Electronic Supplementary Material (ESI) for ChemComm.

Nickel-Catalyzed Direct C−H Trifluoroethylation of Heteroarenes with Trifluoroethyl Iodide

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Supporting Information

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1. General Information

All the materials and solvents were purchased from commercial suppliers, such as Adamas-beta®, Energy Chemical, TCI , J&K and used without additional purification excepted for ^{t}BuCN which was redistilled by CaH_2 before use. NMR spectra were recorded on a Bruke Avance operating for ^{1}H NMR at 400 MHz, ^{13}C NMR at 100 MHz, ^{19}F NMR at 376 MHz, using TMS as internal standard. The peaks were internally referenced to TMS (0.00 ppm) or residual undeuterated solvent signal of $CDCl_3$ (77.16 ppm for ^{13}C NMR). The following abbreviations (or combinations thereof) were used to explain multiplicities: s = singlet, d = doublet, t = triplet, m = multiplet, b = broad. Mass spectroscopy data of the products were collected on an HRMS-TOF instrument or a low-resolution MS instrument using EI ionization.

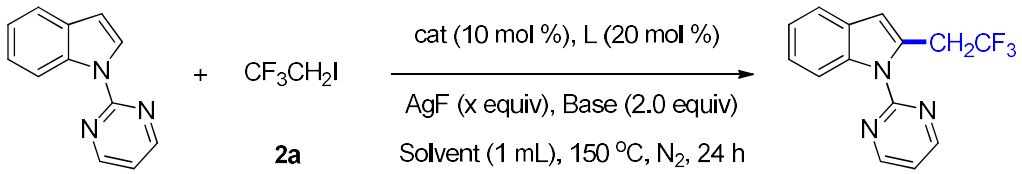
2. Experimental Section

2.1 Preparation of Substrates

All the raw materials were known compounds. Compounds **1a – 1q** were prepared according to the literature procedures [1-5] while compounds **1r – 1x** were reference to the following procedures. [6-7]

2.2 Optimization of Reaction Conditions

Table S1: Optimization of Reaction Conditions[a]

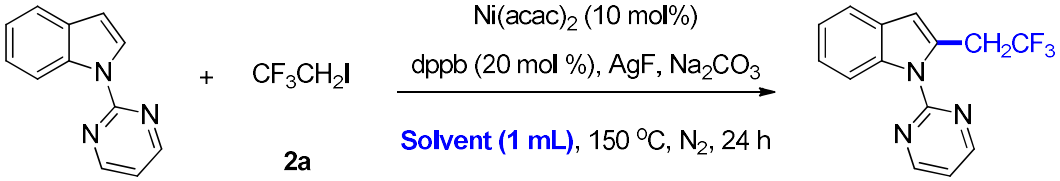


1a **3aa**

Entry	cat	Ligand	AgF (x equiv)	Base	Solvent	Yield (%)[b]
1	$Ni(acac)_2$	dppb	1.0	Na_2CO_3	CH_3CN	25
2	$Ni(acac)_2$	dppb	1.0	Li_2CO_3	CH_3CN	20
3	$Ni(acac)_2$	dppb	1.0	$NaHCO_3$	CH_3CN	23
4	$Ni(acac)_2$	dppb	1.0	$LiOBu^t$	CH_3CN	Trace
5	$Ni(acac)_2$	dppb	1.0	Na_2CO_3	^{t}BuCN	47
6[c]	$Ni(Tfacac)_2{\cdot}2H_2O$	dppb	1.0	Na_2CO_3	^{t}BuCN	60
7	$Ni(Tfacac)_2{\cdot}2H_2O$	dppb	0.7	Na_2CO_3	^{t}BuCN	65
8	$Ni(Tfacac)_2{\cdot}2H_2O$	dppb	0.5	Na_2CO_3	^{t}BuCN	50
9	$Ni(Tfacac)_2{\cdot}2H_2O$	dppe	0.7	Na_2CO_3	^{t}BuCN	36
10	$Ni(Tfacac)_2{\cdot}2H_2O$	dppp	0.7	Na_2CO_3	^{t}BuCN	61
11	$Ni(Tfacac)_2{\cdot}2H_2O$	PhDave-Phos	0.7	Na_2CO_3	^{t}BuCN	59
12[d]	$Ni(Tfacac)_2{\cdot}2H_2O$	dppb	0.7	Na_2CO_3	^{t}BuCN	64
13[e]	**$Ni(Tfacac)_2{\cdot}2H_2O$**	**dppb**	**0.7**	**Na_2CO_3**	**^{t}BuCN**	**74[f]**
14	CuI	2,2'-bipy	0.7	Na_2CO_3	^{t}BuCN	4%
15	$Co(OAc)_2{\cdot}4H_2O$	dppb	0.7	Na_2CO_3	^{t}BuCN	6%
16	---	dppb	0.7	Na_2CO_3	^{t}BuCN	trace

[a]Reaction conditions: **1a** (0.2 mmol), **2a** (1.0 mmol), [Ni] (10 mol%), L (20 mol%), base (0.4 mmol) in 1 mL solvent at 150 °C in N_2 for 24 h. [b]^{1}H NMR yield using CH_2Br_2 as the internal standard. [c]Tf = 1,1,1- Trifluoroacetylacetonate. [d]36 h. [e]reaction was conducted at 160 °C. [f]isolated yield.

Table S2 Screen of Solvent[a]

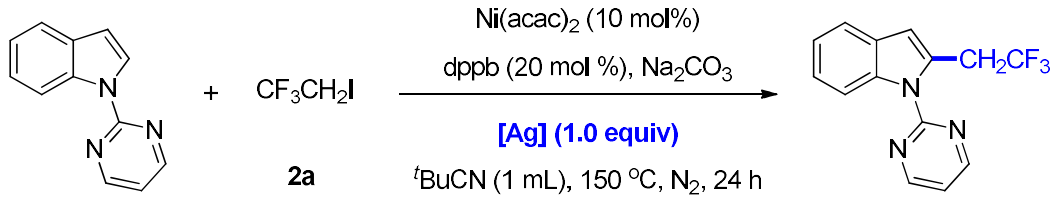


1a **3aa**

Entry	Solvent	Yield[b]
1	^{t}BuCN	47
2	MeCN	25
3	toluene	20
4	1,4-dioxane	15
5	DMF	NR
6	DMSO	16
7	THF	12
8	2-MeTHF	18
9	^{i}PrCN	15
10	^{n}BuCN	22
11	acetone	18

[a]Reaction conditions: **1a** (0.2 mmol), **2a** (1.0 mmol), $Ni(acac)_2$ (10 mol%), dppb (20 mol%), Na_2CO_3 (0.4 mmol), AgF (1.0 equiv) in 1 mL solvent at 150 °C in N_2 for 24 h. [b]^{1}H NMR yield using CH_2Br_2 as the internal standard.

Table S3 Screen of Ag salt[a]

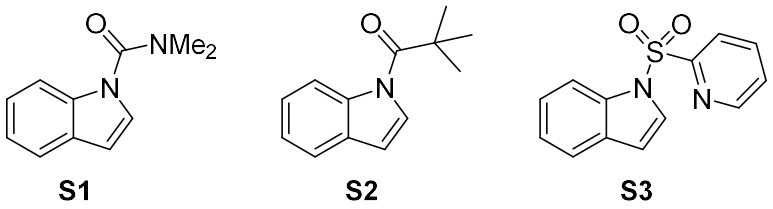


1a **3aa**

Entry	[Ag]	Yield[b]
1	AgF	25
2	Ag_2CO_3	trace
3	Ag_2O	10
4	AgOAc	12
5	$AgVO_3$	9
6	Ag_3PO_4	19
7	$AgSbF_6$	5

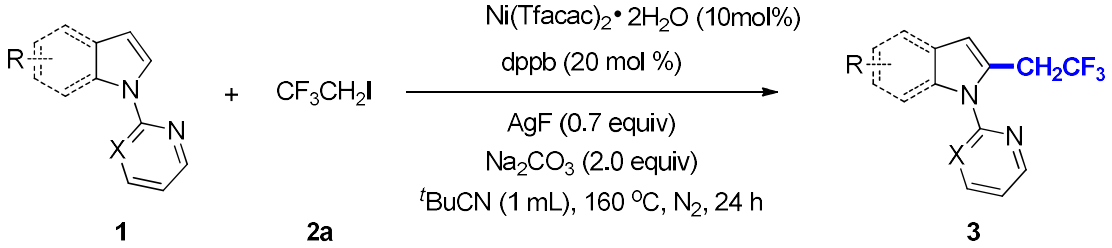
[a]Reaction conditions: **1a** (0.2 mmol), **2a** (1.0 mmol), $Ni(acac)_2$ (10 mol%), dppb (20 mol%), Na_2CO_3 (0.4 mmol) in 1 mL solvent at 150 °C in N_2 for 24 h. [b]^1H NMR yield using CH_2Br_2 as the internal standard.

Table S4 Failed Substrates

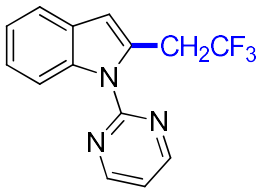


S1 **S2** **S3**

2.3 General Procedure for the Trifluoroethylation

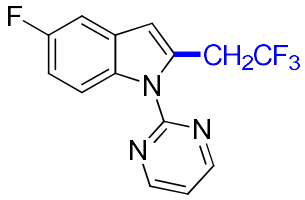


To a 50 mL Schlenk tube was added substrate **1** (0.2 mmol), CF_3CH_2I (1.0 mmol), Na_2CO_3 (42.4 mg, 0.4 mmol), dppb (17 mg, 0.04 mmol), $Ni(Tfacac)_2 \cdot 2H_2O$ (8 mg, 0.02 mmol), AgF (17.8 mg, 0.14 mmol) and ^{t}BuCN (1 mL). The vial was evacuated and filled with N_2 (1 atm) and then stirred at 160 °C for 24 h. After cooling to room temperature, the mixture was diluted with ethyl acetate, filtrated through ceilt. After concentration, the resulting residue was purified by preparative TLC using hexane/EtOAc as the eluent to afford the product.



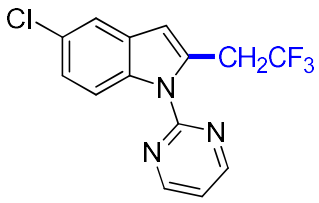
1-(pyrimidin-2-yl)-2-(2,2,2-trifluoroethyl)-1H-indole 3aa

The title compound was isolated by flash chromatography in PE : EA = 10 : 1 as a colorless oil (41 mg, 74%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.76 (d, J = 4.8 Hz, 2H), 8.34 (dd, J = 8.4, 0.4 Hz, 1H), 7.59 (d, J = 7.6 Hz, 1H), 7.30 (td, J = 7.2, 1.2 Hz, 1H), 7.24 – 7.20 (m, 1H), 7.12 (t, J = 4.8 Hz, 1H), 6.75 (s, 1H), 4.29 (q, J = 10.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.30, 158.23, 137.37, 129.23 (q, J = 3.4 Hz), 128.70, 125.53 (q, J = 275.6 Hz), 123.96, 122.38, 120.58, 117.50, 114.43, 110.34, 34.08 (q, J = 30.8 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -64.97; **HRMS** (EI-TOF) calcd for $C_{14}H_{10}F_3N_3$ (M^+): 277.0827, found: 277.0824.



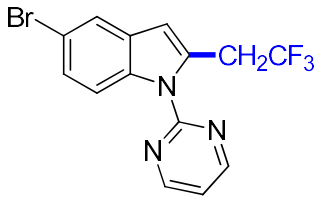
5-fluoro-1-(pyrimidin-2-yl)-2-(2,2,2-trifluoroethyl)-1H-indole 3ba

The title compound was isolated by flash chromatography in PE : EA = 20 : 1 as a colorless oil (41.3 mg, 70%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.77 (d, *J* = 4.8 Hz, 2H), 8.31 (dd, *J* = 9.2, 4.8 Hz, 1H), 7.23 (dd, *J* = 8.8, 2.4 Hz, 1H), 7.16 (t, *J* = 4.8 Hz, 1H), 7.02 (td, *J* = 9.2, 2.4 Hz, 1H), 6.70 (s, 1H), 4.30 (qd, *J* = 10.4, 0.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.34, 158.33, 158.03 (q, *J* = 10.2 Hz), 133.75, 130.92 (q, *J* = 3.4 Hz), 129.36 (q, *J* = 10.1 Hz), 125.44 (q, *J* = 275.6 Hz), 117.65, 115.72 (q, *J* = 9.0 Hz), 111.84 (q, *J* = 24.9 Hz), 110.01 (q, *J* = 3.4 Hz), 105.64 (q, *J* = 23.5 Hz), 34.22 (q, *J* = 30.8 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -64.90, -121.75; **HRMS** (EI-TOF) calcd for $C_{14}H_9F_4N_3$ (M^+): 295.0733, found: 295.0735.



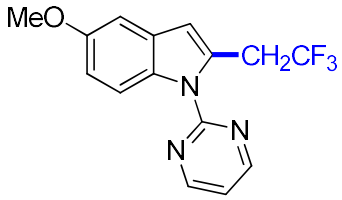
5-chloro-1-(pyrimidin-2-yl)-2-(2,2,2-trifluoroethyl)-1H-indole 3ca

The title compound was isolated by flash chromatography in PE : EA = 20 : 1 as a colorless oil (41.0 mg, 66%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.77 (d, *J* = 4.8 Hz, 2H), 8.28 (d, *J* = 8.8 Hz, 1H), 7.54 (d, *J* = 2.0 Hz, 1H), 7.23 (dd, *J* = 8.8, 2.4 Hz, 1H), 7.17 (t, *J* = 4.8 Hz, 1H), 6.67 (s, 1H), 4.29 (q, *J* = 10.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.35, 157.98, 135.69, 130.72 (q, *J* = 3.3 Hz), 129.80, 127.88, 125.40 (q, *J* = 275.6 Hz), 124.07, 119.97, 117.78, 115.80, 109.57, 34.16 (q, *J* = 30.9 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -64.89; **HRMS** (EI-TOF) calcd for $C_{14}H_9ClF_3N_3$ (M^+): 311.0437, found: 311.0442.



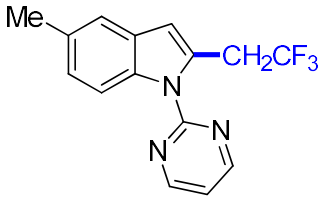
5-bromo-1-(pyrimidin-2-yl)-2-(2,2,2-trifluoroethyl)-1H-indole 3da

The title compound was isolated by flash chromatography in PE : EA = 20 : 1 as a yellow oil (44.9 mg, 63%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.77 (t, *J* = 4.8 Hz, 2H), 8.23 (d, *J* = 8.8 Hz, 1H), 7.70 (d, *J* = 2.0 Hz, 1H), 7.36 (dd, *J* = 8.8, 2.0 Hz, 1H), 7.17 (t, *J* = 4.8 Hz, 1H), 6.67 (s, 1H), 4.29 (qd, *J* = 10.4, 0.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.36, 157.96, 136.02, 130.58 (q, *J* = 3.3 Hz), 130.37, 126.70, 125.39 (q, *J* = 275.6 Hz), 123.06, 117.80, 116.19, 115.54, 109.44, 34.13 (q, *J* = 30.9 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -64.88; **HRMS** (EI-TOF) calcd for $C_{14}H_9BrF_3N_3$ (M^+): 354.9932, found: 354.9938.



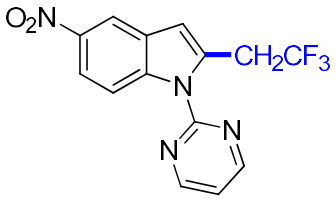
5-methoxy-1-(pyrimidin-2-yl)-2-(2,2,2-trifluoroethyl)-1H-indole 3e

The title compound was isolated by flash chromatography in PE : EA = 10 : 1 as a colorless oil (32.0 mg, 52%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.75 (d, *J* = 4.8 Hz, 2H), 8.29 (d, *J* = 9.2 Hz, 1H), 7.12 (t, *J* = 4.8 Hz, 1H), 7.04 (d, *J* = 2.8 Hz, 1H), 6.93 (dd, *J* = 9.2, 2.8 Hz, 1H), 6.67 (s, 1H), 4.30 (qd, *J* = 10.4, 0.4 Hz, 2H), 3.86 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.26, 158.22, 155.76, 132.26, 129.81 (q, *J* = 3.4 Hz), 129.45, 125.55 (q, *J* =275.6 Hz), 117.23, 115.68, 113.26, 110.27, 102.56, 55.84, 34.26 (q, *J* = 30.7 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -64.94l; **HRMS** (EI-TOF) calcd for $C_{15}H_{12}F_3N_3O$ (M^+): 307.0932, found: 307.0935.



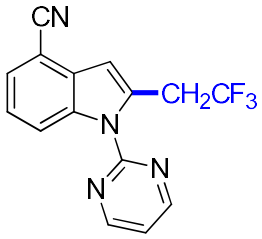
5-methyl-1-(pyrimidin-2-yl)-2-(2,2,2-trifluoroethyl)-1H-indole 3fa

The title compound was isolated by flash chromatography in PE : EA = 20 : 1 as a colorless oil (30.8 mg, 53%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.75 (d, *J* = 5.2 Hz, 2H), 8.24 (d, *J* = 8.4 Hz, 1H), 7.37 – 7.36 (m, 1H), 7.11 (t, *J* = 4.8 Hz, 2H), 6.66 (s, 1H), 4.29 (qd, *J* = 10.4, 0.4 Hz, 2H), 2.44 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.33, 158.22, 135.68, 131.78, 129.24 (q, *J* = 3.4 Hz), 128.96, 125.57 (q, *J* = 275.7 Hz), 125.41, 120.36, 117.24, 114.29, 110.18, 34.18 (q, *J* = 30.8 Hz), 21.41; ^{19}F NMR (377 MHz, $CDCl_3$) δ -64.99; **HRMS** (EI-TOF) calcd for $C_{15}H_{12}F_3N_3$ (M^+): 291.0983, found: 291.0989.



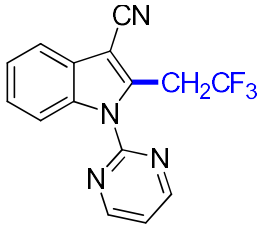
5-nitro-1-(pyrimidin-2-yl)-2-(2,2,2-trifluoroethyl)-1H-indole 3ga

The title compound was isolated by flash chromatography in PE : EA = 10 : 1 as a yellow solid (30.3 mg, 47%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.87 (d, *J* = 4.8 Hz, 2H), 8.52 (d, *J* = 2.0 Hz, 1H), 8.38 (d, *J* = 9.2 Hz, 1H), 8.17 (dd, *J* = 9.6, 2.4 Hz, 1H), 7.32 (t, *J* = 4.8 Hz, 1H), 6.89 (s, 1H), 4.32 (q, *J* = 10.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.68, 157.55, 143.47, 140.17, 132.75 (q, *J* = 3.5 Hz), 128.16, 125.17 (q, *J* = 275.7 Hz), 119.15, 118.75, 117.13, 114.68, 110.84, 34.09 (q, *J* = 31.2 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -64.85; **HRMS** (EI-TOF) calcd for $C_{14}H_9F_3N_4O_2$ (M^+): 322.0678, found: 322.0680.



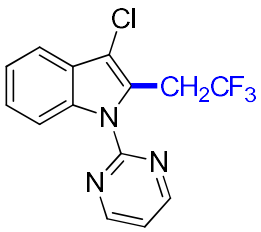
1-(pyrimidin-2-yl)-2-(2,2,2-trifluoroethyl)-1H-indole-4-carbonitrile 3ha

The title compound was isolated by flash chromatography in PE : EA = 10 : 1 as a colorless solid (34.4 mg, 52%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.84 (d, *J* = 4.8 Hz, 2H), 8.55 (d, *J* = 8.4 Hz, 1H), 7.55 (dd, *J* = 7.4, 0.8 Hz, 1H), 7.32 (dd, *J* = 8.4, 7.2 Hz, 1H), 7.28 (t, *J* = 4.8 Hz, 1H), 6.96 (s, 1H), 4.34 (q, *J* = 10.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.57, 157.59, 136.96, 132.34 (q, *J* = 3.3 Hz), 130.17, 127.14, 125.15 (q, *J* = 275.7 Hz), 123.65, 119.33, 118.46, 118.21, 108.19, 103.16, 34.07 (q, *J* = 31.1 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -64.74; **HRMS** (EI-TOF) calcd for $C_{15}H_9F_3N_4$ (M^+): 302.0779, found: 302.0782.



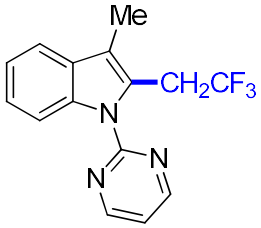
1-(pyrimidin-2-yl)-2-(2,2,2-trifluoroethyl)-1H-indole-3-carbonitrile 3ia

The title compound was isolated by flash chromatography in PE : EA = 10 : 1 as a colorless oil (32.6 mg, 52%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.88 (d, *J* = 4.8 Hz, 2H), 8.25 (dd, *J* = 7.2, 0.8 Hz, 1H), 7.77 – 7.75 (m, 1H), 7.44 – 7.38 (m, 2H), 7.35 (t, *J* = 4.8 Hz, 1H), 4.57 (q, *J* = 9.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.80, 157.20, 136.89 (q, *J* = 3.2 Hz), 136.47, 126.75, 126.01, 124.56 (q, *J* = 276.8 Hz), 124.17, 119.56, 119.39, 114.91, 114.47, 95.48, 32.48 (q, *J* = 31.9 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -64.36; **HRMS** (EI-TOF) calcd for $C_{15}H_9F_3N_4$ (M^+): 302.0779, found: 302.0782.



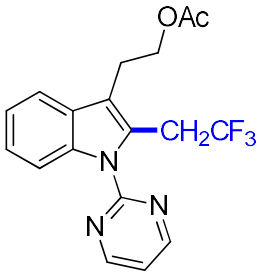
3-chloro-1-(pyrimidin-2-yl)-2-(2,2,2-trifluoroethyl)-1H-indole 3ja

The title compound was isolated by flash chromatography in PE : Acetone = 50 : 1 as a colorless oil (46.0 mg, 74%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.79 (d, *J* = 4.8 Hz, 2H), 8.38 (d, *J* = 8.4 Hz, 1H), 7.68 (dd, *J* = 7.6, 0.4 Hz, 1H), 7.39 (ddd, *J* = 8.5, 7.2, 1.4 Hz, 1H), 7.33 (td, *J* = 8.0, 0.8 Hz, 1H), 7.18 (t, *J* = 4.8 Hz, 1H), 4.53 (q, *J* = 10.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.35, 157.99, 135.92, 126.34, 125.41, 125.35 (q, *J* = 276.8 Hz), 124.87 (q, *J* = 3.2 Hz), 122.88, 118.51, 117.88, 114.64, 30.82 (q, *J* = 31.4 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -64.49; **HRMS** (EI-TOF) calcd for $C_{14}H_9ClF_3N_3$ (M^+): 311.0437, found: 311.0434.



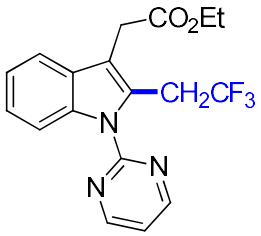
3-methyl-1-(pyrimidin-2-yl)-2-(2,2,2-trifluoroethyl)-1H-indole 3ka

The title compound was isolated by flash chromatography in PE : Acetone = 50 : 1 as a colorless oil (43.7 mg, 75%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.74 (d, *J* = 4.8 Hz, 2H), 8.32 (d, *J* = 8.4 Hz, 1H), 7.58 – 7.56 (m, 1H), 7.31 (td, *J* = 7.2, 1.2 Hz, 1H), 7.26 – 7.22 (m, 1H), 7.09 (t, *J* = 4.8 Hz, 1H), 4.41 (q, *J* = 10.4 Hz, 2H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.42, 158.20, 136.92, 129.69, 125.87 (q, *J* = 276.4 Hz), 124.92 (q, *J* = 3.1 Hz), 124.26, 121.94, 118.83, 118.27, 117.14, 114.28, 30.76 (q, *J* = 30.7 Hz), 9.07; ^{19}F NMR (377 MHz, $CDCl_3$) δ -64.82; **HRMS** (EI-TOF) calcd for $C_{15}H_{12}F_3N_3$ (M^+): 291.0983, found: 291.0984.



2-(1-(pyrimidin-2-yl)-2-(2,2,2-trifluoroethyl)-1H-indol-3-yl)ethyl acetate 3la

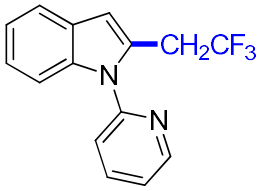
The title compound was isolated by flash chromatography in PE : Acetone = 5 : 1 as a colorless oil (56.0 mg, 77%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.77 (d, *J* = 4.8 Hz, 2H), 8.28 (d, *J* = 8.4 Hz, 1H), 7.66 (d, *J* = 7.6 Hz, 1H), 7.32 (td, *J* = 7.2, 1.2 Hz, 1H), 7.27 – 7.23 (m, 1H), 7.14 (t, *J* = 4.8 Hz, 1H), 4.45 (q, *J* = 10.4 Hz, 2H), 4.33 (t, *J* = 7.2 Hz, 2H), 3.16 (t, *J* = 7.2 Hz, 2H), 2.06 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.15, 158.30, 137.03, 128.72, 126.05 (q, *J* = 3.1 Hz), 125.42 (q, *J* = 276.3 Hz), 124.40, 122.17, 118.89, 117.89, 117.55, 114.20, 63.83, 30.60 (q, *J* = 30.8 Hz), 24.05, 21.10; ^{19}F NMR (377 MHz, $CDCl_3$) δ -64.62; **HRMS** (EI-TOF) calcd for $C_{18}H_{16}F_3N_3O_2$ (M^+): 363.1195, found: 363.1196.



ethyl 2-(1-(pyrimidin-2-yl)-2-(2,2,2-trifluoroethyl)-1H-indol-3-yl)acetate 3ma

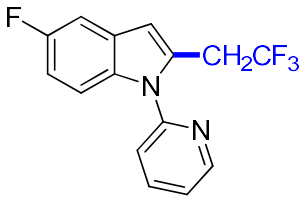
The title compound was isolated by flash chromatography in PE : DCM = 1 : 1 as a yellow oil (48.6 mg, 67%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.78 (d, *J* = 4.8 Hz, 2H), 8.29 (d, *J* = 8.0 Hz, 1H), 7.65 (d, *J* = 7.6 Hz, 1H), 7.34 - 7.30 (m, 1H), 7.28 – 7.24 (m, 1H), 7.15 (t, *J* = 4.8 Hz, 1H), 4.51 (q, *J* = 10.4 Hz, 2H), 4.15 (q, *J* = 6.8 Hz, 2H), 3.82 (s, 2H), 1.23 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.89, 158.30, 136.90, 128.70, 126.66 (q, *J* = 3.1 Hz), 125.55 (q, *J* = 276.4 Hz), 124.45, 122.29, 119.11, 117.62, 115.17, 114.25, 61.19, 30.70 (q, *J* = 30.8 Hz), 30.62, 14.26; ^{19}F NMR

(377 MHz, $CDCl_3$) δ -64.59; **HRMS** (EI-TOF) calcd for $C_{18}H_{16}F_3N_3O_2$ (M^+): 363.1195, found: 363.1198.



1-(pyridin-2-yl)-2-(2,2,2-trifluoroethyl)-1H-indole 3na

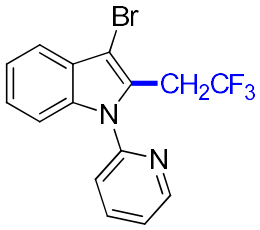
The title compound was isolated by flash chromatography in PE : Acetone = 100 : 1 as a yellow oil (34.3 mg, 62%). ^1H NMR (400 MHz, $CDCl_3$) δ 8.63 (ddd, J = 4.8, 2.0, 0.8 Hz, 1H), 7.91 (td, J = 7.6, 2.0 Hz, 1H), 7.65 – 7.63 (m, 1H), 7.52 (d, J = 8.0 Hz, 1H), 7.38 – 7.36 (m, 1H), 7.32 (ddd, J = 7.2, 4.8, 0.8 Hz, 1H), 7.22 – 7.15 (m, 2H), 6.74 (s, 1H), 3.91 (q, J = 10.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.10, 149.81, 138.72, 137.37, 129.04 (q, J = 3.3 Hz), 128.19, 125.33 (q, J = 275.4 Hz), 123.09, 122.41, 121.32, 121.17, 120.95, 110.38, 106.94, 32.47 (q, J = 31.2 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -65.20; **HRMS** (EI-TOF) calcd for $C_{15}H_{11}F_3N_2$ (M^+): 276.0874, found: 276.0877.



5-fluoro-1-(pyridin-2-yl)-2-(2,2,2-trifluoroethyl)-1H-indole 3oa

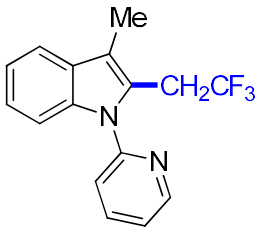
The title compound was isolated by flash chromatography in PE : Acetone = 100 : 1 then PE : DCM = 2 ： 1 as a colorless oil (35.3 mg, 60%). ^1H NMR (400 MHz, $CDCl_3$) δ 8.66 – 8.64 (m, 1H), 7.93 (td, J = 7.6, 2.0 Hz, 1H), 7.49 (d, J = 8.0 Hz, 1H), 7.36 (ddd, J = 7.6, 5.2, 1.2 Hz, 1H), 7.30 – 7.26 (m, 2H), 6.94 (td, J = 9.2, 2.8 Hz, 1H), 6.70 (s, 1H), 3.88 (q, J = 10.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.72 (d, J = 235.0 Hz), 150.89, 149.93, 138.89, 133.96, 130.63 (q, J = 3.3 Hz), 128.59 (d, J = 10.3 Hz), 125.21 (q, J = 275.4 Hz), 122.67, 121.08, 111.36 (d, J = 16.5 Hz), 111.19, 106.68

(d, J = 3.9 Hz), 105.84 (d, J = 23.5 Hz), 32.51 (q, J = 31.3 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -65.12, -123.06; **HRMS** (EI-TOF) calcd for $C_{15}H_{10}F_4N_2$ (M^+): 294.0780, found: 294.0778.



3-bromo-1-(pyridin-2-yl)-2-(2,2,2-trifluoroethyl)-1H-indole 3pa

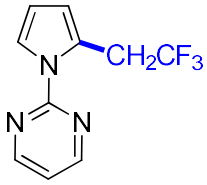
The title compound was isolated by flash chromatography in PE : Acetone = 100 : 1 as a yellow oil (53.3 mg, 75%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.62 (ddd, J = 5.2, 2.0, 0.8 Hz, 1H), 7.92 (td, J = 7.6, 2.0 Hz, 1H), 7.66 – 7.62 (m, 1H), 7.52 (d, J = 8.0 Hz, 1H), 7.38 - 7.33 (m, 2H), 7.29 - 7.24 (m, 2H), 4.13 (q, J = 10.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.84, 149.88, 138.87, 136.57, 127.20, 126.77 (q, J = 3.2 Hz), 125.08 (q, J = 276.8 Hz), 124.53, 122.84, 122.00, 121.15, 119.92, 110.49, 98.75, 30.65 (q, J = 31.7 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -64.55; **HRMS** (EI-TOF) calcd for $C_{15}H_{10}BrF_3N_2$ (M^+): 353.9979, found: 353.9978.



3-methyl-1-(pyridin-2-yl)-2-(2,2,2-trifluoroethyl)-1H-indole 3qa

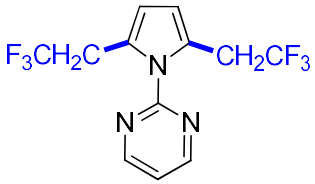
The title compound was isolated by flash chromatography in PE : Acetone = 50 : 1 as a yellow oil (40.1 mg, 69%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60 (ddd, J = 4.8, 2.0, 0.8 Hz, 1H), 7.88 (td, J = 8.0, 2.0 Hz, 1H), 7.62 – 7.59 (m, 1H), 7.51 (d, J = 8.0 Hz, 1H), 7.36 – 7.34 (m, 1H), 7.28 (ddd, J = 7.6, 4.8, 1.2 Hz, 1H), 7.23 – 7.17 (m, 2H), 4.01 (q, J = 10.8 Hz, 2H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.55, 149.66,

138.62, 136.99, 128.88, 125.65 (q, J = 276.3 Hz), 125.05 (q, J = 3.0 Hz), 123.32, 122.05, 121.21, 120.75, 119.23, 115.25, 110.11, 29.74 (q, J = 31.1 Hz), 8.97; ^{19}F NMR (377 MHz, $CDCl_3$) δ -65.04; **HRMS** (EI-TOF) calcd for $C_{16}H_{13}F_3N_2$ (M^+): 290.1031, found: 290.1036.



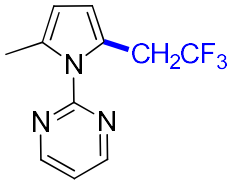
2-(2-(2,2,2-trifluoroethyl)-1H-pyrrol-1-yl)pyrimidine 3ra

The title compound was isolated by flash chromatography in PE : Acetone = 50 : 1 as a yellow oil (12.7 mg, 28%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64 (d, J = 4.8 Hz, 2H), 7.82 (dd, J = 3.2, 2.0 Hz, 1H), 7.08 (t, J = 4.8 Hz, 1H), 6.35 (s, 1H), 6.27 (t, J = 3.2 Hz, 1H), 4.25 (q, J = 10.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.21, 157.76, 125.61 (q, J = 275.4 Hz), 122.87 (q, J = 3.6 Hz), 122.76, 117.56, 115.82, 110.19, 33.59 (q, J = 30.6 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -66.09; **HRMS** (EI-TOF) calcd for $C_{10}H_8F_3N_3$ (M^+): 227.0670, found: 227.0674.



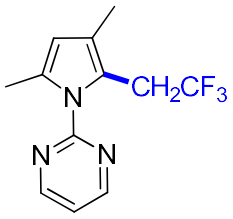
2-(2,5-bis(2,2,2-trifluoroethyl)-1H-pyrrol-1-yl)pyrimidine 3ra'

The title compound was isolated by flash chromatography in PE : Acetone = 50 : 1 as a yellow oil (35.0 mg, 57%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.79 (d, J = 4.8 Hz, 2H), 7.26 -7.24 (m, 1H), 6.30 (s, 2H), 3.91 (q, J = 10.4 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.72, 157.66, 125.31 (q, J = 275.4 Hz), 124.14 (q, J = 3.4 Hz), 119.00, 113.27, 32.68 (q, J = 31.0 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -66.09; **HRMS** (EI-TOF) calcd for $C_{12}H_9F_6N_3$ (M^+): 309.0701, found: 309.0707.



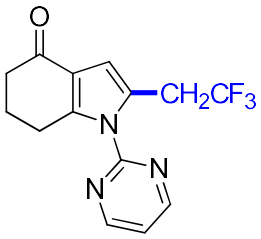
2-(2-methyl-5-(2,2,2-trifluoroethyl)-1H-pyrrol-1-yl)pyrimidine 3sa

The title compound was isolated by flash chromatography in PE : Acetone = 50 : 1 as a yellow oil (25.1 mg, 52%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.78 (d, *J* = 4.8 Hz, 2H), 7.21 (t, *J* = 4.8 Hz, 1H), 6.21 (d, *J* = 3.6 Hz, 1H), 5.99 (dd, *J* = 3.6, 1.2 Hz, 1H), 3.86 (q, *J* = 10.4 Hz, 2H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.47, 157.99, 132.45, 125.50 (q, *J* = 275.4 Hz), 121.60 (q, *J* = 3.3 Hz), 118.50, 113.00, 109.36, 32.72 (q, *J* = 30.9 Hz), 14.80; ^{19}F NMR (377 MHz, $CDCl_3$) δ -66.21; **HRMS** (EI-TOF) calcd for $C_{11}H_{10}F_3N_3$ (M^+): 241.0827, found: 241.0831.



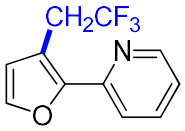
2-(3,5-dimethyl-2-(2,2,2-trifluoroethyl)-1H-pyrrol-1-yl)pyrimidine 3ta

The title compound was isolated by flash chromatography in PE : Acetone = 50 : 1 as a yellow oil (25.5 mg, 50%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.75 (d, *J* = 4.8 Hz, 2H), 7.17 (t, *J* = 4.8 Hz, 1H), 5.89 (s, 1H), 3.91 (q, *J* = 10.8 Hz, 2H), 2.34 (d, *J* = 0.4 Hz, 3H), 2.07 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.38, 158.14, 131.54, 125.85 (q, *J* = 276.2 Hz), 122.03, 118.18, 117.56 (q, *J* = 3.0 Hz), 111.98, 26.77 (q, *J* = 30.8 Hz), 14.58, 11.25; ^{19}F NMR (377 MHz, $CDCl_3$) δ -66.13; **HRMS** (EI-TOF) calcd for $C_{12}H_{12}F_3N_3$ (M^+): 255.0983, found: 255.0982.



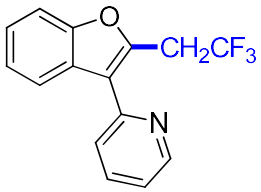
1-(pyrimidin-2-yl)-2-(2,2,2-trifluoroethyl)-6,7-dihydro-1H-indol-4(5H)-one 3ua

The title compound was isolated by flash chromatography in PE : DCM = 1 : 5 as a yellow solid (20.7 mg, 35%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.83 (d, *J* = 4.8 Hz, 2H), 7.32 (t, *J* = 4.8 Hz, 1H), 6.72 (s, 1H), 3.94 (q, *J* = 10.0 Hz, 2H), 3.03 (t, *J* = 6.0 Hz, 2H), 2.53 (t, *J* = 6.0 Hz, 2H), 2.17 – 2.10 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.78, 158.71, 157.00, 146.58, 125.18 (q, *J* = 275.5 Hz), 124.00 (q, *J* = 3.3 Hz), 121.93, 119.41, 110.59, 37.90, 32.61 (q, *J* = 31.2 Hz), 24.78, 23.91; ^{19}F NMR (377 MHz, $CDCl_3$) δ -65.91; **HRMS** (EI-TOF) calcd for $C_{14}H_{12}F_3N_3O$ (M^+): 295.0932, found: 295.0935.



