Aqueous Benzylic C–H Trifluoromethylation for Late-Stage Functionalization

Shuo Guo, Deyaa I. AbuSalim and Silas P. Cook*

Department of Chemistry, Indiana University,

800 East Kirkwood Avenue, Bloomington, IN 47405-7102

Supporting Information

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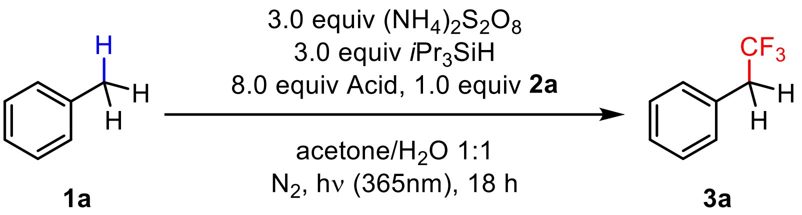
General Methods.

All the reactions were carried out in glassware fitted with rubber septa under a nitrogen atmosphere unless otherwise stated. Analytical grade solvents and commercially available reagents were purchased from commercial sources and used directly without further purification unless otherwise stated. HPLC Acetone (≥99.9%) was obtained from Sigma-Aldrich. PhenCu(CF_3) was purchased from Strem Chemicals, Inc. *p*-Xylene-α,α,α-d_3 was purchased from C/D/N Isotopes Inc. Light irradiation was performed with a Lixada LED lamp (5 W, λ = 365nm). Thin-layer chromatography (TLC) was carried out on Merck 60 F254 precoated, glass silica gel plates which were visualized with either ultraviolet light or stained with $KMnO_4$. Flash chromatography was performed using ZEOprep 60 ECO 40-63 μm silica gel. Automated column chromatography was performed on a Biotage Isolera One using Biotage Snap KPSil cartridges (25g or 50g SiO_2), Biotage Snap Ultra cartridges (25g or 50g SiO_2), Yamzen universal columns (16g 40μm SiO_2), or RediSepR$_f$ columns (24g or 40g SiO_2) monitoring wavelengths 254nm and 280nm unless otherwise noted. ^{1}H-NMR and ^{13}C-NMR spectra were recorded at room temperature using a Varian I400 (^{1}H-NMR at 400MHz and ^{13}C-NMR at 100MHz), Varian VXR400 (^{1}H-NMR at 400MHz and ^{13}C-NMR at 100MHz), Varian I500 (^{1}H-NMR at 500MHz and ^{13}C-NMR at 125MHz), Varian I600 (^{1}H-NMR at 600MHz). ^{19}F-NMR spectra were recorded at room temperature using a VarianI400 or VXR400 (^{19}F-NMR at 376 MHz). Chemical shifts are reported in ppm with reference to solvent signals [^{1}H-NMR: $CDCl_3$ (7.26 ppm); ^{13}C-NMR: $CDCl_3$ (77.16 ppm)]. Signal patterns are indicated as s, singlet; d, doublet; t, triplet; q, quartet; and m, multiplet. High Resolution Mass (HRMS) analysis was obtained using Electron Impact Ionization (EI) and reported as m/z (relative intensity) for the molecular ion [M], or with Electrospray Ionization (ESI) and reporting the molecular ion $[M+H]^+$ or a suitable fragment ion.

Optimization of Pertinent Reaction Conditions.

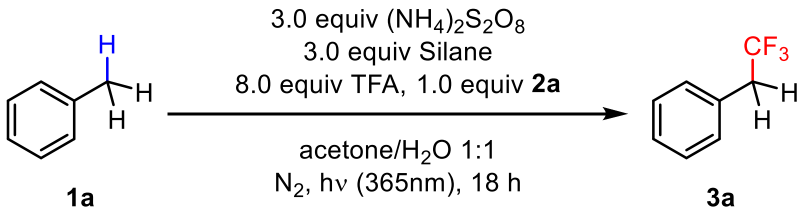
Table S1. *Evaluation of Acids*



Entry	Acid	Yield of **3a** (^{19}F NMR)
1	without Acid	62%
2	CCl_3COOH	58%
3	AcOH	59%
4	MsOH	71%
5	CH_3CF_2COOH	59%
6	**TFA**	**99%**
7	HCOOH	65%
8	PhCOOH	24%

Procedure: In a N_2 glovebox, to a 2.0 mL screw-cap test tube equipped with a stir bar was added $(NH_4)_2S_2O_8$ (27.3 mg, 0.12 mmol, 3.0 equiv) and bpyCu(CF_3)$_3$ (17.1 mg, 0.04 mmol, 1.0 equiv). Acetone (0.20 mL) and toluene **1a** (8.5 µL, 0.08 mmol, 2.0 equiv) were added via syringe, followed by *i*-Pr_3SiH (24.7 µL, 0.12 mmol, 3.0 equiv). The tube was sealed with a PTFE lined screw cap, brought outside the glovebox. Degassed H_2O (0.20 mL) and the desired acid (0.12 mmol, 8.0 equiv) were added under N_2 atmosphere. Then the reaction mixture was irradiated with a 5 W LED lamp (centered at 365 nm and placed 15-20 cm away from the reaction vial) at room temperature for 18 h. The reaction mixture was quenched with saturated aqueous $NaHCO_3$ (4 mL). 1-bromo-4-fluorobenzene (6.0 µL, 0.059 mmol, internal standard) and acetone-*d*$_6$ (0.6 mL) were added. The NMR yield of (2,2,2-trifluoroethyl)benzene **3a** was determined by comparing the integration of the ^{19}F NMR benzene **3a** with that of 1-bromo-4-fluorobenzene (-115.7 ppm).

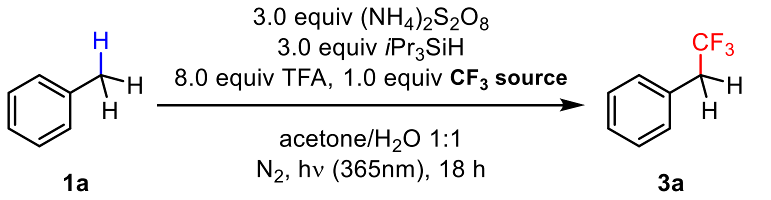
Table S2. *Evaluation of Silanes*



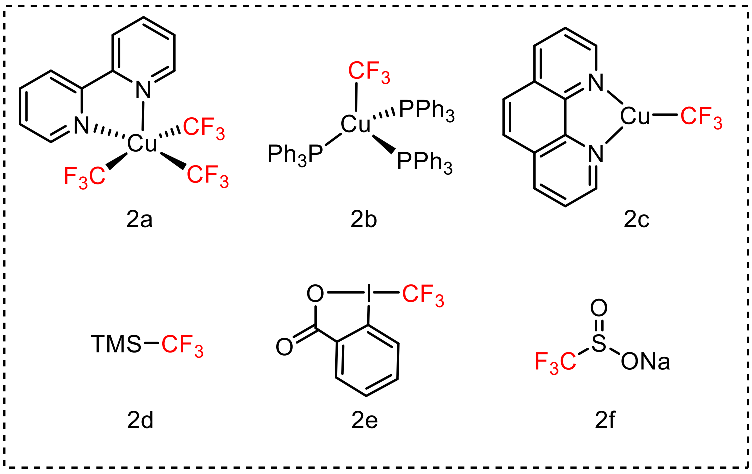
Entry	Silane	Yield of **3a**[b] (^{19}F NMR)
1	without Silane	78%
2	Me_2EtSiH	22%
3	$MeEt_2SiH$	35%
4	Et_3SiH	60%
5	***i*-Pr$_3$SiH**	**99%**
6	*t*-BuMe$_2$SiH	81%
7	*t*-Bu$_2$MeSiH	91%
8	$(TMS)_3SiH$	92%
9	$(EtO)_3SiH$	56%
10	PHMS	70%

Procedure: In a N_2 glovebox, to a 2.0 mL screw-cap test tube equipped with a stir bar was added $(NH_4)_2S_2O_8$ (27.3 mg, 0.12 mmol, 3.0 equiv) and bpyCu$(CF_3)_3$ (17.1 mg, 0.04 mmol, 1.0 equiv). Acetone (0.20 mL) and toluene **1a** (8.5 µL, 0.08 mmol, 2.0 equiv) were added via syringe, followed by the desired silane (0.12 mmol, 3.0 equiv). The tube was sealed with a PTFE lined screw cap, brought outside the glovebox. Degassed H_2O (0.20 mL) and trifluoroacetic acid (24.5 µL, 0.12 mmol, 8.0 equiv) were added under N_2 atmosphere. The reaction mixture was irradiated with a 5 W LED lamp (centered at 365 nm and placed 15-20 cm away from the reaction vial) at room temperature for 18 h. Then the reaction mixture was quenched with saturated aqueous $NaHCO_3$ (4 mL), 1-bromo-4-fluorobenzene (6.0 µL, 0.059 mmol, internal standard) and acetone-*d*$_6$ (0.6 mL) were added. The yield of (2,2,2-trifluoroethyl)benzene **3a** was determined by comparing the integration of the ^{19}F NMR (2,2,2-trifluoroethyl)benzene **3a** with that of 1-bromo-4-fluorobenzene (-115.7 ppm).

Table S3. *Evaluation of* CF_3 *sources*

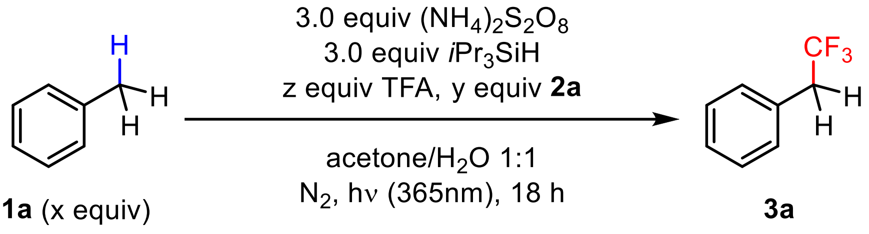


Entry	CF_3 source	Yield of **3a** (^{19}F NMR)
1	**2a**	**99%**
2	2b	0%
3	2c	4%
4	2d	0%
5	2e	0%
6	2f	0%



Procedure: In a N_2 glovebox, to a 2.0 mL screw-cap test tube equipped with a stir bar was added $(NH_4)_2S_2O_8$ (27.3 mg, 0.12 mmol, 3.0 equiv) and CF_3 source (0.04 mmol, 1.0 equiv) (if solid). Acetone (0.20 mL) and toluene **1a** (8.5 μL, 0.08 mmol, 2.0 equiv) were added via syringe, followed by *i*-Pr_3SiH (24.7 μL, 0.12 mmol, 3.0 equiv) and CF_3 source (0.04 mmol, 1.0 equiv) (if liquid). The tube was sealed with a PTFE lined screw cap, brought outside the glovebox. Degassed H_2O (0.20 mL) and trifluoroacetic acid (24.5 μL, 0.12 mmol, 8.0 equiv) were added under N_2 atmosphere. The reaction mixture was irradiated with a 5 W LED lamp (centered at 365 nm and placed 15-20 cm away from the reaction vial) at room temperature for 18 h. Then the reaction mixture was quenched with saturated aqueous $NaHCO_3$ (4 mL), 1-bromo-4-fluorobenzene (6.0 μL, 0.059 mmol, internal standard) and acetone-d_6 (0.6 mL) were added. The yield of (2,2,2-trifluoroethyl)benzene **3a** was determined by comparing the integration of the ^{19}F NMR (2,2,2-trifluoroethyl)benzene **3a** with that of 1-bromo-4-fluorobenzene (-115.7 ppm).

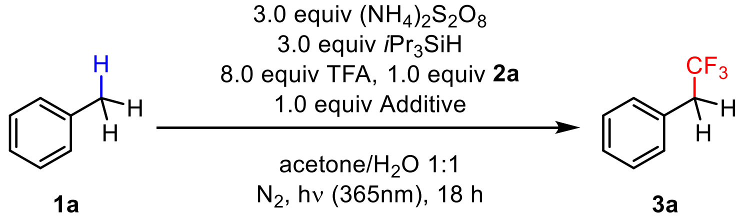
Table S4. *Ratiometric studies.*

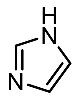
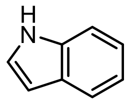
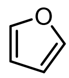
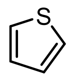
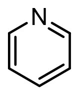
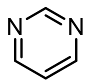
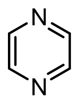


Entry	X	y	z	Yield of **3a** (^{19}F NMR)
1	1.0	1.5	4.0	46%
2	1.0	1.5	8.0	45%
3	**2.0**	**1.0**	**8.0**	**99%**
4	2.0	1.0	6.0	97%
5	2.0	1.0	4.0	85%
6	2.0	1.0	2.0	65%
8	2.0	1.0	0.0	62%

Procedure: In a N_2 glovebox, to a 2.0 mL screw-cap test tube equipped with a stir bar was added $(NH_4)_2S_2O_8$ (27.3 mg, 0.12 mmol, 3.0 equiv) and bpyCu$(CF_3)_3$ (y equiv). Acetone (0.20 mL) and toluene **1a** (x equiv) were added via syringe, followed by the *i*-Pr_3SiH (24.7 µL, 0.12 mmol, 3.0 equiv). The tube was sealed with a PTFE lined screw cap, brought outside the glovebox. Degassed H_2O (0.20 mL) and trifluoroacetic acid (z equiv) were added under N_2 atmosphere. The reaction mixture was irradiated with a 5 W LED lamp (centered at 365 nm and placed 15-20 cm away from the reaction vial) at room temperature for 18 h. Then the reaction mixture was quenched with saturated aqueous $NaHCO_3$ (4 mL), 1-bromo-4-fluorobenzene (6.0 µL, 0.059 mmol, internal standard) and acetone-*d*$_6$ (0.6 mL) were added. The yield of (2,2,2-trifluoroethyl)benzene **3a** was determined by comparing the integration of the ^{19}F NMR (2,2,2-trifluoroethyl)benzene **3a** with that of 1-bromo-4-fluorobenzene (-115.7 ppm).

Table S5. *Heterocycle Screen.*

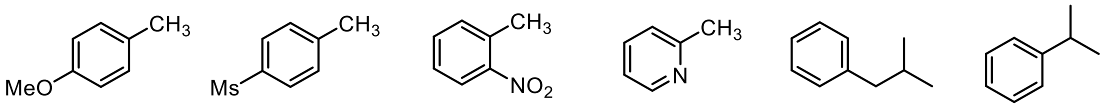


Entry	Additive	Yield of **3a** (^{19}F NMR)
1	None	99%
2		79%
3		6%
4		72%
5		99%
6		99%
7		94%
8		69%

Procedure: In a N_2 glovebox, to a 2.0 mL screw-cap test tube equipped with a stir bar was added $(NH_4)_2S_2O_8$ (27.3 mg, 0.12 mmol, 3.0 equiv), bpyCu$(CF_3)_3$ (17.1 mg, 0.04 mmol, 1.0 equiv) and additive (0.04 mmol, 1.0 equiv). Acetone (0.20 mL) and toluene **1a** (8.5 µL, 0.08 mmol, 2.0 equiv) were added via syringe, followed by the *i*-Pr_3SiH (24.7 µL, 0.12 mmol, 3.0 equiv). The tube was sealed with a PTFE lined screw cap, brought outside the glovebox. Degassed H_2O (0.20 mL) and trifluoroacetic acid (24.5 µL, 0.12 mmol, 8.0 equiv) were added under N_2 atmosphere. The reaction mixture was irradiated with a 5 W LED lamp (centered at 365 nm and placed 15-20 cm away from the reaction vial) at room temperature for 18 h. Then the reaction mixture was quenched with saturated aqueous $NaHCO_3$ (4 mL), 1-bromo-4-fluorobenzene (6.0 µL, 0.059 mmol, internal standard) and acetone-*d*$_6$ (0.6 mL) were added. The yield of (2,2,2-trifluoroethyl)benzene **3a** was determined by comparing the integration of the ^{19}F NMR (2,2,2-trifluoroethyl)benzene **3a** with that of 1-bromo-4-fluorobenzene (-115.7 ppm).

Unreactive substrates

Table S6. Unreactive substrates.



0%	7%	0%	0%	6%	0%[a]

[a] 2-Phenylpropan-2-ol is the main by-product.

Computational Details.

A. Computational Methods

All calculations were performed by using DFT, as implemented in the Jaguar 9.1 suite of ab initio quantum chemistry programs.[1] Geometry optimizations were performed with the M06 functional[2] using the 6-31G** basis set. Cu was represented by using the Los Alamos LACVP[3] basis set that included relativistic core potentials. More accurate single-point energies were computed from the optimized geometries by using Dunning's correlation-consistent triple-ζ basis set, cc-pVTZ(-f),[4] which included a double set of polarization functions. Cu was represented by using a modified version of LACVP, designated as LACV3P, in which the exponents were decontracted to match the effective core potential with triple-ζ quality. Vibrational frequencies were computed at theM06/6-31G** level of theory to derive the zero-point energy (ZPE) and vibrational entropy corrections from unscaled frequencies. Entropy herein referred specifically to the vibrational/rotational/translational entropy of the solutes because the continuum model included the entropy of the solvent implicitly. All intermediates were confirmed as local minima on the potential energy surface with zero imaginary frequencies. Transition states were confirmed to possess only one imaginary frequency. Solvation energies were evaluated by using a self-consistent reaction field (SCRF)[5-7] approach based on accurate numerical solutions of the linearized Poisson–Boltzmann equation. Solvation calculations were carried out on the optimized gas-phase geometries by using a dielectric constant of ε = 20.7. The change in solution-phase free energy, ΔG(sol), was calculated from Equations (S1)–(S5).

$$G(sol) = G(gas) + \Delta G(solv) \quad (S1)$$

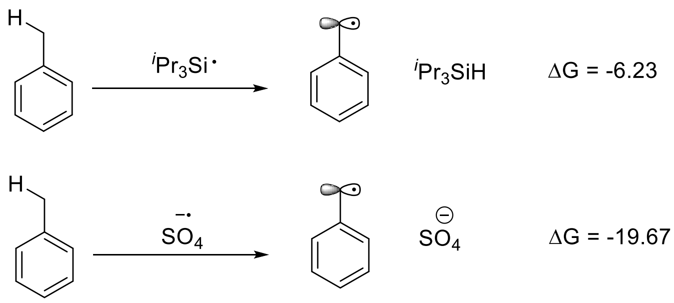
$$G(gas) = H(gas) - TS(gas) \quad (S2)$$

$$H(gas) = E(SCF) + ZPE \quad (S3)$$

$$\Delta E(SCF) = \Sigma E(SCF) \text{ for products} - \Sigma E(SCF) \text{ for reactants} \quad (S4)$$

$$\Delta G(sol) = \Sigma G(sol) \text{ for products} - \Sigma G(sol) \text{ for reactants} \qquad \text{(S5)}$$

A. C-H Abstraction from toluene.



Scheme S1. Benzylic C-H abstraction was significantly more thermodynamically favorable for sulfate radical anion, calculated at -19.67 kcal/mol; in comparison with triisopropylsilyl radical, which was favored by only -6.23 kcal/mol. This is in line with experimental observations where no product formation is observed in the absence of persulfate.

Energies were computed (with uM06/cc-pVTZ(f)−LACV3P**//uM06/LACVP** level of theory).

B. Assessment of outer sphere CF_3 abstraction mechanisms.

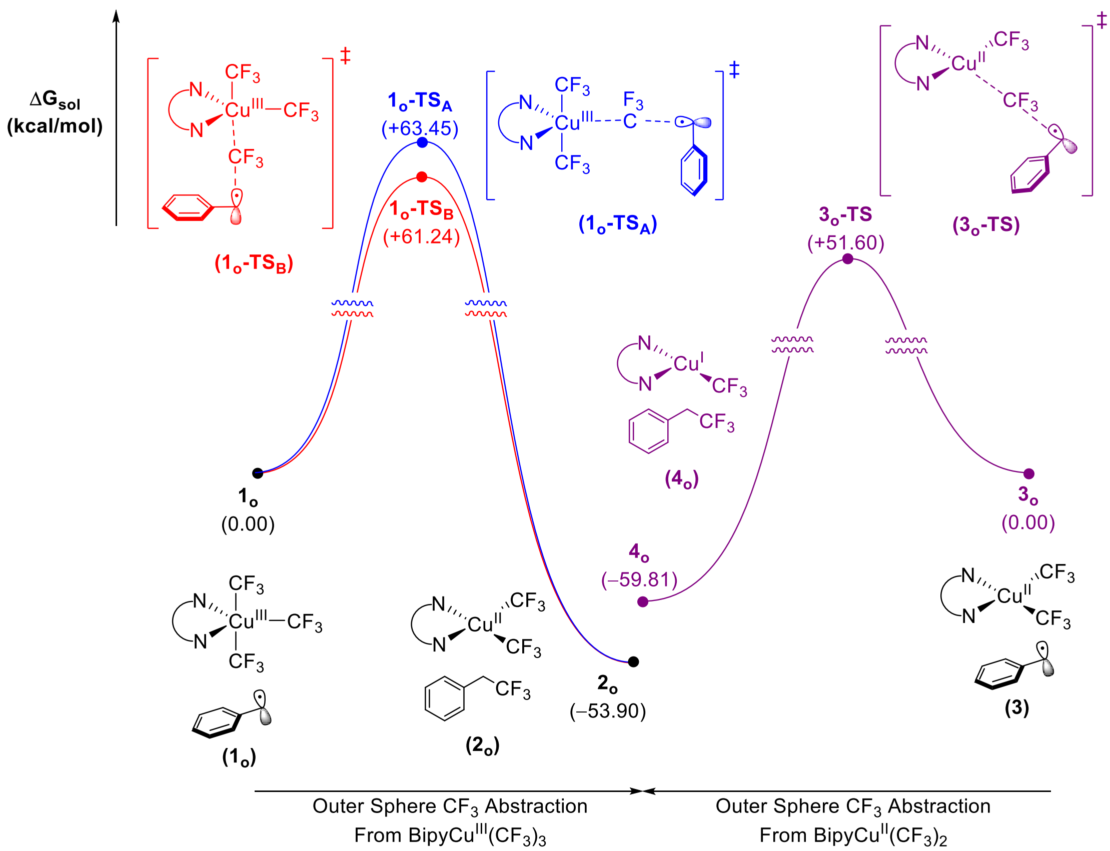
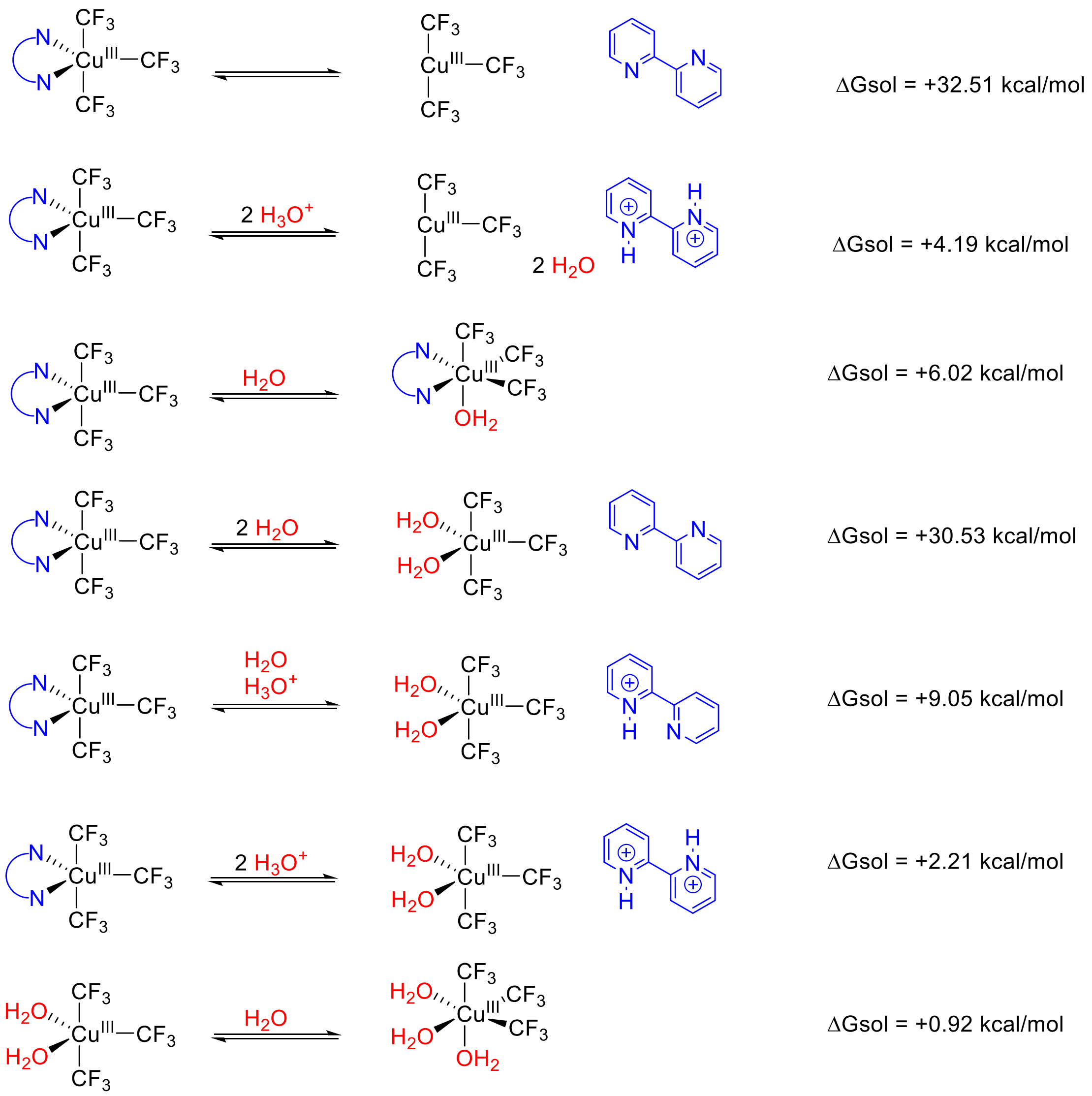


Figure S1. Energy diagram for outer sphere mechanisms involving toluyl radical and different copper species. The barrier for the abstraction of CF_3 from $bipyCu^{III}(CF_3)_3$ **(1_o)** was calculated at +63.5 kcal/mol and +61.2 kcal/mol for **1_o-TS_A** and **1_oTS_B**, respectively. In addition, the barrier **3_o-TS** of abstracting CF_3 from $bipyCu^{II}(CF_3)_2$ **(3_o)** was calculated at

+51.6 kcal/mol. These barriers were deemed too high for the reaction conditions and hence, the outer sphere mechanism was dismissed in favor of the inner sphere one.

Energies were computed (with uM06/cc-pVTZ(f)−LACV3P**//uM06/LACVP** level of theory).

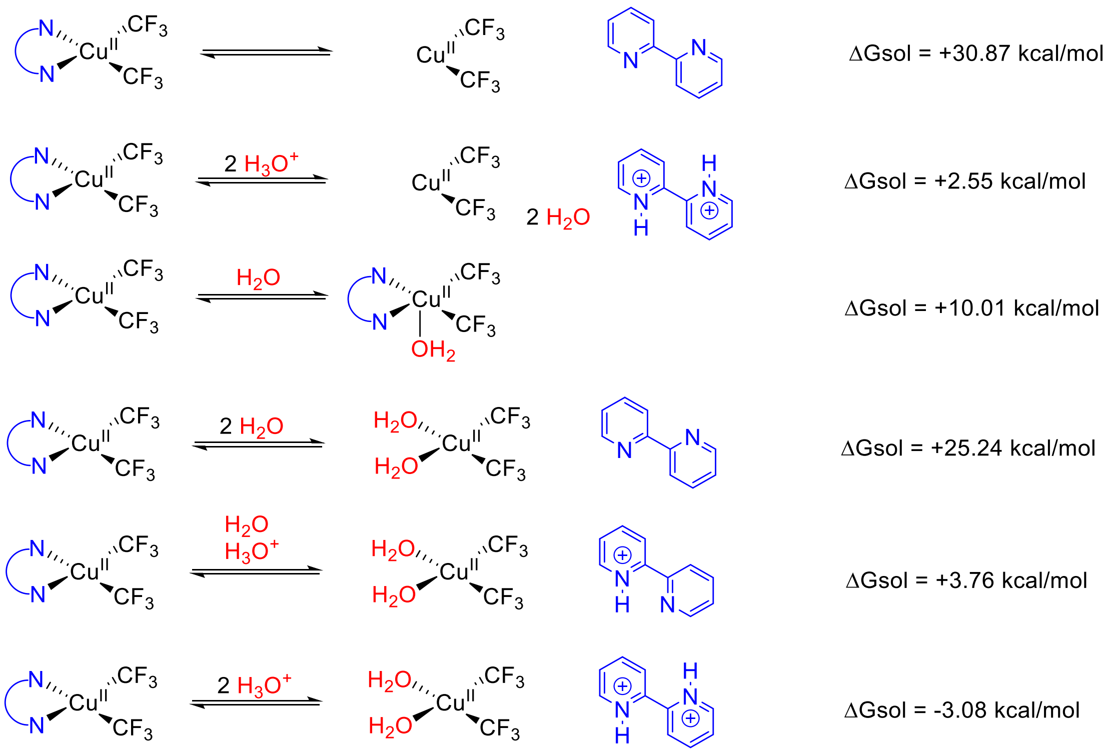
C. Assessment of the ligation of Grushin's complex in a H_2O/TFA mixture



Scheme S2. As expected the Grushin complex does not freely dissociate from the free-base bipy ligand, as this is thermodynamically uphill by +32.5 kcal/mol. Yet, in the presence of a strong acid, like TFA, the diprotonation of bipy can result in a ligand exchange with water to form the bishydrate, calculated at +2.2 kcal/mol or the production of unligated copper(III) which was thermodynamically unfavored by about +4.2 kcal/mol.

Energies were computed (with uM06/cc-pVTZ(f)−LACV3P**//uM06/LACVP** level of theory).

D. Assessment of the ligation of $Cu^{II}(CF_3)_2$ complex in a H_2O/TFA mixture



Scheme S3. In line with the calculated results for the Grushin complex, $Cu^{II}(CF_3)_2$ gains +30.9 kcal/mol with the loss of free-base bipy. Once again, in the presence of TFA, the diprotonation of bipy and exchange with water results in the bishydrate, calculated at -3.08 kcal/mol or the production of unligated copper(II) which was thermodynamically unfavored by only +2.55 kcal/mol.

Energies were computed (with uM06/cc-pVTZ(f)−LACV3P**//uM06/LACVP** level of theory).

E. Assessment of the ligation of $Cu^{II}(CF_3)_2$ complex in a H_2O/TFA mixture

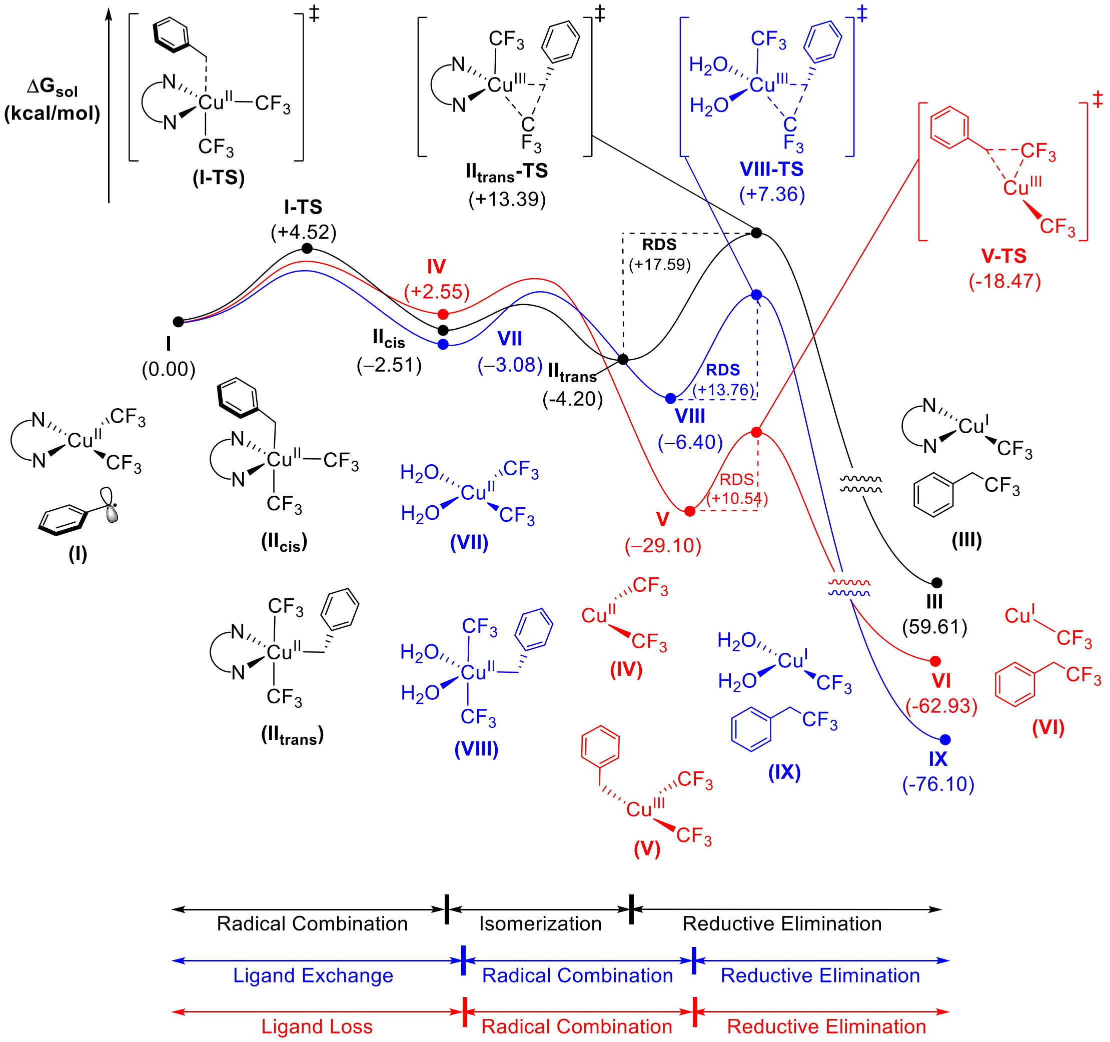


Figure S2. Based on the ligation study (Scheme S2 and S3) we deemed it appropriate not only to study the bipy complex (shown in black), but also to expand our study to include the bishydrate (blue) and unligated (red) copper systems. Interestingly when assessing the rate determining step in these processes, unligated copper species **V** had the lowest barrier to reductive elimination **V-TS** of +10.5kcal/mol. In contrast, the bishydrate species VIII has a barrier of 13.7 kcal/mol and the bipy ligated system $\mathbf{II_{trans}}$ has to overcome 17.6 kcal/mol for the reductive elimination event.

Energies were computed (with uM06/cc-pVTZ(f)−LACV3P**//uM06/LACVP** level of theory).

F. Computed energy components for DFT-optimized structures

Table S7. Computed energy components.

	E(SCF)/(eV) cc-pvtz(-f)/LACV3P**	ZPE/(kcal/mol) **6-31G**/LACVP****	S(gas)/(kcal/mol) **6-31G**/LACVP****	G(solv)/(kcalmol) **6-31G**/LACVP****
Ligands				
bipy – Conformation 1	-13473.4	98.452	94.351	-11.22
BIPY – Conformation 2	-13473.8	98.977	92.766	-6.65
$bipyH^+$ – Conformation 1	-13484.2	107.564	92.964	-49.53
$bipyH^+$ – Conformation 2	-13483.9	107.357	89.039	-53.09
$bipyH_2^{2+}$ – Conformation 1	-13490.1	115.696	94.634	-180.94
$bipyH_2^{2+}$ – Conformation 2	-13490.2	115.778	94.28	-180.19
H_3O^+	-2086.97	21.626	48.459	-96
H_2O	-2079.39	13.688	45.075	-9.53
Radicals				
Toluyl radical	-7368.02	71.548	76.54	-3.19
Secondary radical	-8437.36	89.176	85.884	-3.04
Tertiary radical	-9506.67	106.391	89.411	-3.21
$(^i pr)_3Si$ radical	-17548	175.638	121.367	-1.18
SO_4 radical anion	-19021.7	9.079	71.008	-61.52
CF_3 Radical	-9185.25	7.931	65.323	-0.29
Organic Molecules				
1° Product	-16557.2	84.205	95.879	-4.36
2° Product	-17626.5	101.787	102.501	-4.05
3° Product	-18695.7	119.352	106.293	-3.95
Toluene	-7385.73	79.909	79.365	-2.94
Ethylbenzene				
Cumene				
$(^i Pr)_3SiH$	-17565.9	181.595	119.695	-1.16

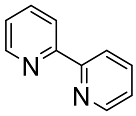
CF_3H	-9203.67	16.182	64.108	-2.56
SO_4 anion	-19039.9	16.522	69.014	-68.68
Toluene	-7385.73	79.853	74.283	-2.94
Copper(III) Complexes				
(bipy)Cu(CF3)3	-46374.7	126.817	160.405	-13.62
bipy$Cu^{III}(CF_3)_2$(toluyl) – Isomer 1	-44556.9	191.535	171.28	-13.84
bipy$Cu^{III}(CF_3)_2$(toluyl) – Isomer 2	-44557.1	192.036	171.654	-11.86
bipy$Cu^{III}(CF_3)_2$(ethylbenzyl) – Isomer 1 Conformer 1	-45626	209.183	175.556	-14.41
bipy$Cu^{III}(CF_3)_2$(ethylbenzyl) – Isomer 1 Conformer 2	-45625.8	209.035	184.922	-14.7
bipy$Cu^{III}(CF_3)_2$(ethylbenzyl) – Isomer 1 Conformer 3	-45626	209.357	178.875	-13.58
bipy$Cu^{III}(CF_3)_2$(ethylbenzyl) – Isomer 2 Conformer 1	-45626.2	209.273	186.896	-13.33
bipy$Cu^{III}(CF_3)_2$(ethylbenzyl) – Isomer 2 Conformer 2	-45626.1	209.466	185.861	-12.16
bipy$Cu^{III}(CF_3)_2$(ethylbenzyl) – Isomer 2 Conformer 3	-45626.2	209.283	180.541	-13.51
bipy$Cu^{III}(CF_3)_2$(cumenyl) – Isomer 1 Confromer 1	-46695.1	226.906	185.918	-13.93
bipy$Cu^{III}(CF_3)_2$(cumenyl) – Isomer 1 Conformer 2	-46695.1	226.72	188.439	-13.15
bipy$Cu^{III}(CF_3)_2$(cumenyl) – Isomer 1 Conformer 3	-46695.1	226.801	190.097	-13.35
bipy$Cu^{III}(CF_3)_2$(cumenyl) – Isomer 2 Conformer 1	-46694.8	226.833	187.784	-14.83
$Cu^{II}(CF_3)_2(CH_2Ph)$	-31082.1	91.128	134.927	-9.13
bipy$Cu^{III}(CF_3)_3(OH_2)$	-48453.4	141.399	189.855	-14.36

$(H_2O)_2Cu^{III}(CF_3)_3$	-37059.3	58.869	137.045	-14.75
$(H_2O)_3Cu^{III}(CF_3)_3$	-39139.4	74.487	154.47	-15.64
Copper(II) Species				
$Cu^{II}(CF_3)_2$	-23712	16.8	105.566	-6.55
$((H_2O)_2Cu^{II}(CF_3)_2$	-27872.5	48.973	129.167	-16.98
bipy$Cu^{II}(CF_3)_2$ – Isomer 1	-37187.7	116.989	153.538	-14.27
bipy$Cu^{II}(CF_3)_2$ – Isomer 2	-37187.3	116.755	154.476	-14.04
bipy$Cu^{II}(CF_3)_2(OH_2)$	-39267.6	132.931	159.07	-15.61
Copper(I) Species				
(bipy)Cu(CF3)	-28001.2	108.259	131.217	-15.26
(H2O)2Cu(CF3)	-16606.2	24.142	92.343	-18.39
Cu(CF3)	-14525.7	8.476	74.895	-9.81
Transition States				
Reductive Elimination (primary) Transition State 1	-44556	191.112	178.285	-16.33
Reductive Elimination (primary) Transition State 2	-44556.1	191.427	177.926	-12.87
Reductive Elimination (primary) Water Ligand Transition State	-35241.2	123.736	150.531	-13.97
Reductive Elimination (primary) Unligated Transition State	-31081.6	91.335	127.375	-11.36
Outer Sphere ‘equatorial’ Cu(III) Transition State	-53740.3	197.718	208.783	-17.15
Outer Sphere ‘Axial’ Cu(III) Transition State	-53740.4	197.341	209.057	-16.75
Outer Sphere ‘Axial’ Cu(III) Transition State	-44554.1	188.787	187.46	-17.03
Reductive Elimination (secondary) Transition State 1	-45625.2	208.631	176.062	-16.19

Reductive Elimination (secondary) Transition State 2	-45625.2	208.665	178.706	-16.09
Reductive Elimination (secondary) Transition State 3	-45625.2	208.638	181.108	-12.92
Reductive Elimination (secondary) Transition State 4	-45625.2	209.134	176.951	-12.89
Reductive Elimination (secondary) Transition State 5	-45625.2	208.96	184.381	-13
Reductive Elimination (tertiary) Transition State 1	-46694.2	225.842	188.202	-16.24
Reductive Elimination (tertiary) Transition State 2	-46694	225.876	183.418	-15.19
Reductive Elimination (tertiary) Transition State 3	-46694.2	225.739	186.683	-16.4

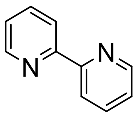
G. Cartesian coordinates for the M06-minimized structures:

Ligands:



bipy – Conformation 1

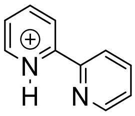
N	1.007953400	-1.315162100	0.097705446
C	1.095210400	-2.639139000	0.122001540
H	0.146611800	-3.178904800	0.193866010
C	2.297207400	-3.343074000	0.065241240
H	2.307344200	-4.429423000	0.093369960
C	3.473711300	-2.607346800	-0.031776390
H	4.442746000	-3.103745200	-0.086588800
C	3.398577000	-1.222765400	-0.066439930
H	4.316288000	-0.642503440	-0.164100080
C	2.140316700	-0.602536800	0.007081670
N	0.746750400	1.364391900	-0.101171140
C	1.995621600	0.883215100	-0.015191414
C	3.110753300	1.734790600	0.053800750
H	4.123888500	1.343701800	0.147793550
C	2.916722000	3.107667200	0.019708500
H	3.771879000	3.781940000	0.071218700
C	1.620382900	3.602908600	-0.072574740
H	1.421652400	4.670960400	-0.100165890
C	0.576556700	2.680344300	-0.125206290
H	-0.458691600	3.026413000	-0.193430830



bipy – Conformation 2

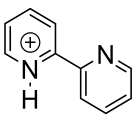
N	2.196564260	-1.209571002	-1.190634246
C	2.325047735	-2.532506896	-1.206279140
H	2.368535333	-3.000931422	-2.190759838
C	2.403207629	-3.314565306	-0.057879713
H	2.507758985	-4.393447200	-0.131880042
C	2.343170154	-2.672947609	1.173184588
H	2.399909367	-3.241247400	2.098907214
C	2.209289899	-1.292951843	1.208515290
H	2.156920688	-0.739246911	2.140557337
C	2.139354566	-0.597182741	0.000197097
N	1.938668694	1.490441742	1.182334602
C	1.995914730	0.878099023	-0.008469161
C	1.926009935	1.573867303	-1.216792123

