-tetrahydroisoquinolin-4-yl)methanone (**3ma**)*



Purification by column chromatography on silica gel (eluting with pentane/ethyl acetate = 5/1, v/v) afforded the title compound as a pale yellow oil (3.6 mg, 15% yield); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.35 (s, 1H), 8.24 (s, 1H), 7.78 – 7.68 (m, 2H), 7.55 (t, *J* = 7.4 Hz, 1H), 7.41 (t, *J* = 7.8 Hz, 2H), 2.77 (t, *J* = 6.3 Hz, 22H), 2.68 (t, *J* = 6.3 Hz, 2H), 1.83 – 1.73 (m, 2H), 1.72 – 1.68 (m, 2H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 196.8, 151.9, 146.0, 145.5, 137.4, 133.8, 130.9, 130.2, 128.8, 128.2, 26.8, 26.7, 22.3, 22.2. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{16}H_{16}NO$ 238.1227, found 238.1223.

*2-(5-benzoylpyridin-3-yl)-2-methyl-1-(pyridin-3-yl)propan-1-one (**3na**)*



Purification by column chromatography on silica gel (eluting with pentane/ethyl acetate = 4/1, v/v) afforded the title compound as an orange solid (8.9 mg, 27% yield); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.83 (d, *J* = 1.8 Hz, 1H), 8.70 (d, *J* = 2.3 Hz, 1H), 8.65 (d, *J* = 1.9 Hz, 1H), 8.57 (dd, *J* = 4.8, 1.5 Hz, 1H), 7.97 (t, *J* = 2.1 Hz, 1H), 7.80 (dt, *J* = 8.0, 1.8 Hz, 1H), 7.64 (d, *J* = 7.3 Hz, 2H), 7.56 (t, *J* = 7.4 Hz, 1H), 7.41 (t, *J* = 7.8 Hz, 2H), 7.22 (dd, *J* = 8.0, 4.8 Hz, 1H), 1.66 (s, 6H); ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 200.7, 194.5, 152.7, 151.0, 150.7, 149.7, 140.4, 137.2, 136.6, 134.5, 133.5, 133.4, 130.8, 130.1, 128.8, 123.5, 50.5, 27.6. HRMS (ESI-TOF) *m/z* $[M + H]^+$ calcd for $C_{21}H_{19}N_2O_2$ 331.1442, found 331.1432.

13. Computational Study

Density functional theory (DFT) calculations were performed using Gaussian 16 rev. A.03 software[13]，using the hybrid exchange-correlation functional B3LYP[14-16]. Grimme's D3 empirical dispersion correction with Becke–Johnson damping (GD3BJ)[17,18] was included to account for dispersion interactions. The Karlsruhe-family basis set def2-SVP[19] were used for all the gas-phase optimizations. Minima and transition structures on the potential energy surface (PES) were confirmed as such by harmonic frequency analysis, showing respectively zero and one imaginary

frequency. Intrinsic reaction coordinate (IRC) analyses were performed to confirm that the found TSs connect to the right reactants and products. To improve on the accuracy of the corrected Gibbs energy profile, single point (SP) calculations were performed at B3LYP-GD3(BJ) level with def2-TZVP basis set[19]. The implicit SMD continuum solvation model[20] for acetonitrile solvent is used to account for the effect of solvent on the potential energy surface.

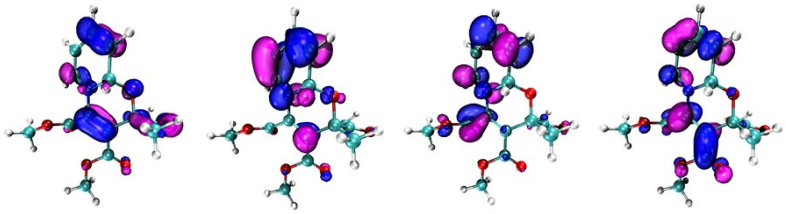
Time-dependent density functional theory (TD-DFT) calculations were performed at TD-B3LYP-GD3(BJ)/def2-SVP level based on the optimized structure. The calculations of spin-orbit coupling (SOC) between triplets and singlets were carried out at B3LYP-D3/def2-TZVP level utilizing orca 6.1.0[21]. SOC provides the relativistic coupling between electronic states of different spin multiplicities and is therefore a key factor governing spin-forbidden intersystem crossing (ISC) from singlet to triplet excited states. In general, a larger SOC matrix element indicates stronger singlet–triplet coupling and thus a higher probability of ISC, while the singlet–triplet energy gap also affects the ISC efficiency. Therefore, the calculated SOC matrix elements were used here as qualitative theoretical descriptors to evaluate the relative propensity for singlet–triplet intersystem crossing in the present system. This treatment is consistent with recent computational analyses[22] in which SOC matrix elements and singlet–triplet energy gaps were used to rationalize enhanced ISC and triplet-state accessibility in photoactive systems. Molecular orbital localization (MOL) analysis was performed with Multiwfn 3.8 (dev)[23] and the VMD 1.9.3[24] were used to visualize the frontier molecular orbitals.

Table S6. The singlet excited state transition configurations of **1a** according to TD-DFT calculations. % Constitution for each orbitals pair is in parentheses.

Singlet excite state	Energy (kcal/mol)	Wavelength (nm)	Oscillator Strength (*f*)	Transition configuration
S_1	78.9	362	0.308	HOMO → LUMO (99.2%)
S_2	98.0	292	0.027	HOMO → LUMO + 1 (86.5%) HOMO - 1 → LUMO (10.5%)
S_3	107.9	265	0.089	HOMO - 1 → LUMO (65.3%) HOMO → LUMO + 2 (22.7%)
S_4	113.5	252	0.001	HOMO - 2 → LUMO (38.8%) HOMO - 3→ LUMO (26.8%) HOMO - 4 → LUMO (20.4%) HOMO → LUMO + 2 (5.9%)

Table S7. Calculated spin-orbital coupling constant of **1a**.

SOC (cm^{-1})			
S_0, T_1	S_0, T_2	S_1, T_1	S_1, T_2
1.380	3.080	2.235	2.685



HOMO-1	HOMO	LUMO+1	LUMO
-7.07 eV	-5.85 eV	-1.00 eV	-1.95 eV

Figure S10. Frontier molecular orbitals of **1a**.

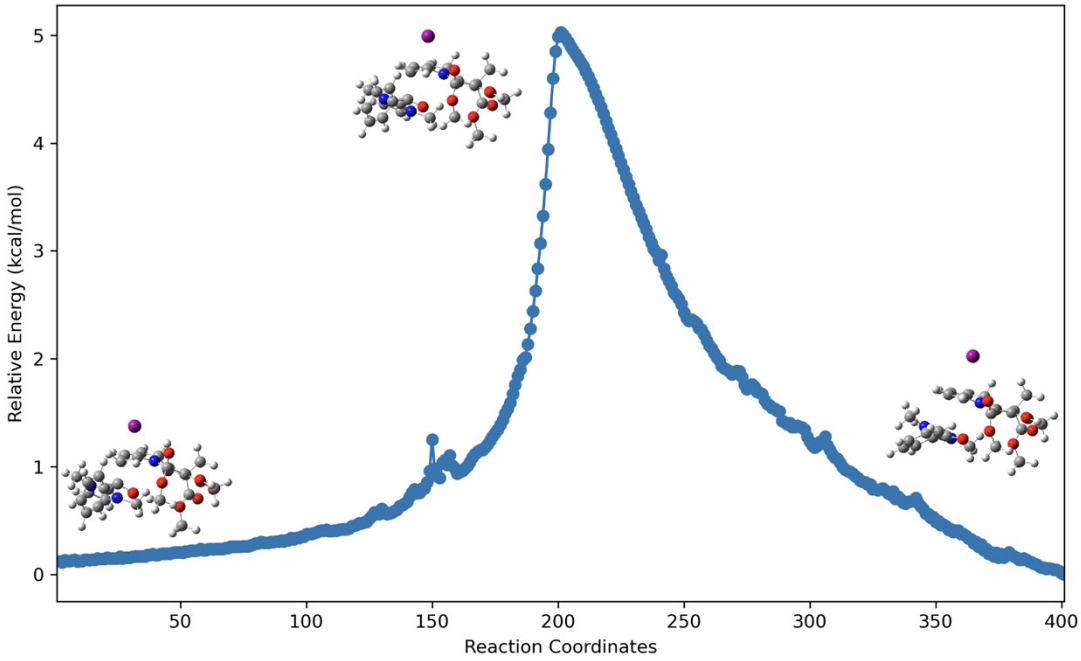


Figure S11. Intrinsic reaction coordinate of **TS-1**.

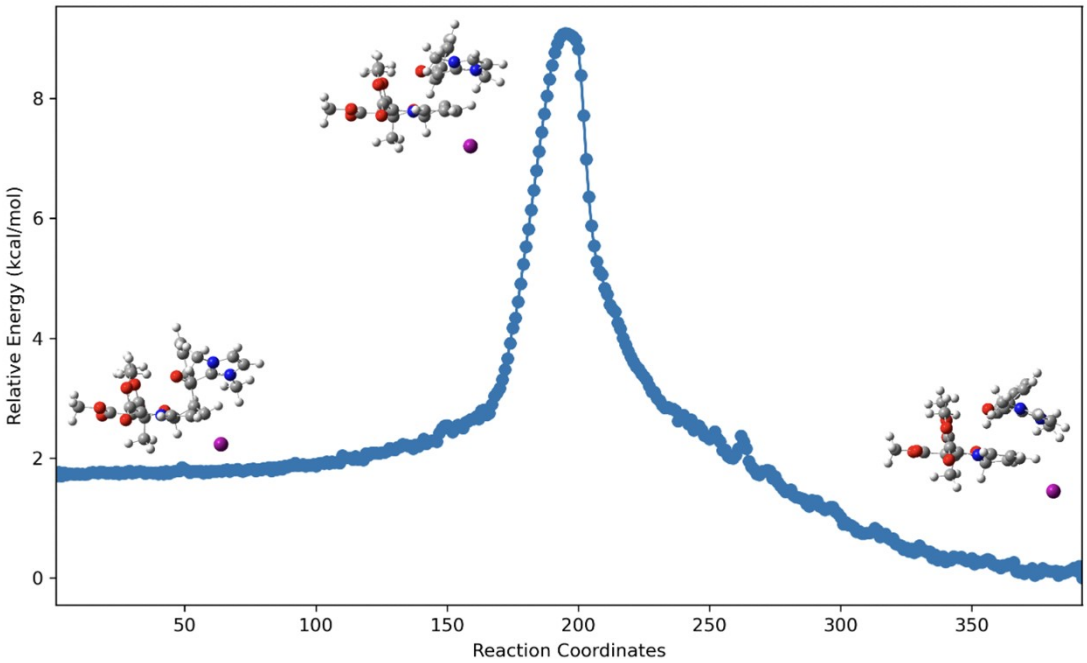


Figure S12. Intrinsic reaction coordinate of **TS-1'**.

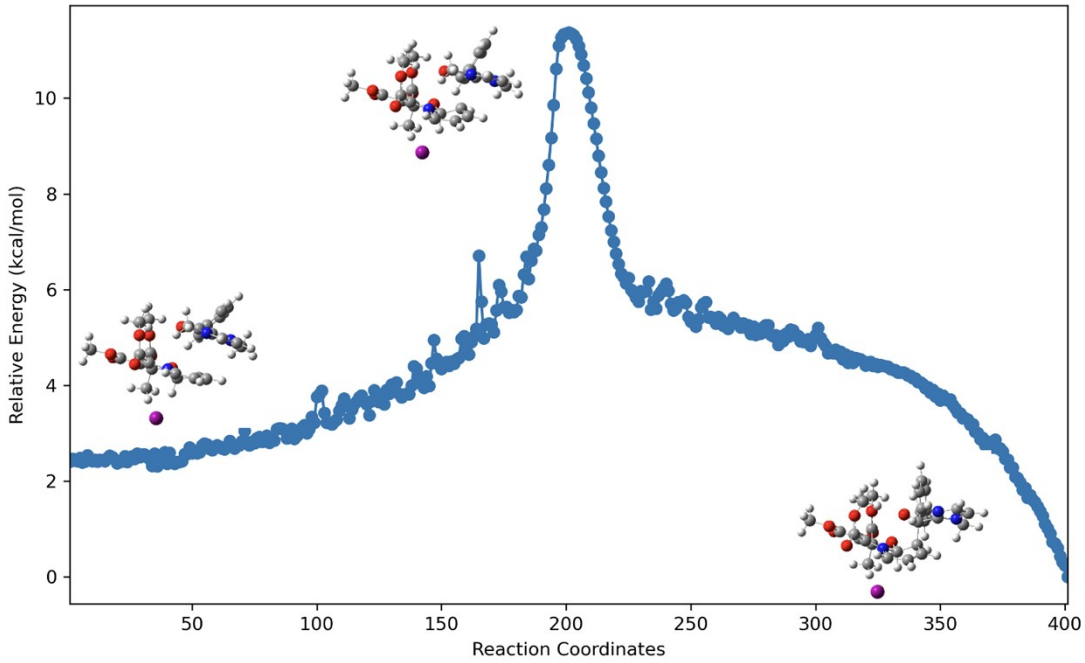


Figure S13. Intrinsic reaction coordinate of **TS-1''**.

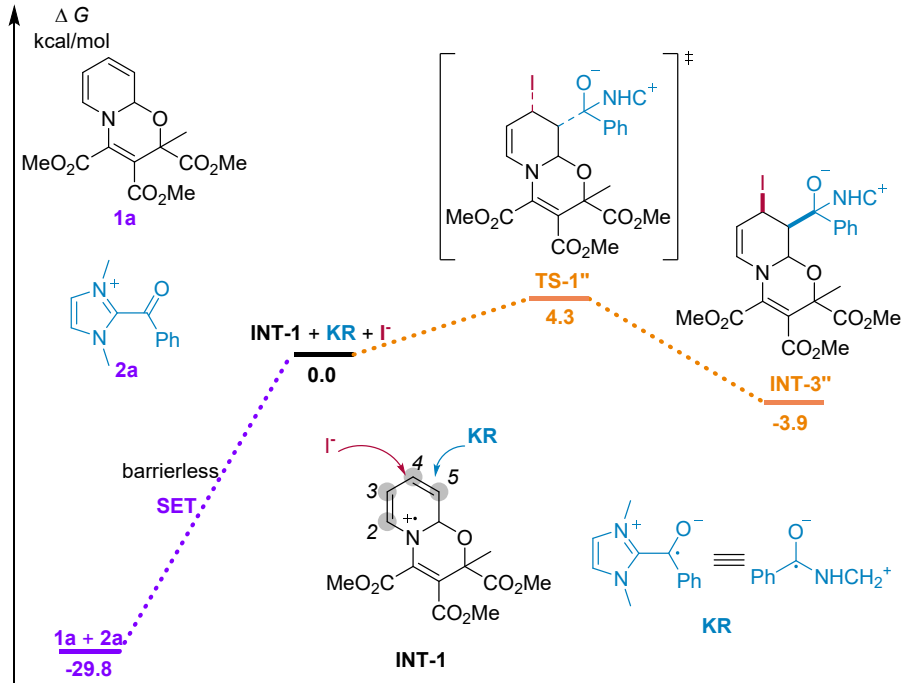


Figure S14. Pathway C: iodide attack at C4 and the barrierless SET process

Cartesian coordinate

NHC

Zero-point correction= 0.126265 (Hartree/Particle)

Thermal correction to Energy= 0.133244

Thermal correction to Enthalpy= 0.134188

Thermal correction to Gibbs Free Energy= 0.095301

Sum of electronic and zero-point Energies=			-304.470999
Sum of electronic and thermal Energies=			-304.464019
Sum of electronic and thermal Enthalpies=			-304.463075
Sum of electronic and thermal Free Energies=			-304.501963
C	0.00005000	-0.98185300	-0.00024800
N	1.06347300	-0.12289400	-0.00050500
C	0.68024500	1.21332800	-0.00017100
C	-0.68034500	1.21333600	0.00025400
N	-1.06348000	-0.12282600	0.00013200
C	2.44163600	-0.57045800	0.00023800
C	-2.44157000	-0.57053400	0.00006700
H	1.38957200	2.03755200	0.00027100
H	-1.38961700	2.03763700	-0.00030500
H	2.43534500	-1.66687400	0.00014800
H	2.97511400	-0.21069500	-0.89460300
H	2.97404400	-0.21135600	0.89605600
H	-2.97466000	-0.21053200	0.89505500
H	-2.97430700	-0.21164600	-0.89558600
H	-2.43553500	-1.66696400	0.00074500

INT-1

Zero-point correction=			0.311728 (Hartree/Particle)
Thermal correction to Energy=			0.334566
Thermal correction to Enthalpy=			0.335510
Thermal correction to Gibbs Free Energy=			0.258367
Sum of electronic and zero-point Energies=			-1161.763903
Sum of electronic and thermal Energies=			-1161.741065
Sum of electronic and thermal Enthalpies=			-1161.740120
Sum of electronic and thermal Free Energies=			-1161.817264
C	-3.52193300	-1.58067500	0.69190100
C	-2.63796200	-0.49873900	0.74531400
N	-1.57514700	-0.42106000	-0.05900900
C	-1.22411100	-1.51830600	-1.01516900
C	-2.19263700	-2.65457000	-1.00038000
C	-3.29342200	-2.66338100	-0.19588700
C	-0.64572200	0.63330500	-0.09446700
C	0.60766500	0.36992700	-0.55956600
C	1.10633300	-1.04514200	-0.76947900
O	0.03397000	-1.99852100	-0.69337500
C	1.88810800	-1.24727500	-2.06355500
C	-1.02798800	2.04859900	0.23257300
O	-0.19150900	2.90589900	0.36907200
O	-2.34105200	2.23869900	0.31888800
C	-2.77944400	3.59616600	0.55282700
C	1.51649800	1.47231800	-1.07702700

O	1.32353300	1.76906500	-2.22772800
O	2.51895500	1.93310200	-0.36516300
C	2.60954000	1.77587000	1.05332500
C	2.01470200	-1.35659000	0.46189900
O	3.20902800	-1.43778100	0.39449700
O	1.28770900	-1.47236400	1.57033800
C	2.01154400	-1.79103800	2.77387300
H	-4.37635200	-1.58161200	1.36994600
H	-2.79012400	0.32391400	1.44141100
H	-1.22857900	-1.03274300	-2.01346100
H	-1.94712700	-3.48417900	-1.66673400
H	-3.98503200	-3.50776900	-0.21176500
H	1.28718500	-0.94192700	-2.93020500
H	2.81344700	-0.65849300	-2.05052900
H	2.15633200	-2.30846200	-2.14463000
H	-3.87249900	3.55142300	0.59753500
H	-2.35980300	3.96991500	1.49660400
H	-2.44715500	4.23982900	-0.27269900
H	3.56855600	1.29097900	1.27517500
H	2.56899600	2.77621900	1.50264600
H	1.78171100	1.17178900	1.44970700
H	1.25971500	-1.86541700	3.56688600
H	2.54462500	-2.74410700	2.65362800
H	2.74003500	-0.99954000	3.00022400

INT-2

Zero-point correction= 0.545201 (Hartree/Particle)
Thermal correction to Energy= 0.585001
Thermal correction to Enthalpy= 0.585945
Thermal correction to Gibbs Free Energy= 0.468476
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Sum of electronic and thermal Energies= -2108.966277
Sum of electronic and thermal Enthalpies= -2108.965333
Sum of electronic and thermal Free Energies= -2109.082802

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C	-0.53975800	1.33804300	0.71394700
N	0.47432300	0.60737100	0.13317600
C	0.92109500	0.95566900	-1.23566600
C	-0.17363900	1.56964000	-2.04908200
C	-1.22311600	2.16807000	-1.46172400
C	1.31325700	-0.24191900	0.82272700
C	2.38095000	-0.83375100	0.20724300
C	2.57811100	-0.74169400	-1.29602100
O	1.38725300	-0.20029200	-1.88760300
C	-2.52851900	-1.02026800	-0.08200400

C	-2.89999500	-0.51136800	-1.42330500
C	-3.49849200	-0.98776800	1.04072900
O	-1.42807800	-1.56096700	0.03209300
C	-2.99576900	-0.92379900	2.35388600
C	-3.86827100	-0.95548800	3.43877200
C	-5.24739400	-1.08521500	3.23241400
C	-5.75006700	-1.19809200	1.93262700
C	-4.88096000	-1.14991100	0.84218100
N	-2.30347200	-0.95207300	-2.56431900
C	-2.83331000	-0.28213000	-3.64124300
C	-3.76801400	0.58958900	-3.16369400
N	-3.80571100	0.44246100	-1.79304900
C	-1.23921000	-1.95625500	-2.67447500
C	-4.54202200	1.34831700	-0.91800200
C	0.96283700	-0.45468800	2.29150100
O	1.03546800	0.43632300	3.09121200
O	0.40812500	-1.62784700	2.64412100
C	0.48230600	-2.83164900	1.88081100
C	3.35412600	-1.67242300	0.91085700
O	4.17377700	-2.37534000	0.35011700
O	3.25838600	-1.59689600	2.25159000
C	4.15170700	-2.40427000	3.01180300
C	2.64193000	-2.15594700	-1.91854800
O	3.36136800	-2.47864900	-2.82371200
O	1.71880900	-2.97560600	-1.37595300
C	1.73188200	-4.31957000	-1.84943800
H	-2.11324300	2.72530200	0.49233700
H	1.74056000	1.69372100	-1.10913600
H	0.00872800	1.61114800	-3.12417300
H	-1.94916700	2.71944300	-2.06351600
H	-1.91896000	-0.85670100	2.51121900
H	-3.46951900	-0.88401800	4.45296100
H	-5.92853000	-1.11310600	4.08593100
H	-6.82140300	-1.33570500	1.76900100
H	-5.27743200	-1.27573500	-0.16791300
H	-2.49588700	-0.47044300	-4.65575400
H	-4.38841400	1.31585800	-3.67991100
H	-0.29851700	-1.54736500	-2.28642200
H	-1.50635300	-2.84929700	-2.09959900
H	-1.13938700	-2.20911400	-3.73740300
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H	-4.59783700	2.32848400	-1.40867700
H	-5.55491700	0.97635300	-0.71780300
H	1.31604000	-3.44008900	2.26247300

H	-0.46555900	-3.36068100	2.04147700
H	0.60985100	-2.64545300	0.81043300
H	3.91143400	-2.21144000	4.06390300
H	4.01515800	-3.47021600	2.77254800
H	5.19530300	-2.13039100	2.79879400
H	0.92874700	-4.84109500	-1.31369400
H	1.55854000	-4.35657000	-2.93561100
H	2.70300700	-4.78947100	-1.63416900
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H	3.89271000	0.06607200	-2.80238100
H	3.75260200	1.08101800	-1.32241400
H	4.71363800	-0.42325800	-1.29806500
H	-0.62313900	1.26963600	1.79519400
I	1.59590300	4.13073300	0.42229100

INT-2'

Zero-point correction= 0.545271 (Hartree/Particle)
Thermal correction to Energy= 0.584783
Thermal correction to Enthalpy= 0.585727
Thermal correction to Gibbs Free Energy= 0.469825
Sum of electronic and zero-point Energies= -2109.006500
Sum of electronic and thermal Energies= -2108.966988
Sum of electronic and thermal Enthalpies= -2108.966044
Sum of electronic and thermal Free Energies= -2109.081946

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N	0.32381200	0.49147500	-0.41256100
C	0.71064400	0.17711800	-1.80856400
C	-0.48576400	-0.02099000	-2.68818900
C	-1.67527000	0.52445900	-2.37291900
C	1.31860700	0.31267500	0.53266400
C	2.52618300	-0.22418300	0.18088800
C	2.73983300	-0.87339400	-1.17491500
O	1.47449100	-0.99509100	-1.83574600
C	-2.30603100	-1.10450800	0.83794700
C	-3.33610600	-0.10789900	1.21894500
C	-2.57214300	-2.16621300	-0.15957900
C	-1.48058800	-2.63386700	-0.91737500
C	-1.66051700	-3.67301500	-1.82852400
C	-2.91226400	-4.28081200	-1.97015400
C	-3.99006300	-3.85150500	-1.18652300
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C	-4.85425200	0.02392900	-0.81071700
C	0.96730000	0.67964800	1.97039100
O	0.53679800	1.76588100	2.27292800
O	1.06161800	-0.26004400	2.91688500
C	1.37553600	-1.63165700	2.68643000
C	3.67840700	-0.28571700	1.08846500
O	4.62437600	-1.03480900	0.93391200
O	3.60136000	0.59385500	2.10236000
C	4.63740100	0.54671300	3.07723700
C	3.15159200	-2.35583600	-1.00580600
O	3.97584200	-2.91860000	-1.67310200
O	2.40004600	-2.96767500	-0.07408500
C	2.68513200	-4.34683600	0.14505200
H	-2.66669500	1.92023800	-0.97467600
H	1.30588800	1.04850100	-2.15599200
H	-0.30450200	-0.57134000	-3.61214000
H	-2.52013400	0.43409100	-3.06023300
H	-0.49818700	-2.17965900	-0.79533200
H	-0.81270100	-4.01020700	-2.42905600
H	-3.04692900	-5.10004600	-2.68031700
H	-4.95960500	-4.34836300	-1.26827800
H	-4.65604900	-2.49370500	0.34718800
H	-4.50459100	2.11797400	3.30128700
H	-5.98533600	1.79008800	0.97426100
H	-1.97508400	-0.54283700	3.60306200
H	-1.38943200	1.08777800	3.20540800
H	-2.74184500	0.88729400	4.37555900
H	-5.62478900	-0.75727400	-0.84737200
H	-5.24320600	0.94658300	-1.26093400
H	-3.97970500	-0.30993600	-1.37474200
H	2.45957300	-1.79651300	2.77266200
H	0.86372500	-2.19301000	3.47978100
H	1.02652700	-1.97652000	1.70964100
H	4.39736300	1.32456900	3.81140000
H	4.67339600	-0.44105500	3.56293900
H	5.61501900	0.74210100	2.61284900
H	1.98216100	-4.68595000	0.91604000
H	2.54720200	-4.92654300	-0.77981400
H	3.72298300	-4.47330500	0.48756800
C	3.76158300	-0.15286900	-2.04964300
H	3.86032600	-0.68204700	-3.00656100
H	3.45054700	0.88639600	-2.22293600