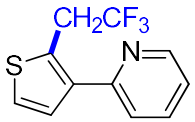
2-(3-(2,2,2-trifluoroethyl)furan-2-yl)pyridine 3va

The title compound was isolated by flash chromatography in PE : Acetone = 10 : 1 as a colorless oil (25.0 mg, 55%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.61 – 8.59 (m, 1H), 7.74 – 7.66 (m, 2H), 7.16 (ddd, *J* = 7.2, 4.8, 1.2 Hz, 1H), 7.02 (d, *J* = 3.2 Hz, 1H), 6.47 (d, *J* = 3.2 Hz, 1H), 3.57 (q, *J* = 10.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.01, 149.77, 149.08, 145.23 (q, *J* = 3.7 Hz), 136.80, 124.63 (q, *J* = 275.4 Hz), 122.25, 118.75, 112.38, 109.66, 33.90 (q, *J* = 32.0 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -65.63; **HRMS** (EI-TOF) calcd for $C_{11}H_8F_3NO$ (M^+): 227.0558, found: 227.0562.



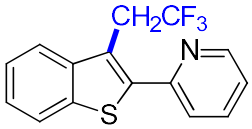
2-(2-(2,2,2-trifluoroethyl)benzofuran-3-yl)pyridine 3wa

The title compound was isolated by flash chromatography in PE : DCM = 4 : 1 as a yellow oil (26.6 mg, 48%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.74 – 8.73 (m, 1H), 7.85 – 7.81 (m, 2H), 7.70 (d, *J* = 7.6 Hz, 1H), 7.56 (d, *J* = 8.0 Hz, 1H), 7.38 (td, *J* = 7.2, 1.2 Hz, 1H), 7.35 – 7.27 (m, 2H), 4.15 (q, *J* = 10.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.83, 151.68, 150.19, 146.06 (q, *J* = 3.7 Hz), 136.93, 126.81, 125.24, 125.02 (q, *J* = 276.6 Hz), 123.56, 123.25, 122.33, 120.60, 120.55, 111.74, 32.80 (q, *J* = 31.6 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.83; **HRMS** (EI-TOF) calcd for $C_{15}H_{10}F_3NO$ (M^+): 277.0714, found: 277.0718.



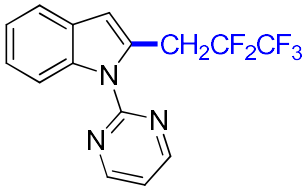
2-(2-(2,2,2-trifluoroethyl)thiophen-3-yl)pyridine 3xa

The title compound was isolated by flash chromatography in PE : EA = 10 : 1 as a yellow oil (42.7 mg, 88%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 (ddd, *J* = 4.8, 1.6, 0.8 Hz, 1H), 7.74 (td, *J* = 8.0, 2.0 Hz, 1H), 7.48 (d, *J* = 8.0 Hz, 1H), 7.33 (d, *J* = 5.2 Hz, 1H), 7.28 (d, *J* = 5.2 Hz, 1H), 7.21 (ddd, *J* = 7.6, 4.8, 1.2 Hz, 1H), 4.22 (q, *J* = 10.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.72, 149.49, 140.51, 136.91, 129.33 (q, *J* = 3.2 Hz), 128.57, 125.51 (q, *J* = 275.7 Hz), 125.21, 122.94, 122.04, 32.90 (q, *J* = 31.2 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -65.72; **HRMS** (EI-TOF) calcd for $C_{11}H_8F_3NS$ (M^+): 243.0330, found: 243.0334.



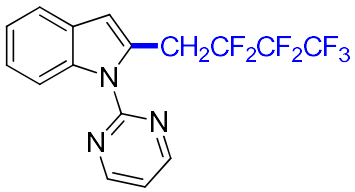
2-(3-(2,2,2-trifluoroethyl)benzo[b]thiophen-2-yl)pyridine 3ya

The title compound was isolated by flash chromatography in PE : Acetone = 100 : 1 as a yellow oil (19.8 mg, 34%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.70 (ddd, *J* = 4.8, 2.0, 0.8 Hz, 1H), 7.87 – 7.82 (m, 2H), 7.77 (td, *J* = 7.6, 2.0 Hz, 1H), 7.67 (dt, *J* = 8.0, 0.8 Hz, 1H), 7.47 – 7.38 (m, 2H), 7.28 – 7.26 (m, 1H), 4.33 (q, *J* = 10.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.06, 149.76, 142.07, 140.78, 138.91, 137.06, 126.14 (q, *J* = 276.6 Hz), 125.50, 124.88, 123.70, 122.90, 122.43, 31.24 (q, *J* = 30.6 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -63.55; **HRMS** (EI-TOF) calcd for $C_{15}H_{10}F_3NS$ (M^+): 293.0486, found: 293.0486.



2-(2,2,3,3,3-pentafluoropropyl)-1-(pyrimidin-2-yl)-1H-indole 3ab

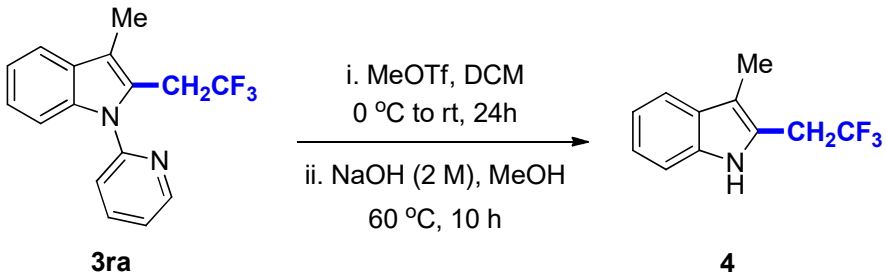
The title compound was isolated by flash chromatography in PE : Acetone = 100 : 1 as a yellow oil (45.2 mg, 69%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.75 (d, *J* = 4.8 Hz, 2H), 8.35 (dd, *J* = 8.4, 0.8 Hz, 1H), 7.60 ((d, *J* = 7.6 Hz, 2H), 7.32 – 7.28 (m, 1H), 7.25 – 7.21 (m, 1H), 7.13 (t, *J* = 4.8 Hz, 1H), 6.75 (s, 1H), 4.32 (t, *J* = 18.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.33, 158.23, 137.56, 128.63, 128.07, 124.02, 122.38, 120.57, 117.53, 114.49, 111.45, 30.61 (t, *J* = 21.5 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -85.29, -116.20; **HRMS** (EI-TOF) calcd for $C_{15}H_{10}F_5N_3$ (M^+): 327.0795, found: 327.0800.



2-(2,2,3,3,4,4,4-heptafluorobutyl)-1-(pyrimidin-2-yl)-1H-indole 3ac

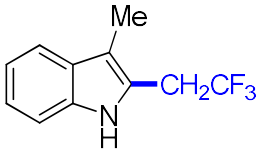
The title compound was isolated by flash chromatography in PE : Acetone = 100 : 1 as a colorless oil (45.1 mg, 60%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.77 (d, *J* = 4.8 Hz, 2H), 8.36 (dd, *J* = 8.4, 0.8 Hz, 1H), 7.60 (dd, *J* = 7.2, 0.8 Hz, 1H), 7.31 (ddd, *J* = 8.5, 7.2, 1.2 Hz, 1H), 7.25 – 7.21 (m, 1H), 7.15 (t, *J* = 4.8 Hz, 1H), 6.76 (s, 1H), 4.37 (t, *J* = 18.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.37, 158.23, 137.61, 128.64, 127.90, 124.03, 122.38, 120.57, 117.54, 114.54, 111.73, 30.59 (q, *J* = 21.5 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ -80.49 (t, *J* = 9.8 Hz), -113.14 (qt, *J* = 9.8, 2.3 Hz), -127.85 (q, *J* = 2.3 Hz); **HRMS** (EI-TOF) calcd for $C_{16}H_{10}F_7N_3$ (M^+): 377.0763, found: 377.0761.

2.4 Removal of 2-Pyridinyl Director [8]



3ra **4**

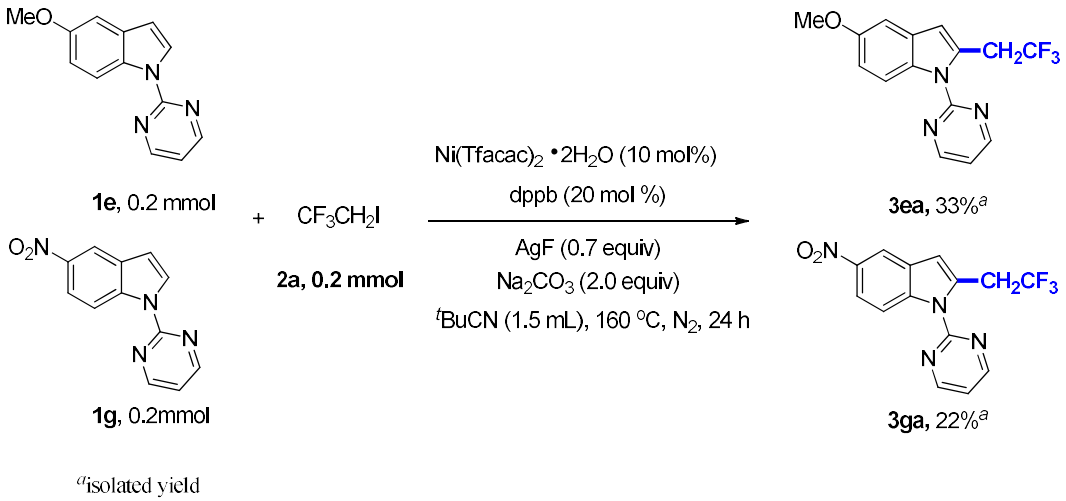
Methyl trifluoromethanesulfonate (27 μL, 0.24 mmol) was added dropwise to a solution of **3ra** (59.6 mg, 0.20 mmol) in dry CH_2Cl_2 (5.0 mL) at 0 °C, and the resulting solution was stirred for 24 h at room temperature. Then the solvent was removed under vacuum, and the residue was dissolved in MeOH (3.0 mL). A 2 M aq. NaOH solution (1.2 mL) was added, and stirring was continued at 60 °C for 12 h. The solvents were removed, and the resulting residue was extracted with EtOAc (2 × 15 mL). The combined organic layers were washed with brine, dried over $MgSO_4$, and concentrated in vacuo. The residue was purified by flash chromatography, affording the desired product **4** (30.7 mg, 72%) as a yellow solid.



3-methyl-2-(2,2,2-trifluoroethyl)-1H-indole 4

The title compound was isolated by flash chromatography in PE : DCM = 5 : 1 as a yellow solid (30.7 mg, 72%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (s, 1H), 7.54 (d, J = 8.0 Hz, 1H), 7.30 (d, J = 8.0 Hz, 1H), 7.22 – 7.18 (m, 1H), 7.14 - 7.11 (m, 1H), 3.50 (q, J = 10.8 Hz, 2H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.00, 128.66, 125.58 (q, J = 275.8 Hz), 122.73, 119.68, 119.04, 111.98, 110.82, 31.64 (q, J = 31.2 Hz), 8.54; ^{19}F NMR (376 MHz, $CDCl_3$) δ -65.08; **HRMS** (EI-TOF) calcd for $C_{11}H_{10}F_3N$ (M^+): 213.0765, found: 213.0766.

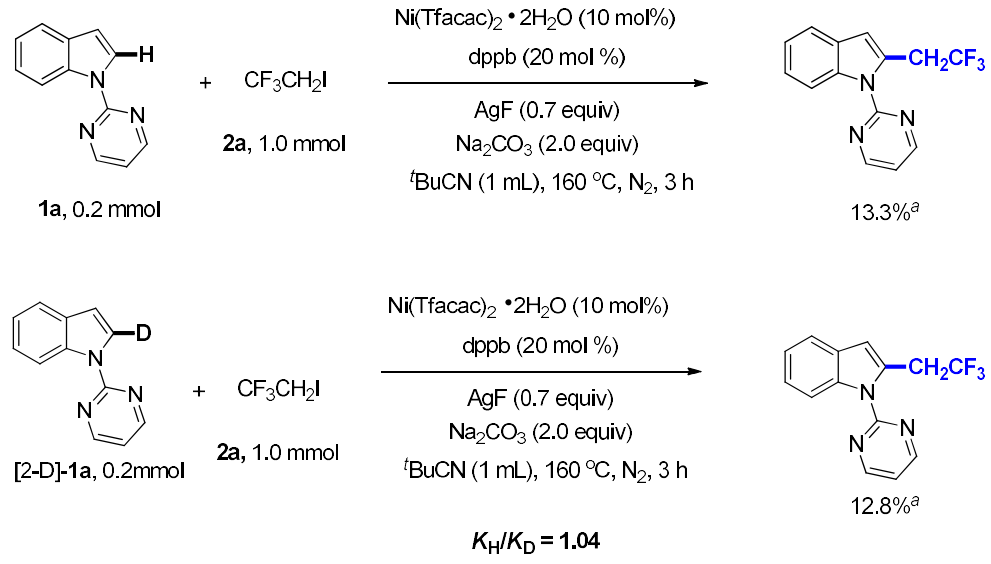
2.5 Intermolecular competition experiment



[a]isolated yield

To a 50 mL Schlenk tube was added substrate **1e** (0.2 mmol), **1g** (0.2 mmol), CF_3CH_2I (0.2 mmol), Na_2CO_3 (42.4 mg, 0.4 mmol), dppb (17 mg, 0.04 mmol), $Ni(Tfacac)_2 \cdot 2H_2O$ (8 mg, 0.02 mmol), AgF (17.8 mg, 0.14 mmol) and ^{t}BuCN (1.5 mL). The vial was evacuated and filled with N_2 (1 atm) and then stirred at 160 °C for 24 h. After cooling to room temperature, the mixture was diluted with ethyl acetate, filtrated through ceilt. After concentration, the resulting residue was purified by preparative TLC using PE/EA as the eluent to afford the product.

2.6 Intermolecular kinetic isotopic effect experiment

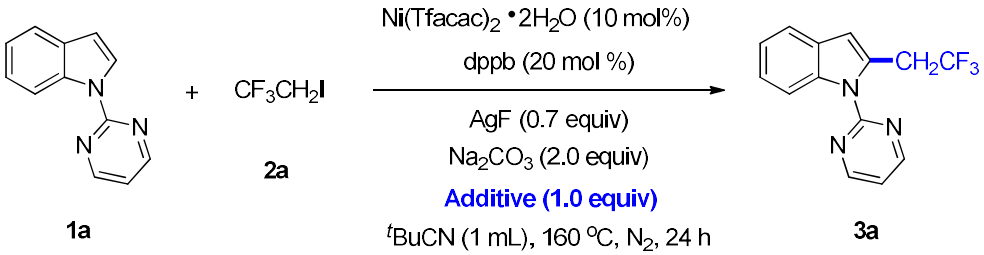


K_H/K_D = 1.04

[a]^{1}H NMR yield using CH_2Br_2 as internal standard.

A mixture of **1a** (0.2 mmol) or [2-D]-**1a** (0.2 mmol), CF_3CH_2I (1.0 mmol), Na_2CO_3 (42.4 mg, 0.4 mmol), dppb (17 mg, 0.04 mmol), $Ni(Tfacac)_2 \cdot 2H_2O$ (8 mg, 0.02 mmol), AgF (17.8 mg, 0.14 mmol) was combined in ^{t}BuCN (1.0 mL) in **two paralleled** dried Schlenk tube which was evacuated and filled with N_2 (1 atm) and then stirred at 160 °C for 3 h. After cooling to room temperature, the mixture was diluted with ethyl acetate, filtrated through ceilt. After concentration, the resulting residue was analyzed with NMR using CH_2Br_2 as the internal standard.

2.7 Radical Scavenger experiments



Additive	2a, yield (%)[a]
hydroquinone	trace
TEMPO	0%
1,4-diphenylethylene	6%

[a] ^{1}H NMR yield using CH_2Br_2 as the internal standard.

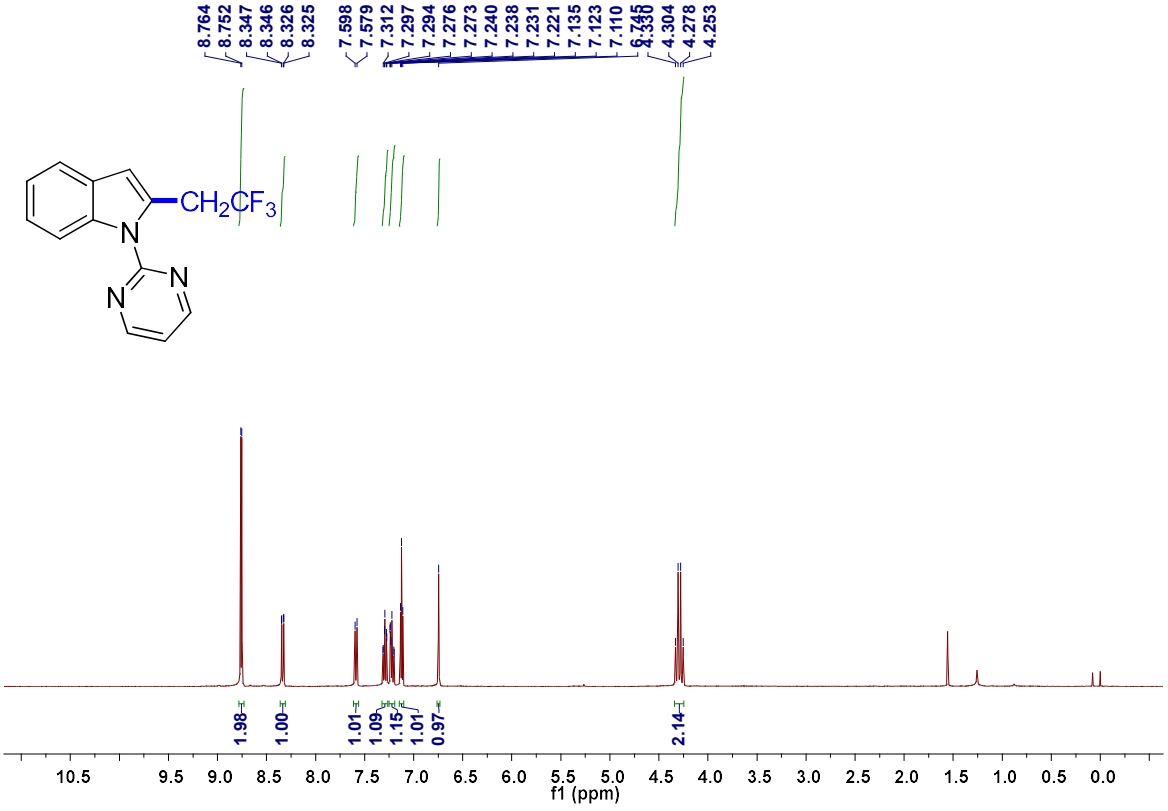
To a 50 mL Schlenk tube was added substrate **1a** (0.2 mmol), CF_3CH_2I (1.0 mmol), Na_2CO_3 (42.4 mg, 0.4 mmol), dppb (17 mg, 0.04 mmol), additive (1.0 equiv), $Ni(Tfacac)_2 \cdot 2H_2O$ (8 mg, 0.02 mmol), AgF (17.8 mg, 0.14 mmol) and ^{t}BuCN (1 mL). The vial was evacuated and filled with N_2 (1 atm) and then stirred at 160 °C for 24 h. After cooling to room temperature, the mixture was diluted with ethyl acetate, filtrated through ceilt. After concentration, the resulting residue was analyzed with NMR using CH_2Br_2 as the internal standard.

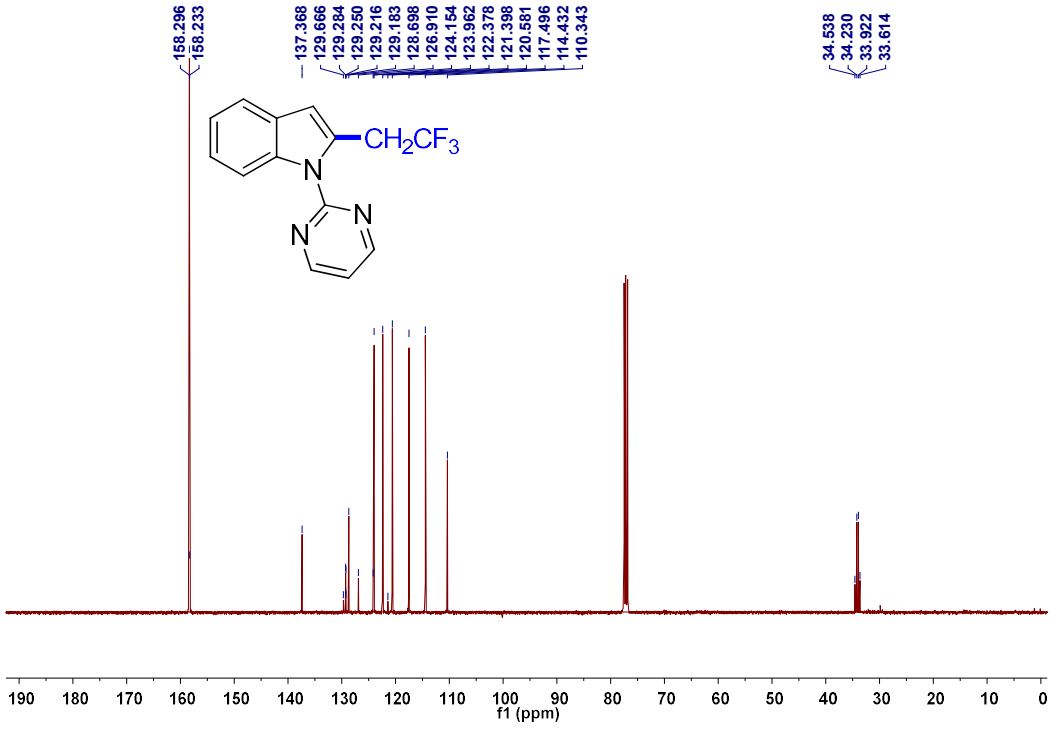
3. References:

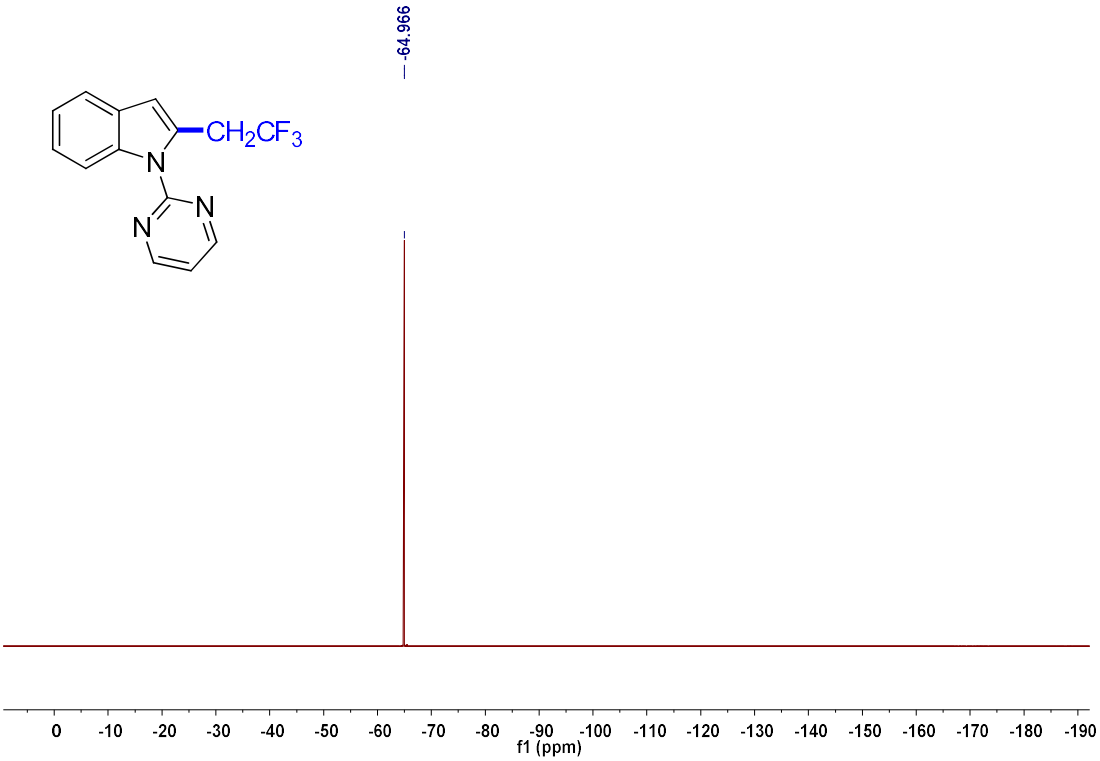
1. L. Ackermann, A. V. Lygin, *Org. Lett.* 2011, **13**, 3332-3335.
2. M. Moselage, N. Sauermann, S. C. Richter, L. Ackermann, *Angew. Chem., Int. Ed.* 2015, **54**, 6352-6355.
3. M.-Z. Lu, P. Lu, Y.-H. Xu, T.-P. Loh, *Org. Lett.* 2014, **16**, 2614–2617.
4. A. B. Pawar, S. Chang, *Org. Lett.* 2015, **17**, 660–663.
5. C.-D. Shao, G.-F. Shi, Y.-H. Zhang, S.-L. Pan, X.-H. Guan, *Org. Lett.* 2015, **17**, 2652-2655.
6. R. Cano, D. J. Ramón, M. Yus, *J. Org. Chem.*, 2011, **76 (2)**, 654–660.
7. J. Pospech, A. Tlili, A. Spannenberg, H. Neumann, M. Beller, *Chem. Eur. J.* 2014, **20**, 3135 – 3141.
8. V. K. Tiwari, N. Kamal, M. Kapur, *Org. Lett.*, **2015**, *17* (7), 1766–1769.

4. NMR Spectra

3aa



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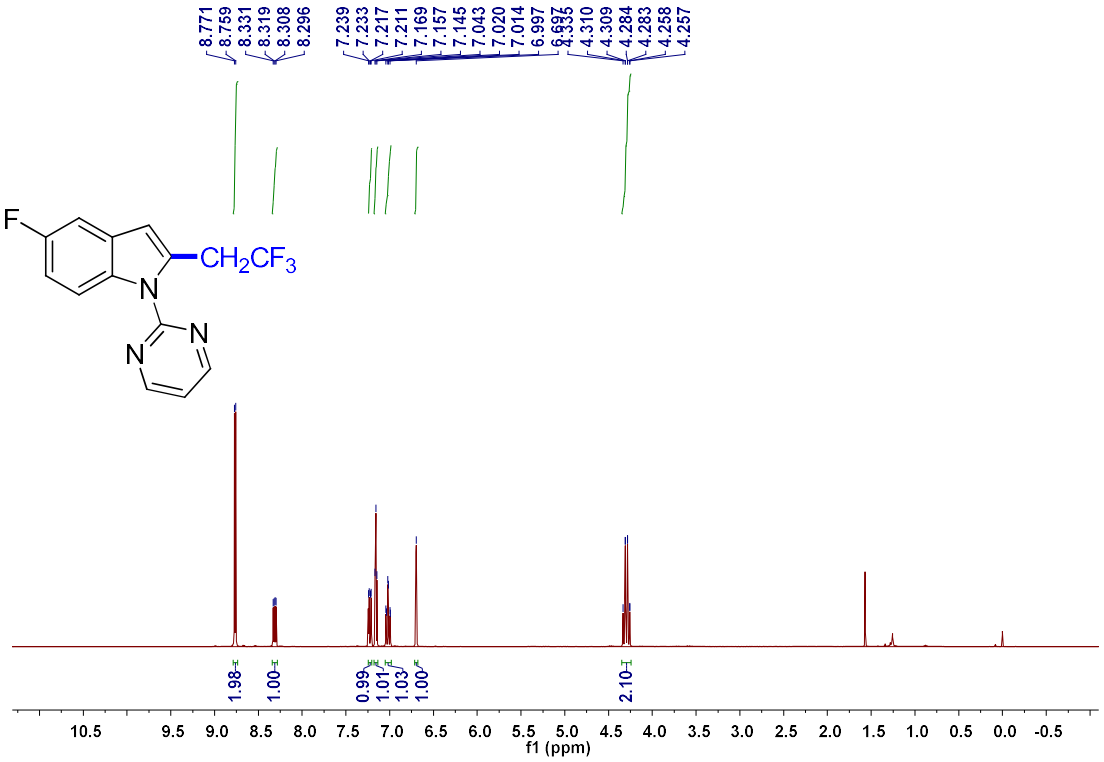
N
N
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)

3ba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8.296
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7.233
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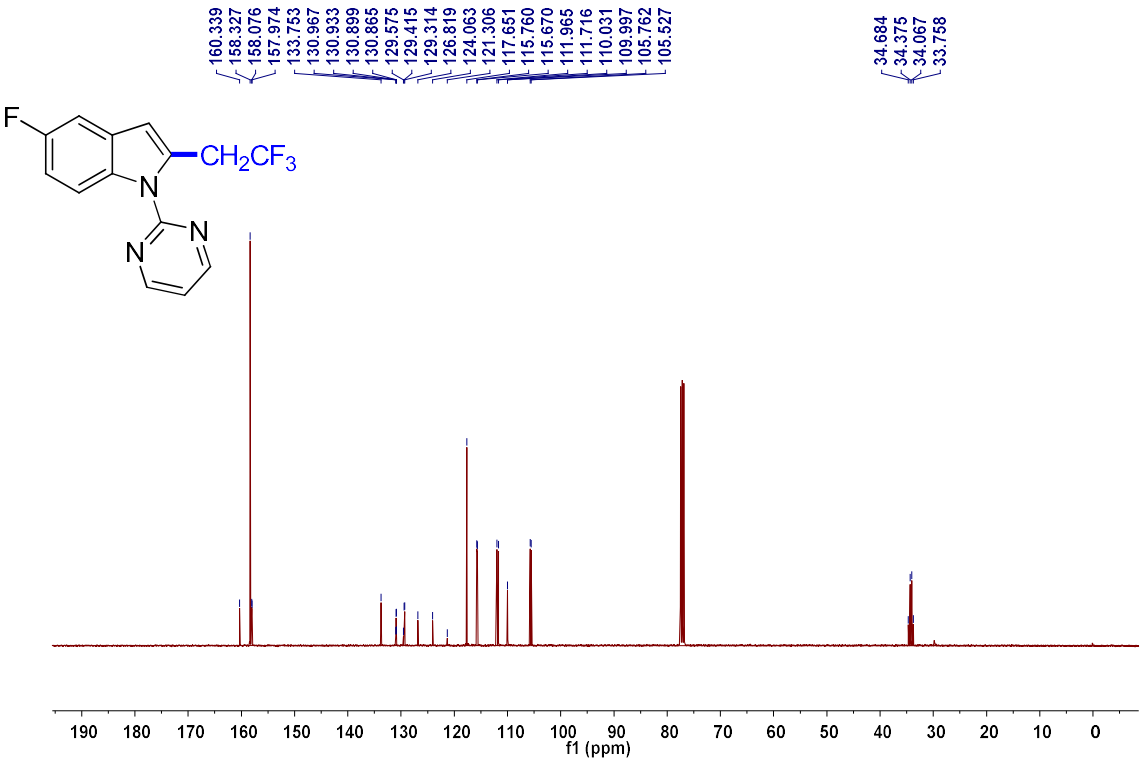
7.211
7.169
7.157
7.145
7.043
7.020
7.014
6.997
6.697
4.335
4.310
4.309
4.284
4.283
4.258
4.257
F
CH2CF3
N
N
N
1.98
1.00
0.99
1.01
1.03
1.00
2.10
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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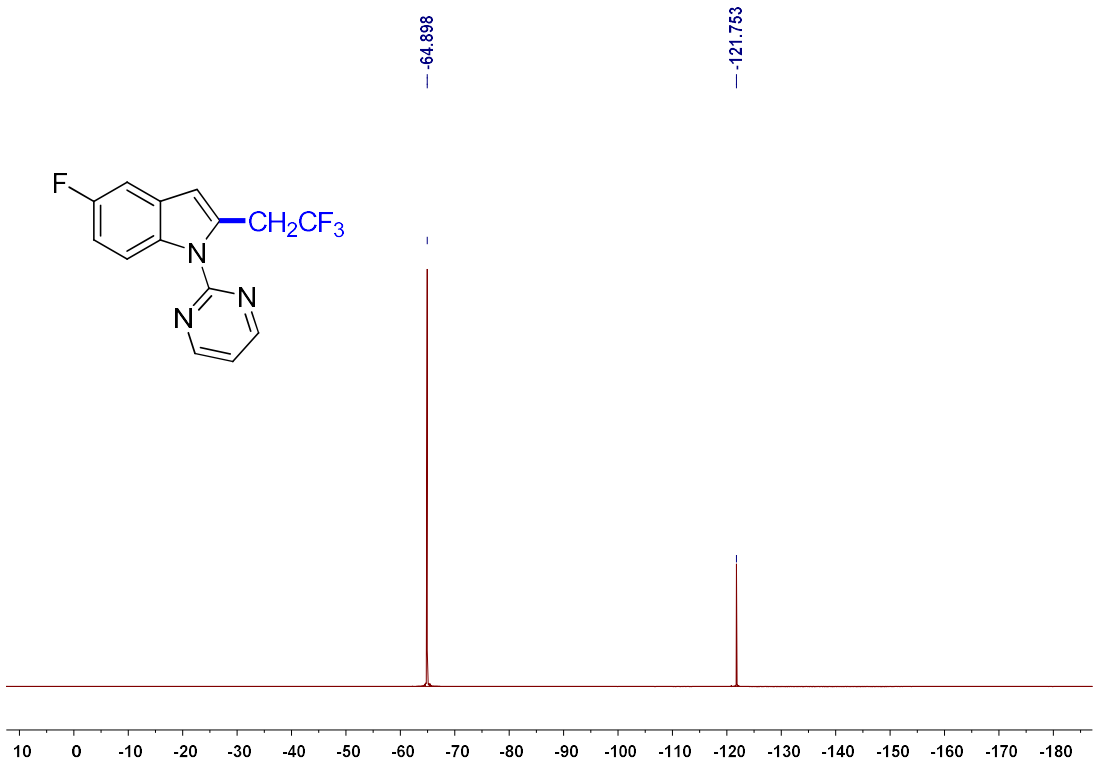
158.327
158.076
157.974
133.753
130.967
130.933
130.899
130.865
129.575
129.415
129.314
126.819
124.063
121.306
117.651
115.760
115.670
111.965
111.716
110.031
109.997
105.762
105.527
34.684
34.375
34.067
33.758
F
CH2CF3
N
N
N
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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-60
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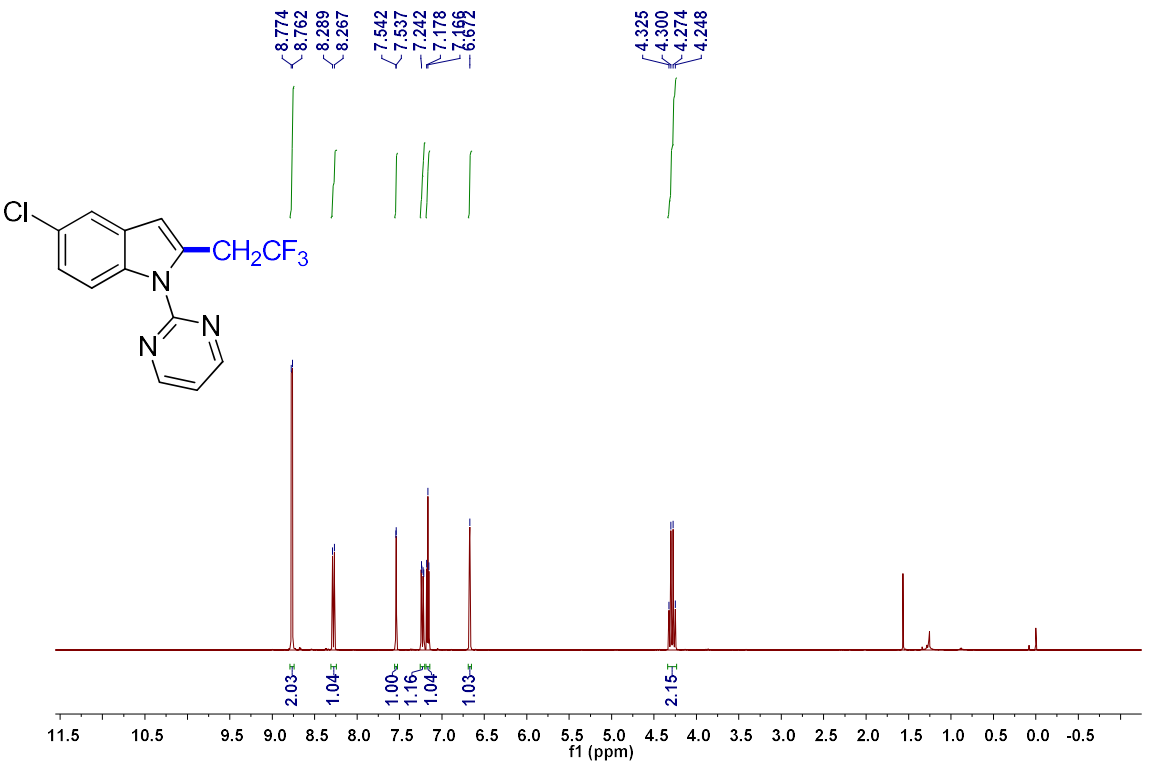
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180