H	1.977786313	1.020173525	-2.148879450
C	1.791711443	2.953832730	-1.181403265
H	1.734420428	3.522100583	-2.107111693
C	1.731720582	3.595429156	0.049688865
H	1.626823666	4.674281799	0.123636971
C	1.809991698	2.813349376	1.198056981
H	1.766301564	3.281683945	2.182578856



bipyH⁺ – Conformation 1

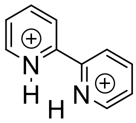
C	1.033599533	-2.564085821	0.043254926
H	0.059194590	-3.048301910	0.051407292
C	2.206530901	-3.321966325	0.057480273
H	2.154694720	-4.406104209	0.076803832
C	3.426269782	-2.663219925	0.046966568
H	4.358658342	-3.220455736	0.058235082
C	3.442250630	-1.272255651	0.022041102
H	4.386233123	-0.734721594	0.014389543
C	2.220506113	-0.608686719	0.008848178
N	0.846404708	1.332115860	-0.022198367
C	2.111244991	0.857930121	-0.016795641
C	3.149875144	1.782296825	-0.036304945
H	4.179920114	1.441166351	-0.033966853
C	2.855986449	3.137795265	-0.059876074
H	3.666012902	3.861781910	-0.075483993
C	1.530694124	3.577557120	-0.064060172
H	1.282684850	4.632867334	-0.082313890
C	0.525390627	2.635635865	-0.044829560
H	-0.531572082	2.878016709	-0.046791328
H	0.139507763	0.582492772	-0.008329753



bipyH⁺ – Conformation 2

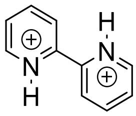
N	2.256437176	-1.126307703	-1.191303391
C	2.354132379	-2.440942833	-1.323320843
H	2.381123774	-2.823490321	-2.342309250
C	2.420587090	-3.315173767	-0.235644028
H	2.499955156	-4.385860910	-0.396204112
C	2.382528411	-2.783023377	1.043665919

H	2.431366131	-3.426980015	1.917013612
C	2.280208709	-1.404757091	1.194860631
H	2.250415856	-0.991965866	2.201809041
C	2.220232069	-0.616701692	0.045736394
N	2.066351918	1.507270603	1.263017632
C	2.111357128	0.850234920	0.078758485
C	2.050738663	1.619031369	-1.080474568
H	2.086798699	1.093382758	-2.028618874
C	1.948471880	2.997080062	-0.994386796
H	1.901548770	3.589333669	-1.904236287
C	1.905280547	3.629373880	0.252125588
H	1.825315736	4.706705424	0.343945672
C	1.966699818	2.850676794	1.381034471
H	1.940321109	3.247356541	2.389969889
H	2.109321560	0.962682190	2.119301574



bipyH_2^{2+} – Conformation 1

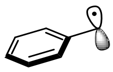
N	1.140630981	-1.375832539	-0.457110721
C	1.190442217	-2.723929467	-0.456394847
H	0.337397143	-3.244744836	-0.881260769
C	2.300990723	-3.368667732	0.056113421
H	2.335729436	-4.453734946	0.057290570
C	3.355187339	-2.605078688	0.545560405
H	4.241354258	-3.090308395	0.947597778
C	3.276887559	-1.209054930	0.529145176
H	4.080915697	-0.601865472	0.935553552
C	2.147839414	-0.593125233	0.023752339
N	0.866036428	1.450767869	0.453948057
C	2.005263902	0.875835751	-0.025594658
C	2.992523815	1.696244146	-0.537317963
H	3.898915867	1.254900227	-0.942190252
C	2.799139247	3.081017931	-0.558889611
H	3.573213842	3.726625449	-0.966729709
C	1.618170927	3.628263642	-0.069155149
H	1.441588339	4.699401587	-0.076601728
C	0.654669163	2.783076904	0.449479301
H	-0.281749290	3.130600331	0.875868545
H	0.169409082	0.869343366	0.918261327
H	0.340953246	-0.938850768	-0.913536522



bipyH_2^{2+} – Conformation 2

N	2.651244698	-1.247330087	-1.040720161
C	2.786156743	-2.586419061	-1.095937776
H	3.200734892	-2.998189605	-2.011379070
C	2.415265510	-3.358548366	-0.009612490
H	2.523797692	-4.437604788	-0.057892343
C	1.909878807	-2.727124650	1.121040896
H	1.604319167	-3.313798357	1.983989812
C	1.775131717	-1.335628737	1.144581994
H	1.331049947	-0.842616755	2.005538363
C	2.152399579	-0.591354423	0.041382297
N	2.368772362	1.615252461	1.036248041
C	2.005605608	0.874570293	-0.045088433
C	1.485680905	1.530570765	-1.146340027
H	1.145810500	0.960616120	-2.007221031
C	1.344396520	2.921441664	-1.121684410
H	0.926196598	3.437060124	-1.982764195
C	1.719252014	3.639319112	0.008267919
H	1.613179380	4.718571457	0.057644032
C	2.238338595	2.954700556	1.092546597
H	2.566904567	3.439367124	2.007214942
H	2.786537859	1.146050757	1.839090073
H	2.964220667	-0.706324604	-1.845999663

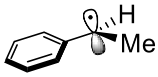
Radicals:



Toluyl Radical

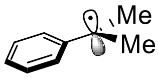
C	-1.192643927	-0.977670185	-2.037633647
H	-1.599509101	-1.876209848	-1.581429386
H	-1.747221968	-0.050108050	-1.921822835
C	0.006793127	-1.014139360	-2.760528015
C	0.736244087	-2.222685976	-2.922116657
C	0.540741442	0.157424747	-3.361927602
C	1.917105875	-2.251861967	-3.637460308
C	1.722644638	0.116815624	-4.075019086
C	2.421176644	-1.085325196	-4.219867663
H	0.344399318	-3.132532486	-2.469136051
H	-0.003042214	1.094676962	-3.250542717
H	2.458434940	-3.189086079	-3.747783550

H	2.112130411	1.026652222	-4.526807351
H	3.351679032	-1.112696215	-4.781752026



Ethylbenzyl radical

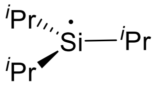
C	-1.193099221	-0.938003774	-2.039569869
H	-1.549503663	-1.873008390	-1.607247862
C	0.011047604	-0.977917999	-2.769992610
C	0.723829877	-2.197403040	-2.910514604
C	0.561391729	0.171897339	-3.392275963
C	1.905798742	-2.260576919	-3.621887200
C	1.745362737	0.098172468	-4.102769214
C	2.428789197	-1.113422572	-4.224911616
H	0.317574013	-3.093069454	-2.441541772
H	0.040438609	1.123970661	-3.309316600
H	2.431742257	-3.208720811	-3.712575694
H	2.146912127	0.994372321	-4.571400417
H	3.359691147	-1.163685739	-4.784574943
C	-2.005568682	0.291189668	-1.833208714
H	-2.379847282	0.699306423	-2.784482792
H	-2.873384506	0.093951780	-1.198350653
H	-1.422055560	1.092731208	-1.357298692



Cumenyl Radical

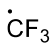
C	-1.198892779	-0.993795329	-2.006078643
C	0.013058496	-1.033063928	-2.750600470
C	0.757238363	-2.227137138	-2.944910516
C	0.538227918	0.143129319	-3.350832290
C	1.932797923	-2.236972263	-3.672540996
C	1.714852155	0.122914656	-4.077126926
C	2.427167960	-1.064647178	-4.246133954
H	0.399709385	-3.161771945	-2.520171497
H	0.005155060	1.084405621	-3.239210937
H	2.474309490	-3.172489467	-3.798652359
H	2.084814508	1.045243547	-4.520622485
H	3.352067155	-1.077425549	-4.817511950
C	-1.967422036	0.283091215	-1.875224691
H	-2.299887150	0.671098131	-2.849801876
H	-2.861903358	0.143237549	-1.259001680
H	-1.371119114	1.082256310	-1.411148271

C	-1.801017067	-2.194003462	-1.356227344
H	-2.703631620	-2.528375319	-1.892698200
H	-1.126276277	-3.051278775	-1.291644126
H	-2.129084159	-1.956107009	-0.334666544



Triisopropylsilyl radical

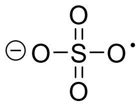
Si	0.107207734	0.349892916	0.075374927
C	-0.347012937	2.207760965	0.199616924
H	0.599833557	2.765084836	0.314827328
C	0.445790974	-0.352827617	1.824735790
H	-0.478072861	-0.187420402	2.401264999
C	1.623642242	0.000087496	-1.049680409
H	2.492421564	-0.005650898	-0.366904740
C	1.517408780	-1.378475301	-1.703310984
H	2.423250811	-1.616280846	-2.279576917
H	1.366894309	-2.183466813	-0.973709303
H	0.668123427	-1.409428350	-2.399807724
C	1.863873519	1.061276138	-2.117470391
H	2.768905041	0.833704036	-2.698622671
H	1.028581777	1.094994974	-2.831348909
H	1.985145557	2.067506240	-1.698636384
C	0.737915063	-1.850538370	1.809592820
H	0.855643518	-2.243231752	2.829451596
H	-0.058513113	-2.424881571	1.319659014
H	1.675433878	-2.065036415	1.277317875
C	1.584961369	0.402203297	2.513229058
H	1.756947105	0.017319998	3.529262575
H	2.528681381	0.280722274	1.962805908
H	1.391933581	1.478981146	2.597933773
C	-1.056547457	2.704092397	-1.059433384
H	-0.453996732	2.574087260	-1.965611165
H	-1.998685403	2.159041755	-1.210661275
H	-1.306221529	3.771679349	-0.977877418
C	-1.223259221	2.473950711	1.421998986
H	-2.146417549	1.877483636	1.379765145
H	-0.721587615	2.235279889	2.367457101
H	-1.524871725	3.529970643	1.466499583



CF_3 Radical

C	-0.734080476	-0.247521538	-2.066017087
F	-1.362971034	-1.332317710	-2.465994315

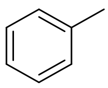
F	0.525800640	-0.258728642	-2.444571133
F	-1.346406289	0.842890988	-2.476172001



Sulfonate radical anion

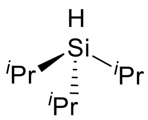
S	2.344938497	-0.041639618	-1.934056920
O	1.220676352	-0.024689333	-0.894456606
O	2.362693916	1.190230492	-2.731094518
O	3.468836905	-0.057883684	-0.893874290
O	2.326781860	-1.273548535	-2.731391099

Organic Molecules:



Toluene

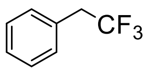
C	0.140775177	1.024325053	-2.250702030
C	-1.060244481	1.024255129	-1.537415085
C	1.336635112	1.024448238	-1.533240847
C	-1.065615214	1.024492593	-0.148093845
C	1.336824208	1.024699356	-0.141592340
C	0.135009381	1.024716133	0.556154536
H	-2.003384997	1.023976734	-2.084061618
H	2.281548813	1.024356233	-2.075358580
H	-2.011984359	1.024415522	0.388930606
H	2.281228996	1.024797842	0.398850663
H	0.132505041	1.024824286	1.643795596
C	0.134018195	1.024592424	-3.752207011
H	1.151210656	1.015211365	-4.157255731
H	-0.392409845	0.147833121	-4.148297623
H	-0.375735767	1.911292798	-4.148102723



Triisopropylsilane

Si	0.132273050	0.362128447	0.087497882

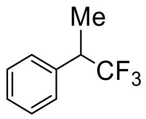
C	-0.355260742	2.197742529	0.207977347
H	0.560973421	2.795770567	0.343583665
C	0.471833940	-0.335471312	1.823343553
H	-0.453347345	-0.162773344	2.397369277
C	1.624958647	0.013920750	-1.049643253
H	2.510480696	0.003711391	-0.391163318
C	1.492778448	-1.367564616	-1.694804025
H	2.381496382	-1.613921418	-2.292979885
H	1.355185160	-2.170452518	-0.960331789
H	0.626875846	-1.395762237	-2.370599950
C	1.857959682	1.064207503	-2.132995483
H	2.755321228	0.828699589	-2.722471325
H	1.015700598	1.094562396	-2.838941810
H	1.985993963	2.074207247	-1.725403772
C	0.742204517	-1.838752110	1.807264954
H	0.839671488	-2.236488293	2.827225087
H	-0.056005442	-2.401571630	1.306131372
H	1.684079451	-2.065716058	1.287786124
C	1.613932158	0.402609292	2.520555865
H	1.772732850	0.022292373	3.539372273
H	2.561447663	0.265783891	1.980035965
H	1.436740065	1.482898667	2.597067170
C	-1.063250376	2.665343931	-1.064537601
H	-0.433837193	2.581961676	-1.957905536
H	-1.970222346	2.071063963	-1.244013853
H	-1.376412961	3.715528250	-0.979915917
C	-1.269894993	2.427568614	1.411731267
H	-2.167168642	1.793703784	1.350250757
H	-0.778732051	2.208478668	2.367452598
H	-1.617482627	3.469513727	1.450896781
H	-1.058228935	-0.355825879	-0.476124785



Primary Product

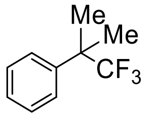
C	-0.773797589	-0.379235268	0.765510160
F	-1.914364681	-0.304227717	1.462949828
F	-0.031454316	-1.345989336	1.315126961
F	-0.120790518	0.774779159	0.932772183
C	-1.053792941	-0.656102585	-0.688961929
H	-1.619957822	-1.594073651	-0.729205107
H	-1.714164389	0.143564881	-1.043847436
C	0.202478755	-0.737185998	-1.507156153

C	0.874077646	-1.950672251	-1.651707266
C	0.733922321	0.406496124	-2.101568563
C	2.051078921	-2.022535525	-2.387005083
C	1.910674695	0.337584399	-2.837684937
C	2.570642621	-0.878124426	-2.982859416
H	0.468405090	-2.844253249	-1.179167968
H	0.218519863	1.358661460	-1.980825651
H	2.564013747	-2.975234594	-2.496057093
H	2.313811269	1.235796697	-3.299596530
H	3.489504052	-0.933876727	-3.561832310



Secondary Product

C	-0.782187483	-0.375636640	0.739596254
F	-1.904234400	-0.392530888	1.473640439
F	0.044930027	-1.287987992	1.258270803
F	-0.216205038	0.825974951	0.905602295
C	-1.079199342	-0.660734130	-0.718197860
H	-1.527555776	-1.665233174	-0.716881124
C	0.206217818	-0.722451002	-1.511054648
C	0.835330435	-1.951675789	-1.708141353
C	0.804284463	0.426873452	-2.028261328
C	2.027432717	-2.037384155	-2.416465839
C	1.997537686	0.345118219	-2.736844127
C	2.611636644	-0.886756582	-2.934528482
H	0.380958453	-2.852613946	-1.296865101
H	0.339006026	1.398222073	-1.874968879
H	2.501042724	-3.005168059	-2.564415138
H	2.450983262	1.250032252	-3.134918254
H	3.543830585	-0.949787895	-3.491112234
C	-2.101281117	0.336207160	-1.250382162
H	-2.272610225	0.167976228	-2.317418155
H	-3.054114463	0.235674991	-0.723200426
H	-1.758500773	1.367825805	-1.118860051

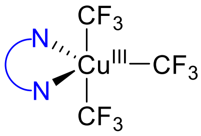


Tertiary Product

C	-1.409895521	-1.804215900	0.027649364
F	-2.618112328	-1.869368514	0.608326414
F	-0.890966654	-3.037285400	0.068907761

F	-0.644682707	-1.022431604	0.797588528
C	-1.505956236	-1.268891034	-1.398345941
C	-0.095031488	-1.211224296	-1.983688873
C	0.509221165	-2.357540764	-2.509298072
C	0.643886569	-0.026268651	-1.986483929
C	1.795964544	-2.317465871	-3.031371438
C	1.931242486	0.018531136	-2.509863851
C	2.513339363	-1.126999052	-3.037119109
H	-0.024571233	-3.304025791	-2.510252144
H	0.216109266	0.885302041	-1.578484544
H	2.239439051	-3.224769877	-3.435387908
H	2.480430408	0.957374773	-2.502627954
H	3.519706785	-1.093522559	-3.447926069
C	-2.414574970	-2.200839481	-2.206242332
H	-2.435876123	-1.875033568	-3.251764665
H	-2.083043620	-3.242292285	-2.178590666
H	-3.436142078	-2.170521731	-1.813737992
C	-2.166963593	0.110050113	-1.336466100
H	-2.173377687	0.563783045	-2.333400702
H	-3.202276814	0.016654085	-0.995153996
H	-1.653931032	0.789299500	-0.649349559

Cu(III) Complexes:

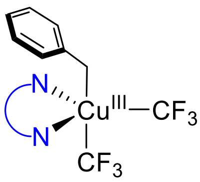


Grushin's Reagent

bipy$Cu^{III}(CF_3)_3$

Cu	-0.717828211	-0.245194336	0.002560647
N	1.038629502	-1.294371079	0.014444416
C	1.064990821	-2.624792574	0.039578925
H	0.096680991	-3.123428301	0.045385533
C	2.253678739	-3.340464040	0.057540725
H	2.238537266	-4.425395877	0.077619859
C	3.446063841	-2.628858048	0.049668112
H	4.400254048	-3.149098056	0.063658830
C	3.412254551	-1.242090773	0.024697920
H	4.337884185	-0.674837579	0.020075347
C	2.181770010	-0.590181414	0.007555931
N	0.790723863	1.348245490	-0.019264091
C	2.045963219	0.886610532	-0.017176876

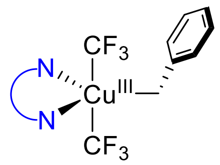
C	3.131854169	1.759219584	-0.038104510
H	4.152415121	1.388162285	-0.037883989
C	2.889413173	3.126523012	-0.060906822
H	3.721999790	3.825191518	-0.077529670
C	1.580606570	3.590585536	-0.063012596
H	1.355399819	4.652430218	-0.080968877
C	0.553580670	2.654553911	-0.042007358
H	-0.496138052	2.945789763	-0.043597682
C	-0.749053924	-0.247913193	-1.970276743
C	-2.628593598	0.194576579	0.001598651
C	-0.744434187	-0.218476497	1.975604161
F	-1.351876447	-1.332735980	-2.484628169
F	0.511232815	-0.257467591	-2.467494920
F	-1.333475341	0.842295589	-2.495087028
F	-2.666218019	1.541924455	0.001297957
F	-3.313966396	-0.225366299	-1.061529632
F	-3.311517663	-0.225703120	1.066350823
F	-1.339424138	0.869827520	2.491099232
F	-1.333581350	-1.304801327	2.503450436
F	0.517266662	-0.208237311	2.469500057



bipyCu^{III}(CF$_3$)$_2$(toluyl) – Isomer 1

Cu	-0.870105625	-0.536634880	0.008203650
N	1.018956878	-1.273521414	0.006190180
C	1.265723293	-2.547839115	0.305823036
H	0.400294378	-3.152238623	0.576486332
C	2.545145989	-3.082985201	0.275386463
H	2.708902912	-4.126613694	0.525090205
C	3.595730228	-2.246147397	-0.079482808
H	4.614252250	-2.623991320	-0.121005897
C	3.336931728	-0.916244610	-0.372615325
H	4.152252688	-0.250343611	-0.636812934
C	2.026049337	-0.445587930	-0.314949771
N	0.376310126	1.280099249	-0.383500767
C	1.662818008	0.969077556	-0.572967655
C	2.587157494	1.931026606	-0.981751009
H	3.628945286	1.674437150	-1.151069687
C	2.146908655	3.228844465	-1.195815292
H	2.847340743	3.992803461	-1.524333023

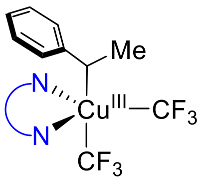
C	0.808215860	3.542049424	-0.987422493
H	0.432168091	4.548951457	-1.141588214
C	-0.045810786	2.526296965	-0.575393963
H	-1.105838345	2.698909218	-0.392147641
C	-2.804686468	-0.257612449	0.141904920
C	-0.688944376	-0.153006255	1.975135358
F	-2.984696088	1.056555050	-0.140484931
F	-3.583997262	-0.937308026	-0.713603930
F	-3.333832807	-0.472772652	1.348343438
F	-1.326997961	0.972275522	2.349432709
F	-1.147030921	-1.157178978	2.748787119
F	0.603226287	0.029084183	2.349226907
C	-1.206517510	-0.952226593	-1.970151455
H	-1.739075863	-1.905136751	-1.909596783
H	-1.881997014	-0.148524399	-2.271934572
C	0.021480790	-1.005001753	-2.762412327
C	0.731625158	-2.207138176	-2.931904309
C	0.548987139	0.144282103	-3.373351988
C	1.917092405	-2.252952504	-3.649879800
C	1.734504717	0.100644598	-4.096337109
C	2.432777363	-1.095518069	-4.231833492
H	0.331666018	-3.117772698	-2.483840738
H	0.010500898	1.087452269	-3.270427405
H	2.444174416	-3.199159749	-3.762194937
H	2.117207176	1.010417997	-4.556461920
H	3.361907986	-1.130754332	-4.796786845



bipyCu^{III}(CF$_3$)$_2$(toluyl) – Isomer 2

Cu	-1.078890143	-0.473175659	-0.009044739
N	0.898721208	-1.192561745	0.079897056
C	1.098389208	-2.509251649	0.148815173
H	0.203699568	-3.125396126	0.184026242
C	2.363994542	-3.075597332	0.172639436
H	2.480571867	-4.153009698	0.229121178
C	3.461470115	-2.227665968	0.116779526
H	4.473663112	-2.624788601	0.124637683
C	3.254056518	-0.859889214	0.049187320
H	4.104995430	-0.188563819	-0.001817589
C	1.951414715	-0.359965534	0.037887719

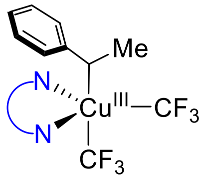
N	0.381107048	1.448460271	-0.112524290
C	1.669437297	1.093971193	-0.020242765
C	2.693558278	2.041843701	0.026088884
H	3.734077275	1.744936878	0.114452825
C	2.369689448	3.389063747	-0.033820238
H	3.153405363	4.142383783	0.001027440
C	1.036084169	3.753061008	-0.134877312
H	0.732584531	4.794787031	-0.184708971
C	0.079005449	2.743716890	-0.168331366
H	-0.977251890	2.989348690	-0.245427991
C	-1.024917212	-0.858142081	-1.965939714
C	-1.094596315	-0.544625016	1.982053459
F	-2.076239638	-0.629469536	-2.789338866
F	0.022870041	-0.230220740	-2.546988465
F	-0.772182087	-2.192851730	-2.091481471
F	-2.152338028	-0.148578005	2.726910591
F	-0.908637210	-1.856148221	2.305975769
F	-0.032175240	0.116513883	2.496597287
C	-3.024887334	-0.130555020	-0.065043593
H	-3.406437588	-0.543775866	0.866777235
H	-3.365329839	-0.674627416	-0.944140356
C	-3.151826851	1.334037300	-0.171737042
C	-3.157033353	1.970212622	-1.423957019
C	-3.279728267	2.133865859	0.975757595
C	-3.301030653	3.347927602	-1.523228683
C	-3.422507683	3.511544307	0.873568015
C	-3.436046448	4.126589879	-0.376020394
H	-3.035034961	1.367288418	-2.319532196
H	-3.254796772	1.658308049	1.952156940
H	-3.304496101	3.818858295	-2.504120722
H	-3.522588686	4.110514907	1.776440996
H	-3.547262588	5.206005081	-0.455532293



bipyCu^{III}(CF$_3$)$_2$(ethylbenzyl) – Isomer 1 Conformer 1

Cu	-0.966202305	-0.143453071	-0.095445006
N	0.999298068	-1.222902776	0.127281084
C	1.189440716	-2.488513401	0.482515054
H	0.307467820	-3.016850893	0.846102780
C	2.432953399	-3.104056561	0.396817246

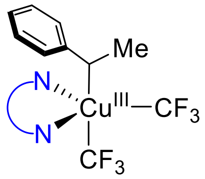
H	2.555930797	-4.142095032	0.691445345
C	3.503492165	-2.355006413	-0.077375321
H	4.490287956	-2.802130545	-0.170231605
C	3.307208284	-1.027356416	-0.431199402
H	4.135235732	-0.436242613	-0.810272872
C	2.027303944	-0.486805802	-0.305730121
N	0.413460236	1.276372864	-0.554202485
C	1.707945131	0.926200141	-0.616973566
C	2.685602520	1.870903909	-0.926902358
H	3.732180311	1.585649701	-0.970748537
C	2.310537005	3.182036670	-1.171718159
H	3.062617607	3.927153614	-1.418335882
C	0.969021100	3.534553579	-1.080251144
H	0.635544713	4.554129525	-1.245847177
C	0.054018561	2.543963518	-0.757522071
H	-1.008225786	2.763905615	-0.655342972
C	-2.690744219	-0.998407015	0.305425376
C	-0.779547133	0.296849301	1.895559175
F	-3.549471080	-0.036282341	0.688164161
F	-3.337099203	-1.683642996	-0.661910452
F	-2.566263009	-1.867136968	1.319673196
F	-1.803054024	0.980907581	2.439710966
F	-0.611499794	-0.810403794	2.649200386
F	0.327330888	1.051853716	2.133604553
C	-1.294762010	-0.551640342	-2.108865352
C	-0.025662072	-0.701620733	-2.835986717
C	0.600637983	-1.960546620	-2.875696946
C	0.605295853	0.349015896	-3.521676326
C	1.802611740	-2.156270137	-3.536901853
C	1.812135330	0.156271110	-4.185188154
C	2.423387148	-1.093237363	-4.191943968
H	0.120060709	-2.794708936	-2.363087646
H	0.146286555	1.337089308	-3.532127065
H	2.260362588	-3.144134715	-3.544085567
H	2.277457883	0.992025832	-4.705500874
H	3.365774074	-1.242878354	-4.714674894
C	-2.235465470	0.537077228	-2.567376257
H	-2.459134059	0.438142146	-3.641974423
H	-3.183534812	0.489981715	-2.023261735
H	-1.826796240	1.547769165	-2.430935320
H	-1.797837428	-1.515011998	-2.039959169



bipyCu^{III}(CF$_3$)$_2$(ethylbenzyl) – Isomer 1 Confromer 2

Cu	-1.032306932	-0.685476051	-0.002180594
N	0.930044864	-1.348649433	-0.084545519
C	1.291888985	-2.547356184	0.369236031
H	0.491998727	-3.167992761	0.771949113
C	2.607472837	-2.987985389	0.335850471
H	2.865030517	-3.974519974	0.708141277
C	3.571206128	-2.131567216	-0.181853595
H	4.614031770	-2.435377181	-0.227311385
C	3.193686007	-0.876658048	-0.636363107
H	3.941041751	-0.193741670	-1.028435940
C	1.851996215	-0.503005913	-0.574696037
N	0.049321174	1.037732408	-0.837197011
C	1.354262341	0.818876931	-1.030135616
C	2.163938698	1.778804285	-1.635741328
H	3.221135094	1.598376955	-1.808379597
C	1.590967547	2.983229247	-2.025208494
H	2.202969566	3.746523773	-2.499657568
C	0.236816641	3.201062507	-1.807401717
H	-0.242792489	4.129042389	-2.103456953
C	-0.503198265	2.186531222	-1.210697112
H	-1.575844062	2.275904988	-1.036731351
C	-2.945357185	-0.551065271	0.397153799
C	-0.610742142	0.034250715	1.849639533
F	-3.289295570	0.703740185	0.019135524
F	-3.824593488	-1.372672135	-0.211761050
F	-3.235667343	-0.659034434	1.699745819
F	-1.325250829	1.118574089	2.205155520
F	-0.792558609	-0.902166987	2.806127413
F	0.690923716	0.415576587	1.974041714
C	-1.343255060	-1.521983239	-1.880127739
C	-1.861450284	-0.524757622	-2.835067901
C	-0.958247265	0.168465863	-3.660105943
C	-3.224523468	-0.219448212	-2.976185842
C	-1.384060892	1.134674094	-4.560724701
C	-3.651727772	0.746540543	-3.876628255
C	-2.738140418	1.435236470	-4.670764731
H	0.105835447	-0.063076551	-3.585019410
H	-3.952903367	-0.722021526	-2.346800629

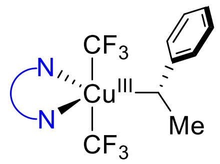
H	-0.654214238	1.653579410	-5.180340435
H	-4.714135210	0.967832216	-3.958115971
H	-3.079721276	2.192459733	-5.373127435
C	-2.018714231	-2.870176976	-1.813207396
H	-1.809837753	-3.437015273	-2.734145354
H	-1.642258057	-3.467550463	-0.971997787
H	-3.101996766	-2.803616748	-1.706187785
H	-0.275460962	-1.663154654	-2.083049669



bipyCu^{III}(CF$_3$)$_2$(ethylbenzyl) – Isomer 1 Confromer 3

Cu	-1.019079686	-0.491156439	-0.064166936
N	0.787318266	-1.376236290	-0.198003104
C	0.917207504	-2.677485522	0.066914548
H	-0.000804956	-3.218093102	0.289522317
C	2.147837694	-3.318123442	0.053561839
H	2.208252718	-4.380721417	0.267088743
C	3.275876500	-2.566588846	-0.241873158
H	4.259624194	-3.028872622	-0.266192383
C	3.139505127	-1.209495726	-0.498703942
H	4.017241645	-0.608842334	-0.714530860
C	1.873983458	-0.627706195	-0.461494793
N	0.391402710	1.247758026	-0.524438517
C	1.648340958	0.820773846	-0.691204423
C	2.669738359	1.698041912	-1.057626080
H	3.687465374	1.348681372	-1.205232887
C	2.364289432	3.039066908	-1.241507705
H	3.144285790	3.739345861	-1.530204881
C	1.058296083	3.474035618	-1.053507480
H	0.784691499	4.516747551	-1.184041609
C	0.100279674	2.533588194	-0.692544753
H	-0.941449131	2.806962791	-0.528654522
C	-2.835379676	0.160351742	0.274677138
C	-0.626668133	-0.327338009	1.932485882
F	-2.733305300	1.464508094	0.612148467
F	-3.767169236	0.121390051	-0.702969373
F	-3.396579994	-0.487325284	1.308295901
F	-1.339739667	0.513843147	2.693184781
F	-0.800867604	-1.568929279	2.460812634
F	0.672651827	-0.011504664	2.178482618

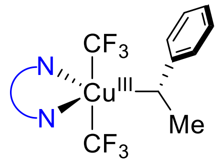
C	-1.503970976	-1.031885671	-1.997792773
C	-1.511983371	-2.501315224	-1.890012687
C	-0.565819916	-3.316311907	-2.532081769
C	-2.474611325	-3.136385489	-1.082074294
C	-0.584083394	-4.699410398	-2.379413000
C	-2.485544509	-4.513939176	-0.922808122
C	-1.537417727	-5.306798609	-1.570249580
H	0.196939603	-2.861848765	-3.162353473
H	-3.210996613	-2.521889905	-0.564730010
H	0.158447541	-5.306011902	-2.895311178
H	-3.238401776	-4.974673894	-0.286699890
H	-1.546269481	-6.387168538	-1.444669555
C	-0.573893637	-0.410686795	-3.005210238
H	-0.676148974	0.679490182	-3.013759861
H	0.484831444	-0.641972393	-2.826438722
H	-0.807993378	-0.769788360	-4.020716108
H	-2.512160950	-0.636719237	-2.093198935



bipyCu^{III}(CF$_3$)$_2$(ethylbenzyl) – Isomer 2 Conformer 1

Cu	-0.513169006	-0.576207636	0.137135367
N	1.081209003	-1.837395618	-0.489395438
C	1.036119038	-3.157750295	-0.334358803
H	0.122669866	-3.554697195	0.107781069
C	2.082131839	-3.984993758	-0.720392996
H	2.015122493	-5.058538711	-0.574311820
C	3.201222593	-3.397929219	-1.295456469
H	4.043254254	-4.007731541	-1.613130837
C	3.238518844	-2.021222207	-1.466465640
H	4.107302930	-1.554937763	-1.921022629
C	2.151349723	-1.255796368	-1.048394685
N	0.985936085	0.815205373	-0.741738247
C	2.102212953	0.222703028	-1.182703124
C	3.146755576	0.972338824	-1.721943699
H	4.053624258	0.494318388	-2.079875149
C	3.017289132	2.352384023	-1.793983707
H	3.822032488	2.952659423	-2.210868303
C	1.857091851	2.955013957	-1.326371814
H	1.721260064	4.031620051	-1.362349331
C	0.863747545	2.136136232	-0.803647113

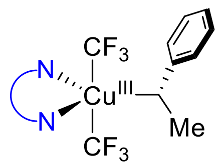
H	-0.068375076	2.547873562	-0.415917422
C	-1.401078427	-0.990588833	-1.598077043
C	0.359101500	-0.215437815	1.884777551
F	-0.519735412	-0.778675733	-2.613663725
F	-1.678746066	-2.320246883	-1.643419057
F	-2.534533288	-0.367420707	-2.000225861
F	0.088175507	1.034988957	2.340266052
F	0.035780495	-1.058567532	2.900511969
F	1.710091907	-0.275021276	1.803168969
C	-2.266703433	-0.320329602	1.133201118
C	-3.016851254	-1.571739815	0.923855273
C	-4.173405193	-1.651722998	0.143713181
C	-2.545038869	-2.741219245	1.541422551
C	-4.820267265	-2.868548418	-0.037467971
C	-3.182676956	-3.955595711	1.350119242
C	-4.323667197	-4.025767583	0.551674955
H	-4.558802667	-0.758887273	-0.342183198
H	-1.651041539	-2.673586071	2.162527274
H	-5.717768162	-2.913485414	-0.651053018
H	-2.796423913	-4.852841527	1.830290294
H	-4.827364992	-4.977675268	0.398477111
C	-2.836360118	0.998931474	0.692137473
H	-2.162135716	1.810250737	0.990326580
H	-3.002905170	1.052360933	-0.386643752
H	-3.800383218	1.181262949	1.193964636
H	-1.922436695	-0.266349517	2.164648762



bipyCu^{III}(CF$_3$)$_2$(ethylbenzyl) – Isomer 2 Conformer 2

Cu	-0.619932742	-0.793286322	0.084600535
N	1.277995532	-1.684492213	-0.269270149
C	1.516403696	-2.949428406	0.060793244
H	0.714107709	-3.466240882	0.585398355
C	2.718270567	-3.579609604	-0.231482873
H	2.877192519	-4.616095037	0.049684048
C	3.696903745	-2.844539113	-0.886754269
H	4.653701542	-3.297187900	-1.134862900
C	3.445121163	-1.522747925	-1.226457824
H	4.204236071	-0.941865390	-1.740144735
C	2.209259552	-0.962282261	-0.905702608

N	0.608694763	0.822116012	-0.898050491
C	1.839363877	0.433718636	-1.253142554
C	2.703566030	1.298556335	-1.924308088
H	3.702758752	0.983876114	-2.209937425
C	2.266498731	2.579629773	-2.230442873
H	2.925586815	3.268841984	-2.752731084
C	0.983345834	2.966609462	-1.867848144
H	0.603749511	3.957996800	-2.096207039
C	0.184121399	2.045793784	-1.201163168
H	-0.832527568	2.291893701	-0.891674644
C	-1.225417172	-1.323808462	-1.764705880
C	0.065867343	-0.459195507	1.935264487
F	-1.649688302	-0.247245659	-2.471611231
F	-0.198229386	-1.830969039	-2.491393569
F	-2.218467812	-2.241894450	-1.881931659
F	-0.514603351	0.370911805	2.837780703
F	0.133161943	-1.670101458	2.560561563
F	1.347300896	-0.018559376	1.867526996
C	-2.584846117	-0.664736644	0.612898306
C	-2.946433546	0.737958127	0.309800823
C	-2.645228347	1.804856184	1.171038431
C	-3.645973878	1.025673909	-0.872398576
C	-3.015829421	3.104510712	0.850686018
C	-4.021420555	2.324352479	-1.189009682
C	-3.702679328	3.373672694	-0.331249914
H	-2.088897056	1.612457150	2.082805148
H	-3.885891384	0.210890213	-1.552085826
H	-2.764861084	3.915730083	1.531053790
H	-4.563925400	2.517868976	-2.112074724
H	-3.993539031	4.392426500	-0.578172837
C	-2.873916770	-1.193680332	1.993352704
H	-2.511857744	-0.549852072	2.795198970
H	-3.966074985	-1.285129661	2.099797781
H	-2.445192083	-2.189709904	2.139734236
H	-3.003109994	-1.339645115	-0.133911280

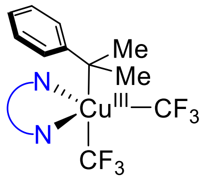


bipyCu^{III}(CF$_3$)$_2$(ethylbenzyl) – Isomer 2 Conformer 3

Cu	-0.551882989	-0.804453059	0.168943694
N	1.037840824	-1.936858832	-0.968571806

C	0.963133843	-3.192404641	-1.393868666
H	0.025844368	-3.710584744	-1.190905748
C	2.008351479	-3.820676244	-2.060093977
H	1.911201098	-4.850154077	-2.391310391
C	3.168740458	-3.091893523	-2.283455970
H	4.013301718	-3.542340929	-2.798944626
C	3.244671234	-1.777692685	-1.843419883
H	4.148906346	-1.201228084	-2.014554848
C	2.149320168	-1.222485218	-1.182644582
N	1.023223474	0.566044689	-0.039281752
C	2.134187389	0.174402362	-0.678015148
C	3.201343604	1.055316292	-0.844689198
H	4.103306349	0.745943208	-1.363426589
C	3.101804271	2.343500808	-0.338510322
H	3.926414562	3.040904213	-0.463011326
C	1.945679259	2.729536980	0.326448740
H	1.833213660	3.726900303	0.739803662
C	0.925559206	1.797125497	0.455382752
H	-0.002239549	2.029411359	0.977392455
C	-1.310754120	-0.315077943	-1.598019034
C	0.191349934	-1.248403236	1.964833834
F	-2.276061734	0.642213906	-1.580798968
F	-0.366988275	0.156448071	-2.446757806
F	-1.858192092	-1.380520313	-2.236531985
F	0.056476953	-0.166144282	2.775295747
F	-0.249657651	-2.304016806	2.689435949
F	1.535121788	-1.449366081	1.862354973
C	-2.438300275	-1.371145622	0.653269316
C	-2.788043754	-0.601198612	1.861722560
C	-2.976605037	0.784399609	1.733904493
C	-2.948441595	-1.179883169	3.123741778
C	-3.276416286	1.568649602	2.835352635
C	-3.261140133	-0.393936441	4.226504130
C	-3.414937929	0.981082663	4.091992730
H	-2.863321050	1.232690529	0.746024197
H	-2.810397044	-2.250809361	3.247759859
H	-3.410042410	2.642220971	2.716971337
H	-3.378797451	-0.860351025	5.202435159
H	-3.650038374	1.593225525	4.959905471
C	-2.449851377	-2.874165166	0.672146656
H	-1.732575026	-3.295875067	1.380149482
H	-3.452168410	-3.240471245	0.945952433
H	-2.232654833	-3.258811971	-0.330587153

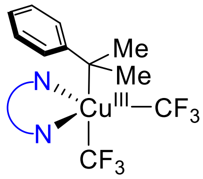
H	-3.002416786	-0.989847012	-0.195636698



bipyCu^{III}(CF$_3$)$_2$(cumenyl) – Isomer 1 Confromer 1

Cu	-0.929240906	-0.527991477	-0.029233794
N	0.934626895	-1.316821535	-0.077102456
C	1.158718058	-2.591942374	0.236692186
H	0.281390644	-3.183009774	0.498559439
C	2.430615896	-3.145017276	0.235545781
H	2.573656635	-4.189542560	0.493992344
C	3.500068988	-2.324064275	-0.098276190
H	4.513935529	-2.715810607	-0.116723106
C	3.265607777	-0.990448418	-0.396154123
H	4.096190204	-0.335779090	-0.639596016
C	1.961323458	-0.500647320	-0.367367523
N	0.344049138	1.257473065	-0.452182792
C	1.629126971	0.923615457	-0.613834536
C	2.583408086	1.875087347	-0.975203097
H	3.624138355	1.600769557	-1.121550565
C	2.176057714	3.185696482	-1.174885576
H	2.900926535	3.941221020	-1.468357174
C	0.839362466	3.523043018	-0.992670158
H	0.489040226	4.541345658	-1.132389298
C	-0.045327570	2.517728597	-0.622108440
H	-1.104542018	2.710905555	-0.453786865
C	-2.837421662	-0.171091151	0.338082124
C	-0.544616474	-0.123453250	1.945105952
F	-3.008797164	1.151146620	0.075947593
F	-3.795977060	-0.813571452	-0.367562292
F	-3.202605339	-0.357291099	1.611860337
F	-1.136503699	1.003300662	2.379409313
F	-0.932311457	-1.130494664	2.752760323
F	0.776995536	0.053876007	2.207963560
C	-1.294532398	-1.031908060	-2.084066379
C	0.016768210	-1.021807002	-2.795676390
C	0.775586547	-2.192112473	-2.991672545
C	0.537930988	0.155246270	-3.364007041
C	1.982501522	-2.180479813	-3.677356726
C	1.743761936	0.170493985	-4.053738949
C	2.483512158	-0.996266423	-4.210336369

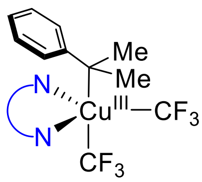
H	0.414465484	-3.141336962	-2.603431564
H	-0.008711631	1.090043180	-3.259493670
H	2.534363476	-3.110922971	-3.801945039
H	2.106849805	1.108825586	-4.470797424
H	3.426793522	-0.987319197	-4.752399622
C	-2.255773202	-0.021677812	-2.691527136
H	-2.265189739	-0.130771863	-3.788376806
H	-3.273907376	-0.163605795	-2.332469055
H	-1.979077907	1.016830641	-2.474498191
C	-1.900459474	-2.418645390	-1.969095115
H	-2.023586078	-2.872460702	-2.968006090
H	-1.281172258	-3.110698279	-1.382934955
H	-2.881949718	-2.381138826	-1.496214875



bipyCu^{III}(CF$_3$)$_2$(cumenyl) – Isomer 1 Confromer 2

Cu	-1.039281473	-0.552827799	-0.032050606
N	0.838643374	-1.368828164	-0.069329806
C	1.009324763	-2.665494404	0.206344250
H	0.104462606	-3.257129508	0.311066737
C	2.259551109	-3.243546195	0.361814075
H	2.339070097	-4.305525691	0.572278880
C	3.376941610	-2.429935101	0.253668185
H	4.376702392	-2.835720395	0.385886081
C	3.203247889	-1.081452015	-0.020324462
H	4.066307863	-0.427375416	-0.086533302
C	1.917774542	-0.569013984	-0.189670916
N	0.433576266	1.305978139	-0.412967635
C	1.690054358	0.860764093	-0.520125296
C	2.723705138	1.696746174	-0.948888030
H	3.736966669	1.324827991	-1.067455357
C	2.434377003	3.019885951	-1.250039230
H	3.224009645	3.685958070	-1.588936297
C	1.129339523	3.476383505	-1.122564515
H	0.862695881	4.504056979	-1.351401675
C	0.158612266	2.574864237	-0.701733018
H	-0.884542106	2.869603376	-0.601149604
C	-2.565338013	0.639285304	0.077252881
C	-0.993243198	-0.728936088	1.996672413
F	-2.709355220	1.452910849	-0.997922665