H	4.74043500	-0.14947800	-1.55272000
H	-0.85230400	1.82098600	0.70498700
I	0.50662800	3.90325800	-1.32839900
O	-1.23070700	-1.07278600	1.44335100

TS-1

Zero-point correction=	0.544989 (Hartree/Particle)
Thermal correction to Energy=	0.583464
Thermal correction to Enthalpy=	0.584408
Thermal correction to Gibbs Free Energy=	0.472349
Sum of electronic and zero-point Energies=	-2108.997377
Sum of electronic and thermal Energies=	-2108.958903
Sum of electronic and thermal Enthalpies=	-2108.957959
Sum of electronic and thermal Free Energies=	-2109.070018

C	-1.79036700	0.49924500	-0.96644000
C	-0.67136300	1.26126500	-0.38867100
N	0.58785100	0.68055700	-0.56496200
C	0.96019200	0.17888900	-1.89367800
C	-0.22144300	-0.26655500	-2.69339400
C	-1.48162900	-0.11040100	-2.25715300
C	1.60621000	0.76598200	0.35433800
C	2.83722100	0.22634100	0.10082600
C	3.07796300	-0.63153700	-1.12819600
O	1.82195700	-0.92606000	-1.75927200
C	-1.99560200	-0.91707300	0.50971100
C	-2.38469300	-2.03434700	-0.43619000
C	-3.15988300	-0.42731300	1.37735800
O	-0.89586100	-1.07741300	1.11534700
C	-3.47533300	0.91959100	1.59444800
C	-4.48084500	1.27937100	2.49685000
C	-5.18632100	0.30005600	3.19974500
C	-4.86703200	-1.04733200	3.00698300
C	-3.85665700	-1.40185800	2.11112900
N	-1.55040200	-3.02376300	-0.82428600
C	-2.17759300	-3.80852900	-1.77439000
C	-3.42515100	-3.29756500	-1.96401600
N	-3.54252400	-2.20169200	-1.12671100
C	-0.16634200	-3.24944700	-0.38254100
C	-4.72899100	-1.35465200	-1.06145800
C	1.27115400	1.53080700	1.63349900
O	1.12737100	2.72336300	1.60040700
O	1.05295700	0.84257700	2.75210000
C	1.30879600	-0.55258000	2.90060000
C	3.96917300	0.30070900	1.02669200
O	4.98869200	-0.35327700	0.89897700

O	3.78558000	1.16276000	2.04219800
C	4.82090800	1.24973200	3.01465600
C	3.57127100	-2.03868200	-0.71451600
O	4.38364000	-2.68640600	-1.31712800
O	2.90824400	-2.49295200	0.36505900
C	3.31541400	-3.76863000	0.85108000
H	-2.73346200	1.04794000	-0.94945000
H	1.49242200	1.00275600	-2.41118900
H	0.01679900	-0.72076300	-3.65658600
H	-2.30708600	-0.45081700	-2.88883300
H	-2.94248700	1.71052900	1.06694100
H	-4.71047400	2.33646700	2.65011900
H	-5.97402500	0.58503500	3.90104800
H	-5.40009800	-1.82330100	3.56235400
H	-3.59673100	-2.45650100	1.98003200
H	-1.68132800	-4.65914200	-2.23090900
H	-4.23474000	-3.61538700	-2.61386200
H	0.48945200	-2.46169000	-0.76869800
H	-0.12177900	-3.23337800	0.70812700
H	0.14303500	-4.22531100	-0.77965800
H	-4.43683700	-0.29993600	-1.03932800
H	-5.33436600	-1.54569900	-1.95622600
H	-5.31373200	-1.56998300	-0.15777800
H	2.23891800	-0.67475000	3.47778400
H	0.45905000	-0.97508700	3.44917400
H	1.38909600	-1.06755500	1.93905300
H	4.47416600	1.97556000	3.75961500
H	4.99900700	0.27010400	3.48411900
H	5.75965600	1.58978200	2.55281600
H	2.67020100	-3.98877200	1.71064800
H	3.20080300	-4.54022700	0.07483000
H	4.37022600	-3.73805800	1.16228400
C	4.05979000	-0.02448500	-2.12662600
H	4.19771600	-0.71357000	-2.97031100
H	3.68528800	0.94230800	-2.49016400
H	5.03132000	0.13471900	-1.64130900
H	-0.81919900	1.60390700	0.63231300
I	-0.70243400	3.44053500	-1.43152100

TS-1'

Zero-point correction=	0.544606 (Hartree/Particle)
Thermal correction to Energy=	0.583207
Thermal correction to Enthalpy=	0.584151
Thermal correction to Gibbs Free Energy=	0.471582
Sum of electronic and zero-point Energies=	-2108.990122

Sum of electronic and thermal Energies= -2108.951521
Sum of electronic and thermal Enthalpies= -2108.950577
Sum of electronic and thermal Free Energies= -2109.063146

C	-0.28611900	-2.99252500	-0.22713200
C	-1.29149400	-2.02202200	0.17384300
N	-0.96105200	-0.68718100	-0.00144300
C	-0.17012300	-0.41498400	-1.23130900
C	1.11032500	-1.21874600	-1.19364800
C	0.83967500	-2.60178000	-0.88944800
C	-1.65401100	0.35314800	0.59002000
C	-1.72738700	1.58032200	0.00903300
C	-0.96710600	1.86144800	-1.26789000
O	0.11675500	0.92951100	-1.37308100
C	2.28117100	-0.29368600	0.41383500
C	2.79011500	-1.64272800	0.84822700
C	3.33244700	0.58078800	-0.26508600
C	3.08520600	1.36627300	-1.39770400
C	4.05856300	2.24939200	-1.87323900
C	5.29073100	2.36804000	-1.22385100
C	5.54008500	1.60373300	-0.08072800
C	4.56434100	0.72451700	0.39529400
N	2.30369900	-2.32004400	1.91448300
C	2.90937800	-3.56285900	1.98671600
C	3.78507700	-3.64725400	0.94939600
N	3.70571200	-2.45228000	0.25373800
C	1.29833000	-1.85975600	2.87879100
C	4.44482200	-2.18071400	-0.97382500
C	-2.25705000	0.01119900	1.94640100
O	-3.19955000	-0.72657900	2.06146300
O	-1.59004600	0.43072300	3.02980400
C	-0.61290500	1.48248700	3.01155700
C	-2.54578100	2.68564400	0.51969000
O	-2.63562500	3.76614700	-0.02792300
O	-3.21937400	2.38154600	1.64565300
C	-4.08139100	3.38444600	2.17475400
C	-0.17087000	3.18435700	-1.16855100
O	0.05742300	3.90981800	-2.10042000
O	0.34466000	3.34069300	0.05502800
C	1.24916800	4.42789600	0.22446900
H	-0.49305400	-4.04020400	-0.00893300
H	-0.81171600	-0.76697300	-2.06879900
H	1.73664300	-1.03466800	-2.07149400
H	1.57769900	-3.36420700	-1.15435300
H	2.11754300	1.30437500	-1.88923500

H	3.84355500	2.85505800	-2.75706400
H	6.04882900	3.05907700	-1.60015900
H	6.49173800	1.69939900	0.44837500
H	4.75979500	0.14824600	1.30481200
H	2.65892300	-4.27705800	2.76475000
H	4.45181100	-4.44766700	0.64356000
H	1.68833500	-1.01901700	3.46258200
H	0.40236700	-1.52182900	2.35602300
H	1.06726100	-2.70654000	3.53758700
H	5.33182700	-1.56601900	-0.77203500
H	4.74416000	-3.14079800	-1.41298200
H	3.80614900	-1.63966500	-1.67910500
H	-1.12636900	2.45387600	3.02966100
H	-0.03764000	1.36094800	3.93902700
H	0.06211000	1.41082900	2.15110500
H	-4.53858700	2.94731200	3.07024000
H	-3.51227700	4.29025600	2.43319800
H	-4.85501700	3.65522500	1.44125700
H	1.55343300	4.40874900	1.27775900
H	2.12873300	4.29669600	-0.42372100
H	0.76007600	5.38215000	-0.02114200
C	-1.84594400	1.84812600	-2.51307000
H	-1.23246300	2.06158100	-3.39870000
H	-2.34059400	0.87205800	-2.61899600
H	-2.61721000	2.62474900	-2.42470800
H	-1.88500800	-2.22984300	1.06170300
I	-3.24343400	-2.50875600	-1.33391000
O	1.49661900	0.27513400	1.21076600

INT-3

Zero-point correction= 0.546120 (Hartree/Particle)
Thermal correction to Energy= 0.584708
Thermal correction to Enthalpy= 0.585652
Thermal correction to Gibbs Free Energy= 0.472808
Sum of electronic and zero-point Energies= -2109.004622
Sum of electronic and thermal Energies= -2108.966033
Sum of electronic and thermal Enthalpies= -2108.965089
Sum of electronic and thermal Free Energies= -2109.077933

C	1.69123400	-0.42761100	-0.85883700
C	0.51126100	-1.28821400	-0.44685400
N	-0.73254900	-0.72364800	-0.73723000
C	-0.98026000	-0.04398100	-2.00755200
C	0.27154800	0.28995700	-2.75351700
C	1.48681100	0.13083500	-2.22877000
C	-1.81028100	-0.79598600	0.11136900

C	-2.92645400	-0.03988000	-0.10531300
C	-2.95395000	1.03353500	-1.17964200
O	-1.66029800	1.16473700	-1.78926900
C	1.84098900	0.73072300	0.27863200
C	2.67666800	1.85460000	-0.42582100
C	2.67011900	0.20495700	1.48402400
O	0.68889700	1.20576500	0.69836900
C	3.09134700	-1.11620500	1.67211700
C	3.75493200	-1.49406900	2.84720200
C	4.01962800	-0.55368100	3.84224500
C	3.59327600	0.76973300	3.66760600
C	2.91132100	1.13501200	2.50888400
N	2.15550400	2.98847600	-0.93980500
C	3.16265700	3.75181200	-1.50081400
C	4.32886600	3.07104400	-1.32805900
N	4.01120900	1.89686600	-0.66525000
C	0.73455200	3.36814300	-1.00006600
C	5.00316300	0.89368700	-0.28550200
C	-1.69085400	-1.84753000	1.21321600
O	-1.83808000	-3.00831300	0.94135800
O	-1.32664900	-1.45452500	2.43264200
C	-1.19229300	-0.06115300	2.76570800
C	-4.10408000	-0.06577600	0.76572900
O	-5.01522300	0.73822900	0.69886600
O	-4.08151100	-1.05865300	1.67467300
C	-5.16156100	-1.11582000	2.59894600
C	-3.13076000	2.43195800	-0.54043500
O	-3.70177800	3.35328400	-1.06248700
O	-2.47962000	2.51796200	0.62634000
C	-2.50528800	3.78471600	1.27242300
H	2.59657500	-1.04429600	-0.87007100
H	-1.61531700	-0.72194700	-2.61420500
H	0.11761600	0.69920200	-3.75417100
H	2.37055800	0.40830400	-2.81056200
H	2.91434500	-1.88085700	0.91354500
H	4.06366900	-2.53401300	2.97865400
H	4.54351800	-0.84862200	4.75449300
H	3.78205100	1.51270600	4.44695800
H	2.53072800	2.15168900	2.38634000
H	2.95768600	4.70813500	-1.97243700
H	5.34854100	3.31765300	-1.60828200
H	0.19970100	2.68211300	-0.32511600
H	0.64695100	4.41966000	-0.69360400
H	0.37096500	3.23912000	-2.02747900

H	4.65687700	-0.10903100	-0.55750000
H	5.93130200	1.11258200	-0.82789200
H	5.18448900	0.91955800	0.79641400
H	-2.18221800	0.41655500	2.79583300
H	-0.75129300	-0.04943900	3.77071700
H	-0.52705300	0.46087300	2.05670000
H	-4.95006200	-1.96688800	3.25712100
H	-5.22661000	-0.18435700	3.18174000
H	-6.11617800	-1.26412200	2.07249700
H	-1.87700000	3.68277500	2.16544100
H	-2.10657600	4.56870800	0.61067700
H	-3.53507400	4.05436400	1.55223500
C	-4.01723500	0.81212700	-2.25195900
H	-3.99641000	1.65187000	-2.95908100
H	-3.82258500	-0.12905000	-2.78599300
H	-5.01259000	0.76053100	-1.79334100
H	0.56570200	-1.59952100	0.59646900
I	0.80302800	-3.35304900	-1.48667600

INT-3'

Zero-point correction=	0.546282 (Hartree/Particle)
Thermal correction to Energy=	0.584697
Thermal correction to Enthalpy=	0.585641
Thermal correction to Gibbs Free Energy=	0.473585
Sum of electronic and zero-point Energies=	-2109.003851
Sum of electronic and thermal Energies=	-2108.965436
Sum of electronic and thermal Enthalpies=	-2108.964492
Sum of electronic and thermal Free Energies=	-2109.076548

C	-0.11336300	-3.05137600	0.03435000
C	-1.21634000	-2.13656700	0.36210300
N	-1.00350200	-0.80553000	0.09146000
C	-0.15789000	-0.53974900	-1.09025500
C	1.22509300	-1.18246000	-0.90606400
C	1.00989300	-2.62777400	-0.56711100
C	-1.74184800	0.21800100	0.65443900
C	-1.89871800	1.40506400	0.01201800
C	-1.18389400	1.63334700	-1.30114500
O	-0.00940900	0.80964300	-1.32299300
C	2.09053000	-0.45989100	0.24017000
C	3.31971300	-1.45713700	0.48127200
C	2.74947200	0.87968400	-0.21792100
C	2.74292500	1.41585300	-1.50972100
C	3.36216700	2.64021300	-1.78135300
C	4.01261100	3.34318500	-0.76478200
C	4.01813200	2.82075000	0.53339600

C	3.38024800	1.60905600	0.80071400
N	3.44024800	-2.27302200	1.55175400
C	4.63184500	-2.97129300	1.48511500
C	5.26031300	-2.58103400	0.34417800
N	4.43639700	-1.65080100	-0.26793000
C	2.45378000	-2.49580500	2.61774500
C	4.79681500	-0.98747700	-1.51773700
C	-2.32258900	-0.10070400	2.02658000
O	-3.25646800	-0.85039100	2.15615100
O	-1.68143400	0.39245200	3.08209700
C	-0.58567200	1.31829900	2.95662400
C	-2.76644700	2.49397700	0.47364200
O	-2.97613900	3.50295400	-0.17070400
O	-3.33139600	2.26297300	1.67170400
C	-4.23817200	3.24594000	2.16112200
C	-0.54771800	3.04224700	-1.35194000
O	-0.47362900	3.72164700	-2.34118500
O	0.00040100	3.35514100	-0.17273800
C	0.65465000	4.61852800	-0.09765000
H	-0.27109000	-4.10240400	0.28140100
H	-0.66459600	-1.04625900	-1.93873100
H	1.73619300	-1.11773600	-1.87970300
H	1.80370200	-3.34509500	-0.79279600
H	2.23182900	0.90168500	-2.32177700
H	3.32228000	3.05003100	-2.79355000
H	4.49872600	4.29824600	-0.97871300
H	4.51066800	3.36735100	1.34204400
H	3.33180400	1.21085000	1.81615000
H	4.91998300	-3.68330900	2.25262400
H	6.21490600	-2.87437000	-0.08215100
H	2.96074800	-2.40132700	3.58810100
H	1.68262700	-1.72084100	2.47451000
H	2.03763700	-3.50692900	2.50848800
H	5.11242200	0.04637000	-1.33171900
H	5.61672700	-1.55447500	-1.97608900
H	3.94500900	-0.97476400	-2.20484300
H	-0.96553600	2.30746900	2.66576100
H	-0.14898700	1.37850200	3.96209300
H	0.16965100	0.95516700	2.24133900
H	-4.58256000	2.87934600	3.13526300
H	-3.73571600	4.21889700	2.26897700
H	-5.08817100	3.36552100	1.47303900
H	1.11753600	4.66253500	0.89518200
H	1.42549700	4.70062400	-0.87575700

H	-0.07591600	5.43231000	-0.22267700
C	-2.06707400	1.39238100	-2.51893700
H	-1.48958400	1.56670600	-3.43701600
H	-2.46319400	0.36653500	-2.50665700
H	-2.91198200	2.09354700	-2.49796100
H	-1.77622000	-2.33369700	1.27494700
I	-3.00552900	-2.96394900	-1.12065500
O	1.41630800	-0.30157400	1.35702000

TS-2

Zero-point correction= 0.545195 (Hartree/Particle)
Thermal correction to Energy= 0.583675
Thermal correction to Enthalpy= 0.584619
Thermal correction to Gibbs Free Energy= 0.471218
Sum of electronic and zero-point Energies= -2108.996472
Sum of electronic and thermal Energies= -2108.957992
Sum of electronic and thermal Enthalpies= -2108.957048
Sum of electronic and thermal Free Energies= -2109.070449

C	-1.58511100	0.49002700	-0.93528200
C	-0.36566900	1.26881400	-0.45789100
N	0.83792600	0.58489800	-0.64998600
C	1.13626500	0.01139100	-1.96615900
C	-0.09908000	-0.33944200	-2.73374300
C	-1.33062900	-0.12160400	-2.27564500
C	1.87983600	0.61127900	0.24657000
C	3.04520000	-0.05421900	0.00103600
C	3.18408600	-0.95813700	-1.21111300
O	1.89869300	-1.15111800	-1.82369500
C	-1.87964700	-0.59231600	0.16432600
C	-3.46189500	-1.51231500	-0.66289100
C	-2.56715600	-0.05329700	1.42168900
O	-1.01621500	-1.48316800	0.34745400
C	-2.93265500	1.28514200	1.61549900
C	-3.52508300	1.69432200	2.81566100
C	-3.77108200	0.76845100	3.83042000
C	-3.40015200	-0.57004700	3.64802700
C	-2.79019000	-0.96983800	2.46044800
N	-3.30356400	-2.76451300	-1.15019700
C	-4.52234900	-3.41665600	-1.24333500
C	-5.46709100	-2.54451600	-0.79703700
N	-4.79504300	-1.38165200	-0.45131300
C	-2.03644000	-3.34830300	-1.58943000
C	-5.44979700	-0.20604800	0.10502200
C	1.62427000	1.45522400	1.49090600
O	1.75508300	2.64825200	1.46391800

O	1.13181300	0.82780800	2.56166100
C	1.05442500	-0.60499900	2.61803400
C	4.18262300	-0.06912300	0.92517700
O	5.20692900	-0.69510000	0.73119200
O	3.98328500	0.66535600	2.03673400
C	5.04771800	0.71626000	2.98029700
C	3.53587900	-2.39838400	-0.76757000
O	4.20918000	-3.16164900	-1.40742400
O	2.93089000	-2.71794000	0.38504200
C	3.16552300	-4.03790500	0.86632300
H	-2.44345200	1.16807900	-1.00792900
H	1.71409200	0.77971100	-2.52266200
H	0.08711800	-0.79256100	-3.70991300
H	-2.19944600	-0.40131100	-2.87562000
H	-2.76265500	2.03385700	0.83951800
H	-3.79054800	2.74496400	2.95479800
H	-4.23786000	1.08811100	4.76511500
H	-3.57842500	-1.29938500	4.44245500
H	-2.46461300	-2.00057600	2.30793400
H	-4.61131300	-4.43101300	-1.62222800
H	-6.54425500	-2.64825700	-0.70049400
H	-1.21925600	-2.80861700	-1.09322600
H	-2.01888200	-4.41018600	-1.30763700
H	-1.94120500	-3.25898500	-2.68144000
H	-4.94669600	0.69958800	-0.24872700
H	-6.49522100	-0.18960300	-0.23100200
H	-5.41367900	-0.22034300	1.20338000
H	2.06289300	-1.03500600	2.69415300
H	0.48394300	-0.82752100	3.52831300
H	0.52392800	-1.02116900	1.74952400
H	4.69326300	1.35209800	3.80024600
H	5.29039600	-0.29173700	3.34910400
H	5.95103400	1.14708100	2.52340500
H	2.58600800	-4.13326600	1.79265900
H	2.83658900	-4.78634000	0.12996800
H	4.23723500	-4.18892700	1.06569700
C	4.20459700	-0.47172800	-2.23641400
H	4.27010200	-1.19986200	-3.05564300
H	3.90953000	0.51061800	-2.63155800
H	5.19085200	-0.37890900	-1.76435100
H	-0.46498700	1.60965200	0.57258700
I	-0.37613900	3.32956500	-1.52344500

TS-2'

Zero-point correction= 0.545273 (Hartree/Particle)

Thermal correction to Energy= 0.583623
Thermal correction to Enthalpy= 0.584567
Thermal correction to Gibbs Free Energy= 0.472044
Sum of electronic and zero-point Energies= -2109.000804
Sum of electronic and thermal Energies= -2108.962454
Sum of electronic and thermal Enthalpies= -2108.961510
Sum of electronic and thermal Free Energies= -2109.074033

C	1.55462700	-2.18131900	1.32238600
C	0.20146600	-2.23554700	1.40106200
N	-0.63127400	-1.58482900	0.52231300
C	0.00832200	-0.96864400	-0.65971400
C	1.33330200	-0.28659800	-0.29195000
C	2.23150000	-1.31322600	0.37609400
C	-1.99491100	-1.49769500	0.67006400
C	-2.79192700	-0.98186800	-0.30805800
C	-2.16261700	-0.39917800	-1.55334100
O	-0.81046500	-0.02964100	-1.25264700
C	1.12165200	0.99217500	0.65108800
C	2.59895100	1.43626500	1.10150900
C	0.62589000	2.25633400	-0.14071100
C	0.59401400	2.42476900	-1.53114900
C	0.12543200	3.61382000	-2.10087900
C	-0.30712300	4.66275500	-1.28758600
C	-0.29323400	4.50120100	0.10192600
C	0.15692900	3.30623400	0.66270900
N	2.98312400	1.62741300	2.38375100
C	4.30219700	2.04290800	2.42811200
C	4.74589200	2.10043300	1.14482200
N	3.68647200	1.72517200	0.33691400
C	2.18750300	1.42848000	3.60376300
C	3.81160800	1.62121800	-1.11452800
C	-2.51757800	-2.01581700	2.00378900
O	-2.65955700	-3.19362300	2.20958300
O	-2.69049700	-1.10979600	2.96122800
C	-2.54421700	0.29805000	2.69006100
C	-4.25180200	-0.92778900	-0.24242500
O	-4.95553900	-0.55742800	-1.16289400
O	-4.75471100	-1.32379500	0.94325500
C	-6.17230000	-1.35221200	1.06782100
C	-2.77262100	0.98257700	-1.89195300
O	-2.94443400	1.39342400	-3.00902700
O	-2.99315100	1.69379000	-0.78123400
C	-3.53021700	3.00065500	-0.97052100
H	2.14274800	-2.77899400	2.01904500

H	0.23523100	-1.80008900	-1.35552600
H	1.77329000	0.01901200	-1.24450400
H	0.87641300	1.61081300	-2.19775800
H	0.08142200	3.70771400	-3.18851600
H	-0.67041100	5.59193800	-1.73340400
H	-0.64834500	5.30676800	0.75028100
H	0.12565800	3.14202400	1.74117500
H	4.80167900	2.25550700	3.36837500
H	5.71408300	2.37090200	0.73456300
H	2.00095600	2.40557700	4.07224600
H	1.24653800	0.96037100	3.27247300
H	2.76199000	0.79172200	4.29083400
H	2.94100100	2.07687700	-1.59673900
H	4.71286400	2.16776900	-1.41716300
H	3.90913400	0.56977400	-1.42306300
H	-3.38551200	0.64875100	2.07614100
H	-2.58046600	0.78331700	3.67387300
H	-1.58434100	0.52292600	2.19550000
H	-6.37871700	-1.69724100	2.08791600
H	-6.59768400	-0.35064700	0.90467600
H	-6.61351900	-2.04217500	0.33309900
H	-3.56210800	3.46308400	0.02300700
H	-2.88724500	3.58806700	-1.63926700
H	-4.54113800	2.93596600	-1.40098600
C	-2.23447200	-1.31956300	-2.76600300
H	-1.77175300	-0.82898300	-3.63284400
H	-1.72453500	-2.27077300	-2.55588700
H	-3.28639600	-1.53049600	-2.99936900
O	0.37117900	0.74227000	1.69769200
H	3.16170100	-0.89753500	0.76908700
H	-0.29268700	-2.83335300	2.16553600
I	3.30399400	-2.57198100	-1.31772900

INT-4

Zero-point correction=	0.416533 (Hartree/Particle)
Thermal correction to Energy=	0.447916
Thermal correction to Enthalpy=	0.448860
Thermal correction to Gibbs Free Energy=	0.350422
Sum of electronic and zero-point Energies=	-1804.511950
Sum of electronic and thermal Energies=	-1804.480567
Sum of electronic and thermal Enthalpies=	-1804.479623
Sum of electronic and thermal Free Energies=	-1804.578061