3ca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7.537
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7.178
7.166
6.672
4.325
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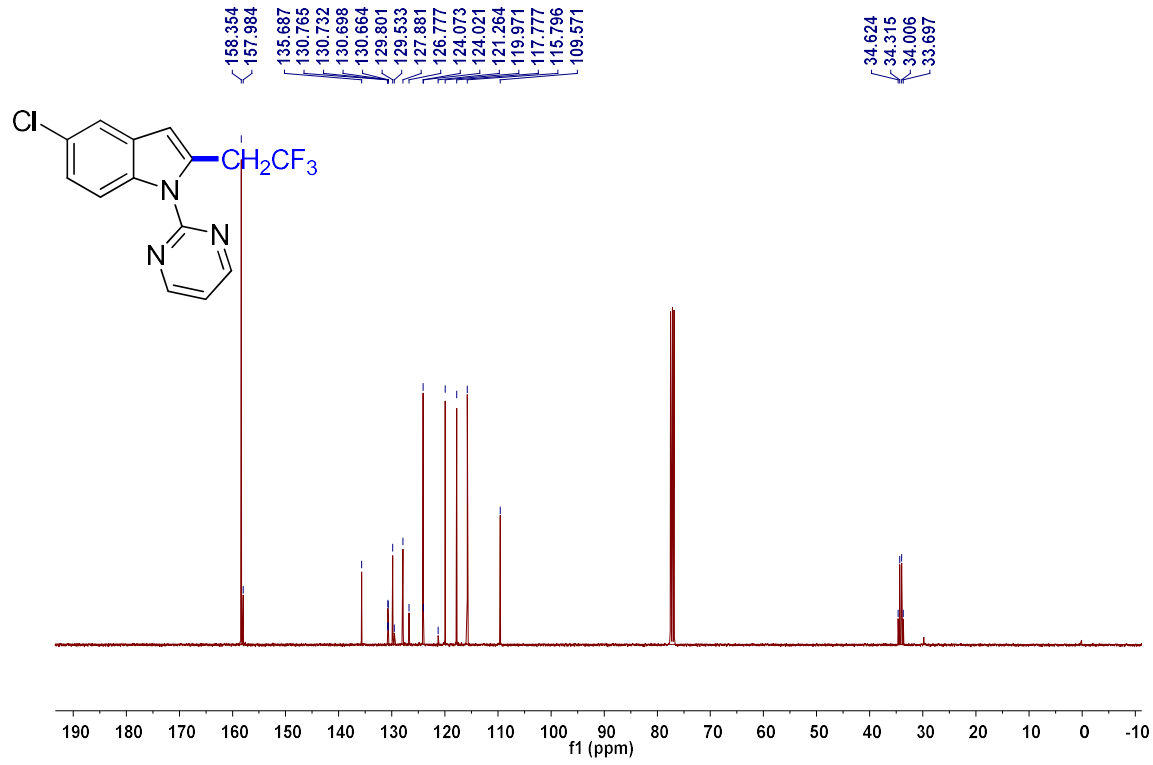
4.274
4.248
Cl
CH2CF3
N
N
N
2.03
1.04
1.00
1.16
1.04
1.03
2.15
f1 (ppm)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124.021
121.264
119.971
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Cl
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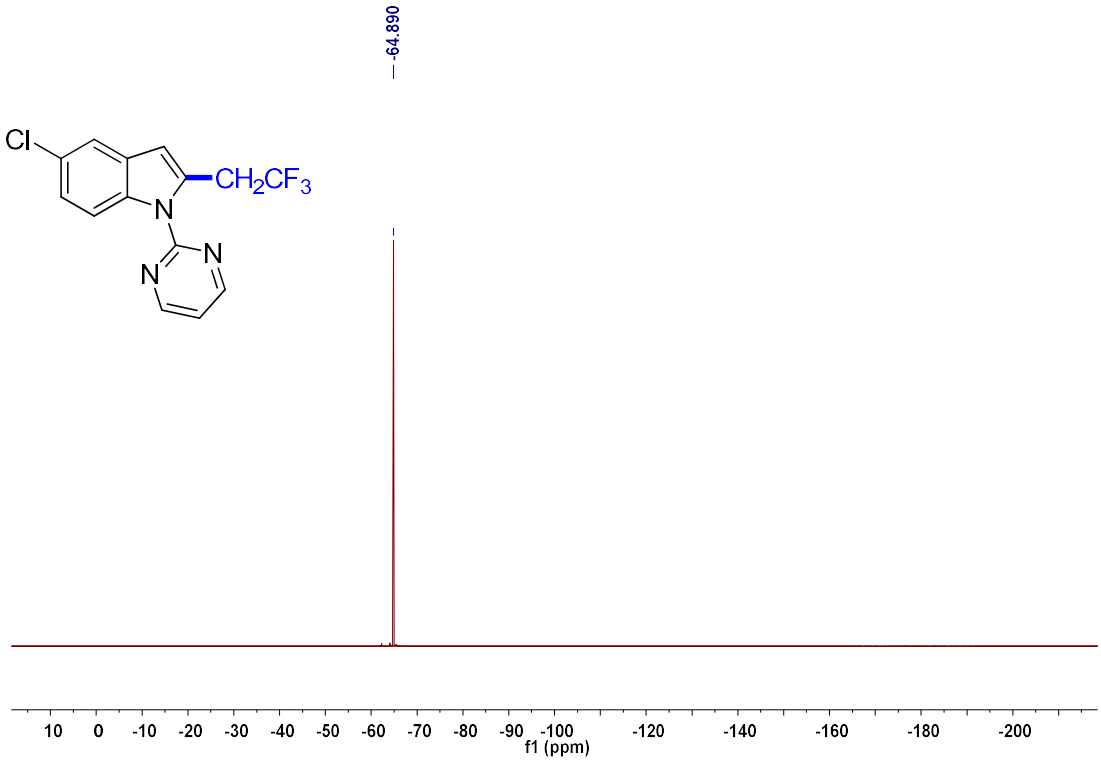
N
N
N
f1 (ppm)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-80
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-160
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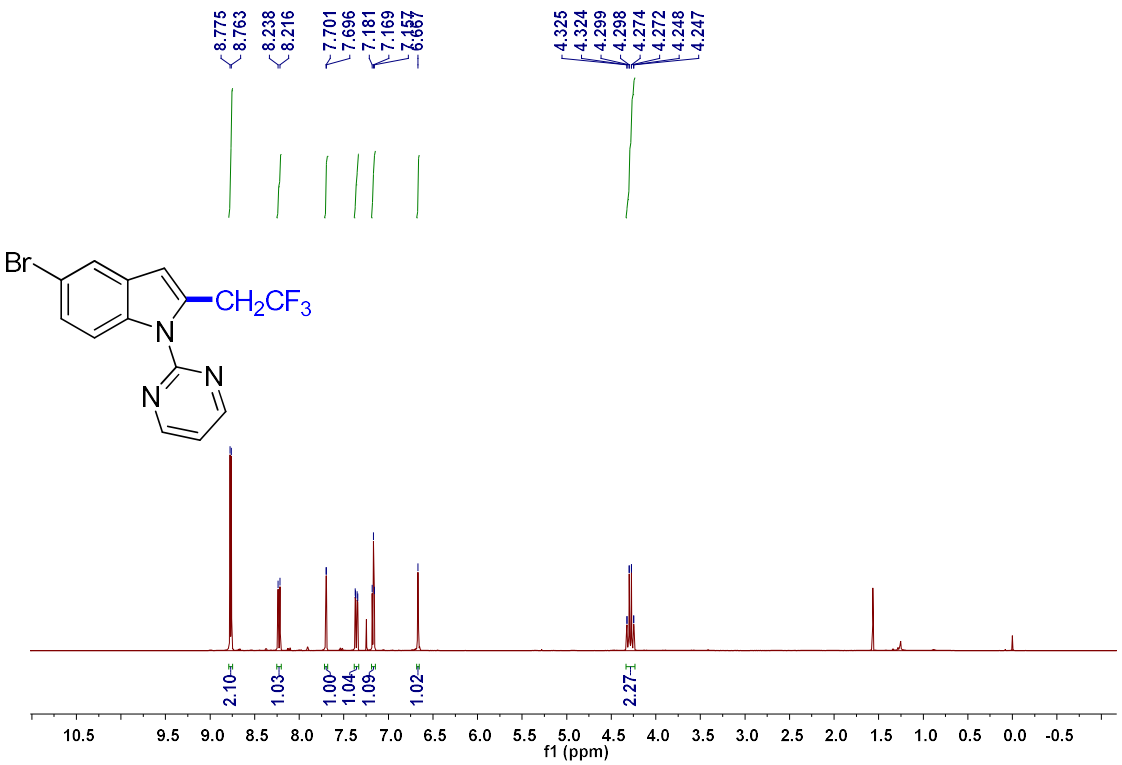
-200
f1 (ppm)

3da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7.169
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4.299
4.298
4.274
4.272
4.248
4.247
Br
CH2CF3
N
N
N
2.10
1.03
1.00
1.04
1.09
1.02
2.27
10.5
9.5
9.0
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8.0
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7.0
6.5
6.0
5.5
5.0
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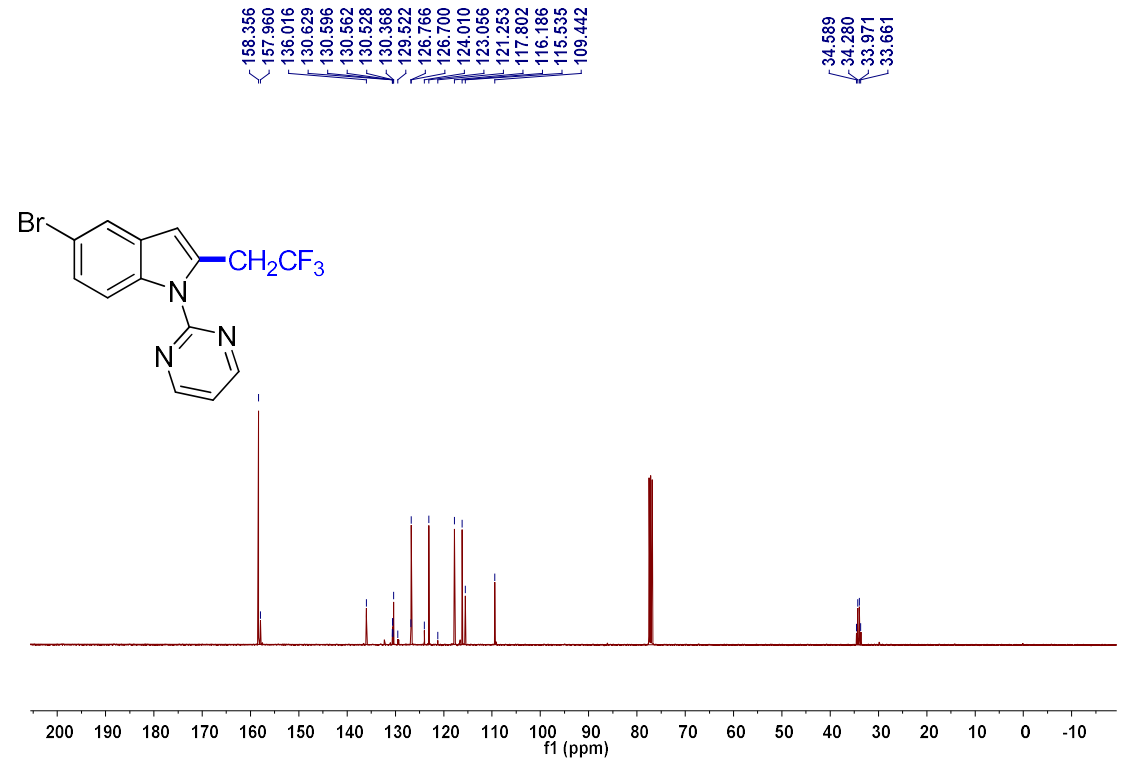
f1 (ppm)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123.056
121.253
117.802
116.186
115.535
109.442
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33.661
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N
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200
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180
170
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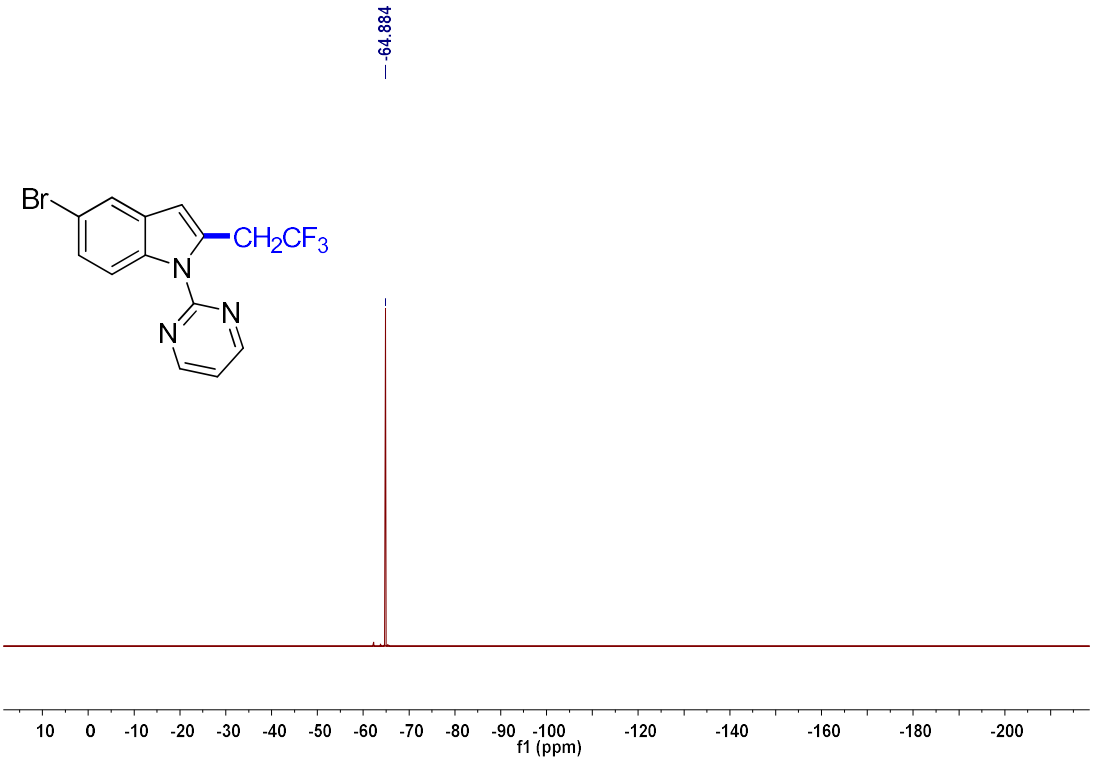
f1 (ppm)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-160
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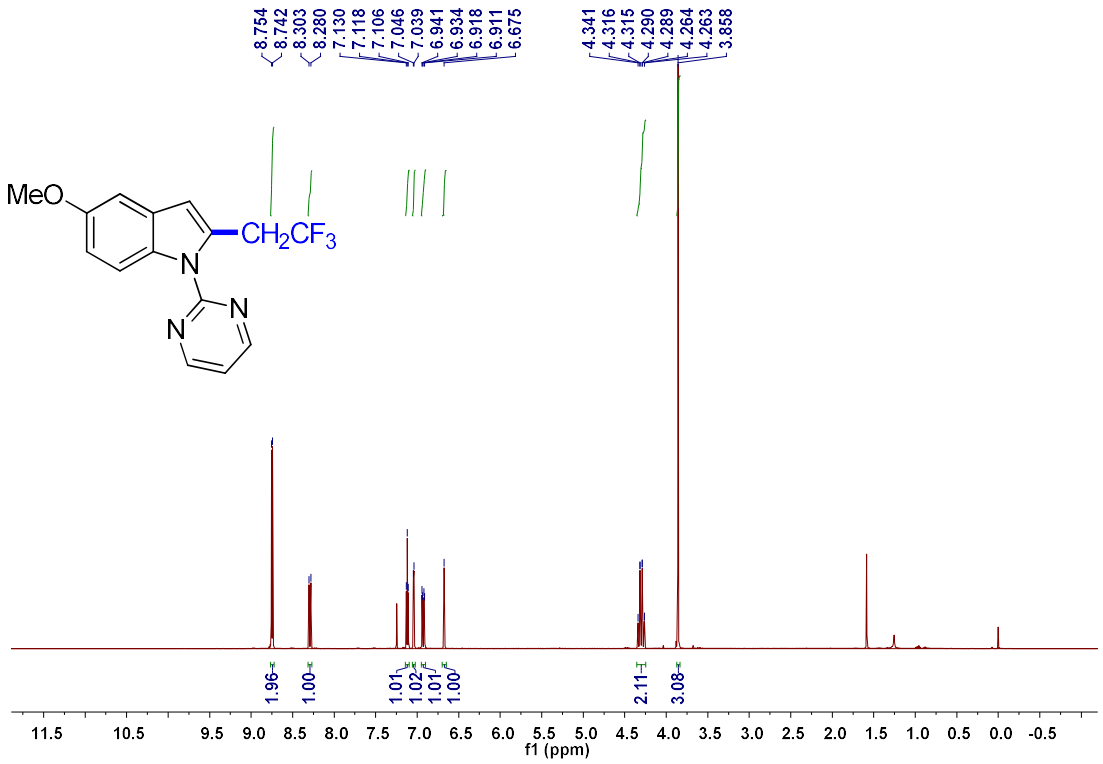
-200
f1 (ppm)

3ea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6.918
6.911
6.675
4.341
4.316
4.315
4.290
4.289
4.264
4.263
3.858
MeO
CH2CF3
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N
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1.02
1.01
1.00
2.11
3.08
11.5
10.5
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8.0
7.5
7.0
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6.0
5.5
5.0
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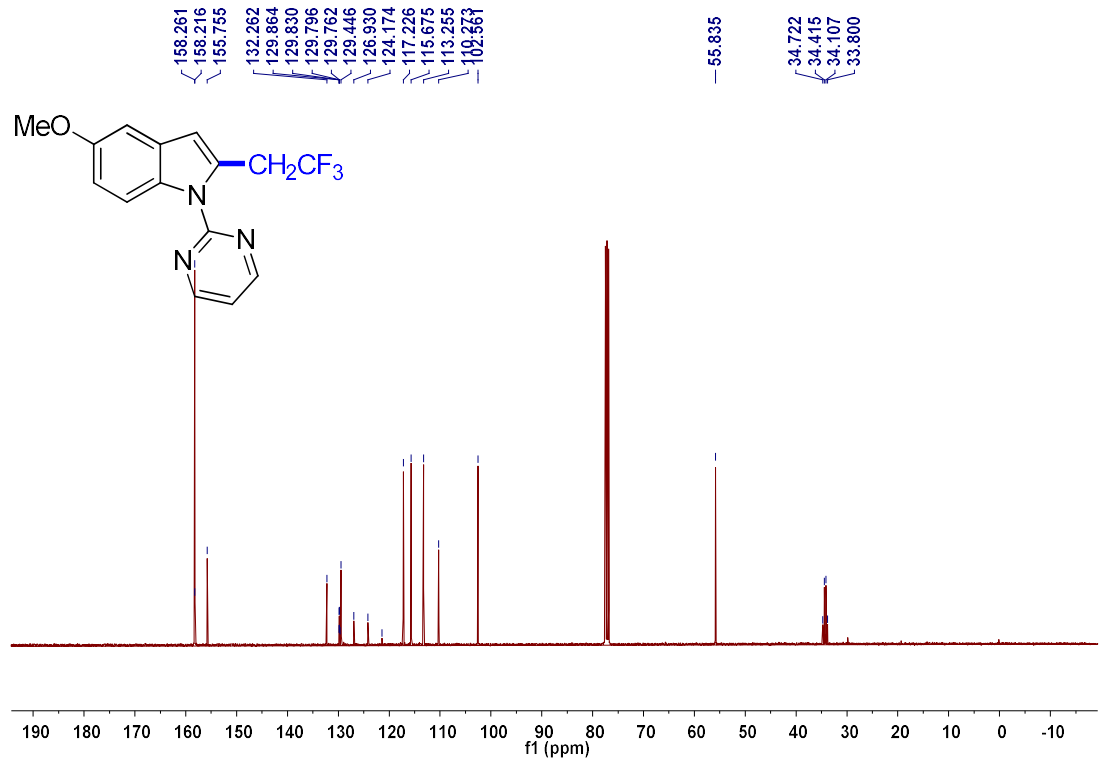
f1 (ppm)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34.107
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N
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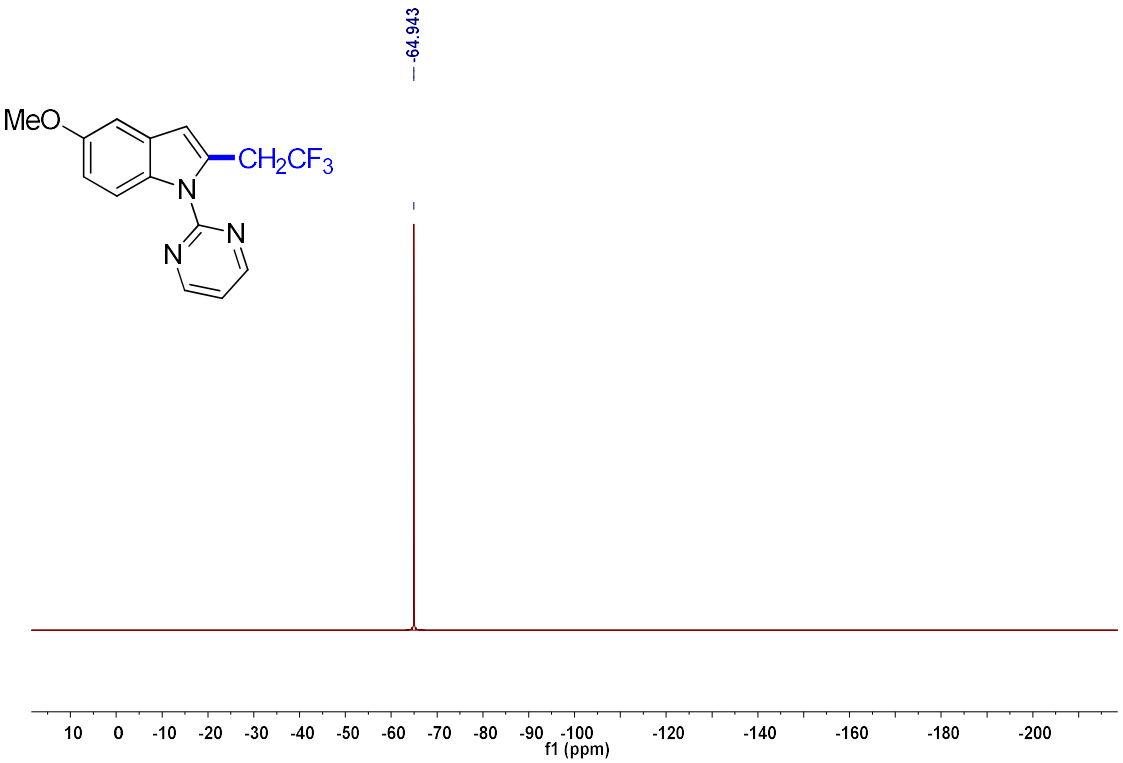
f1 (ppm)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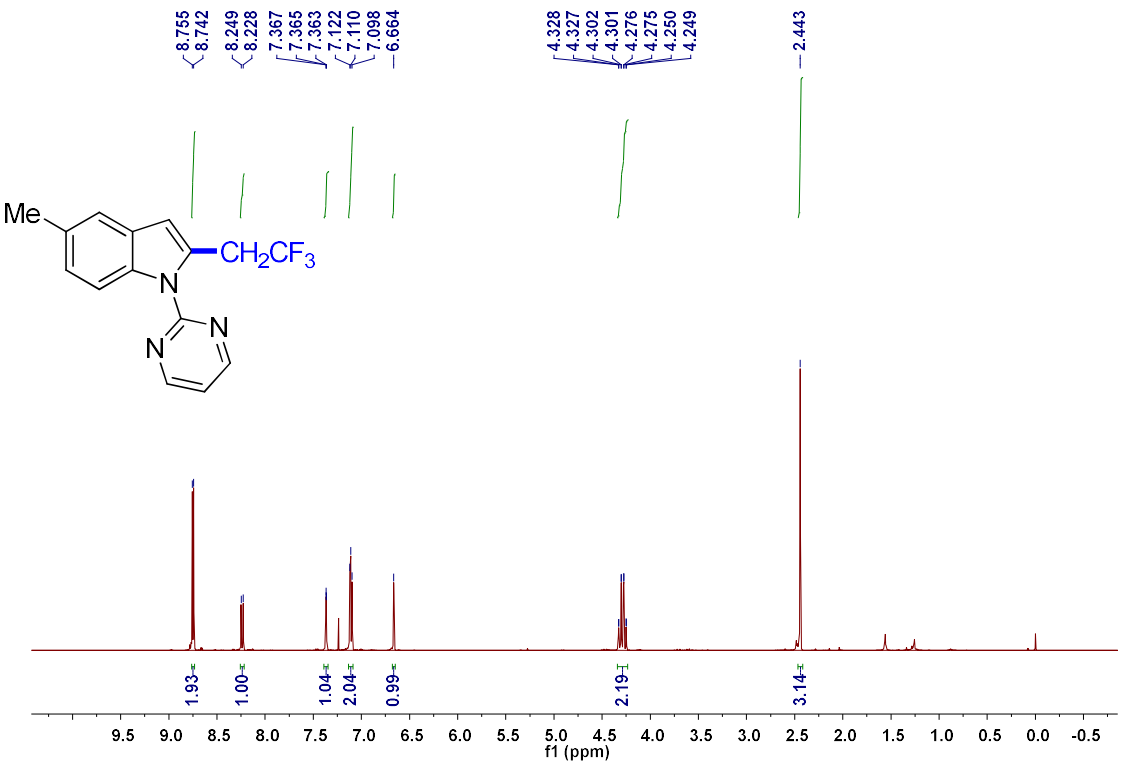
-200
f1 (ppm)

3fa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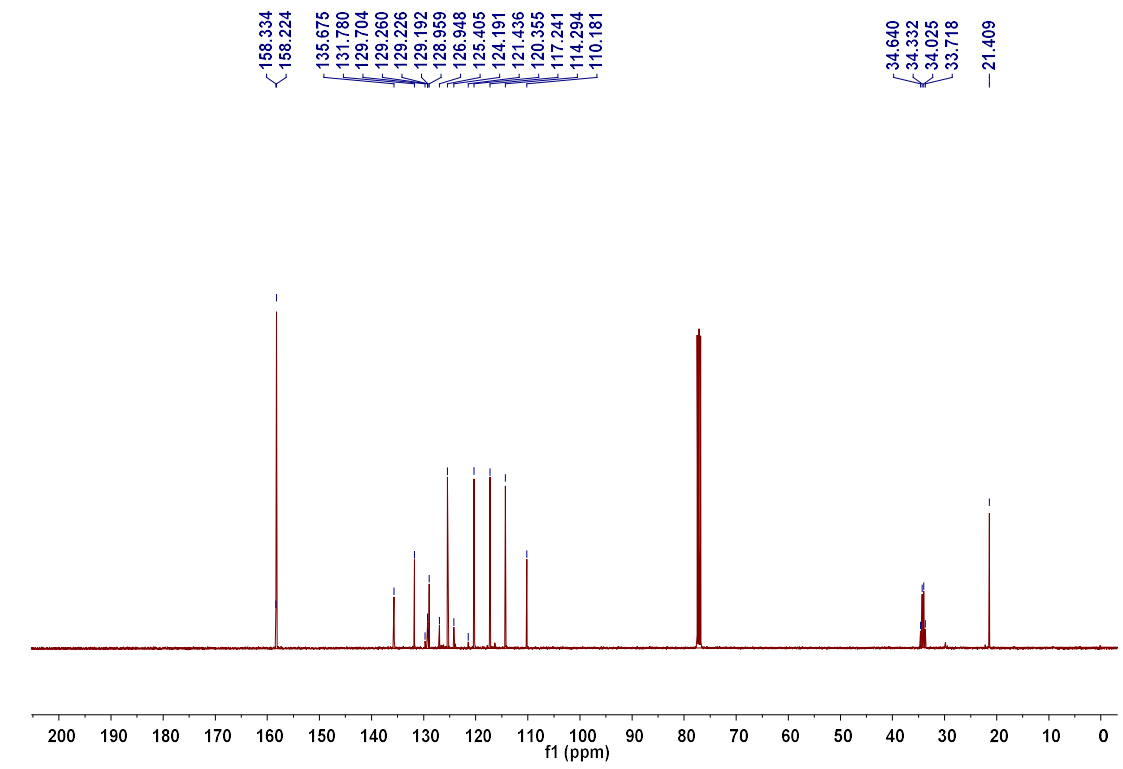
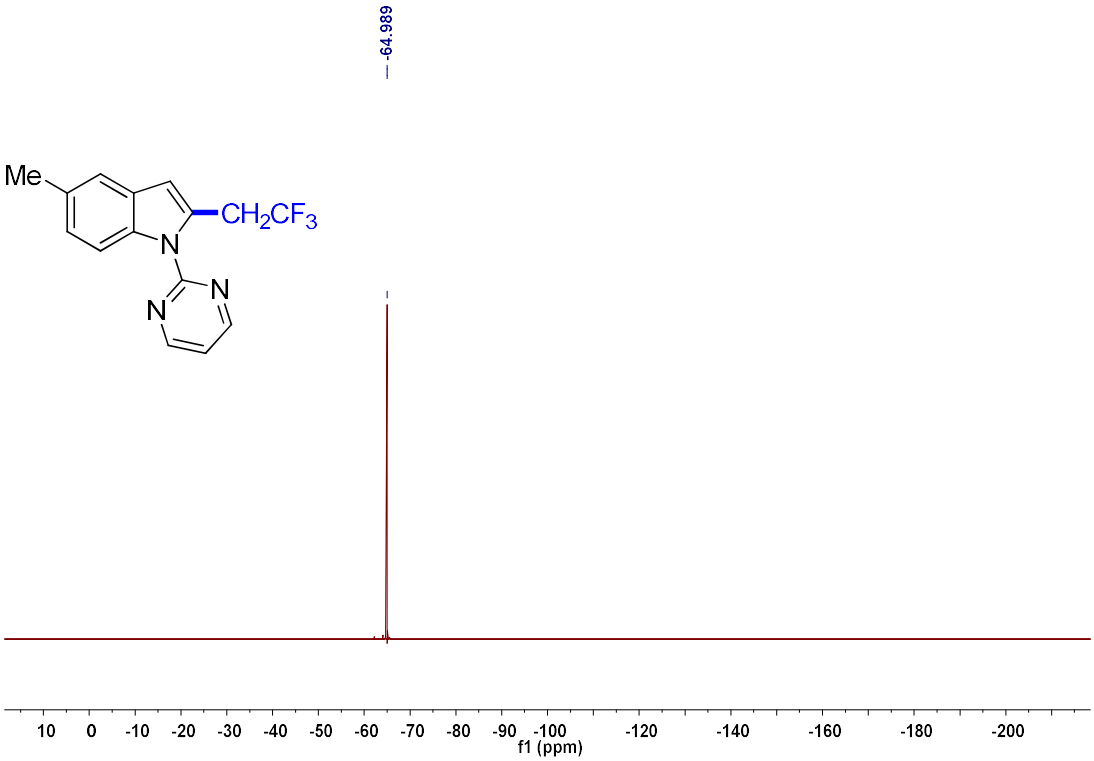
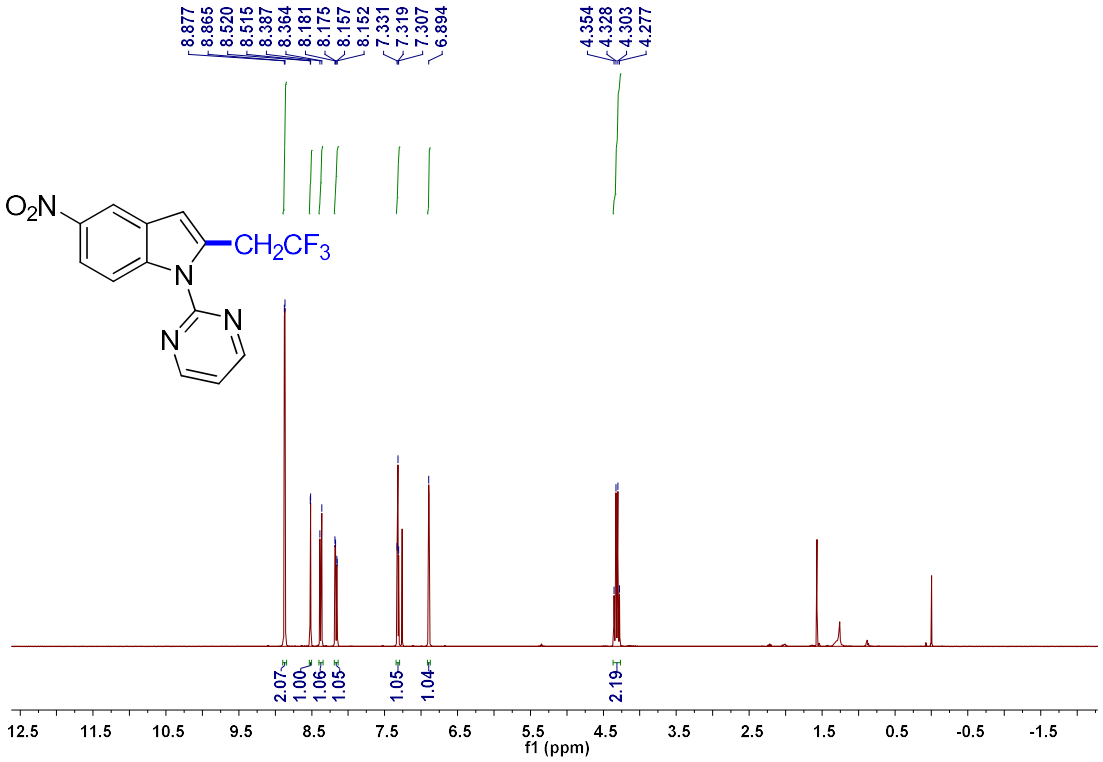
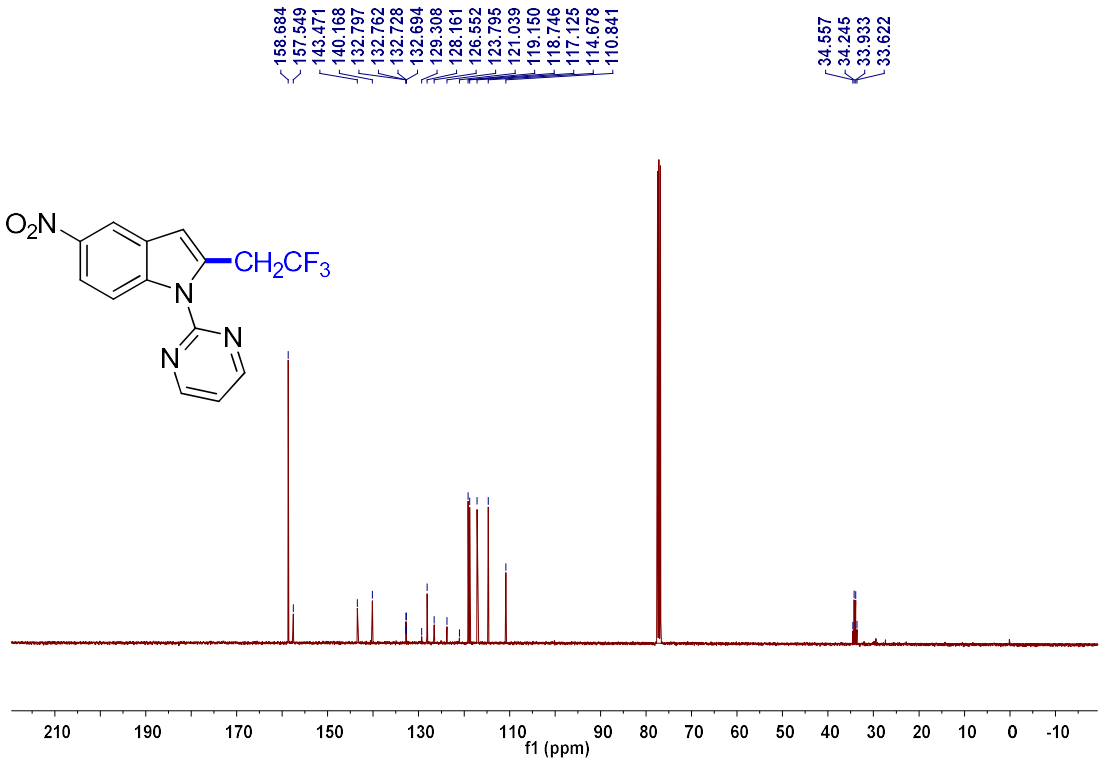
4.302
4.301
4.276
4.275
4.250
4.249
2.443
Me
CH2CF3
N
N
N
1.93
1.00
1.04
2.04
0.99
2.19
3.14
f1 (ppm)

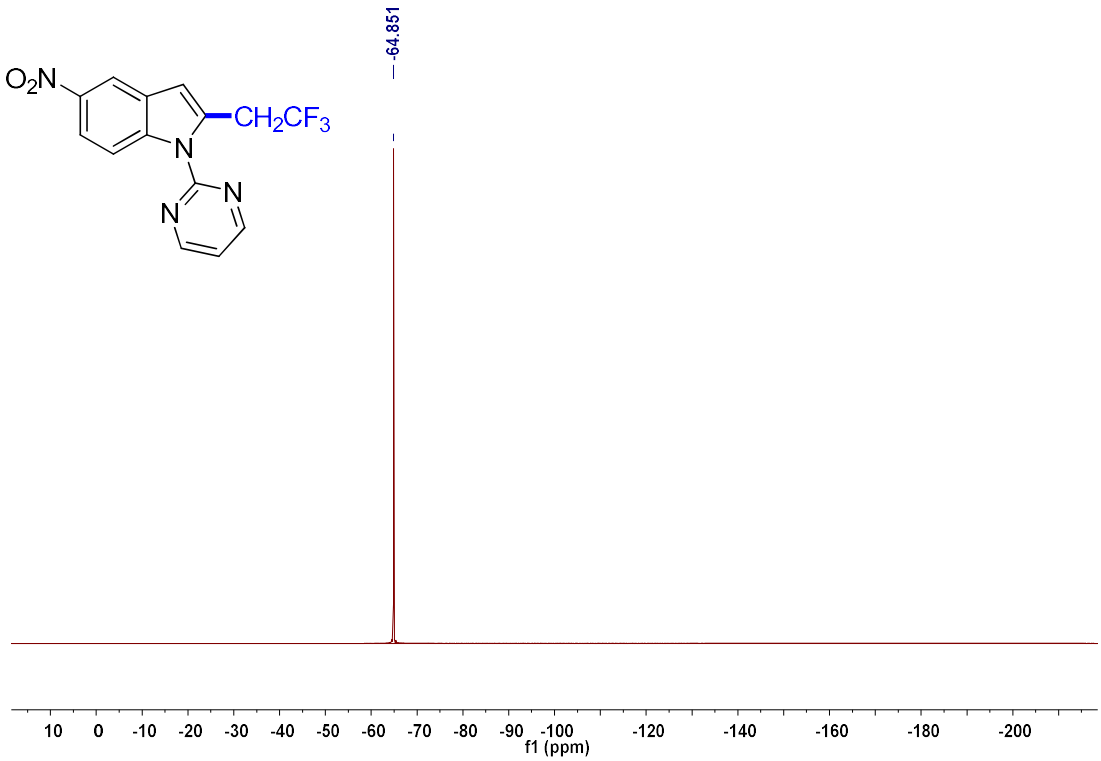

158.334
158.224
135.675
131.780
129.704
129.260
129.226
129.192
128.959
126.948
125.405
124.191
121.436
120.355
117.241
114.294
110.181
34.640
34.332
34.025
33.718
21.409
f1 (ppm)