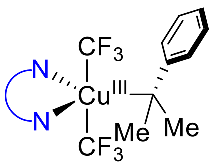
F	-3.747755710	0.051039382	0.290303420
F	-2.350553701	1.496770457	1.090962210
F	-0.054246301	0.078387268	2.544046962
F	-2.126109212	-0.517723780	2.689436590
F	-0.618666294	-2.001374214	2.331278088
C	-1.584302650	-1.097409833	-2.012460888
C	-1.406847629	-2.554349516	-1.769651233
C	-0.454661273	-3.329758542	-2.450349455
C	-2.245346095	-3.216524688	-0.852780454
C	-0.357819516	-4.701240111	-2.239770053
C	-2.134766363	-4.583407850	-0.629282633
C	-1.193393621	-5.337714368	-1.326875195
H	0.210730609	-2.855740511	-3.169464454
H	-2.985216537	-2.637277152	-0.299827066
H	0.378245657	-5.277944046	-2.797180678
H	-2.793619957	-5.062700134	0.091405847
H	-1.115281489	-6.409799037	-1.162079330
C	-2.993847240	-0.836992964	-2.524216079
H	-3.130687997	-1.426746538	-3.446442490
H	-3.779608853	-1.139958447	-1.827484711
H	-3.151037792	0.212942291	-2.776648142
C	-0.579579137	-0.442120307	-2.927726699
H	-0.719467924	0.645360585	-2.917828921
H	0.461027345	-0.655517303	-2.657928099
H	-0.729622527	-0.773864473	-3.971134661



bipyCu^{III}(CF$_3$)$_2$(cumenyl) – Isomer 1 Confromer 3

Cu	-1.109207651	-0.627811479	-0.076788303
N	0.869099798	-1.183194263	-0.068809323
C	1.233606493	-2.426797485	0.253724220
H	0.424975786	-3.115334033	0.489216835
C	2.557993613	-2.836864052	0.285644699
H	2.805980365	-3.862455036	0.540129165
C	3.543669965	-1.904388861	-0.010821532
H	4.595253247	-2.180477224	0.004965757
C	3.169037049	-0.606694798	-0.317881872
H	3.925720856	0.144319802	-0.522762287
C	1.815890552	-0.268490643	-0.344247757
N	0.071269421	1.357880042	-0.422516026

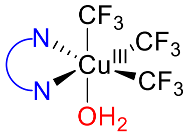
C	1.356860661	1.098048457	-0.683648224
C	2.194801613	2.051322364	-1.266001458
H	3.227387566	1.821859715	-1.512539589
C	1.674084923	3.306612438	-1.553660767
H	2.304881674	4.065436116	-2.010629752
C	0.343380615	3.574889628	-1.260619268
H	-0.098833775	4.543107483	-1.475562176
C	-0.424920523	2.558147673	-0.702046921
H	-1.482480742	2.695156847	-0.479172843
C	-2.976043609	-0.160494383	0.195797011
C	-0.872449793	-0.553860130	1.960789420
F	-3.805933630	-0.077358905	-0.853411390
F	-3.559594932	-1.012730221	1.053136002
F	-2.991354760	1.070714080	0.749432527
F	0.334228181	-0.054781688	2.327944783
F	-1.755471528	0.006878095	2.790831931
F	-0.830918905	-1.882862353	2.297808480
C	-1.400515996	-1.308863015	-2.069777155
C	-1.928017551	-0.242426373	-2.971288921
C	-3.195023027	-0.319649867	-3.564813362
C	-1.110919402	0.830134443	-3.365320217
C	-3.629738816	0.632827097	-4.478750162
C	-1.545309272	1.790600849	-4.266726650
C	-2.813805051	1.701775409	-4.832043019
H	-3.858525388	-1.141035245	-3.306967451
H	-0.106491444	0.917137474	-2.956537855
H	-4.619711187	0.534654660	-4.919697608
H	-0.880601287	2.611123295	-4.534395605
H	-3.156727405	2.448697121	-5.544137642
C	-2.307472172	-2.504840260	-1.840593329
H	-2.426551510	-3.084437547	-2.774004509
H	-1.855360099	-3.189729981	-1.108435270
H	-3.301568894	-2.242136867	-1.472888012
C	-0.085485664	-1.825654092	-2.654602088
H	0.708655689	-1.073585334	-2.728133384
H	0.311975570	-2.685754558	-2.104424595
H	-0.282830240	-2.170301621	-3.683997870



bipyCu^{III}(CF$_3$)$_2$(cumenyl) – Isomer 2 Conformer 1

Cu	-1.008438515	-0.404962471	-0.104320004
N	0.996849037	-1.342807653	0.299140757
C	1.208506177	-2.499454511	0.914125201
H	0.317087844	-3.050336373	1.215127893
C	2.482748224	-2.995433626	1.162084765
H	2.614540977	-3.948819099	1.664568466
C	3.567198177	-2.233734953	0.749531506
H	4.583536985	-2.578414546	0.922845084
C	3.345092097	-1.020444424	0.112619534
H	4.188682267	-0.416424956	-0.206640197
C	2.034350055	-0.596836752	-0.100920044
N	0.403138744	0.985645664	-0.881336282
C	1.704516644	0.685595307	-0.775127886
C	2.674268752	1.544837325	-1.290311542
H	3.730411749	1.306516881	-1.213630080
C	2.273397097	2.717341308	-1.916366714
H	3.017361578	3.397938359	-2.322985528
C	0.920021888	3.007183336	-2.026083820
H	0.568832856	3.909947124	-2.516529318
C	0.014220860	2.099880009	-1.493070889
H	-1.062096675	2.254442608	-1.566068498
C	-0.993623475	-1.154831011	-1.998070637
C	-0.834646819	0.407972645	1.704393014
F	-1.515791822	-0.242762245	-2.857811150
F	0.296465425	-1.318669239	-2.408076575
F	-1.586109957	-2.333292699	-2.314321803
F	-1.662950791	1.432734688	2.011487471
F	-0.934768286	-0.495764226	2.713861935
F	0.410327074	0.932817923	1.854099911
C	-2.948332587	-1.062931010	0.291188394
C	-3.687871744	-0.596552535	-0.916236106
C	-4.292383314	-1.476848684	-1.816799281
C	-3.844795578	0.780825876	-1.133287494
C	-5.006557334	-0.996807769	-2.909010839
C	-4.548231378	1.260224348	-2.225891586
C	-5.131361227	0.369677767	-3.125142534
H	-4.192160639	-2.549941444	-1.675148519
H	-3.373901071	1.478434588	-0.437863547
H	-5.465018896	-1.701030460	-3.600483128
H	-4.642885263	2.333249217	-2.381902042
H	-5.681628448	0.740947623	-3.986768805
C	-3.625729374	-0.520327689	1.536227040
H	-4.635075109	-0.963391395	1.548811638

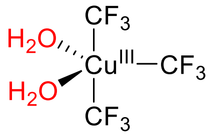
H	-3.114984432	-0.814858029	2.453855412
H	-3.750061701	0.562846738	1.536977558
C	-2.717352871	-2.547212021	0.461906267
H	-3.683468100	-3.056772888	0.622327423
H	-2.219810312	-3.015674768	-0.388047172
H	-2.125074753	-2.716654900	1.370083244



bipyCu^{III}(CF$_3$)$_3$(OH$_2$)

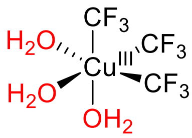
Cu	-0.514137840	0.047063589	-0.346956425
N	1.366912075	-0.996244471	-0.320553251
C	1.492875516	-2.311298642	-0.491054704
H	0.590624505	-2.841715188	-0.783991316
C	2.697436815	-2.975760716	-0.307463073
H	2.757355988	-4.048583763	-0.461802145
C	3.803034550	-2.234268900	0.085653585
H	4.762467193	-2.717002497	0.253731787
C	3.670789428	-0.865850954	0.272676454
H	4.521333608	-0.276913479	0.601842952
C	2.430155536	-0.268656331	0.053305229
N	0.924021495	1.594087860	0.187396806
C	2.202417688	1.186765045	0.210892577
C	3.251471178	2.093530946	0.352043366
H	4.283073034	1.755700568	0.348602867
C	2.964024619	3.445610465	0.471151054
H	3.769593847	4.167728722	0.577761207
C	1.640396398	3.858411610	0.439468869
H	1.369919869	4.906625865	0.521744995
C	0.651212393	2.893779748	0.292689250
H	-0.399242196	3.167377324	0.261070673
C	-1.622109987	-1.309739761	-1.491965143
C	-2.199121117	1.255008487	-0.162890821
C	-0.945763403	-0.889400727	1.568316614
F	-2.216386802	-2.307764134	-0.834897834
F	-0.760886996	-1.899964792	-2.389630291
F	-2.554294323	-0.717655927	-2.260237925
F	-2.229821004	2.146199098	-1.208899673
F	-3.392259657	0.666247594	-0.136040209
F	-2.121248317	2.019755075	0.953050829
F	-0.126456541	-0.305923371	2.453566985
F	-2.193401355	-0.749758429	1.990283679

F	-0.654714148	-2.195086575	1.542215659
O	-0.034758099	0.958475464	-2.599114752
H	-0.897070202	1.395462010	-2.564179308
H	-0.196169170	0.126222261	-3.059124585



$(H_2O)_2Cu^{III}(CF_3)_3$

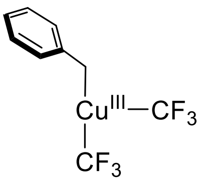
Cu	-0.534961404	-0.074797478	-0.166940080
C	-0.966271041	-1.222727856	-1.717240072
C	0.004935813	1.182815618	1.256319646
C	-1.996210109	1.174102365	-0.592480729
F	-2.214004585	-1.638807640	-1.933353168
F	-0.216728559	-2.368650103	-1.575300325
F	-0.518993796	-0.658949024	-2.860352403
F	0.819679187	0.499001550	2.075987041
F	0.784516976	2.137233026	0.677407314
F	-0.889415390	1.807113431	2.016912565
F	-1.585208030	2.437260925	-0.582320545
F	-2.567213852	0.962778669	-1.771719577
F	-2.924412394	1.009591679	0.349095351
O	1.559217836	-0.229812711	-0.723250995
H	1.602503603	-0.241485817	-1.687243774
O	-0.286608066	-1.839444851	1.051131590
H	-1.051317580	-2.049103601	1.597120803
H	1.953480946	0.604689501	-0.437049335
H	-0.216869136	-2.534944140	0.381612674



$(H_2O)_3Cu^{III}(CF_3)_3$

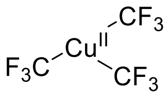
Cu	-0.809537128	-0.504088681	0.031988603
C	-0.718232501	-0.239119096	-1.941976816
C	-2.490321392	0.511865940	0.049905134
C	-0.816815388	-0.455444756	2.012152524
F	-1.562875697	-0.976774342	-2.678712845
F	0.535449957	-0.570645258	-2.373118504
F	-0.881528286	1.048152278	-2.322038754
F	-2.217607010	1.812122227	0.174685380
F	-3.206994059	0.345404072	-1.063599804

F	-3.290540559	0.152496602	1.056516422
F	-0.999810486	0.783540558	2.517656350
F	-1.689025569	-1.267360283	2.612663556
F	0.419871271	-0.833742091	2.451739369
O	0.828374071	-1.633774116	-0.003016888
H	1.347103418	-1.341909303	-0.766212680
O	0.760052672	1.473577361	0.139824634
H	0.360740681	1.905856063	-0.625245989
H	1.322178608	-1.436515483	0.805138239
H	0.306527823	1.854559217	0.901416536
O	-2.250314563	-2.482669992	-0.213276415
H	-2.953124305	-2.348155824	0.431167815
H	-2.638794337	-2.284986089	-1.073213879



Cu^{II}(CF$_3$)$_2$(CH$_2$Ph)

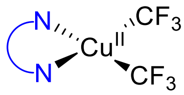
Cu	-0.580445402	0.255454317	0.230758660
C	-2.075361223	1.491392753	0.248735727
C	-0.870097796	-1.059622652	1.657702670
F	-1.621568909	2.770179079	0.308522289
F	-2.732828307	1.386759341	-0.938439287
F	-3.003000196	1.378958346	1.204764068
F	-2.089738819	-0.959529152	2.173746997
F	-0.694484364	-2.341200823	1.310684785
F	0.007917989	-0.778454922	2.638405841
C	1.102165239	-0.734202510	-0.240451497
H	1.724731135	-1.043524733	0.595995929
H	0.743446012	-1.537826707	-0.884158565
C	1.271471261	0.580240701	-0.788606898
C	2.034340035	1.574038114	-0.114270784
C	0.391116798	1.011046561	-1.821919908
C	1.976687495	2.889689566	-0.512593625
C	0.340522492	2.353861355	-2.207643006
C	1.132838455	3.284653961	-1.563996464
H	2.672242399	1.267300737	0.712496328
H	-0.198662716	0.265935734	-2.357582345
H	2.577805810	3.634480545	0.002988282
H	-0.336916181	2.657410793	-3.000454592
H	1.090098611	4.330702549	-1.854794977



Cu^{III}(CF$_3$)$_3$

Cu	-0.881386403	-0.241724912	0.002517777
C	-0.745763809	-0.232753376	-1.913416052
C	-2.791885822	0.209942520	0.003062837
C	-0.741406283	-0.205660430	1.917992525
F	-1.226570422	-1.275906860	-2.585290478
F	0.622271117	-0.323937386	-1.940015764
F	-1.087549369	0.877606168	-2.562887076
F	-2.821995873	1.527865808	0.001074706
F	-3.396094114	-0.261650816	-1.066660933
F	-3.394064054	-0.258405372	1.075365923
F	-1.093243333	0.906580434	2.558320933
F	-1.210819420	-1.247959236	2.599748422
F	0.627419572	-0.283324878	1.942994516

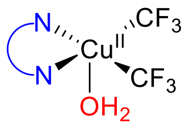
<u>Cu(II) Complexes:</u>



bipyCu^{II}(CF$_3$)$_2$ – Isomer 1

Cu	-0.537436061	-0.031758513	0.568418398
N	1.188465146	-1.177395787	0.253171064
C	1.268995052	-2.488925830	0.484222658
H	0.334913170	-2.981718275	0.744743273
C	2.469158965	-3.181704116	0.405075333
H	2.495224956	-4.250388131	0.593647136
C	3.621384729	-2.472012448	0.092147014
H	4.582882349	-2.976101054	0.036990056
C	3.538532840	-1.106158362	-0.141814048
H	4.433923827	-0.535784549	-0.369556841
C	2.295303884	-0.482658462	-0.061748455
N	0.868464977	1.434083885	0.000178265
C	2.093963600	0.966699558	-0.293018207
C	3.089175881	1.811114118	-0.779945330
H	4.070218253	1.424110833	-1.039401043
C	2.804202183	3.160151527	-0.942227691
H	3.567631589	3.835644794	-1.319680857
C	1.538413905	3.633913316	-0.622537777
H	1.280721753	4.682547738	-0.732730407
C	0.592279316	2.728755800	-0.160761683

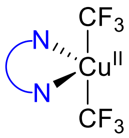
H	-0.421787278	3.031226687	0.091436810
C	-2.192962529	0.973487799	0.125448305
C	-1.416302795	-1.242810932	1.897959615
F	-2.322158486	2.014829927	0.998211571
F	-2.086342916	1.558628735	-1.103558387
F	-3.363510860	0.327170853	0.131099608
F	-2.468053817	-0.780705665	2.581836378
F	-1.825688837	-2.393585267	1.292362553
F	-0.500708455	-1.639867572	2.830109409



bipyCu^{II}(CF$_3$)$_2$(OH$_2$)

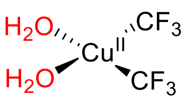
Cu	-0.498348684	0.091373119	0.757577198
N	1.227076059	-1.077559674	0.436256914
C	1.249404041	-2.404912263	0.537099057
H	0.339519799	-2.868455358	0.910504794
C	2.366105601	-3.156018903	0.193343913
H	2.345798480	-4.237408831	0.285747184
C	3.493097988	-2.487911139	-0.264250130
H	4.389163851	-3.038409763	-0.539514613
C	3.465943504	-1.104329234	-0.375871049
H	4.337476173	-0.571704313	-0.743692210
C	2.304274982	-0.422203219	-0.021056958
N	0.945619586	1.537516382	0.182060389
C	2.155649056	1.048495274	-0.137138239
C	3.184644196	1.889889088	-0.553824552
H	4.161240327	1.491596159	-0.811131750
C	2.947441345	3.255246015	-0.635161911
H	3.738967634	3.926555771	-0.958468958
C	1.694665981	3.749492442	-0.299249891
H	1.471038068	4.810606743	-0.348066775
C	0.717756694	2.848844093	0.104543625
H	-0.283067784	3.173845926	0.379738633
C	-2.125894477	1.244488996	0.429072983
C	-1.488138483	-1.179271346	1.976560618
F	-2.229256227	2.362546331	1.189802864
F	-2.040950531	1.713318869	-0.871496859
F	-3.321851975	0.633029394	0.487523993
F	-2.406631087	-0.662766273	2.802519685
F	-2.159825841	-2.111723918	1.211006487

F	-0.662975887	-1.928006950	2.762371122
O	-1.342097699	-1.076374063	-1.350499440
H	-1.795832784	-0.264174306	-1.608415936
H	-1.941694755	-1.498762983	-0.719611305



bipyCu^{II}(CF$_3$)$_2$ – Isomer 2

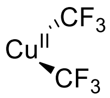
Cu	-0.654903037	-0.194090953	-0.000225431
N	1.146129594	-1.379649641	0.037726096
C	1.204214873	-2.705697616	0.121439189
H	0.248773599	-3.226500939	0.145603186
C	2.407735471	-3.394932607	0.181413109
H	2.417132905	-4.478573845	0.243775675
C	3.583745614	-2.657154530	0.163680959
H	4.549474007	-3.153849893	0.210688174
C	3.518891783	-1.273450777	0.091915737
H	4.434153007	-0.690380894	0.090790893
C	2.271641865	-0.651467074	0.029836647
N	0.869625711	1.307925882	-0.030962322
C	2.119762548	0.826080695	-0.039740467
C	3.211000310	1.692424925	-0.115753750
H	4.227210462	1.311471242	-0.130019236
C	2.987529144	3.060045594	-0.181442934
H	3.828871965	3.745906353	-0.239322655
C	1.684622354	3.540018141	-0.178617657
H	1.469559704	4.602570091	-0.234394101
C	0.650522720	2.617245270	-0.107680418
H	-0.392207231	2.928941892	-0.117599390
C	-0.851863884	-0.026212650	-1.937798452
C	-0.813073425	-0.373453620	1.938655101
F	-1.716970256	-0.883332829	-2.527181222
F	0.308661672	-0.134631450	-2.630717623
F	-1.321615108	1.226382816	-2.217007397
F	-1.834189367	0.317748610	2.497982364
F	-1.030586753	-1.683727911	2.251092461
F	0.297401187	-0.017443292	2.629341917



(H$_2$O)$_2$Cu^{II}(CF$_3$)$_2$

Cu	-0.587198841	0.217633311	0.769321889

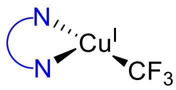
C	-2.378510457	0.907939068	0.168619225
C	-1.337968989	-1.314847508	1.835339645
F	-2.978326149	1.641430761	1.120577899
F	-2.243143159	1.758938689	-0.916963855
F	-3.245943266	-0.030823677	-0.216243012
F	-2.407917022	-1.010447436	2.572184014
F	-1.667326662	-2.362012848	1.063065858
F	-0.396815023	-1.801652665	2.727860801
O	1.380357783	-0.220064745	1.470956627
H	1.938281701	-0.609248412	0.789082962
H	1.156278379	-0.931352100	2.093234203
O	0.409220039	1.665517979	-0.448535772
H	0.827787505	2.365482237	0.063040268
H	-0.365774629	2.057553493	-0.882866211



$Cu^{II}(CF_3)_2$

Cu	-0.807415811	-0.029194473	0.701809225
C	-2.179177077	1.221091387	0.022156208
C	-1.295286785	-1.480628442	1.949862899
F	-2.096959016	2.409678792	0.623723302
F	-2.032784469	1.408457642	-1.294727450
F	-3.391295777	0.720693964	0.243487176
F	-2.474513766	-1.219466819	2.506900523
F	-1.377980380	-2.653434907	1.318137245
F	-0.383804043	-1.594131892	2.923160365

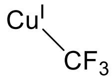
<u>Cu(I) Complexes:</u>



bipyCu^{I}CF3

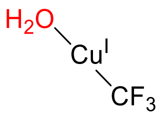
Cu	-0.481270045	0.046984405	0.752348539
N	1.248186235	-1.334461019	0.076288651
C	1.370145089	-2.637117593	0.310934160
H	0.434494871	-3.178670051	0.444338028
C	2.609879521	-3.263786870	0.397712998
H	2.673809314	-4.331847355	0.584968193
C	3.752005480	-2.487166484	0.252756466
H	4.738752243	-2.936794997	0.332124937

C	3.625235440	-1.121854661	0.023227088
H	4.507249302	-0.491911766	-0.056722279
C	2.344051070	-0.580809031	-0.062548990
N	0.883882458	1.326254500	0.101302415
C	2.088685197	0.863636040	-0.285959983
C	3.022420457	1.707767209	-0.881647884
H	3.979505497	1.313132559	-1.210275733
C	2.699505672	3.042354950	-1.083652082
H	3.413227841	3.711073825	-1.557228720
C	1.452202728	3.508099822	-0.687504840
H	1.155317809	4.541603928	-0.834204102
C	0.575311125	2.611477308	-0.095941835
H	-0.414739527	2.917750162	0.235763217
C	-1.956875716	-1.035947328	1.309688203
F	-2.667510960	-0.684980227	2.412516060
F	-2.896740414	-1.231287779	0.337650865
F	-1.508230888	-2.314890036	1.591243922



$Cu^{I}CF_3$

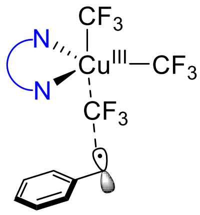
Cu	-0.514152311	0.057060209	0.773816288
C	-1.945661785	-1.099895059	1.291104268
F	-2.595197428	-0.652098209	2.379473166
F	-2.866495628	-1.234085112	0.320067497
F	-1.508954294	-2.337958003	1.582499422



$(H_2O)Cu^{I}CF_3$

Cu	-1.048074023	0.571690605	0.883832341
C	-1.581433271	-1.198371580	1.305628451
F	-2.713462165	-1.261661771	2.050006086
F	-1.829032957	-1.955229041	0.205212900
F	-0.645578533	-1.884160178	2.011846156
O	-0.471489601	2.409878770	0.433332658
H	0.371156456	2.680332801	0.816602532
H	-0.417950349	2.579581457	-0.514244157

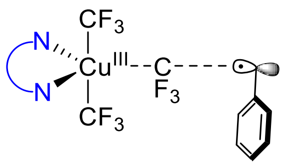
Transition States:



Outer Sphere 'Axial' Cu(III) Transition State

Cu	3.664977980	0.124601838	-1.532708343
N	5.559085113	-0.107932800	-2.334782897
C	6.023496185	-1.294414978	-2.730229495
H	5.310503889	-2.116237539	-2.709002433
C	7.337215118	-1.485178669	-3.134275559
H	7.673405323	-2.465913912	-3.455787084
C	8.198226821	-0.395403167	-3.105250842
H	9.237094107	-0.502693782	-3.407449728
C	7.721830624	0.835617619	-2.678582756
H	8.388079155	1.691820440	-2.637351022
C	6.386036467	0.953419623	-2.297440125
N	4.513369390	2.163096867	-1.442912192
C	5.793018270	2.230639239	-1.833434375
C	6.496437081	3.434389465	-1.800709027
H	7.530552817	3.492942033	-2.127005227
C	5.845845662	4.573574072	-1.345762521
H	6.374030202	5.523316020	-1.312800506
C	4.520500224	4.489824078	-0.937207393
H	3.984864626	5.361686657	-0.574188435
C	3.889627466	3.253326552	-1.005376844
H	2.852508190	3.110743967	-0.702402609
C	3.021879100	1.065539115	-4.029695369
C	1.759376462	0.008291423	-1.113333994
C	4.300694807	-0.794754269	0.202735873
F	2.548827478	-0.132290222	-4.260152219
F	4.253320605	1.345124864	-4.380315034
F	2.261882775	2.022181610	-3.573066689
F	1.500448671	0.966021588	-0.174239783
F	0.878197049	0.250769418	-2.117288952
F	1.368323614	-1.159116867	-0.570389366
F	3.478609308	-0.817574575	1.250961491
F	4.672322550	-2.072397392	-0.043353111
F	5.426136139	-0.150577569	0.607083565
C	2.303356072	1.613319808	-6.286755113
H	1.260991625	1.491527847	-5.999774017
H	2.806550224	0.743847503	-6.705246812
C	2.853257908	2.901426203	-6.463105385

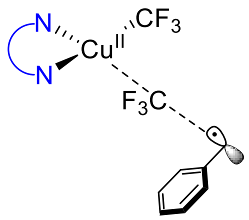
C	2.150550502	4.062224315	-6.056666083
C	4.154773149	3.073791191	-6.995248906
C	2.715072205	5.317795398	-6.187800269
C	4.710582504	4.333395462	-7.124348025
C	3.996395450	5.464458973	-6.723318683
H	1.151585332	3.947270637	-5.638109481
H	4.711539172	2.190719140	-7.307828164
H	2.155178356	6.196747333	-5.874361753
H	5.708568576	4.443307445	-7.544044984
H	4.434295847	6.454310706	-6.830749711



Outer Sphere 'equatorial' Cu(III) Transition State

Cu	3.819250942	1.057845947	-1.026788449
N	5.195730353	-0.547419183	-1.768780695
C	4.819543905	-1.738399299	-2.219738308
H	3.765555008	-1.981788921	-2.101219826
C	5.709271416	-2.631569102	-2.800568741
H	5.364381226	-3.597938223	-3.155414157
C	7.038101484	-2.246296038	-2.915571804
H	7.767290643	-2.909244016	-3.373882808
C	7.430793499	-1.002091017	-2.443230130
H	8.464319927	-0.686434909	-2.542966513
C	6.475780080	-0.167254414	-1.860657149
N	5.785972115	1.948172227	-0.939876054
C	6.811767754	1.174377634	-1.315183249
C	8.125622820	1.625031311	-1.184739999
H	8.962704290	0.992530506	-1.462610077
C	8.355970500	2.893056231	-0.671359650
H	9.374389713	3.256585082	-0.559218543
C	7.280350700	3.688802736	-0.300364291
H	7.420147917	4.687037672	0.103414682
C	6.003665683	3.163249372	-0.449429590
H	5.117293534	3.730109966	-0.165626971
C	3.449889909	1.706357966	-2.856062923
C	1.215461864	0.224000868	-1.016635783
C	3.878086602	0.386641752	0.819456620
F	2.973852655	0.707367935	-3.664514588
F	4.577540977	2.138083013	-3.485152698

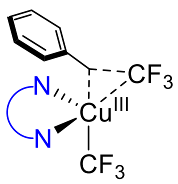
F	2.561129447	2.727020731	-2.989655483
F	0.846275199	1.367370587	-1.503099129
F	1.700270214	-0.712294111	-1.784273727
F	1.096364490	0.002552905	0.250305765
F	3.111417697	1.034295647	1.735079553
F	3.479715394	-0.921047323	0.881770028
F	5.134054942	0.386256219	1.341329649
C	-0.897556893	-0.653045098	-1.468676591
H	-0.602759055	-1.675037711	-1.232921720
H	-0.843372247	-0.361533030	-2.516645630
C	-1.757725207	0.047330348	-0.590540697
C	-2.005365601	-0.426436188	0.720317328
C	-2.345442587	1.277443847	-0.973434348
C	-2.802489940	0.289462585	1.594182307
C	-3.143408634	1.985568488	-0.093767006
C	-3.375904571	1.497779722	1.193930745
H	-1.555724906	-1.369329859	1.029193728
H	-2.163499989	1.653455064	-1.979300276
H	-2.982918862	-0.090215584	2.597256805
H	-3.590388589	2.926763948	-0.405364595
H	-4.001697008	2.058789332	1.884347042



Outer Sphere Cu(II) Transition State

Cu	-0.278203066	0.652505010	1.685521394
N	-0.041770268	-0.802706434	-0.028843187
C	-0.347649838	-2.096040348	-0.037102246
H	-0.948120483	-2.437742777	0.806180728
C	0.072845227	-2.948197642	-1.054127877
H	-0.197587955	-3.999857812	-1.038994430
C	0.847161981	-2.417943507	-2.078269942
H	1.204788700	-3.052793614	-2.885145584
C	1.169339827	-1.066215717	-2.064558626
H	1.789184037	-0.644255152	-2.850457333
C	0.694664102	-0.281189970	-1.015439967
N	0.651993532	1.748667715	0.278515352
C	0.945398153	1.177196643	-0.906501365
C	1.419076132	1.937565860	-1.973286605
H	1.631570935	1.468457786	-2.929691480

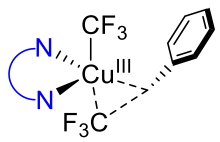
C	1.582099287	3.306337400	-1.813407254
H	1.941990703	3.913450157	-2.640086821
C	1.266906337	3.889109555	-0.592768512
H	1.371764139	4.956969282	-0.428316944
C	0.804496927	3.068146989	0.425583268
H	0.544017915	3.469439347	1.403216068
C	-2.596005279	1.204104933	0.301649761
C	-1.179821521	-0.080009935	3.205940497
F	-2.803221181	2.211808892	1.109519960
F	-2.052708838	1.435112540	-0.870945669
F	-3.084760134	0.023255335	0.561555728
F	-2.358608141	0.514810454	3.548134019
F	-1.532157798	-1.392936294	2.944441429
F	-0.478791534	-0.152754549	4.368842183
C	-4.806869944	1.034702348	-1.907716961
C	-5.282124212	-0.300769401	-1.920943114
C	-4.267424922	1.548387660	-3.114124985
C	-5.233853567	-1.062495286	-3.074045934
C	-4.224121412	0.779341789	-4.262298123
C	-4.710498045	-0.529795250	-4.254411036
H	-5.690379506	-0.718100306	-1.001322689
H	-3.889607607	2.570714141	-3.121111924
H	-5.611166081	-2.083297518	-3.062233481
H	-3.813324003	1.199392189	-5.178514037
H	-4.680928284	-1.130503180	-5.160708483
C	-4.823057036	1.810127801	-0.730695397
H	-4.542116546	2.860566635	-0.761339544
H	-5.327521229	1.453602604	0.164381399



Reductive Elimination (primary) Transition State 1

Cu	-0.617287728	-0.433493346	0.264686230
N	1.295244770	-1.241582816	0.349753339
C	1.518229984	-2.443872786	0.882480591
H	0.631105967	-2.969581436	1.235833376
C	2.794641661	-2.979148519	0.984586875
H	2.940703728	-3.968242142	1.407527814
C	3.867516597	-2.210593674	0.547904594
H	4.884269822	-2.587983575	0.624750791
C	3.635000150	-0.943811395	0.031941304

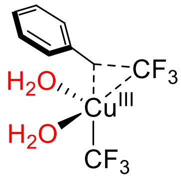
H	4.467565293	-0.316035382	-0.272055599
C	2.321796670	-0.484283592	-0.064081518
N	0.715134105	1.266526197	-0.374532033
C	1.973199768	0.853643070	-0.598214488
C	2.890972559	1.643510122	-1.291196862
H	3.890975984	1.276546340	-1.503780450
C	2.497638031	2.898702288	-1.732101265
H	3.196493741	3.530847410	-2.274446082
C	1.202219136	3.330432835	-1.478252359
H	0.856082579	4.306895414	-1.804063191
C	0.342595589	2.471495909	-0.804719736
H	-0.690111729	2.749515060	-0.600120740
C	-2.375436331	0.346823585	-0.516653725
C	-1.315581886	-1.110276017	2.015215392
F	-2.650312421	1.056287490	-1.637757417
F	-3.440843902	-0.384815748	-0.223541354
F	-2.293001320	1.328019558	0.421829616
F	-0.409947191	-1.140932972	3.039164197
F	-2.464741884	-0.681439807	2.581167444
F	-1.547675404	-2.472459335	1.762132519
C	-1.368451002	-1.089350922	-1.634484974
H	-1.245961603	-2.038257404	-1.090433371
H	-2.351977126	-1.093928015	-2.097803306
C	-0.278891579	-0.773645886	-2.577065349
C	0.836020890	-1.620441631	-2.665848545
C	-0.335694481	0.331316329	-3.439082826
C	1.862002061	-1.366824013	-3.566768917
C	0.697831275	0.592458546	-4.328404790
C	1.803736116	-0.251172200	-4.396098410
H	0.890552879	-2.495103658	-2.018187068
H	-1.195300458	0.994717344	-3.397061125
H	2.712148064	-2.044529872	-3.617932029
H	0.636445612	1.461440074	-4.980688581
H	2.608077777	-0.046360579	-5.099302674



Reductive Elimination (primary) Transition State 2

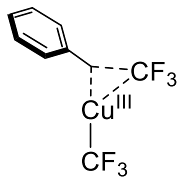
Cu	-0.957413025	-0.428262541	0.097747769
N	1.044889512	-1.201117063	-0.044573437
C	1.257003745	-2.503145899	0.145273718

H	0.373056275	-3.137820281	0.111399547
C	2.517022351	-3.034852907	0.381257356
H	2.642576313	-4.103011830	0.528373516
C	3.595794500	-2.162562872	0.440734512
H	4.598549563	-2.531478373	0.642098407
C	3.378106071	-0.805696202	0.257538845
H	4.204134831	-0.106233244	0.337802770
C	2.082072236	-0.351260915	0.008082698
N	0.493770795	1.449079947	-0.053796068
C	1.779892538	1.089238628	-0.167456542
C	2.787514342	2.023515594	-0.416059837
H	3.818848123	1.710007927	-0.545132684
C	2.453929785	3.365906958	-0.517936199
H	3.223895428	4.108756089	-0.713004678
C	1.126683278	3.738678063	-0.366927208
H	0.817074322	4.778131841	-0.427846659
C	0.183844065	2.741128343	-0.142694338
H	-0.867819632	2.992574412	-0.020326826
C	-1.457693447	-0.653248954	-1.976401734
C	-1.176675577	-0.675680999	2.066462642
F	-2.316099073	-0.459662449	-2.995403264
F	-0.349246907	-0.002204079	-2.372713142
F	-1.200748855	-1.972892523	-1.965495087
F	-2.482371825	-0.778234705	2.517007560
F	-0.565435455	-1.784281382	2.582249584
F	-0.664848655	0.362869760	2.791821638
C	-2.916338026	-0.133287544	-0.574916386
H	-3.132582804	-0.666381243	0.356646213
H	-3.539915892	-0.547101495	-1.363007972
C	-3.025284558	1.339950545	-0.443006972
C	-3.093919319	2.172097481	-1.567725116
C	-3.098328958	1.921206540	0.830568521
C	-3.240984823	3.546420098	-1.423339627
C	-3.257544218	3.294626682	0.970632834
C	-3.327521429	4.112790348	-0.154309674
H	-3.032045062	1.734115935	-2.561402956
H	-3.021340111	1.281766775	1.707458440
H	-3.292578216	4.178818626	-2.307184464
H	-3.318504825	3.728742940	1.966005853
H	-3.447086425	5.188444215	-0.042466239



Reductive Elimination (primary) Water Ligand Transition State

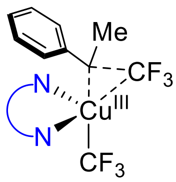
Cu	-1.132572145	-0.338682768	0.224607746
C	-0.025773674	-1.916773661	-0.274653225
C	-1.608775529	-0.043709560	2.263830899
F	-0.363320313	-2.371226527	-1.549582209
F	1.292817883	-1.505347020	-0.458704114
F	0.070252234	-3.034095637	0.461401316
F	-1.375110389	1.092854754	2.923674549
F	-2.658478715	-0.662030794	2.809543921
F	-0.540898072	-0.823451348	2.559754998
O	0.833204557	1.067595233	0.632895616
H	1.248501741	0.506733975	-0.038796092
H	1.125903006	0.670818680	1.460970110
O	-0.769490039	0.319955301	-1.983216218
H	-1.635359679	0.342820938	-2.410122174
H	-0.424071728	-0.561551874	-2.199524666
C	-2.616730968	0.918235278	0.800408159
H	-2.036518554	1.777426392	0.437935358
H	-3.190242274	1.221083509	1.672872060
C	-3.468305349	0.247769085	-0.226048994
C	-3.693723472	0.881378827	-1.457517203
C	-4.076700657	-0.991115468	0.014105697
C	-4.508672751	0.294567146	-2.418467652
C	-4.875928794	-1.582239024	-0.957449612
C	-5.095684665	-0.944211614	-2.173279768
H	-3.233030004	1.851005181	-1.648264354
H	-3.908144865	-1.496528078	0.961854333
H	-4.686154162	0.805133955	-3.362390863
H	-5.328399892	-2.551224166	-0.761676771
H	-5.722881223	-1.410187723	-2.929304405



Reductive Elimination (primary) Unligated Transition State

Cu	-0.833783778	0.372705001	0.204075699
C	-2.331491954	1.551631923	0.343334507
C	-0.347181856	-1.227049674	1.493050629

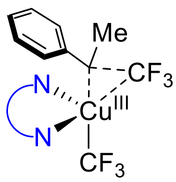
F	-1.928605005	2.851935178	0.229586783
F	-3.241386272	1.378094349	-0.654978934
F	-3.040447598	1.493945969	1.493141315
F	-1.612192368	-1.335734009	1.911520094
F	0.095544616	-2.478863615	1.373812443
F	0.354871171	-0.617999101	2.452927897
C	0.844652600	-0.726825634	-0.216377760
H	1.621161345	-1.097616329	0.447053054
H	0.485557397	-1.487702864	-0.912140665
C	1.114215528	0.603515252	-0.772278415
C	1.847610545	1.542490478	-0.017055004
C	0.518559980	1.020260310	-1.980896525
C	2.013773082	2.835292420	-0.480093089
C	0.695090882	2.321208305	-2.438871618
C	1.441030315	3.224348386	-1.692370447
H	2.274325109	1.233632726	0.936299168
H	-0.060582354	0.305204941	-2.564048041
H	2.585212443	3.551389523	0.104668391
H	0.237925548	2.631490311	-3.374257971
H	1.570266255	4.243607764	-2.047555978



Reductive Elimination (secondary) Transition State 1

Cu	-0.700045013	-0.046739924	0.142133345
N	1.184345503	-1.208972790	0.374764790
C	1.285528702	-2.498703251	0.698476924
H	0.402219105	-2.946067633	1.147520576
C	2.436257748	-3.244216333	0.477615146
H	2.469944783	-4.292410304	0.759476675
C	3.523672319	-2.615497380	-0.114467437
H	4.438614700	-3.165437756	-0.320883012
C	3.428143072	-1.272033919	-0.443916901
H	4.260258855	-0.769103223	-0.927239663
C	2.240811687	-0.590547870	-0.176937429
N	0.828585663	1.339524880	-0.349012159
C	2.071735142	0.852646466	-0.473127443
C	3.134617530	1.677287897	-0.840837963
H	4.144702271	1.286404869	-0.915177594
C	2.888708771	3.017800375	-1.100004224
H	3.703130326	3.672767854	-1.399981854

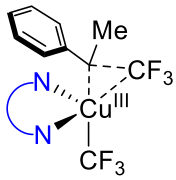
C	1.600654893	3.514968226	-0.947983576
H	1.372486175	4.562513308	-1.120287813
C	0.600154825	2.637940509	-0.549917167
H	-0.422134548	2.965285314	-0.364971123
C	-1.920323077	-1.770737618	0.033897015
C	-1.880433042	1.061863045	1.362787500
F	-3.244165862	-1.725769133	-0.068865726
F	-1.503473308	-2.955394702	-0.485192519
F	-1.669202775	-1.931821943	1.363417594
F	-2.142168785	2.309129829	0.783342943
F	-3.125517295	0.595240726	1.663732610
F	-1.331927845	1.383630705	2.567141321
C	-1.631645970	-0.749254245	-1.799123217
C	-0.346555373	-0.747439580	-2.539238592
C	0.374578770	-1.940371646	-2.711159009
C	0.144664046	0.408855233	-3.164283597
C	1.553065802	-1.965567740	-3.442502550
C	1.320334442	0.379822140	-3.904121384
C	2.039764807	-0.803838492	-4.039169265
H	0.000912024	-2.852095311	-2.250996361
H	-0.404408080	1.343924158	-3.077367244
H	2.094751411	-2.903290291	-3.552181259
H	1.674586801	1.292499447	-4.380144456
H	2.958961579	-0.826414315	-4.620271625
C	-2.511740999	0.470926339	-1.842703075
H	-2.886921160	0.602175053	-2.868690025
H	-3.371773625	0.346972756	-1.180150030
H	-2.013057903	1.396785705	-1.541411196
H	-2.198129205	-1.637261328	-2.073917772



Reductive Elimination (secondary) Transition State 2

Cu	-0.940957921	-0.632447699	0.122280315
N	1.072235248	-1.454401081	-0.081344522
C	1.301409384	-2.690154770	0.365188931
H	0.424223892	-3.237309296	0.704831473
C	2.575847908	-3.240783709	0.418745750
H	2.717574258	-4.253041332	0.784952709
C	3.650785670	-2.460881468	0.013720608
H	4.665738536	-2.849112726	0.054724502

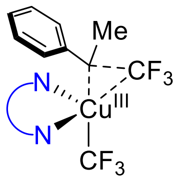
C	3.417840910	-1.164512730	-0.422046323
H	4.247510372	-0.519215686	-0.697004929
C	2.106326104	-0.691168505	-0.458972339
N	0.604689348	1.172512099	-0.455796021
C	1.782784849	0.692198271	-0.878097144
C	2.650437440	1.446567727	-1.670789763
H	3.578276709	1.018232367	-2.040238372
C	2.292603047	2.745110403	-2.005674034
H	2.946252794	3.349940946	-2.629355115
C	1.088257645	3.254018981	-1.537945610
H	0.774105432	4.267832569	-1.769587371
C	0.277420444	2.424511375	-0.770072515
H	-0.687131063	2.769578539	-0.398884091
C	-2.635680541	0.611709741	-0.247505334
C	-1.196131038	-1.156132597	2.017622256
F	-2.204431502	1.403695370	0.762732861
F	-3.098678030	1.517574188	-1.141797574
F	-3.697096648	-0.068312605	0.187019812
F	-2.282180541	-0.735743755	2.712603461
F	-1.214041913	-2.535310356	2.168497527
F	-0.124178035	-0.766816136	2.777580494
C	-1.960625972	-0.556813138	-1.848719110
C	-1.597885729	-1.998510045	-1.741058104
C	-0.567323962	-2.566551462	-2.506330401
C	-2.339035805	-2.837661249	-0.892370453
C	-0.298249679	-3.925343341	-2.433914517
C	-2.045810765	-4.193494869	-0.802135427
C	-1.030145223	-4.744271099	-1.575686282
H	0.027146129	-1.939557669	-3.167704492
H	-3.139207193	-2.410406063	-0.291122550
H	0.493821024	-4.348499509	-3.048500442
H	-2.617514176	-4.818303514	-0.120685681
H	-0.809413410	-5.807407207	-1.514149177
C	-1.214140329	0.278871097	-2.852767653
H	-1.499890068	1.330469847	-2.782680292
H	-0.126768189	0.211225265	-2.744095457
H	-1.471367108	-0.060520568	-3.866978410
H	-3.036843794	-0.490788560	-2.012414521