C	-2.04198800	-0.74929800	1.47422400
C	-1.30689600	-0.81055600	0.13501400
N	0.07877000	-0.66011400	0.28180300

C	0.76428000	-1.63083300	1.15075900
C	-0.02850700	-1.87671100	2.39897300
C	-1.28828200	-1.47126900	2.55229100
C	0.85610500	0.06412400	-0.59936900
C	2.21234100	-0.02316700	-0.59875600
C	2.91926600	-0.89541400	0.42150300
O	2.01879000	-1.15081700	1.51550800
C	-2.22039000	0.75173800	1.81228400
C	-3.20816200	1.53862200	1.01351000
O	-1.52734900	1.27471400	2.66082100
C	-4.06984100	0.96047600	0.06492000
C	-4.94432900	1.76159300	-0.67054000
C	-4.96977200	3.14332000	-0.46454700
C	-4.11978300	3.72674900	0.48244800
C	-3.24588000	2.92961800	1.21580100
C	0.05491300	1.01293300	-1.47809600
O	-0.42828500	0.67142700	-2.52185800
O	-0.21453000	2.20931600	-0.93832400
C	0.47133000	2.66945400	0.23276100
C	3.07520600	0.75302100	-1.49816800
O	4.27336500	0.58575600	-1.59589600
O	2.40826000	1.69226900	-2.19563400
C	3.15216800	2.43644600	-3.15795600
C	4.04349400	-0.09918500	1.12502800
O	5.08549500	-0.57166400	1.48989600
O	3.67618100	1.17279700	1.34055200
C	4.63941900	1.99339500	2.00085900
H	-3.03771900	-1.19695500	1.35395700
H	0.85709100	-2.57201800	0.56810700
H	0.50763900	-2.41269600	3.18488600
H	-1.81215300	-1.64864100	3.49431200
H	-4.06843000	-0.11588400	-0.11597400
H	-5.60553300	1.30420400	-1.40943300
H	-5.65292900	3.76829800	-1.04450900
H	-4.14009800	4.80699300	0.64351700
H	-2.57135000	3.35876000	1.95840600
H	1.53038500	2.85286400	0.00634200
H	-0.02373200	3.60653100	0.51379700
H	0.39108100	1.95558700	1.06371300
H	2.43753800	3.12420800	-3.62496600
H	3.96649300	2.99333100	-2.67135400
H	3.58765900	1.76514800	-3.91254800
H	4.17711700	2.98201500	2.10858900
H	4.89240000	1.57866700	2.98761300

H	5.55849900	2.06157200	1.39990700
C	3.48642300	-2.18616200	-0.15906800
H	3.99439800	-2.75312300	0.63232400
H	2.68711500	-2.79399100	-0.60547200
H	4.21498900	-1.94076200	-0.94277600
H	-1.70723200	-0.11176700	-0.59855900
I	-1.85767400	-2.77462800	-0.93823100

INT-4'

Zero-point correction=	0.416583 (Hartree/Particle)
Thermal correction to Energy=	0.447930
Thermal correction to Enthalpy=	0.448874
Thermal correction to Gibbs Free Energy=	0.351408
Sum of electronic and zero-point Energies=	-1804.521296
Sum of electronic and thermal Energies=	-1804.489949
Sum of electronic and thermal Enthalpies=	-1804.489005
Sum of electronic and thermal Free Energies=	-1804.586471

C	-1.97753300	-2.56082300	1.10005200
C	-2.18430100	-1.12574400	0.82025200
N	-1.05321500	-0.45878700	0.34164900
C	-0.25183100	-1.23045200	-0.62196900
C	0.28354800	-2.49843800	0.07083100
C	-0.84241800	-3.19513500	0.78044100
C	-0.89070600	0.91063300	0.43303500
C	-0.05058100	1.58882200	-0.38946500
C	0.68217400	0.84411300	-1.48225700
O	0.84750900	-0.52320300	-1.06917200
C	1.41164800	-2.09914900	1.05235400
C	2.83032300	-2.04238200	0.58954900
C	3.22518600	-2.26075200	-0.74036000
C	4.56790900	-2.15147800	-1.10397600
C	5.53112600	-1.83005200	-0.14341000
C	5.14784900	-1.61224600	1.18521600
C	3.80727000	-1.71510800	1.54688200
C	-1.75977300	1.57984600	1.49199600
O	-2.86090900	1.97682300	1.22808400
O	-1.28557300	1.60144600	2.74001700
C	0.05766700	1.19021200	3.02543400
C	0.18333500	3.03539600	-0.31234100
O	0.75958300	3.66900600	-1.17225300
O	-0.28797500	3.58823600	0.81985100
C	-0.20780800	5.00801000	0.92983500
C	2.16013300	1.28415100	-1.58223100
O	2.77415100	1.38886800	-2.60935700
O	2.69129100	1.42468000	-0.36101400

C	4.08411600	1.73307700	-0.31588400
H	-2.80149000	-3.07986900	1.59253700
H	-0.93277000	-1.51682800	-1.44911800
H	0.68588900	-3.15127000	-0.71633100
H	-0.70476400	-4.24392000	1.05305400
H	2.48608300	-2.48039700	-1.50881200
H	4.86159600	-2.30928800	-2.14381600
H	6.58195700	-1.74617400	-0.43110000
H	5.89885100	-1.35971900	1.93742600
H	3.48225900	-1.54130700	2.57366900
H	0.77600200	1.76905700	2.42845900
H	0.21074400	1.39947500	4.09117500
H	0.19640500	0.11689500	2.83755800
H	-0.65155100	5.26033500	1.89994700
H	0.83950200	5.34068900	0.88257600
H	-0.76812400	5.49023900	0.11542400
H	4.35044000	1.78379400	0.74626600
H	4.66611100	0.94469500	-0.81385600
H	4.27978400	2.69520100	-0.81191400
C	-0.00974500	0.94068300	-2.83497100
H	0.56503900	0.38448500	-3.58782700
H	-1.03305600	0.54359100	-2.76729300
H	-0.06261900	1.99447500	-3.13916400
H	-2.70459000	-0.58083800	1.61011000
I	-3.91826500	-1.05257200	-0.79187500
O	1.11609000	-1.81018300	2.19693700

INT-5

Zero-point correction= 0.403581 (Hartree/Particle)
Thermal correction to Energy= 0.432974
Thermal correction to Enthalpy= 0.433919
Thermal correction to Gibbs Free Energy= 0.340982
Sum of electronic and zero-point Energies= -1506.118576
Sum of electronic and thermal Energies= -1506.089182
Sum of electronic and thermal Enthalpies= -1506.088238
Sum of electronic and thermal Free Energies= -1506.181174

C	-2.07083400	-1.74827800	-0.55094800
C	-1.27903200	-0.66740500	-0.29370000
N	0.03440800	-0.61620500	-0.67188400
C	0.73400600	-1.74519100	-1.30840900
C	-0.15625200	-2.92823000	-1.50062800
C	-1.45375600	-2.92143100	-1.15086400
C	0.86633300	0.45675600	-0.39333900
C	2.21583600	0.30028500	-0.42287700
C	2.85246900	-1.08246900	-0.45134100

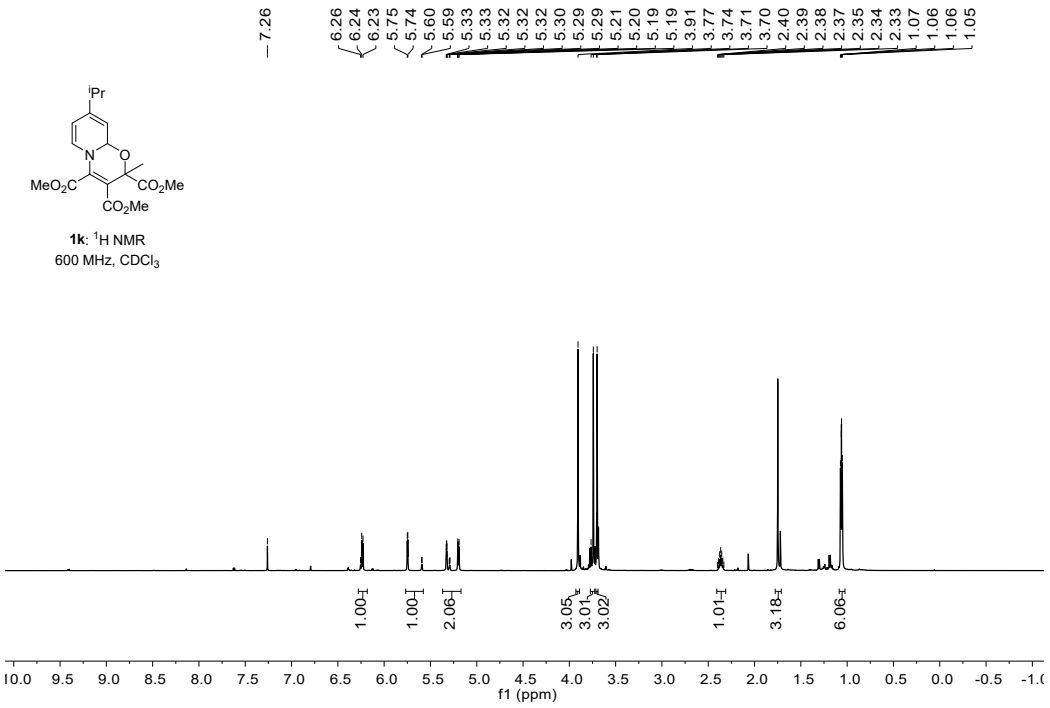
O	1.84189700	-2.09917100	-0.51168300
C	3.86450200	-1.27000800	-1.57789700
C	-3.48638100	-1.81531800	-0.12807700
C	-4.22416500	-0.54637700	0.20440600
C	-4.04521900	0.65343900	-0.50467900
C	-4.80209500	1.78302400	-0.18205100
C	-5.73688900	1.72917100	0.85500100
C	-5.93071900	0.53352300	1.55575400
C	-5.18999900	-0.59922100	1.22242700
O	-4.05909500	-2.89216300	-0.04021100
C	0.18231500	1.75665000	-0.03646800
O	0.26822600	2.29735200	1.03405700
O	-0.59049100	2.18030700	-1.04558800
C	-1.33672000	3.37593700	-0.80065000
C	3.13860200	1.43575400	-0.23100700
O	4.25112700	1.32851300	0.23730400
O	2.62157500	2.60727700	-0.64647300
C	3.37483300	3.77676800	-0.32946400
C	3.53241600	-1.36265200	0.91370000
O	4.56895400	-1.95755100	1.04028100
O	2.78643500	-0.91170000	1.92447700
C	3.30945600	-1.12556900	3.23464400
H	-1.64645700	0.19315900	0.26159300
H	1.11381300	-1.36471300	-2.27877200
H	0.32243800	-3.80401800	-1.94236900
H	-2.08880100	-3.79742300	-1.29247300
H	3.36908300	-1.16947200	-2.55440300
H	4.66675200	-0.52456200	-1.50475200
H	4.31036500	-2.26899900	-1.49164400
H	-3.33329300	0.69880300	-1.33038200
H	-4.66846900	2.70639400	-0.75084200
H	-6.32300800	2.61522400	1.11048100
H	-6.66794000	0.48518000	2.36062800
H	-5.34496800	-1.54669100	1.74171300
H	-1.88737700	3.58409600	-1.72540800
H	-2.03437500	3.22947900	0.03699000
H	-0.65980700	4.20798800	-0.55880100
H	2.83503300	4.61840800	-0.77963800
H	3.44099500	3.90628500	0.76134800
H	4.39233000	3.70654900	-0.73999900
H	2.57876100	-0.69328500	3.92848700
H	3.43878300	-2.20032500	3.43108500
H	4.28402800	-0.62652200	3.34184600

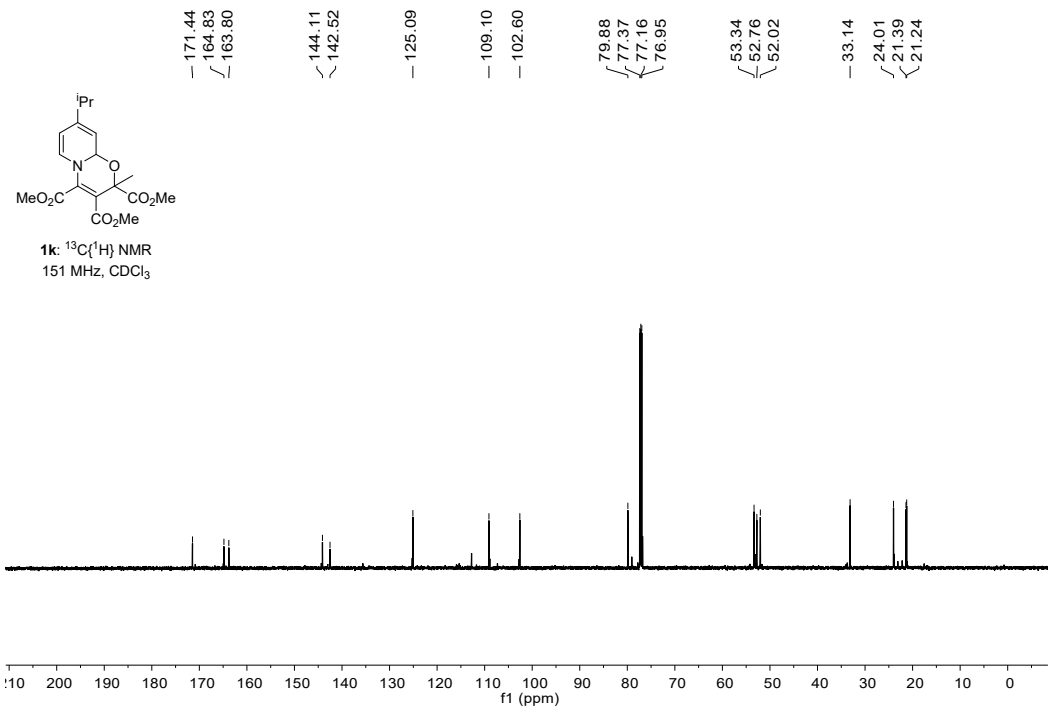
INT-5'

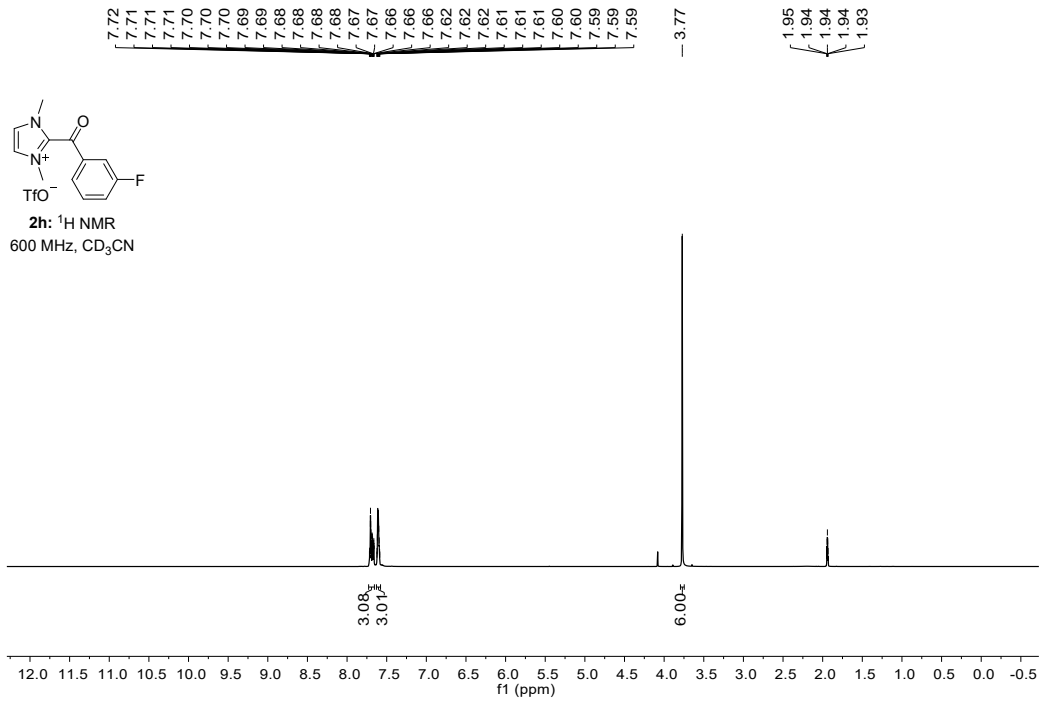
Zero-point correction=			0.403965 (Hartree/Particle)
Thermal correction to Energy=			0.433178
Thermal correction to Enthalpy=			0.434122
Thermal correction to Gibbs Free Energy=			0.341581
Sum of electronic and zero-point Energies=			-1506.113727
Sum of electronic and thermal Energies=			-1506.084514
Sum of electronic and thermal Enthalpies=			-1506.083569
Sum of electronic and thermal Free Energies=			-1506.176110
C	-0.31477100	3.25704300	1.54470000
N	0.43650700	1.50317900	0.11208900
C	-0.81188900	0.75633900	0.24539300
C	-1.94063600	1.63366200	0.70388700
C	-1.65240800	2.79021500	1.37168700
C	1.47674800	0.71695700	-0.40259000
C	1.41273800	-0.62380900	-0.23341200
C	0.42054700	-1.24928800	0.73759000
O	-0.57987900	-0.31647200	1.16677800
C	-0.21916000	-2.51653400	0.17766900
C	-3.37040100	1.37862900	0.36623100
C	-3.79179900	0.11159900	-0.32103300
C	-4.74922900	0.21228500	-1.34522500
C	-5.22118100	-0.93248300	-1.98419100
C	-4.76741200	-2.19527000	-1.58451100
C	-3.84084900	-2.30414200	-0.54526800
C	-3.34813200	-1.15583800	0.08085700
C	0.68479400	2.61105800	0.88586800
O	-4.21820900	2.23157000	0.59140200
C	2.61366000	1.37161700	-1.12457100
O	3.69450400	0.85967700	-1.29254500
O	2.29350000	2.59880300	-1.55752200
C	3.32153300	3.30814500	-2.25150400
C	2.42535700	-1.55743600	-0.80649500
O	3.07974600	-2.30696100	-0.12032800
O	2.46973400	-1.51117200	-2.14094700
C	3.52947100	-2.24479900	-2.75691700
C	1.17426100	-1.58013600	2.05428700
O	1.06006900	-2.61541800	2.65328500
O	1.91425900	-0.54456900	2.45753800
C	2.63926200	-0.72878500	3.67332300
H	-0.09555600	4.15098000	2.12736800
H	-1.02297600	0.31273800	-0.74227900
H	-2.49758800	3.39243000	1.71292800
H	-0.79251400	-2.28451200	-0.72966700
H	0.54973100	-3.26455300	-0.05625000

H	-0.88656600	-2.94847800	0.93370300
H	-5.11510700	1.20210800	-1.62415100
H	-5.95286800	-0.84424000	-2.79092400
H	-5.14427900	-3.09398900	-2.07898500
H	-3.49851800	-3.28829000	-0.21621100
H	-2.63217000	-1.23760000	0.89653200
H	1.72127100	2.94495900	0.91746000
H	2.89862800	4.28808200	-2.50107900
H	4.21250800	3.42017200	-1.61597100
H	3.61072500	2.76913000	-3.16567000
H	3.36118300	-2.17514900	-3.83808900
H	4.49574100	-1.79100300	-2.48990300
H	3.52225600	-3.29430000	-2.42949300
H	3.18111600	0.20786600	3.85022700
H	1.95272700	-0.93901200	4.50676600
H	3.34390500	-1.56743600	3.57313600

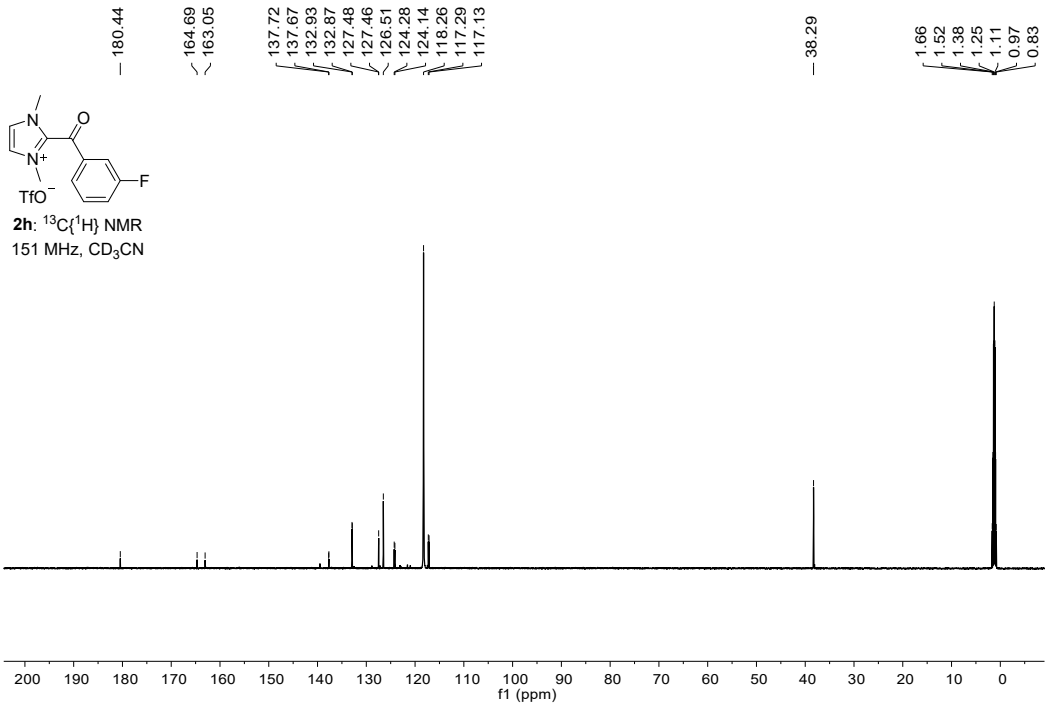
14. ^{1}H, ^{13}C, and ^{19}F NMR spectra



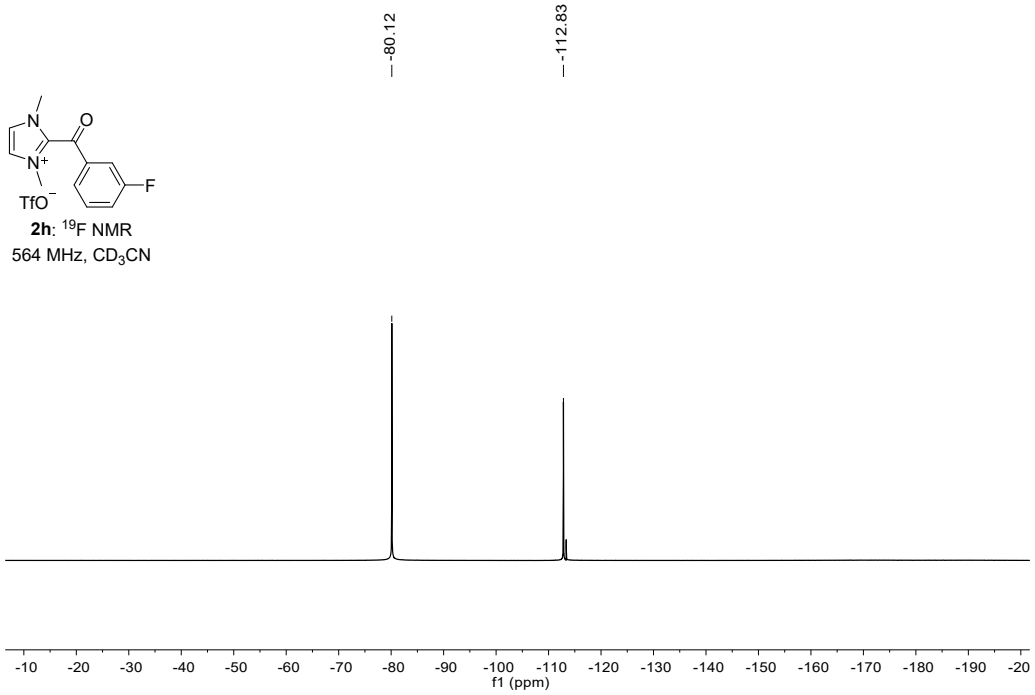




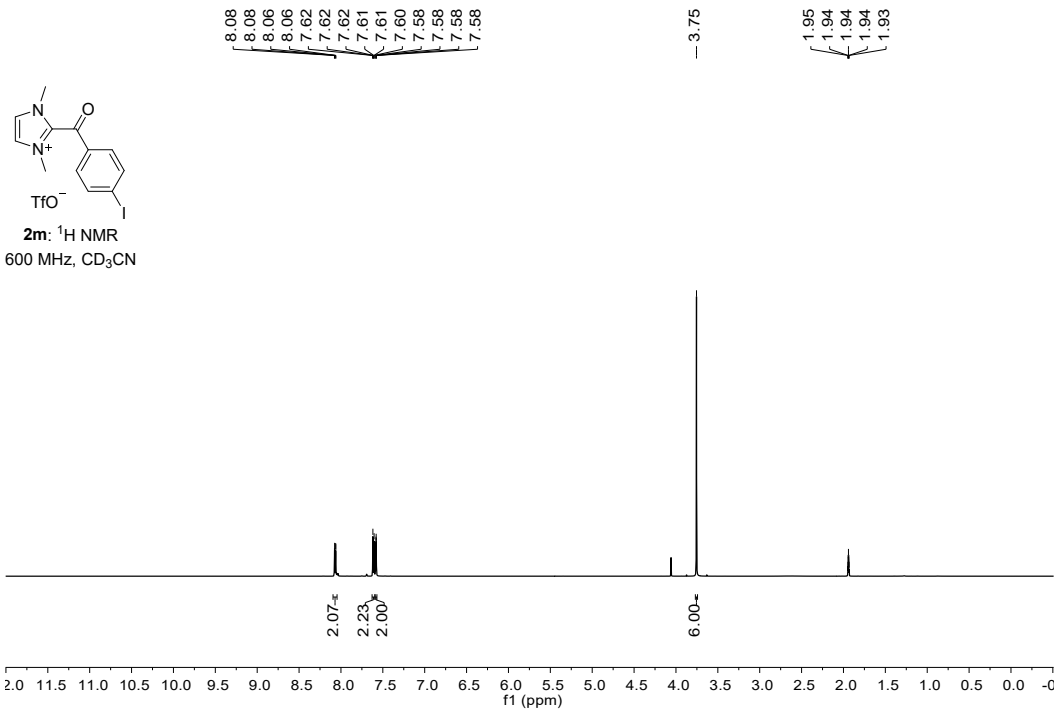
2h: ^{1}H NMR
600 MHz, CD_3CN



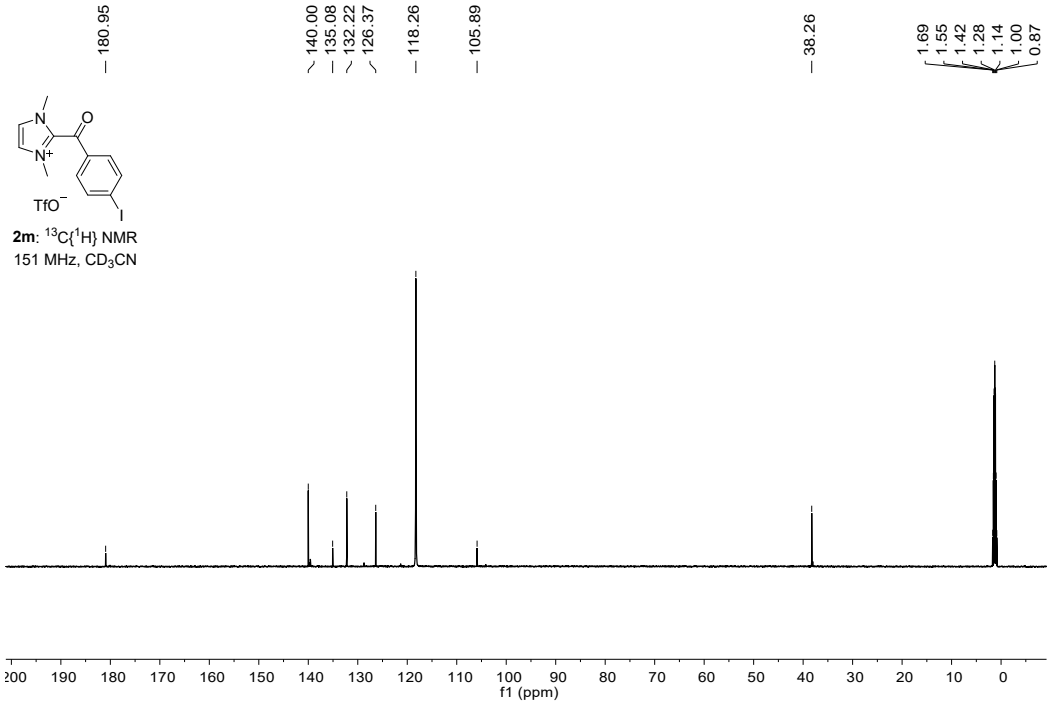
2h: $^{13}C\{^{1}H\}$ NMR
151 MHz, CD_3CN