-64.989
Me
CH2CF3
N
N
N
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)

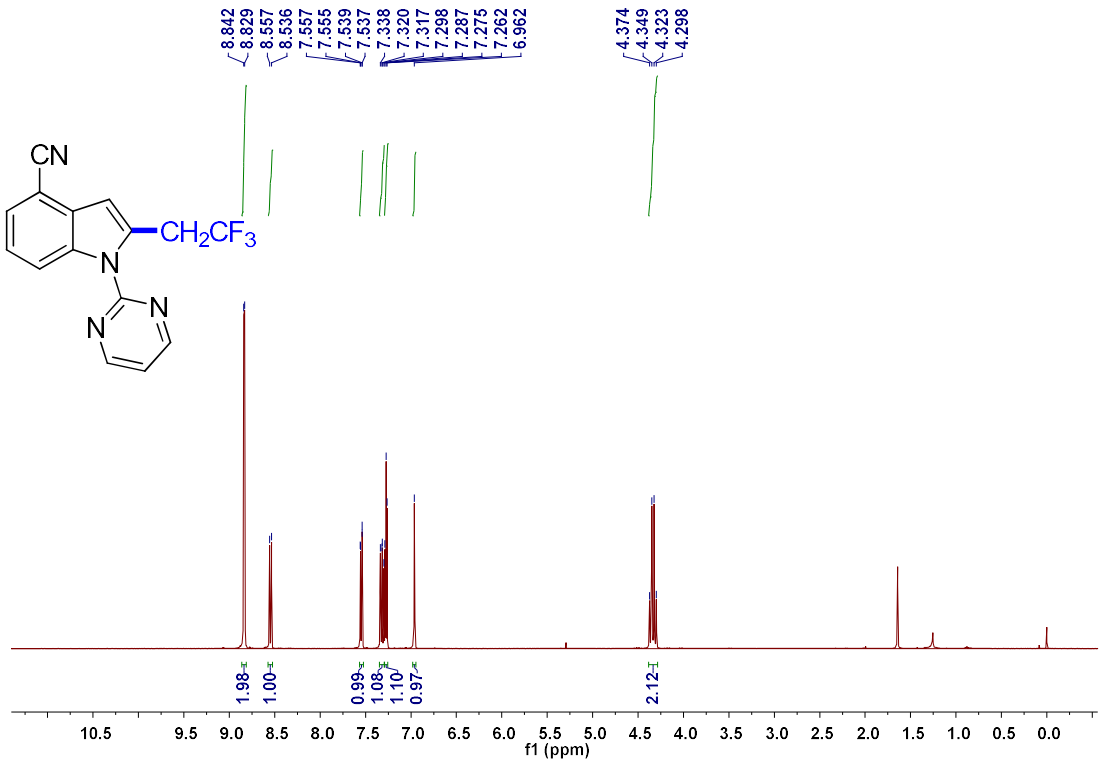
3ga

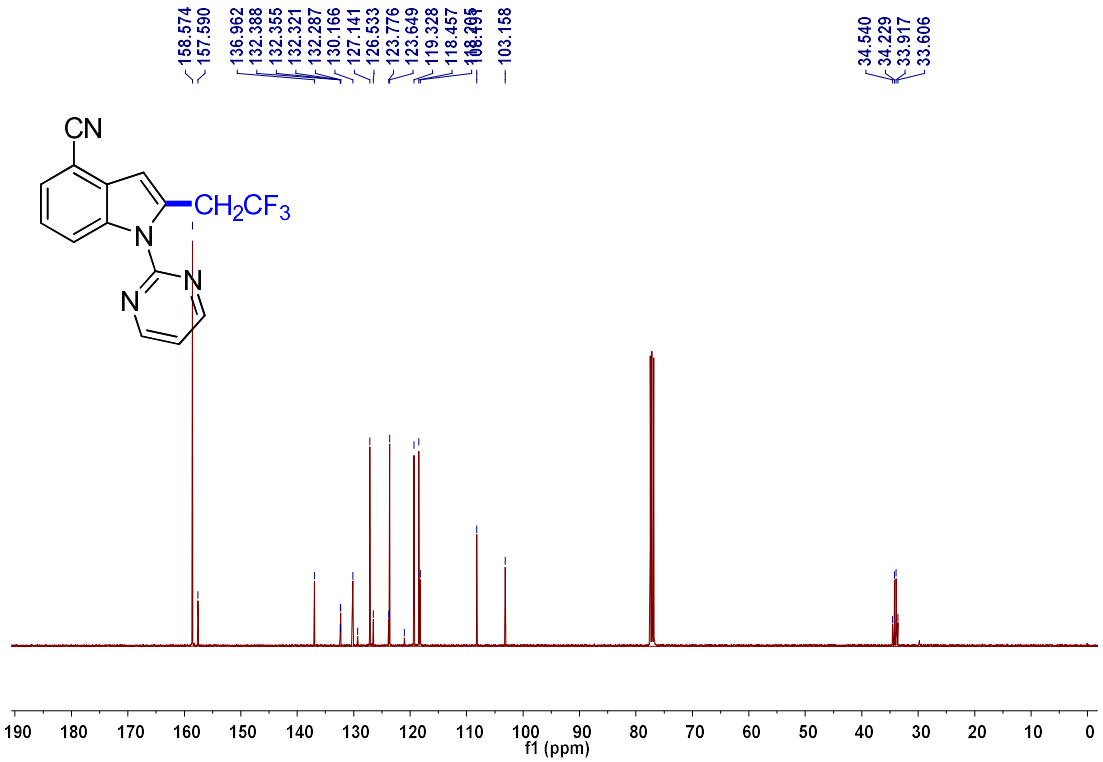

8.877
8.865
8.520
8.515
8.387
8.364
8.181
8.175
8.157
8.152
7.331
7.319
7.307
6.894
4.354
4.328
4.303
4.277
O2N
CH2CF3
N
N
N
2.07
1.00
1.06
1.05
1.05
1.04
2.19
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
-1.5
f1 (ppm)

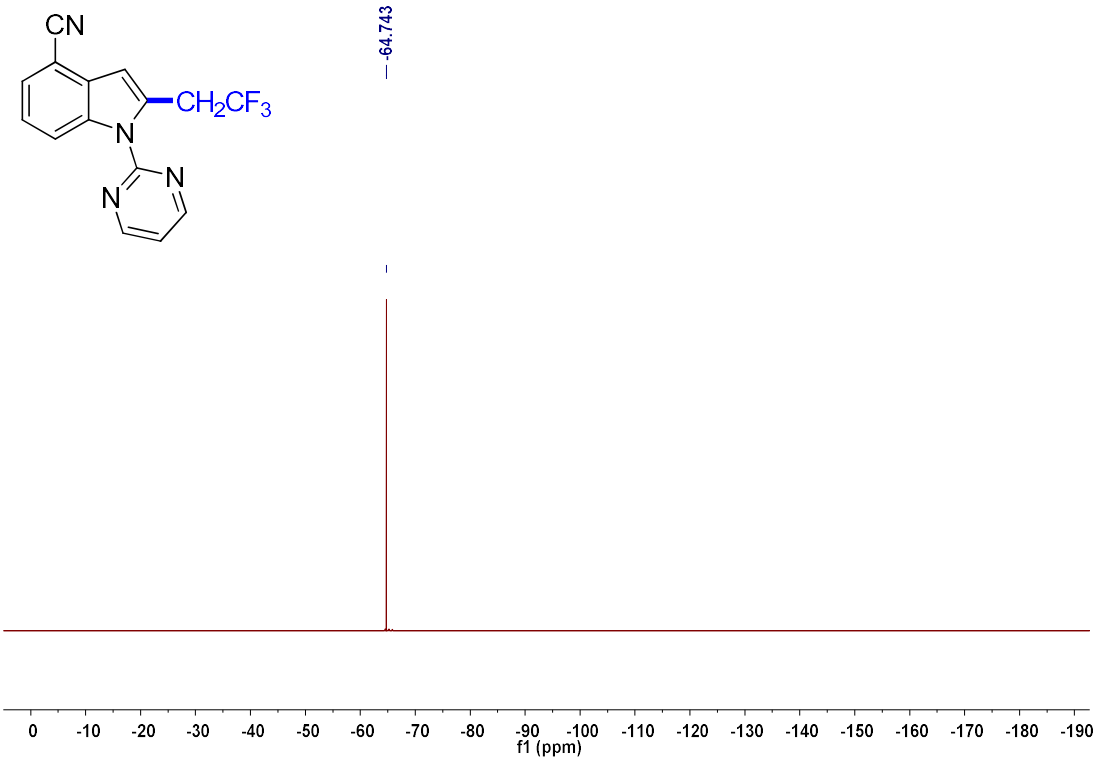

158.684
157.549
143.471
140.168
132.797
132.762
132.728
132.694
129.308
128.161
126.552
123.795
121.039
119.150
118.746
117.125
114.678
110.841
34.557
34.245
33.933
33.622
O2N
CH2CF3
N
N
N
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


O2N
CH2CF3
N
N
N
-64.851
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)

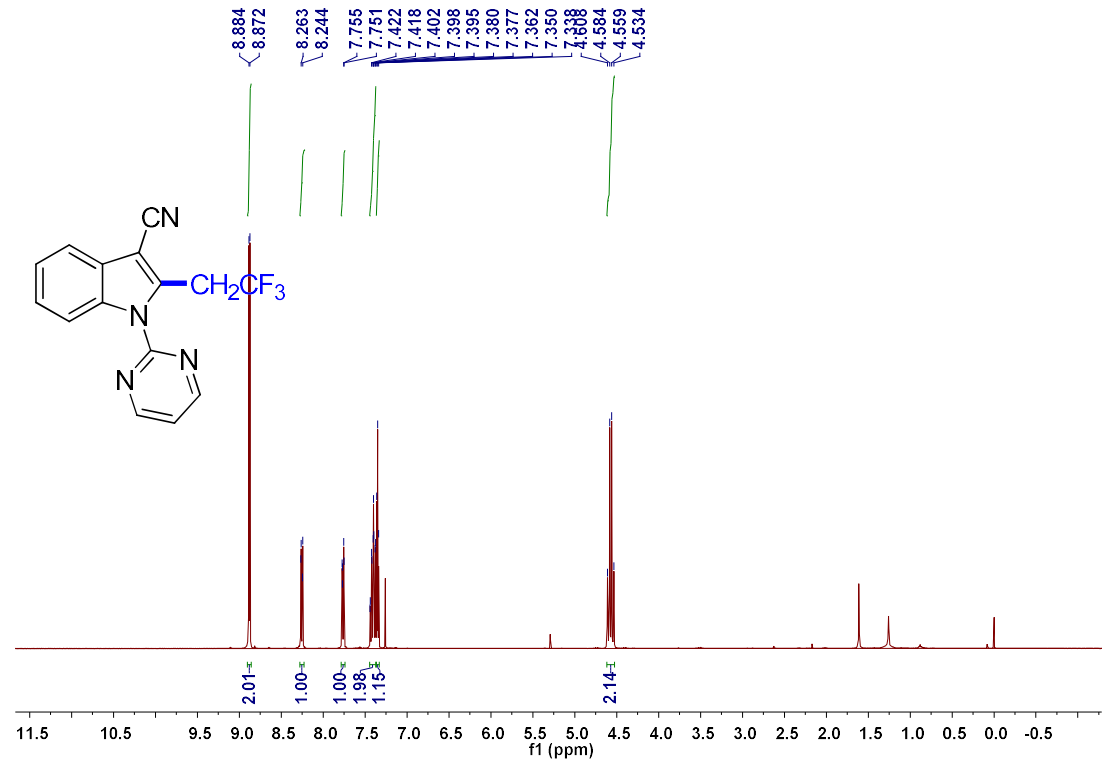
3ha

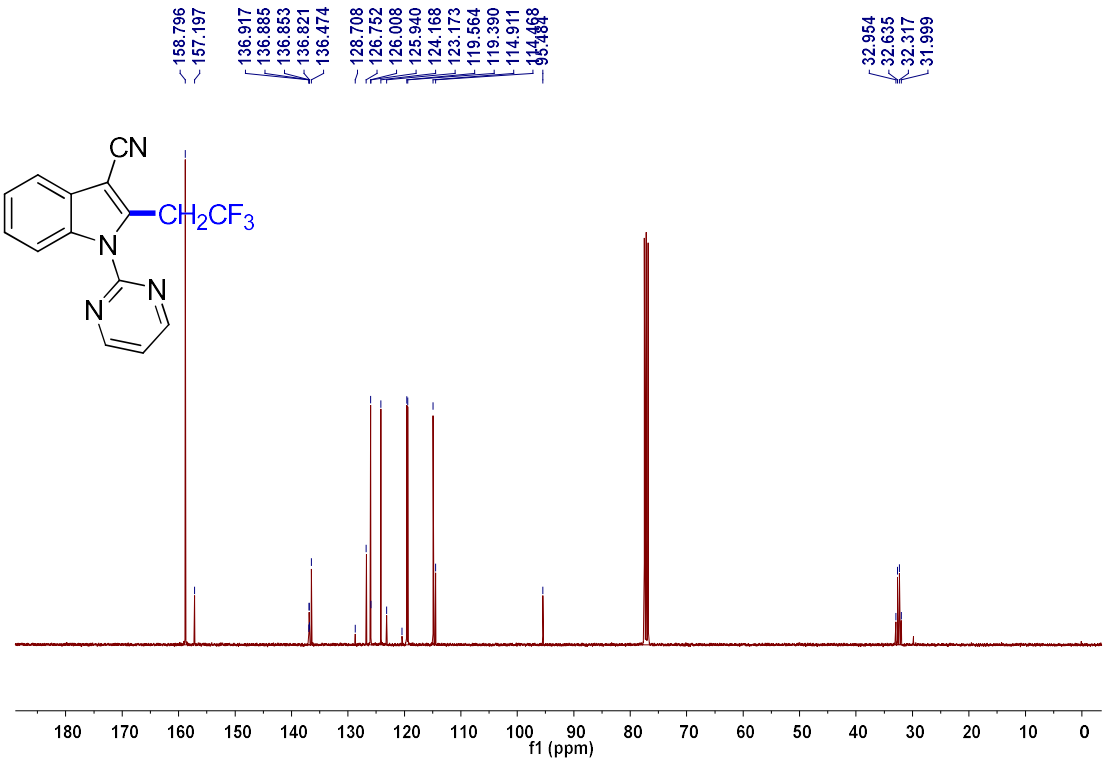

8.842
8.829
8.557
8.536
7.557
7.555
7.539
7.537
7.338
7.320
7.317
7.298
7.287
7.275
7.262
6.962
4.374
4.349
4.323
4.298
CN
CH2CF3
N
N
N
1.98
1.00
0.99
1.08
1.10
0.97
2.12
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

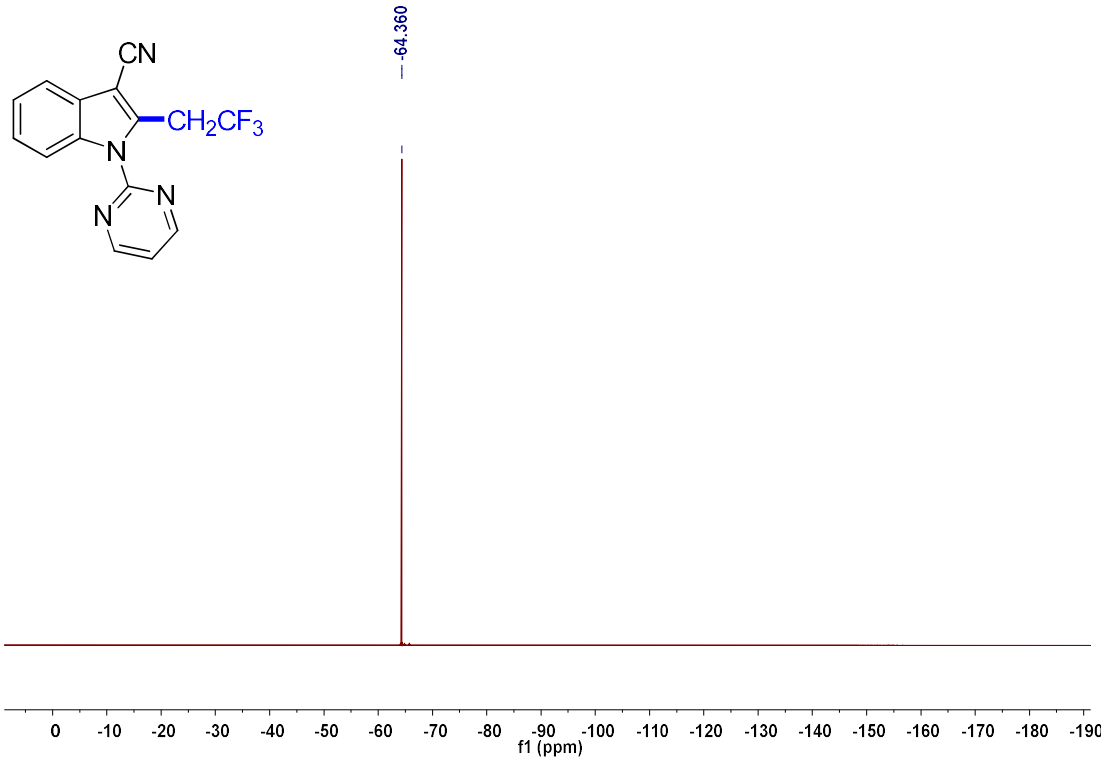

158.574
157.590
136.962
132.388
132.355
132.321
132.287
130.166
127.141
126.533
123.776
123.649
119.328
118.457
103.158
34.540
34.229
33.917
33.606
CN
CH2CF3
N
N
N
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


CN
CH2CF3
N
N
N
-64.743
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)

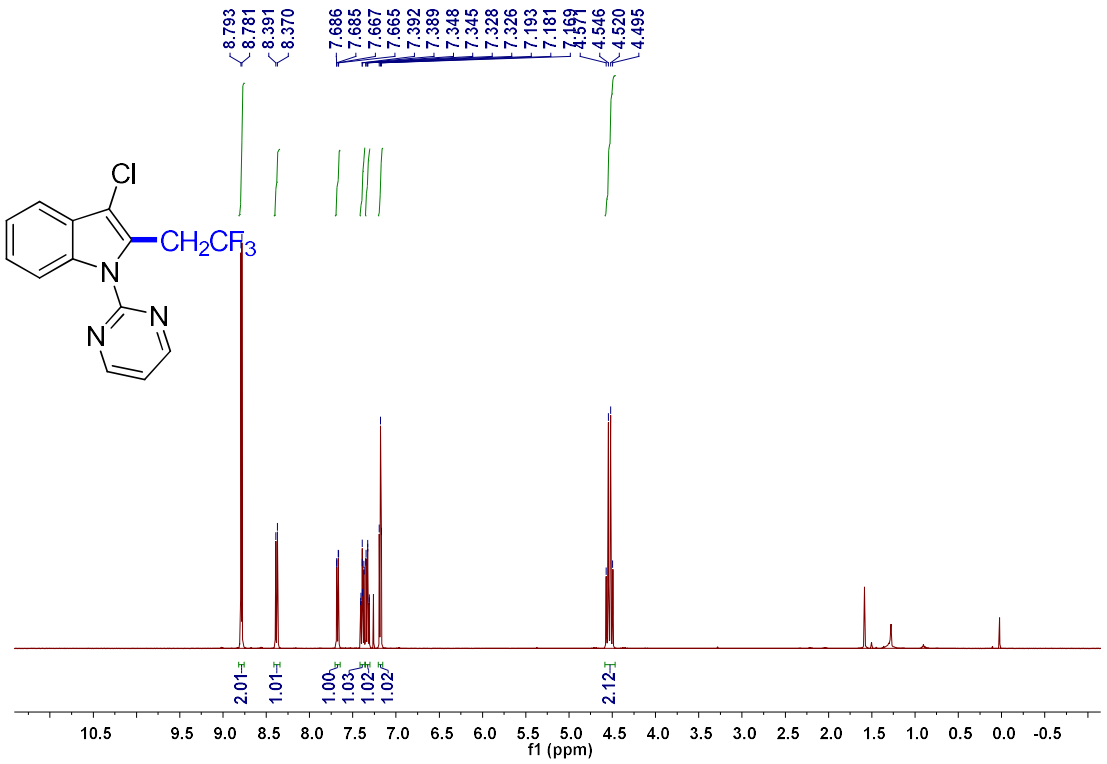
3ia

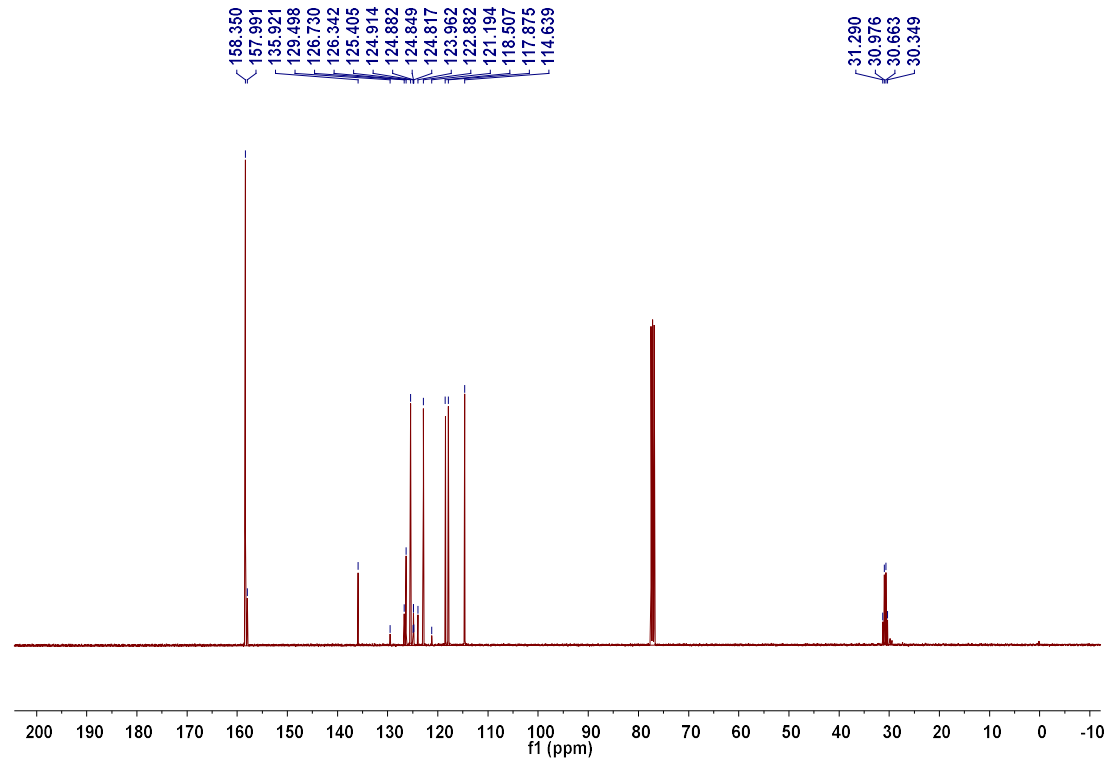

8.884
8.872
8.263
8.244
7.755
7.751
7.422
7.418
7.402
7.398
7.395
7.380
7.377
7.362
7.350
4.584
4.559
4.534
CN
CH2CF3
N
N
N
2.01
1.00
1.00
1.98
1.15
2.14
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

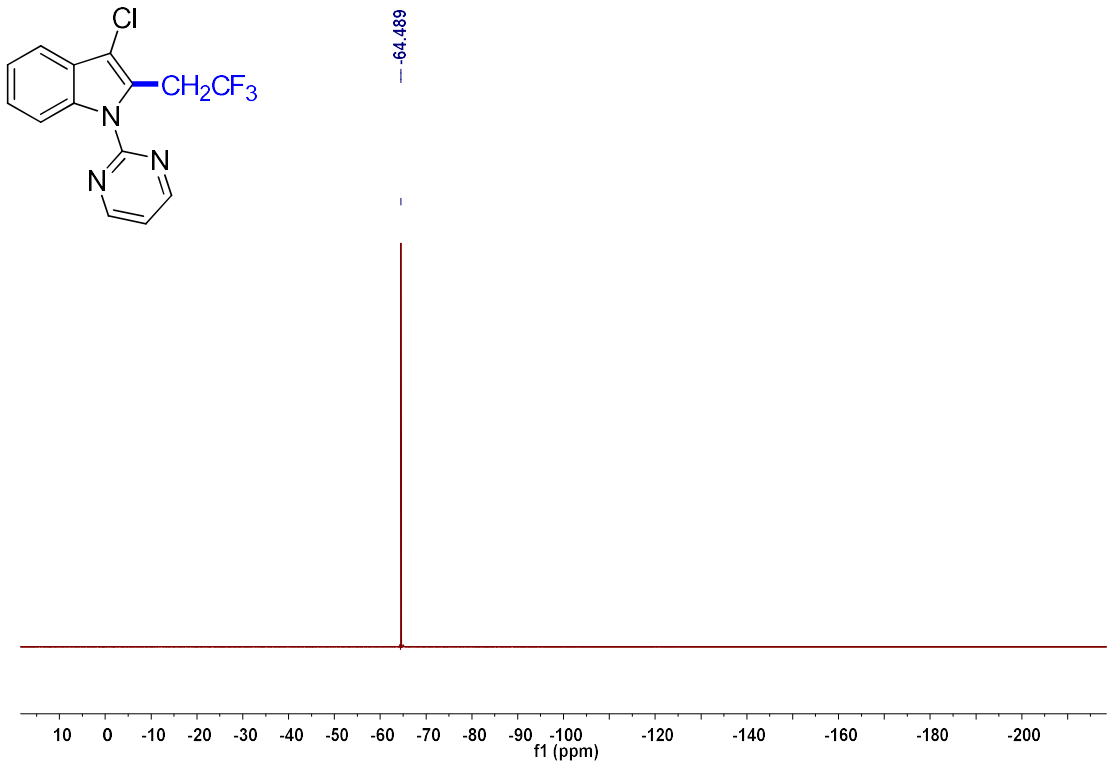

158.796
157.197
136.917
136.885
136.853
136.821
136.474
128.708
126.752
126.008
125.940
124.168
123.173
119.564
119.390
114.911
32.954
32.635
32.317
31.999
CN
CH2CF3
N
N
N
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


CN
CH2CF3
N
N
N
-64.360
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)

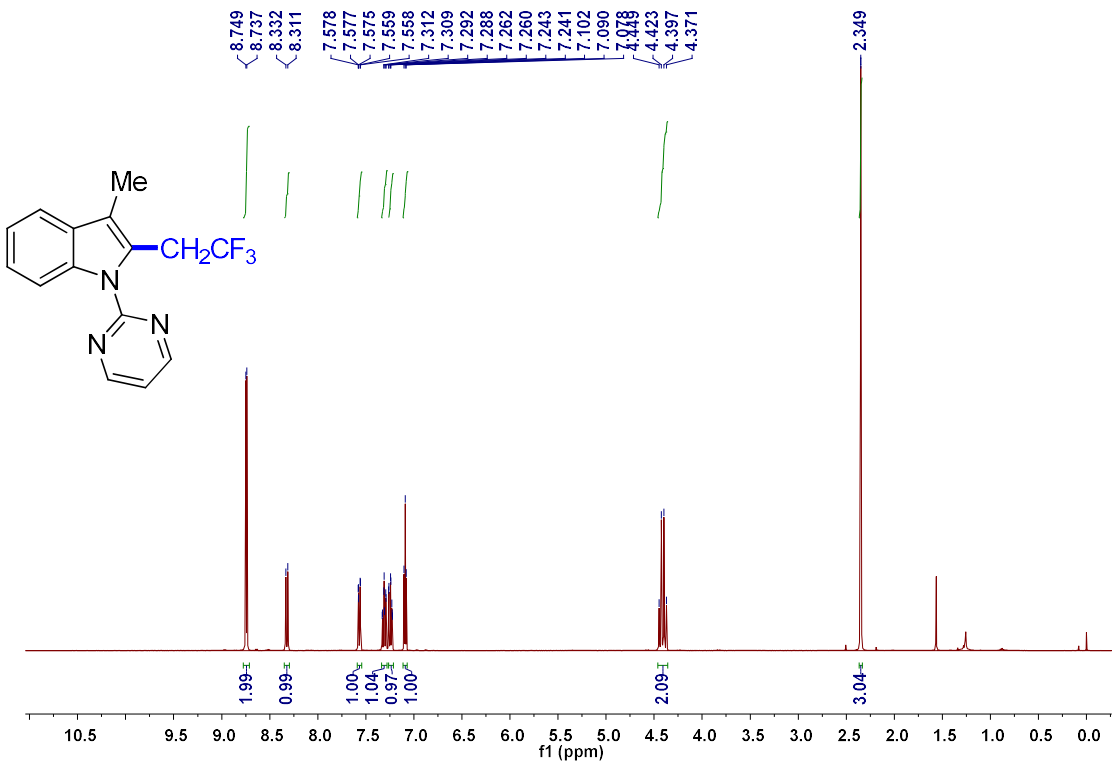
3ja

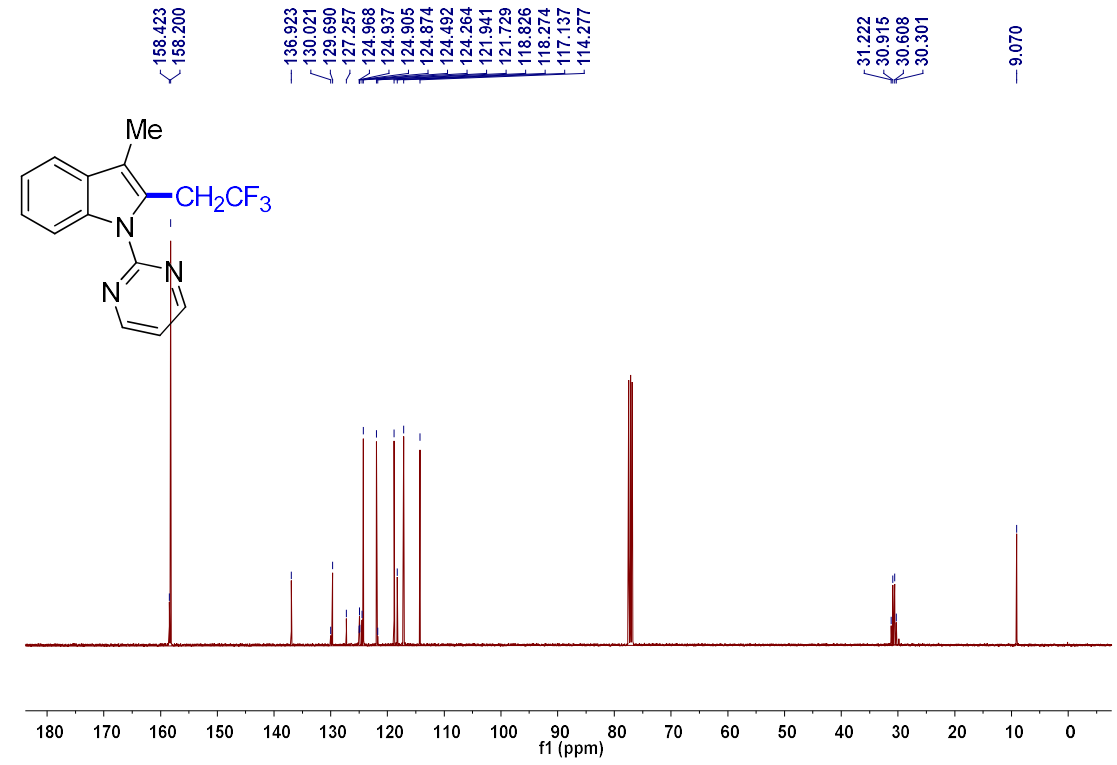

8.793
8.781
8.391
8.370
7.686
7.685
7.667
7.665
7.392
7.389
7.348
7.345
7.328
7.326
7.193
7.181
4.546
4.520
4.495
Cl
CH2CF3
N
N
N
2.01
1.01
1.00
1.03
1.02
1.02
2.12
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

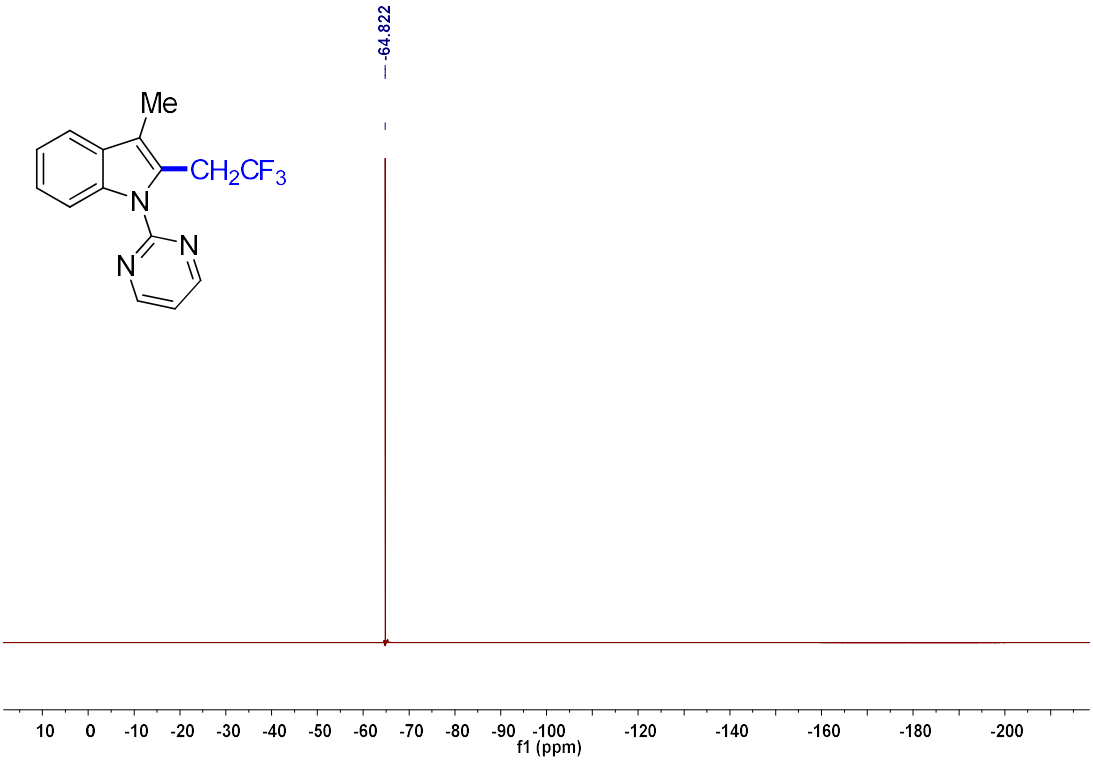

158.350
157.991
135.921
129.498
126.730
126.342
125.405
124.914
124.882
124.849
124.817
123.962
122.882
121.194
118.507
117.875
114.639
31.290
30.976
30.663
30.349
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


Cl
CH2CF3
N
N
N
-64.489
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)

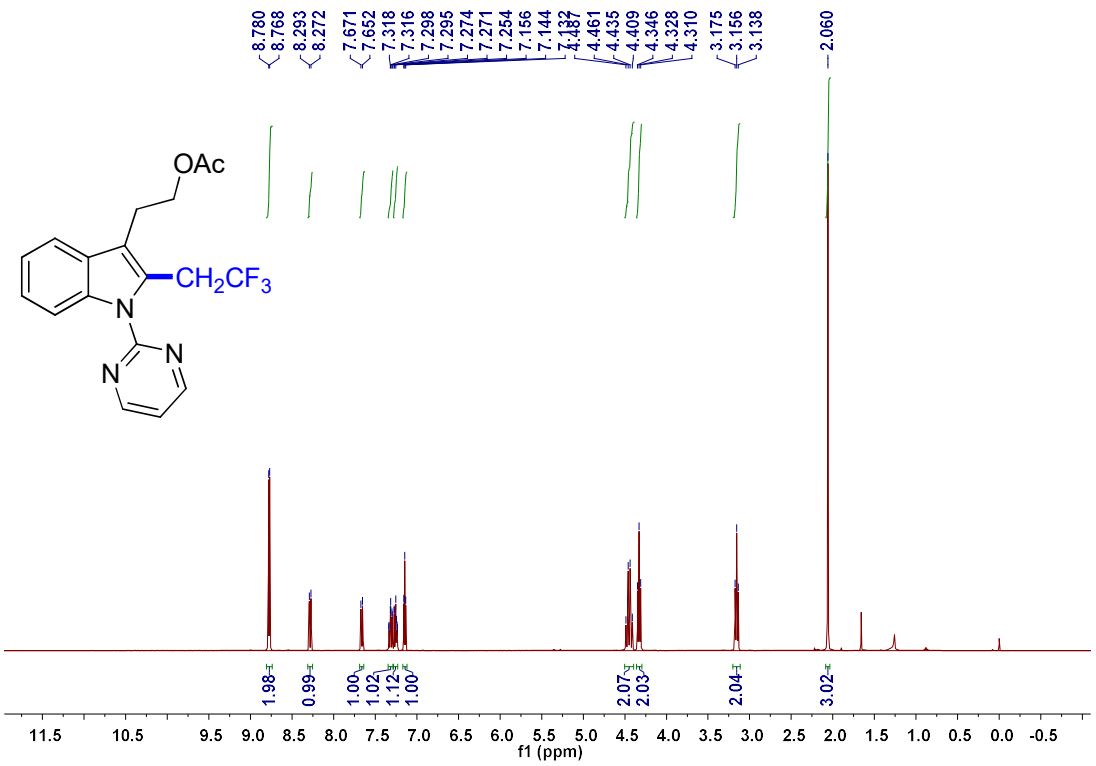
3ka

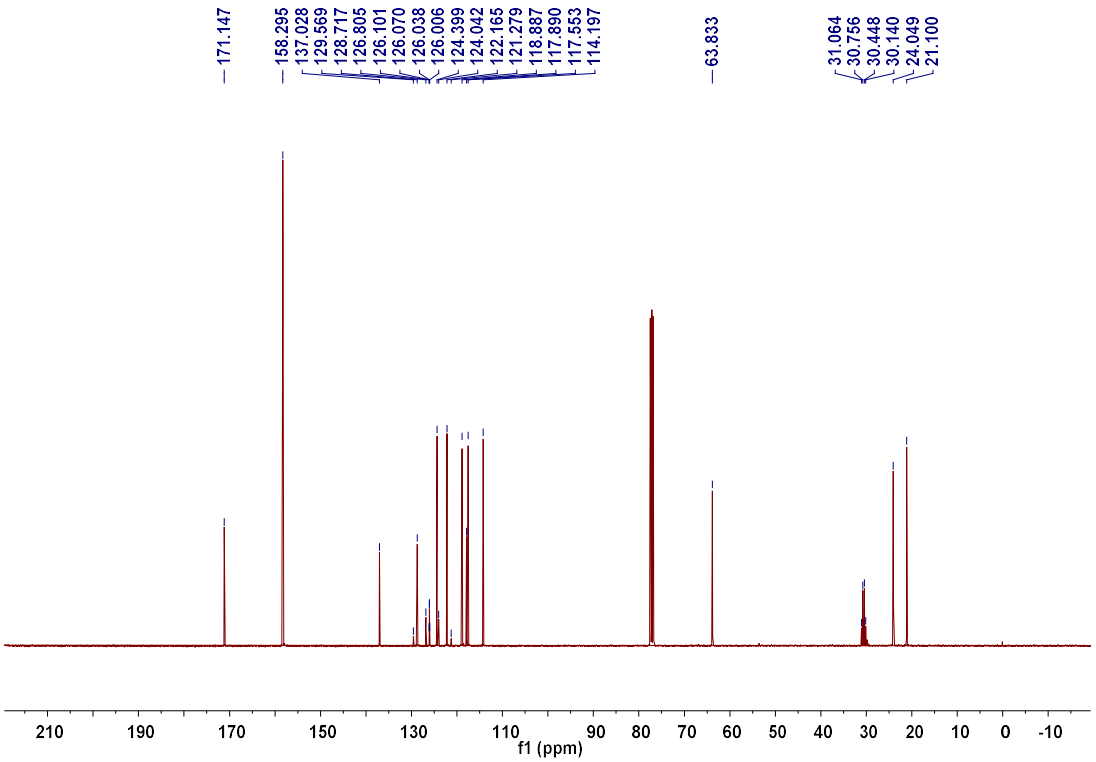

8.749
8.737
8.332
8.311
7.578
7.577
7.575
7.559
7.558
7.312
7.309
7.292
7.288
7.262
7.260
7.243
7.241
7.102
7.090
4.423
4.397
4.371
2.349
Me
CH2CF3
N
N
N
1.99
0.99
1.00
1.04
0.97
1.00
2.09
3.04
f1 (ppm)