Reductive Elimination (secondary) Transition State 3

Cu	-0.494724550	-0.298852547	0.002850065
N	0.689359281	-2.047248021	-0.709474559
C	0.352533160	-3.335365009	-0.714081091
H	-0.668085581	-3.565756536	-0.407109481
C	1.236480188	-4.343813978	-1.078807412
H	0.917579010	-5.381811678	-1.067462071
C	2.522009479	-3.983746349	-1.459890966
H	3.243876697	-4.738515005	-1.762300392
C	2.874121974	-2.642252040	-1.464341345
H	3.864865138	-2.337912808	-1.788907471
C	1.929681021	-1.691522140	-1.076903897
N	1.179135591	0.588364279	-1.045365797
C	2.234679583	-0.239256487	-1.074886289
C	3.539334156	0.252160690	-1.086340628
H	4.387777680	-0.425336097	-1.064746125
C	3.742858518	1.625017256	-1.086370626
H	4.752995567	2.026890444	-1.085887503
C	2.644165261	2.473644551	-1.072827668
H	2.760212742	3.553233215	-1.067552875
C	1.379458621	1.903868550	-1.038590180
H	0.482378362	2.520051478	-0.993567775
C	-1.968553582	-0.081447889	-1.522566541
C	0.390968548	0.022374473	1.795080329
F	-1.834341416	1.249786992	-1.686436517
F	-1.135289015	-0.682130079	-2.400194907
F	-3.181722301	-0.401162672	-2.001491544
F	1.148105327	1.156269535	1.899061394
F	-0.472135348	0.102006676	2.877751846
F	1.252653544	-0.984417183	2.148454563
C	-2.600569541	-0.400891672	0.516082367
C	-2.774499751	-1.867301349	0.673778897
C	-3.665444870	-2.618665235	-0.102366732
C	-2.046532494	-2.522813448	1.679429762
C	-3.812894975	-3.984056225	0.111439380
C	-2.204162706	-3.885126039	1.897199977
C	-3.085977434	-4.622739841	1.111600163
H	-4.239022667	-2.135426805	-0.887500920
H	-1.350529831	-1.948282245	2.288421885
H	-4.506750024	-4.551950753	-0.504675639
H	-1.634154336	-4.371411224	2.685701507
H	-3.208079961	-5.690709301	1.279148006
C	-3.831171371	0.466199693	0.384380933
H	-3.563936124	1.501678905	0.154509552

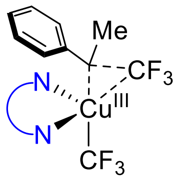
H	-4.561566712	0.121693956	-0.347643120
H	-4.315919250	0.467170217	1.370010560
H	-2.045436983	-0.003096720	1.371548334



Reductive Elimination (secondary) Transition State 4

Cu	-0.551514317	-0.688805044	0.178558953
N	1.499757126	-1.558293355	-0.200522684
C	1.890370057	-2.737443199	0.269405030
H	1.204368178	-3.218195913	0.964799697
C	3.103696413	-3.317737290	-0.080274621
H	3.382939753	-4.288210522	0.319051223
C	3.932917863	-2.624862036	-0.951984753
H	4.885965193	-3.046189287	-1.262115077
C	3.533157795	-1.384202181	-1.428241032
H	4.166220168	-0.837733700	-2.120956594
C	2.299054097	-0.872704168	-1.022641042
N	0.499818666	0.716231381	-1.247138660
C	1.796134810	0.447247497	-1.477278683
C	2.632761261	1.371123527	-2.105841297
H	3.686642898	1.154177029	-2.249657647
C	2.110200814	2.585680130	-2.523280660
H	2.749264432	3.318175716	-3.010494082
C	0.765825083	2.849524773	-2.304316892
H	0.309506345	3.784368397	-2.616255575
C	0.004572687	1.884662631	-1.656802170
H	-1.053613929	2.052073274	-1.460866672
C	-1.695703664	-1.638664381	-1.458400930
C	0.017476422	-0.516798188	2.109465406
F	-2.068276603	-0.845732628	-2.472583942
F	-0.506226671	-2.161287641	-1.837932295
F	-2.510021377	-2.709489104	-1.439956566
F	-0.736649958	0.060940585	3.117320344
F	0.237420402	-1.791931397	2.601618145
F	1.230295213	0.097537379	2.231839052
C	-2.748126601	-0.682716009	0.025023083
C	-2.842010027	0.805634804	0.000200901
C	-2.421536930	1.628478181	1.055232608
C	-3.479577971	1.407342880	-1.096187794
C	-2.624339818	3.001723165	1.000324680

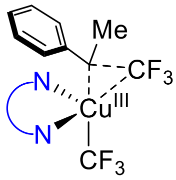
C	-3.677326080	2.781641553	-1.150066707
C	-3.245957103	3.585954670	-0.100117218
H	-1.927252650	1.195773094	1.919096594
H	-3.823000174	0.782886978	-1.918261280
H	-2.293390948	3.621357423	1.830649399
H	-4.177432826	3.222577544	-2.009752758
H	-3.402209308	4.662197850	-0.134149351
C	-2.984098575	-1.435606535	1.315056086
H	-2.429904757	-1.042813768	2.167148778
H	-4.059946775	-1.386827832	1.542274391
H	-2.726753572	-2.492720434	1.192310834
H	-3.487888002	-1.038326558	-0.690871583



Reductive Elimination (secondary) Transition State 5

Cu	-0.551514317	-0.688805044	0.178558953
N	1.499757126	-1.558293355	-0.200522684
C	1.890370057	-2.737443199	0.269405030
H	1.204368178	-3.218195913	0.964799697
C	3.103696413	-3.317737290	-0.080274621
H	3.382939753	-4.288210522	0.319051223
C	3.932917863	-2.624862036	-0.951984753
H	4.885965193	-3.046189287	-1.262115077
C	3.533157795	-1.384202181	-1.428241032
H	4.166220168	-0.837733700	-2.120956594
C	2.299054097	-0.872704168	-1.022641042
N	0.499818666	0.716231381	-1.247138660
C	1.796134810	0.447247497	-1.477278683
C	2.632761261	1.371123527	-2.105841297
H	3.686642898	1.154177029	-2.249657647
C	2.110200814	2.585680130	-2.523280660
H	2.749264432	3.318175716	-3.010494082
C	0.765825083	2.849524773	-2.304316892
H	0.309506345	3.784368397	-2.616255575
C	0.004572687	1.884662631	-1.656802170
H	-1.053613929	2.052073274	-1.460866672
C	-1.695703664	-1.638664381	-1.458400930
C	0.017476422	-0.516798188	2.109465406
F	-2.068276603	-0.845732628	-2.472583942

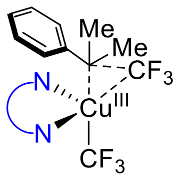
F	-0.506226671	-2.161287641	-1.837932295
F	-2.510021377	-2.709489104	-1.439956566
F	-0.736649958	0.060940585	3.117320344
F	0.237420402	-1.791931397	2.601618145
F	1.230295213	0.097537379	2.231839052
C	-2.748126601	-0.682716009	0.025023083
C	-2.842010027	0.805634804	0.000200901
C	-2.421536930	1.628478181	1.055232608
C	-3.479577971	1.407342880	-1.096187794
C	-2.624339818	3.001723165	1.000324680
C	-3.677326080	2.781641553	-1.150066707
C	-3.245957103	3.585954670	-0.100117218
H	-1.927252650	1.195773094	1.919096594
H	-3.823000174	0.782886978	-1.918261280
H	-2.293390948	3.621357423	1.830649399
H	-4.177432826	3.222577544	-2.009752758
H	-3.402209308	4.662197850	-0.134149351
C	-2.984098575	-1.435606535	1.315056086
H	-2.429904757	-1.042813768	2.167148778
H	-4.059946775	-1.386827832	1.542274391
H	-2.726753572	-2.492720434	1.192310834
H	-3.487888002	-1.038326558	-0.690871583



Reductive Elimination (secondary) Transition State 6

Cu	-0.499695001	-1.144474536	0.286382732
N	1.074807587	-1.734385211	-1.104193966
C	1.125364861	-2.890073660	-1.759699949
H	0.285596173	-3.565465901	-1.599131348
C	2.170179927	-3.227565725	-2.609435446
H	2.171342927	-4.181664010	-3.128046764
C	3.194584961	-2.305499595	-2.779484837
H	4.024726486	-2.517843253	-3.448738570
C	3.148831181	-1.104057357	-2.087467273
H	3.936284629	-0.368504111	-2.222835090
C	2.072000826	-0.849029310	-1.236790517
N	0.792041148	0.643003075	0.155327961
C	1.974472296	0.392318724	-0.425994369
C	3.067762283	1.238350195	-0.237645418
H	4.031375670	1.011955432	-0.683890323

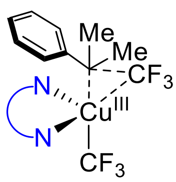
C	2.920843527	2.361358231	0.563336073
H	3.763678982	3.029226540	0.725034241
C	1.695401374	2.607660864	1.167214066
H	1.543981172	3.468013650	1.812054149
C	0.660195689	1.709285182	0.941757555
H	-0.316804793	1.840134368	1.409376801
C	-1.884865221	-0.890082299	-1.415500543
C	0.413794106	-1.726412448	2.009121815
F	-3.035422791	-0.311147335	-1.828012532
F	-0.948732951	-0.135381303	-2.023858378
F	-1.851790033	-2.108755873	-1.980583910
F	0.611671854	-0.670223679	2.865528944
F	-0.114835960	-2.701031505	2.833804874
F	1.682704118	-2.174810169	1.755977769
C	-2.641637276	-1.298190679	0.483567262
C	-2.624476600	-0.169000065	1.458307694
C	-2.970214840	1.114769560	1.010455082
C	-2.336009026	-0.350241974	2.814885647
C	-3.014793501	2.187276555	1.890299810
C	-2.393062194	0.722921563	3.694355773
C	-2.727121042	1.994520137	3.239269639
H	-3.202769836	1.264475897	-0.042312108



Reductive Elimination (tertiary) Transition State 1

Cu	-1.020475406	-0.649567068	0.281111370
N	0.996514964	-1.489837094	0.414807023
C	1.165718417	-2.657631076	1.031161405
H	0.275707341	-3.072022135	1.502840665
C	2.397308496	-3.302681140	1.081056273
H	2.492742479	-4.257915367	1.588395806
C	3.487210758	-2.689674718	0.481210778
H	4.469634734	-3.155080411	0.506303547
C	3.318561163	-1.453544323	-0.129429271
H	4.170493605	-0.930560688	-0.554703033
C	2.049584750	-0.878758574	-0.144485615
N	0.671705765	1.068395473	-0.324671549
C	1.798137030	0.462472350	-0.725365423
C	2.684283547	1.064164775	-1.622455459
H	3.564191449	0.533673314	-1.976075230

C	2.411575787	2.349417164	-2.072118184
H	3.083032743	2.838123195	-2.774022566
C	1.270215848	2.995609574	-1.615910876
H	1.025104674	4.004840317	-1.934485851
C	0.425851614	2.305950432	-0.751441351
H	-0.501454576	2.753317279	-0.396152601
C	-2.543528468	0.776908390	-0.228379925
C	-1.653703136	-1.185716245	2.091296023
F	-2.823170166	1.753895393	-1.132105562
F	-3.716071276	0.248247213	0.123601050
F	-2.098220185	1.510387131	0.830699388
F	-0.701342383	-0.857469791	3.017060890
F	-2.811295748	-0.708681232	2.600255387
F	-1.771313803	-2.563828603	2.217882874
C	-1.899367831	-0.537606878	-2.043089353
C	-1.274931513	-1.861446535	-1.813840399
C	-0.078289322	-2.241481732	-2.451201412
C	-1.916466892	-2.811210274	-0.992180189
C	0.445623140	-3.512324782	-2.279372686
C	-1.372047065	-4.076535083	-0.806645487
C	-0.195663870	-4.434918256	-1.453341856
H	0.441086977	-1.537619343	-3.097582785
H	-2.835663120	-2.542917314	-0.474801746
H	1.365699360	-3.786703127	-2.791912506
H	-1.873217187	-4.777287093	-0.143215025
H	0.225655009	-5.428023725	-1.313500327
C	-3.350306693	-0.658546231	-2.451959307
H	-3.362018998	-1.211298821	-3.404563185
H	-3.960372069	-1.221040503	-1.743257335
H	-3.817166572	0.313982920	-2.617860883
C	-1.142523475	0.407750552	-2.931308421
H	-1.588482225	1.403609838	-2.921515134
H	-0.084554279	0.495413666	-2.674716132
H	-1.206472206	0.034010301	-3.966736469

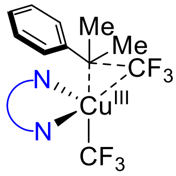


Reductive Elimination (tertiary) Transition State 2

Cu	-0.792217893	-0.184376770	-0.168529691
N	1.021662247	-1.359928054	0.468048640
C	1.006186223	-2.456858990	1.223335563

H	0.022373956	-2.865203279	1.458239951
C	2.152259774	-3.075556639	1.702242434
H	2.080015703	-3.971362533	2.311427958
C	3.377501956	-2.512475616	1.373617044
H	4.306380748	-2.961331229	1.716494884
C	3.403713213	-1.360293099	0.603934884
H	4.356807470	-0.909266801	0.346975909
C	2.203209318	-0.794926057	0.167313815
N	0.963802802	0.893041446	-1.012094381
C	2.169766937	0.463487441	-0.624270382
C	3.325566394	1.184646102	-0.933431964
H	4.305714304	0.838541466	-0.620586975
C	3.211736122	2.369475510	-1.645177534
H	4.101385975	2.941824206	-1.896258589
C	1.952276162	2.816375784	-2.020984106
H	1.818746594	3.744407065	-2.568770750
C	0.854760736	2.040676608	-1.674525854
H	-0.157477729	2.344580226	-1.934575478
C	-1.265532891	-0.981946305	-2.119513554
C	-1.098394099	1.151725412	1.305991037
F	-1.305008748	0.288807940	-2.573092363
F	-0.034046834	-1.486603539	-2.323499025
F	-2.041130980	-1.649006965	-2.984413518
F	-2.357086944	1.701762638	1.475727193
F	-0.814746722	0.622673566	2.542570031
F	-0.281923860	2.247298012	1.222677746
C	-2.551538703	-1.655332086	-0.453683704
C	-3.787558634	-1.118059865	-1.099864657
C	-4.676793154	-1.945848926	-1.787762521
C	-4.098943228	0.239686292	-0.962476226
C	-5.850313398	-1.431003156	-2.326770445
C	-5.264266793	0.753236691	-1.511597414
C	-6.145237811	-0.079645429	-2.196076620
H	-4.452244618	-3.003341960	-1.911526540
H	-3.413337946	0.892177861	-0.421821586
H	-6.532541591	-2.090452159	-2.858832083
H	-5.486276471	1.812396999	-1.403184218
H	-7.058769291	0.324661918	-2.626006402
C	-2.669061879	-1.474410459	1.066041178
H	-3.445468786	-2.194648441	1.378822263
H	-1.753962047	-1.715222534	1.617486650
H	-2.995399456	-0.481178330	1.368958659
C	-2.176476688	-3.103395753	-0.710432573

H	-2.875683583	-3.752561943	-0.164751265
H	-2.191972999	-3.398169207	-1.758686993
H	-1.174815498	-3.306313033	-0.316959017



Reductive Elimination (tertiary) Transition State 3

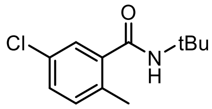
Cu	-0.596649113	-0.375033245	0.148255195
N	1.357500845	-1.241078748	0.163005372
C	1.609840690	-2.509158936	0.488231301
H	0.750202194	-3.086649506	0.823583586
C	2.885998846	-3.053535396	0.431662793
H	3.048006533	-4.095120629	0.692581290
C	3.935914059	-2.227936555	0.051580628
H	4.952374590	-2.610875884	0.001713307
C	3.679289867	-0.897277994	-0.244631941
H	4.497741115	-0.234952356	-0.508867536
C	2.366523898	-0.429413343	-0.183557023
N	0.727603507	1.323870964	-0.228378597
C	2.002362466	0.979562363	-0.470267817
C	2.926819841	1.906786430	-0.951257130
H	3.949516315	1.612133183	-1.166393044
C	2.519369632	3.213212987	-1.174158216
H	3.225002039	3.948641412	-1.552857150
C	1.202919471	3.565727004	-0.906427231
H	0.843420262	4.578981098	-1.058828881
C	0.341708658	2.583680767	-0.435685107
H	-0.700179996	2.802887469	-0.215718977
C	-2.380546853	0.574379856	-0.408989881
C	-1.345568761	-1.241770142	1.835314656
F	-2.447713927	1.514708445	-1.390594476
F	-3.591510936	0.038046540	-0.268444216
F	-2.225889783	1.357904107	0.708732764
F	-0.741295445	-0.779764650	2.966767162
F	-2.676197731	-1.174295905	2.099398450
F	-1.082990784	-2.613440627	1.863849233
C	-1.746891361	-1.044231413	-1.900694408
C	-0.421400120	-0.884554455	-2.555611316
C	0.458502298	-1.968099316	-2.698909311
C	-0.056504586	0.336682503	-3.147197384
C	1.661925534	-1.828915482	-3.380270906

C	1.148221372	0.476141135	-3.818675454
C	2.018523400	-0.605921141	-3.938365179
H	0.198128620	-2.935101304	-2.273760584
H	-0.717814534	1.193661720	-3.039031851
H	2.324550429	-2.687288140	-3.475809994
H	1.412254083	1.440125973	-4.250179246
H	2.960721861	-0.498104380	-4.471379482
C	-2.867173524	-0.693666711	-2.857612913
H	-2.826324545	-1.452021690	-3.656367372
H	-3.852251088	-0.751553796	-2.391065146
H	-2.752413669	0.279953283	-3.334657002
C	-2.039721366	-2.337025581	-1.189622375
H	-2.244987121	-3.121097278	-1.936906860
H	-1.241046197	-2.690179787	-0.532443185
H	-2.934655463	-2.229776306	-0.568959795

Synthesis and Characterization of Substrates.

Copper complexes (bpy)Cu(CF_3)$_3$[8-9] and [(Ph_3P)$_3$Cu(CF_3)][10] were synthesized followed by the reported procedures. The following compounds were synthesized according to the literature procedures: *N*-(*tert*-butyl)-2-methylbenzamide (**1k**),[11] *N*-butyl-2-methylbenzamide (**1l**),[12] *N*-benzyl-2-methylbenzamide (**1n**),[13] *N*-(pyridin-2-ylmethyl)-2-methylbenzamide (**1q**),[14] 5-phenylhexanenitrile (**1x**),[15] 1-(4-Chlorophenyl)-3-phenylpropan-1-one (**1cc**),[16] and *N*-(*tert*-butyl)-3-phenylbutanamide (**1dd**)[17]

***N*-(*tert*-Butyl)-5-chloro-2-methylbenzamide (1o)**

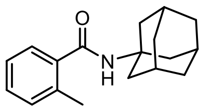


1o

To a round-bottom flask with a stir bar was added 5-chloro-2-methylbenzoic acid (0.853 g, 5.00 mmol, 1.0 equiv) and DCM (17 mL, 0.3 M). *N*, *N*-Dimethylformamide (19.4 µL; 0.25 mmol, 0.05 equiv) was added at rt. Oxalyl chloride (643 µL; 7.5 mmol, 1.50 equiv) was added dropwise. The reaction was stirred at room temperature until bubbling stopped. Without transferring from the reaction flask, volatile components were removed by rotary evaporation and high vacuum. The crude reaction product, a yellow oily solid, was dissolved in DCM (17 mL, 0.3 M). *tert*-Butylamine (788 µL; 7.5 mmol, 1.5 equiv), followed by triethylamine (1.39 mL, 10 mmol, 2.0 equiv), were added at room temperature, and the reaction was stirred for 3 hours. The reaction mixture was diluted with EtOAc and the organic layer was washed with water. The organic layer was concentrated under vacuum. The amide was purified by silica column chromatography (10% EtOAc in hexanes) to provide *N*-(*tert*-butyl)-5-chloro-2-methylbenzamide **1o** (1.050 g, 93% yield) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.19 (m, 2H), 7.12 (d, *J* = 8.2 Hz, 1H), 5.52 (br, 1H), 2.38 (s, 3H), 1.46 (s, 9H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 168.3, 139.3, 134.1, 132.3, 131.4, 129.39, 126.6, 52.1, 28.9, 19.1.
HRMS (ESI): Calcd. for $C_{12}H_{16}ONClNa$ $[M+Na]^+$, 248.0813. Found: 248.0812.
TLC: R_f = 0.28, 15% EtOAc in hexanes.

***N*-1-Adamantyl-2-methylbenzamide (1p)**

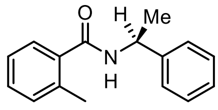


1p

To a round-bottom flask with a stir bar was added *o*-Toluoyl chloride (0.853 g, 5.00 mmol, 1.0 equiv) and DCM (17.0 mL, 0.3 M). 1-Adamantylamine (1.13 mg; 7.5 mmol, 1.5 equiv), followed by triethylamine (1.39 mL, 10 mmol, 2.0 equiv), were added at room temperature, and the reaction was stirred for 5 hours. The reaction mixture was then diluted with EtOAc and washed with water. Thereafter the organic layer was concentrated under vacuum. The amide was purified by silica column chromatography (10% EtOAc in hexanes) to provide *N*-1-Adamantyl-2-methylbenzamide (**1p**) (1.27 g, 94% yield) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (d, *J* = 7.6 Hz, 1H), 7.30 – 7.13 (m, 3H), 5.40 (br, 1H), 2.43 (s, 3H), 2.12 (s, 9H), 1.81 – 1.66 (m, 6H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 169.5, 138.0, 135.5, 130.8, 129.4, 126.5, 125.7, 52.5, 41.8, 36.4, 29.6, 19.7.
HRMS (ESI): Calcd. for $C_{18}H_{23}ONNa$ $[M+Na]^+$, 292.1672. Found: 292.1672.
TLC: R_f = 0.30, 20% EtOAc in hexanes.

(*S*)-2-Methyl-*N*-(1-phenylethyl)benzamide (1r)

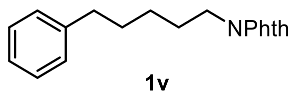


1r

To a round-bottom flask with a stir bar was added o-Toluoyl chloride (0.853 g, 5.00 mmol, 1.0 equiv) and DCM (17.0 mL, 0.3 M). (*S*)-1-phenylethan-1-amine (909 mg; 7.5 mmol, 1.5 equiv), followed by triethylamine (1.39 mL, 10 mmol, 2.0 equiv), were added at room temperature, and the reaction was stirred for 5 hours. The reaction mixture was then diluted with EtOAc and washed with water. The organic layer was concentrated under vacuum. The amide was purified by silica column chromatography (20% EtOAc in hexanes) to provide (*S*)-2-methyl-*N*-(1-phenylethyl)benzamide (**1r**) (0.972 g, 81% yield) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.10 (m, 9H), 5.96 (br, *J* = 6.0 Hz, 1H), 5.44 – 5.19 (m, 1H), 2.43 (s, 3H), 1.60 (d, *J* = 6.9 Hz, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 169.2, 143.2, 136.6, 136.2, 131.1, 129.9, 128.8, 127.5, 126.7, 126.3, 125.8, 49.2, 21.9, 19.9.
HRMS (ESI): Calcd. for $C_{16}H_{17}ONNa$ $[M+Na]^+$, 262.1202. Found: 262.1202.
TLC: R_f = 0.23, 20% EtOAc in hexanes.

***N*-Phthaloyl-5-phenylhexan-1-amine (1v)**[18]

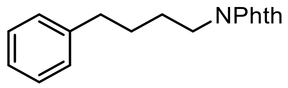


1v

(5-Bromopentyl)benzene (0.681 g, 3 mmol) and potassium phthalimide (0.556 g, 3 mmol) were then dissolved in 20 mL DMF. The stirred solution was heated for 15 hours. After filtration, the mixture was washed with 50 mL brine and was extracted with 50 mL Et_2O. The solution was dried over Na_2SO_4 and the solvent was removed by evaporation under vacuum. The product was purified by silica column chromatography (20% EtOAc in hexanes) or Biotage flash chromatography to afford *N*-Phthaloyl-5-phenylhexan-1-amine **1v** (0.671g, 76% yield) as an off-white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 – 7.80 (m, 2H), 7.76 – 7.68 (m, 2H), 7.29 – 7.21 (m, 2H), 7.21 – 7.08 (m, 3H), 3.68 (t, J = 7.3 Hz, 2H), 2.60 (t, J = 7.7 Hz, 2H), 1.79 – 1.59 (m, 4H), 1.46 – 1.29 (m, 2H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 168.5, 142.5, 133.9, 132.3, 128.5, 128.3, 125.7, 123.2, 38.0, 35.8, 31.1, 28.5, 26.6.
TLC: R_f = 0.25, 30% EtOAc in hexanes.

***N*-Phthaloyl-4-phenylpentan-1-amine (1w)[19]**

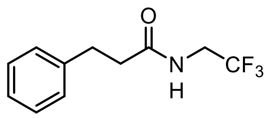


1w

(4-Bromopentyl)benzene (0.639 g, 3 mmol) and potassium phthalimide (0.556 g, 3 mmol) were then dissolved in 20 mL DMF. With stirring, the solution was heated for 15 hours. After filtration, the mixture was washed with 50 mL brine and was extracted with 50 mL Et_2O. The solution was dried over Na_2SO_4 and removal of the solvent with evaporation. The product was purified by silica column chromatography (20% EtOAc in hexanes) or Biotage flash chromatography to afford *N*-Phthaloyl-4-phenylpentan-1-amine **1w** (0.604 g, 72% yield) as an off-white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 – 7.78 (m, 2H), 7.76 – 7.60 (m, 2H), 7.30 – 7.21 (m, 2H), 7.21 – 7.09 (m, 3H), 3.71 (t, J = 6.9 Hz, 2H), 2.66 (t, J = 7.3 Hz, 2H), 1.86 – 1.59 (m, 4H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 168.5, 142.1, 134.0, 132.3, 128.5, 128.4, 125.9, 123.3, 37.9, 35.5, 28.8, 28.3.
TLC: R_f = 0.25, 30% EtOAc in hexanes.

3-Phenyl-*N*-(2,2,2-trifluoroethyl)butanamide (1z)

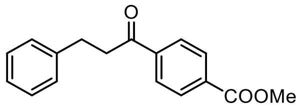


1z

To a round-bottom flask with a stir bar was added 3-Phenylpropanoic acid (0.751 g, 5.00 mmol, 1.0 equiv) and DCM (17 mL, 0.3 M). *N*, *N*-Dimethylformamide (19.4 µL; 0.25 mmol, 0.05 equiv) was added at rt. Oxalyl chloride (643 µL; 7.5 mmol, 1.50 equiv) was added dropwise. The reaction was stirred at room temperature until bubbling stopped. Without transferring from the reaction flask, volatile components were removed by rotary evaporation and high vacuum. The crude reaction product was dissolved in DCM (17 mL, 0.3 M) and stirred. 2,2,2-Trifluoroethylamine hydrochloride (1.02 g, 7.5 mmol, 1.5 equiv), followed by triethylamine (1.39 mL, 10 mmol, 2.0 equiv), were added at room temperature, and the reaction was stirred for 3 hours. The reaction mixture was then diluted with EtOAc and washed with water. Thre organic layer was concentrated under vacuum. The amide was purified by silica column chromatography (20% EtOAc in hexanes) to provide 3-Phenyl-*N*-(2,2,2-trifluoroethyl)-butanamide **1y** (1.09 g, 94% yield) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.24 (m, 2H), 7.25 – 7.14 (m, 3H), 5.53 (br, 1H), 3.88 (qd, *J* = 9.1, 6.6 Hz, 2H), 2.99 (t, *J* = 7.6 Hz, 2H), 2.56 (t, *J* = 7.6 Hz, 2H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 172.8, 140.4, 128.7, 128.3, 126.5, 124.1 (q, *J* = 278.5 Hz), 40.6 (q, *J* = 34.7 Hz), 38.0, 31.4.
^{19}F NMR (376 MHz, $CDCl_3$) δ -72.59 (t, *J* = 9.1 Hz).
HRMS (ESI): Calcd. for $C_{11}H_{13}ONF_3$ $[M+H]^+$, 232.0944. Found: 232.0941.
TLC: R_f = 0.15, 30% EtOAc in hexanes.

Methyl-4-(3-phenylbutanoyl)benzoate (1bb)[20]

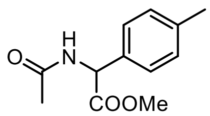


1bb

In a glovebox, to a stirred solution of methyl-4-(1-hydroxyallyl)benzoate (721 mg, 3.75 mmol, 1.25 equiv) in CH_3CN (1.88 mL, 2 M) were added the iodobenzene (334 μL, 3 mmol, 1 equiv), triethylamine (523 μL, 3.75 mmol, 1.25 equiv), and $Pd(OAc)_2$ (6.7 mg, 0.03 mmol, 0.01 equiv). The reaction was capped and removed from the glovebox. The mixture was heated at 100 °C After 24 hours, the mixture was diluted with diethyl ether, passed through a small plug of silica gel and eluted with diethyl ether. The solvent was removed *in vacuo*, and the residue was purified by column chromatography (20% EtOAc in hexanes) to provide methyl-4-(3-phenylbutanoyl)benzoate **(1bb)** (0.635 g, 79% yield) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, *J* = 8.5 Hz, 2H), 8.00 (d, *J* = 8.5 Hz, 2H), 7.42 – 7.07 (m, 5H), 3.95 (s, 3H), 3.33 (t, *J* = 7.6 Hz, 2H), 3.08 (t, *J* = 7.6 Hz, 2H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 198.8, 166.3, 141.1, 140.2, 134.0, 121.0, 128.7, 128.5, 128.1, 126.4, 52.6, 41.0, 30.1.
TLC: R_f = 0.20, 20% EtOAc in hexanes.

2-Acetamido-2-(*p*-tolyl)acetate methylester (7-SM)[21]



7-SM

To a round-bottom flask with a stir bar was added 4-methyl-DL-phenylalanine (1.98 g, 12.0 mmol, 1.0 equiv) and methanol (40 mL) was added. Thionyl chloride (1.31 mL, 18.0 mmol, 1.5 equiv) was added dropwise at 0 °C. After 10 min, the reaction mixture was heated to 75 °C for 2 h. After completion (monitored by TLC), the solvent was removed *in vacuo*. Then the white solid was formed 4-methyl-DL-phenylglycine methylester hydrochloride (2.41 g, 93% yield). To a solution of 4-methyl-DL-phenylglycine methylester hydrochloride (1.0 equiv, 2.16 g, 10 mmol) and $NaHCO_3$ (2.5 equiv, 2.10 g, 25 mmol) in H_2O (20 mL) was added Ac_2O (1.0 equiv, 0.95 mL, 10 mmol) dropwise at 0 °C. After stirring for 3 h at room temperature, the resulting mixture was filtrated. The filtrate was concentrated *in vacuo* and the residue was purified by column chromatography (30% EtOAc in hexanes) to provide 2-acetamido-2-(*p*-tolyl)acetate methylester **(7-SM)** (1.83 g, 83% yield) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24 (d, J = 8.2 Hz, 2H), 7.17 (d, J = 7.9 Hz, 2H), 6.38 (s, 1H), 5.55 (d, J = 7.2 Hz, 1H), 3.72 (s, 3H), 2.34 (s, 3H), 2.03 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 171.8, 169.4, 138.6, 133.7, 129.8, 127.3, 56.3, 52.9, 23.2, 21.3.
HRMS (ESI): Calcd. for $C_{12}H_{15}O_3NNa$ $[M+Na]^+$, 244.0944. Found: 244.0945.
TLC: R_f = 0.18, 40% EtOAc in hexanes.

Experimental Procedures and Characterization.

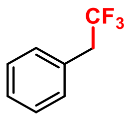
Benzylic C–H Trifluoromethylation. **General Procedure A**

In a N_2 glovebox, to a 6.0 mL screw-cap test tube equipped with a stir bar was added $(NH_4)_2S_2O_8$ (205 mg, 0.900 mmol, 3.0 equiv), bpyCu$(CF_3)_3$ (128 mg, 0.300 mmol, 1.0 equiv) and the reaction substrate (0.600 mmol, 2.0 equiv) (if solid). Acetone (1.50 mL) and the reaction substrate (0.600 mmol, 2.0 equiv) (if liquid) were added via syringe, followed by *i*-Pr_3SiH (185 μL, 0.900 mmol, 3.0 equiv). The tube was sealed with a PTFE lined screw cap, brought outside the glovebox. Degassed H_2O (1.50 mL) and trifluoroacetic acid (184 μL, 2.40 mmol, 8.0 equiv) were added under N_2 atmosphere. Then the reaction mixture was irradiated with a 5 W LED lamp (centered at 365 nm and placed 15-20 cm away from the reaction vial) at room temperature for 18 h. The reaction mixture was quenched with saturated aqueous $NaHCO_3$ (8 mL) and extracted 3 times with EtOAc (15.0 mL) or dichloromethane (15.0 mL). The combined organic layer was dried over $MgSO_4$. The filtrate was concentrated *in vacuo* and the residue was purified by column chromatography on silica gel to give the desired product.

Benzylic C–H Trifluoromethylation. **General Procedure B**

Procedure A wherein *t*-butyldimethylsilane (99.4 μL, 0.600 mmol, 2.0 equiv) was used instead of *i*-Pr_3SiH. $(NH_4)_2S_2O_8$ (273 mg, 1.200 mmol, 4.0 equiv) was used.

(2,2,2-Trifluoroethyl)benzene (3a)[22]

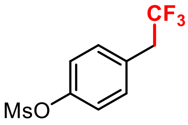


3a

Toluene **1a** (64 μL, 0.600 mmol) was subjected to General Procedure A. After the reaction mixture was quenched with saturated aqueous $NaHCO_3$ (30 mL), 1-bromo-4-fluorobenzene (20.0 μL, 0.197 mmol) and acetone-d_6 (4.0 mL) were added. The yield of (2,2,2-trifluoroethyl)benzene **3a** was determined by comparing the integration of the ^{19}F NMR (2,2,2-trifluoroethyl)benzene **3a** with that of 1-bromo-4-fluorobenzene (99% ^{19}F NMR yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 – 7.27 (m, 5H), 3.37 (q, *J* = 10.8 Hz, 2H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 130.3, 128.8, 128.2, 125.9 (q, *J* = 276.7 Hz), 40.4 (q, *J* = 29.6 Hz).
^{19}F NMR (376 MHz, $CDCl_3$) δ -66.00 (t, *J* = 10.8 Hz).
HRMS (EI): Calcd. for $C_8H_7F_3$ [M], 160.0500. Found: 160.0492.
TLC: R_f = 0.75, hexanes.

4-(2,2,2-Trifluoroethyl)phenyl methanesulfonate (3b)[23]

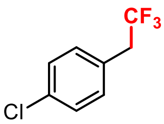


3b

p-Tolylmethanesulfonate **1b** (90.11 µL, 0.600 mmol) was subjected to General Procedure. Silica gel chromatography (Gradient: 30%-80% dichloromethane in hexanes) provided **3b** (36.7 mg, 48% yield) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (d, *J* = 8.4 Hz, 2H), 7.29 (d, *J* = 8.6 Hz, 2H), 3.39 (q, *J* = 10.7 Hz, 2H), 3.16 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 149.2, 132.0, 129.7 (q, *J* = 2.9 Hz), 125.6 (q, *J* = 276.9 Hz), 122.4, 39.7 (q, *J* = 30.1 Hz), 37.6.
^{19}F NMR (376 MHz, $CDCl_3$) δ -65.97 (t, *J* = 10.6 Hz).
HRMS (ESI): Calcd. for $C_9H_{10}O_3F_3S$ $[M+H]^+$, 255.0297. Found: 255.0297.
TLC: R_f = 0.20, 40% dichloromethane in hexanes.

1-Chloro-4-(2,2,2-trifluoroethyl)benzene (3c)[24]

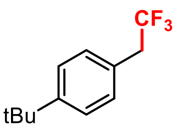


3c

1-Chloro-4-methylbenzene **1c** (70.98 µL, 0.600 mmol) was subjected to General Procedure A. Silica gel chromatography (*n*-pentane) provided **3c** (42.0 mg, 72% yield) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 (d, *J* = 8.4 Hz, 2H), 7.23 (d, *J* = 8.2 Hz, 2H), 3.34 (q, *J* = 10.7 Hz, 2H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 134.4, 131.6, 129.1, 128.7, 125.6 (q, *J* = 276.7 Hz), 39.8 (q, *J* = 30.0 Hz).
^{19}F NMR (376 MHz, $CDCl_3$) δ -66.11 (t, *J* = 10.7 Hz).
HRMS (EI): Calcd. for $C_8H_6ClF_3$ [M], 194.0110. Found: 194.0102.
TLC: R_f = 0.60, hexanes.

1-(*Tert*-butyl)-4-(2,2,2-trifluoroethyl)benzene (3d)[25]

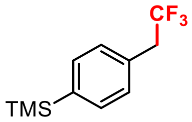


3d

1-(*t*-Butyl)-4-methylbenzene **1d** (103.43 µL, 0.600 mmol) was subjected to General Procedure A. Silica gel chromatography (*n*-pentane) provided **3d** (57.3 mg, 88% yield) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (d, *J* = 8.3 Hz, 2H), 7.23 (d, *J* = 8.1 Hz, 2H), 3.95 – 2.37 (m, 2H), 1.32 (s, 9H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 151.2, 130.0, 127.3 (q, *J* = 2.9 Hz), 126.0 (q, *J* = 276.8 Hz), 125.8, 39.9 (q, *J* = 29.6 Hz), 34.7, 31.5.
^{19}F NMR (376 MHz, $CDCl_3$) δ -66.01 (t, *J* = 10.9 Hz).
TLC: R_f = 0.60, hexanes.

Trimethyl(4-(2,2,2-trifluoroethyl)phenyl)silane (3e)

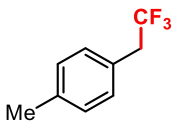


3e

Trimethyl(*p*-tolyl)silane **1e** (113.32 µL, 0.600 mmol) was subjected to General Procedure A. Silica gel chromatography (*n*-pentane) provided **3e** (28.1 mg, 40% yield) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 8.0 Hz, 2H), 7.28 (d, *J* = 7.6 Hz, 2H), 3.36 (q, *J* = 10.8 Hz, 2H), 0.27 (s, 9H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 140.6, 133.8, 130.7 (q, *J* = 2.9 Hz), 129.6, 125.9 (q, *J* = 276.9 Hz), 40.4 (q, *J* = 29.6 Hz), -1.0.
^{19}F NMR (376 MHz, $CDCl_3$) δ -65.84 (t, *J* = 10.9 Hz).
HRMS (EI): Calcd. for $C_{11}H_{15}F_3Si$ [M], 232.0895. Found: 232.0887.
TLC: R_f = 0.70, hexanes.

1-Methyl-4-(2,2,2-trifluoroethyl)benzene (3f)[24]

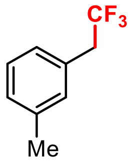


3f

p-Xylene **1f** (73.9 µL, 0.600 mmol) was subjected to General Procedure A. After the reaction mixture was quenched with saturated aqueous $NaHCO_3$ (30 mL), 1-bromo-4-fluorobenzene (20.0 µL, 0.197 mmol) and acetone-d_6 (4.0 mL) were added. The yield of 1-methyl-4-(2,2,2-trifluoroethyl)benzene **3f** was determined by comparing the integration of the ^{19}F NMR 1-methyl-4-(2,2,2-trifluoroethyl)benzene **3f** with that of 1-bromo-4-fluorobenzene (99% ^{19}F NMR yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24 – 7.06 (m, 4H), 3.32 (q, *J* = 10.9 Hz, 2H), 2.35 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 138.0, 130.2, 129.5, 127.3 (q, *J* = 2.9 Hz), 126.0 (q, *J* = 276.7 Hz), 39.98 (q, *J* = 29.6 Hz), 21.24.
^{19}F NMR (376 MHz, $CDCl_3$) δ -66.17 (t, *J* = 10.9 Hz).
HRMS (EI): Calcd. for $C_9H_9F_3$ [M], 174.0656. Found: 174.0648.
TLC: R_f = 0.70, hexanes.

1-Methyl-3-(2,2,2-trifluoroethyl)benzene (3g)

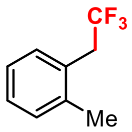


3g

m-Xylene **1g** (73.9 µL, 0.600 mmol) was subjected to General Procedure A. After the reaction mixture was quenched with saturated aqueous $NaHCO_3$ (30 mL), 1-bromo-4-fluorobenzene (20.0 µL, 0.197 mmol) and acetone-d_6 (4.0 mL) were added. The yield of 1-methyl-3-(2,2,2-trifluoroethyl)benzene **3g** was determined by comparing the integration of the ^{19}F NMR 1-methyl-3-(2,2,2-trifluoroethyl)benzene **3g** with that of 1-bromo-4-fluorobenzene (99% ^{19}F NMR yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 – 7.20 (m, 1H), 7.15 (d, J = 7.7 Hz, 1H), 7.12 – 7.05 (m, 2H), 3.33 (q, J = 10.9 Hz, 2H), 2.36 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 138.5, 131.0, 130.2, 129.0, 128.7, 127.3, 126.0 (q, J = 276.8 Hz), 40.3 (q, J = 29.6 Hz), 21.5.
^{19}F NMR (376 MHz, $CDCl_3$) δ -65.93 (t, J = 10.9 Hz).
HRMS (EI): Calcd. for $C_9H_9F_3$ [M], 174.0656. Found: 174.0655.
TLC: R_f = 0.70, hexanes.

1-Methyl-2-(2,2,2-trifluoroethyl)benzene (3h)

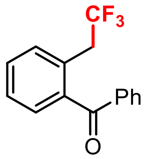


3h

o-Xylene **1h** (73 µL, 0.600 mmol) was subjected to General Procedure A. After the reaction mixture was quenched with saturated aqueous $NaHCO_3$ (30 mL), 1-bromo-4-fluorobenzene (20.0 µL, 0.197 mmol) and acetone-d_6 (4.0 mL) were added. The yield of 1-methyl-2-(2,2,2-trifluoroethyl)benzene **3h** was determined by comparing the integration of the ^{19}F NMR 1-methyl-2-(2,2,2-trifluoroethyl)benzene **3h** with that of 1-bromo-4-fluorobenzene (93% ^{19}F NMR yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 – 7.15 (m, 4H), 3.41 (q, J = 10.8 Hz, 2H), 2.37 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 137.7, 131.3, 130.8, 128.8 (q, J = 2.7 Hz), 128.4, 126.3 (q, J = 277.2 Hz), 126.3, 37.3 (q, J = 29.6 Hz), 19.8.
^{19}F NMR (376 MHz, $CDCl_3$) δ -65.33 (t, J = 10.8 Hz).
HRMS (EI): Calcd. for $C_9H_9F_3$ [M], 174.0656. Found: 174.0649.
TLC: R_f = 0.50, hexanes.