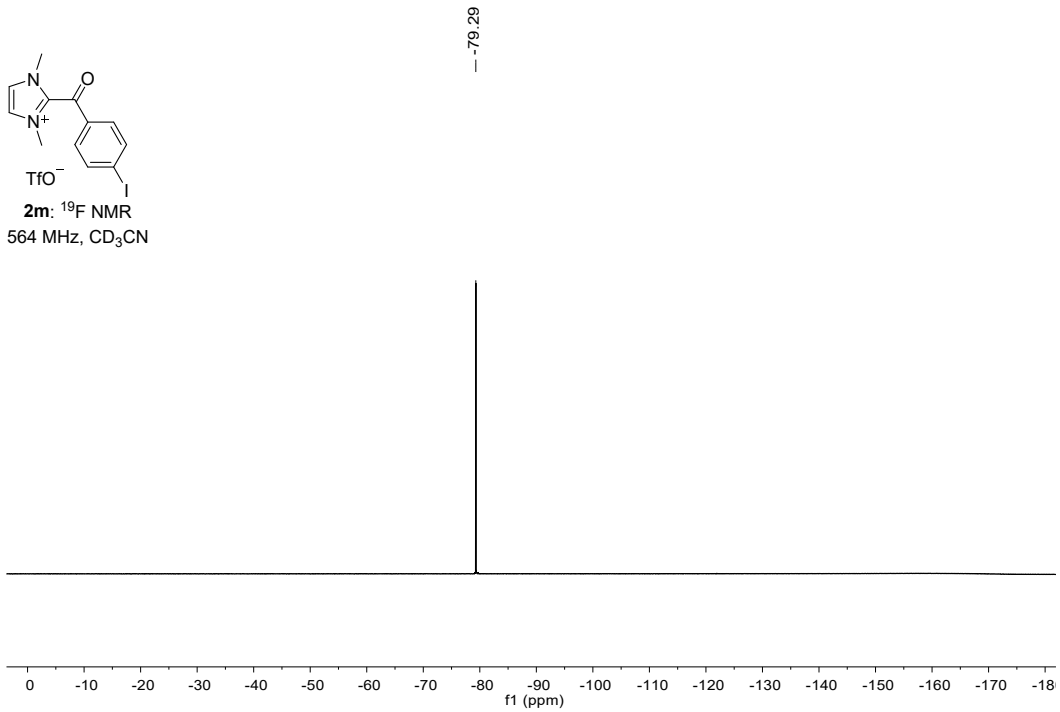
2h: ^{19}F NMR
564 MHz, CD_3CN



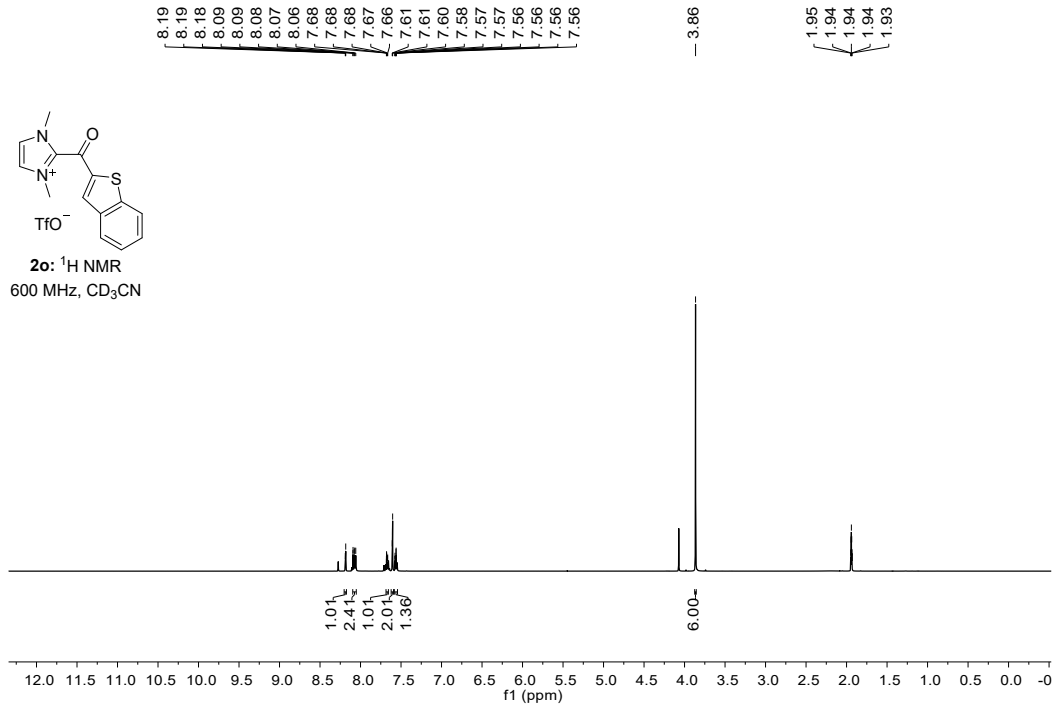
2m: ^{1}H NMR
600 MHz, CD_3CN



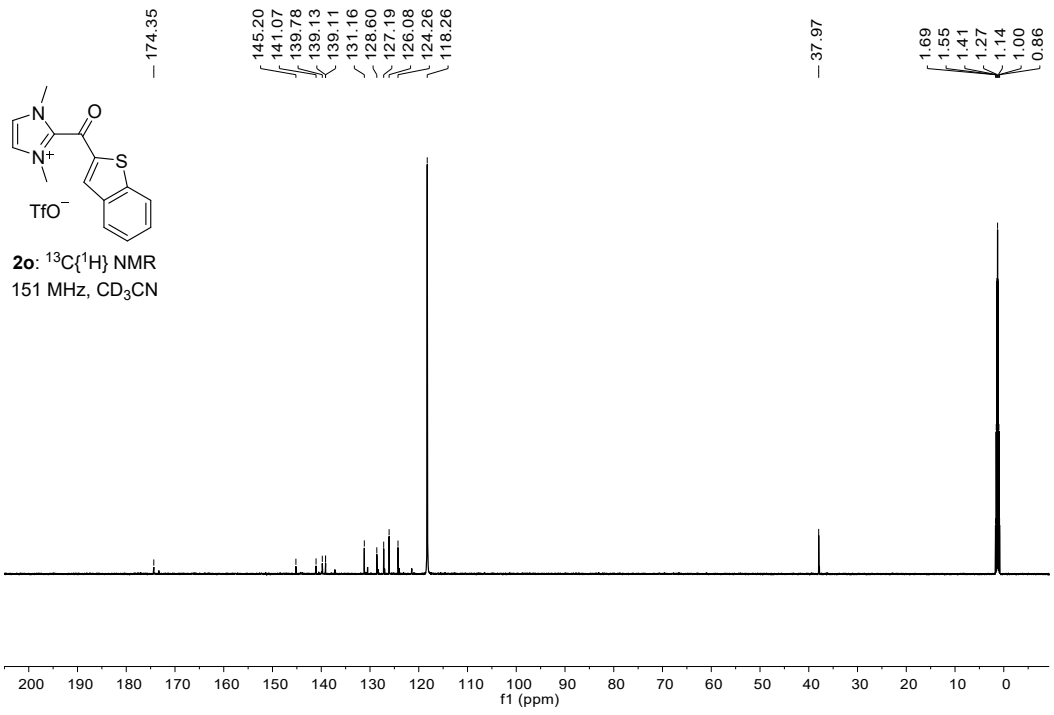
2m: $^{13}C\{^{1}H\}$ NMR
151 MHz, CD_3CN



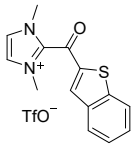
2m: ^{19}F NMR
564 MHz, CD_3CN



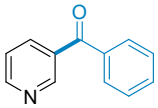
2o: ^{1}H NMR
600 MHz, CD_3CN



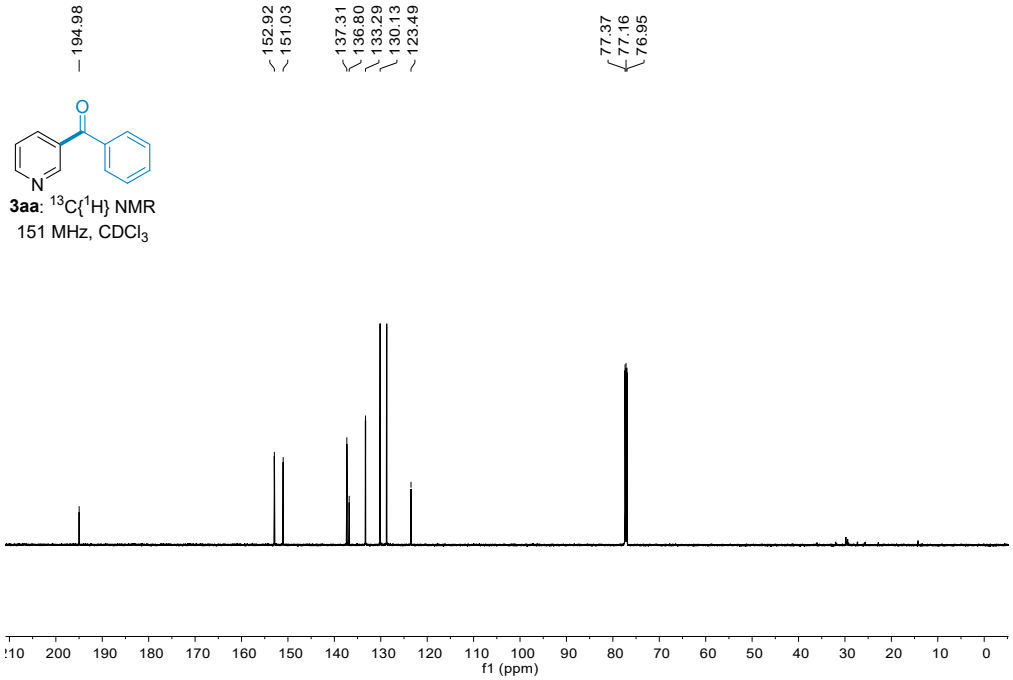
2o: $^{13}C\{^{1}H\}$ NMR
151 MHz, CD_3CN



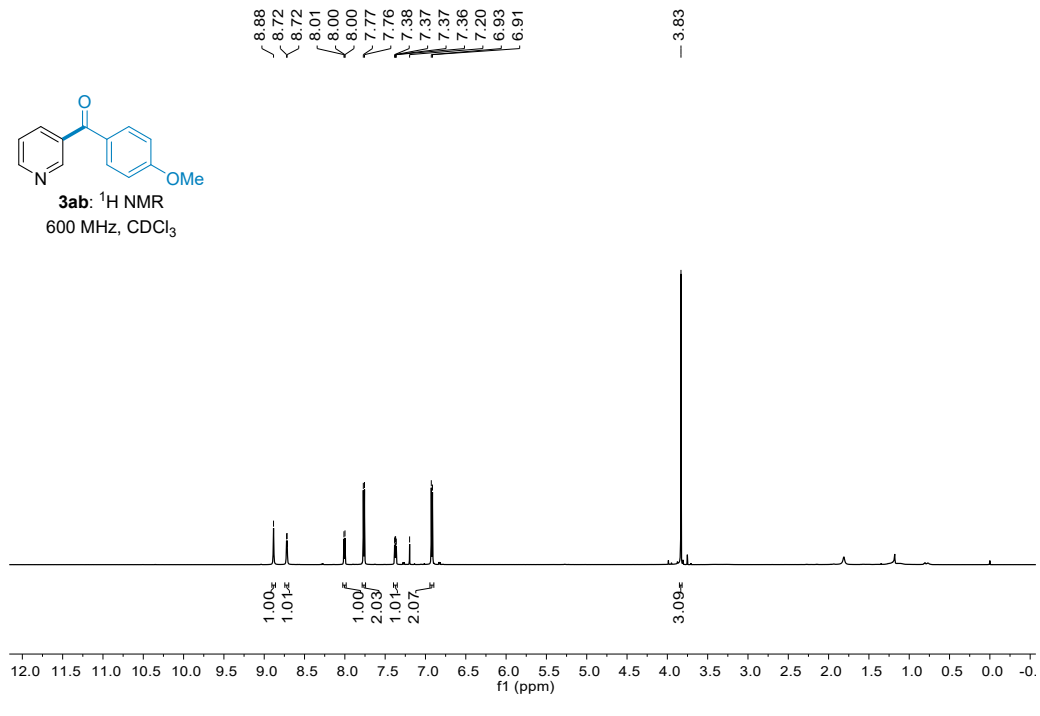
2o: ^{19}F NMR
564 MHz, CD_3CN



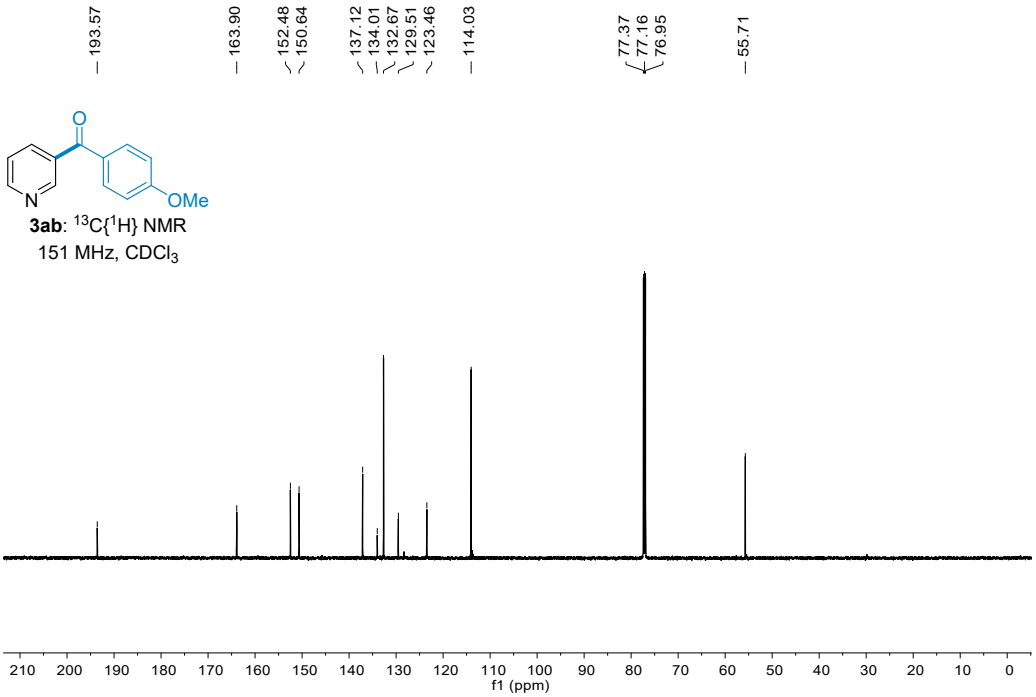
3aa: ^{1}H NMR
600 MHz, $CDCl_3$



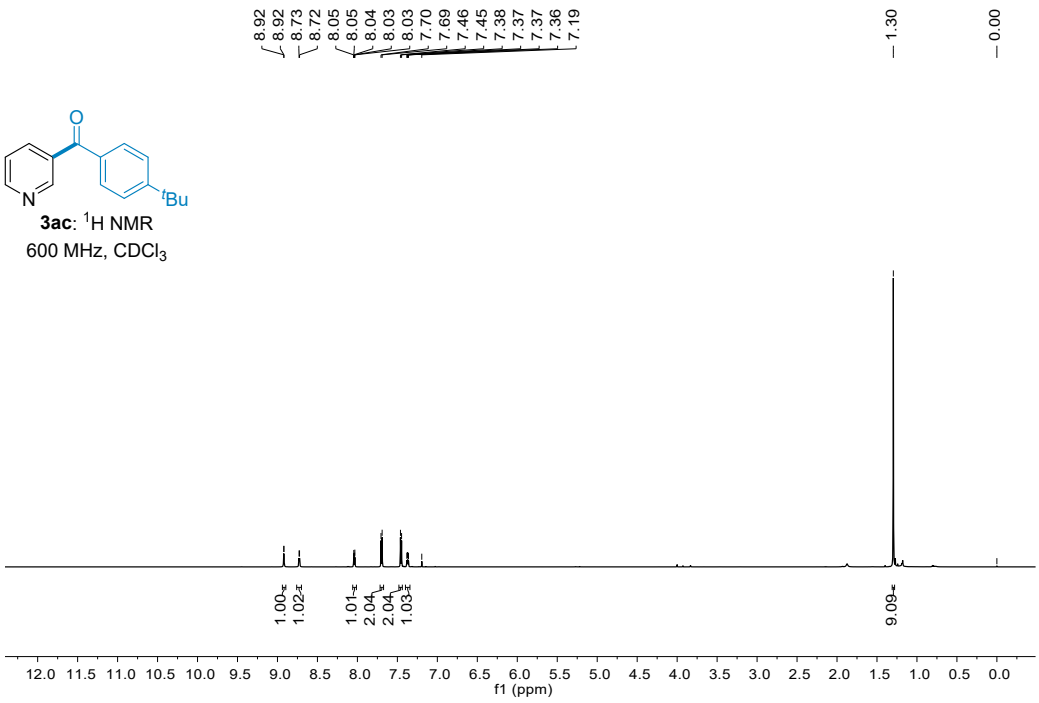
3aa: $^{13}C\{^{1}H\}$ NMR
151 MHz, $CDCl_3$



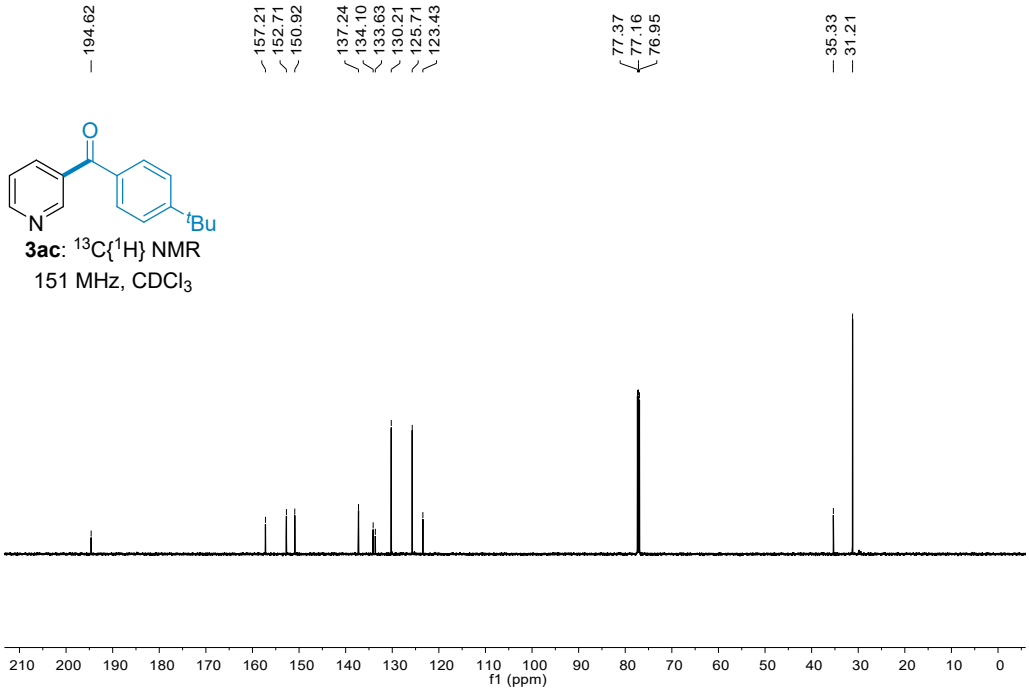
3ab: ^{1}H NMR
600 MHz, $CDCl_3$



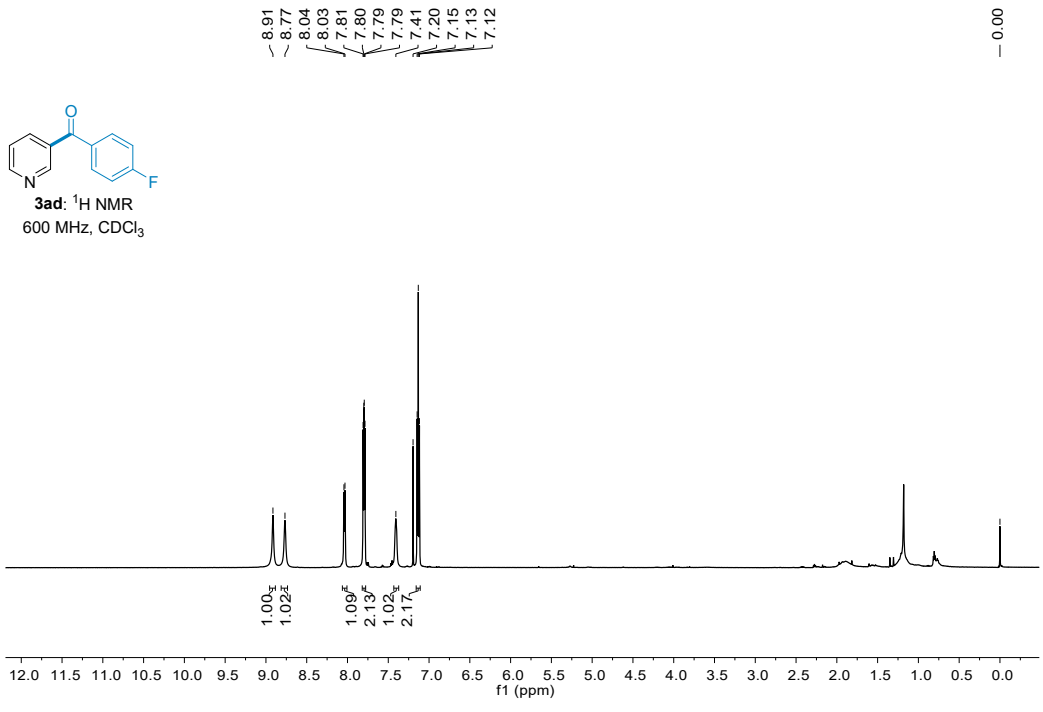
3ab: $^{13}C\{^{1}H\}$ NMR
151 MHz, $CDCl_3$