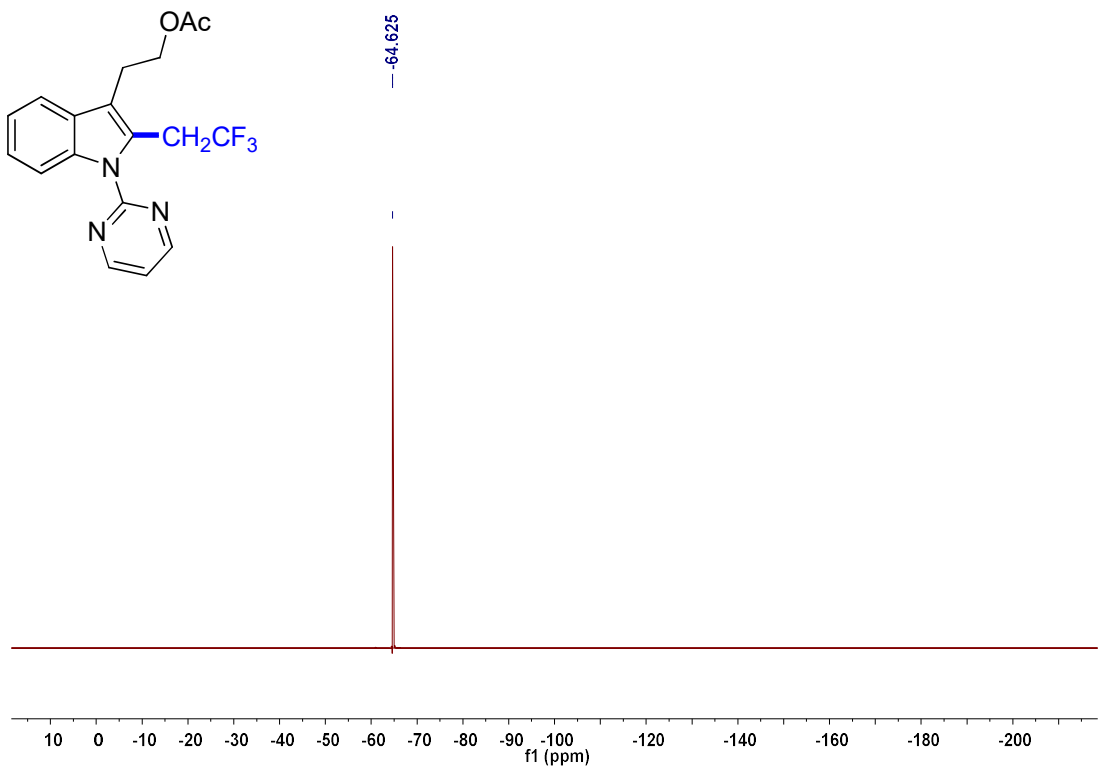

158.423
158.200
136.923
130.021
129.690
127.257
124.968
124.937
124.905
124.874
124.492
124.264
121.941
121.729
118.826
118.274
117.137
114.277
31.222
30.915
30.608
30.301
9.070
Me
CH2CF3
N
N
N
f1 (ppm)


-64.822
Me
CH2CF3
N
N
N
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)

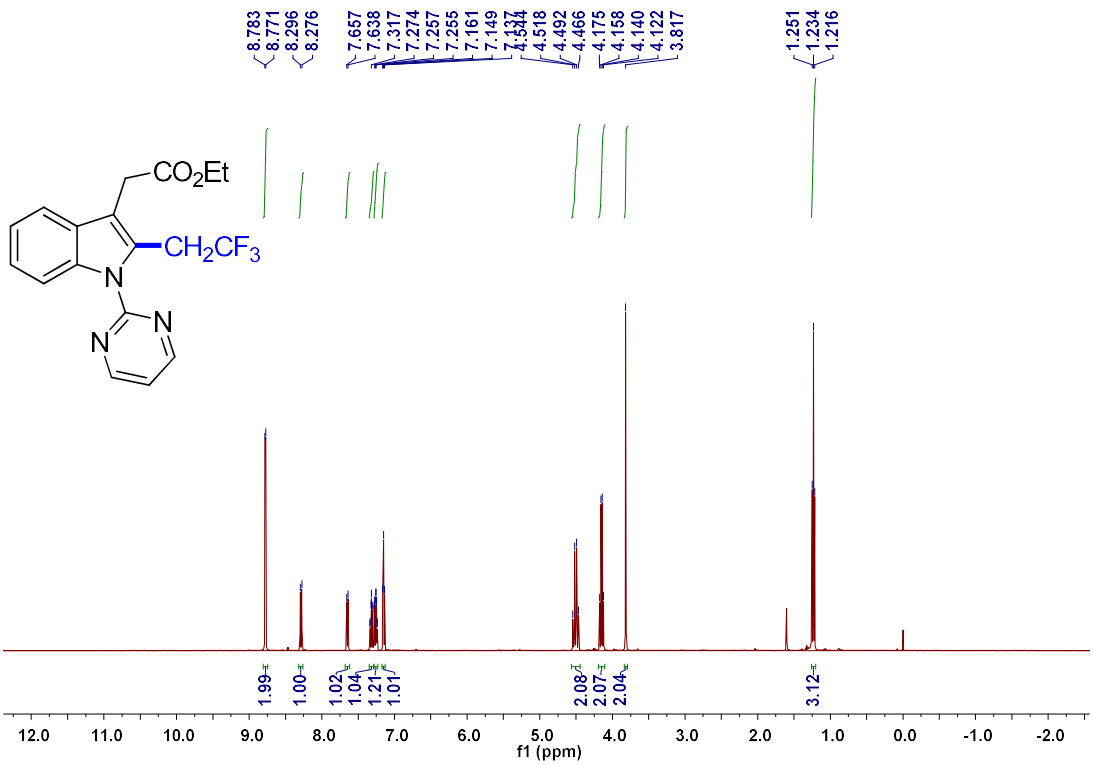
3la

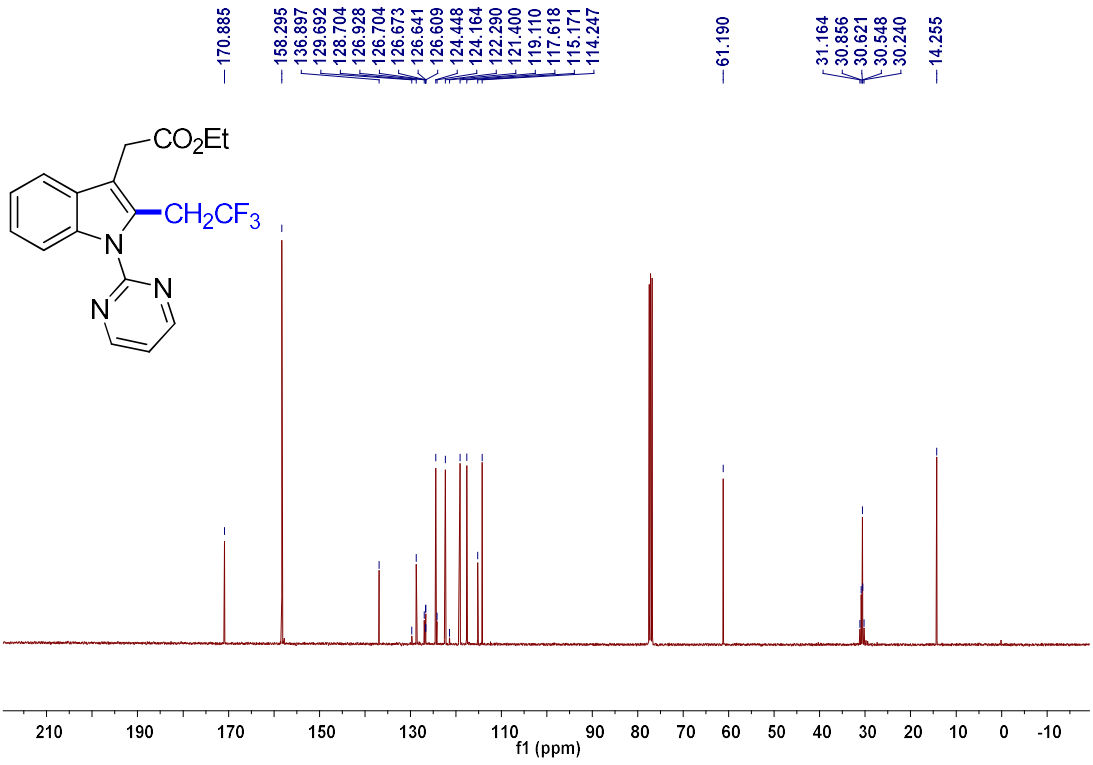

8.780
8.768
8.293
8.272
7.671
7.652
7.318
7.316
7.298
7.295
7.274
7.271
7.254
7.156
7.144
4.461
4.435
4.409
4.346
4.328
4.310
3.175
3.156
3.138
2.060
OAc
CH2CF3
N
N
N
1.98
0.99
1.00
1.02
1.12
1.00
2.07
2.03
2.04
3.02
f1 (ppm)

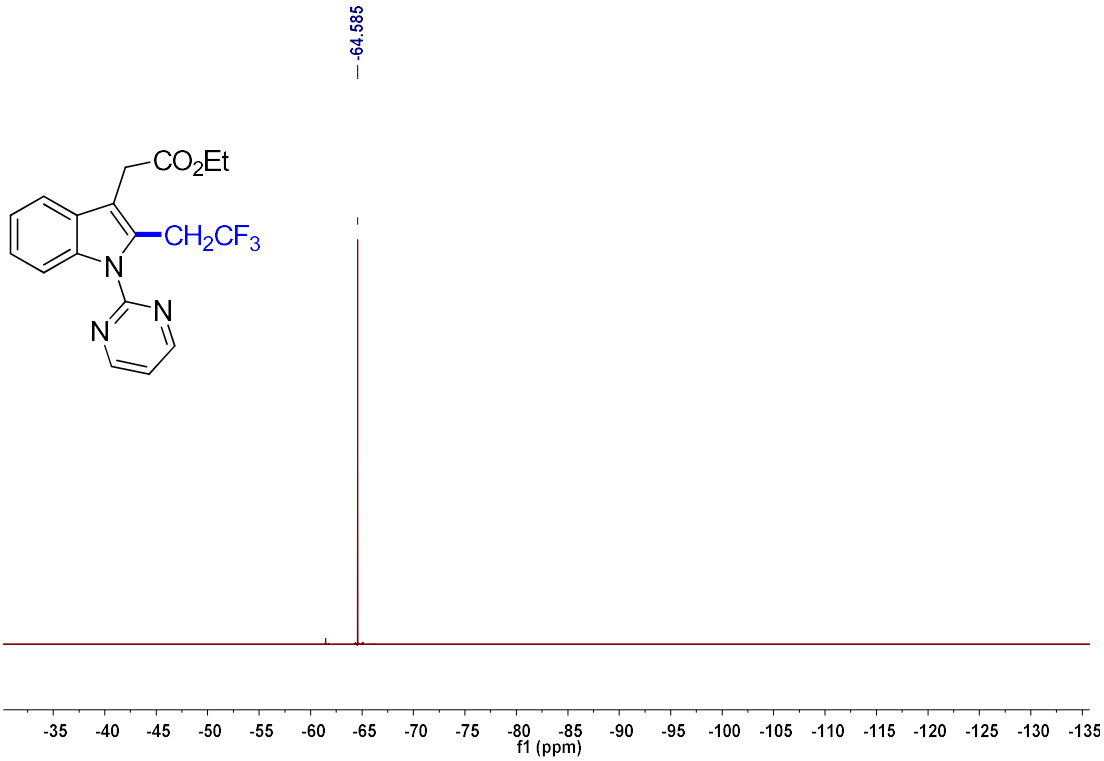

171.147
158.295
137.028
129.569
128.717
126.805
126.101
126.070
126.038
126.006
124.399
124.042
122.165
121.279
118.887
117.890
117.553
114.197
63.833
31.064
30.756
30.448
30.140
24.049
21.100
f1 (ppm)


OAc
CH2CF3
N
N
N
-64.625
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)

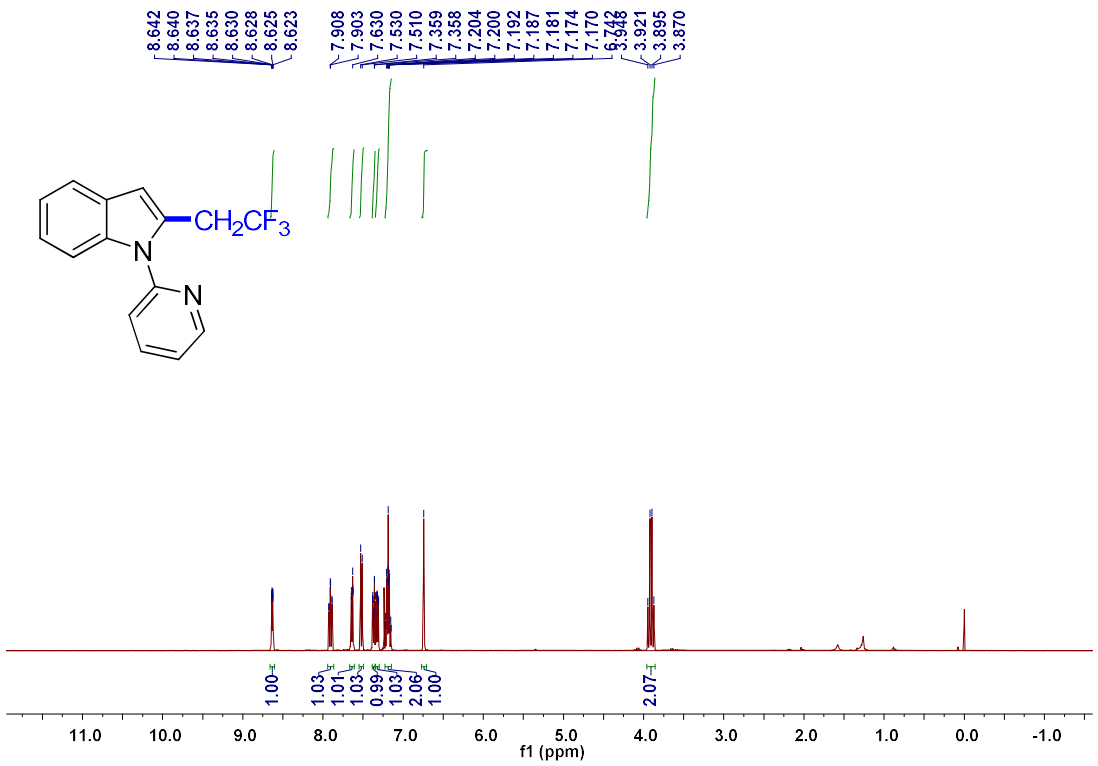
3ma

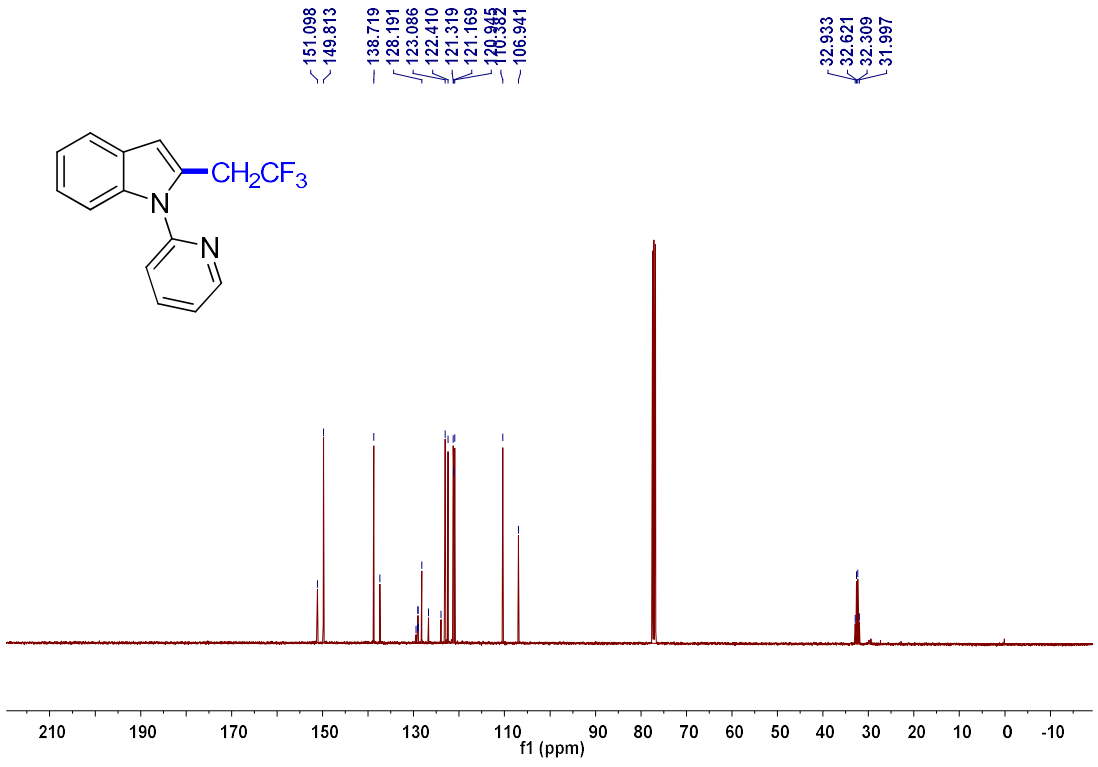

8.783
8.771
8.296
8.276
7.657
7.638
7.317
7.274
7.257
7.255
7.161
7.149
7.137
4.534
4.518
4.492
4.466
4.175
4.158
4.140
4.122
3.817
1.251
1.234
1.216
CO2Et
CH2CF3
N
N
N
1.99
1.00
1.02
1.04
1.21
1.01
2.08
2.07
2.04
3.12
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)

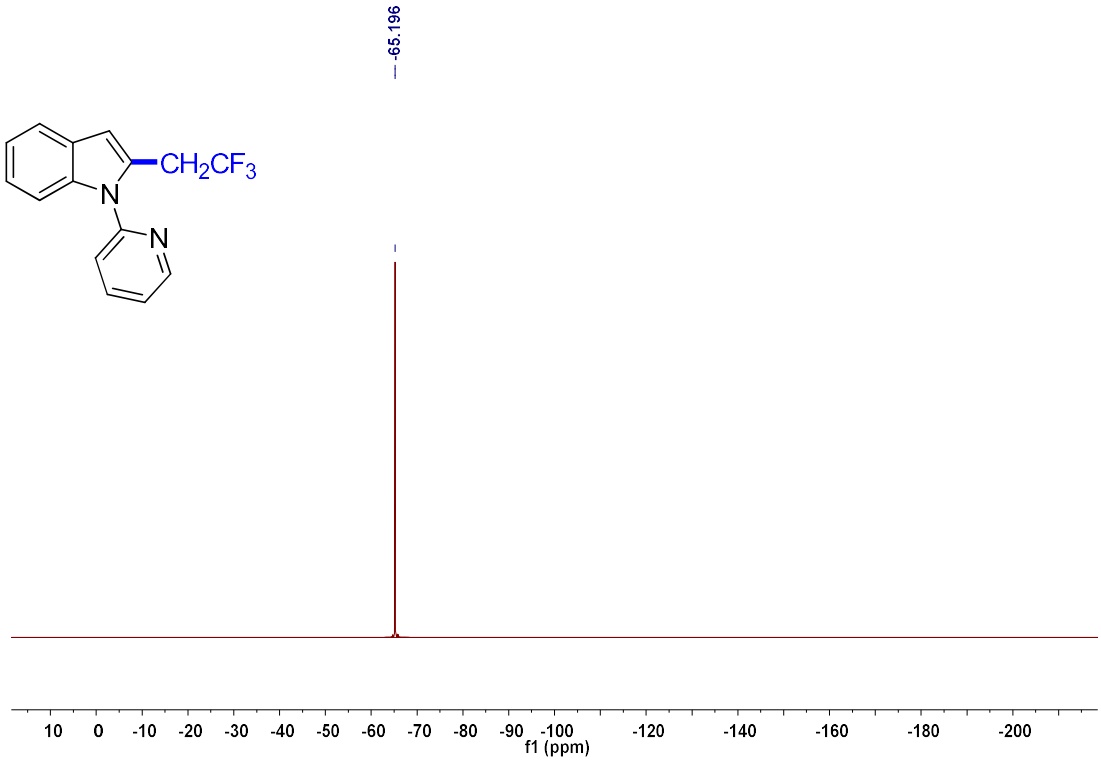

170.885
158.295
136.897
129.692
128.704
126.928
126.704
126.673
126.641
126.609
124.448
124.164
122.290
121.400
119.110
117.618
115.171
114.247
61.190
31.164
30.856
30.621
30.548
30.240
14.255
CO2Et
CH2CF3
N
N
N
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


-64.585
CO2Et
CH2CF3
N
N
N
-35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135
f1 (ppm)

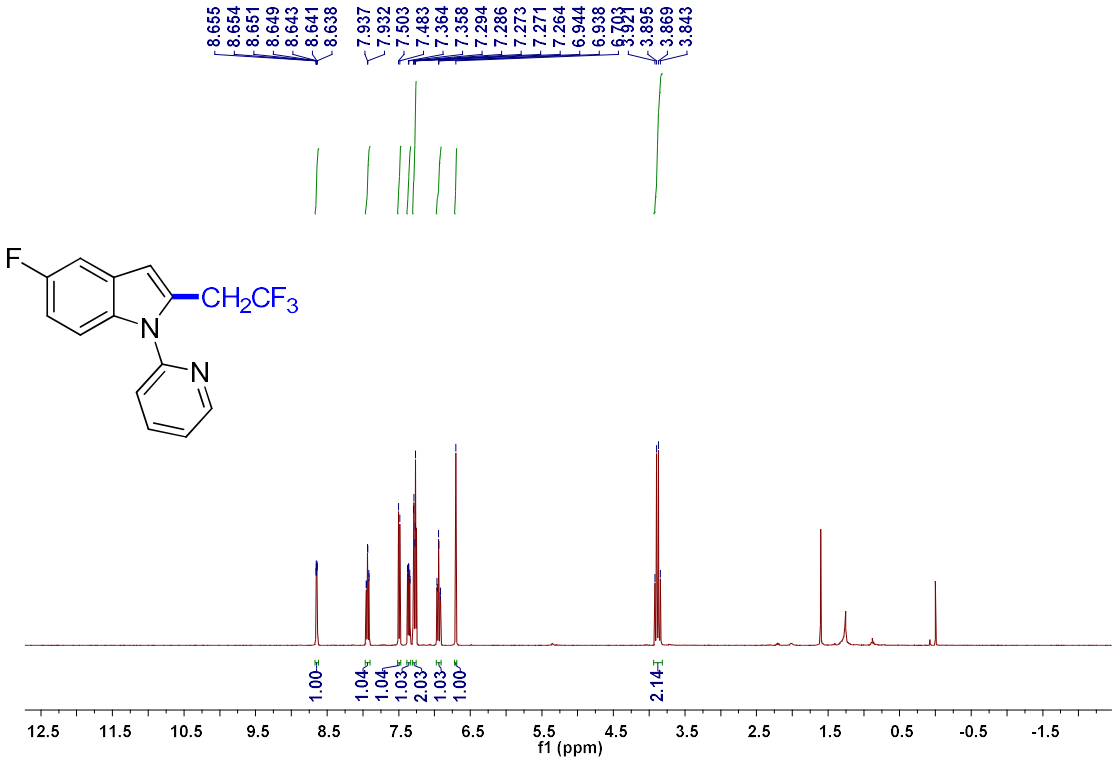
3na

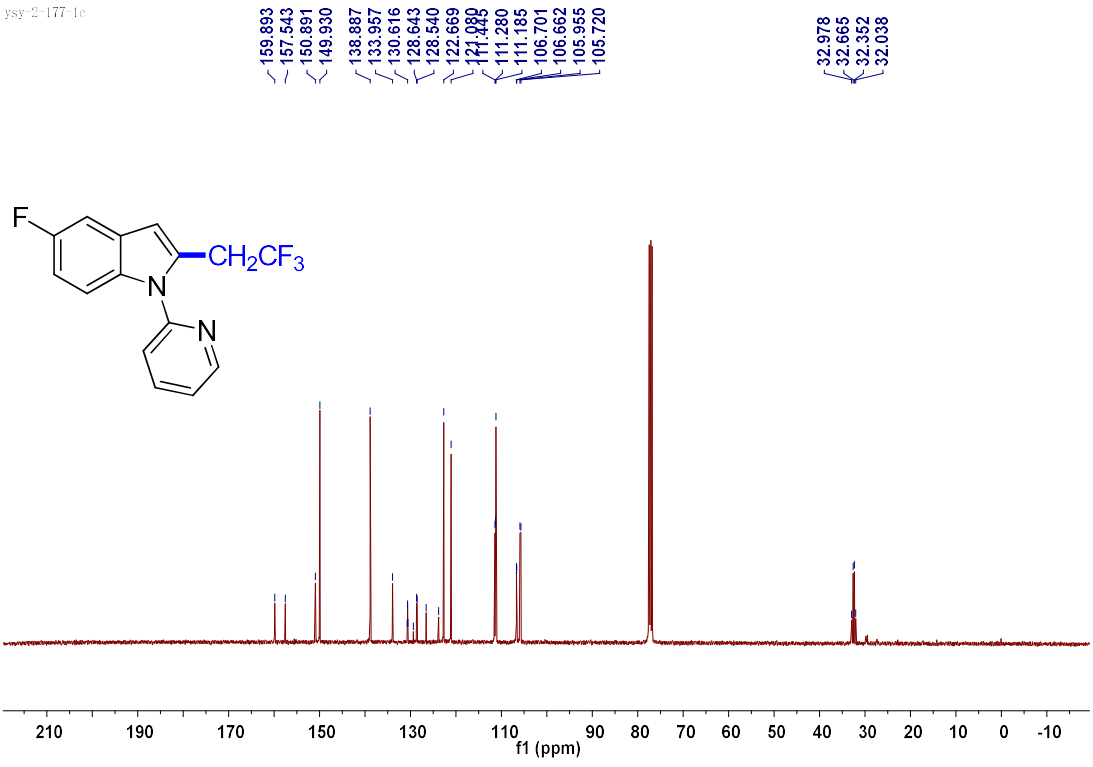

8.642
8.640
8.637
8.635
8.630
8.628
8.625
8.623
7.908
7.903
7.630
7.530
7.510
7.359
7.358
7.204
7.200
7.192
7.187
7.181
7.174
7.170
3.921
3.895
3.870
CH2CF3
N
N
1.00
1.03
1.01
1.03
0.99
1.03
2.06
1.00
2.07
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)

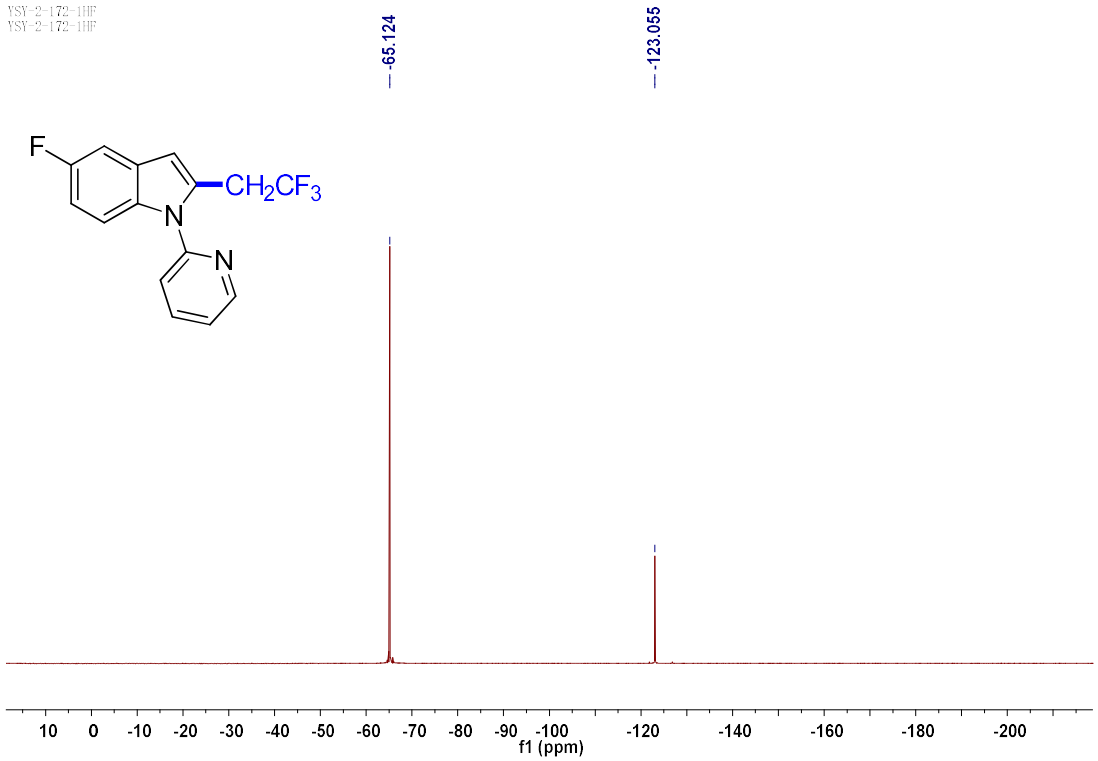

151.098
149.813
138.719
128.191
123.086
122.410
121.319
121.169
106.941
32.933
32.621
32.309
31.997
CH2CF3
N
N
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


-65.196
CH2CF3
N
N
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)

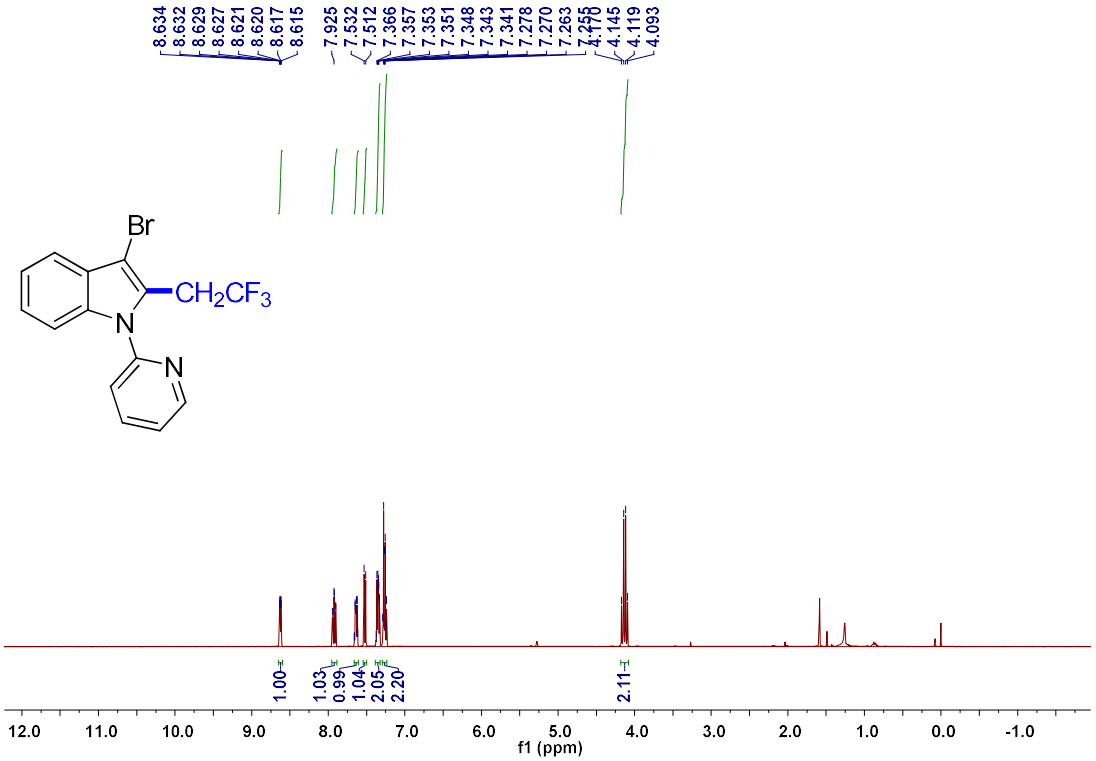
3oa

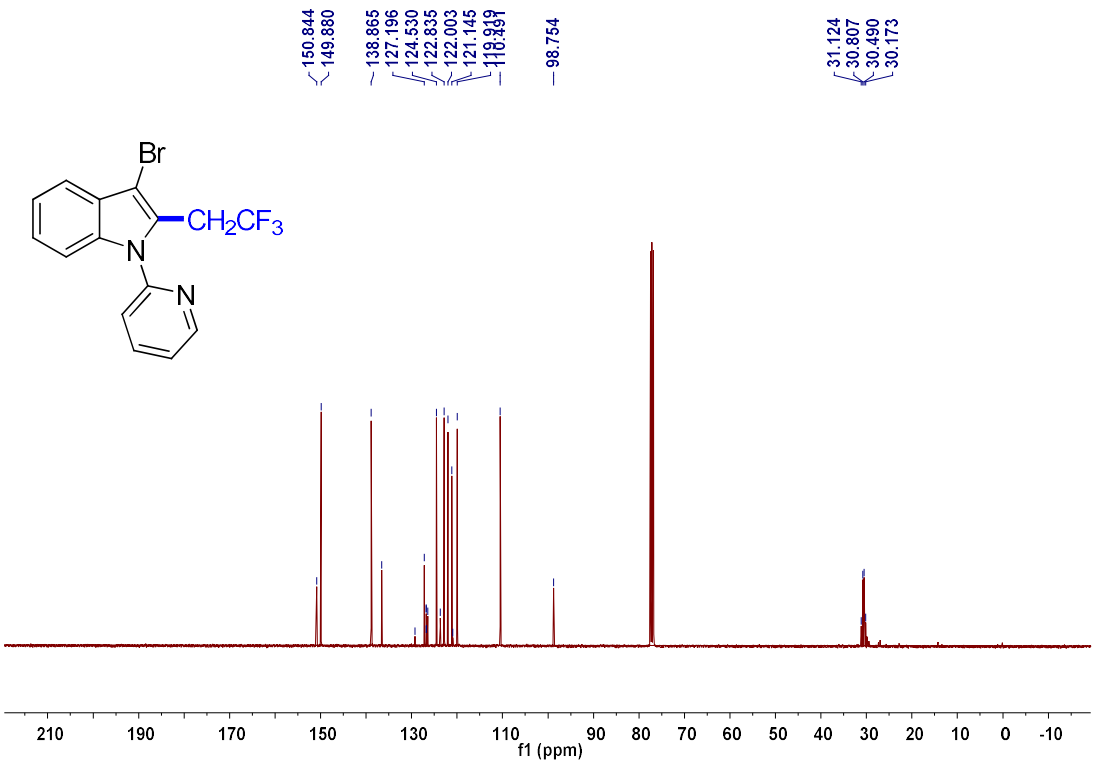

8.655
8.654
8.651
8.649
8.643
8.641
8.638
7.937
7.932
7.503
7.483
7.364
7.358
7.294
7.286
7.273
7.271
7.264
6.944
6.938
3.921
3.895
3.869
3.843
F
CH2CF3
N
N
1.00
1.04
1.04
1.03
2.03
1.03
1.00
2.14
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
-1.5
f1 (ppm)