Phenyl(2-(2,2,2-trifluoroethyl)phenyl)methanone (3i)[26]

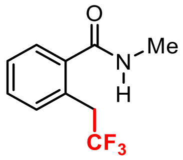


3i

Phenyl(*o*-tolyl)methanone **1i** (106.1 μL, 0.600 mmol) was subjected to General Procedure A. Silica gel chromatography (8% EtOAc in hexanes) provided **3i** (44.7 mg, 56% yield) as a colorless solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 – 7.75 (m, 2H), 7.67 – 7.56 (m, 1H), 7.55 – 7.42 (m, 4H), 7.43 – 7.33 (m, 2H), 3.74 (q, J = 10.8 Hz, 2H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 197.9, 139.7, 137.6, 133.5, 132.6, 130.9, 130.5, 129.9, 129.7, 128.5, 127.5, 125.9 (q, J = 277.2 Hz), 36.2 (q, J = 29.8 Hz).
^{19}F NMR (376 MHz, $CDCl_3$) δ -65.19 (t, J = 10.8 Hz).
HRMS (ESI): Calcd. for $C_{15}H_{12}OF_3$ $[M+H]^+$, 265.0835. Found: 265.0835.
TLC: R_f = 0.35, 10% EtOAc in hexanes.

***N*-methyl-2-(2,2,2-trifluoroethyl)benzamide (3j)**[27]

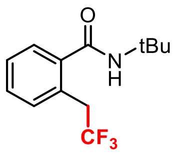


3j

N-methyl-2-methylbenzamide **1j** (89.5 mg, 0.600 mmol) was subjected to General Procedure A. Silica gel chromatography (20% EtOAc in hexanes) provided **3j** (44.9 mg, 69% yield) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 – 7.30 (m, 4H), 5.88 (s, 1H), 3.79 (q, J = 11.0 Hz, 2H), 2.99 (d, J = 4.9 Hz, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 170.3, 137.7, 132.4, 130.3, 128.9 (q, J = 2.9 Hz), 128.3, 127.2, 126.0 (q, J = 277.1 Hz), 36.4 (q, J = 29.7 Hz), 26.8.
^{19}F NMR (376 MHz, $CDCl_3$) δ -65.38 (t, J = 11.0 Hz).
HRMS (ESI): Calcd. for $C_{10}H_{10}ONF_3Na$ $[M+Na]^+$, 240.0607. Found: 240.0608.
TLC: R_f = 0.20, 30% EtOAc in hexanes.

***N*-(*tert*-butyl)-2-(2,2,2-trifluoroethyl)benzamide (3k)**[27]

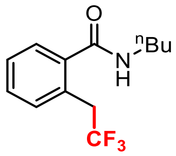


3k

N-(*tert*-butyl)-2-methylbenzamide **1k** (114.8 mg, 0.600 mmol) was subjected to General Procedure A. Silica gel chromatography (15% EtOAc in hexanes) provided **3k** (66.3 mg, 85% yield) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 – 7.27 (m, 4H), 5.68 (br, 1H), 3.77 (q, *J* = 11.0 Hz, 2H), 1.45 (s, 9H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 169.1, 139.0, 132.3, 129.9, 128.4 (q, *J* = 3.0 Hz), 128.3, 127.1, 126.1 (q, *J* = 277.1 Hz), 52.1, 36.2 (q, *J* = 29.7 Hz), 28.8.
^{19}F NMR (376 MHz, $CDCl_3$) δ -65.18 (t, *J* = 11.0 Hz).
HRMS (ESI): Calcd. for $C_{13}H_{17}ONF_3$ $[M+H]^+$, 260.1257. Found: 260.1259.
TLC: R_f = 0.25, 15% EtOAc in hexanes.

_N_-butyl-2-(2,2,2-trifluoroethyl)benzamide (3l)[27]

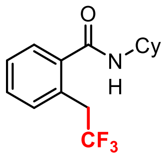


3l

N-butyl-2-methylbenzamide **1l** (114.8 mg, 0.600 mmol) was subjected to General Procedure A. Silica gel chromatography (15% EtOAc in hexanes) provided **3l** (59.1 mg, 76% yield) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 – 7.30 (m, 4H), 5.85 (br, 1H), 3.81 (q, *J* = 11.0 Hz, 2H), 3.45 (dd, *J* = 13.1, 7.1 Hz, 2H), 1.69 – 1.53 (m, 2H), 1.50 – 1.33 (m, 2H), 0.98 (t, *J* = 7.3 Hz, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 169.6, 138.0, 132.4, 130.2, 128.8, 128.3, 127.2, 126.0 (q, *J* = 277.1 Hz), 39.8, 36.3 (q, *J* = 29.6 Hz), 31.7, 20.2, 13.8.
^{19}F NMR (376 MHz, $CDCl_3$) δ -65.30 (t, *J* = 11.0 Hz).
HRMS (ESI): Calcd. for $C_{13}H_{16}ONF_3Na$ $[M+Na]^+$, 282.1076. Found: 282.1078.
TLC: R_f = 0.25, 15% EtOAc in hexanes.

_N_-cyclohexyl-2-(2,2,2-trifluoroethyl)benzamide (3m)[27]

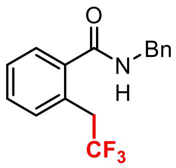


3m

N-cyclohexyl-2-methylbenzamide **1m** (130.4 mg, 0.600 mmol) was subjected to General Procedure A. Silica gel chromatography (15% EtOAc in hexanes) provided **3m** (76.9 mg, 90% yield) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 – 7.39 (m, 2H), 7.36 (d, *J* = 6.5 Hz, 2H), 5.71 (br, 1H), 4.04 – 3.88 (m, 1H), 3.78 (q, *J* = 11.0 Hz, 2H), 2.03 (d, *J* = 9.9 Hz, 2H), 1.83 – 1.69 (m, 2H), 1.71 – 1.60 (m, 1H), 1.51 – 1.34 (m, 2H), 1.33 – 1.09 (m, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 168.7, 138.2, 132.4, 130.1, 128.7 (q, *J* = 2.9 Hz), 128.3, 127.2, 126.1 (q, *J* = 277.1 Hz), 48.8, 36.4 (q, *J* = 29.7 Hz), 33.1, 25.6, 25.0.
^{19}F NMR (376 MHz, $CDCl_3$) δ -65.20 (t, *J* = 11.0 Hz).
HRMS (ESI): Calcd. for $C_{15}H_{18}ONF_3Na$ $[M+Na]^+$, 308.1233. Found: 308.1236.
TLC: R_f = 0.25, 20% EtOAc in hexanes.

_N_-benzyl-2-(2,2,2-trifluoroethyl)benzamide (3n)[27]

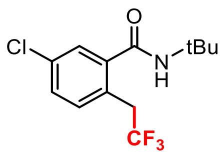


3n

N-benzyl-2-methylbenzamide **1n** (135.2 mg, 0.600 mmol) was subjected to General Procedure A. Silica gel chromatography (Gradient: 5%-30% EtOAc in hexanes) provided **3n** (42.1 mg, 48% yield) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 – 7.28 (m, 9H), 6.14 (br, 1H), 4.62 (d, *J* = 5.7 Hz, 2H), 3.84 (q, *J* = 11.0 Hz, 2H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 169.3, 137.9, 137.4, 132.6, 130.5, 129.1, 129.0, 128.4, 128.1, 127.9, 127.3, 126.1 (q, *J* = 276.8 Hz), 44.3, 36.4 (q, *J* = 29.7 Hz).
^{19}F NMR (376 MHz, $CDCl_3$) δ -65.24 (t, *J* = 11.0 Hz).
HRMS (ESI): Calcd. for $C_{16}H_{14}ONF_3Na$ $[M+Na]^+$, 316.0920. Found: 316.0922.
TLC: R_f = 0.35, 30% EtOAc in hexanes.

_N_-(_tert_-butyl)-5-chloro-2-(2,2,2-trifluoroethyl)benzamide (3o)



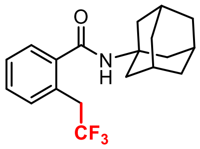
3o

N-(*tert*-butyl)-5-chloro-2-methylbenzamide **1o** (135.4 mg, 0.600 mmol) was subjected to General Procedure A. Silica gel chromatography (10% EtOAc in hexanes) provided **3o** (52.9 mg, 60% yield) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (s, 1H), 7.37 – 7.26 (m, 2H), 5.67 (br, 1H), 3.72 (q, *J* = 10.9 Hz, 2H), 1.45 (s, 9H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 167.6, 140.3, 134.3, 133.6, 129.9, 127.4, 126.9 (q, *J* = 3.0 Hz), 125.8 (q, *J* = 277.2 Hz), 52.4, 35.7 (q, *J* = 30.0 Hz), 28.7.
^{19}F NMR (376 MHz, $CDCl_3$) δ -65.28 (t, *J* = 10.9 Hz).
HRMS (ESI): Calcd. for $C_{13}H_{16}ONClF_3$ $[M+H]^+$, 294.0867. Found: 294.0874.

TLC: R_f = 0.30, 15% EtOAc in hexanes.

***N*-1-adamantyl-2-(2,2,2-trifluoroethyl)benzamide (3p)**[27]

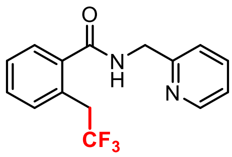


3p

N-1-adamantyl-2-methylbenzamide **1p** (161.6 mg, 0.600 mmol) was subjected to General Procedure A. Silica gel chromatography (3% EtOAc/30% dichloromethane in hexanes)provided **3p** (57.9 mg, 57% yield) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 – 7.28 (m, 4H), 5.52 (br, 1H), 3.77 (q, *J* = 11.0 Hz, 2H), 2.11 (s, 9H), 1.81 – 1.63 (m, 6H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 168.9, 139.1, 132.3, 129.9, 128.4 (q, *J* = 2.8 Hz), 128.3, 127.2, 126.1 (q, *J* = 277.3 Hz), 52.9, 41.6, 36.5, 36.3 (q, *J* = 29.7 Hz), 29.6.
^{19}F NMR (376 MHz, $CDCl_3$) δ -65.02 (t, *J* = 11.0 Hz).
HRMS (ESI): Calcd. for $C_{19}H_{23}ONF_3$ $[M+H]^+$, 338.1726. Found: 338.1730.
TLC: R_f = 0.18, 40% dichloromethane in hexanes.

***N*-(pyridin-2-ylmethyl)-2-(2,2,2-trifluoroethyl)benzamide (3q)**

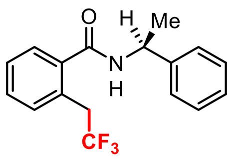


3q

2-Methyl-*N*-(pyridin-2-ylmethyl)benzamide **1q** (135.8 mg, 0.600 mmol) was subjected to General Procedure A. Silica gel chromatography (30% EtOAc in hexanes) provided **3q** (33.7 mg, 38% yield) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 (d, *J* = 4.5 Hz, 1H), 7.82 – 7.63 (m, 1H), 7.59 – 7.54 (m, 1H), 7.49 – 7.35 (m, 3H), 7.33 (d, *J* = 7.8 Hz, 1H), 7.26 – 7.17 (m, 2H), 4.74 (d, *J* = 4.9 Hz, 2H), 3.86 (q, *J* = 11.0 Hz, 2H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 169.5, 156.0, 149.2, 137.4, 137.00, 132.4, 130.4, 129.2 (q, *J* = 3.0 Hz), 128.4, 127.6, 126.1 (q, *J* = 277.3 Hz), 122.6, 122.3, 44.9, 36.4 (q, *J* = 29.7 Hz).
^{19}F NMR (376 MHz, $CDCl_3$) δ -65.24 (t, *J* = 11.0 Hz).
HRMS (ESI): Calcd. for $C_{15}H_{13}ON_2F_3Na$ $[M+Na]^+$, 317.0872. Found: 317.0875.
TLC: R_f = 0.20, 40% EtOAc in hexanes.

(*S*)-*N*-(1-phenylethyl)-2-(2,2,2-trifluoroethyl)benzamide (3r)[27]

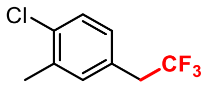


3r

(S)-2-methyl-N-(1-phenylethyl)benzamide **1r** (143.6 mg, 0.600 mmol) was subjected to General Procedure A. Silica gel chromatography (20% EtOAc in hexanes) provided **3r** (59.8 mg, 65% yield) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 – 7.27 (m, 9H), 6.09 (d, J = 7.4 Hz, 1H), 5.44 – 5.21 (m, 1H), 4.02 – 3.79 (m, 1H), 3.77 – 3.56 (m, 1H), 1.60 (d, J = 6.9 Hz, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 168.6, 142.8, 137.6, 132.4, 130.3, 128.9, 128.3, 127.7, 127.3, 126.3, 126.0 (q, J = 277.2 Hz), 49.4, 36.3 (q, J = 29.7 Hz), 21.6.
^{19}F NMR (376 MHz, $CDCl_3$) δ -65.20 (t, J = 11.0 Hz).
HRMS (ESI): Calcd. for $C_{17}H_{16}ONF_3Na$ $[M+Na]^+$, 330.1076. Found: 330.1079.
TLC: R_f = 0.25, 20% EtOAc in hexanes.

1-Chloro-2-methyl-4-(2,2,2-trifluoroethyl)benzene (3s)

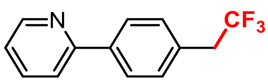


3s

1-Chloro-2,4-dimethylbenzene **1s** (84.4 mg, 0.600 mmol) was subjected to General Procedure A. Silica gel chromatography (*n*-pentane) provided **3s** (28.1 mg, 45% yield) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (d, J = 8.1 Hz, 1H), 7.15 (s, 1H), 7.06 (d, J = 8.1 Hz, 1H), 3.31 (q, J = 10.7 Hz, 2H), 2.38 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 136.6, 134.5, 132.8, 129.5, 128.9, 128.7 (q, J = 2.9 Hz), 125.7 (q, J = 276.7 Hz), 39.8 (q, J = 29.9 Hz), 20.2.
^{19}F NMR (376 MHz, $CDCl_3$) δ -66.04 (t, J = 10.7 Hz).
HRMS (EI): Calcd. for $C_9H_8ClF_3$ [M], 208.0267. Found: 208.0260.
TLC: R_f = 0.5, hexanes.

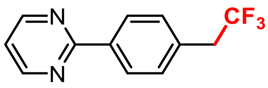
2-(4-(2,2,2-Trifluoroethyl)phenyl)pyridine (3t)



3t

2-(p-Tolyl)pyridine **1t** (101.5 mg, 0.600 mmol) was subjected to General Procedure A. Silica gel chromatography (20% EtOAc in hexanes) provided **3t** (17.3 mg, 24% yield) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.70 (d, J = 4.7 Hz, 1H), 7.99 (d, J = 8.3 Hz, 2H), 7.84 – 7.67 (m, 2H), 7.41 (d, J = 8.1 Hz, 2H), 7.27 – 7.17 (m, 1H), 3.43 (q, J = 10.8 Hz, 2H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 157.0, 149.9, 139.4, 136.9, 131.0 (q, J = 2.9 Hz), 130.7, 127.3, 125.9 (q, J = 276.9 Hz), 122.5, 120.7, 40.2 (q, J = 29.8 Hz).
^{19}F NMR (376 MHz, $CDCl_3$) δ -65.83 (t, J = 10.8 Hz).
HRMS (ESI): Calcd. for $C_{13}H_{11}F_3N$ $[M+H]^+$, 238.0838. Found: 238.0840.
TLC: R_f = 0.25, 30% EtOAc in hexanes.

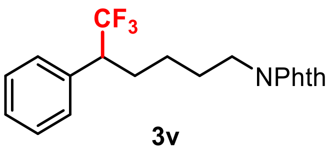


3u

2-(*p*-Tolyl)pyrimidine **1u** (102.1 mg, 0.600 mmol) was subjected to General Procedure A. Silica gel chromatography (25% EtOAc in hexanes) provided **3u** (40.7 mg, 57% yield) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.82 (d, *J* = 4.8 Hz, 2H), 8.44 (d, *J* = 8.3 Hz, 2H), 7.43 (d, *J* = 8.1 Hz, 2H), 7.21 (t, *J* = 4.8 Hz, 1H), 3.45 (q, *J* = 10.8 Hz, 2H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 164.4, 157.4, 137.6, 132.9 (q, *J* = 2.9 Hz), 130.6, 128.6, 125.8 (q, *J* = 276.9 Hz), 119.4, 40.3 (q, *J* = 29.8 Hz).
^{19}F NMR (376 MHz, $CDCl_3$) δ -65.70 (t, *J* = 10.8 Hz).
HRMS (EI): Calcd. for $C_{12}H_9F_3N_2$ [M], 238.0718. Found: 238.0714.
TLC: R_f = 0.30, 30% EtOAc in hexanes.

_N_-Phthaloyl-6,6,6-trifluoro-5-phenylhexan-1-amine (3v)

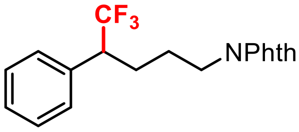


3v

N-Phthaloyl-5-phenylhexan-1-amine **1v** (88.3 mg, 0.600 mmol) was subjected to General Procedure B. Silica gel chromatography (15% EtOAc in hexanes) provided **3v** (32.4 mg, 50% yield) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 – 7.77 (m, 2H), 7.73 – 7.64 (m, 2H), 7.33 – 7.20 (m, 5H), 3.59 (t, *J* = 7.3 Hz, 2H), 3.32 – 3.09 (m, 1H), 2.11 – 1.96 (m, 1H), 1.96 – 1.79 (m, 1H), 1.78 – 1.55 (m, 2H), 1.30 – 1.13 (m, 2H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 168.5, 134.7, 134.0, 132.2, 129.1, 128.8, 128.3, 127.0 (q, *J* = 279.9 Hz), 123.3, 50.1 (q, *J* = 26.5 Hz), 37.6, 28.3 (q, *J* = 2.0 Hz), 28.2, 24.1.
^{19}F NMR (376 MHz, $CDCl_3$) δ -69.81 (d, *J* = 9.3 Hz).
HRMS (ESI): Calcd. for $C_{20}H_{19}O_2NF_3$ $[M+H]^+$, 362.1362. Found: 362.1361.
TLC: R_f = 0.30, 20% EtOAc in hexanes.

_N_-Phthaloyl-5,5,5-trifluoro-4-phenylpentan-1-amine (3w)[28]

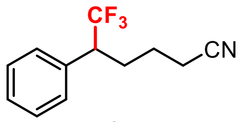


3w

N-Phthaloyl-4-phenylpentan-1-amine **1w** (79.9 mg, 0.600 mmol) was subjected to General Procedure B. Silica gel chromatography (15% EtOAc in hexanes) provided **3w** (24.8 mg, 41% yield) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 – 7.80 (m, 2H), 7.74 – 7.68 (m, 2H), 7.39 – 7.26 (m, 5H), 3.65 (t, J = 7.1 Hz, 2H), 3.39 – 3.11 (m, 1H), 2.11 – 1.98 (m, 1H), 1.98 – 1.85 (m, 1H), 1.67 – 1.48 (m, 2H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 168.4, 134.4, 134.1, 132.2, 129.1, 128.9, 128.4, 126.9 (q, J = 280.0 Hz), 123.4, 49.8 (q, J = 26.7 Hz), 37.5, 26.1 (q, J = 2.2 Hz), 26.0.
^{19}F NMR (376 MHz, $CDCl_3$) δ -69.76 (d, J = 9.2 Hz).
HRMS (ESI): Calcd. for $C_{19}H_{17}O_2NF_3$ $[M+H]^+$, 348.1206. Found: 348.1206.
TLC: R_f = 0.30, 20% EtOAc in hexanes.

6,6,6-Trifluoro-5-phenylhexanenitrile (3x)

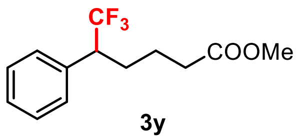


3x

5-Phenylpentanenitrile **1x** (96 mg, 0.600 mmol) was subjected to General Procedure B. Silica gel chromatography (10% EtOAc in hexanes) provided **3x** (43.3 mg, 64% yield) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 – 7.26 (m, 5H), 3.40 – 3.08 (m, 1H), 2.32 (t, J = 7.1 Hz, 2H), 2.23 – 2.11 (m, 1H), 2.10 – 1.98 (m, 1H), 1.70 – 1.46 (m, 2H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 133.9, 129.1, 129.0, 128.7, 126.7 (q, J = 280.0 Hz), 119.0, 49.8 (q, J = 27.0 Hz), 28.0 (q, J = 2.2 Hz), 23.0, 17.2.
^{19}F NMR (376 MHz, $CDCl_3$) δ -69.87 (d, J = 9.1 Hz).
HRMS (EI): Calcd. for $C_{12}H_{12}F_3N$ [M], 227.0924. Found: 227.0919.
TLC: R_f = 0.25, 10% EtOAc in hexanes.

Methyl-6,6,6-trifluoro-5-phenylhexanoate (3y)

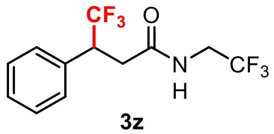


3y

Methyl-5-phenylpentanoate **1y** (115.4 mg, 0.600 mmol) was subjected to General Procedure B. Silica gel chromatography (10% EtOAc in hexanes) provided **3y** (33.4 mg, 43% yield) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.26 (m, 5H), 3.64 (s, 3H), 3.34 – 3.12 (m, 1H), 2.29 (td, J = 7.4, 3.2 Hz, 2H), 2.09 – 1.98 (m, 1H), 1.97 – 1.86 (m, 1H), 1.55 – 1.47 (m, 2H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 173.5, 134.5, 129.1, 128.9, 128.4, 126.9 (q, J = 279.9 Hz), 51.7, 50.1 (q, J = 26.6 Hz), 33.7, 28.3 (q, J = 2.2 Hz), 22.4.
^{19}F NMR (376 MHz, $CDCl_3$) δ -69.89 (d, J = 9.2 Hz).
HRMS (EI): Calcd. for $C_{13}H_{14}F_2O_2$ [M-HF], 240.0962. Found: 240.0959.
TLC: R_f = 0.15, 20% EtOAc in hexanes.

4,4,4-Trifluoro-3-phenyl-*N*-(2,2,2-trifluoroethyl)butanamide (3z)

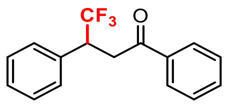


3z

3-Phenyl-*N*-(2,2,2-trifluoroethyl)propanamide **1z** (138 mg, 0.600 mmol) was subjected to General Procedure A. Silica gel chromatography (25% EtOAc in hexanes) provided **3z** (57.2 mg, 64% yield) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 – 7.25 (m, 5H), 5.54 (br, 1H), 4.18 – 3.92 (m, 1H), 3.91 – 3.66 (m, 2H), 2.99 (dd, *J* = 15.0, 4.9 Hz, 1H), 2.73 (dd, *J* = 15.0, 9.6 Hz, 1H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 169.6, 133.8, 129.0 (q, *J* = 12.8 Hz), 128.8, 128.8, 126.3 (q, *J* = 343.8 Hz), 123.9 (q, *J* = 278.4 Hz), 46.4 (q, *J* = 27.8 Hz), 40.8 (q, *J* = 34.9 Hz), 36.5.
^{19}F NMR (376 MHz, $CDCl_3$) δ -69.99 (d, *J* = 9.3 Hz), -72.79 (t, *J* = 9.0 Hz).
HRMS (ESI): Calcd. for $C_{12}H_{11}ONF_6Na$ $[M+Na]^+$, 322.0637. Found: 322.0638.
TLC: R_f = 0.18, 30% EtOAc in hexanes.

4,4,4-Trifluoro-1,3-diphenylbutan-1-one (3aa)[29]

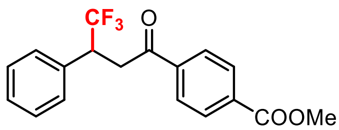


3aa

1,3-Diphenylpropan-1-one **1aa** (126.2 mg, 0.600 mmol) was subjected to General Procedure B. Silica gel chromatography (10% toluene in hexanes) provided **3aa** (35.7 mg, 43% yield) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, *J* = 7.6 Hz, 2H), 7.63 – 7.52 (m, 1H), 7.50 – 7.43 (m, 2H), 7.40 (d, *J* = 7.2 Hz, 2H), 7.37 – 7.28 (m, 3H), 4.38 – 4.10 (m, 1H), 3.70 (dd, *J* = 17.8, 9.1 Hz, 1H), 3.60 (dd, *J* = 17.8, 4.1 Hz, 1H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 195.4, 136.5, 134.7, 133.7, 129.2, 128.9, 128.8, 128.4, 128.2, 127.1 (q, *J* = 279.3 Hz), 45.0 (q, *J* = 27.5 Hz), 38.5.
^{19}F NMR (376 MHz, $CDCl_3$) δ -69.69 (d, *J* = 9.7 Hz).
HRMS (ESI): Calcd. for $C_{16}H_{14}OF_3$ $[M+H]^+$, 279.0991. Found: 279.0991.
TLC: R_f = 0.25, 10% Toluene in hexanes.

Methyl-4-(4,4,4-trifluoro-3-phenylbutanoyl)benzoate (3bb)

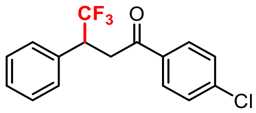


3bb

Methyl-4-(3-phenylpropanoyl)benzoate **1bb** (161 mg, 0.600 mmol) was subjected to General Procedure B. Silica gel chromatography (Gradient: 40%-100% dichloromethane in hexanes) provided **3bb** (31.9 mg, 32% yield) as a white solid.

^{1}**H NMR** (400 MHz, $CDCl_3$) δ 8.11 (d, *J* = 8.5 Hz, 2H), 7.97 (d, *J* = 8.5 Hz, 2H), 7.49 – 7.28 (m, 5H), 4.35 – 4.13 (m, 1H), 3.95 (s, 3H), 3.71 (dd, *J* = 17.9, 8.9 Hz, 1H), 3.62 (dd, *J* = 17.9, 4.3 Hz, 1H).
^{13}**C NMR** (126 MHz, $CDCl_3$) δ 195.0, 166.2, 139.6, 134.5, 134.5, 130.1, 129.1, 128.9, 128.6, 128.1, 127.0 (q, *J* = 279.4 Hz), 52.7, 45.0 (q, *J* = 27.7 Hz), 38.9.
^{19}**F NMR** (376 MHz, $CDCl_3$) δ -69.71 (d, *J* = 9.6 Hz).
HRMS (ESI): Calcd. for $C_{18}H_{16}O_3F_3$ $[M+H]^+$, 337.1046. Found: 337.1047.
TLC: R_f = 0.15, 50% Dichloromethane in hexanes.

1-(4-Chlorophenyl)-4,4,4-trifluoro-3-phenylbutan-1-one (3cc)[30]

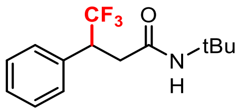


3cc

1-(4-Chlorophenyl)-3-phenylpropan-1-one **1cc** (146 mg, 0.600 mmol) was subjected to General Procedure B. Silica gel chromatography (10% toluene in hexanes) provided **3cc** (36.8 mg, 39% yield) as a white solid.

^{1}**H NMR** (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.6 Hz, 2H), 7.43 (d, *J* = 8.6 Hz, 2H), 7.41 – 7.28 (m, 5H), 4.30 – 4.15 (m, 1H), 3.65 (dd, *J* = 17.7, 9.0 Hz, 1H), 3.56 (dd, *J* = 17.8, 4.2 Hz, 1H).
^{13}**C NMR** (126 MHz, $CDCl_3$) δ 194.3, 140.3, 134.8, 134.5, 129.6 129.2, 129.1, 128.9, 128.5, 127.0 (q, *J* = 279.7 Hz), 45.0 (q, *J* = 27.5 Hz), 38.4.
^{19}**F NMR** (376 MHz, $CDCl_3$) δ -69.71 (d, *J* = 9.6 Hz).
HRMS (ESI): Calcd. for C_{16} $H_{13}OClF_3$ $[M+H]^+$, 313.0602. Found: 313.0603.
TLC: R_f = 0.20, 10% Toluene in hexanes.

***N*-(*tert*-Butyl)-4,4,4-trifluoro-3-phenylbutanamide (3dd)**

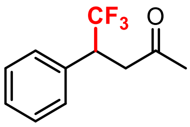


3dd

N-(*tert*-butyl)-3-phenylpropanamide **1dd** (123.1 mg, 0.600 mmol) was subjected to General Procedure A. Silica gel chromatography (10% EtOAc in hexanes) provided **3dd** (64.1 mg, 78% yield) as a white solid.

^{1}**H NMR** (400 MHz, $CDCl_3$) δ 7.52 – 7.27 (m, 5H), 5.08 (s, 1H), 4.08 – 3.74 (m, 1H), 2.81 (dd, *J* = 14.3, 5.1 Hz, 1H), 2.51 (dd, *J* = 14.3, 9.6 Hz, 1H), 1.16 (s, 9H).
^{13}**C NMR** (126 MHz, $CDCl_3$) δ 168.1, 134.4, 129.0, 128.8, 128.5, 126.9 (q, *J* = 279.7 Hz), 51.6, 46.8 (q, *J* = 27.5 Hz), 38.1, 28.6.
^{19}**F NMR** (376 MHz, $CDCl_3$) δ -69.76 (d, *J* = 9.4 Hz).
HRMS (ESI): Calcd. for $C_{14}H_{18}ONF_3Na$ $[M+Na]^+$, 296.1233. Found: 296.1234.
TLC: R_f = 0.25, 10% EtOAc in hexanes.

5,5,5-Trifluoro-4-phenylpentan-2-one (3ee)[31]

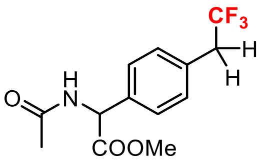


3ee

4-Phenylbutan-2-one **1ee** (90 uL, 0.600 mmol) was subjected to General Procedure B. Silica gel chromatography (Gradient: 30%-80% dichloromethane in hexanes) provided **3ee** (41.5 mg, 64% yield) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.28 (m, 5H), 4.15 – 3.88 (m, 1H), 3.20 – 2.96 (m, 2H), 2.12 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 203.8, 134.5, 129.1, 128.9, 128.5, 126.8 (q, J = 279.4 Hz), 44.7 (q, J = 27.6 Hz), 43.1, 30.5.
^{19}F NMR (376 MHz, $CDCl_3$) δ -70.03 (d, J = 9.6 Hz).
HRMS (EI): Calcd. for $C_{11}H_{11}F_3O$ [M], 216.0762. Found: 216.0761.
TLC: R_f = 0.35, 50% Dichloromethane in hexanes. (visualized with $KMnO_4$).

Methyl-2-acetamido-2-(4-(2,2,2-trifluoroethyl)phenyl)acetate (7)

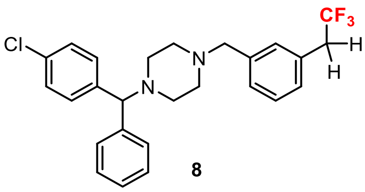


7

2-Acetamido-2-(*p*-tolyl)acetate methylester (132.8 mg, 0.600 mmol) was subjected to General Procedure A. Silica gel chromatography (30% EtOAc in hexanes) provided **7** (52.9 mg, 61% yield) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (d, J = 8.2 Hz, 2H), 7.29 (d, J = 8.1 Hz, 2H), 6.47 (d, J = 5.7 Hz, 1H), 5.60 (d, J = 7.2 Hz, 1H), 3.74 (s, 3H), 3.36 (q, J = 10.8 Hz, 2H), 2.05 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 171.4, 169.5, 136.7, 130.9, 130.7 (q, J = 2.9 Hz), 127.7, 125.7 (q, J = 276.8 Hz), 56.2, 53.1, 40.0 (q, J = 29.9 Hz), 23.2.
^{19}F NMR (376 MHz, $CDCl_3$) δ -65.85 (t, J = 10.8 Hz).
HRMS (EI): Calcd. for $C_{13}H_{14}F_3NO_3$ [M], 289.0926. Found: 289.0923.
TLC: R_f = 0.2, 40% EtOAc in hexanes.

1-((4-Chlorophenyl)(phenyl)methyl)-4-(3-(2,2,2-trifluoroethyl)benzyl)piperazine (8)



8

Meclizine (117.3 mg, 0.300 mmol, 1.0 equiv), $bpyCu(CF_3)_3$ (192 mg, 0.450 mmol, 15 equiv) and trifluoroacetic acid (230 μL, 3.00 mmol, 10.0 equiv) was subjected to General Procedure A. Silica gel chromatography (15% Acetone in hexanes) provided **8** (35.9 mg, 26% yield) as a colorless oil.

¹H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.29 (m, 4H), 7.30 – 7.14 (m, 9H), 4.21 (s, 1H), 3.51 (s, 2H), 3.34 (q, *J* = 10.8 Hz, 2H), 2.39 (d, *J* = 53.2 Hz, 8H).

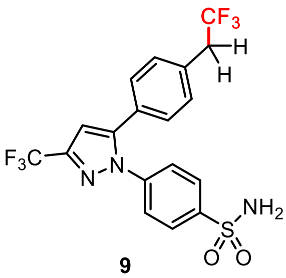
¹³C NMR (126 MHz, $CDCl_3$) δ 142.3, 141.5, 132.6, 131.0, 130.2, 129.4, 129.1, 129.0, 128.8, 128.7, 128.6, 128.0, 127.3, 125.9 (q, *J* = 276.7 Hz), 75.6, 62.9, 53.4, 51.9, 40.3 (q, *J* = 29.7 Hz).

¹⁹F NMR (376 MHz, $CDCl_3$) δ -65.94 (t, *J* = 10.9 Hz).

HRMS (ESI): Calcd. for $C_{26}H_{27}ClF_3N_2$ $[M+H]^+$, 459.1809. Found: 459.1814.

TLC: R_f = 0.25, 20% Acetone in hexanes.

4-(5-(4-(2,2,2-Trifluoroethyl)phenyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl)benzenesulfonamide (9)



9

Celecoxib (228.8 mg, 0.600 mmol) was subjected to General Procedure A. Silica gel chromatography (Gradient: 5%-40% acetone in hexanes) provided **9** (111.0 mg, 82% yield) as a white solid.

¹H NMR (400 MHz, $CDCl_3$) δ 8.39 (d, *J* = 8.6 Hz, 2H), 7.94 (d, *J* = 8.6 Hz, 2H), 7.80 (d, *J* = 8.0 Hz, 2H), 7.76 – 7.67 (m, 3H), 5.45 (s, 2H), 3.87 (q, *J* = 10.7 Hz, 2H).

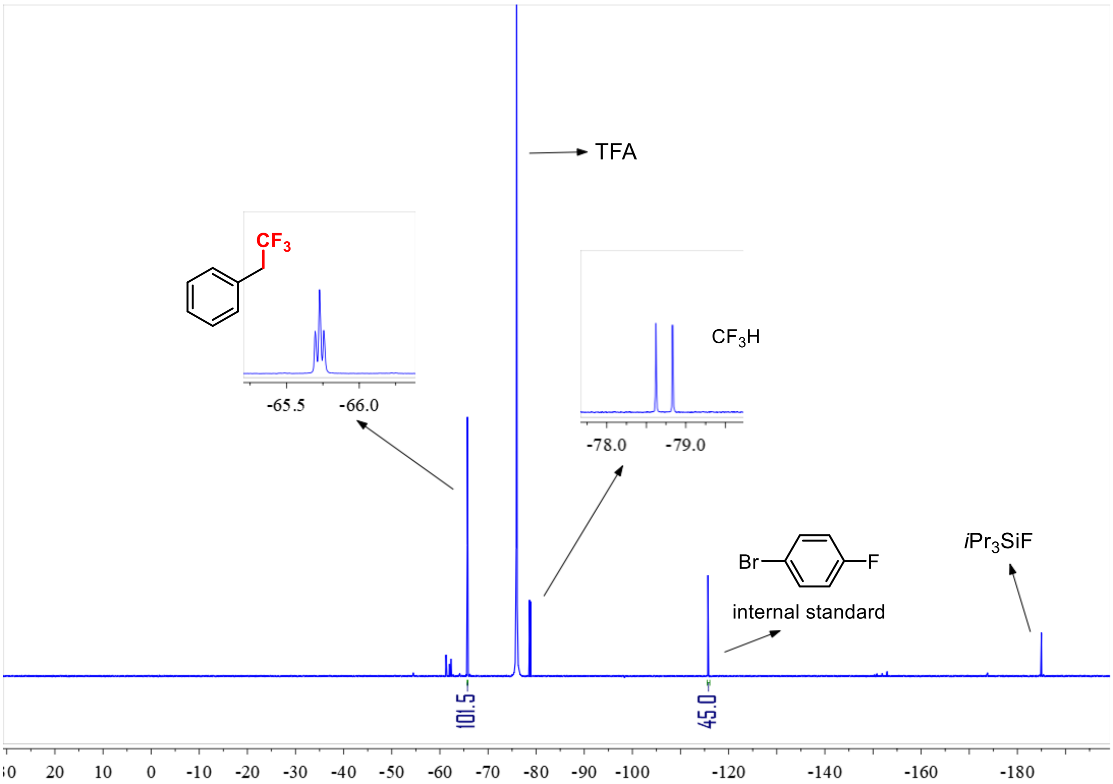
¹³C NMR (126 MHz, $CDCl_3$) δ 144.6, 144.4 (q, *J* = 38.7 Hz), 142.4, 141.8, 131.9 (q, *J* = 2.8 Hz), 131.0, 129.2, 128.6, 127.7, 125.7, 125.6 (q, *J* = 276.9 Hz), 121.1 (q, *J* = 269.3 Hz), 106.9, 40.1 (q, *J* = 30.0 Hz).

¹⁹F NMR (376 MHz, $CDCl_3$) δ -62.53 (s), -65.68 (t, *J* = 10.7 Hz).

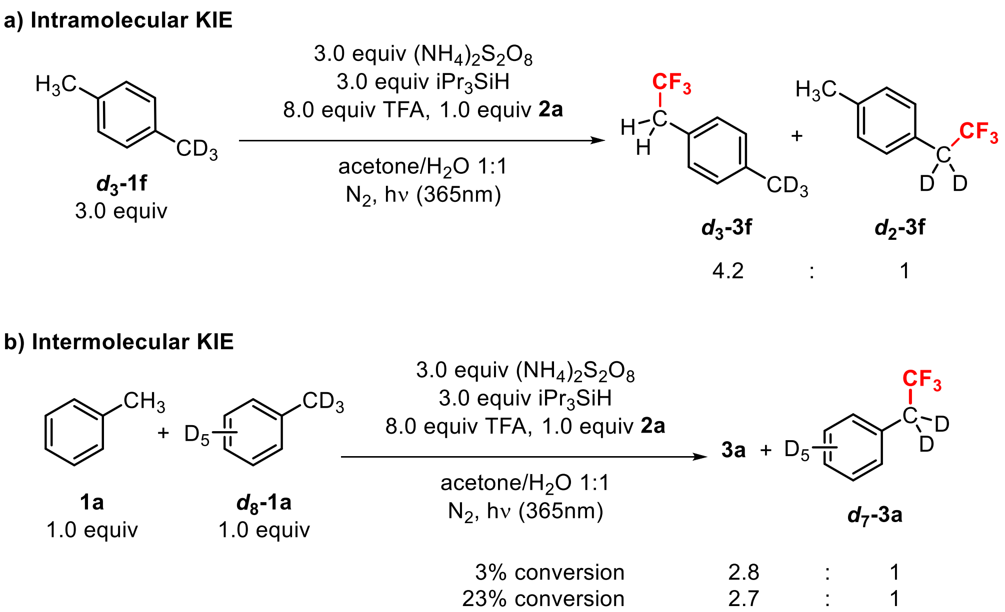
HRMS (ESI): Calcd. for $C_{18}H_{14}O_2N_3F_6S$ $[M+H]^+$, 450.0705. Found: 450.0707.

TLC: R_f = 0.30, 30% acetone in hexanes.

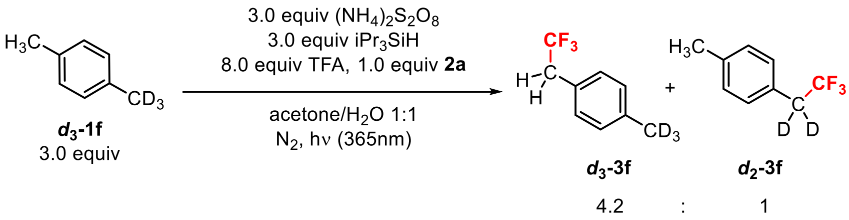
^{19}F NMR spectrum of a reaction mixture



Scheme S4. Kinetic Isotope Effect

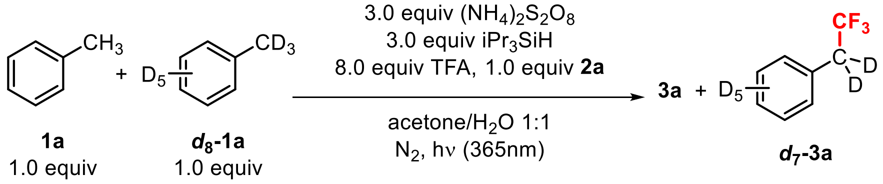


Intramolecular KIE study



In a N_2 glovebox, to a 2.0 mL screw-cap test tube equipped with a stir bar was added $(NH_4)_2S_2O_8$ (27.3 mg, 0.12 mmol, 3.0 equiv) and bpyCu$(CF_3)_3$ (17.1 mg, 0.04 mmol, 1.0 equiv). Acetone (0.20 mL) and *p*-Xylene-α,α,α-*d*$_3$ (***d*$_3$-1f**) (13.1 mg, 0.120 mmol, 3.0 equiv) were added via syringe, followed by *i*-Pr_3SiH (24.7 μL, 0.12 mmol, 3.0 equiv). The tube was sealed with a PTFE lined screw cap, brought outside the glovebox. Degassed H_2O (0.20 mL) and trifluoroacetic acid (24.5 μL, 0.12 mmol, 8.0 equiv) were added under N_2 atmosphere. Then the reaction mixture was irradiated with a 5 W LED lamp (centered at 365 nm and placed 15-20 cm away from the reaction vial) at room temperature for 18 h. After the reaction mixture was quenched with saturated aqueous $NaHCO_3$ (30 mL), 1-bromo-4-fluorobenzene (6.0 μL, 0.056 mmol) and acetone-*d*$_6$ (4.0 mL) was added. The ratio of 1-(methyl-*d*$_3$)-4-(2,2,2-trifluoroethyl)benzene (***d*$_3$-3f**) and 1-methyl-4-(2,2,2-trifluoroethyl-1,1-*d*$_2$)benzene (***d*$_2$-3f**) was determined by comparing with that of 1-bromo-4-fluorobenzene.