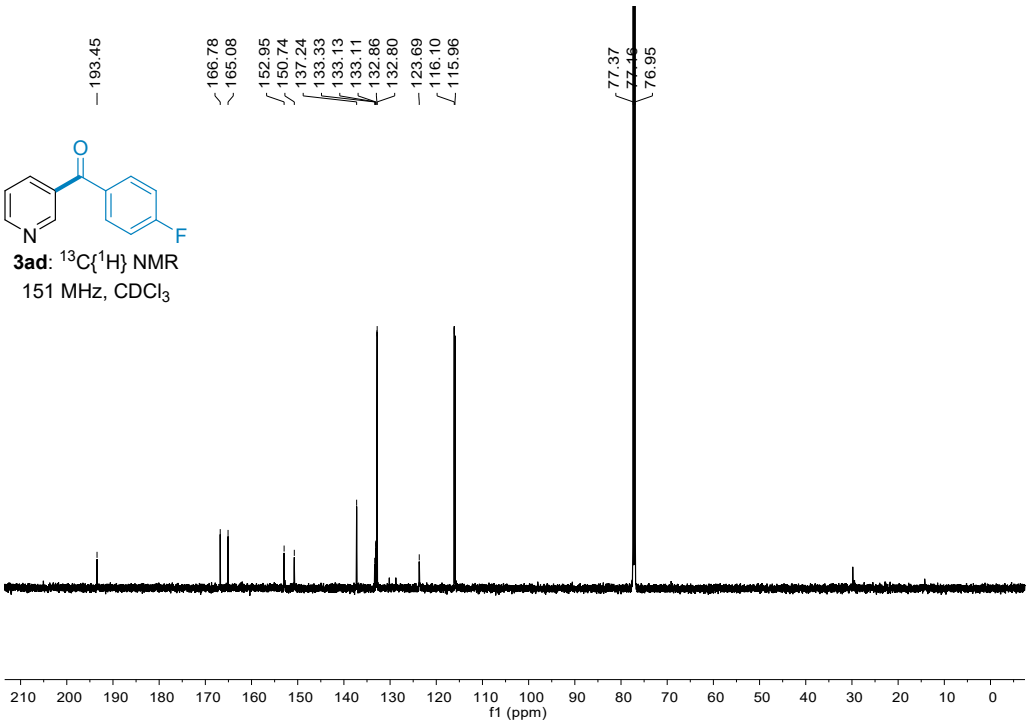
3ac: ^{1}H NMR
600 MHz, $CDCl_3$



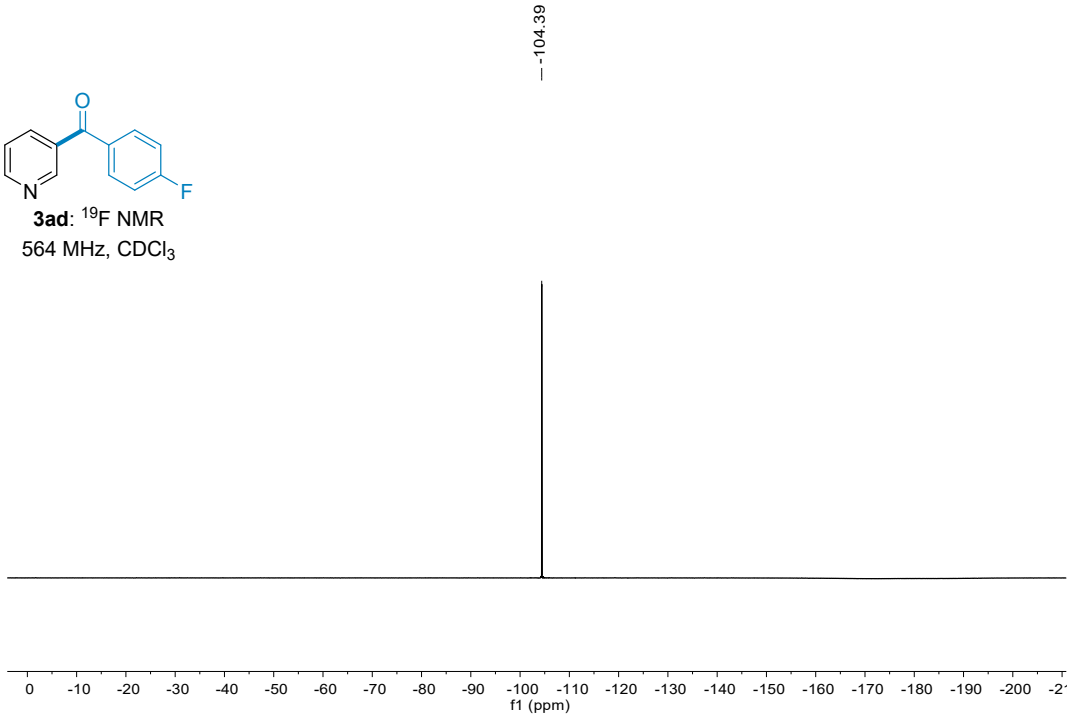
3ac: $^{13}C\{^{1}H\}$ NMR
151 MHz, $CDCl_3$



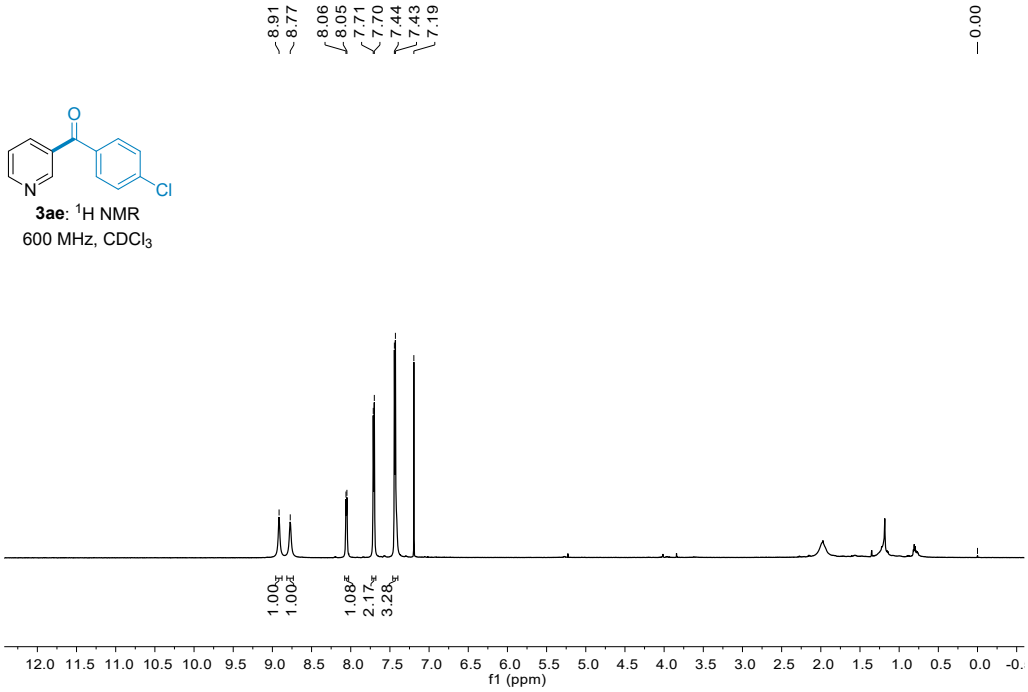
3ad: ^{1}H NMR
600 MHz, $CDCl_3$



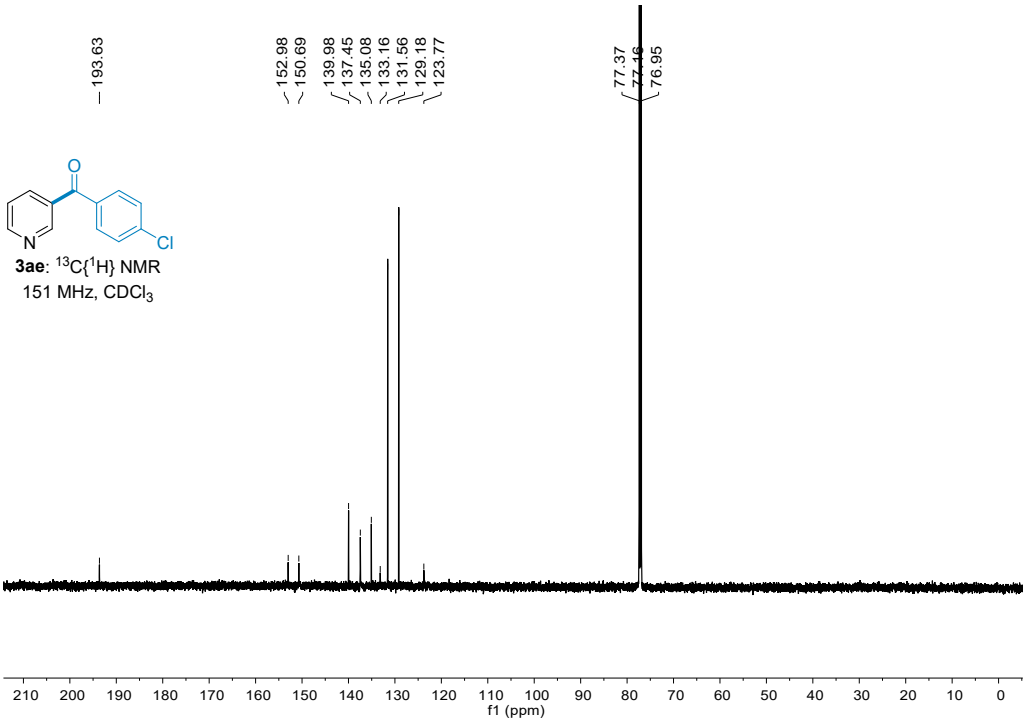
3ad: $^{13}C\{^{1}H\}$ NMR
151 MHz, $CDCl_3$



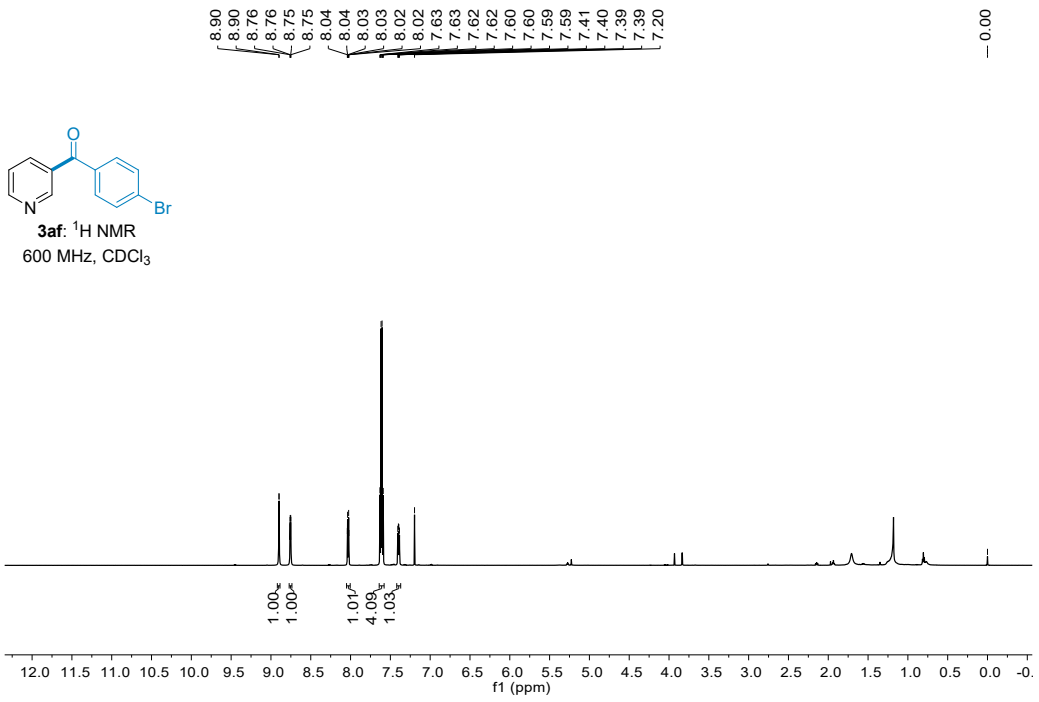
3ad: ^{19}F NMR
564 MHz, $CDCl_3$

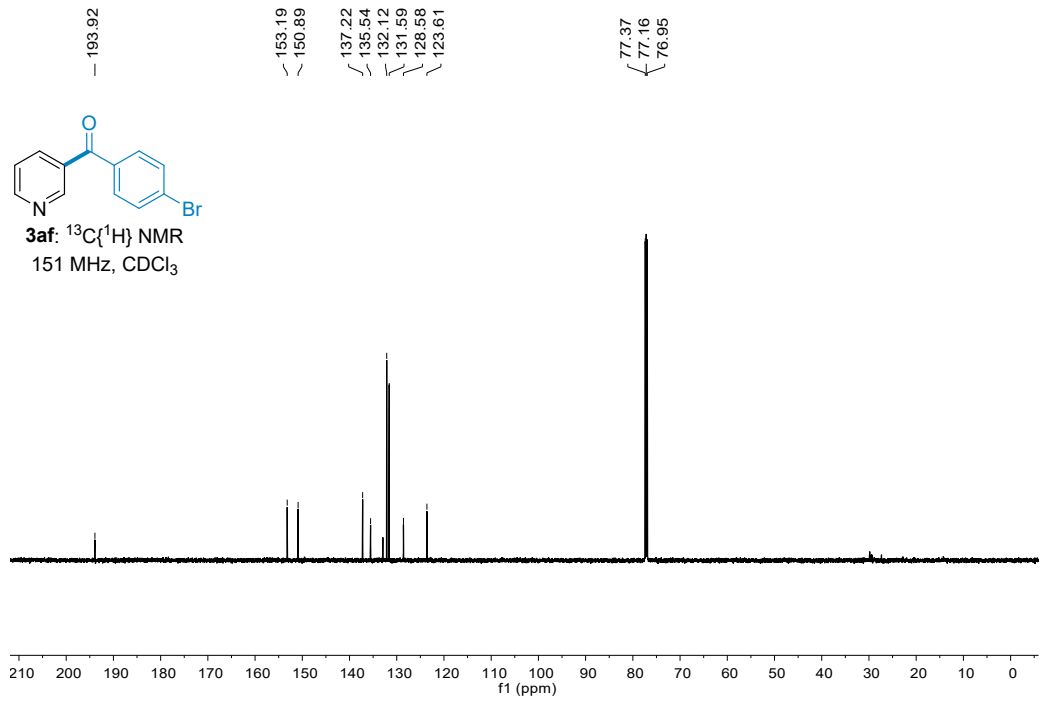


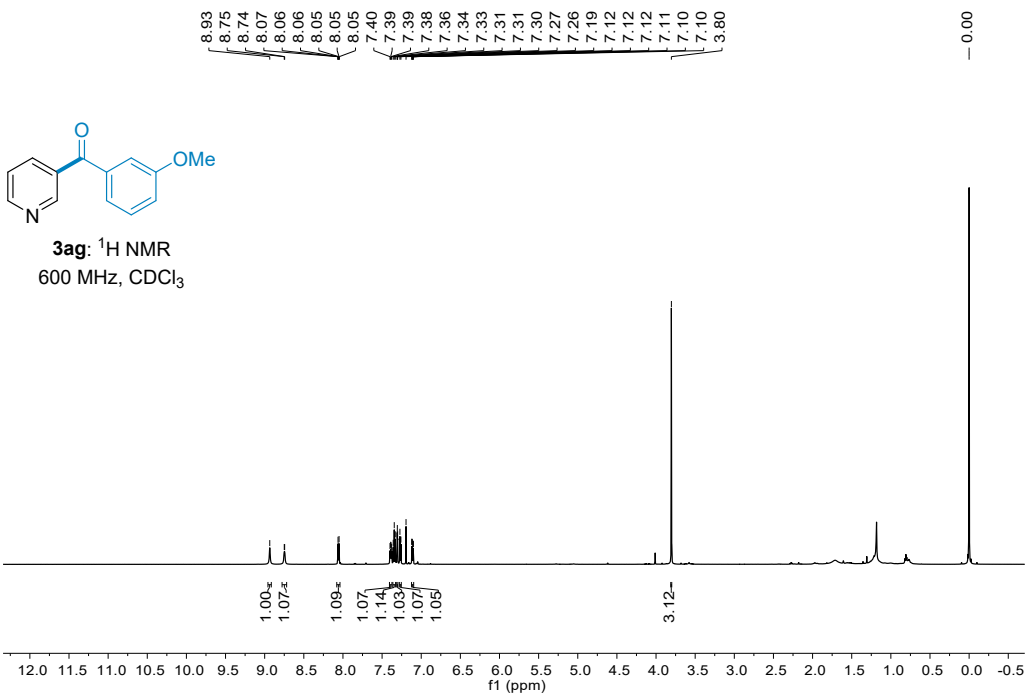
3ae: ^{1}H NMR
600 MHz, $CDCl_3$



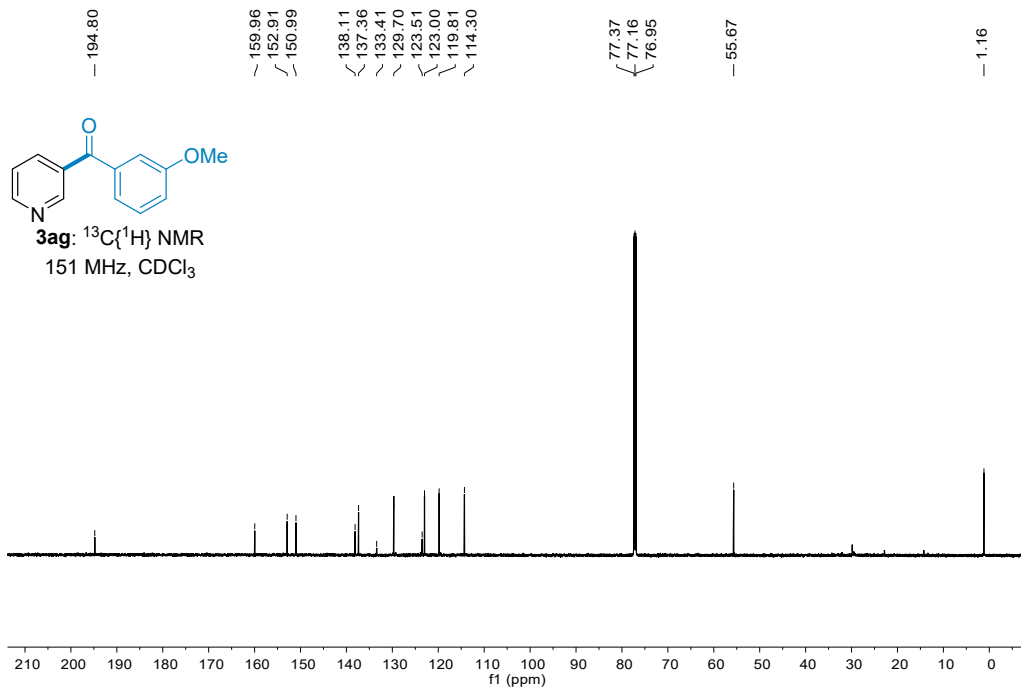
3ae: $^{13}C\{^{1}H\}$ NMR
151 MHz, $CDCl_3$


8.90
8.90
8.76
8.76
8.75
8.75
8.04
8.04
8.03
8.03
8.02
8.02
7.63
7.63
7.62
7.62
7.60
7.60
7.59
7.59
7.41
7.40
7.39
7.39
7.20
0.00
O
N
Br
3af: 1H NMR
600 MHz, CDCl3
1.00
1.00
1.01
4.09
1.03
12.0 11.5 11.0 10.5 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
f1 (ppm)

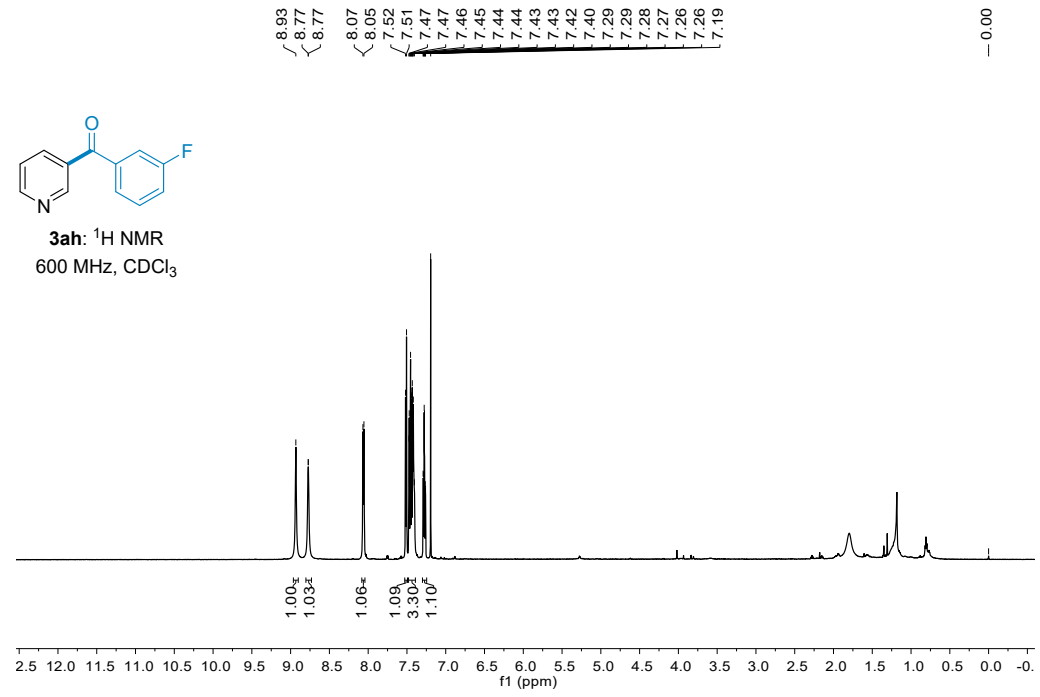

193.92
153.19
150.89
137.22
135.54
132.12
131.59
128.58
123.61
77.37
77.16
76.95
O
N
Br
3af: 13C{1H} NMR
151 MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



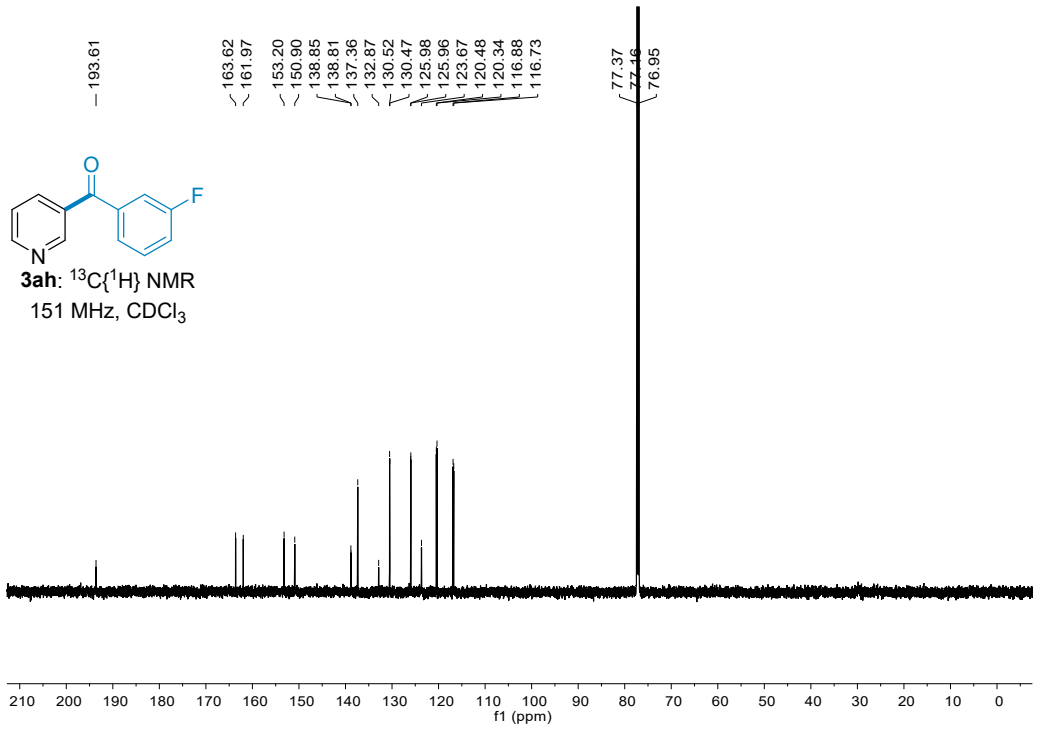
3ag: ^{1}H NMR
600 MHz, $CDCl_3$



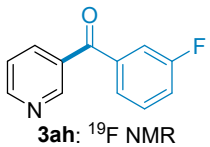
3ag: $^{13}C\{^{1}H\}$ NMR
151 MHz, $CDCl_3$