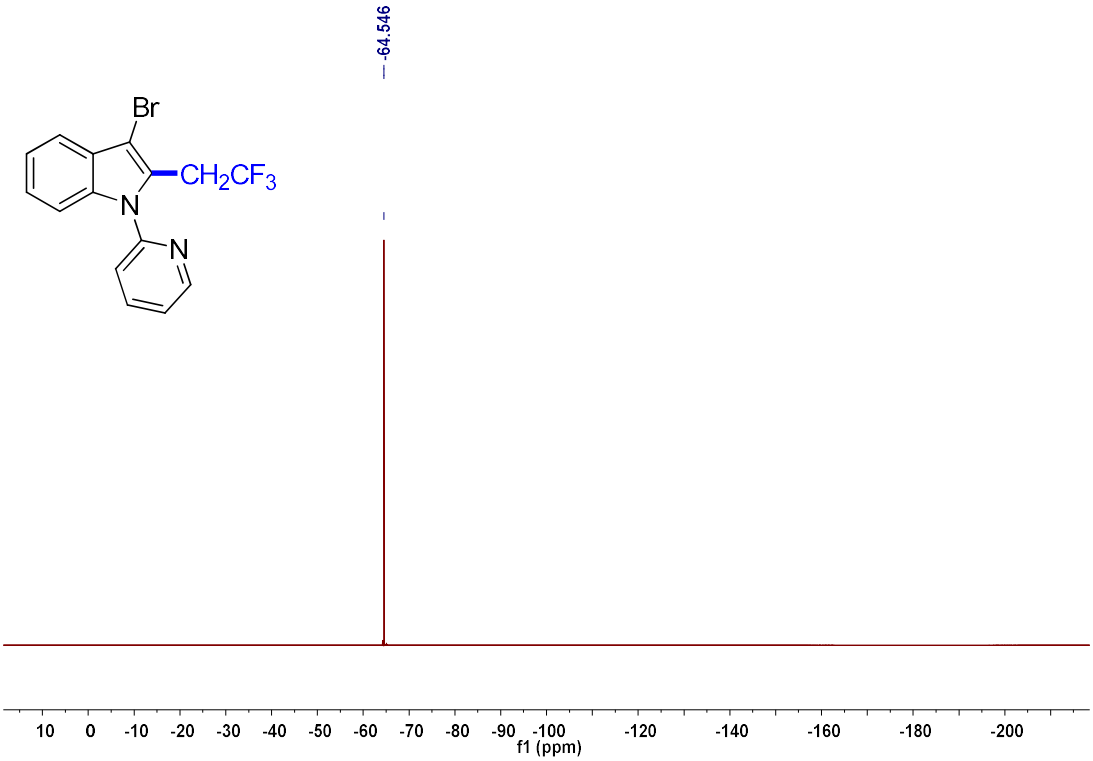

ysy-2-177-1c
159.893
157.543
150.891
149.930
138.887
133.957
130.616
128.643
128.540
122.669
111.280
111.185
106.701
106.662
105.955
105.720
32.978
32.665
32.352
32.038
F
CH2CF3
N
N
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


YSY-2-172-1HF
YSY-2-172-1HF
-65.124
-123.055
F
CH2CF3
N
N
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)

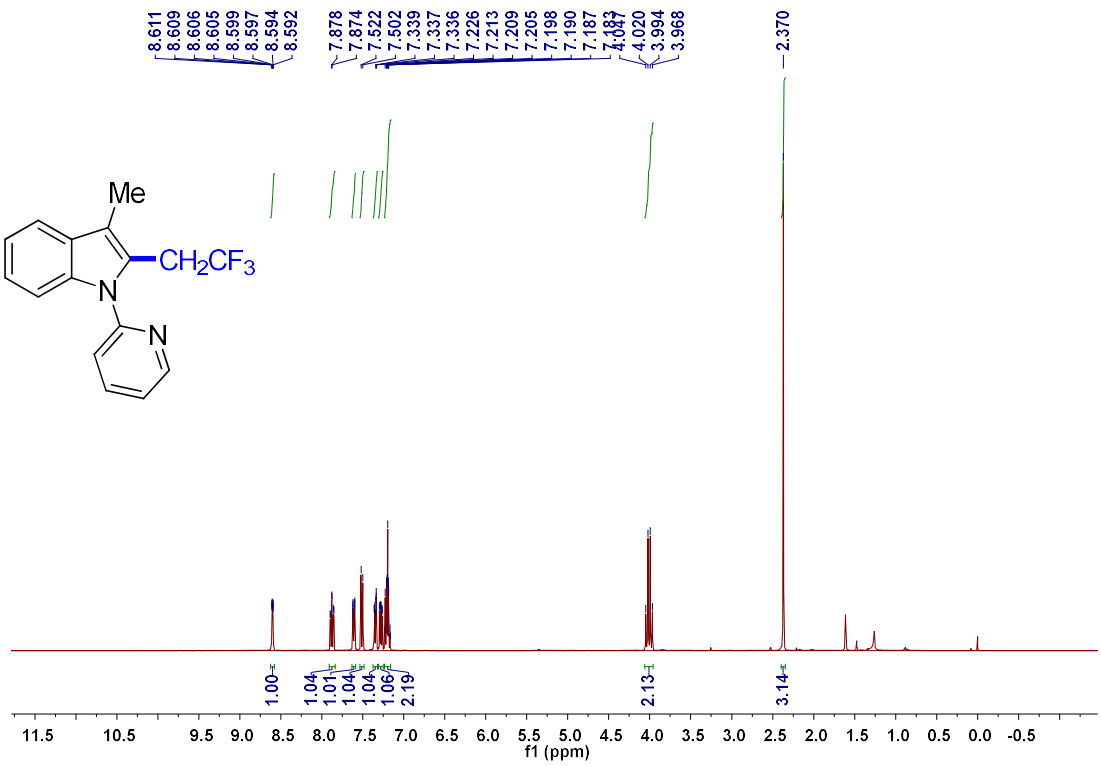
3pa

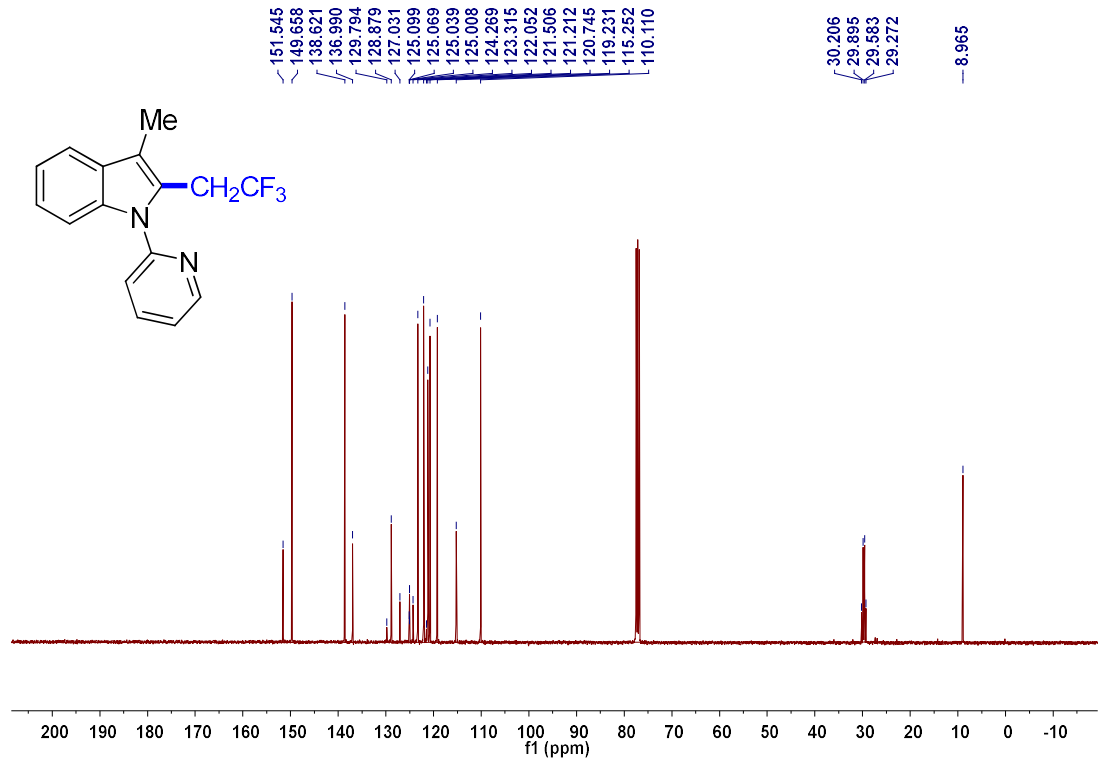

8.634
8.632
8.629
8.627
8.621
8.620
8.617
8.615
7.925
7.532
7.512
7.366
7.357
7.353
7.351
7.348
7.343
7.341
7.278
7.270
7.263
4.145
4.119
4.093
Br
CH2CF3
N
N
1.00
1.03
0.99
1.04
2.05
2.20
2.11
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)

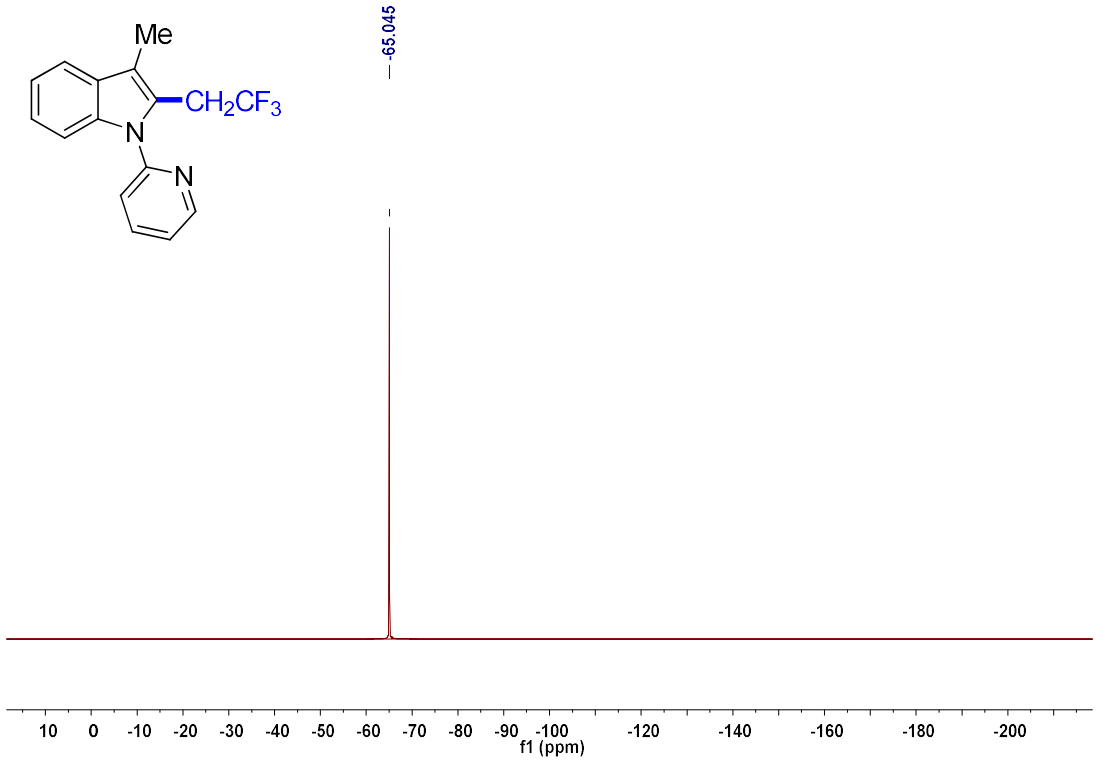

150.844
149.880
138.865
127.196
124.530
122.835
122.003
121.145
110.491
98.754
31.124
30.807
30.490
30.173
Br
CH2CF3
N
N
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


-64.546
Br
CH2CF3
N
N
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)

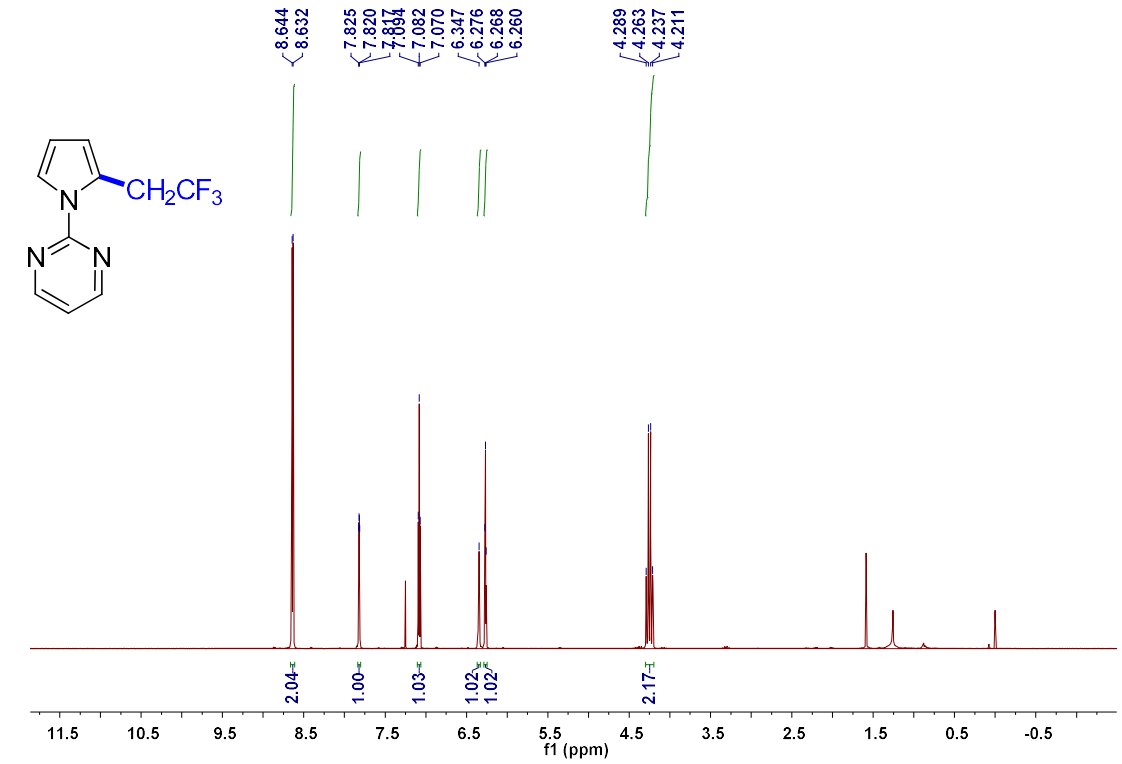
3qa

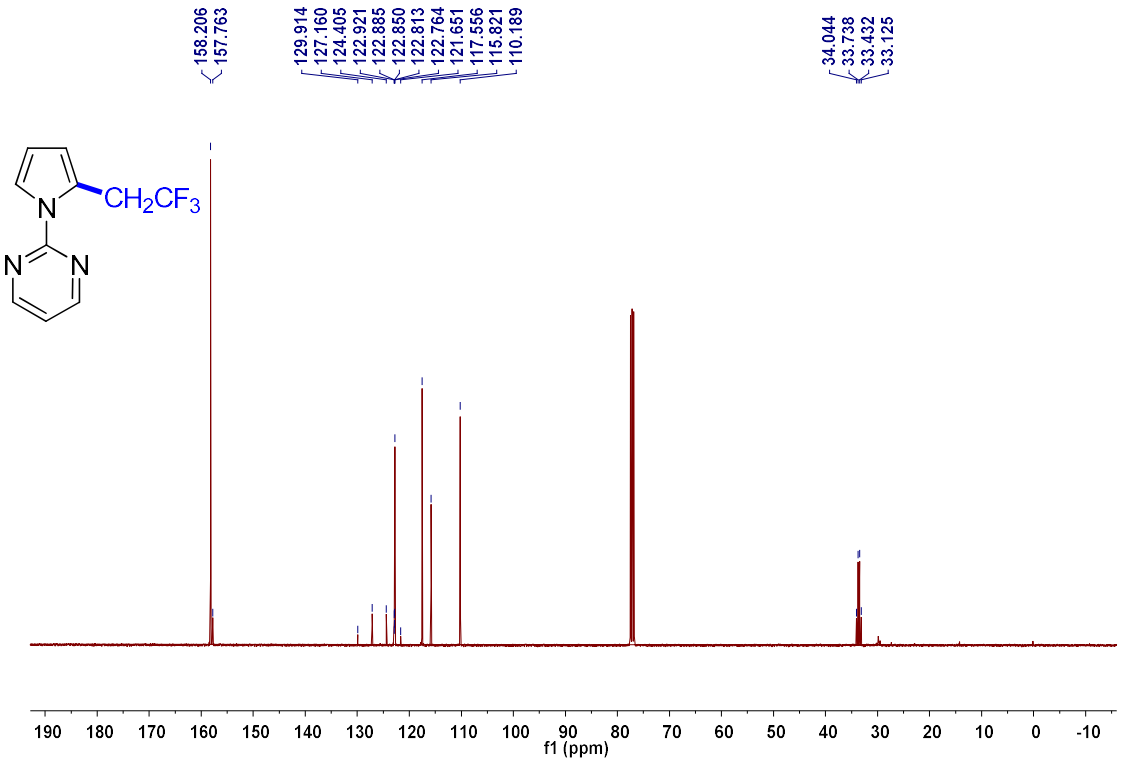

8.611
8.609
8.606
8.605
8.599
8.597
8.594
8.592
7.878
7.874
7.522
7.502
7.339
7.337
7.336
7.226
7.213
7.209
7.205
7.198
7.190
7.187
4.047
4.020
3.994
3.968
2.370
Me
CH2CF3
N
N
1.00
1.04
1.01
1.04
1.04
1.06
2.19
2.13
3.14
11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

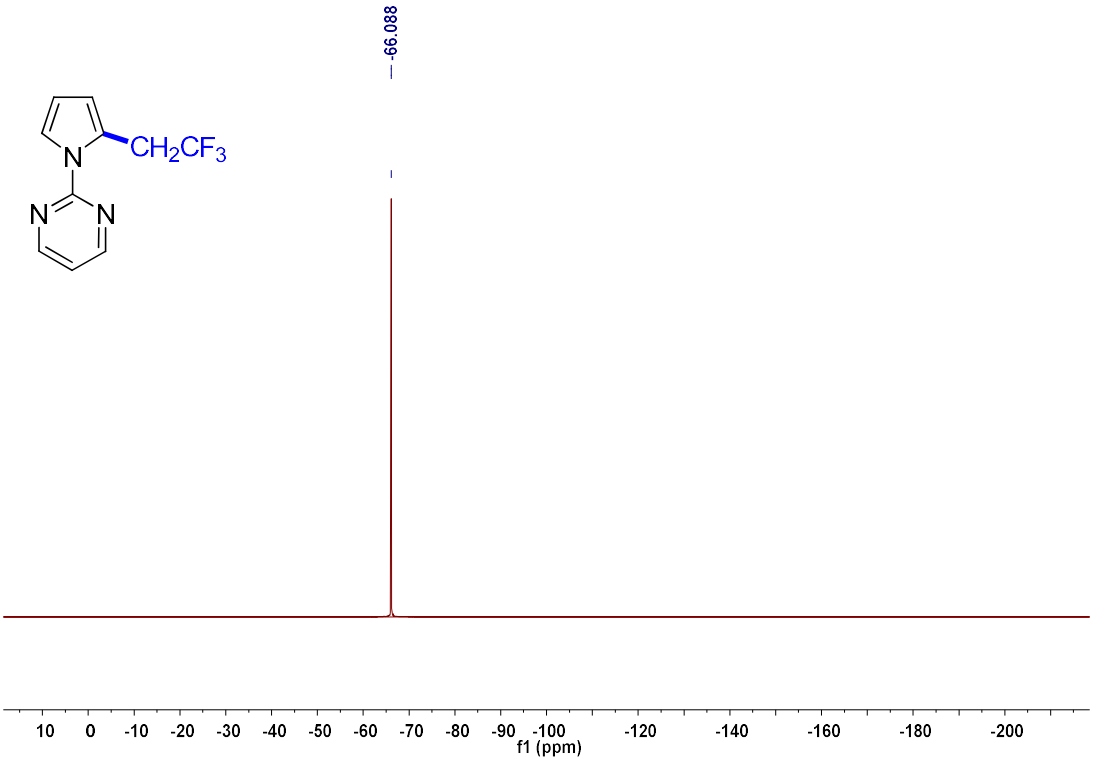

151.545
149.658
138.621
136.990
129.794
128.879
127.031
125.099
125.069
125.039
125.008
124.269
123.315
122.052
121.506
121.212
120.745
119.231
115.252
110.110
30.206
29.895
29.583
29.272
8.965
Me
CH2CF3
N
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


Me
CH2CF3
N
N
-65.045
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)

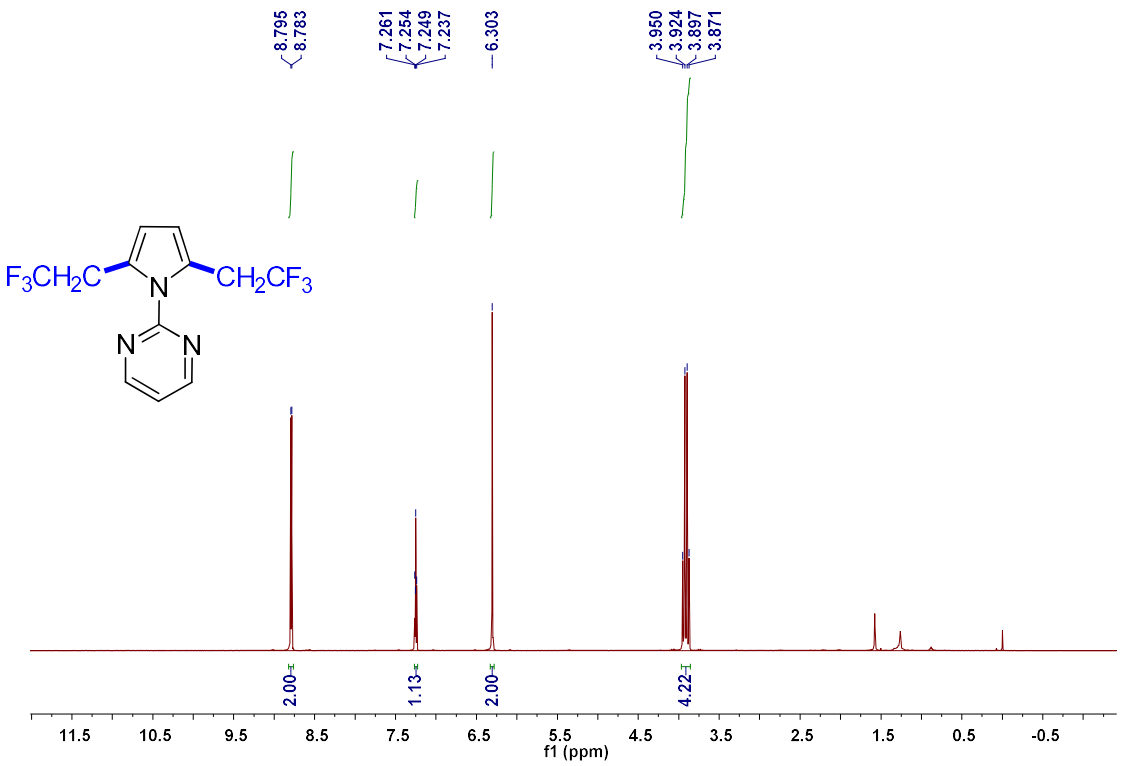
3ra

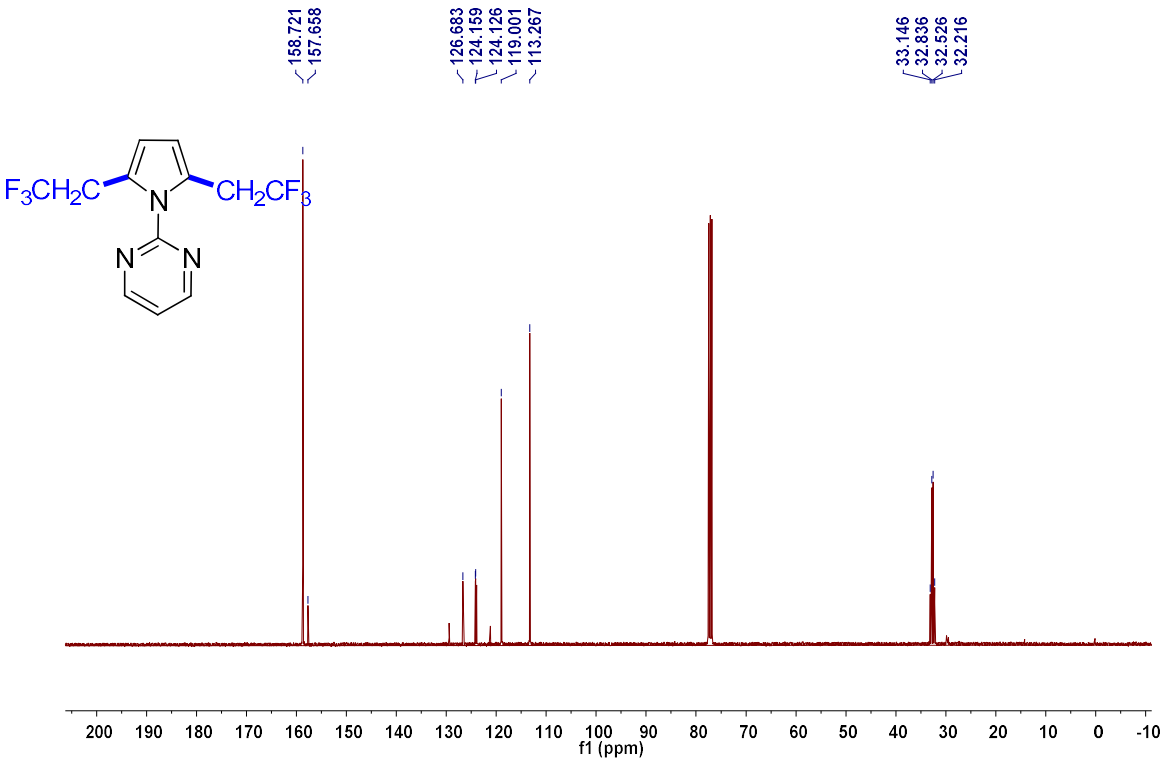

8.644
8.632
7.825
7.820
7.817
7.094
7.082
7.070
6.347
6.276
6.268
6.260
4.289
4.263
4.237
4.211
CH2CF3
N
N
N
2.04
1.00
1.03
1.02
1.02
2.17
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)

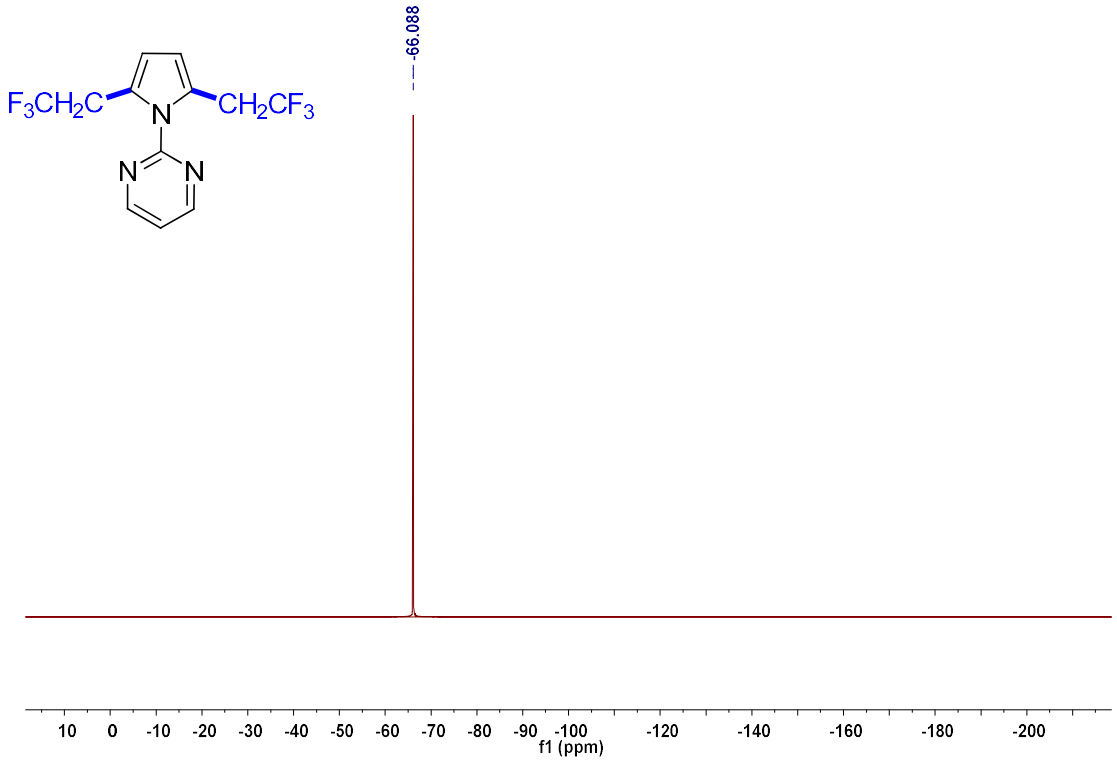

158.206
157.763
129.914
127.160
124.405
122.921
122.885
122.850
122.813
122.764
121.651
117.556
115.821
110.189
34.044
33.738
33.432
33.125
CH2CF3
N
N
N
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


-66.088
CH2CF3
N
N
N
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)

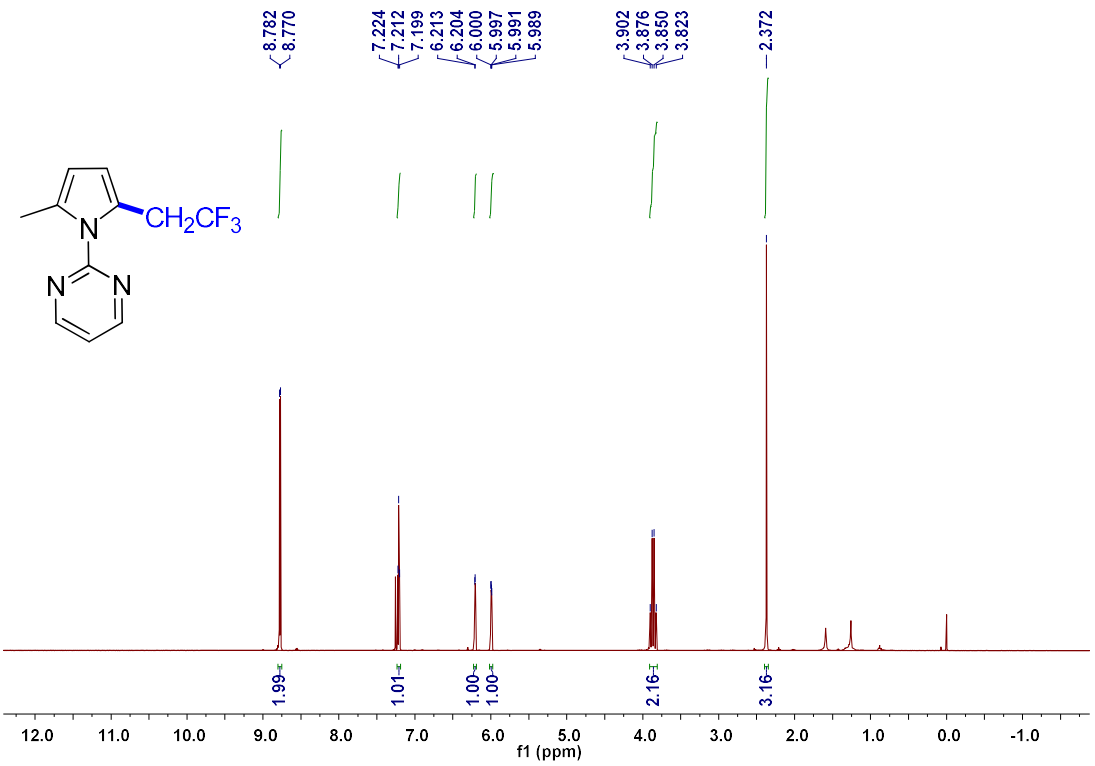
3ra'

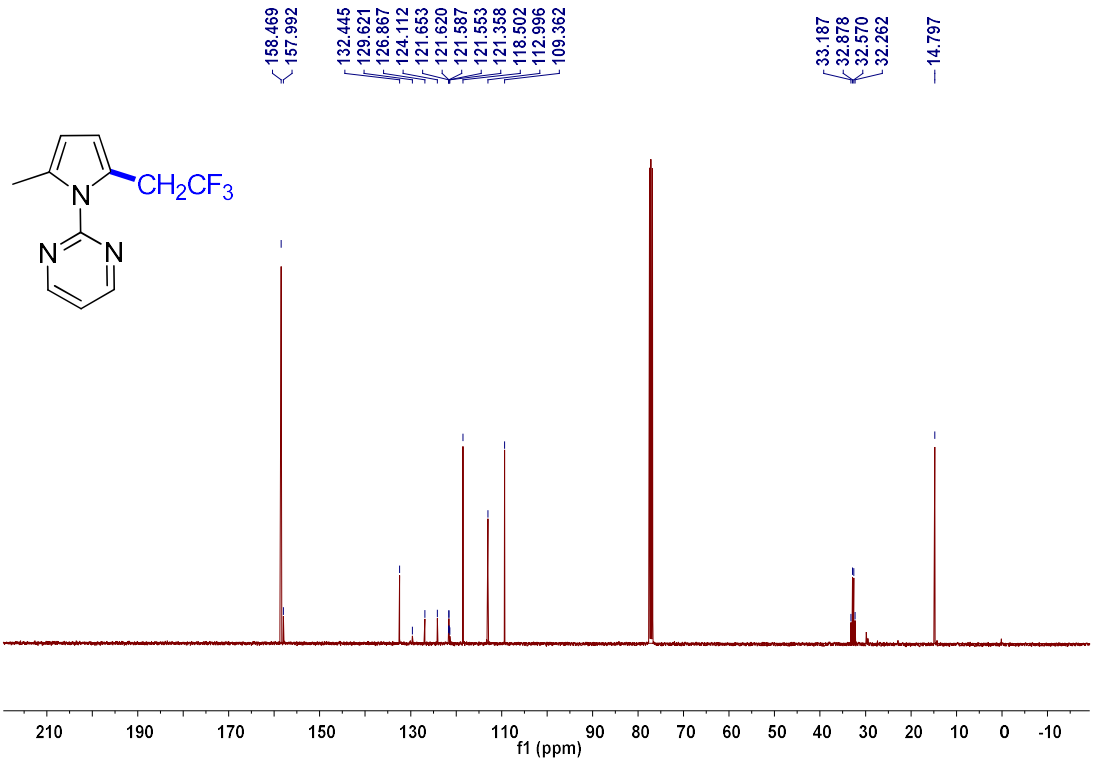

8.795
8.783
7.261
7.254
7.249
7.237
6.303
3.950
3.924
3.897
3.871
F3CH2C
CH2CF3
N
N
N
2.00
1.13
2.00
4.22
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)

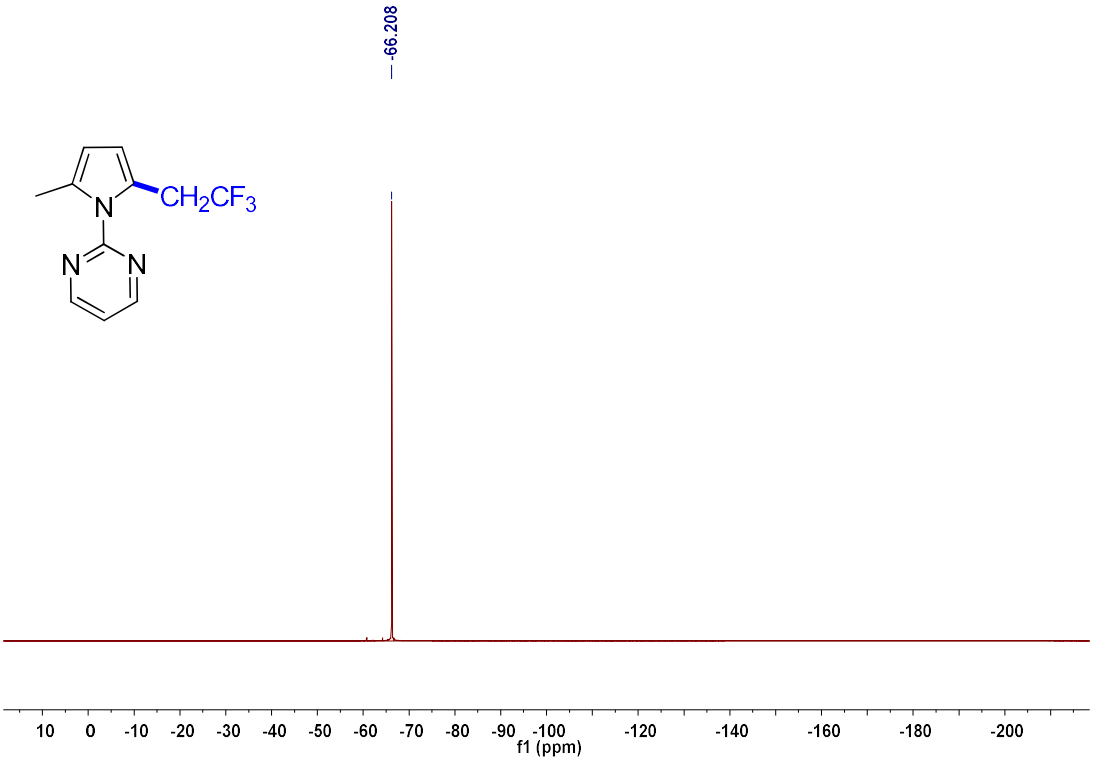

158.721
157.658
126.683
124.159
124.126
119.001
113.267
33.146
32.836
32.526
32.216
F3CH2C
CH2CF3
N
N
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


F3CH2C
CH2CF3
N
N
N
-66.088
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)