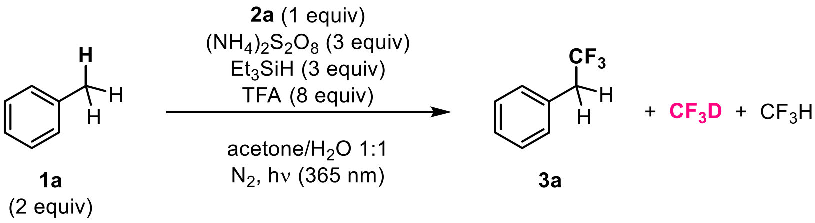
Intermolecular KIE study



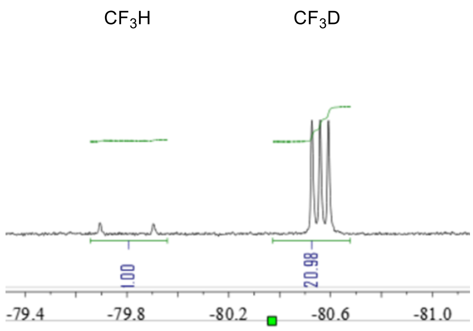
In a N_2 glovebox, to a 2.0 mL screw-cap test tube equipped with a stir bar was added $(NH_4)_2S_2O_8$ (27.3 mg, 0.12 mmol, 3.0 equiv) and bpyCu$(CF_3)_3$ (17.1 mg, 0.04 mmol, 1.0 equiv). Acetone (0.20 mL) and 1:1 mixture of **1a** and *d*$_8$-**1a** (0.04 mmol each) were added via syringe, followed by *i*-Pr_3SiH (24.7 μL, 0.12 mmol, 3.0 equiv). The tube was sealed with a PTFE lined screw cap, brought outside the glovebox. Degassed H_2O (0.20 mL) and trifluoroacetic acid (24.5 μL, 0.12 mmol, 8.0 equiv) were added under N_2 atmosphere. Then the reaction mixture was irradiated with a 5 W LED lamp (centered at 365 nm and placed 15-20 cm away from the reaction vial) at room temperature for 1 hour and 5 hours. After the reaction mixture was quenched with saturated aqueous $NaHCO_3$ (30 mL), 1-bromo-4-fluorobenzene (6.0 μL, 0.056 mmol) and acetone-*d*$_6$ (4.0 mL) was added. The ratio of (2,2,2-trifluoroethyl)benzene **(3a)** and 1-(2,2,2-trifluoroethyl-1,1-*d*$_2$)benzene-2,3,4,5,6-*d*$_5$ **(*d*$_7$-3a)** was determined by comparing with that of 1-bromo-4-fluorobenzene.

	Time (hour)	Conv (%)	KIE (^{19}F NMR)
A	1	3%	2.8
B	5	23%	2.7

Table S8. The isotope labeling experiments



Entry	conditions	Ratio (CF_3D : CF_3H)
1	d_8-**1a** instead of **1a**	0 : 1
2	CD_3COOD instead of TFA	0 : 1
3	Et_3SiD instead of Et_3SiH	21 : 1
4	D_2O instead of H_2O	0 : 1
5	acetone-d_6 instead of acetone	0 : 1



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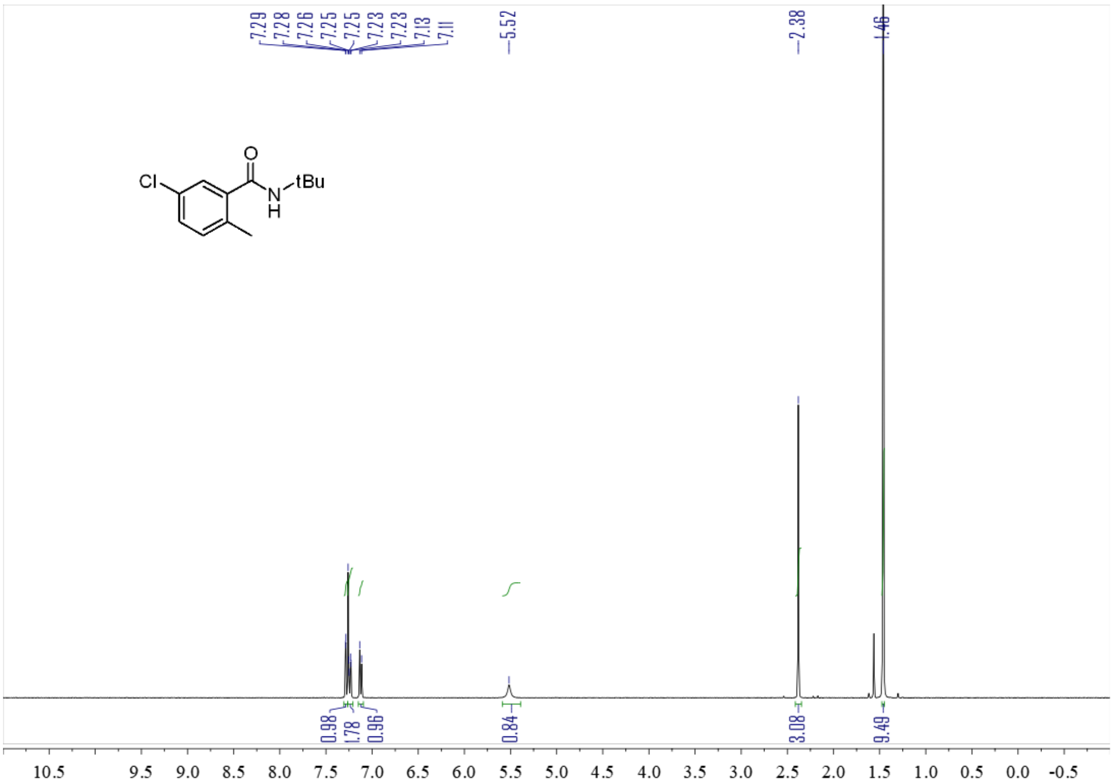
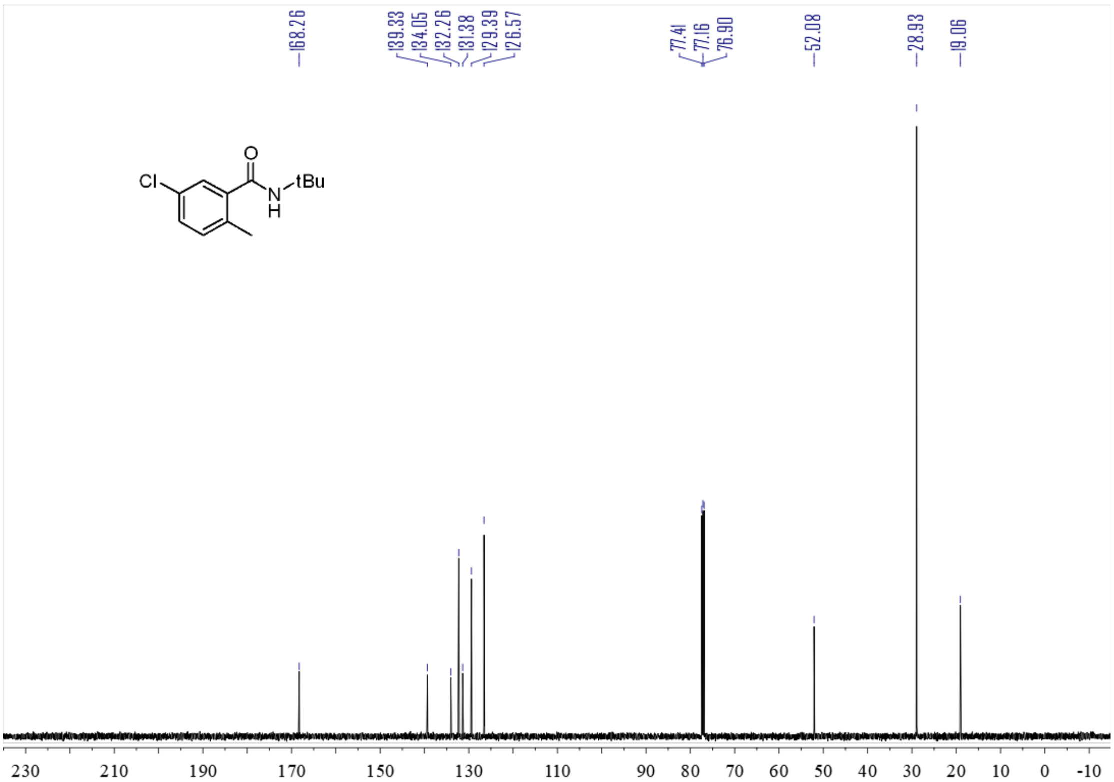
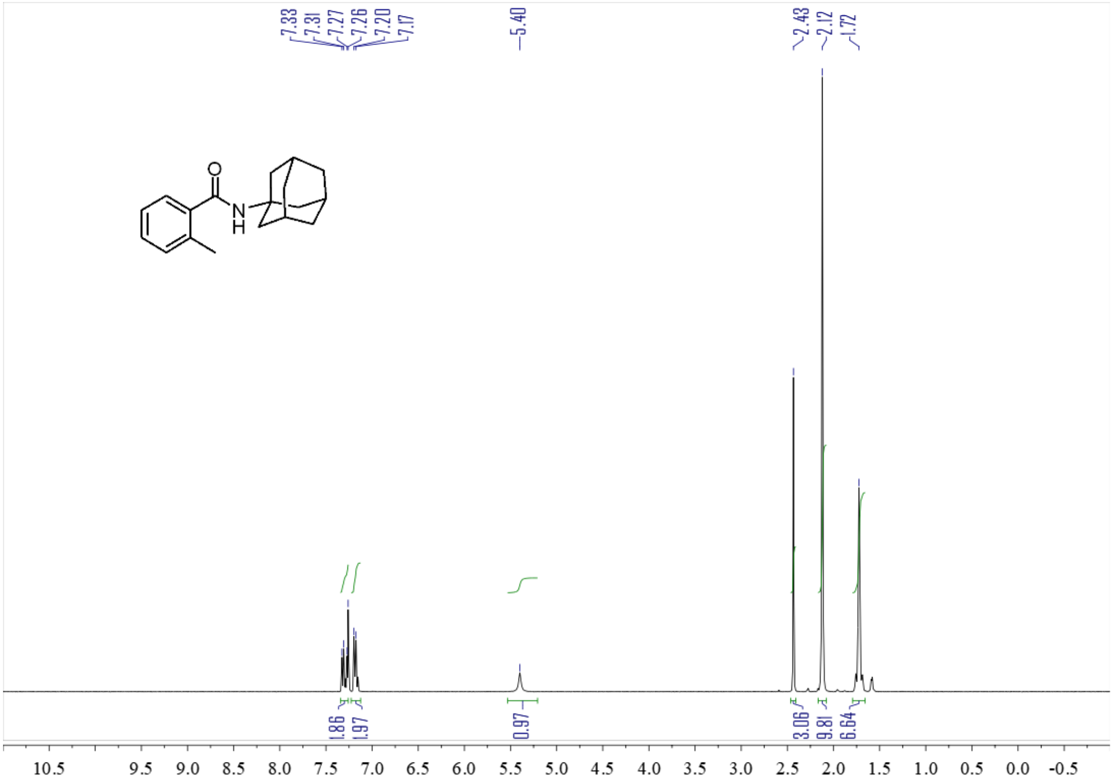
NMR Spectra.



^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of **1o**



^{13}C NMR spectrum (126 MHz, $CDCl_3$, 23 ºC) of **1o**



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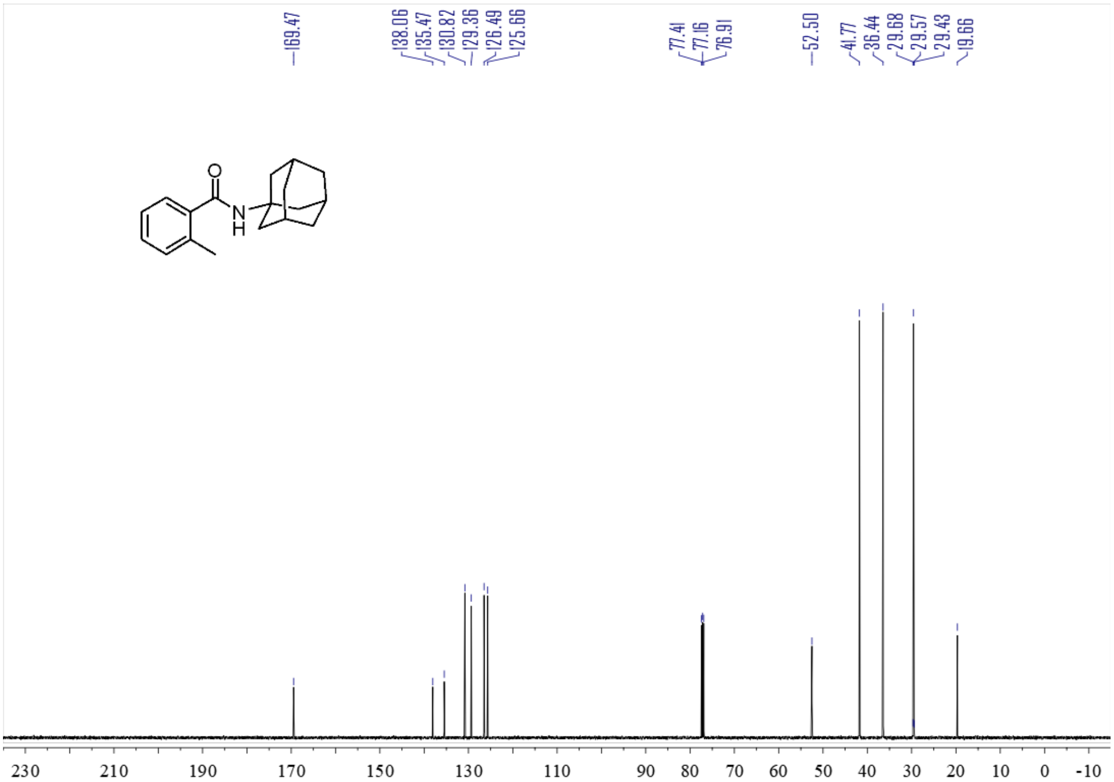
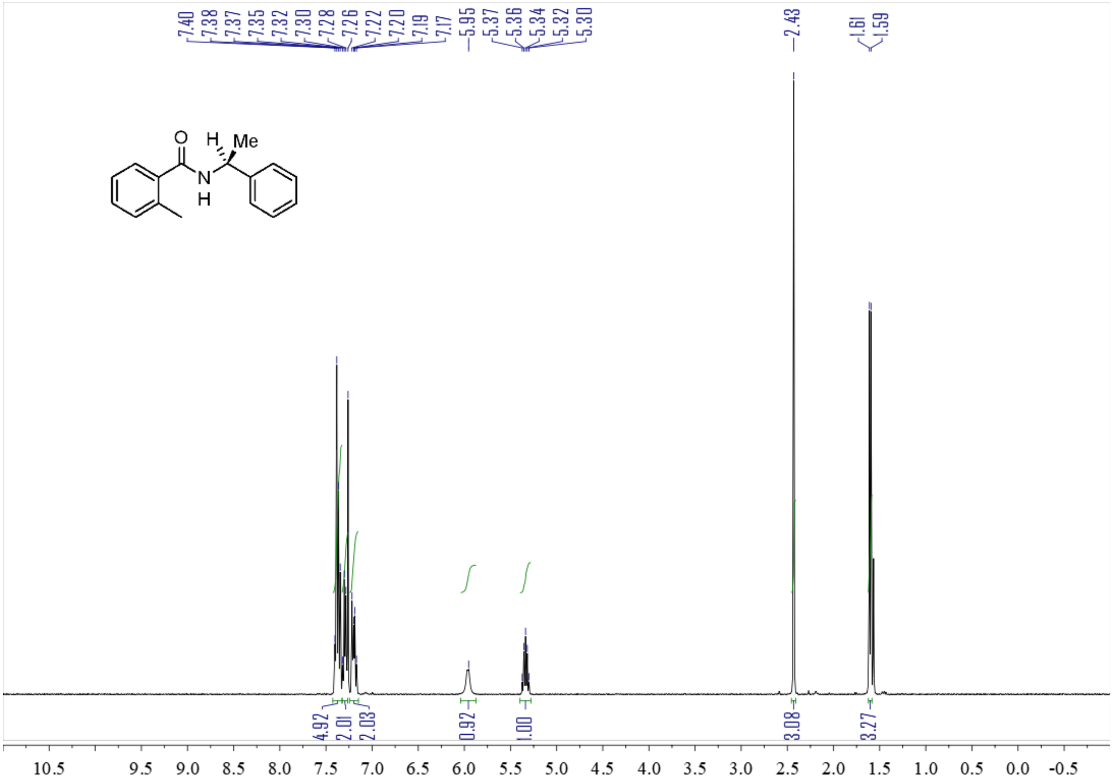


[13]C NMR spectrum (126 MHz, $CDCl_3$, 23 ºC) of **1p**



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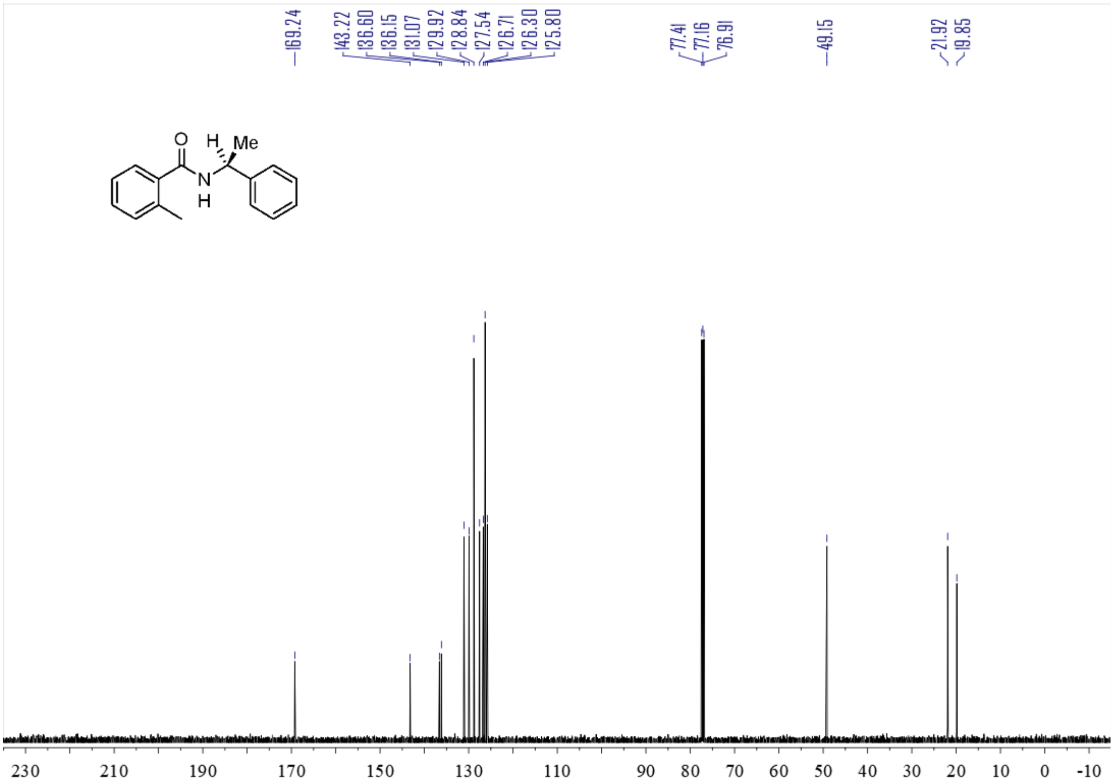
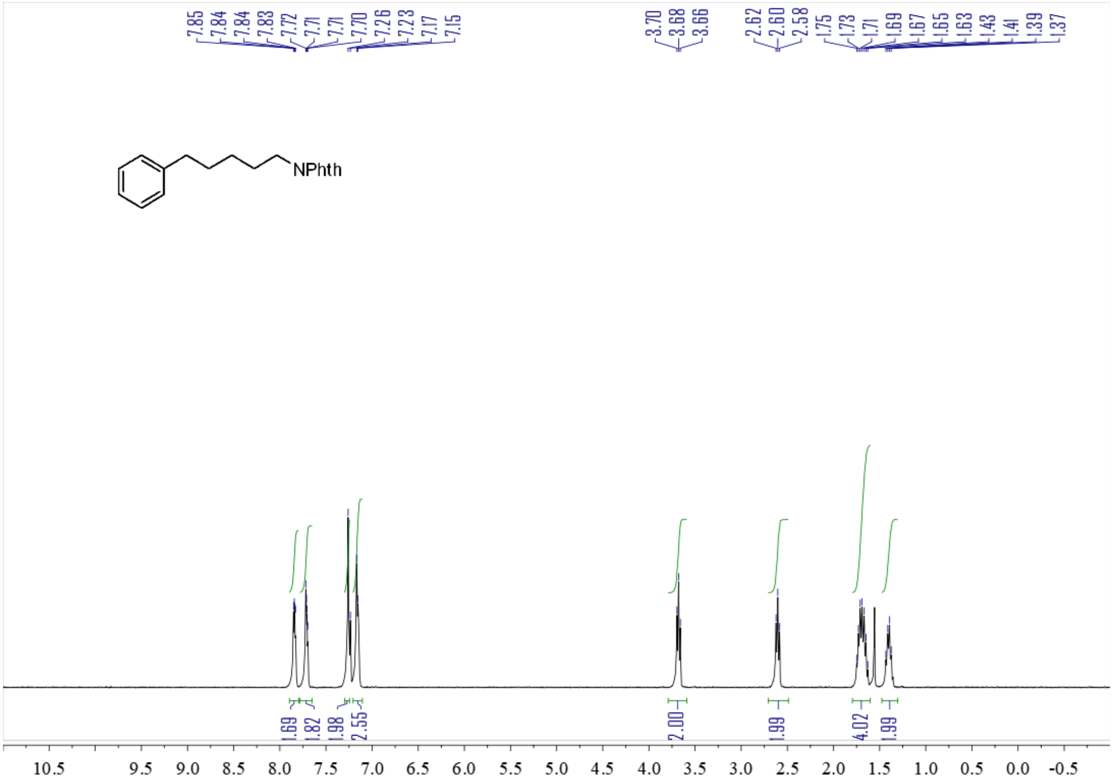
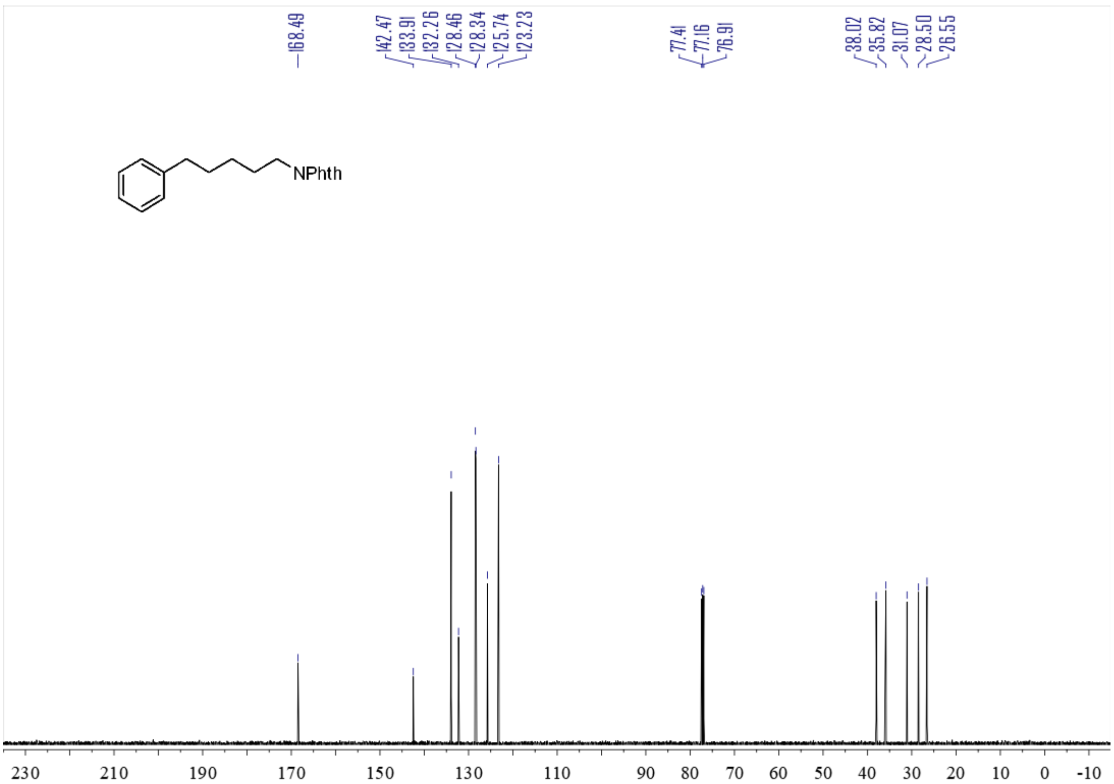


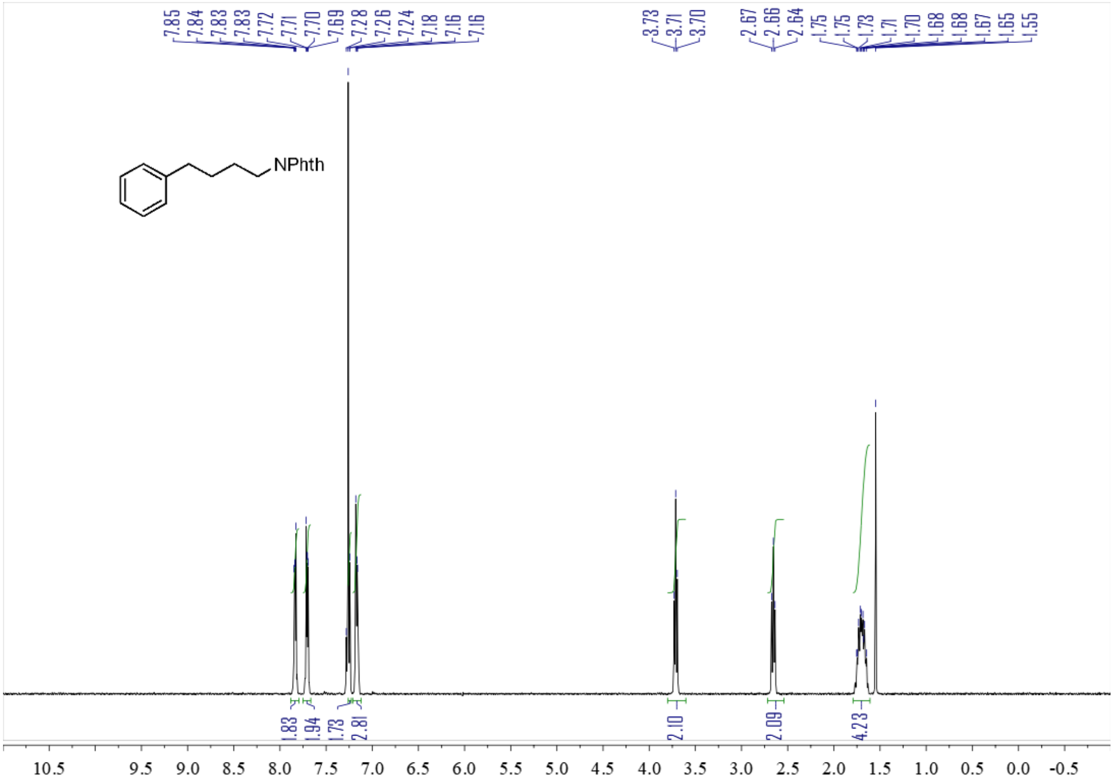
[13]C NMR spectrum (126 MHz, $CDCl_3$, 23 ºC) of **1r**



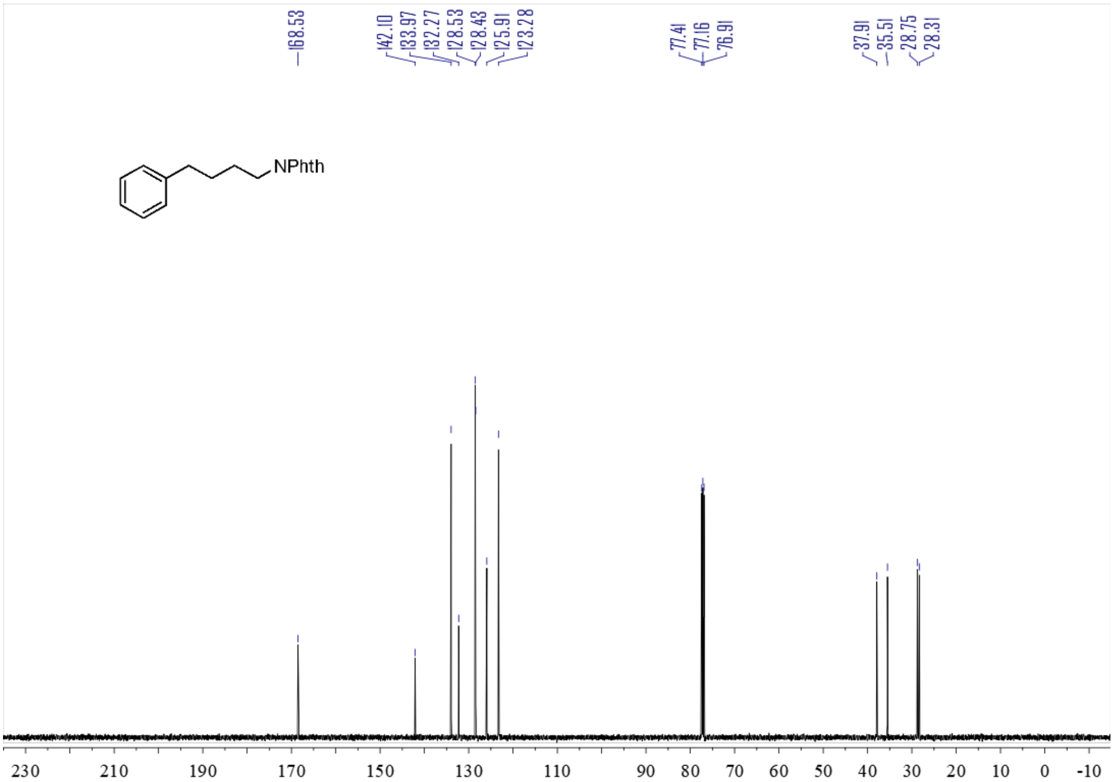
[1]H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of **1v**



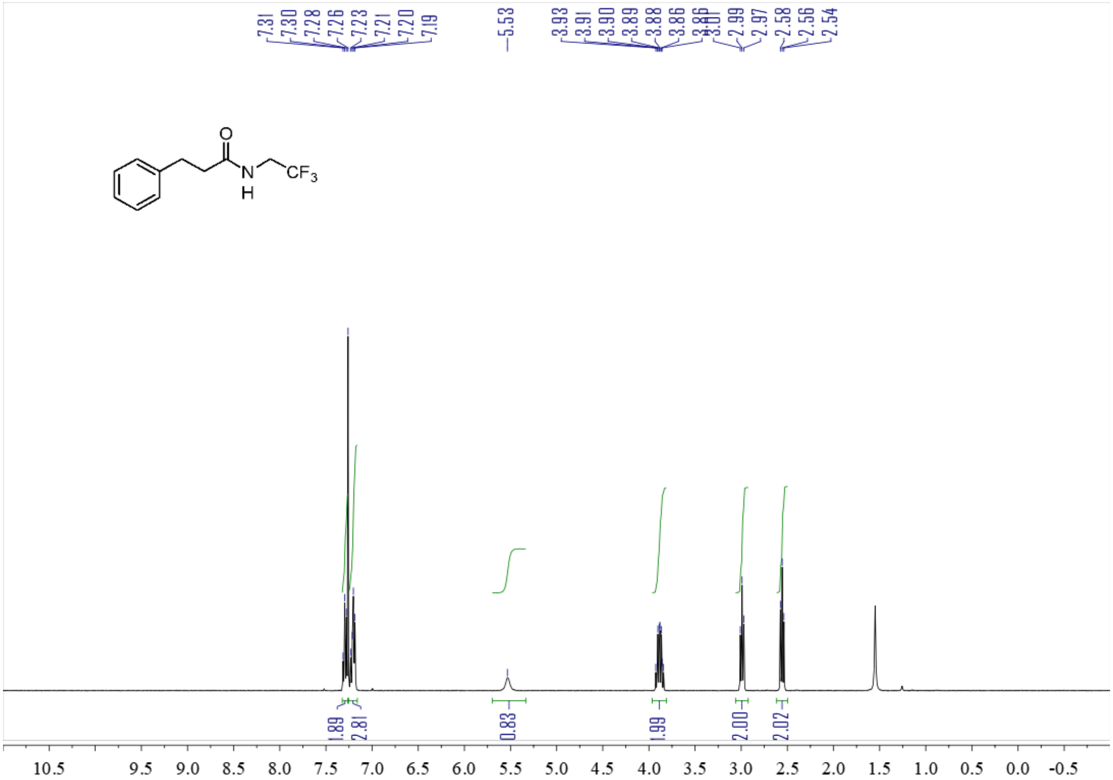
[13]C NMR spectrum (126 MHz, $CDCl_3$, 23 ºC) of **1v**



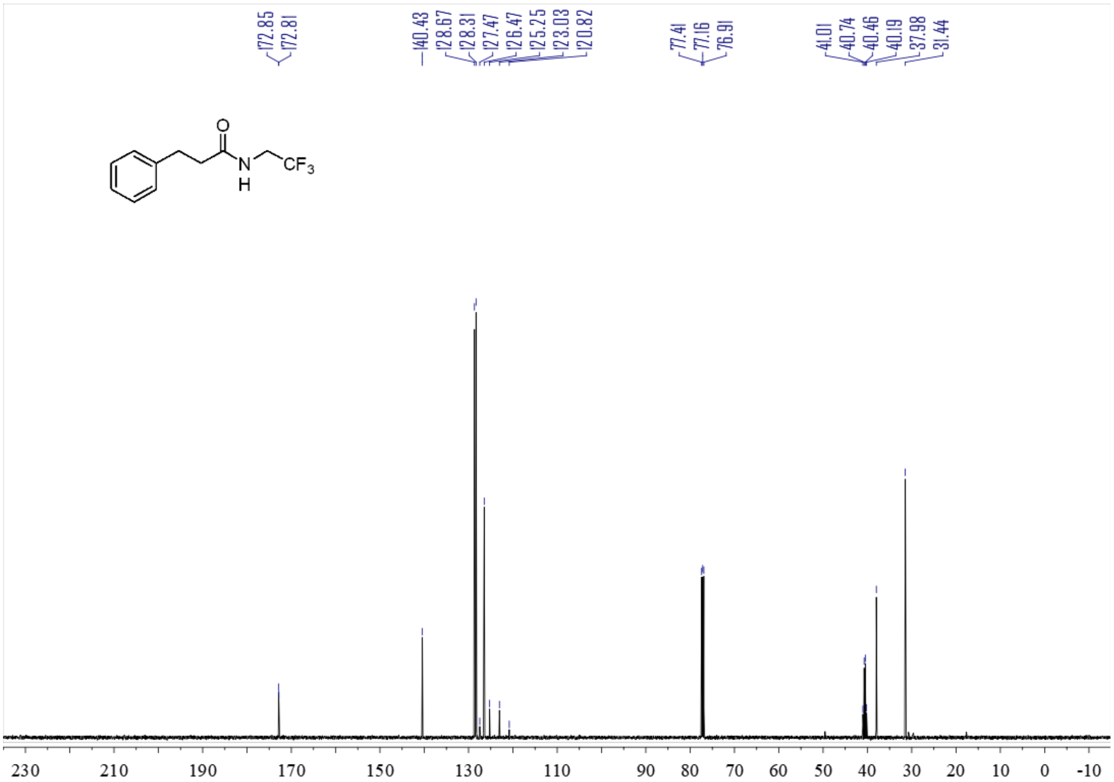
[1]H NMR spectrum (400 MHz, CDCl3, 23 ºC) of **1w**



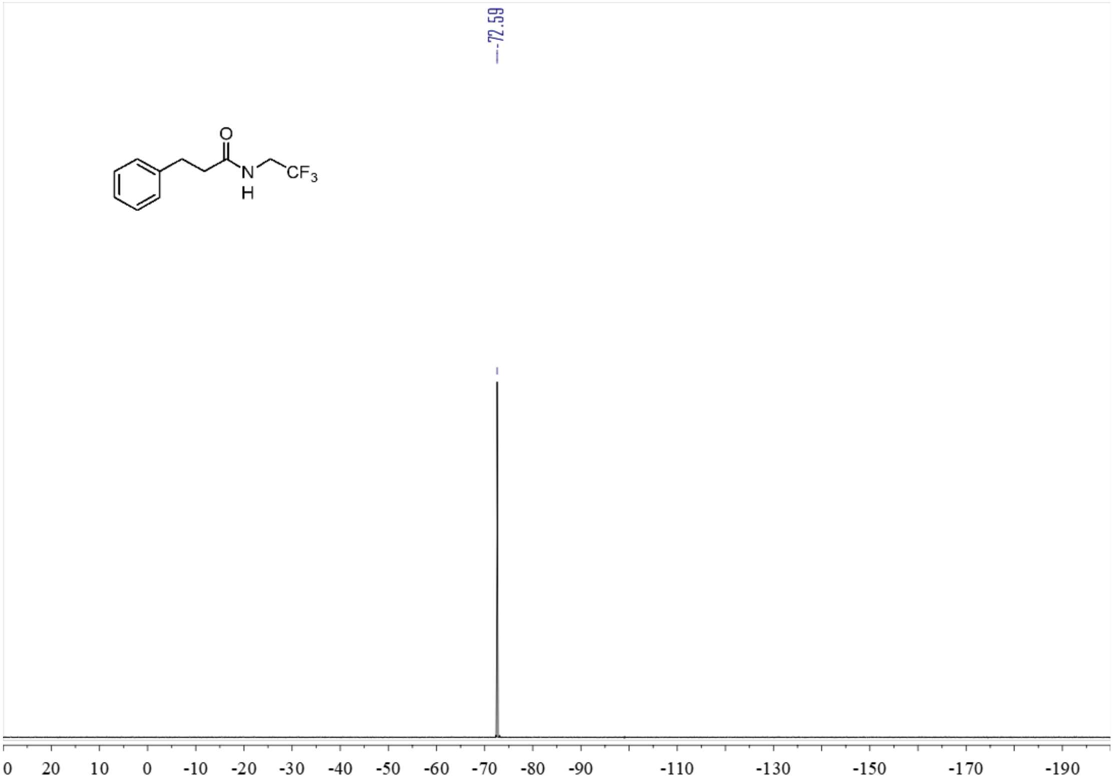
[13]C NMR spectrum (126 MHz, CDCl3, 23 ºC) of **1w**



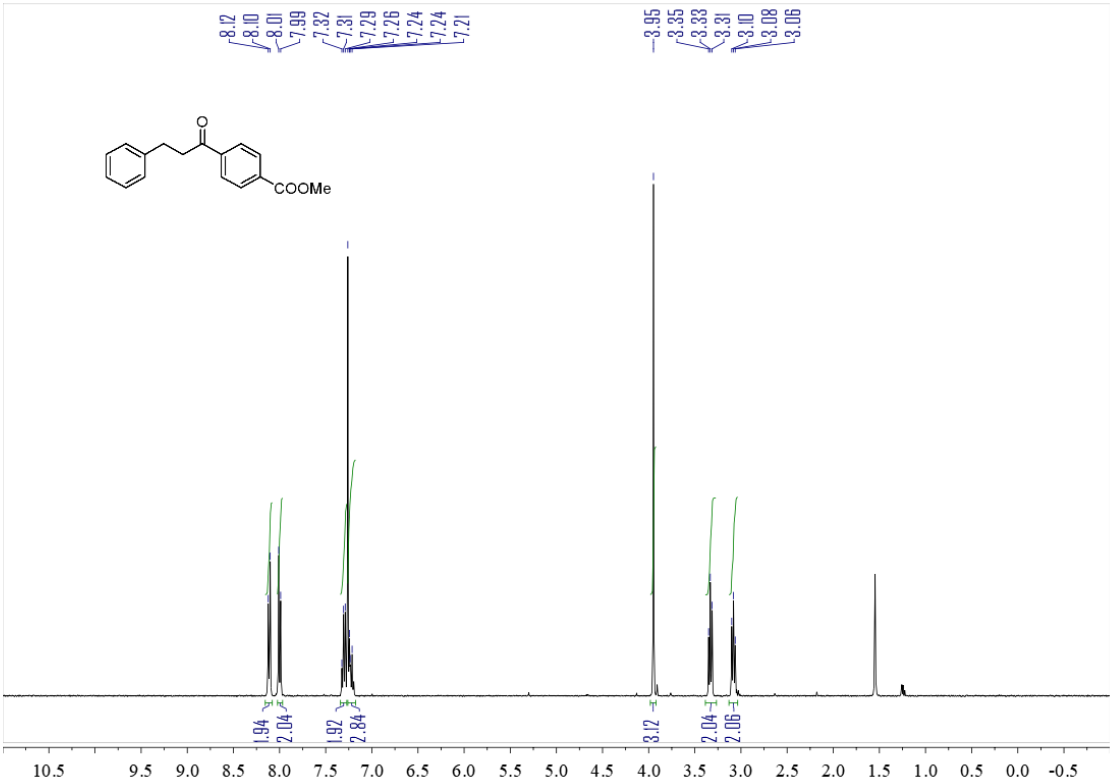
[1]H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of **1z**



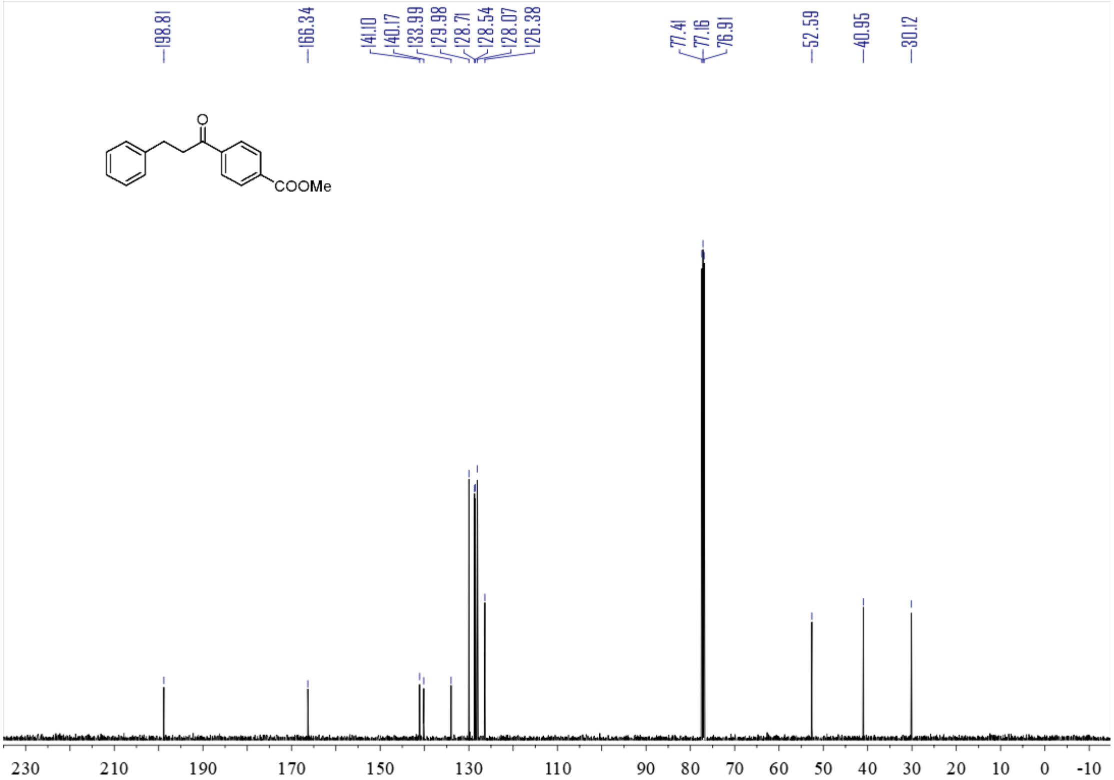
[13]C NMR spectrum (126 MHz, $CDCl_3$, 23 ºC) of **1z**