3ah: ^{1}H NMR
600 MHz, $CDCl_3$

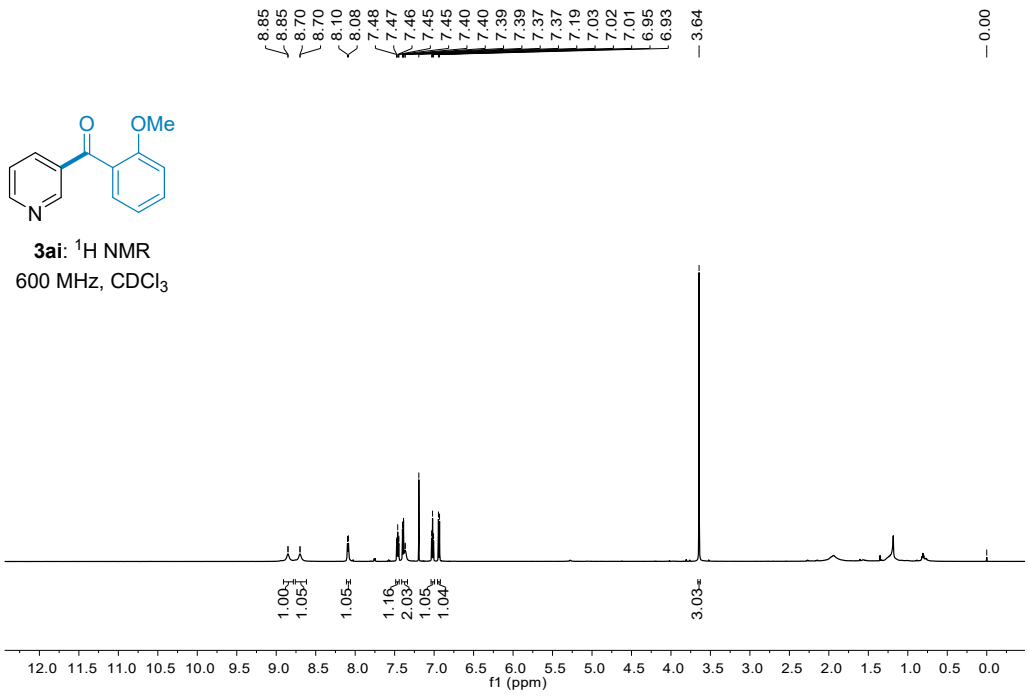


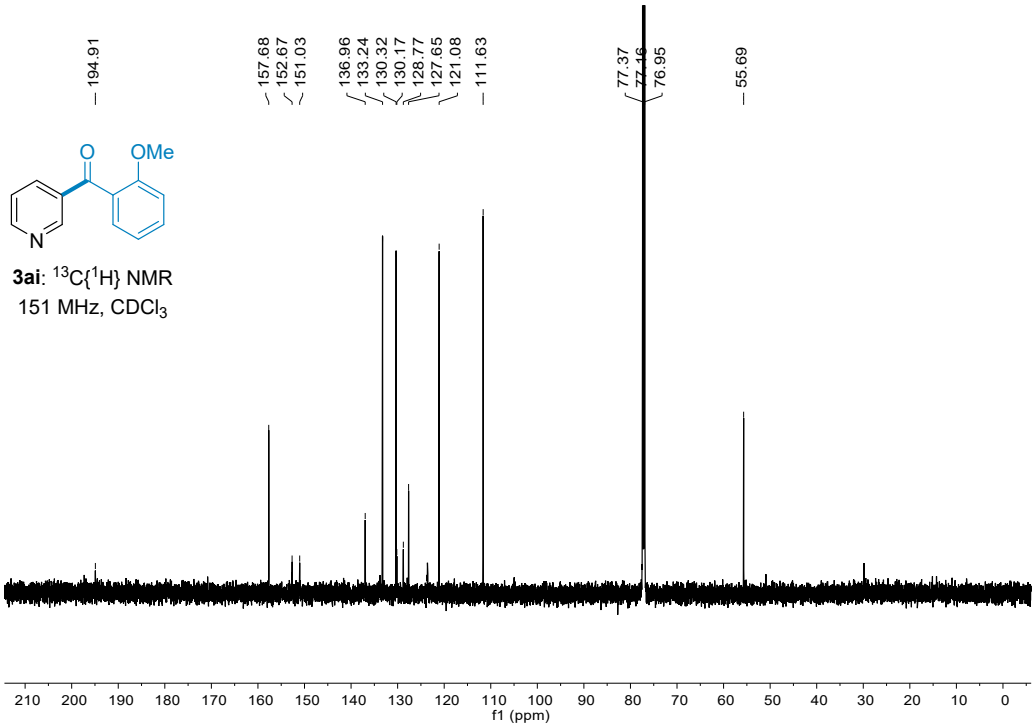
3ah: $^{13}C\{^{1}H\}$ NMR
151 MHz, $CDCl_3$



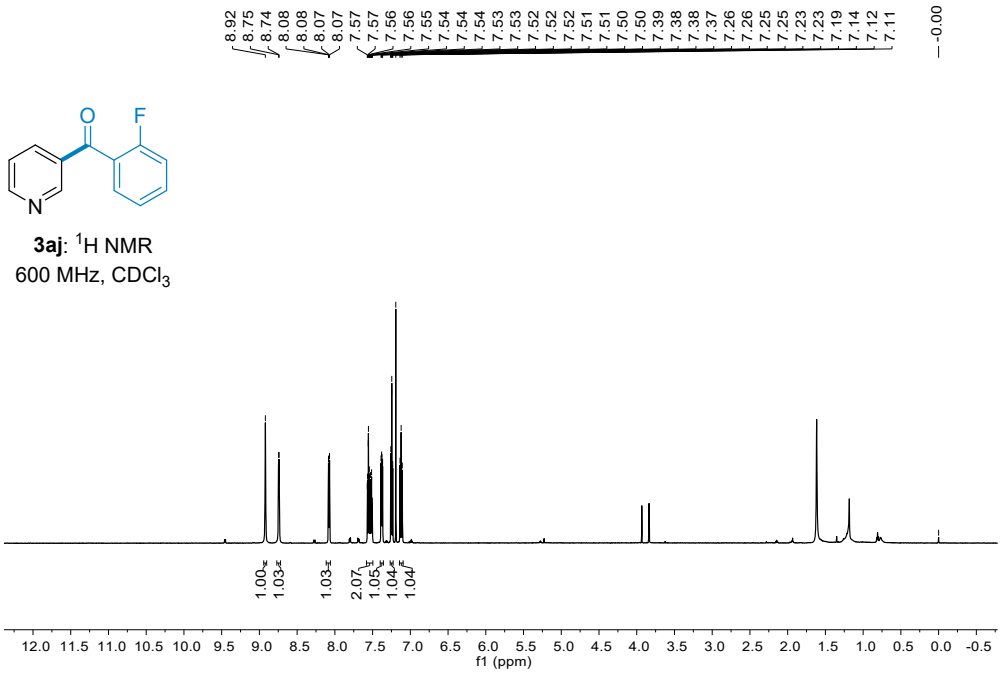
3ah: ^{19}F NMR
564 MHz, $CDCl_3$

3ai: ^{1}H NMR
600 MHz, $CDCl_3$

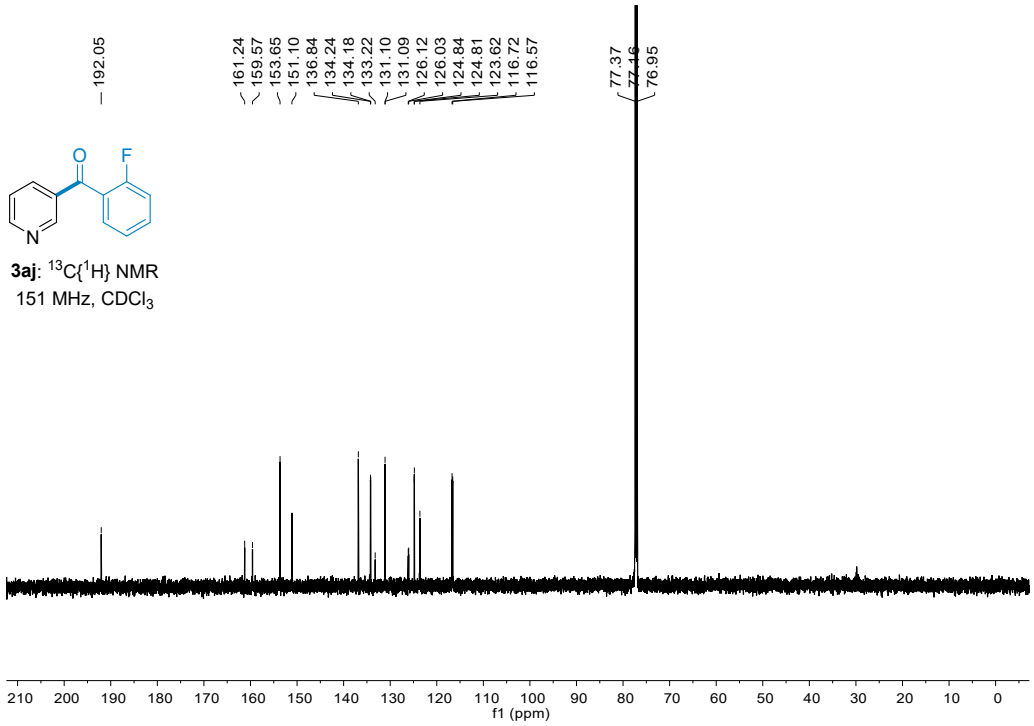




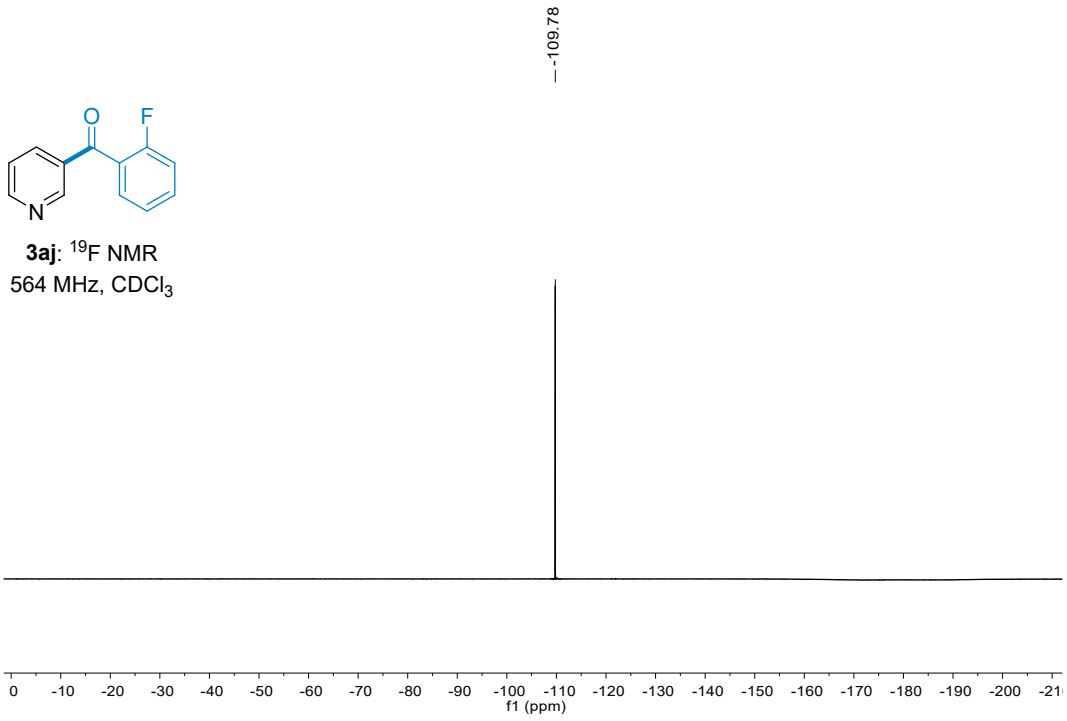
3ai: $^{13}C\{^{1}H\}$ NMR
151 MHz, $CDCl_3$



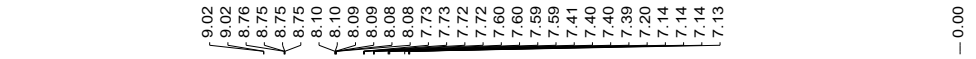
3aj: ^{1}H NMR
600 MHz, $CDCl_3$

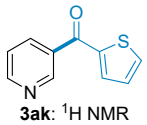


3aj: $^{13}C\{^{1}H\}$ NMR
151 MHz, $CDCl_3$

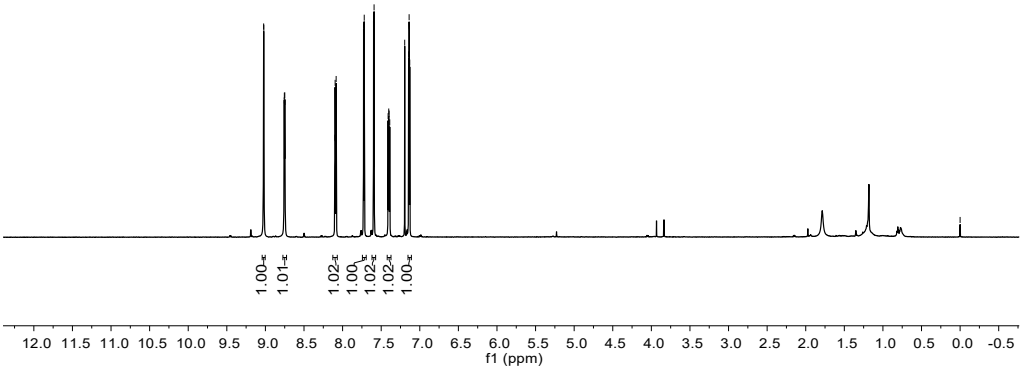


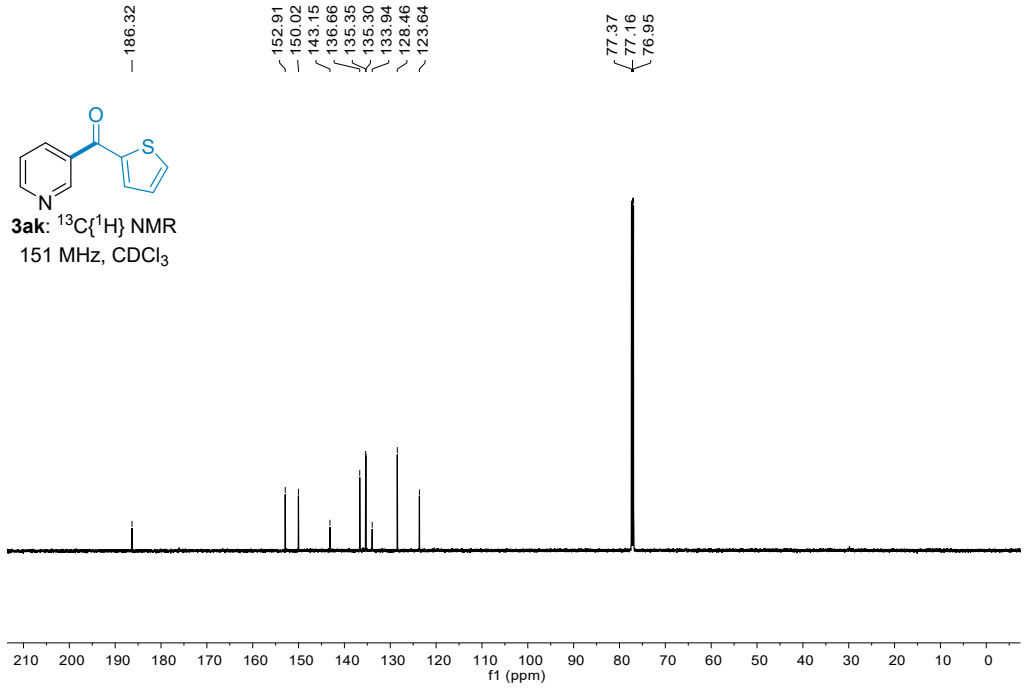
3aj: ^{19}F NMR
564 MHz, $CDCl_3$



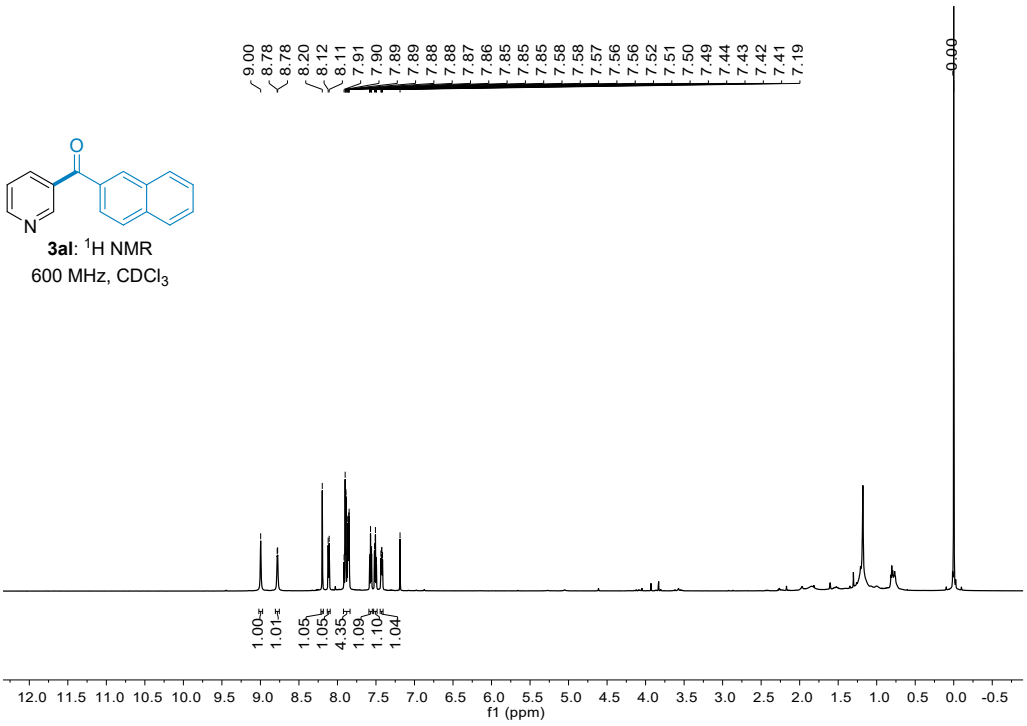


3ak: ^{1}H NMR
600 MHz, $CDCl_3$

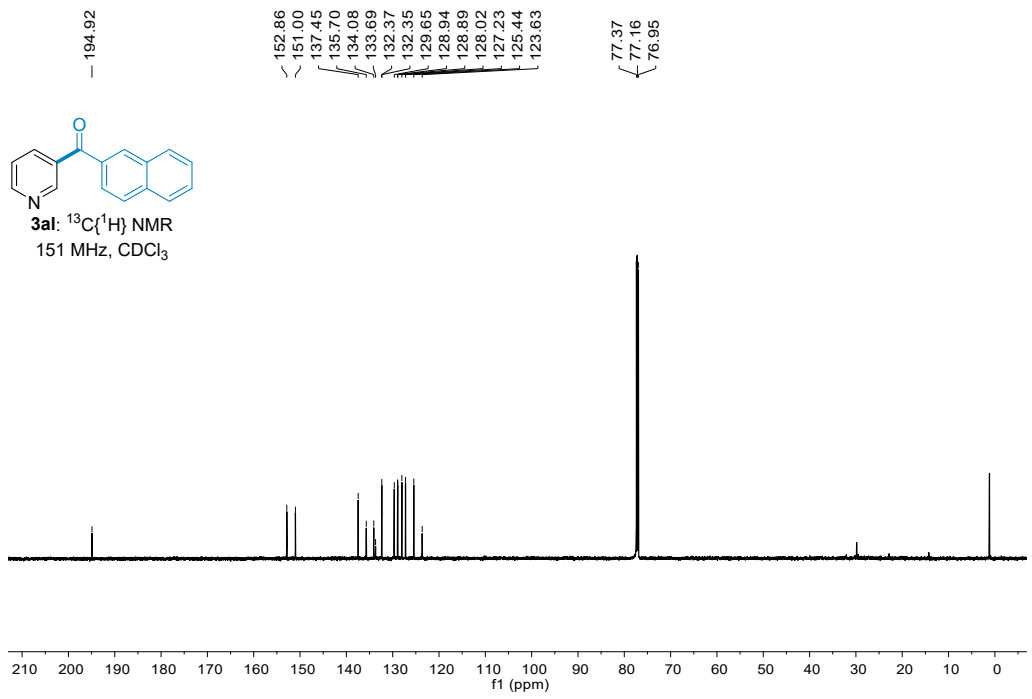




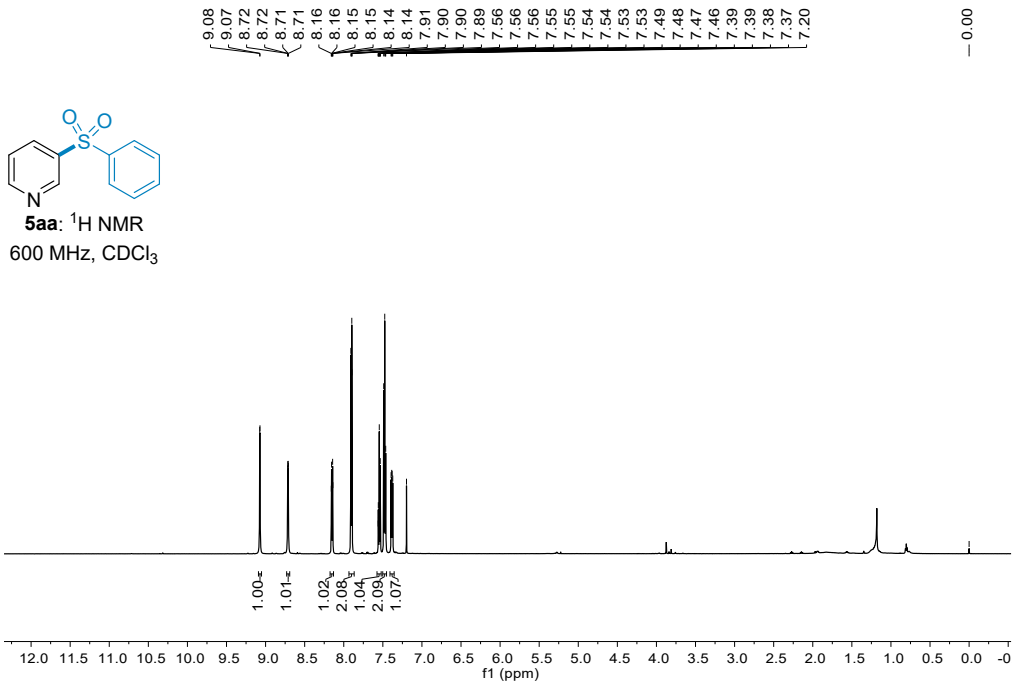
3ak: $^{13}C\{^{1}H\}$ NMR
151 MHz, $CDCl_3$



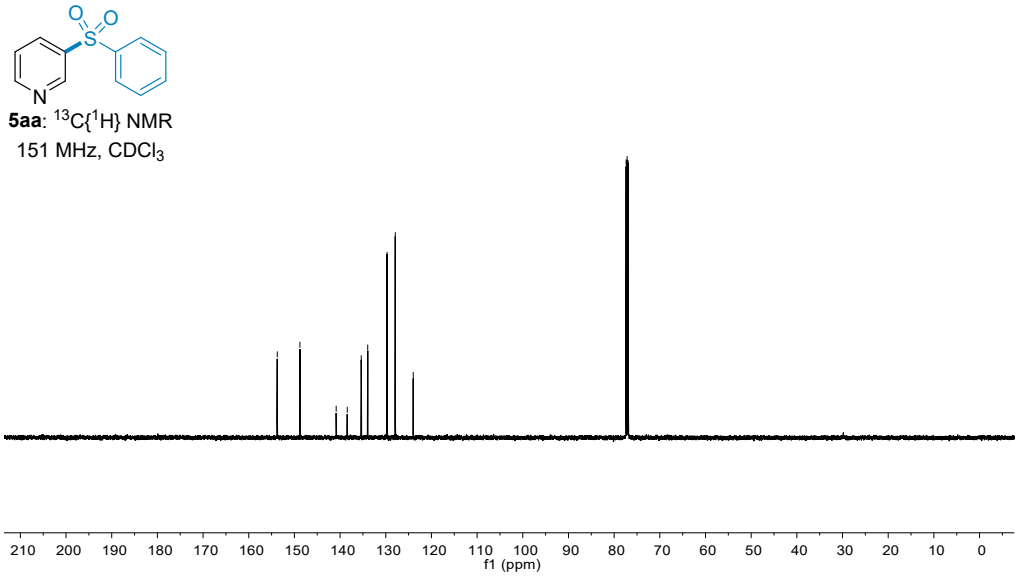
3al: ^{1}H NMR
600 MHz, $CDCl_3$



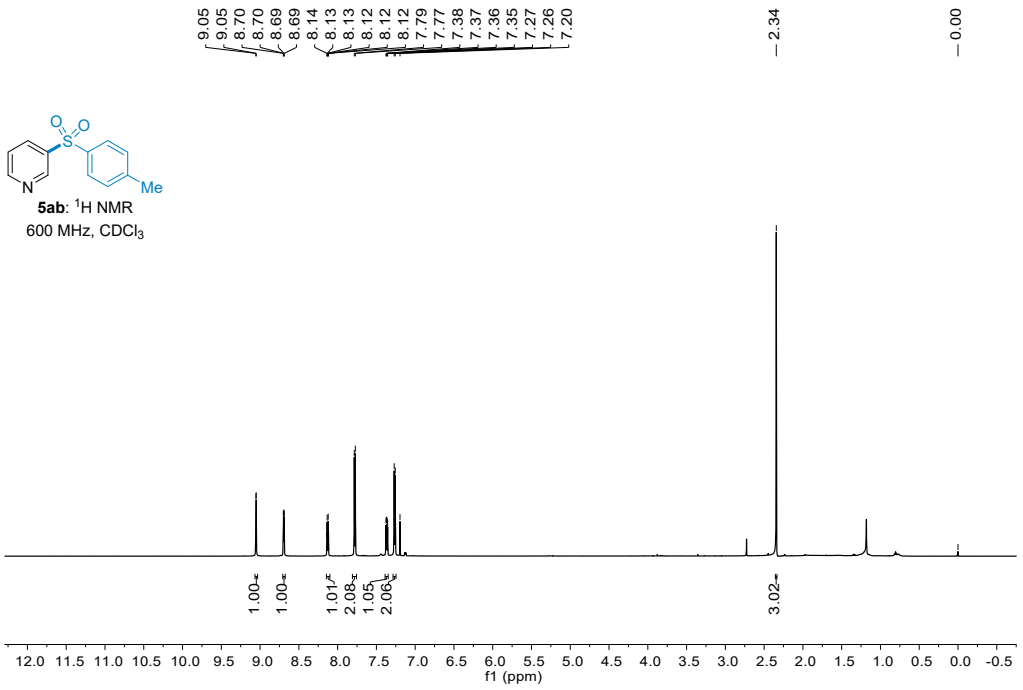
3al: $^{13}C\{^{1}H\}$ NMR
151 MHz, $CDCl_3$