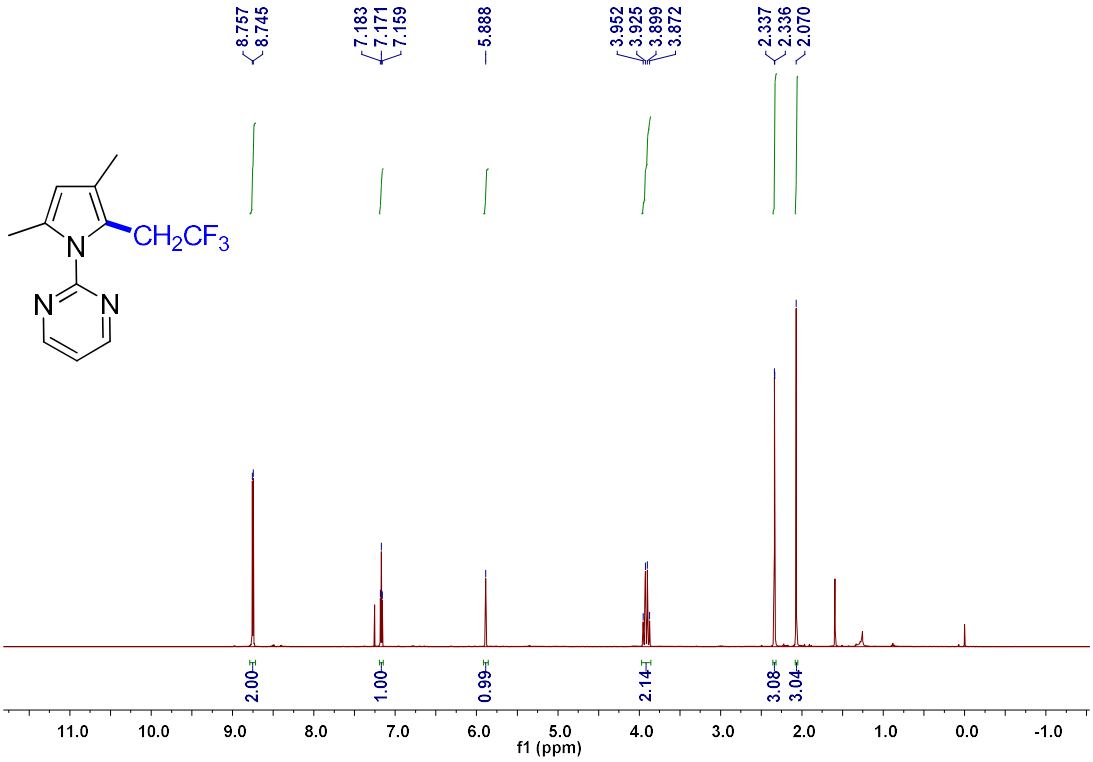
3sa

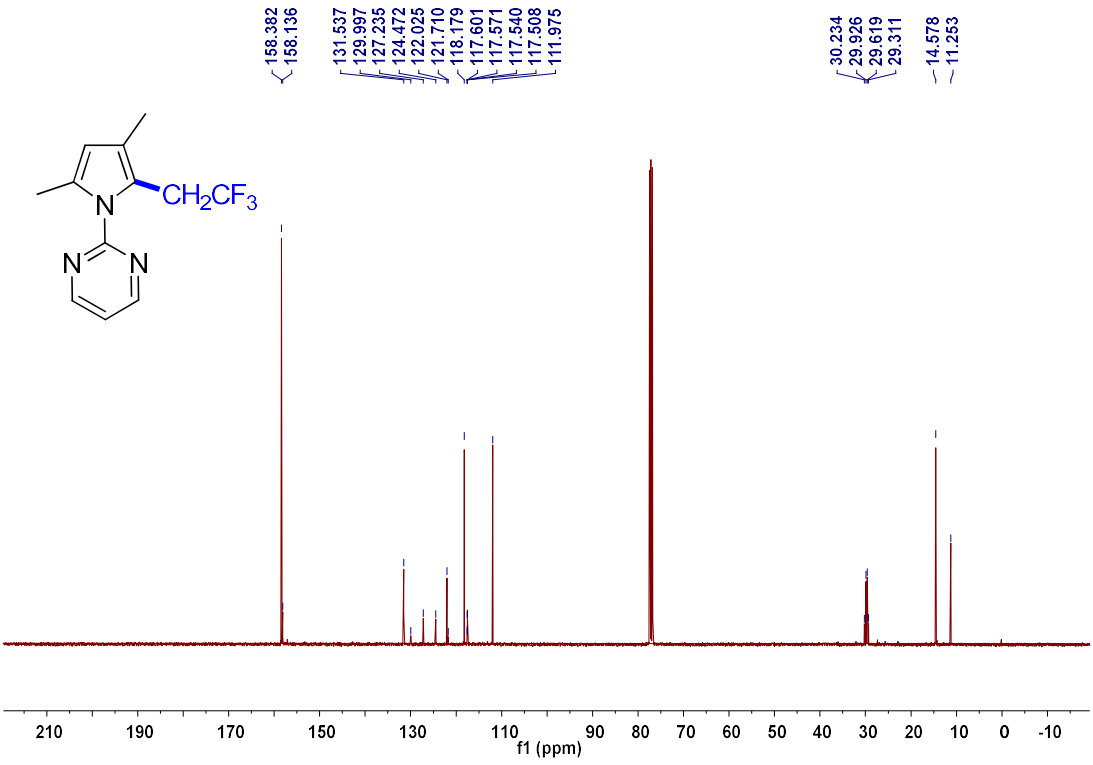

8.782
8.770
7.224
7.212
7.199
6.213
6.204
6.000
5.997
5.991
5.989
3.902
3.876
3.850
3.823
2.372
CH2CF3
N
N
N
1.99
1.01
1.00
1.00
2.16
3.16
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)

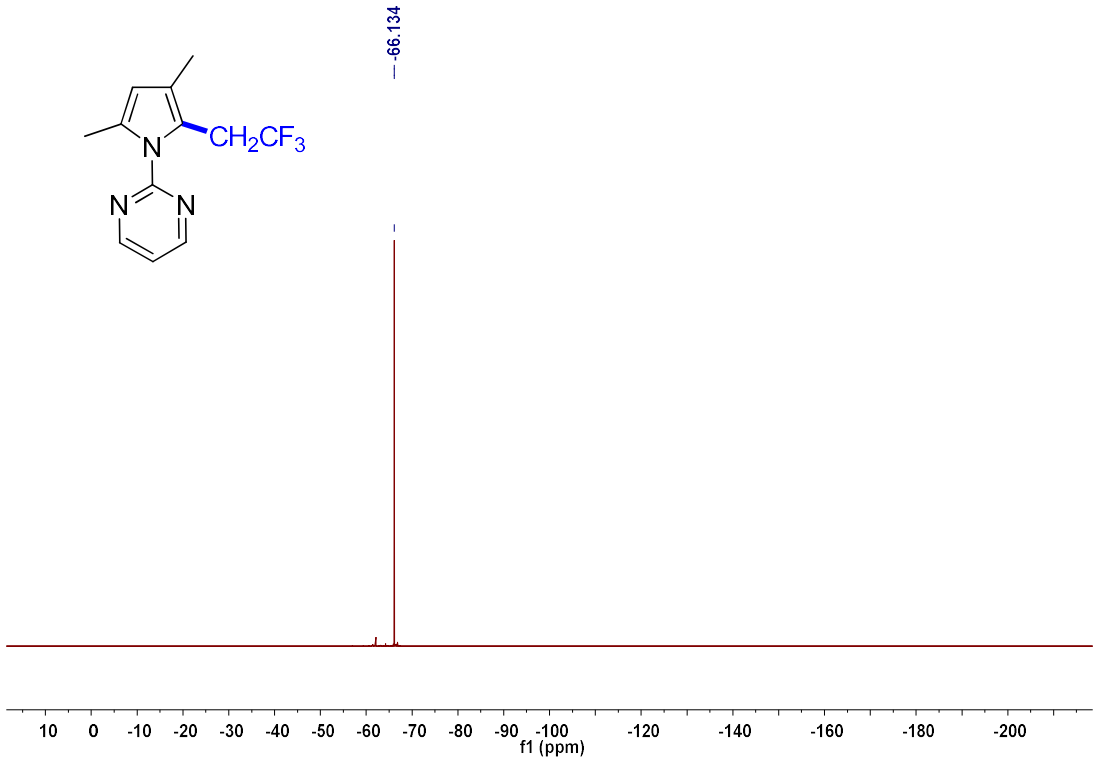

158.469
157.992
132.445
129.621
126.867
124.112
121.653
121.620
121.587
121.553
121.358
118.502
112.996
109.362
33.187
32.878
32.570
32.262
14.797
CH2CF3
N
N
N
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


-66.208
CH2CF3
N
N
N
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)

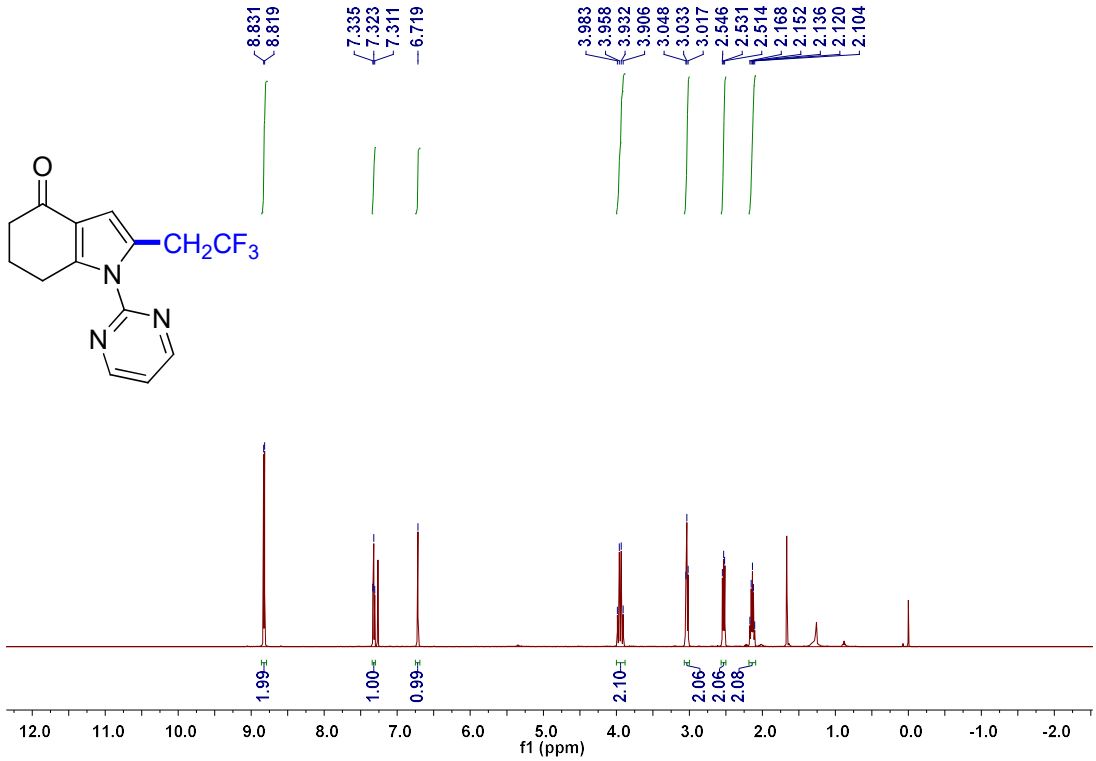
3ta

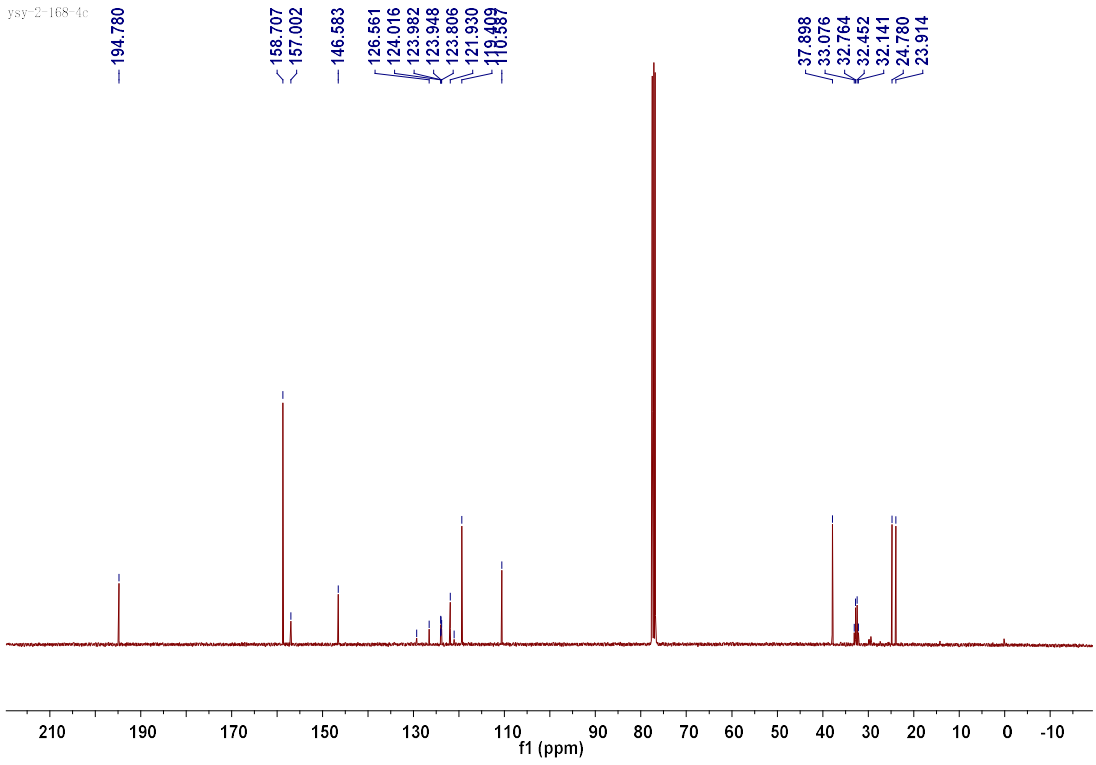

8.757
8.745
7.183
7.171
7.159
5.888
3.952
3.925
3.899
3.872
2.337
2.336
2.070
CH2CF3
N
N
N
2.00
1.00
0.99
2.14
3.08
3.04
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)

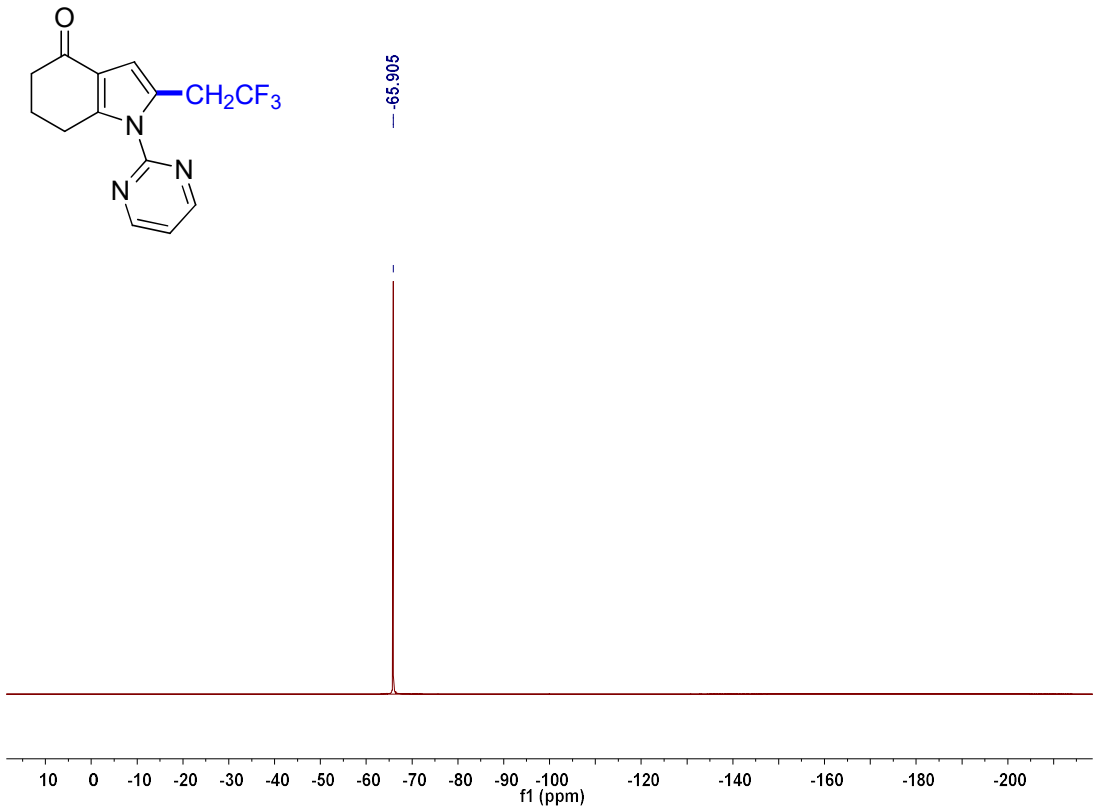

158.382
158.136
131.537
129.997
127.235
124.472
122.025
121.710
118.179
117.601
117.571
117.540
117.508
111.975
30.234
29.926
29.619
29.311
14.578
11.253
CH2CF3
N
N
N
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


-66.134
CH2CF3
N
N
N
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)

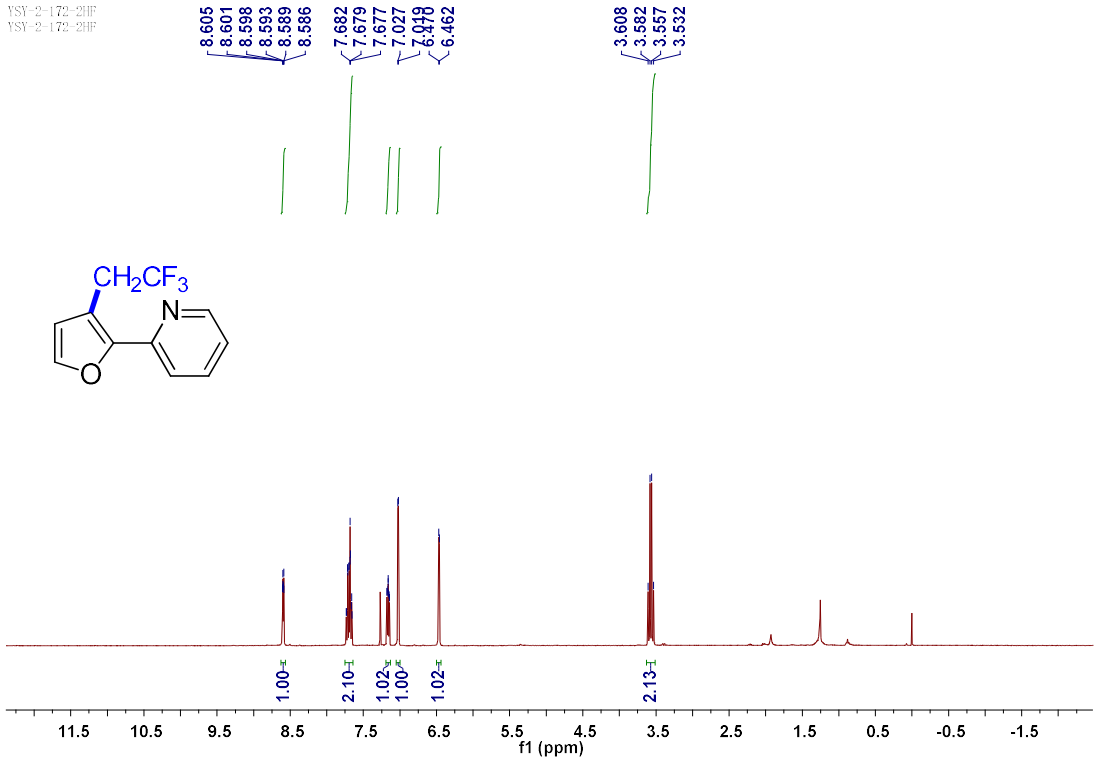
3ua

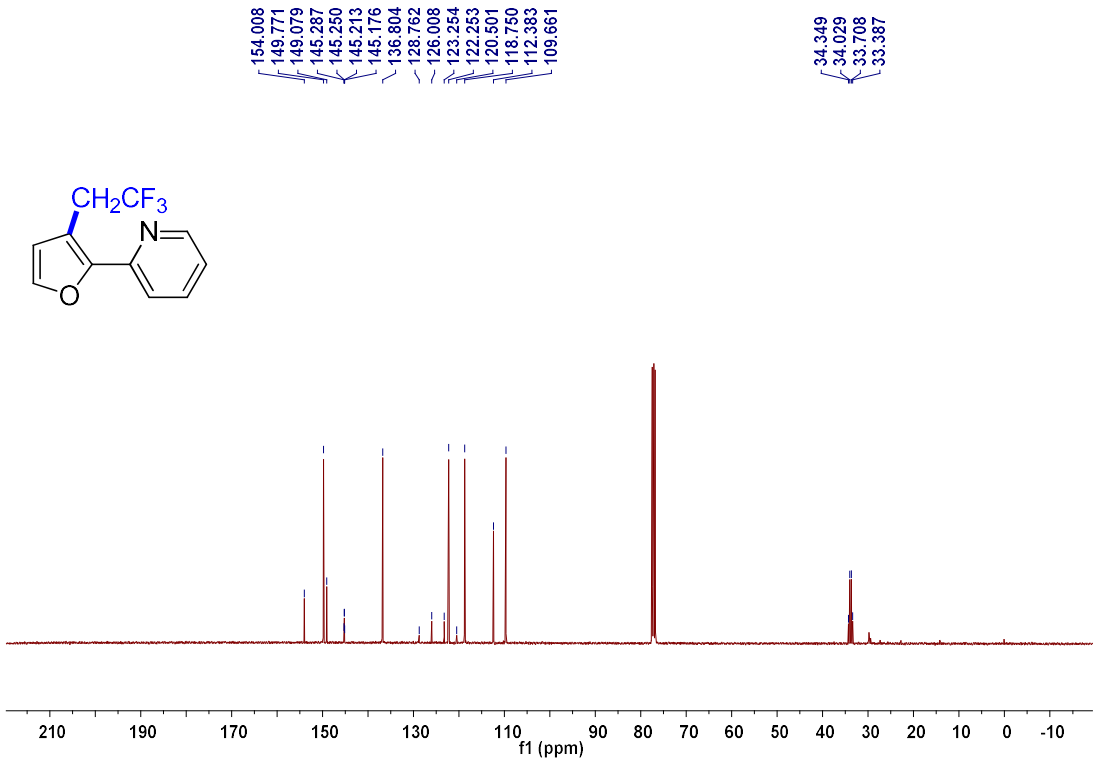

8.831
8.819
7.335
7.323
7.311
6.719
3.983
3.958
3.932
3.906
3.048
3.033
3.017
2.546
2.531
2.514
2.168
2.152
2.136
2.120
2.104
O
CH2CF3
N
N
N
1.99
1.00
0.99
2.10
2.06
2.06
2.08
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)

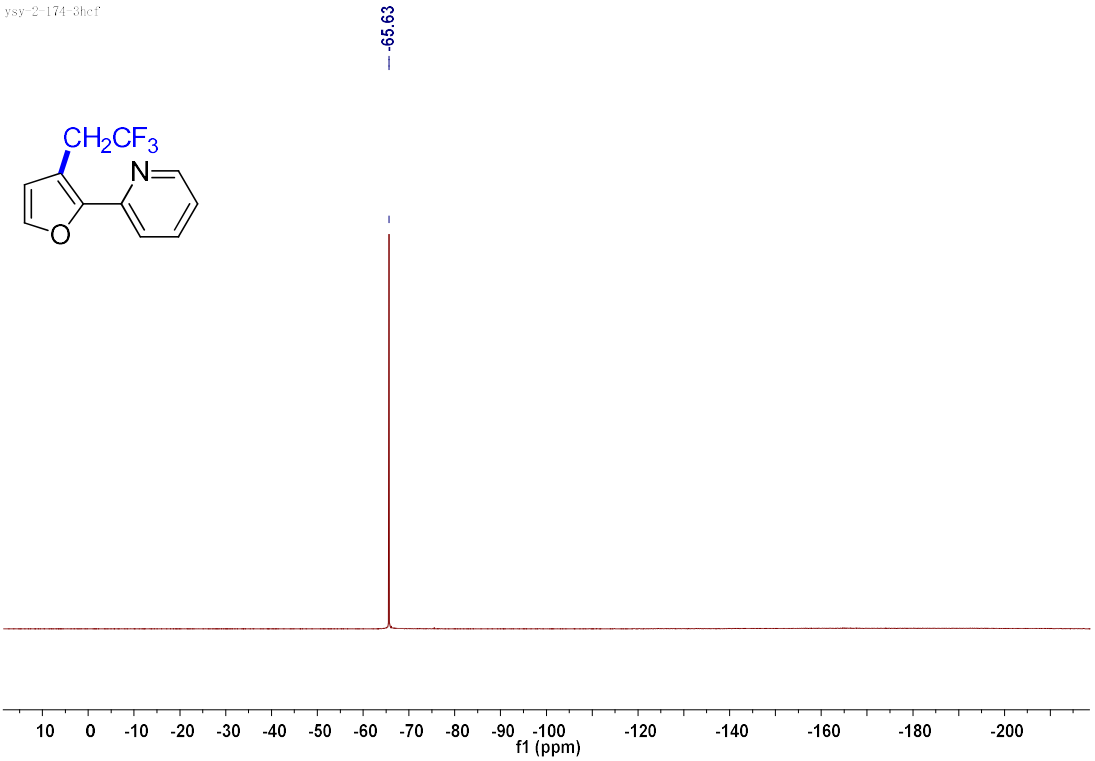

ysy-2-168-4c
194.780
158.707
157.002
146.583
126.561
124.016
123.982
123.948
123.806
121.930
110.587
37.898
33.076
32.764
32.452
32.141
24.780
23.914
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


O
CH2CF3
N
N
N
-65.905
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)

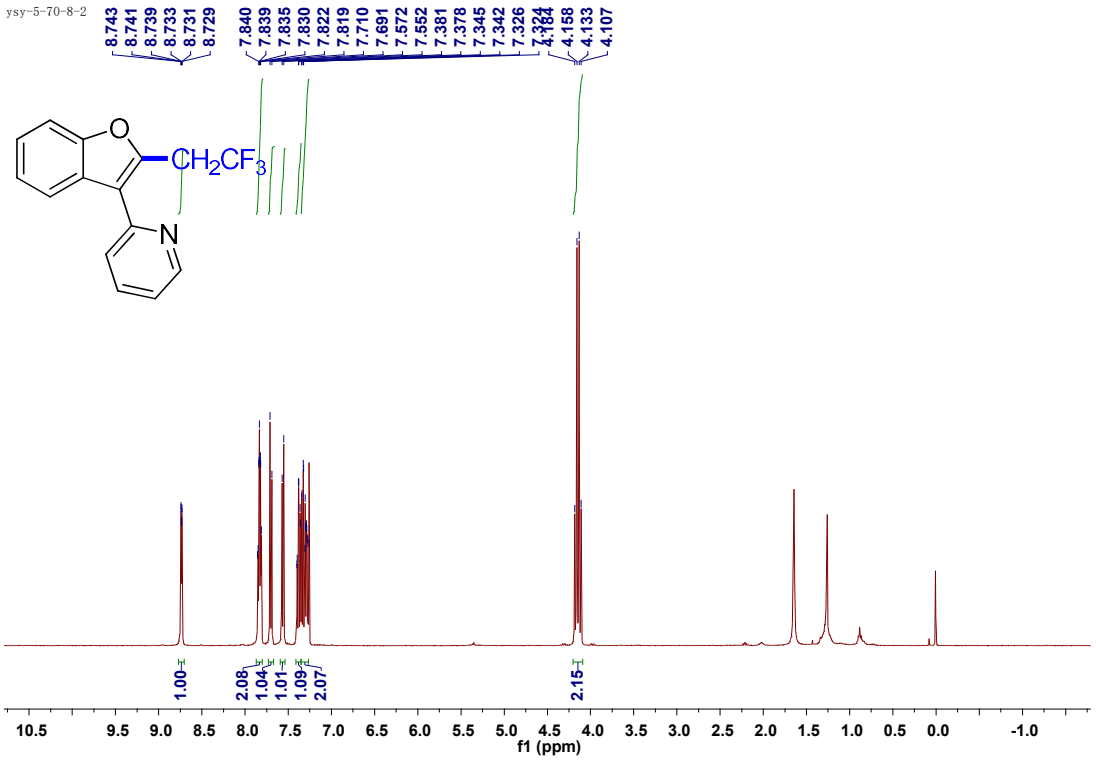
3va

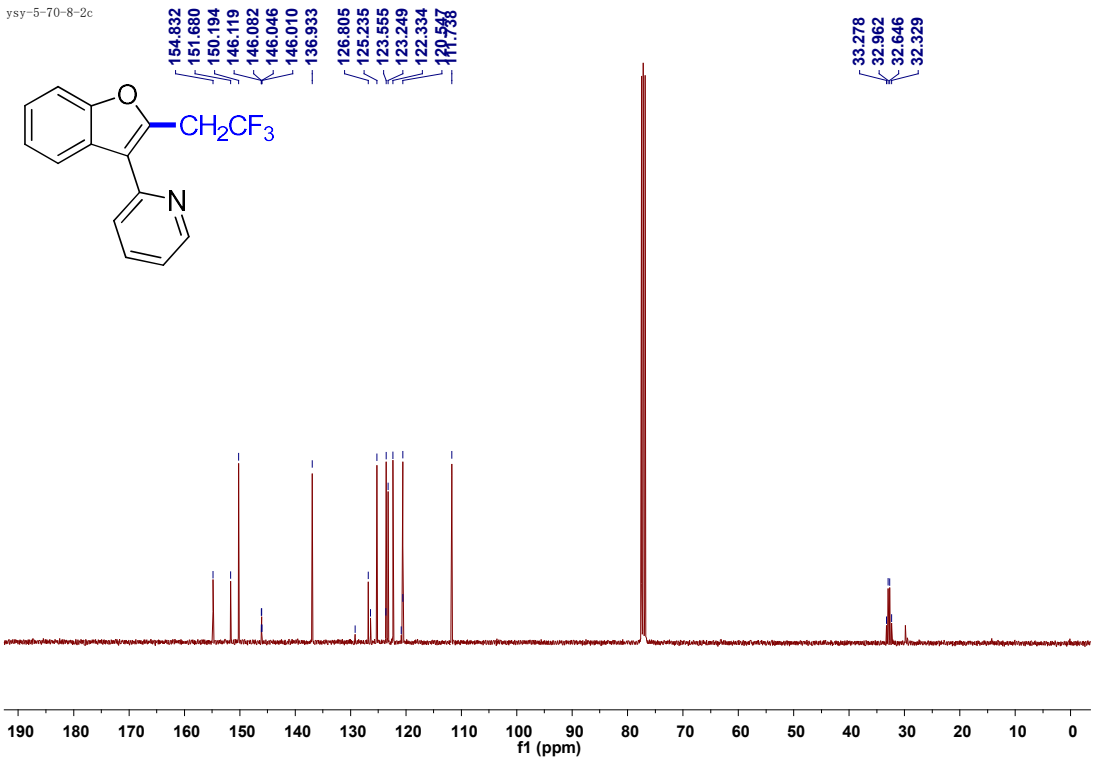

YSY-2-172-2HF
YSY-2-172-2HF
8.605
8.601
8.598
8.593
8.589
8.586
7.682
7.679
7.677
7.027
7.019
7.010
6.470
6.462
3.608
3.582
3.557
3.532
CH2CF3
N
O
1.00
2.10
1.02
1.00
1.02
2.13
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
-1.5
f1 (ppm)

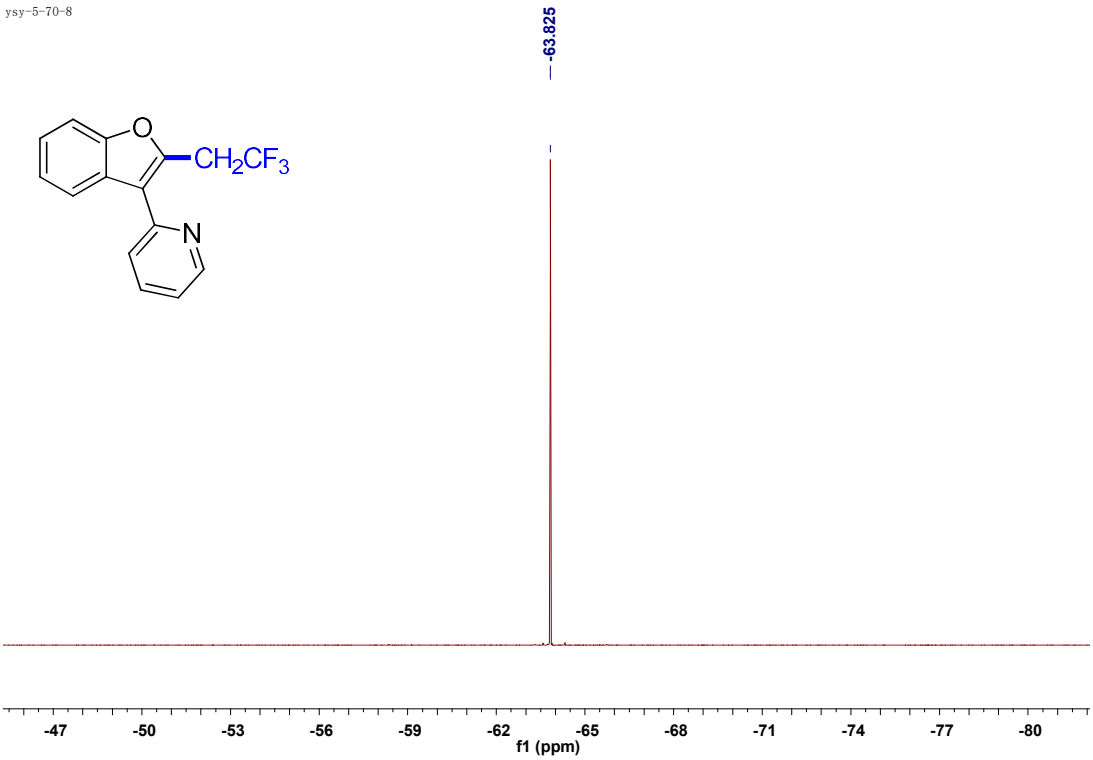

154.008
149.771
149.079
145.287
145.250
145.213
145.176
136.804
128.762
126.008
123.254
122.253
120.501
118.750
112.383
109.661
34.349
34.029
33.708
33.387
CH2CF3
N
O
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


ysy-2-174-3hcf
-65.63
CH2CF3
N
O
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)

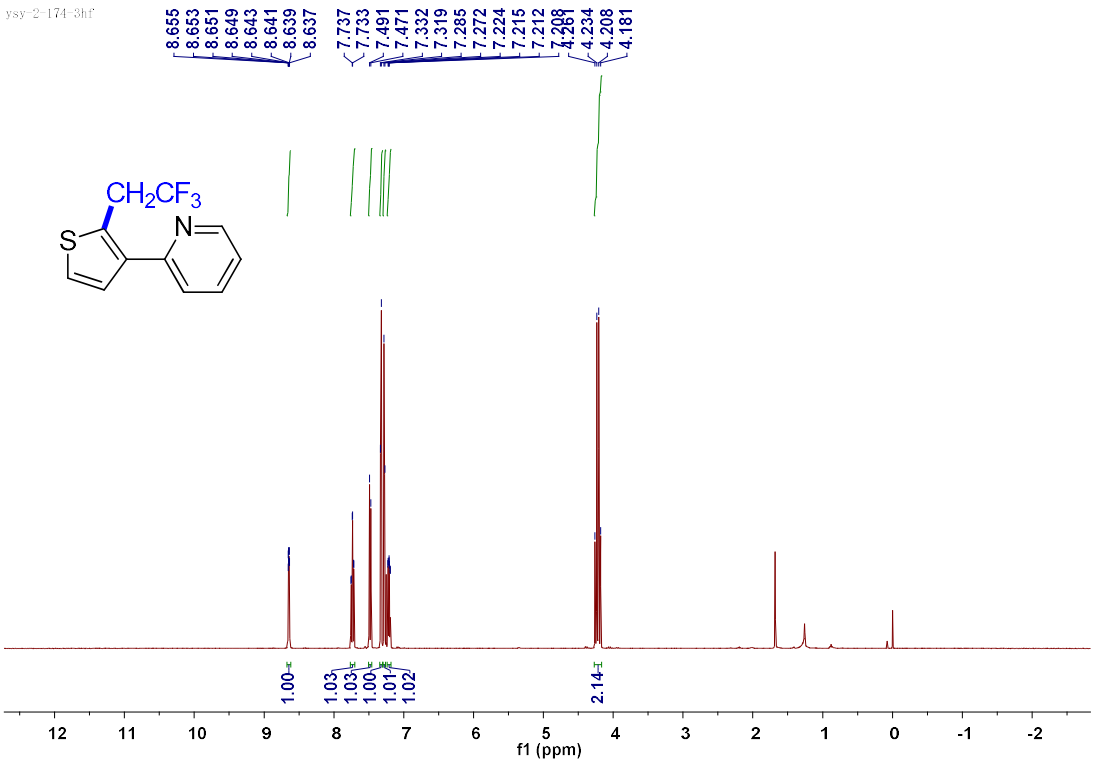
3wa

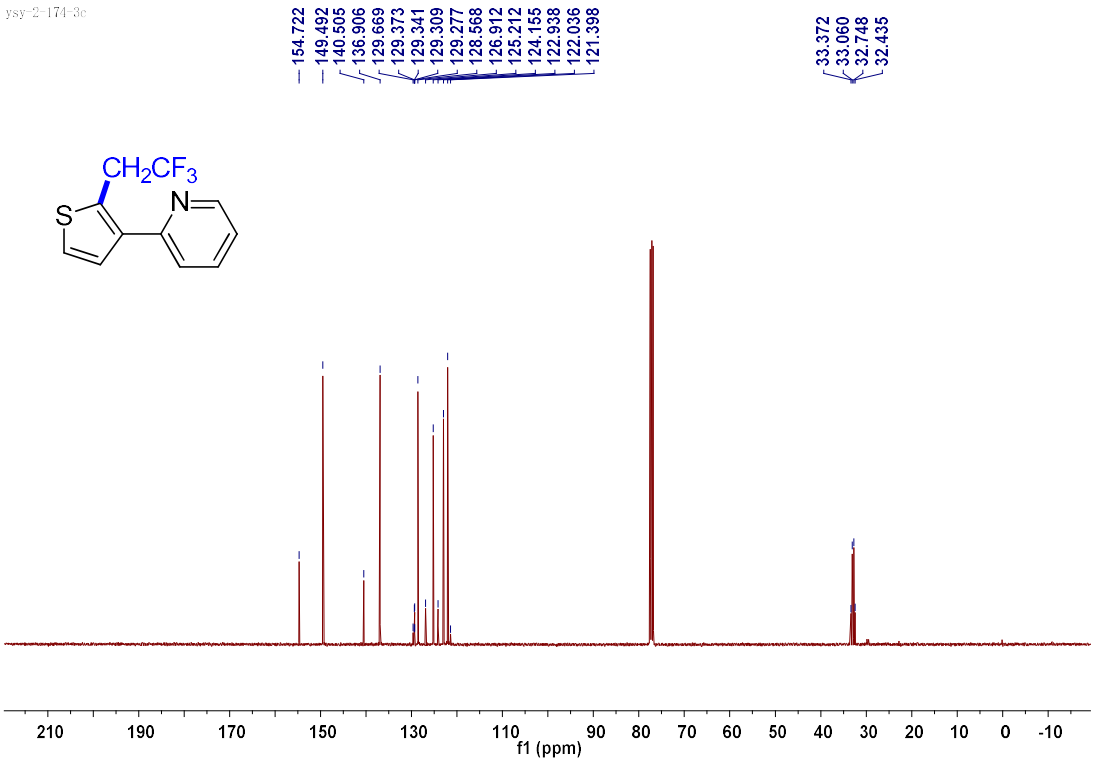

ysy-5-70-8-2
8.743
8.741
8.739
8.733
8.731
8.729
7.840
7.839
7.835
7.830
7.822
7.819
7.710
7.691
7.572
7.552
7.381
7.378
7.345
7.342
7.326
4.158
4.133
4.107
CH2CF3
N
1.00
2.08
1.04
1.01
1.09
2.07
2.15
f1 (ppm)