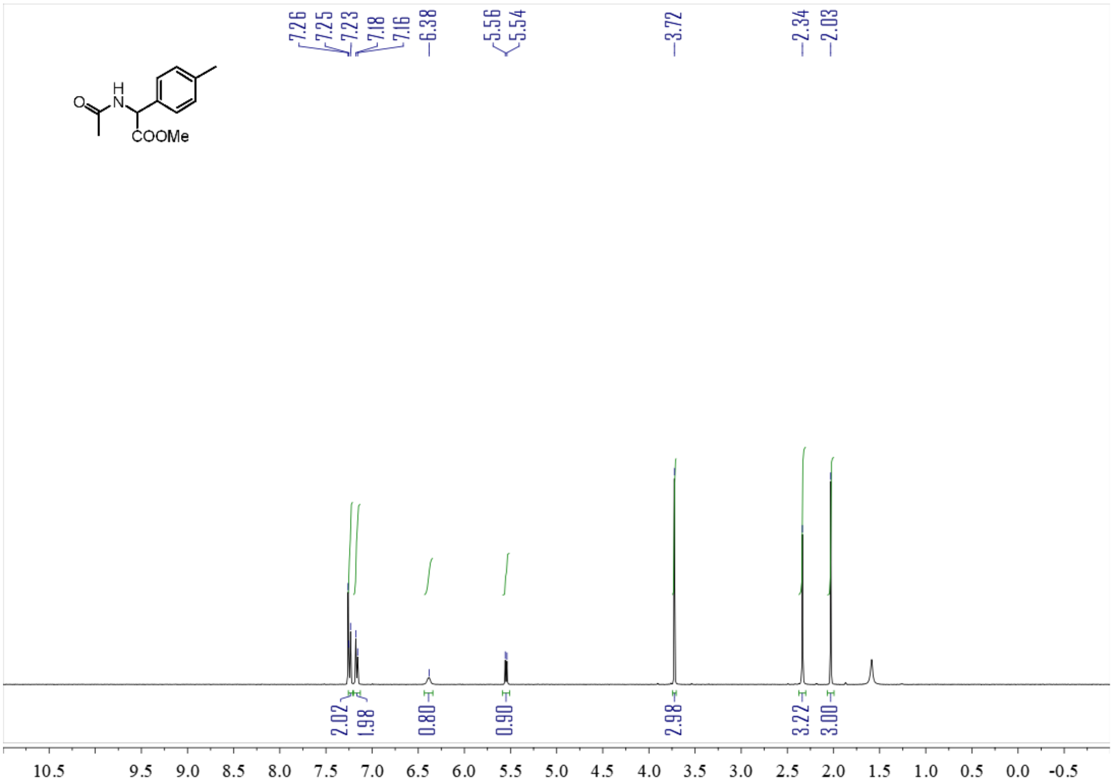
^{19}F NMR spectrum (375 MHz, $CDCl_3$, 23 ºC) of **1z**



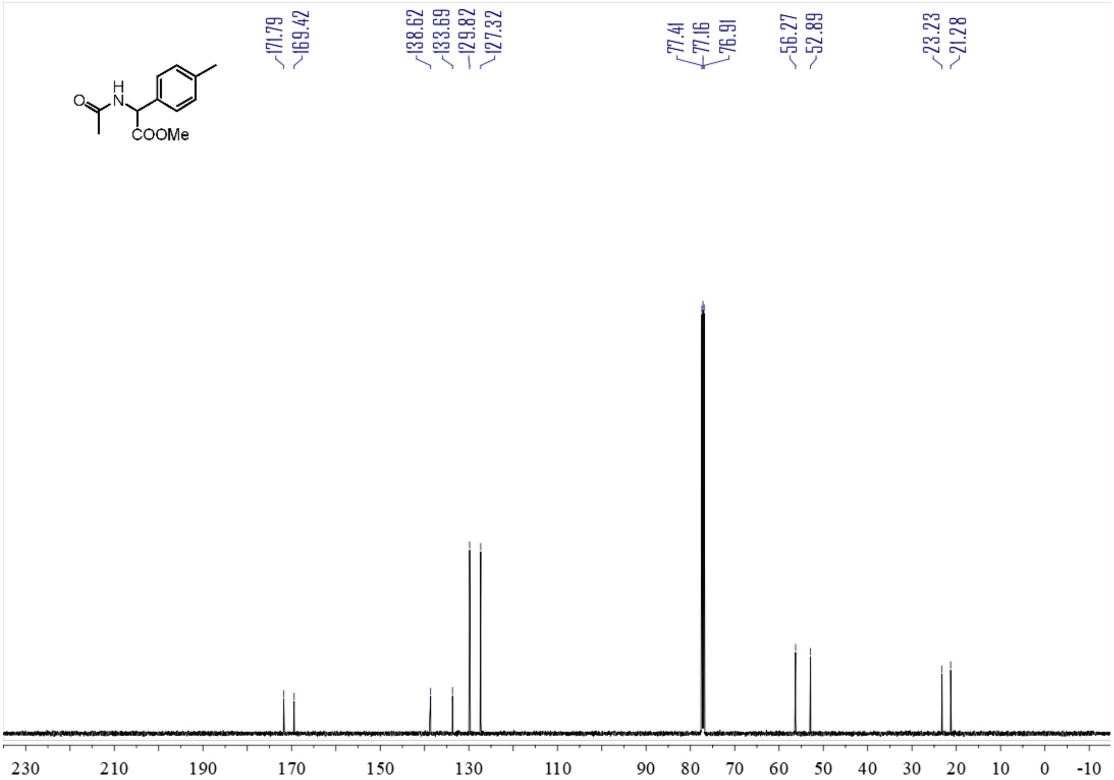
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of **1bb**



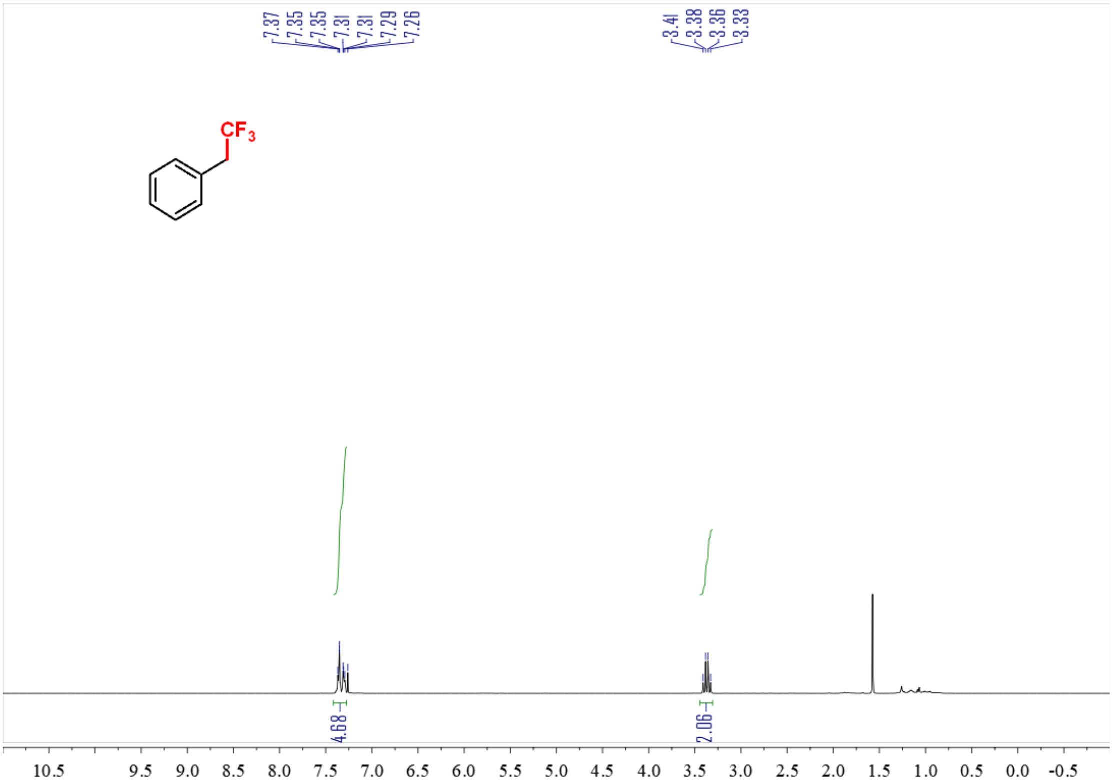
^{13}C NMR spectrum (126 MHz, $CDCl_3$, 23 ºC) of **1bb**



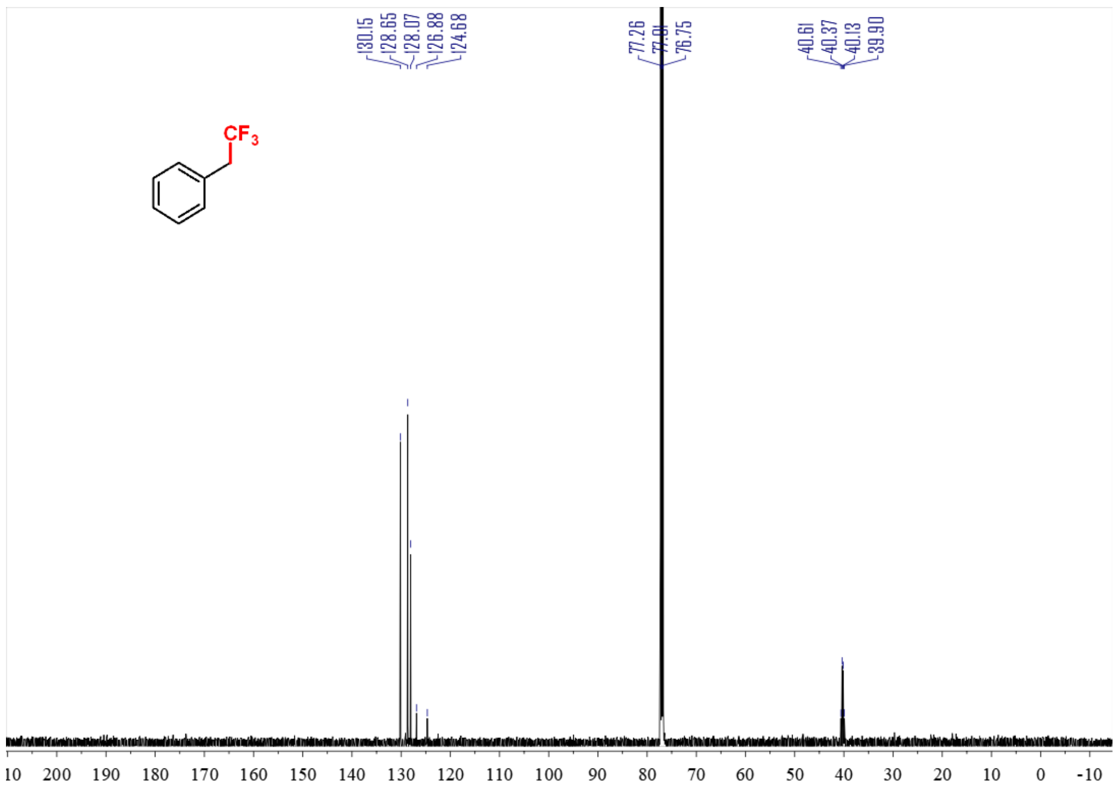
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of **7-SM**



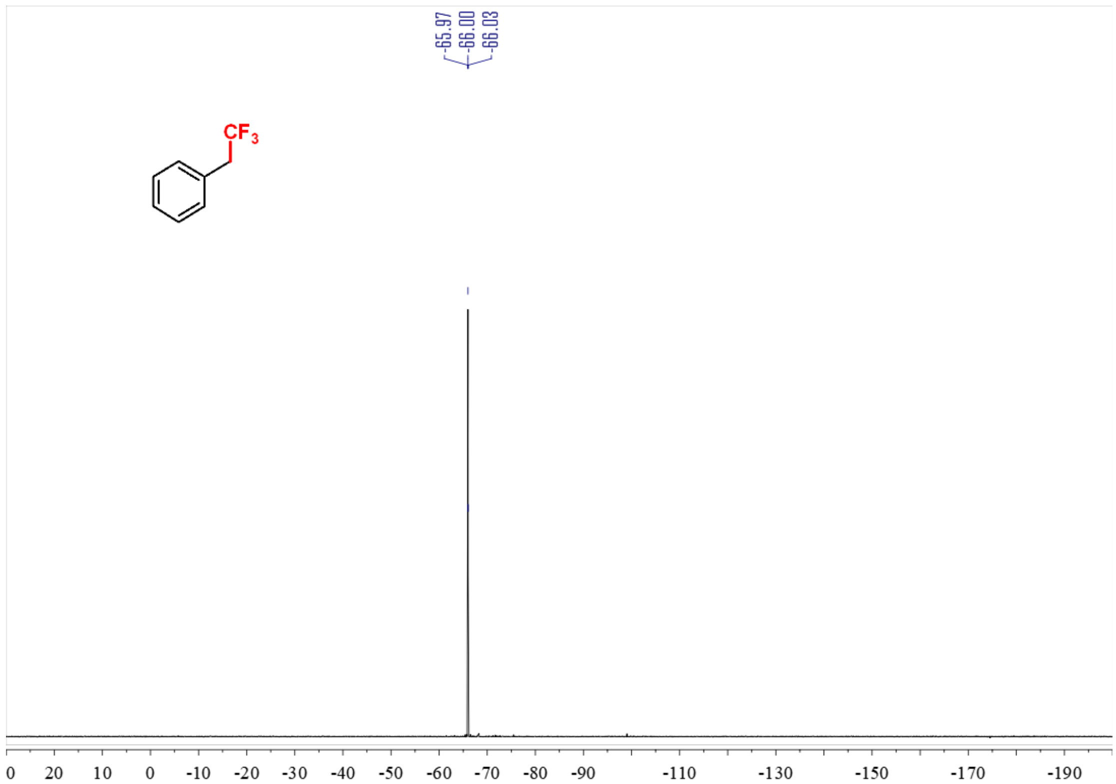
^{13}C NMR spectrum (126 MHz, $CDCl_3$, 23 ºC) of **7-SM**



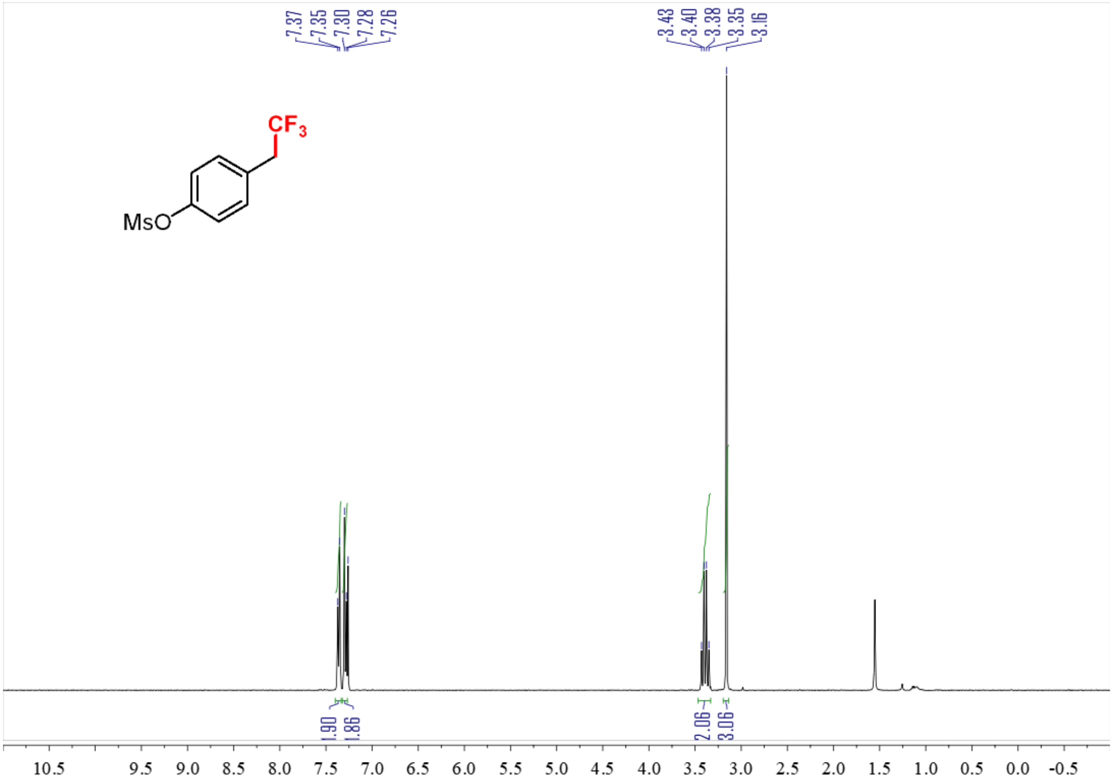
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of **3a**



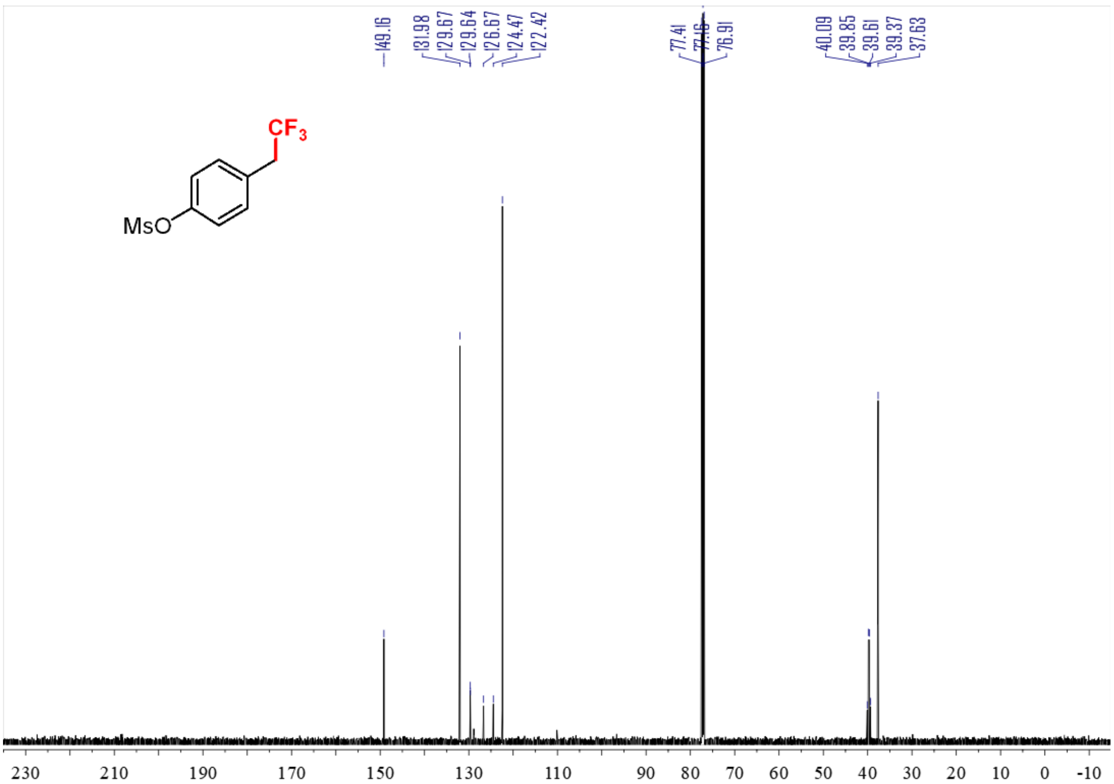
^{13}C NMR spectrum (126 MHz, $CDCl_3$, 23 ºC) of **3a**



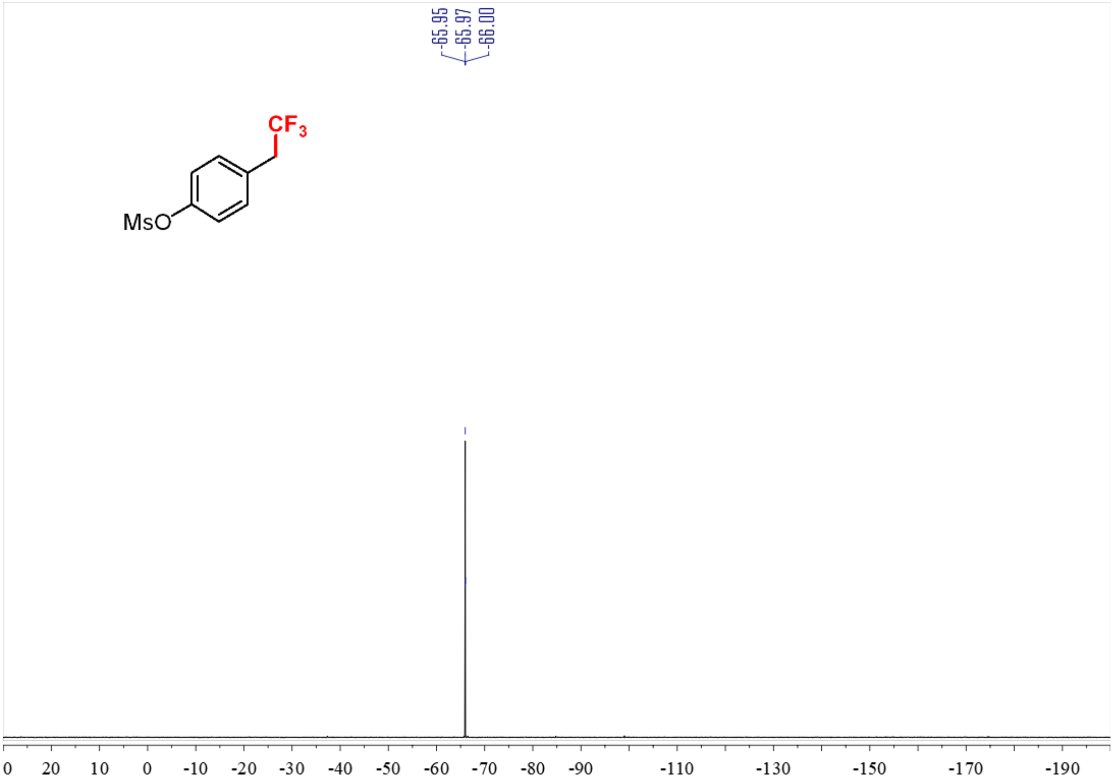
^{19}F NMR spectrum (375 MHz, $CDCl_3$, 23 ºC) of **3a**



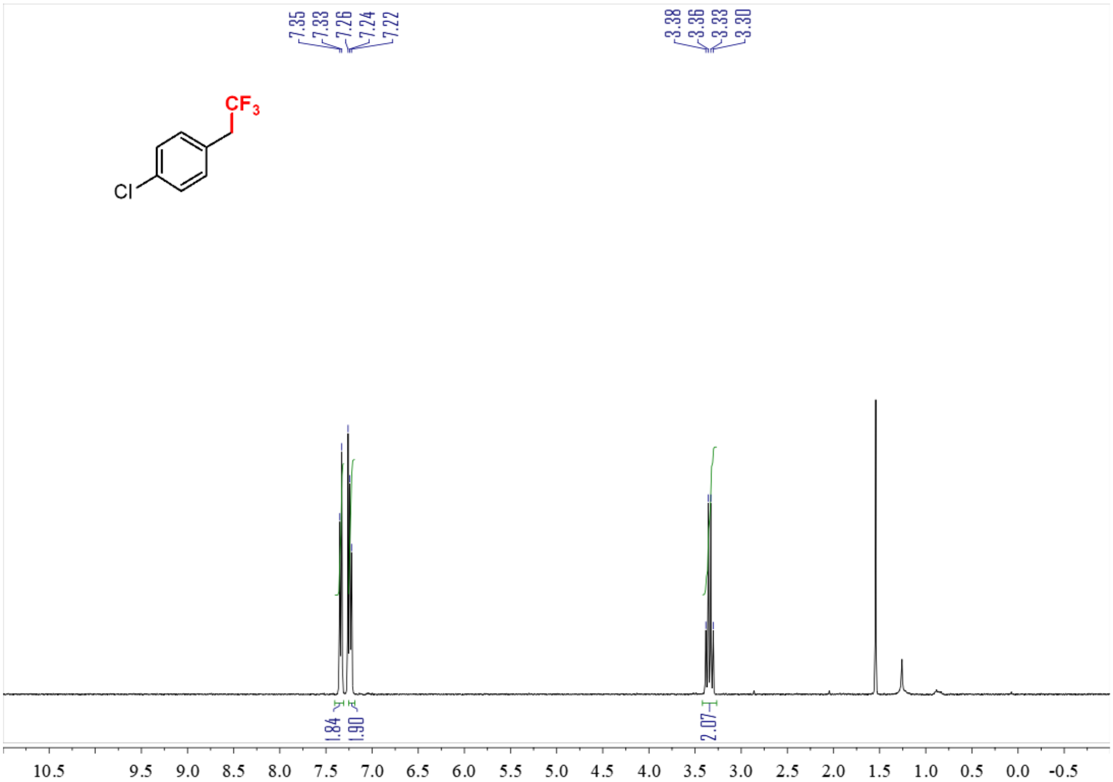
[1]H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of **3b**



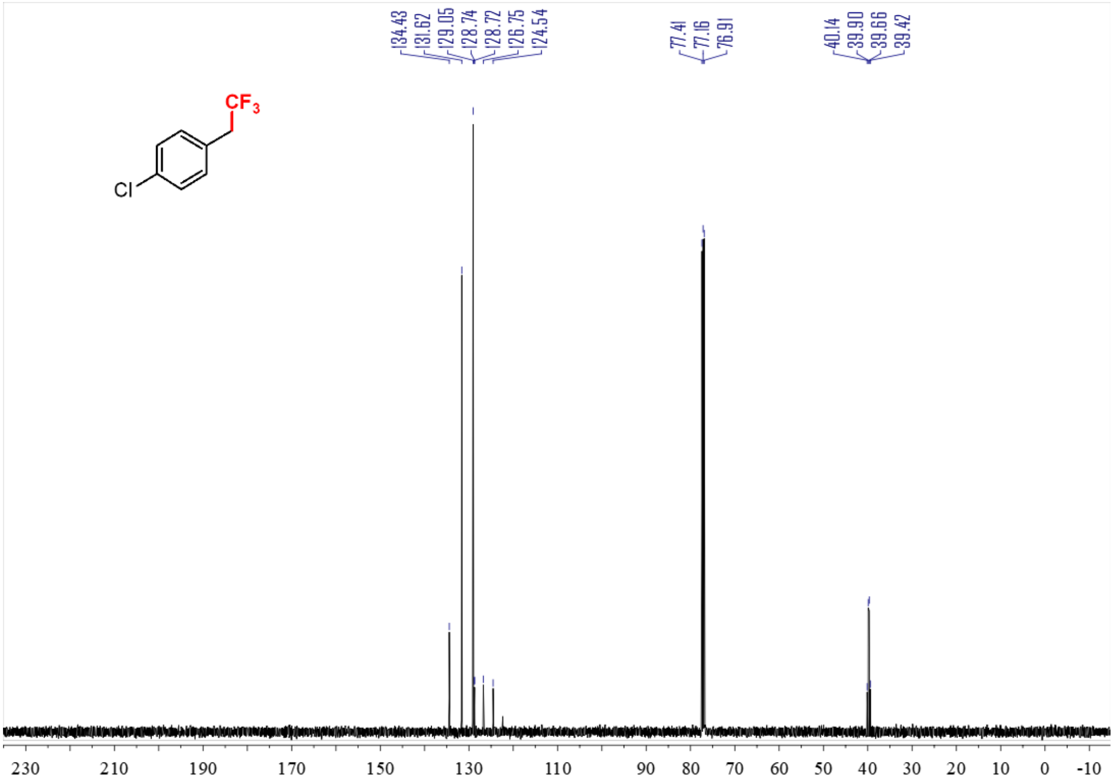
[13]C NMR spectrum (126 MHz, $CDCl_3$, 23 ºC) of **3b**



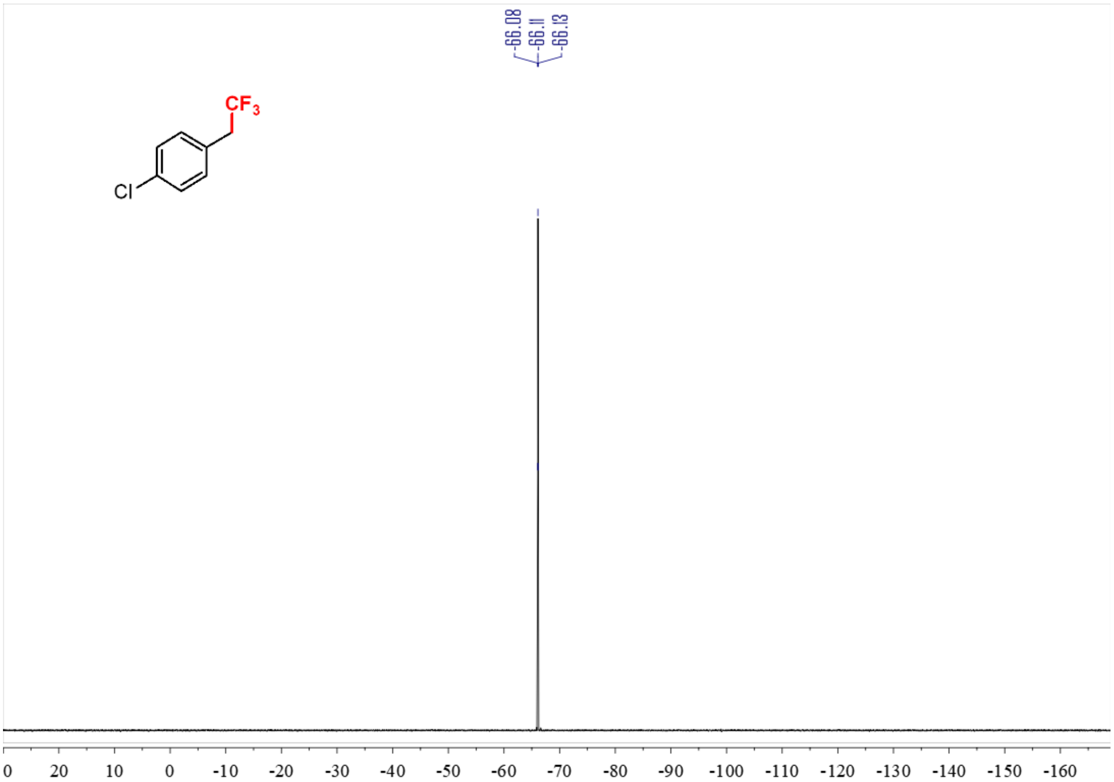
^{19}F NMR spectrum (375 MHz, $CDCl_3$, 23 ºC) of **3b**



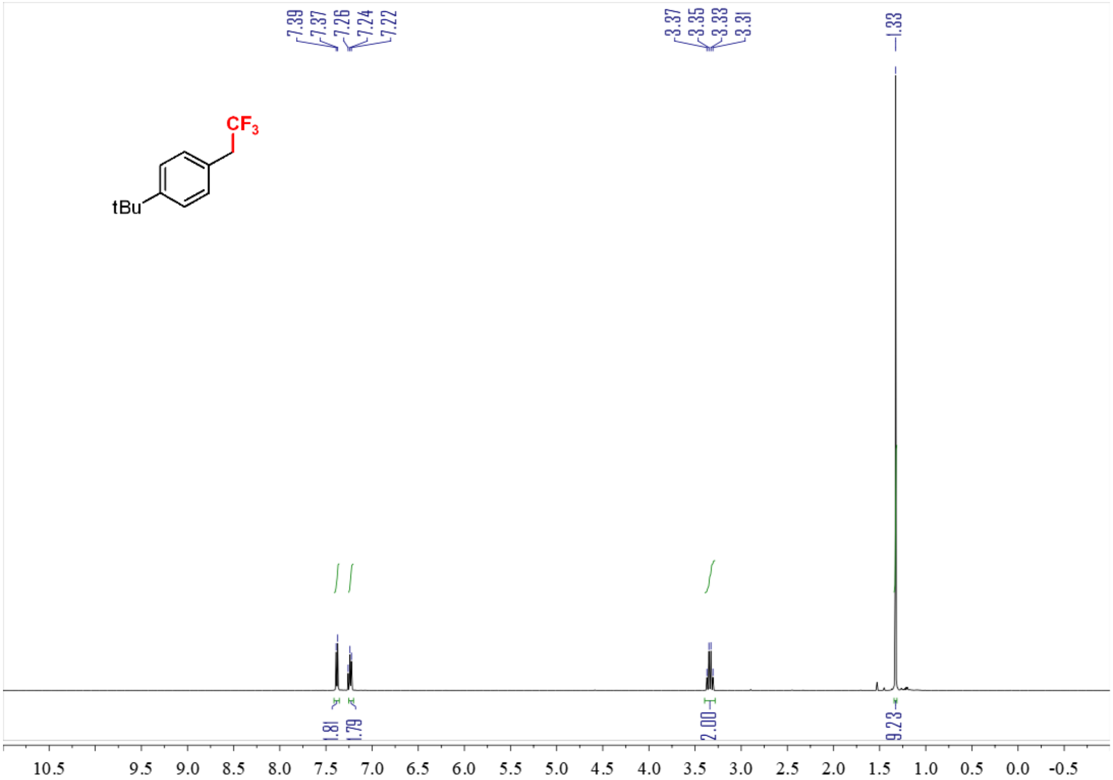
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of **3c**



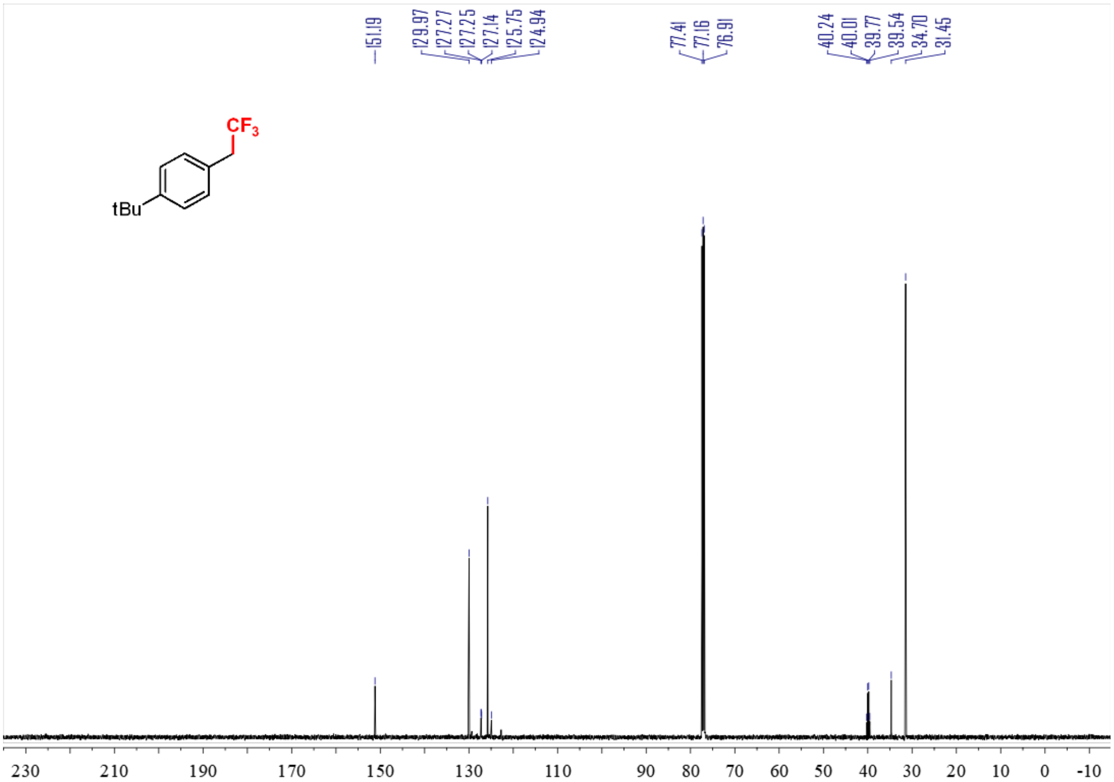
^{13}C NMR spectrum (126 MHz, $CDCl_3$, 23 ºC) of **3c**



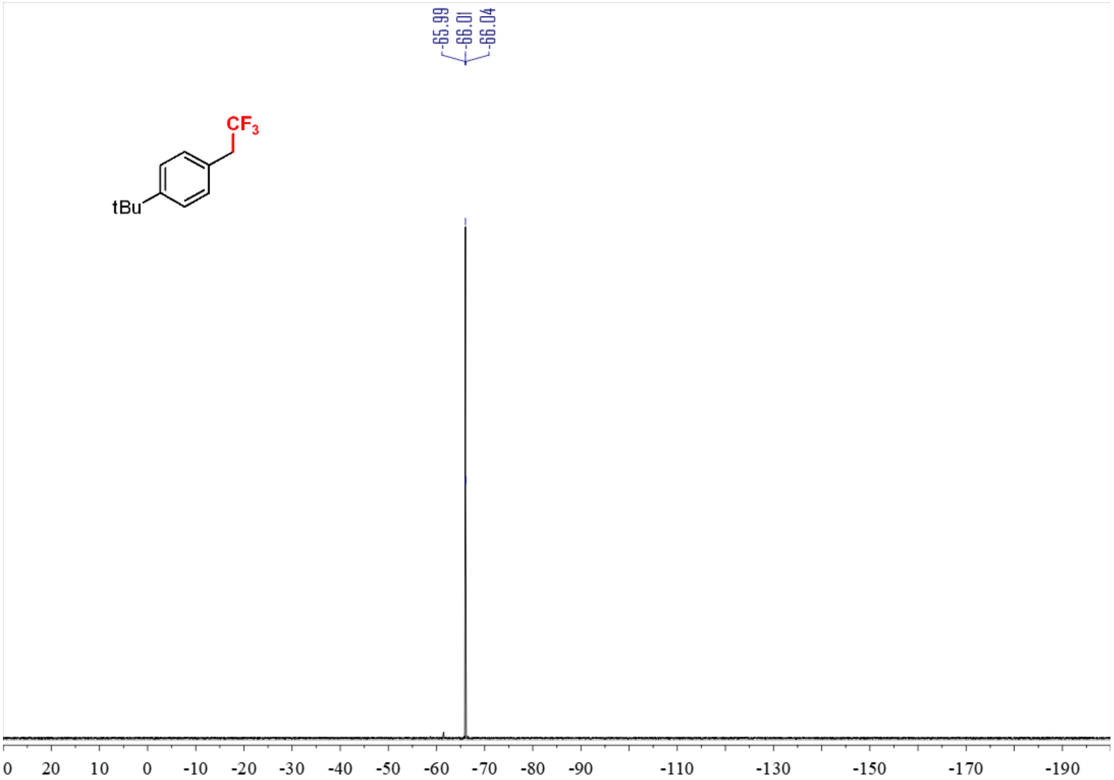
^{19}F NMR spectrum (375 MHz, $CDCl_3$, 23 ºC) of **3c**



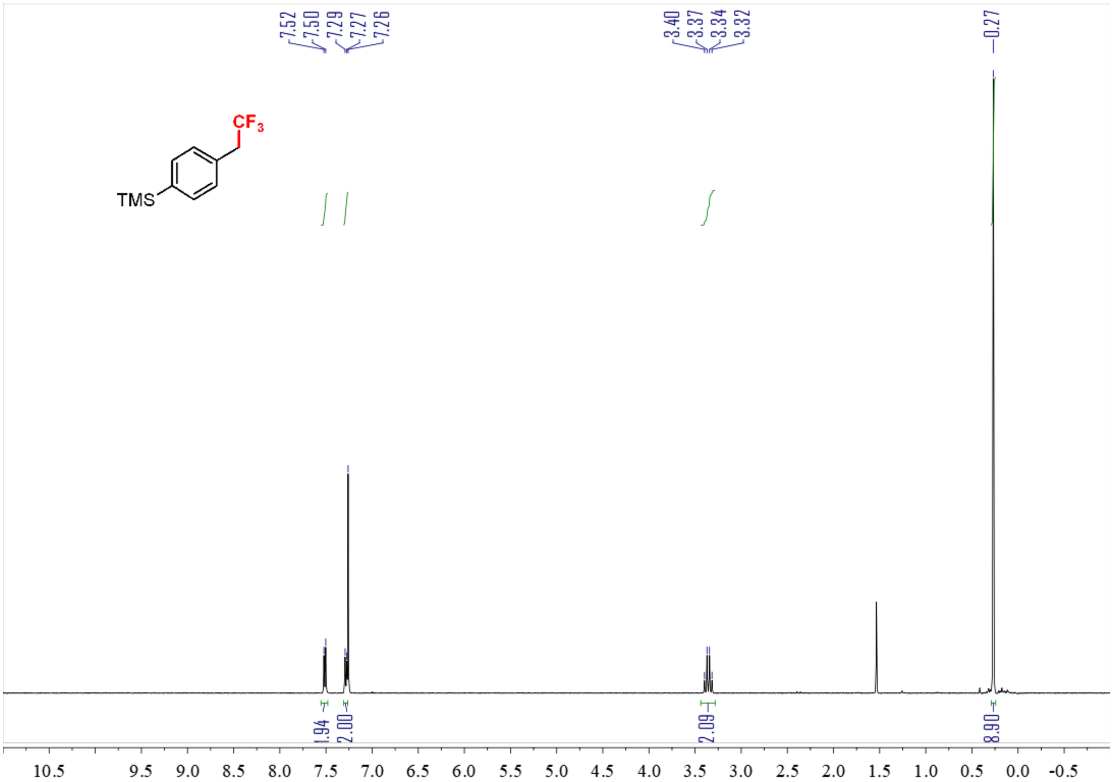
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of **3d**