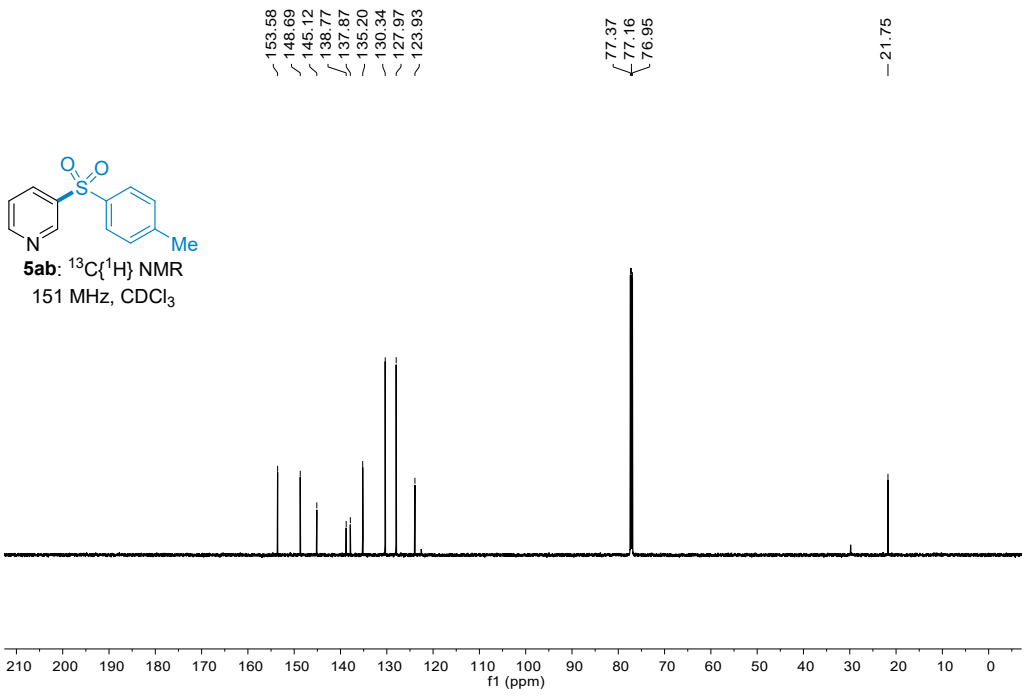
5aa: ^{1}H NMR
600 MHz, $CDCl_3$



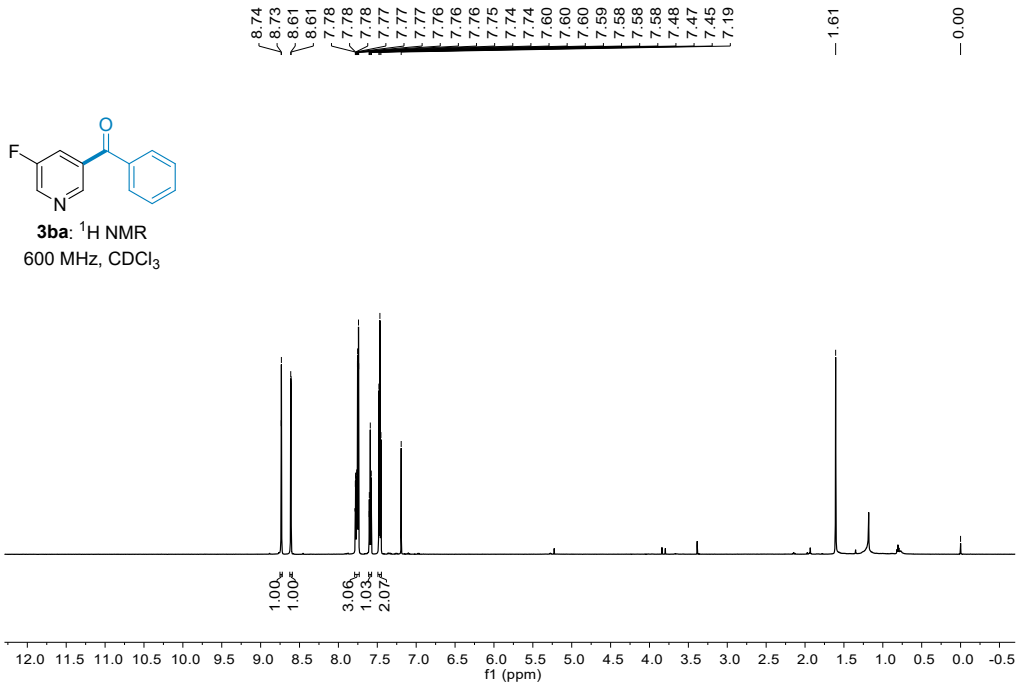
5aa: $^{13}C\{^{1}H\}$ NMR
151 MHz, $CDCl_3$



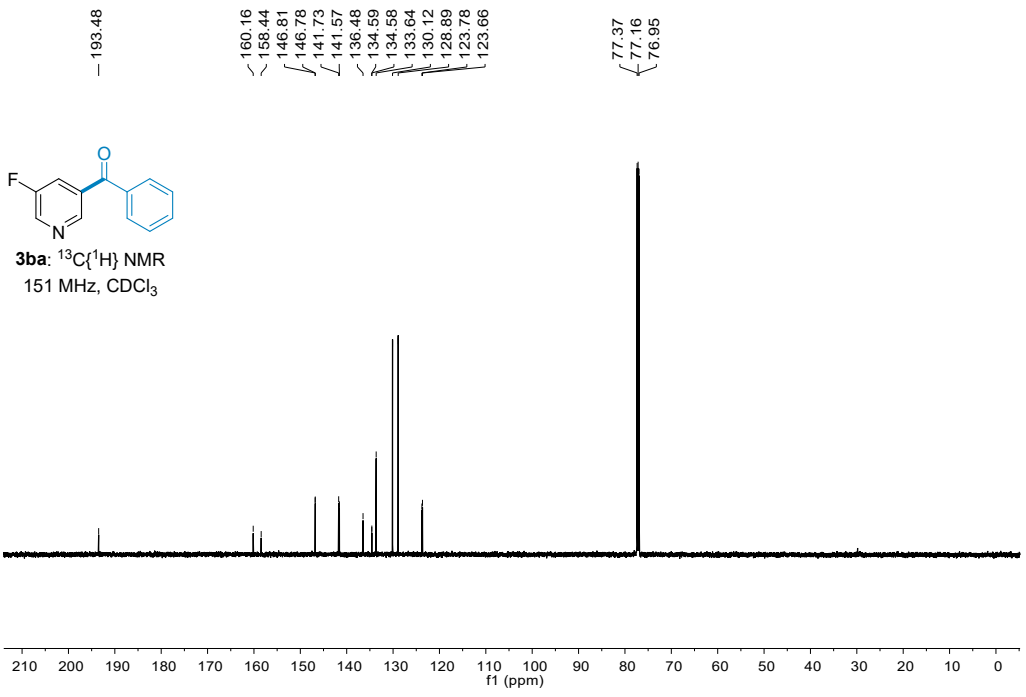
5ab: ^{1}H NMR
600 MHz, $CDCl_3$



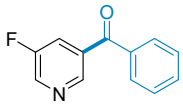
5ab: $^{13}C\{^{1}H\}$ NMR
151 MHz, $CDCl_3$



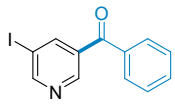
3ba: ^{1}H NMR
600 MHz, $CDCl_3$



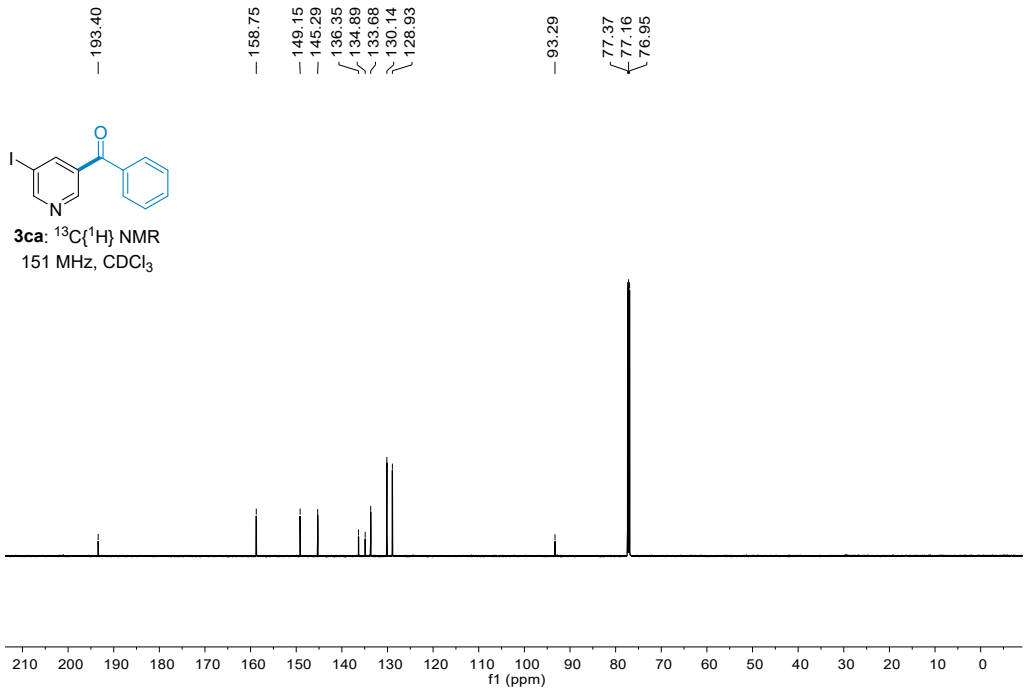
3ba: $^{13}C\{^{1}H\}$ NMR
151 MHz, $CDCl_3$



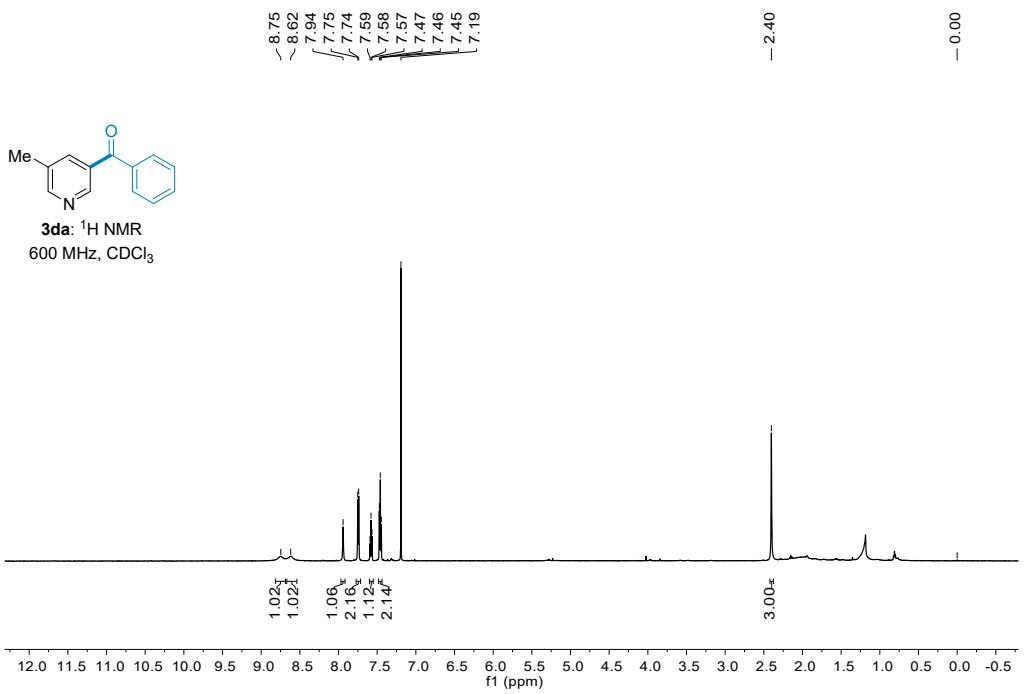
3ba: ^{19}F NMR
564 MHz, $CDCl_3$



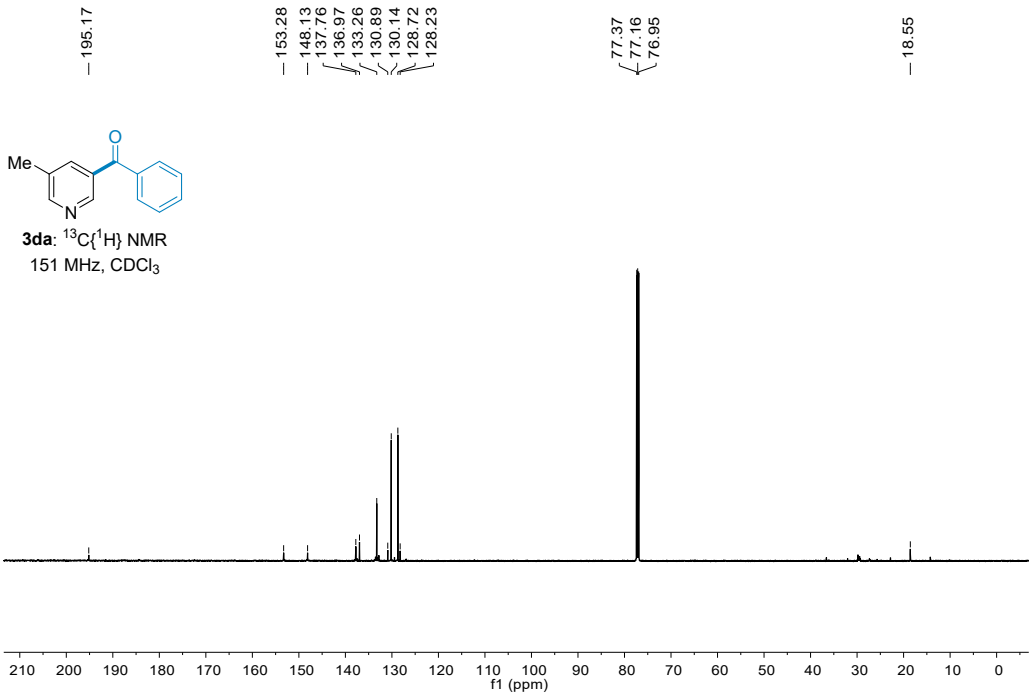
3ca: ^{1}H NMR
600 MHz, $CDCl_3$



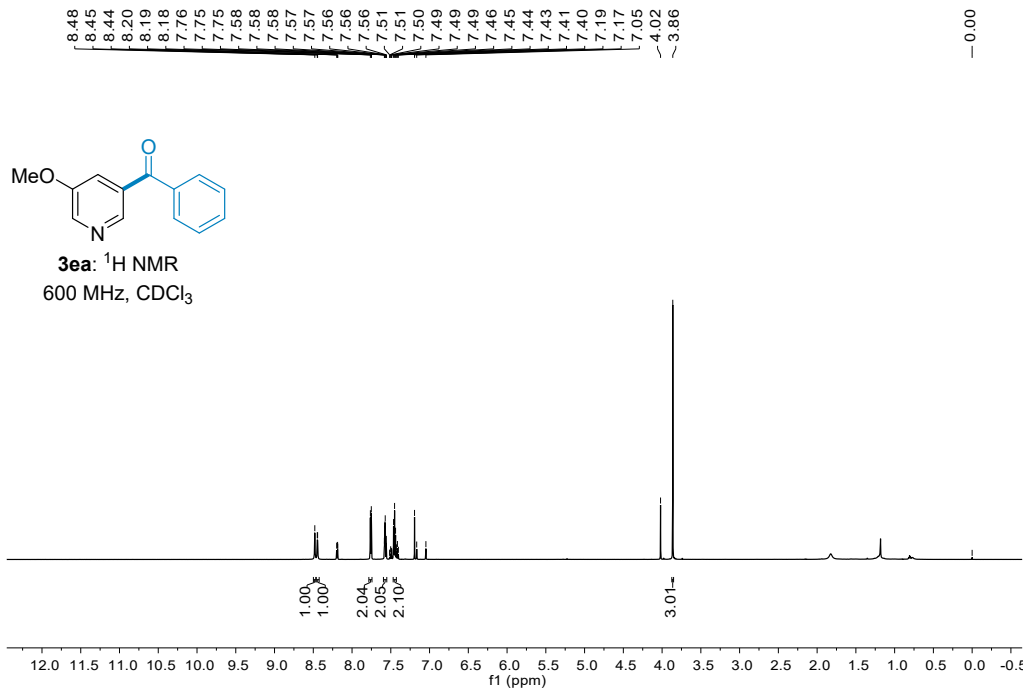
3ca: $^{13}C\{^{1}H\}$ NMR
151 MHz, $CDCl_3$



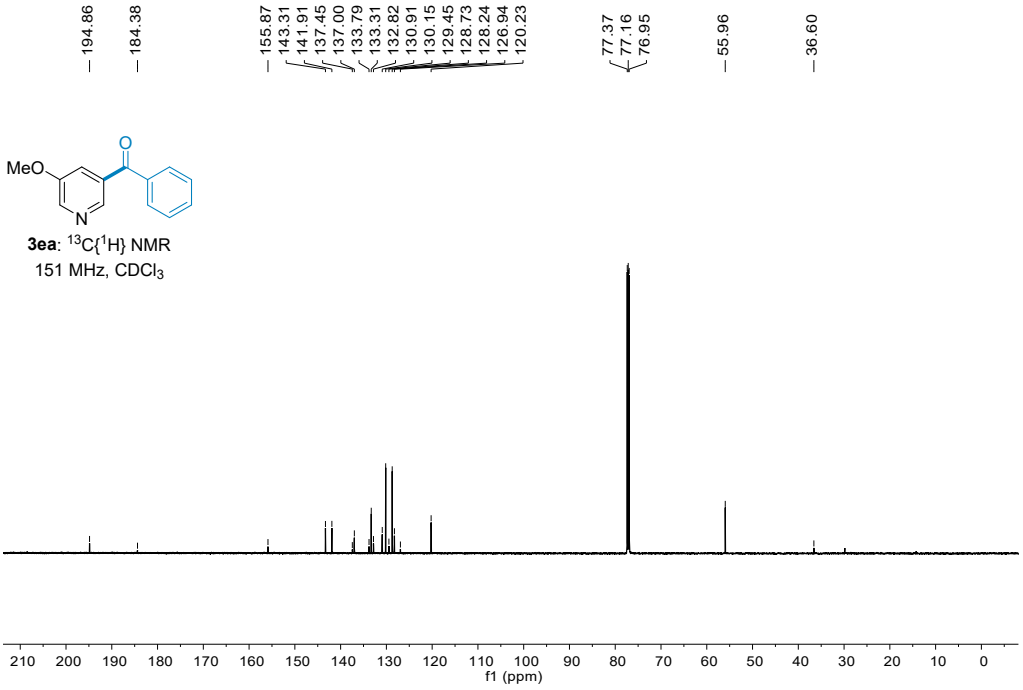
3da: ^{1}H NMR
600 MHz, $CDCl_3$



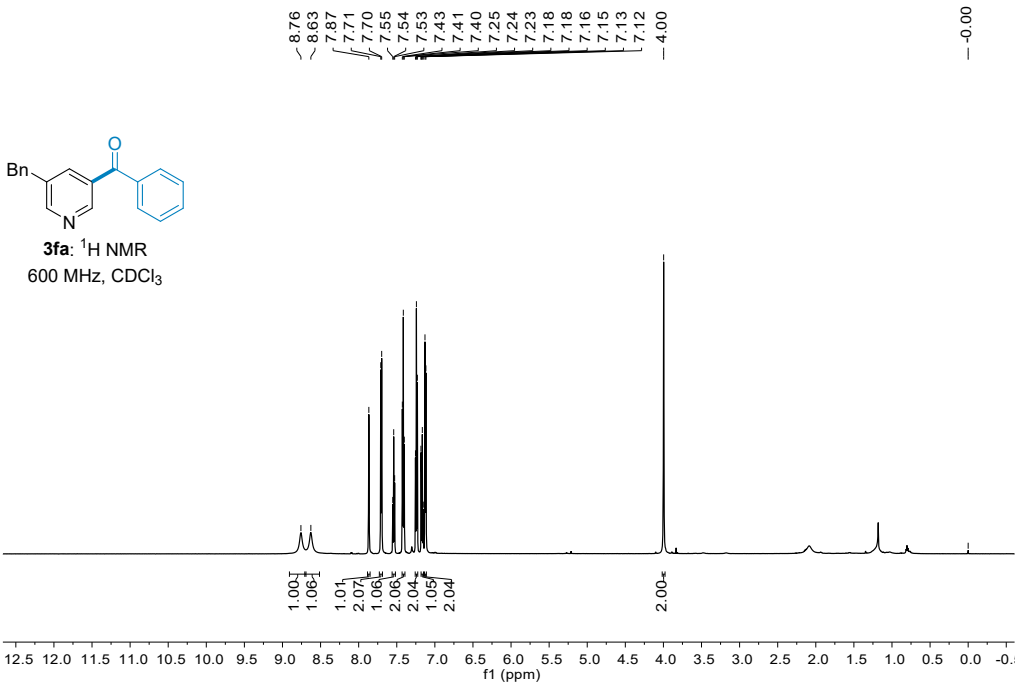
3da: $^{13}C\{^{1}H\}$ NMR
151 MHz, $CDCl_3$



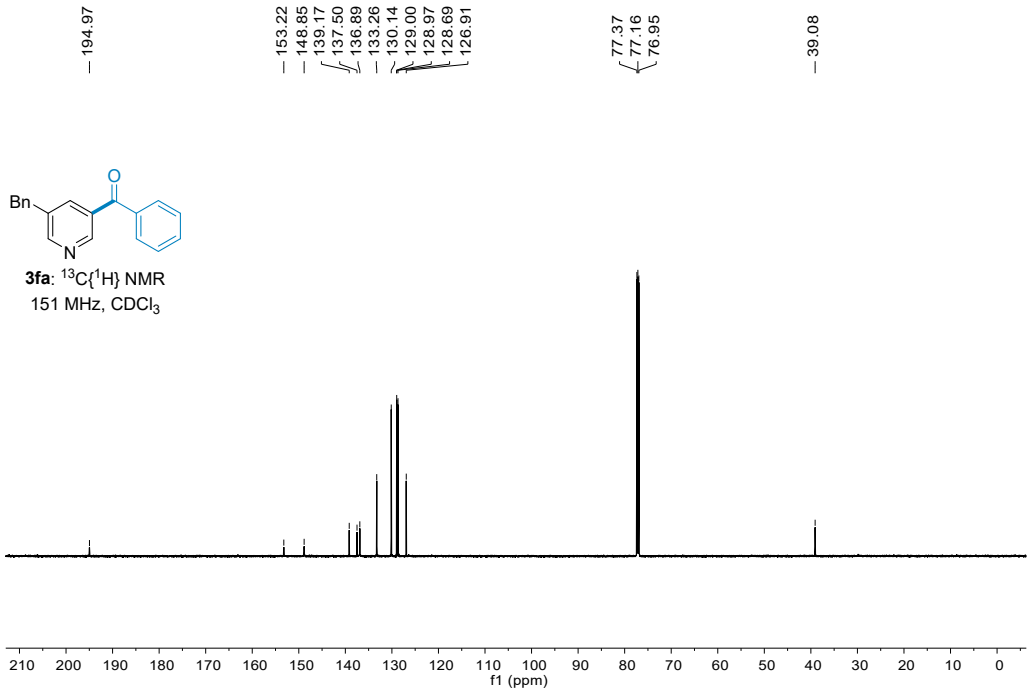
3ea: ^{1}H NMR
600 MHz, $CDCl_3$



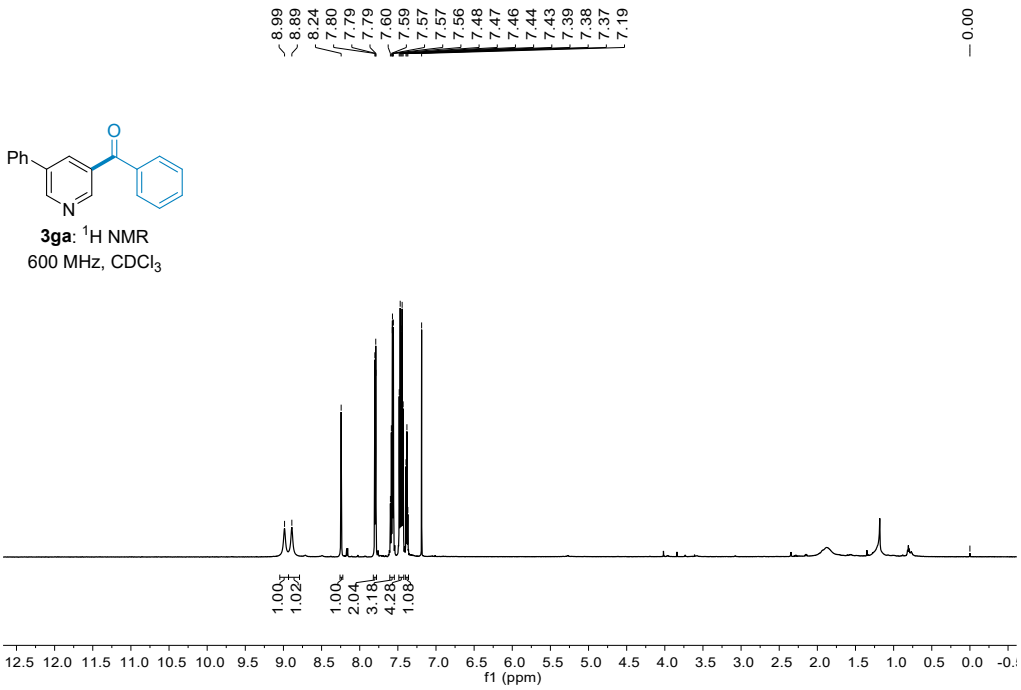
3ea: $^{13}C\{^{1}H\}$ NMR
151 MHz, $CDCl_3$