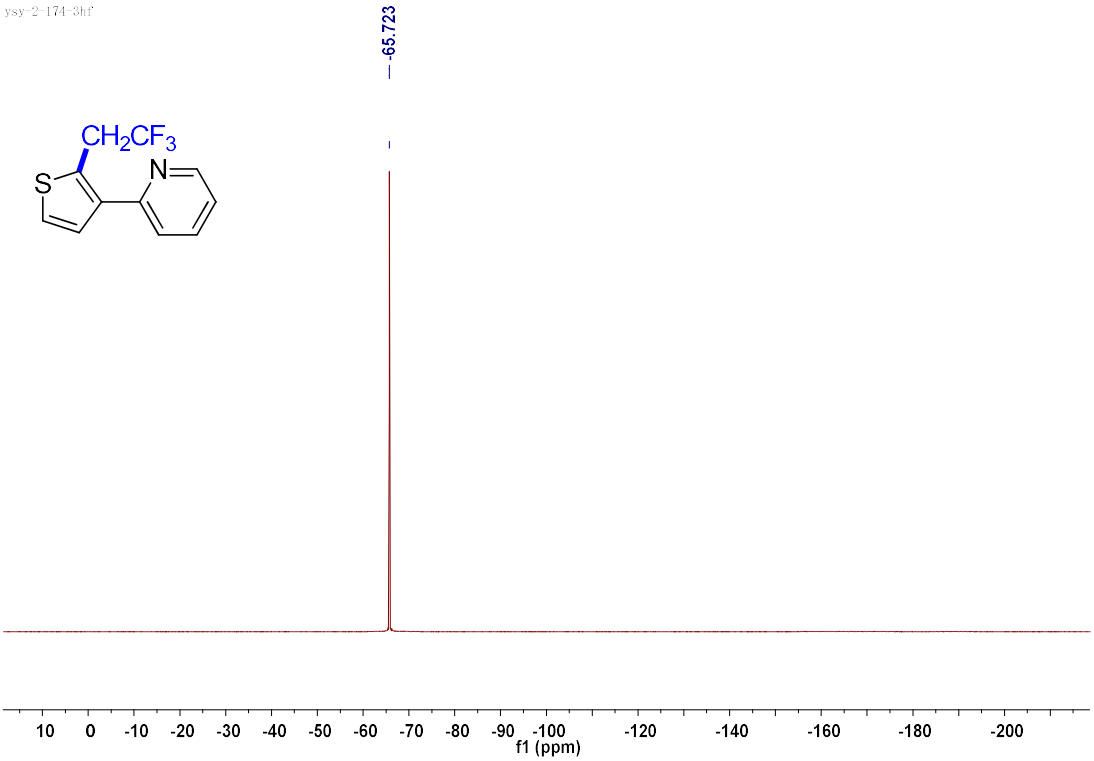

ysy-5-70-8-2c
154.832
151.680
150.194
146.119
146.082
146.046
146.010
136.933
126.805
125.235
123.555
123.249
122.334
33.278
32.962
32.646
32.329
CH2CF3
N
f1 (ppm)


ysy-5-70-8
-63.825
O
CH2CF3
N
-47
-50
-53
-56
-59
-62
-65
-68
-71
-74
-77
-80
f1 (ppm)

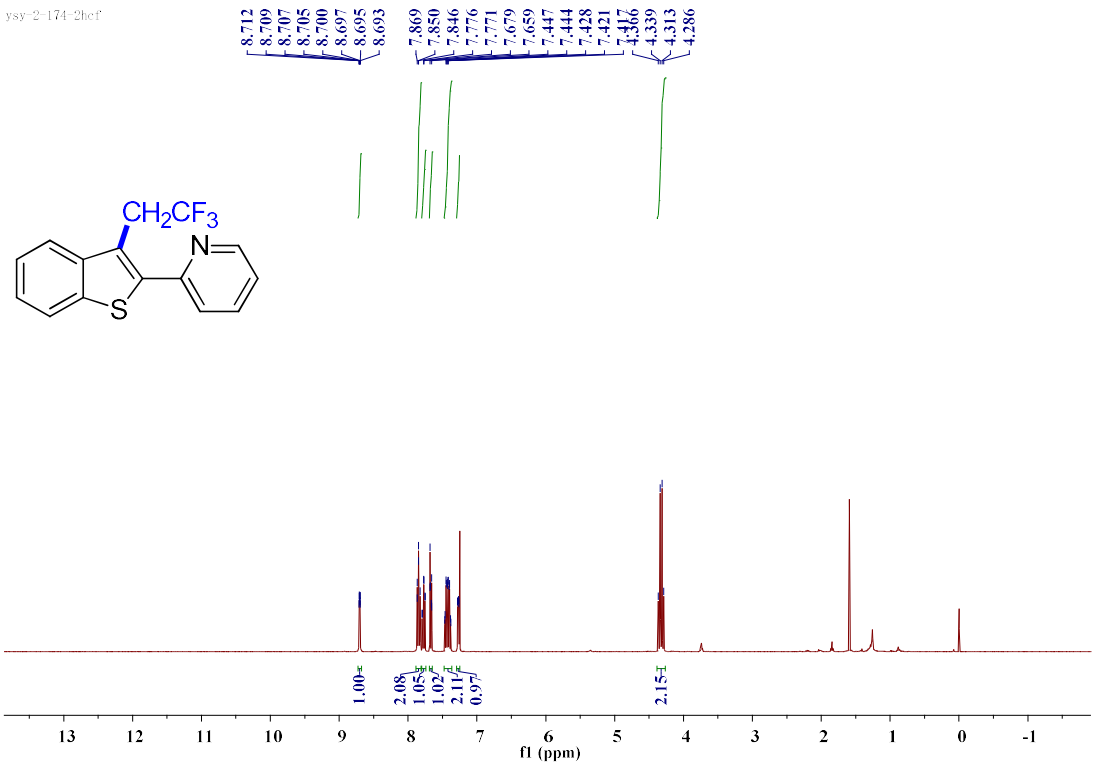
3xa

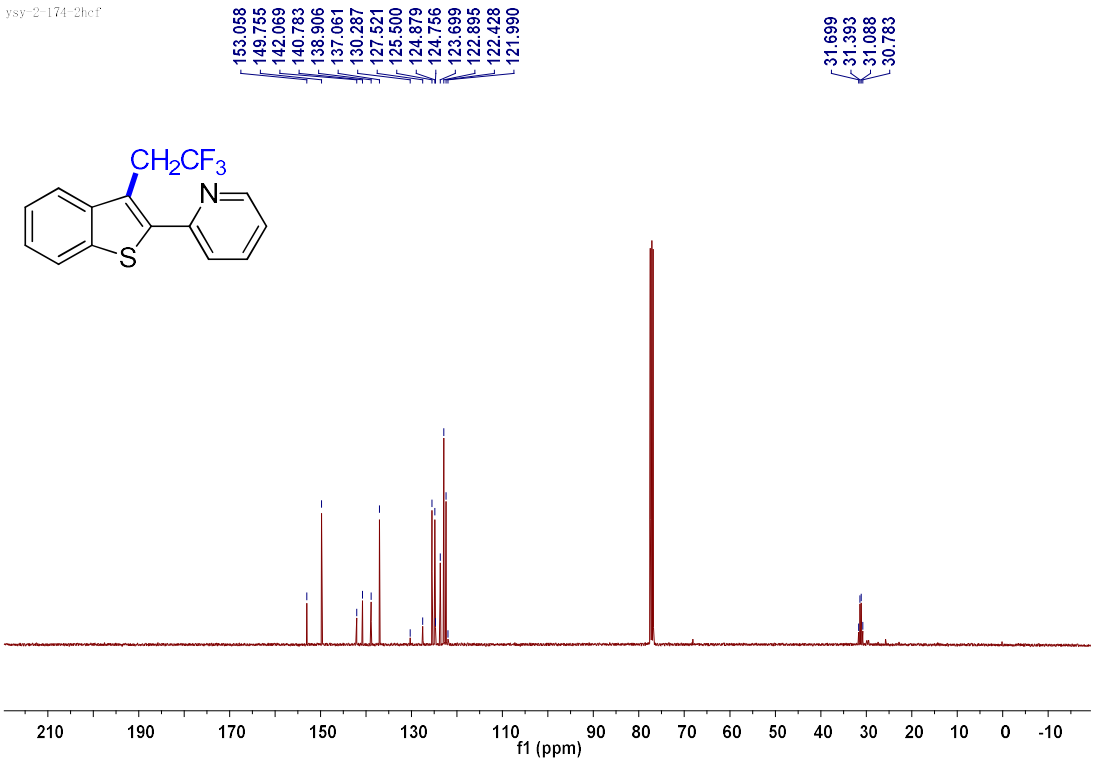

ysy-2-174-3hf
8.655
8.653
8.651
8.649
8.643
8.641
8.639
8.637
7.737
7.733
7.491
7.471
7.332
7.319
7.285
7.272
7.224
7.215
7.212
4.234
4.208
4.181
CH2CF3
S
N
1.00
1.03
1.03
1.00
1.01
1.02
2.14
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
f1 (ppm)

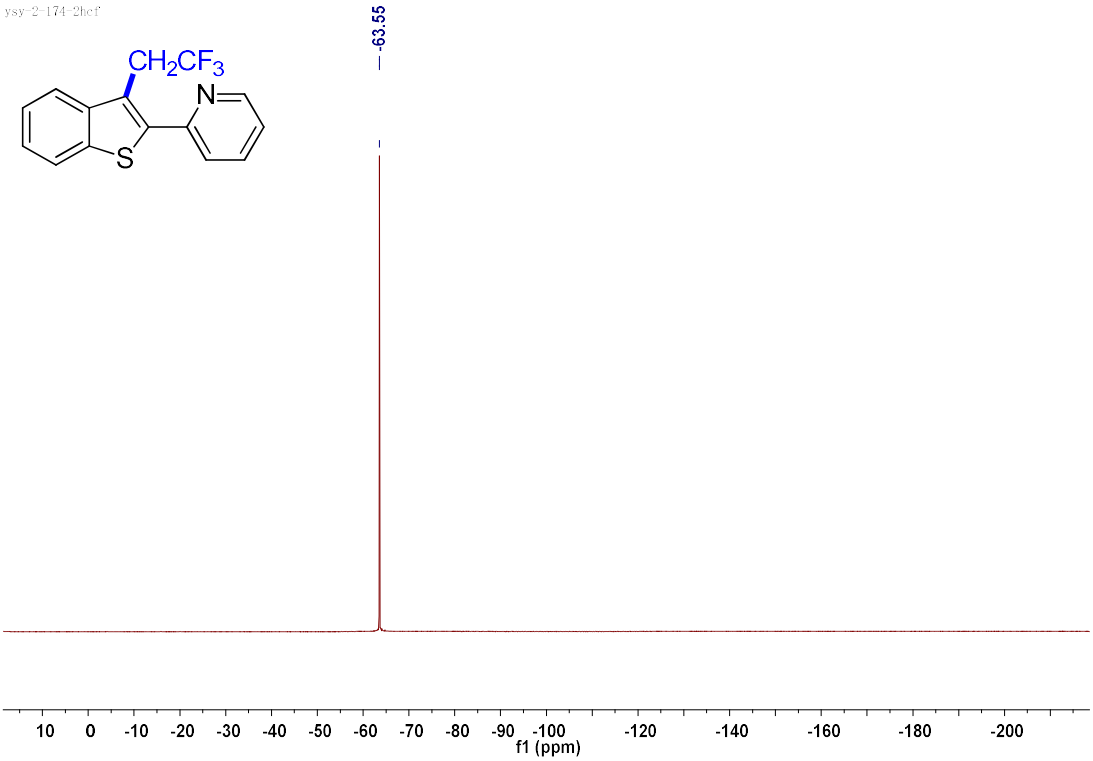

ysy-2-174-3c
154.722
149.492
140.505
136.906
129.669
129.373
129.341
129.309
129.277
128.568
126.912
125.212
124.155
122.938
122.036
121.398
33.372
33.060
32.748
32.435
CH2CF3
S
N
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


ysy-2-174-3hf
-65.723
CH2CF3
S
N
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)

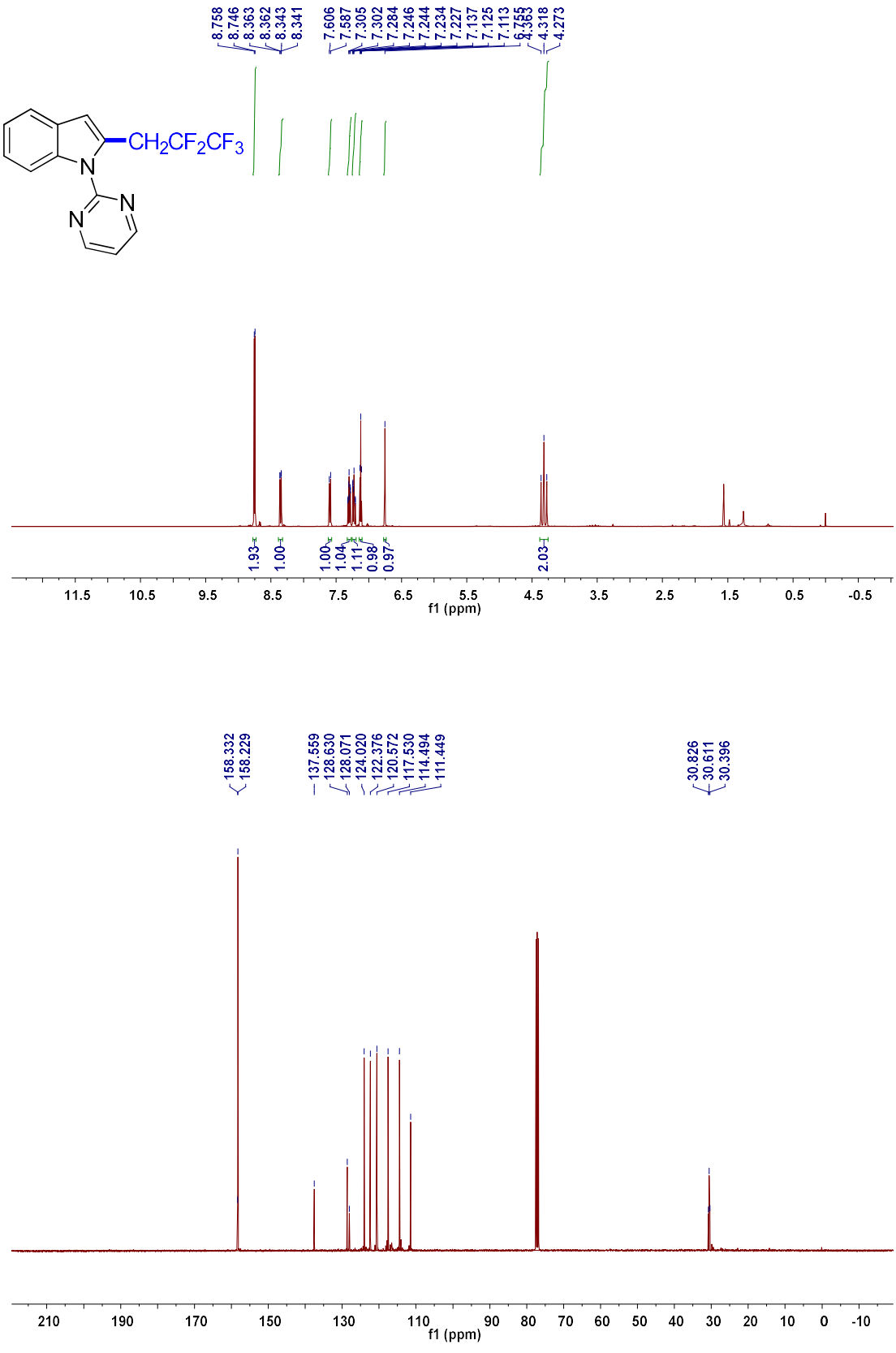
3ya

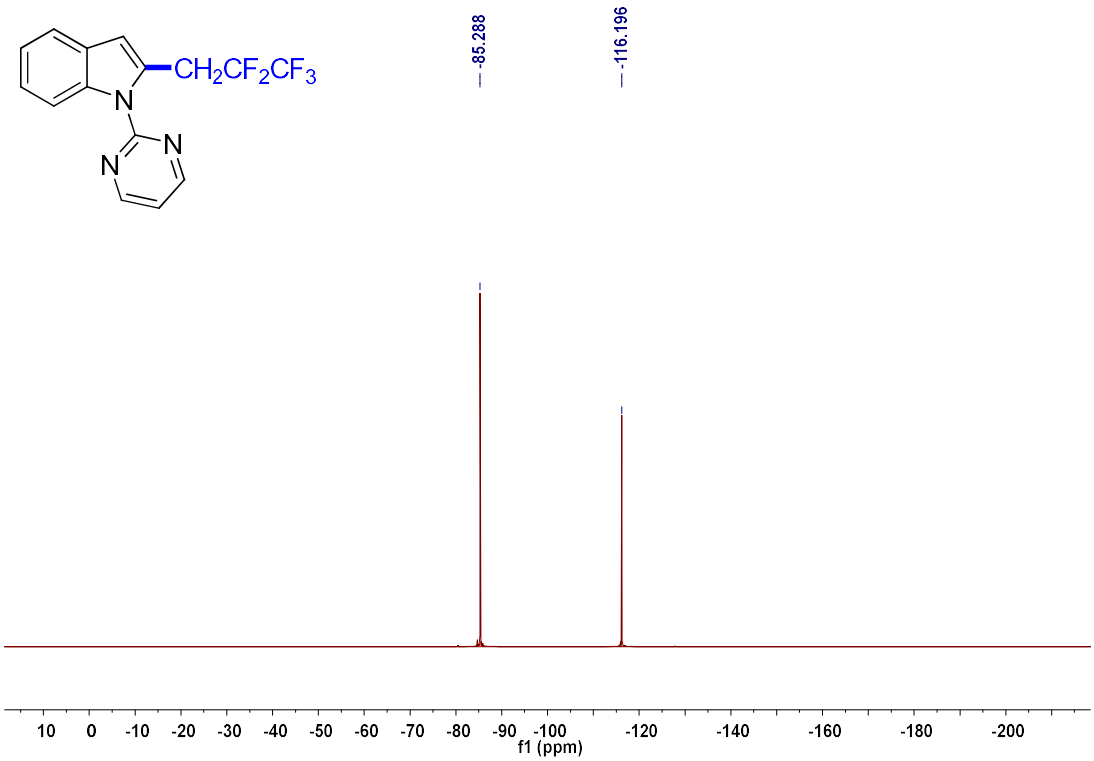

ysy-2-174-2hcf
8.712
8.709
8.707
8.705
8.700
8.697
8.695
8.693
7.869
7.850
7.846
7.776
7.771
7.679
7.659
7.447
7.444
7.428
7.421
4.339
4.313
4.286
CH2CF3
N
S
1.00
2.08
1.05
1.02
2.11
0.97
2.15
f1 (ppm)


ysy-2-174-2hcf
153.058
149.755
142.069
140.783
138.906
137.061
130.287
127.521
125.500
124.879
124.756
123.699
122.895
122.428
121.990
31.699
31.393
31.088
30.783
CH2CF3
N
S
f1 (ppm)

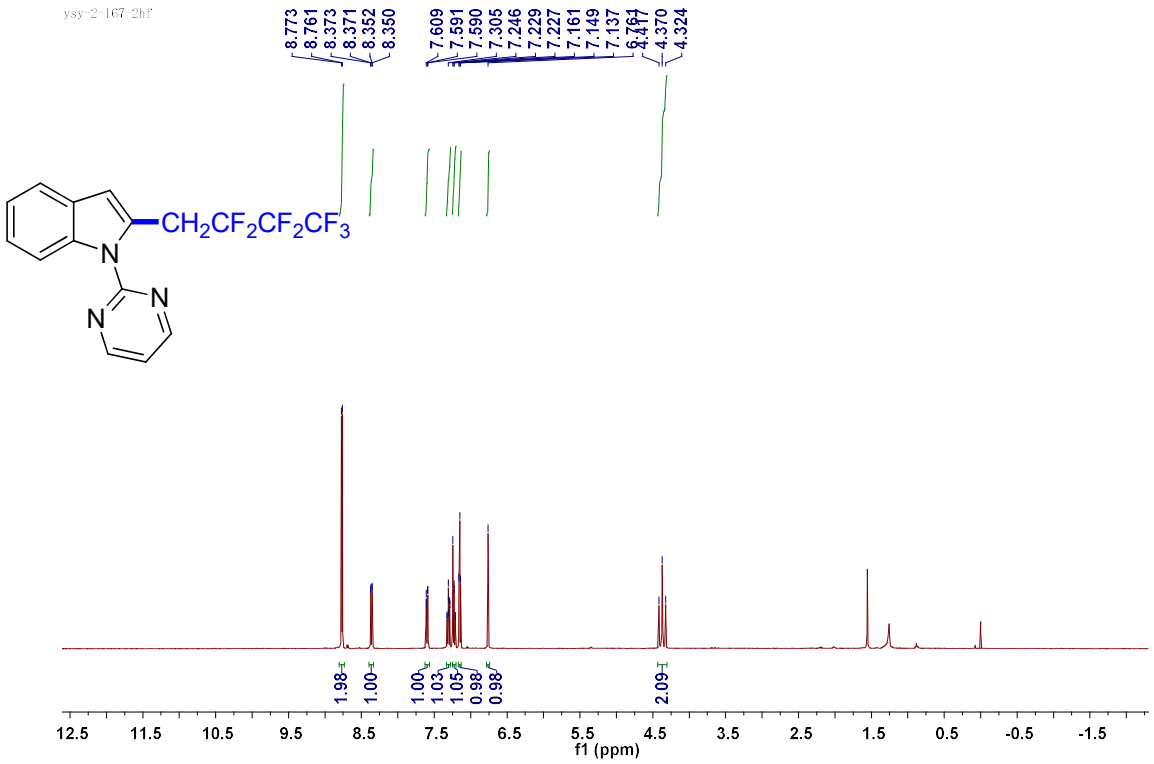

ysy-2-174-2hcf
CH2CF3
N
S
-63.55
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)

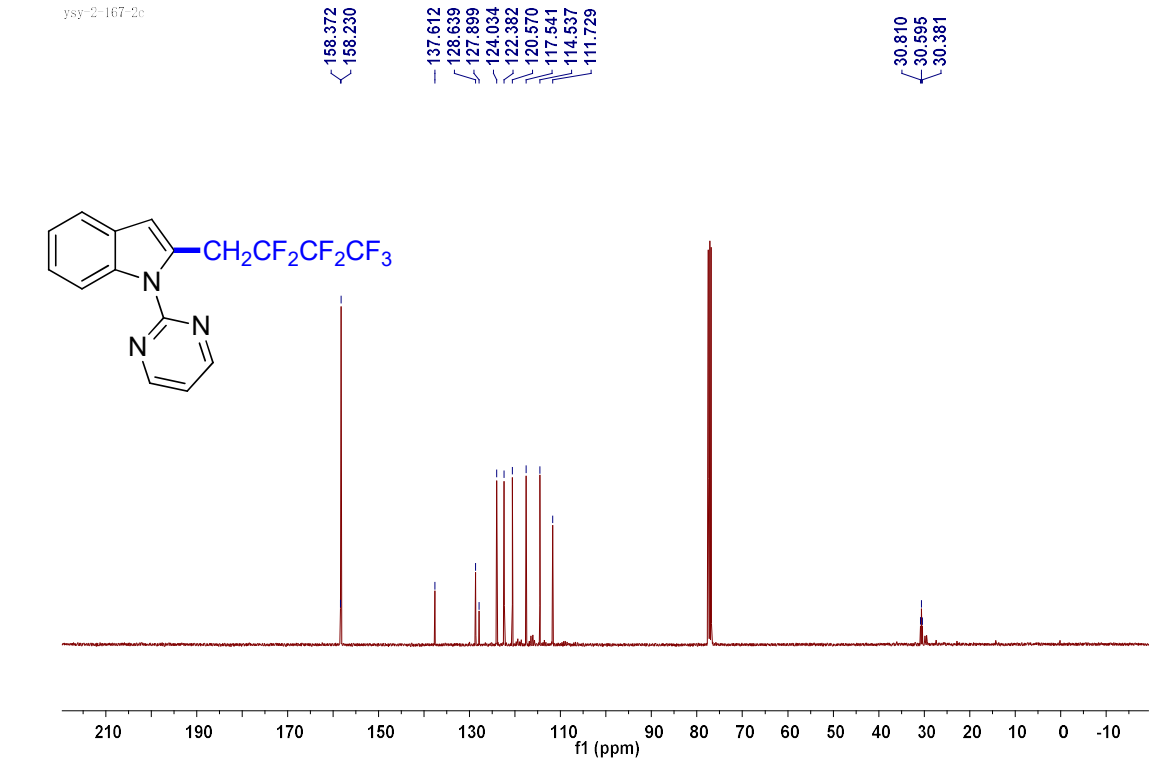
3ab

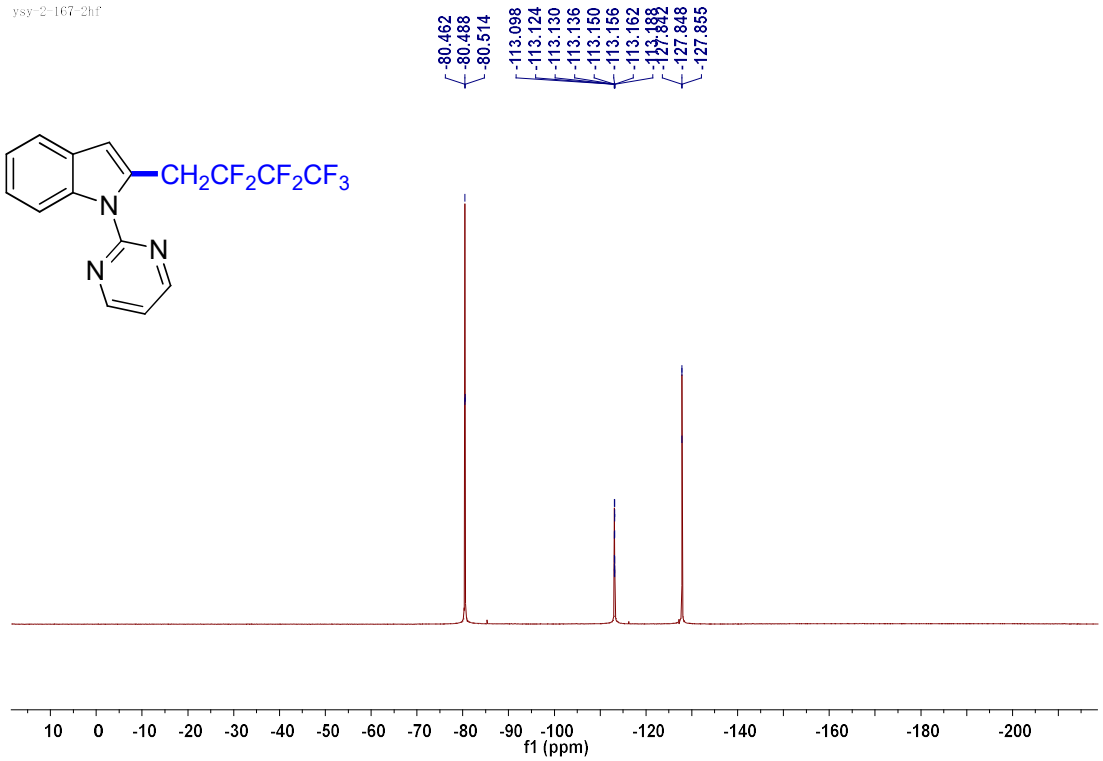

8.758
8.746
8.363
8.362
8.343
8.341
7.606
7.587
7.305
7.302
7.284
7.246
7.244
7.234
7.227
7.137
7.125
7.113
6.755
4.363
4.318
4.273
CH2CF2CF3
N
N
N
1.93
1.00
1.00
1.04
1.11
0.98
0.97
2.03
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)
158.332
158.229
137.559
128.630
128.071
124.020
122.376
120.572
117.530
114.494
111.449
30.826
30.611
30.396
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


CH2CF2CF3
N
N
N
-85.288
-116.196
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)

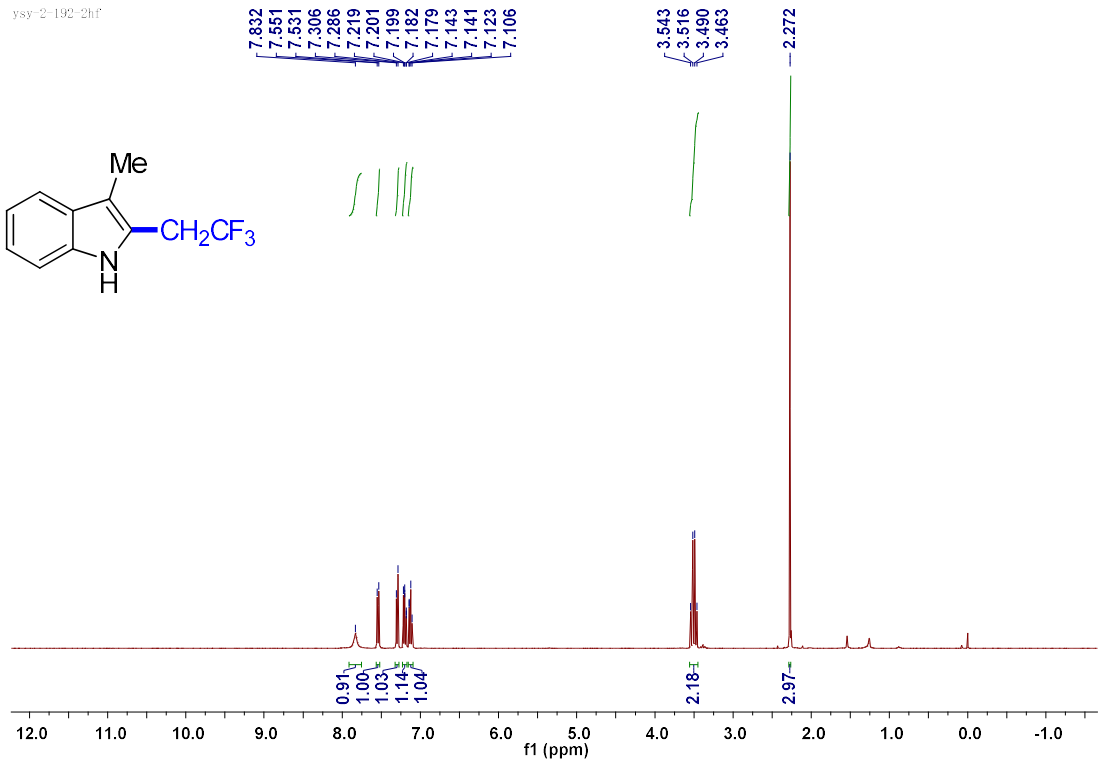
3ac

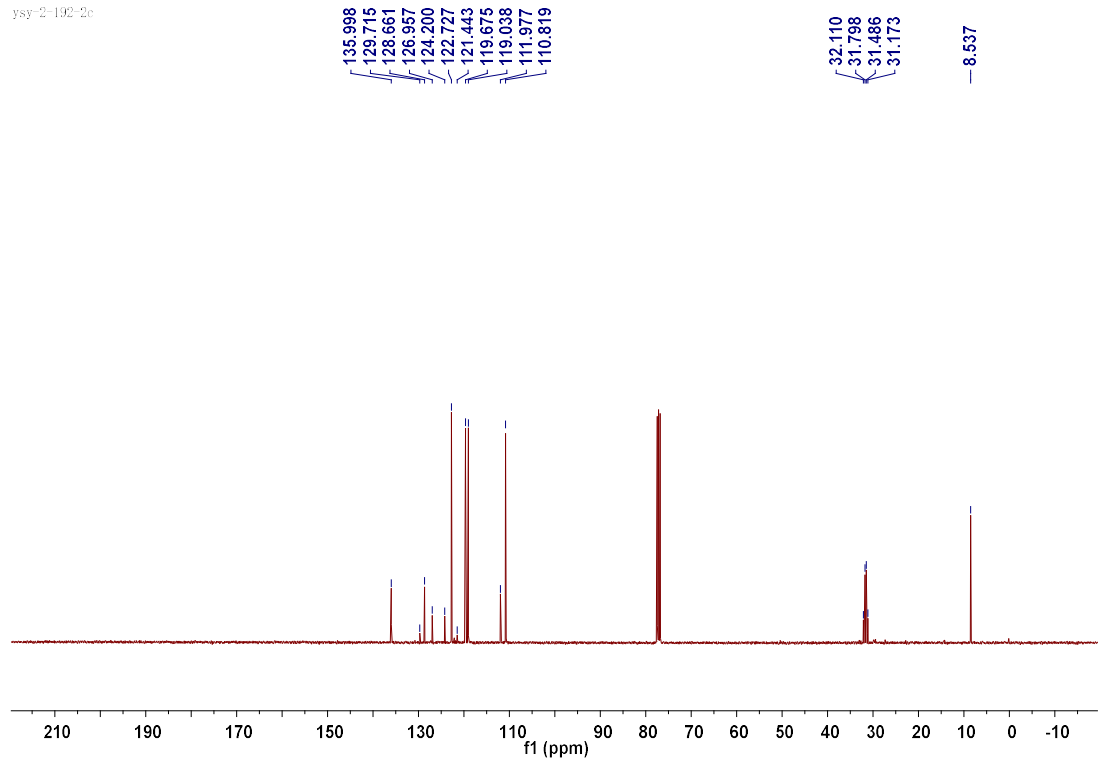

ysy-2-167-2hf
8.773
8.761
8.373
8.371
8.352
8.350
7.609
7.591
7.590
7.305
7.246
7.229
7.227
7.161
7.149
7.137
6.761
6.747
4.370
4.324
CH2CF2CF2CF3
N
N
N
1.98
1.00
1.00
1.03
1.05
0.98
0.98
2.09
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
-1.5
f1 (ppm)

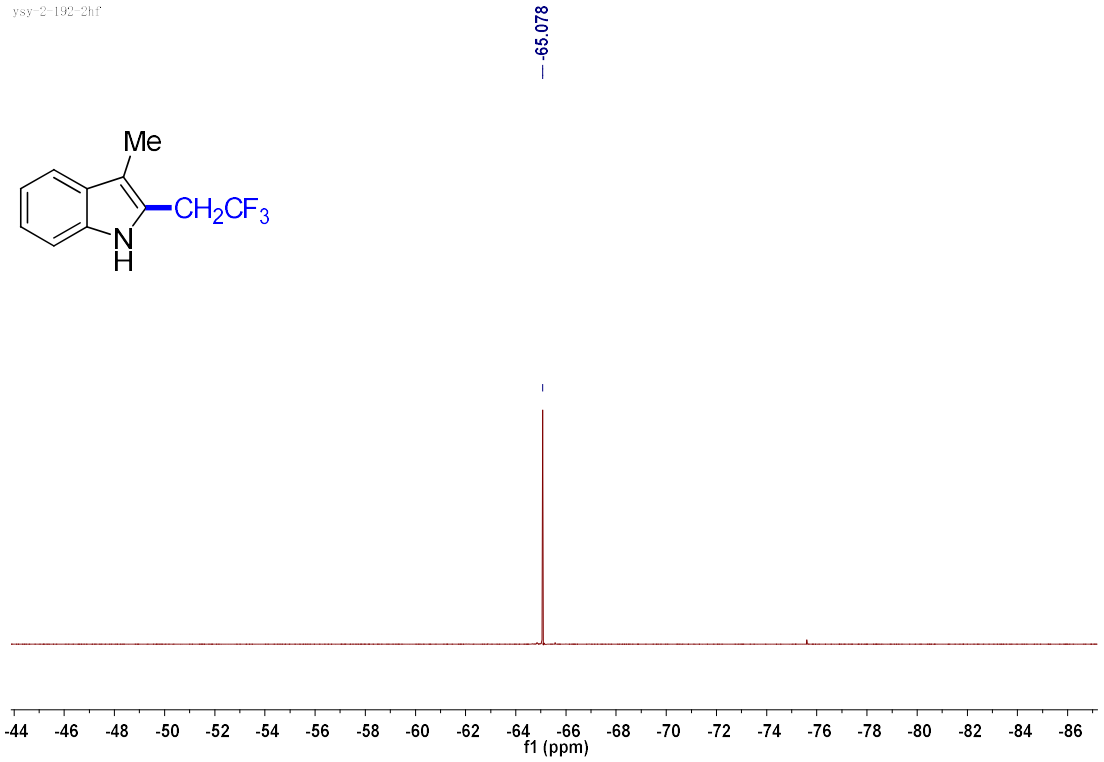

ysy-2-167-2c
158.372
158.230
137.612
128.639
127.899
124.034
122.382
120.570
117.541
114.537
111.729
30.810
30.595
30.381
CH2CF2CF2CF3
N
N
N
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


ysy-2-167-2hf
-80.462
-80.488
-80.514
-113.098
-113.124
-113.130
-113.136
-113.150
-113.156
-113.162
-113.188
-127.842
-127.848
-127.855
CH2CF2CF2CF3
N
N
N
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)

4


ysy-2-192-2hf
7.832
7.551
7.531
7.306
7.286
7.219
7.201
7.199
7.182
7.179
7.143
7.141
7.123
7.106
3.543
3.516
3.490
3.463
2.272
Me
CH2CF3
N
H
0.91
1.00
1.03
1.14
1.04
2.18
2.97
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)


ysy-2-192-2c
135.998
129.715
128.661
126.957
124.200
122.727
121.443
119.675
119.038
111.977
110.819
32.110
31.798
31.486
31.173
8.537
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


ysy-2-192-2hf
-65.078
Me
CH2CF3
N
H
-44 -46 -48 -50 -52 -54 -56 -58 -60 -62 -64 -66 -68 -70 -72 -74 -76 -78 -80 -82 -84 -86
f1 (ppm)