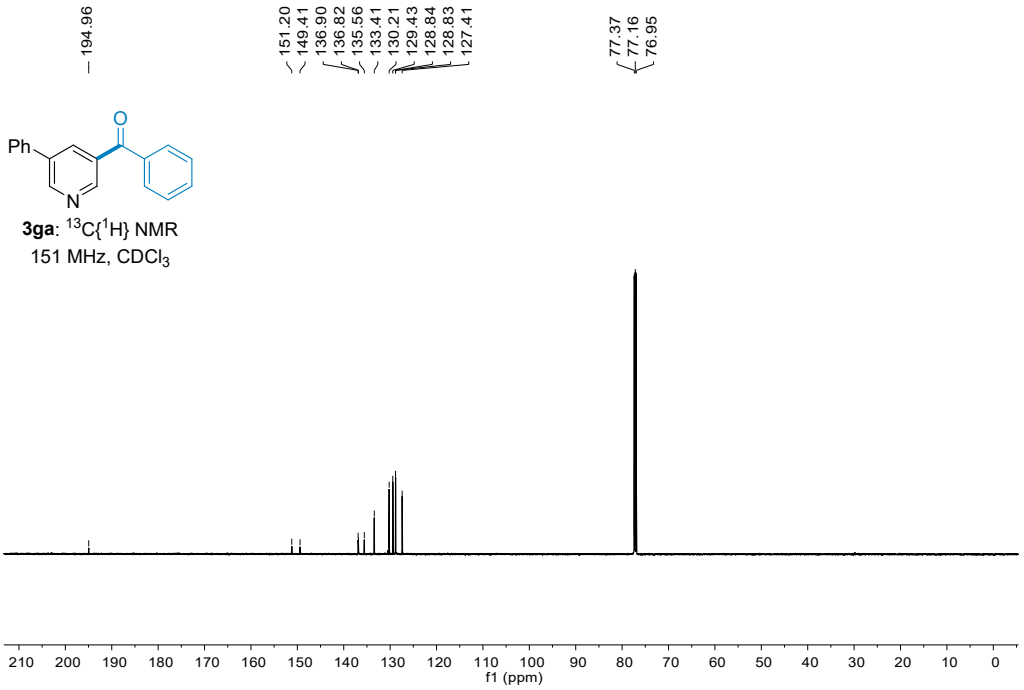
3fa: ^{1}H NMR
600 MHz, $CDCl_3$



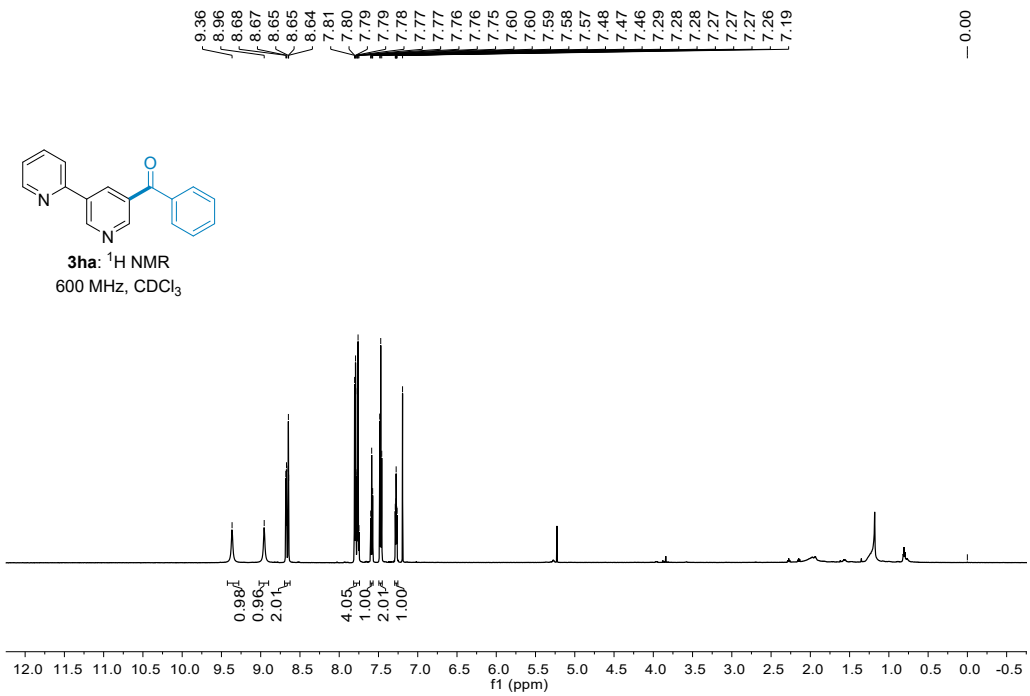
3fa: $^{13}C\{^{1}H\}$ NMR
151 MHz, $CDCl_3$



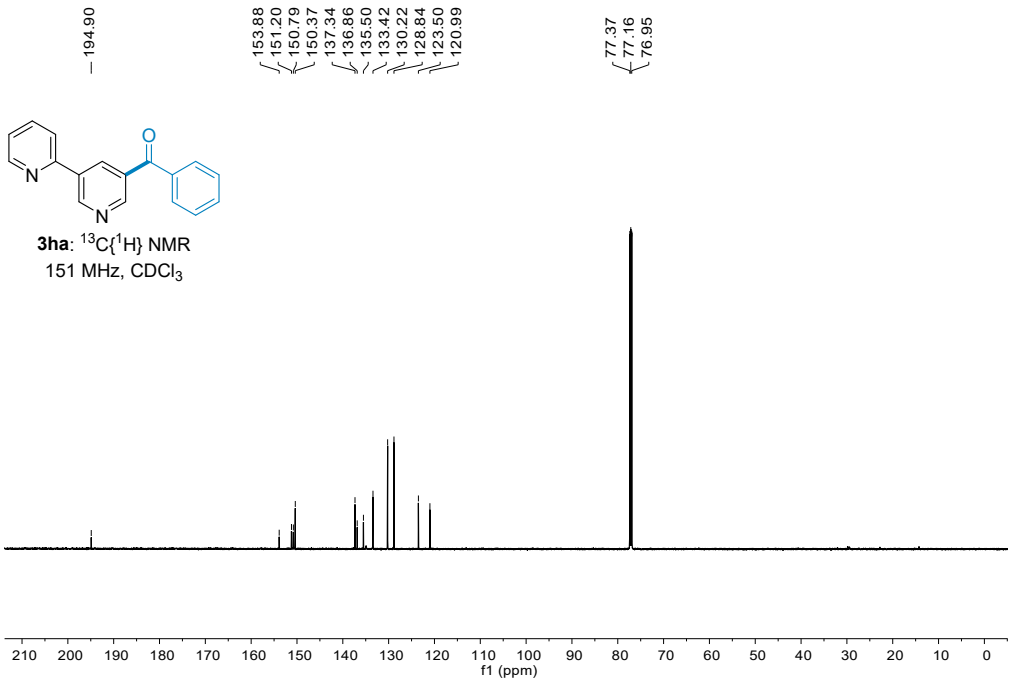
3ga: ^{1}H NMR
600 MHz, $CDCl_3$



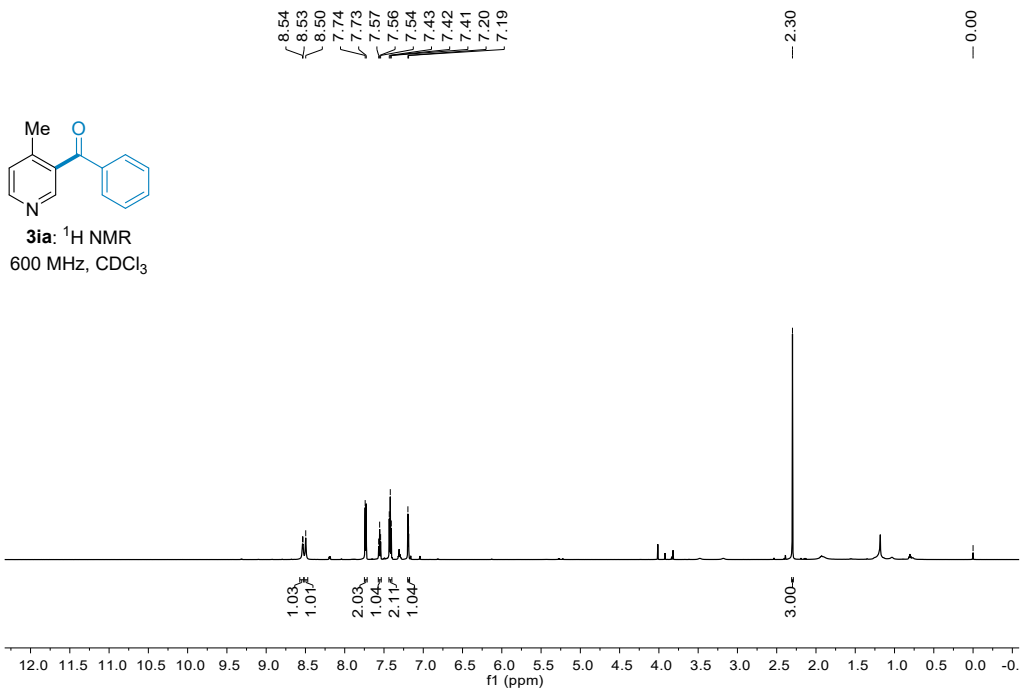
3ga: $^{13}C\{^{1}H\}$ NMR
151 MHz, $CDCl_3$



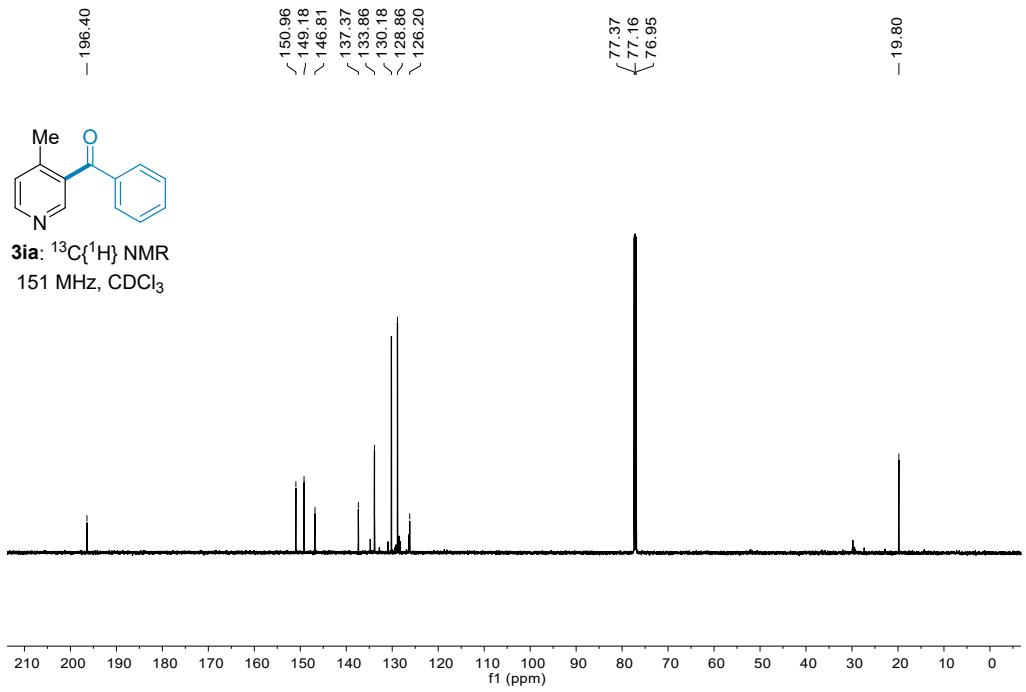
3ha: ^{1}H NMR
600 MHz, $CDCl_3$



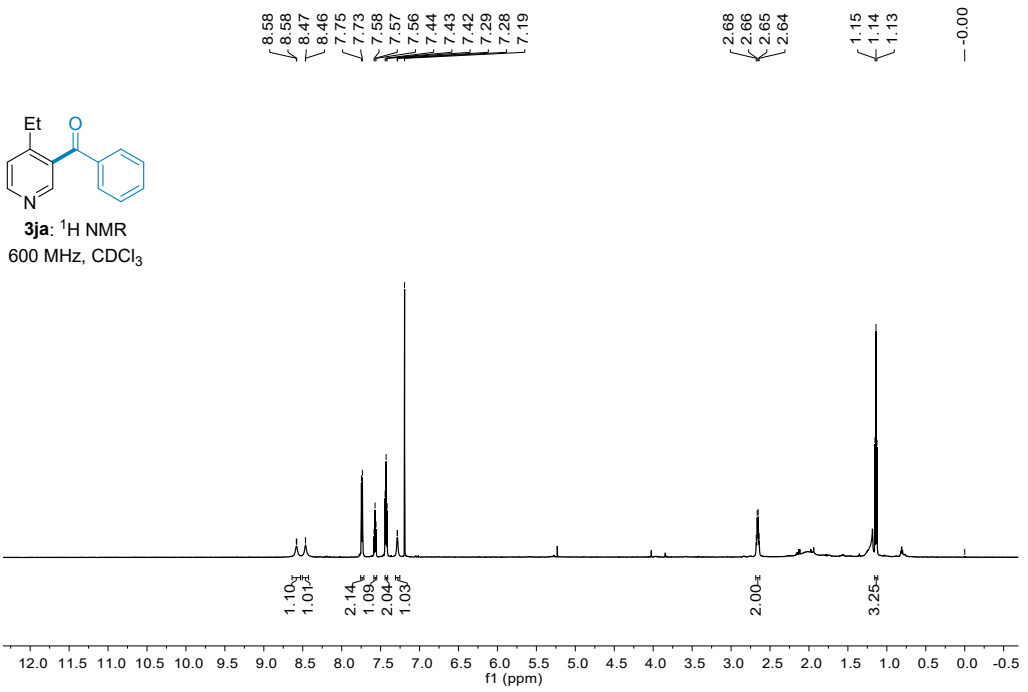
3ha: $^{13}C\{^{1}H\}$ NMR
151 MHz, $CDCl_3$



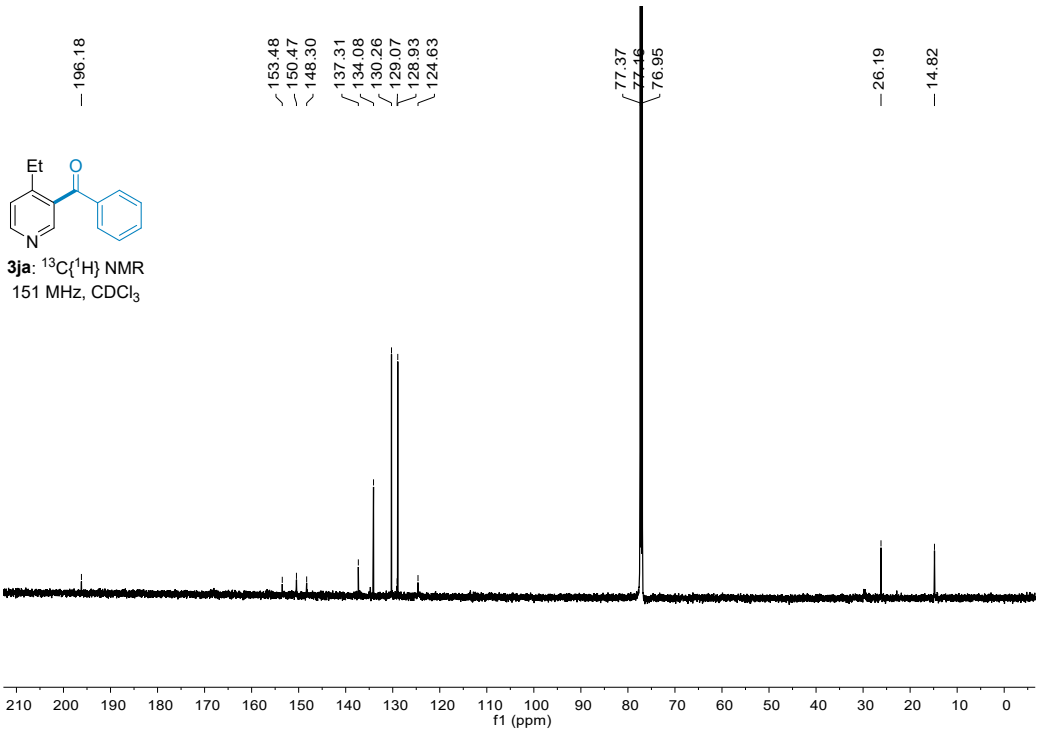
3ia: ^{1}H NMR
600 MHz, $CDCl_3$



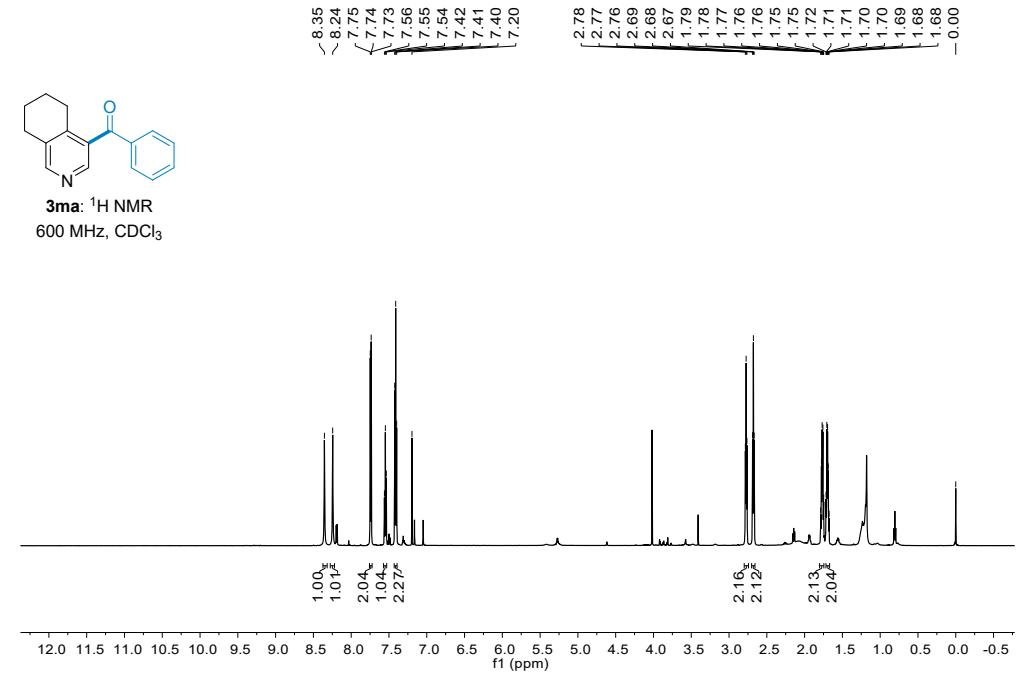
3ia: $^{13}C\{^{1}H\}$ NMR
151 MHz, $CDCl_3$



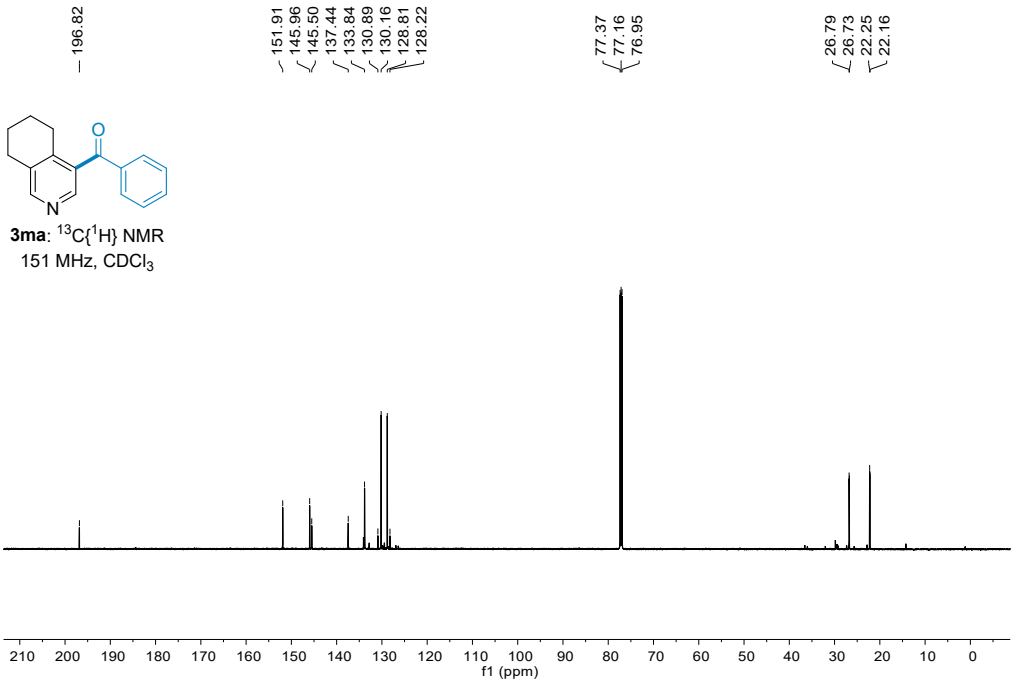
3ja: ^{1}H NMR
600 MHz, $CDCl_3$



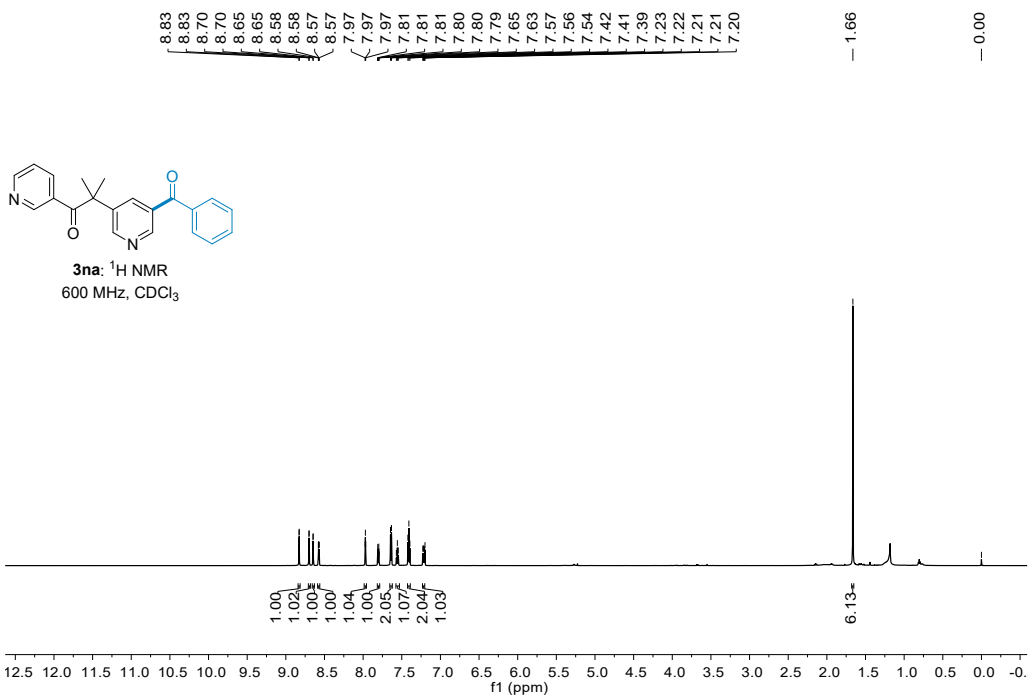
3ja: $^{13}C\{^{1}H\}$ NMR
151 MHz, $CDCl_3$



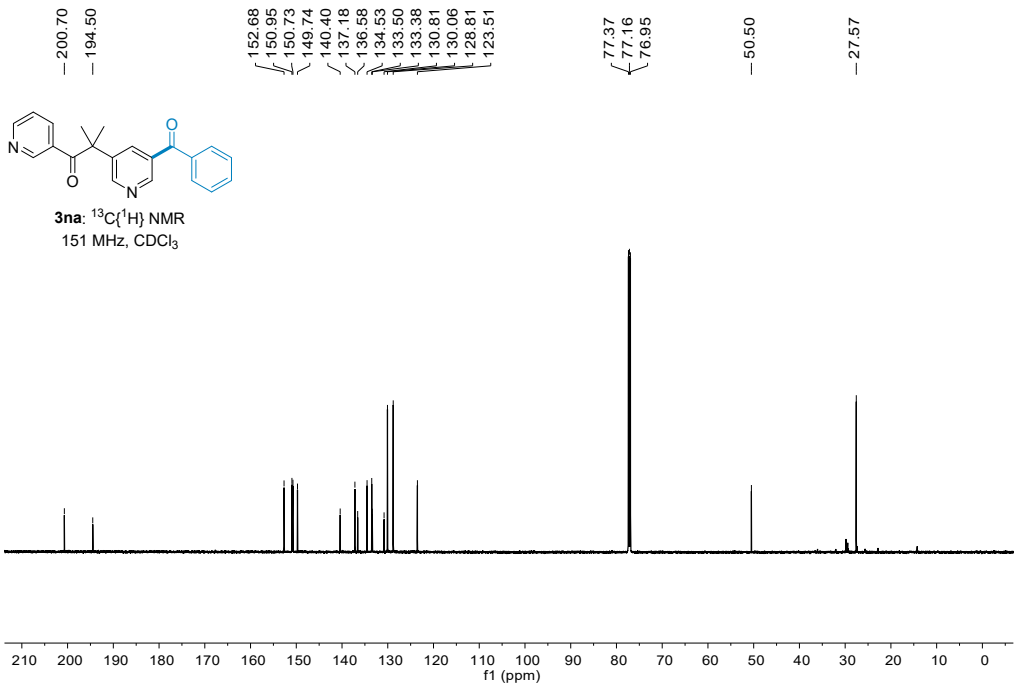
3ma: ^{1}H NMR
600 MHz, $CDCl_3$



3ma: $^{13}C\{^{1}H\}$ NMR
151 MHz, $CDCl_3$



3na: ^{1}H NMR
600 MHz, $CDCl_3$



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