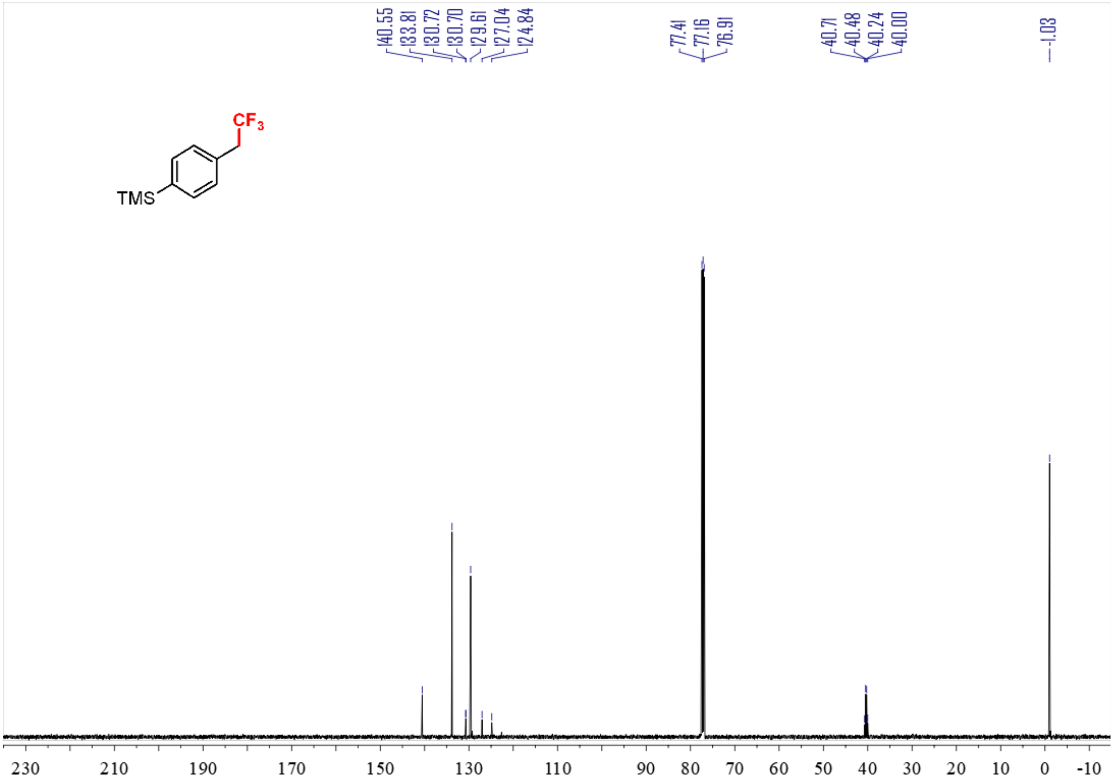
^{13}C NMR spectrum (126 MHz, $CDCl_3$, 23 ºC) of **3d**



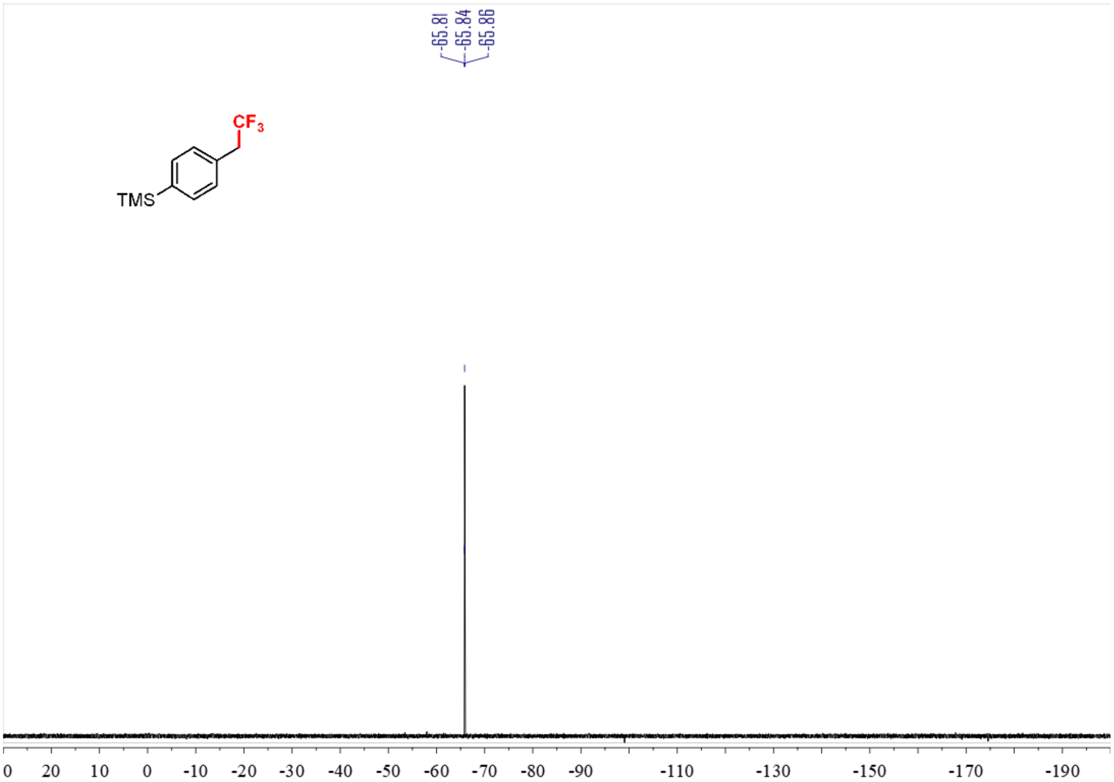
^{19}F NMR spectrum (375 MHz, $CDCl_3$, 23 ºC) of **3d**



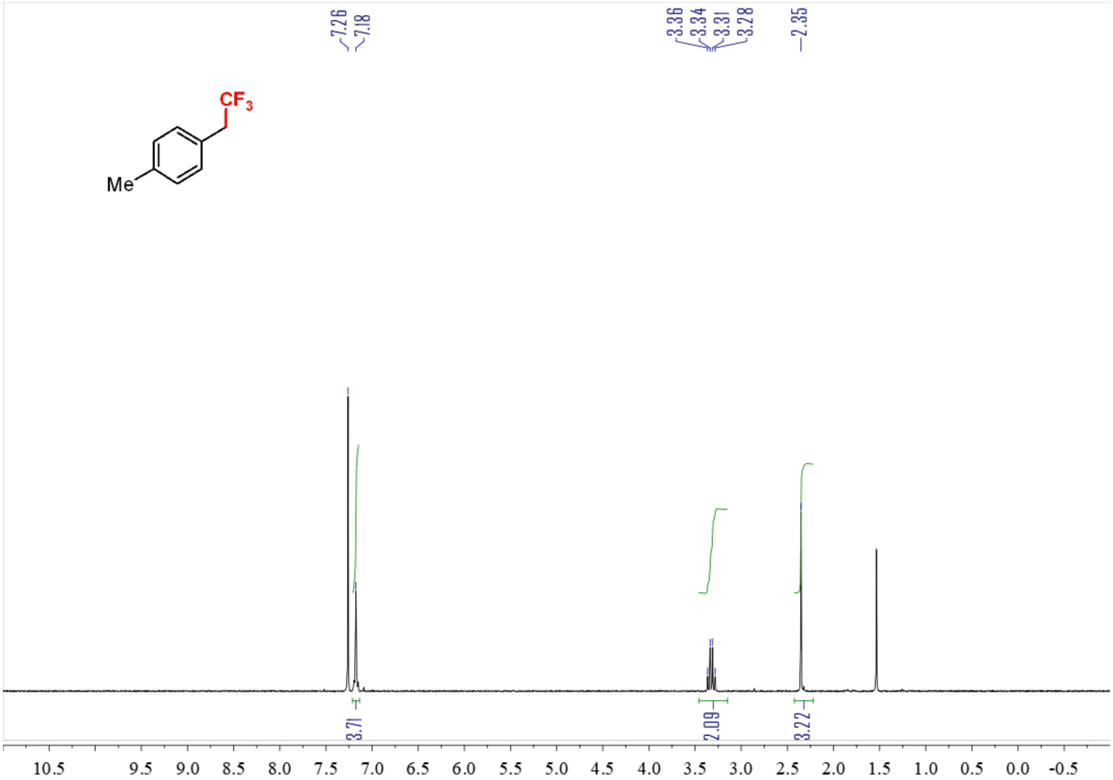
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of **3e**



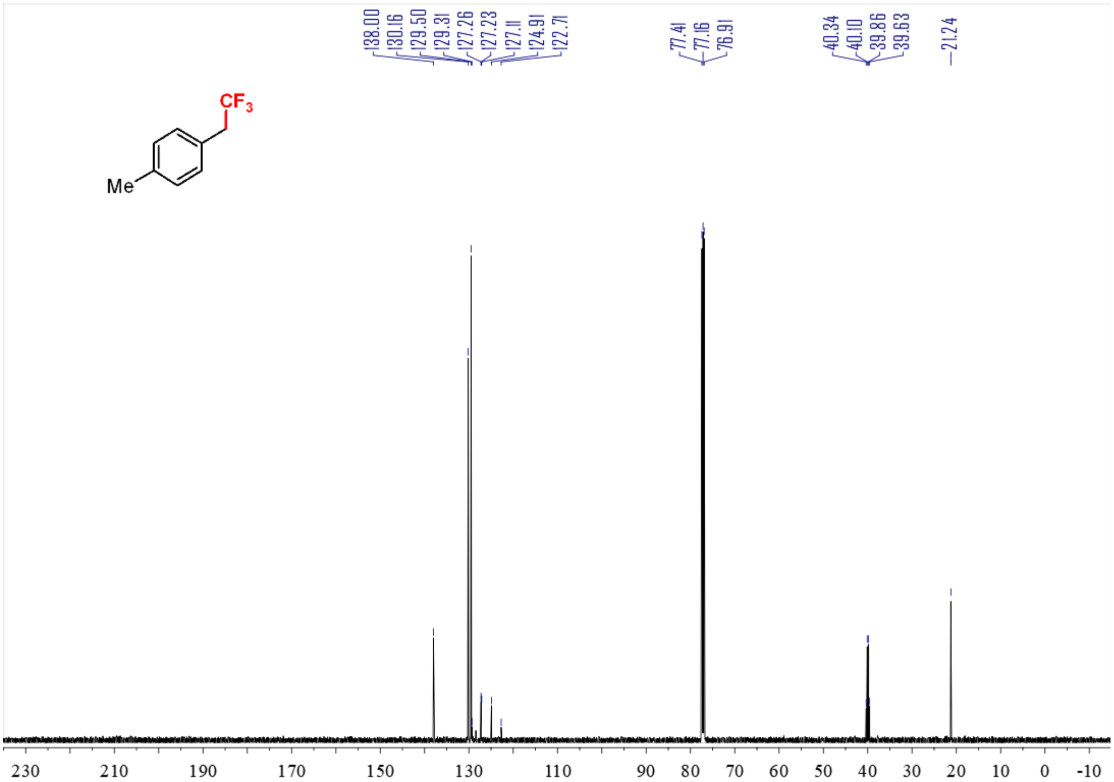
^{13}C NMR spectrum (126 MHz, $CDCl_3$, 23 ºC) of **3e**



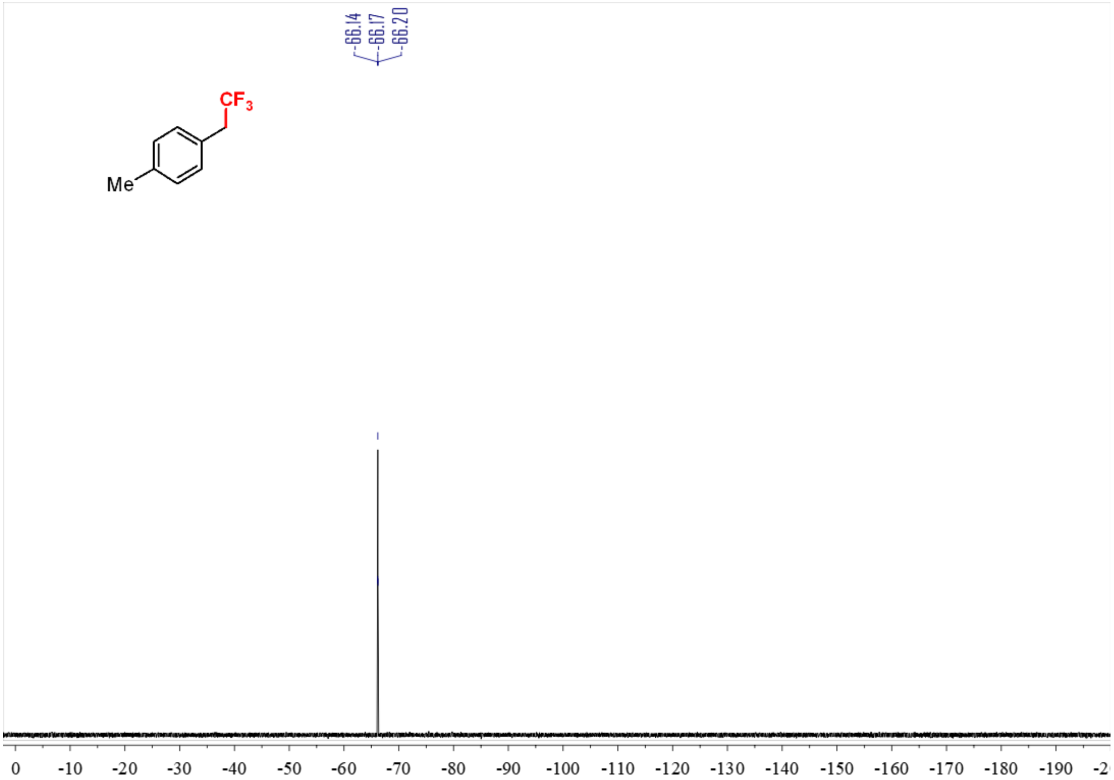
^{19}F NMR spectrum (375 MHz, $CDCl_3$, 23 ºC) of **3e**



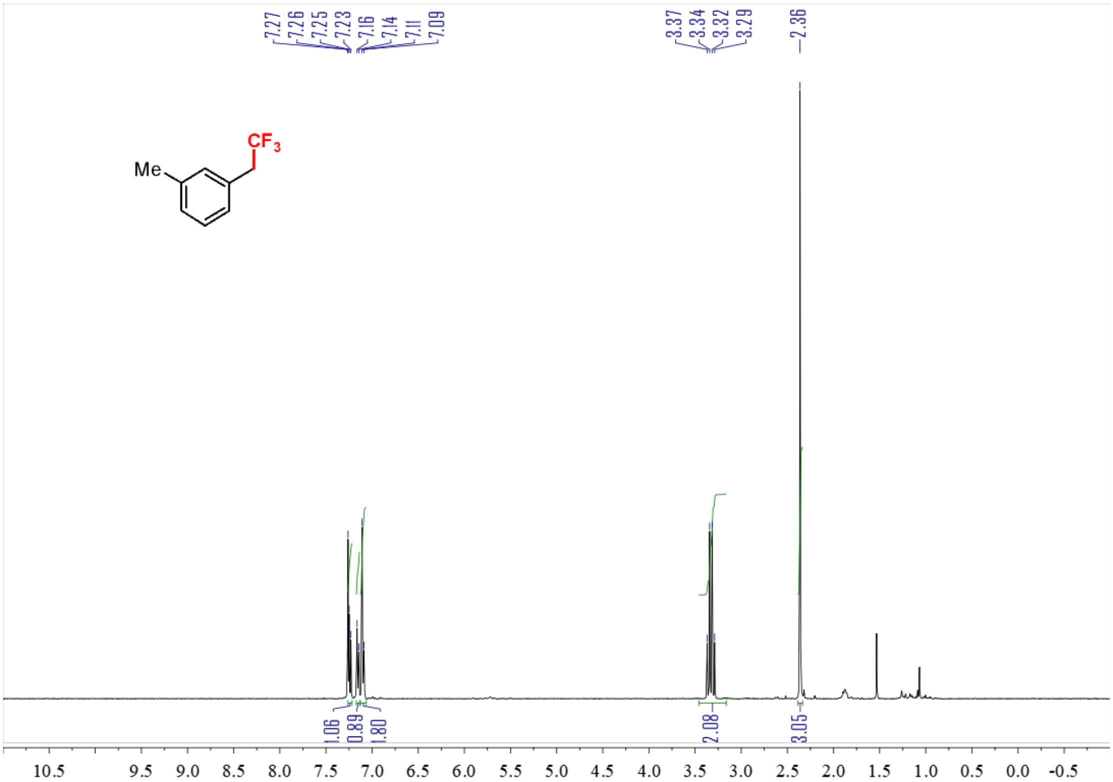
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of **3f**



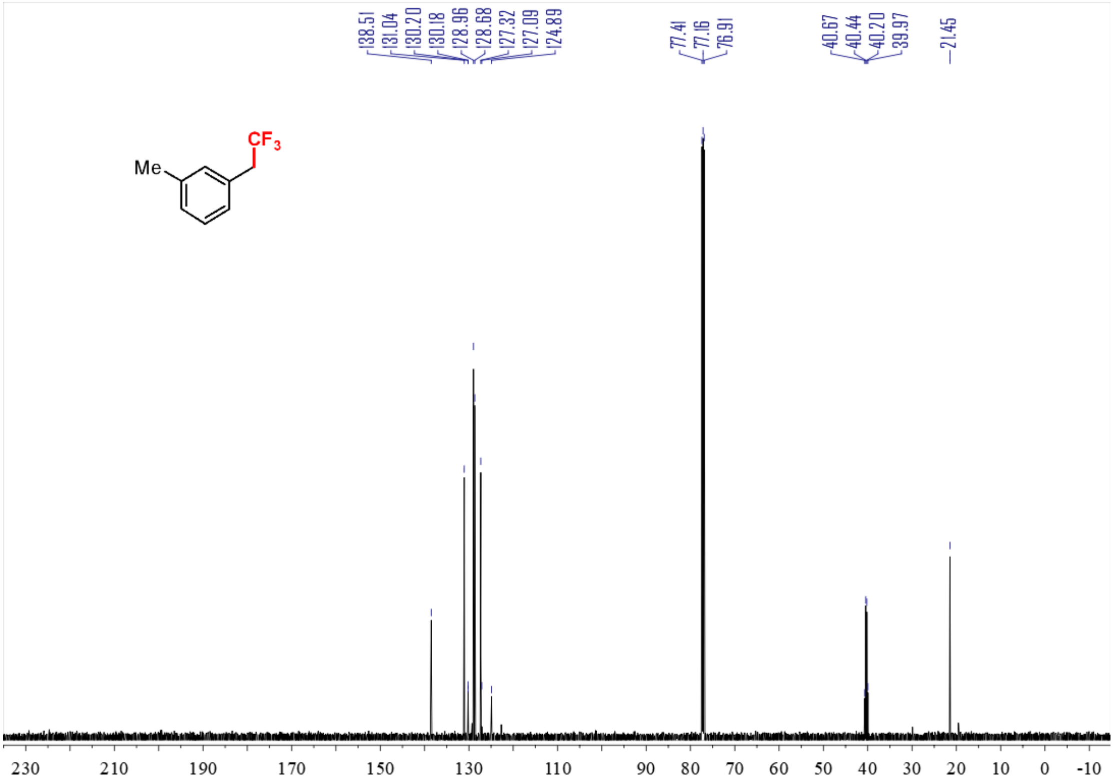
^{13}C NMR spectrum (126 MHz, $CDCl_3$, 23 ºC) of **3f**



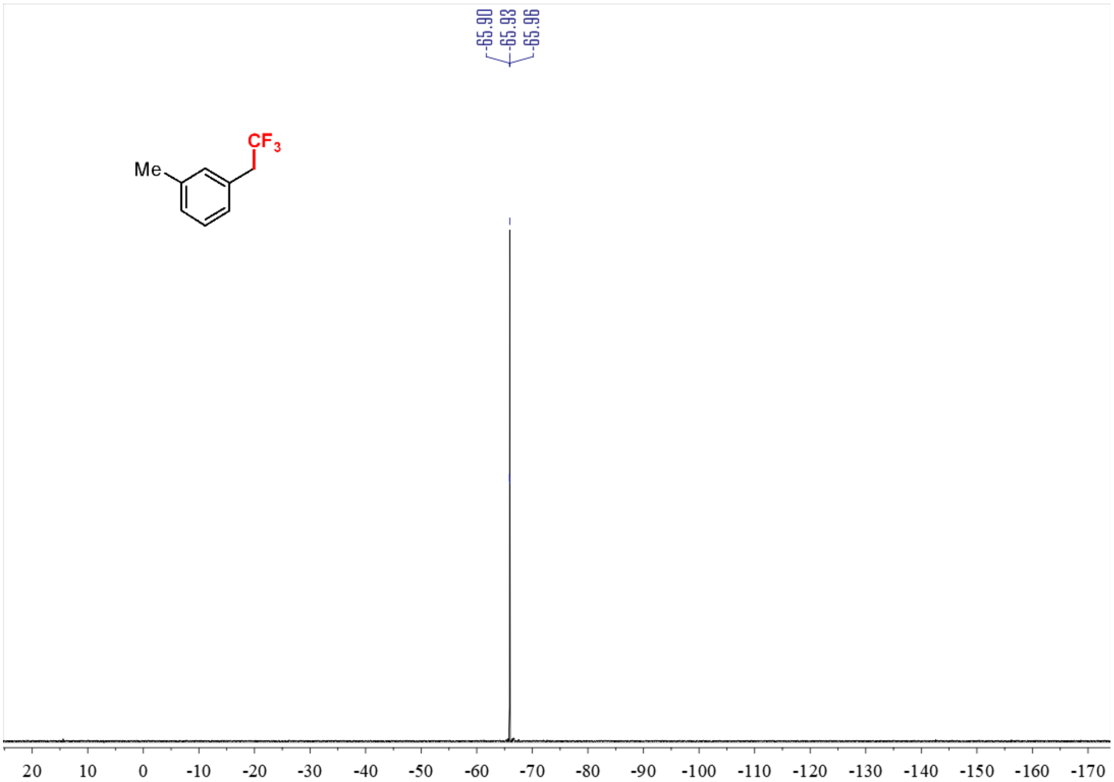
^{19}F NMR spectrum (375 MHz, $CDCl_3$, 23 ºC) of **3f**



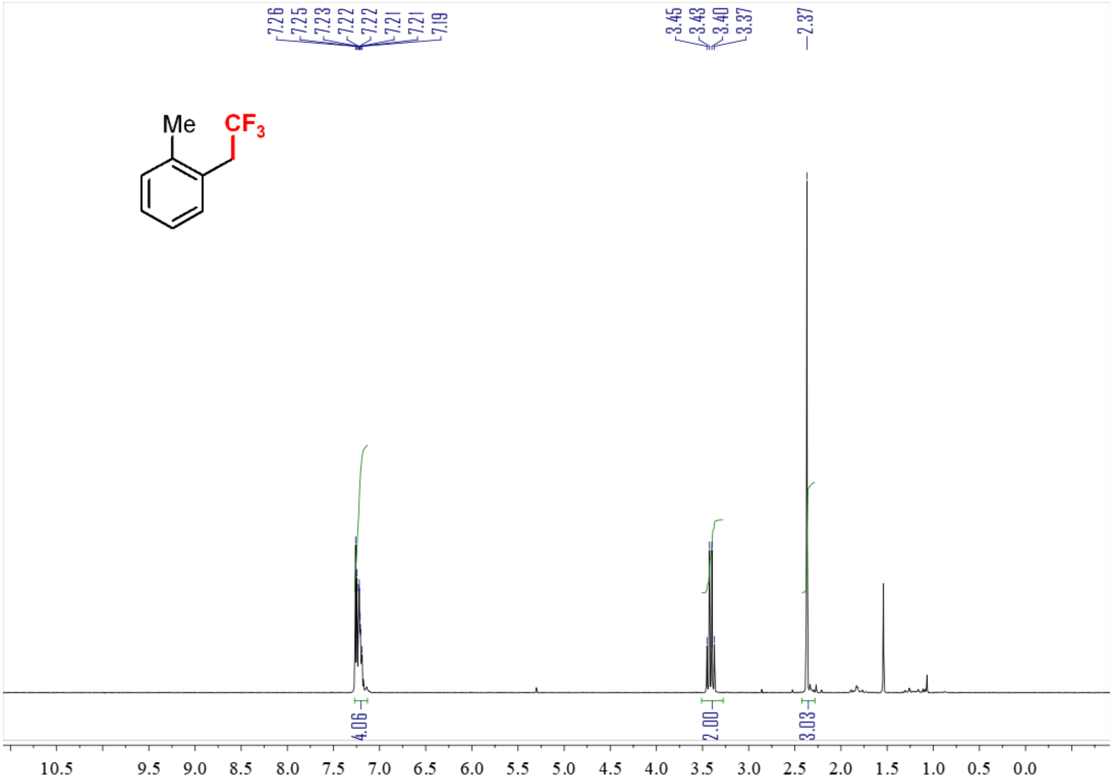
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of **3g**



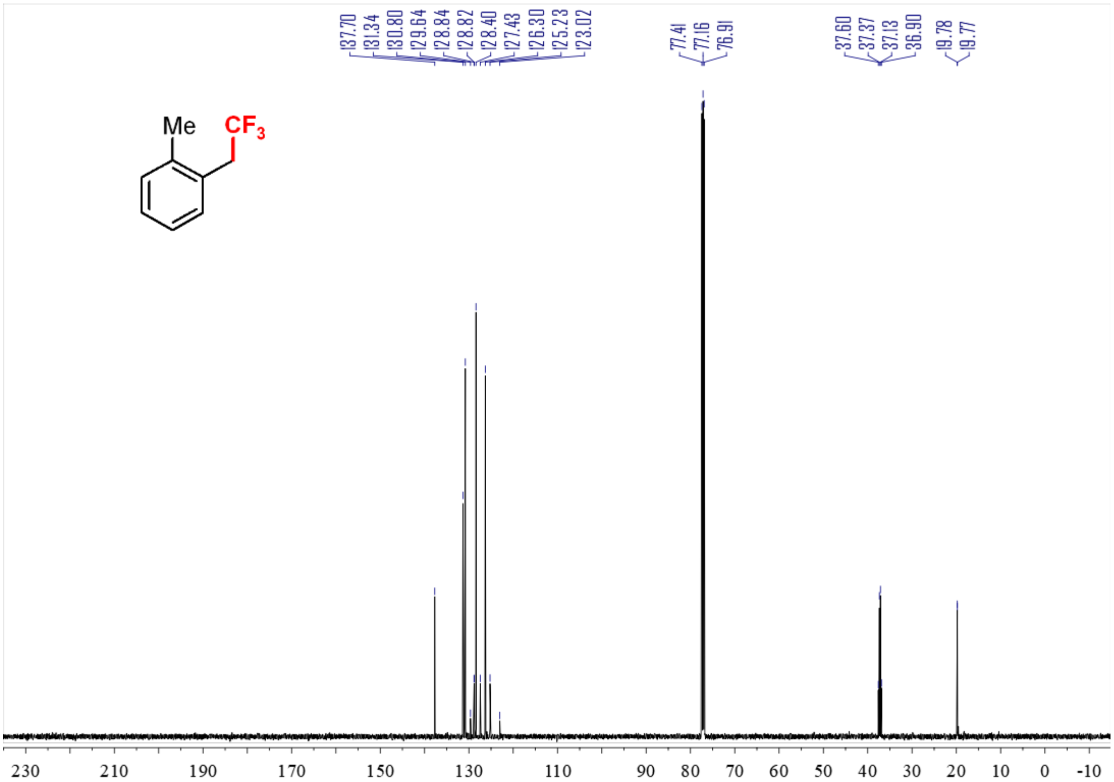
^{13}C NMR spectrum (126 MHz, $CDCl_3$, 23 ºC) of **3g**



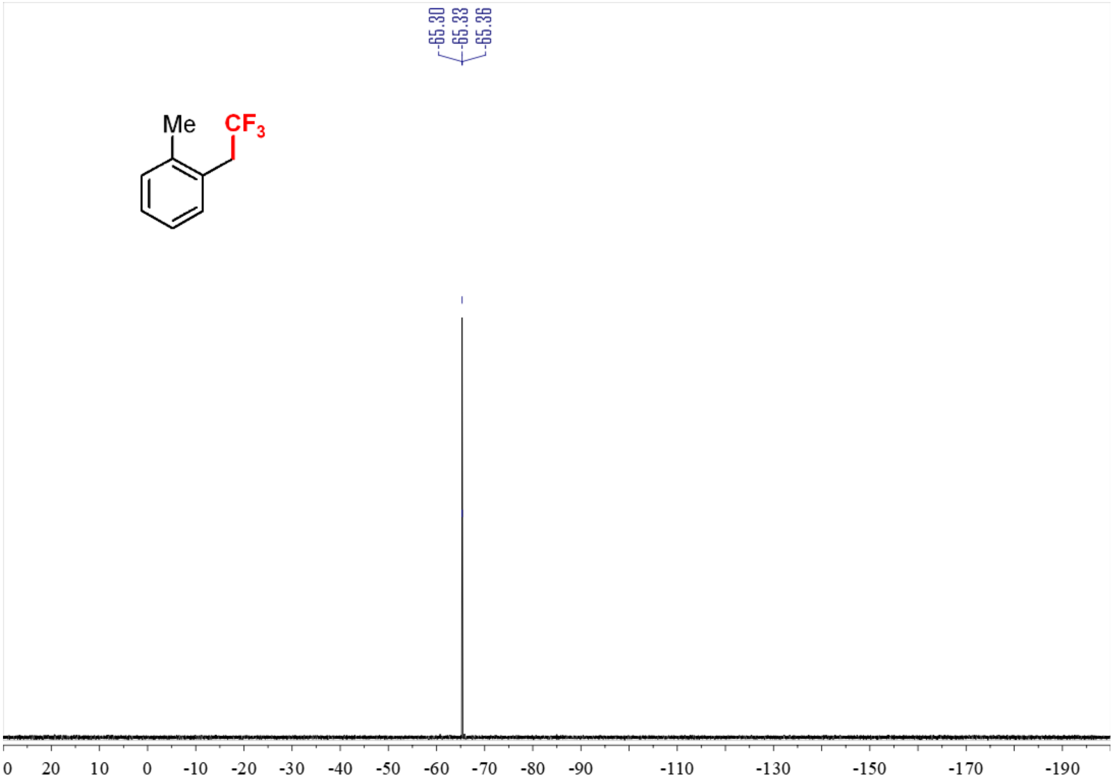
^{19}F NMR spectrum (375 MHz, $CDCl_3$, 23 ºC) of **3g**



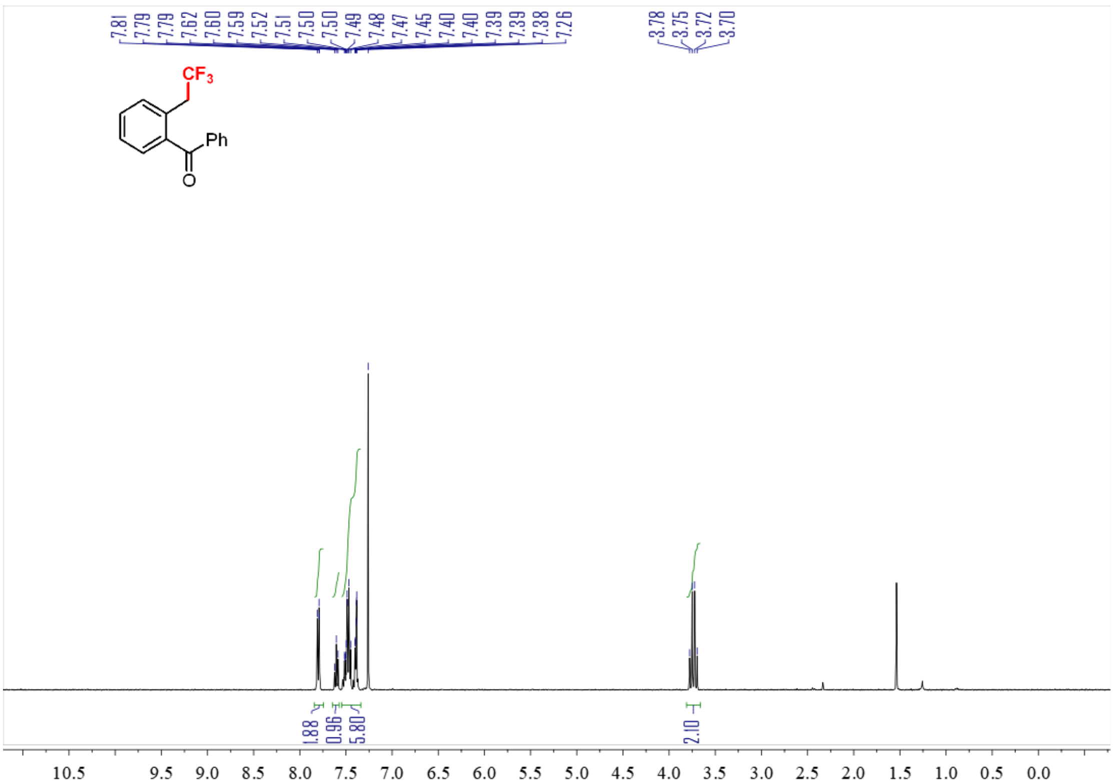
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of **3h**



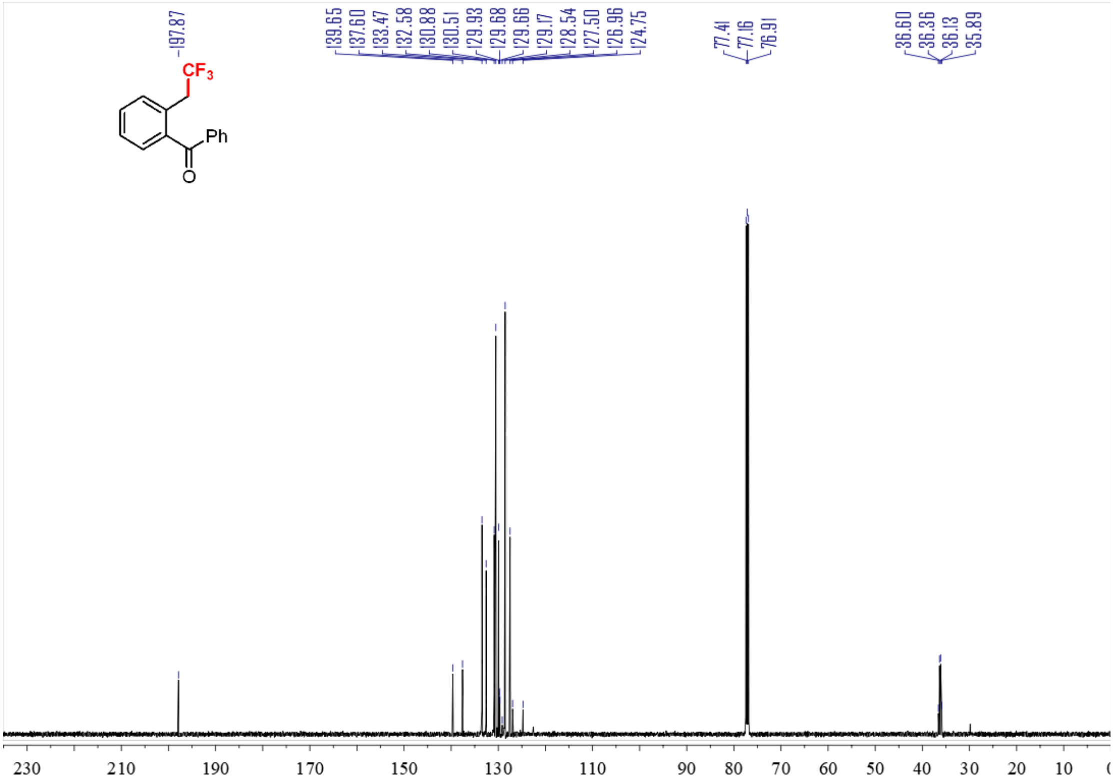
^{13}C NMR spectrum (126 MHz, $CDCl_3$, 23 ºC) of **3h**



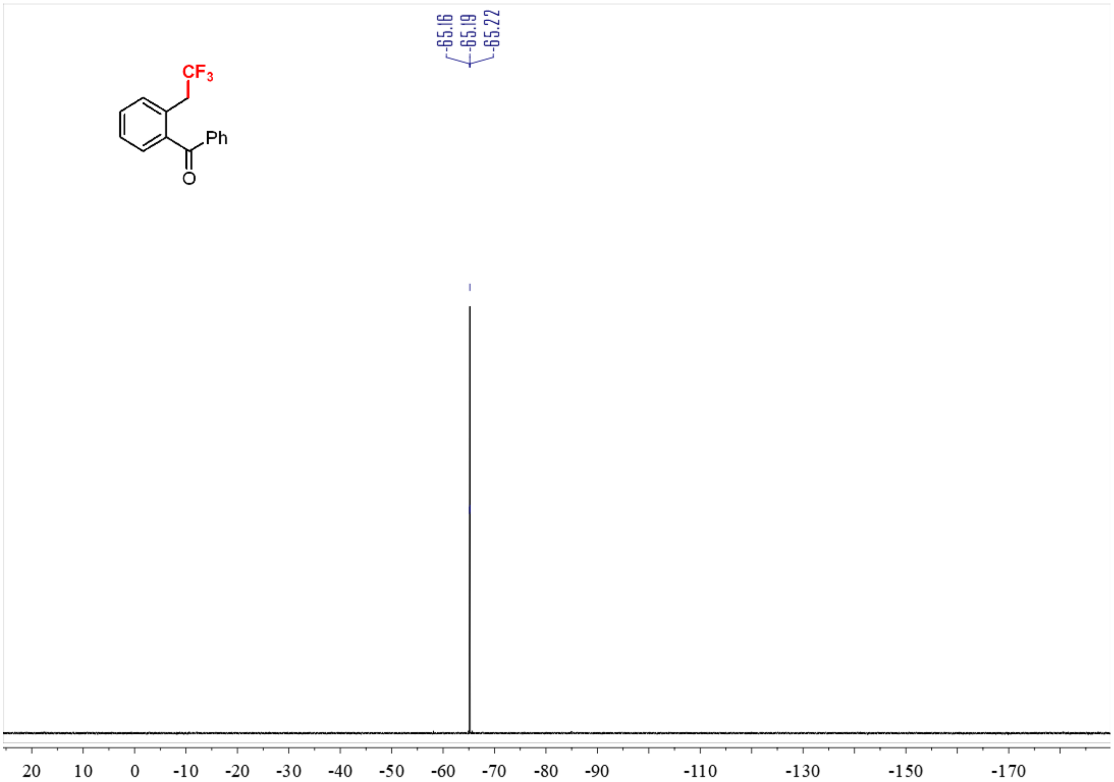
^{19}F NMR spectrum (375 MHz, CDCl$_3$, 23 ºC) of **3h**



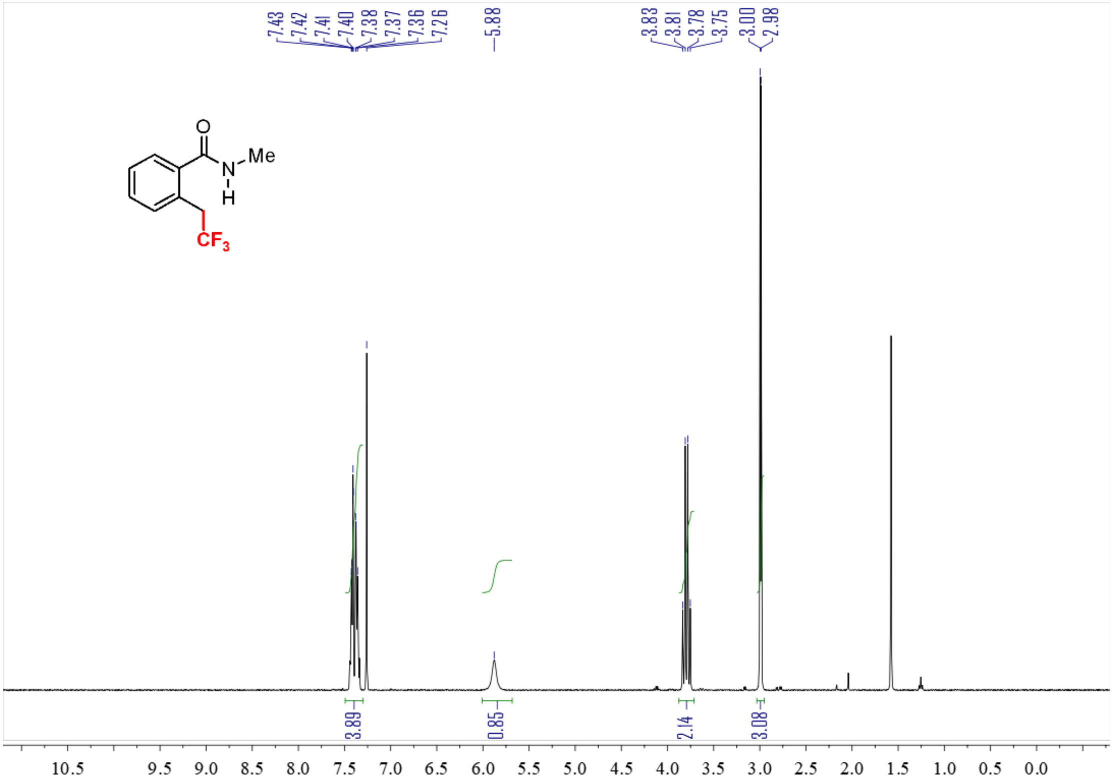
^{1}H NMR spectrum (400 MHz, CDCl$_3$, 23 ºC) of **3i**



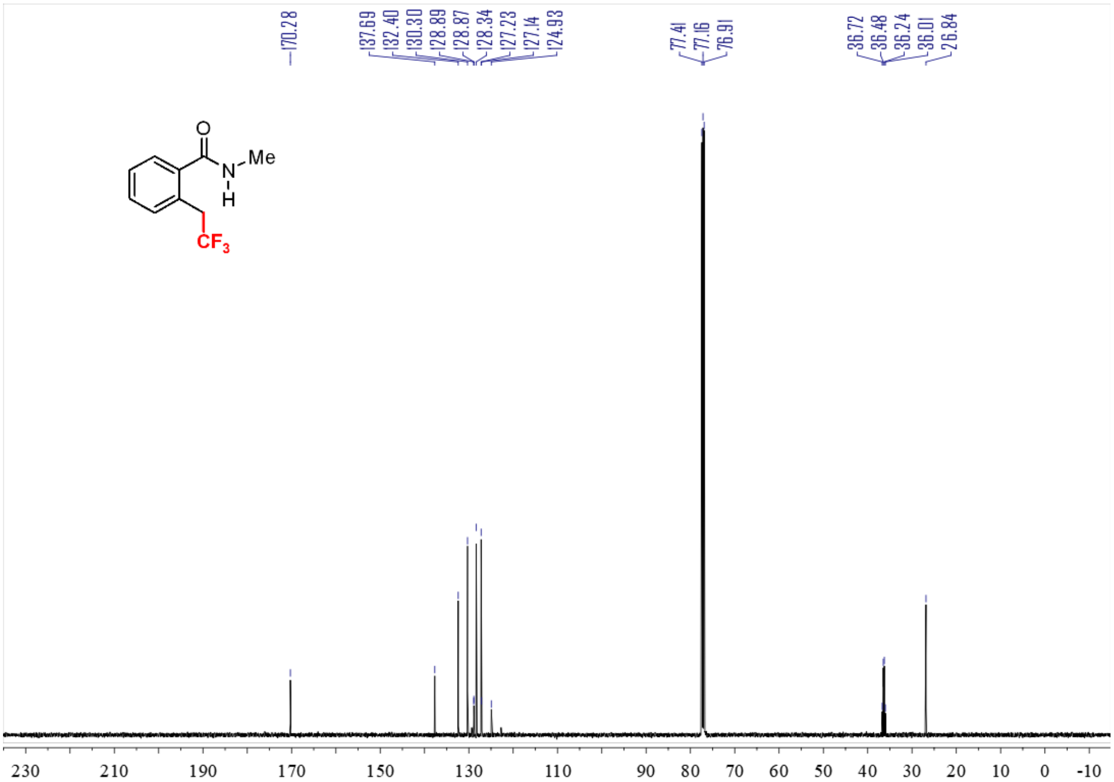
^{13}C NMR spectrum (126 MHz, CDCl₃, 23 ºC) of **3i**



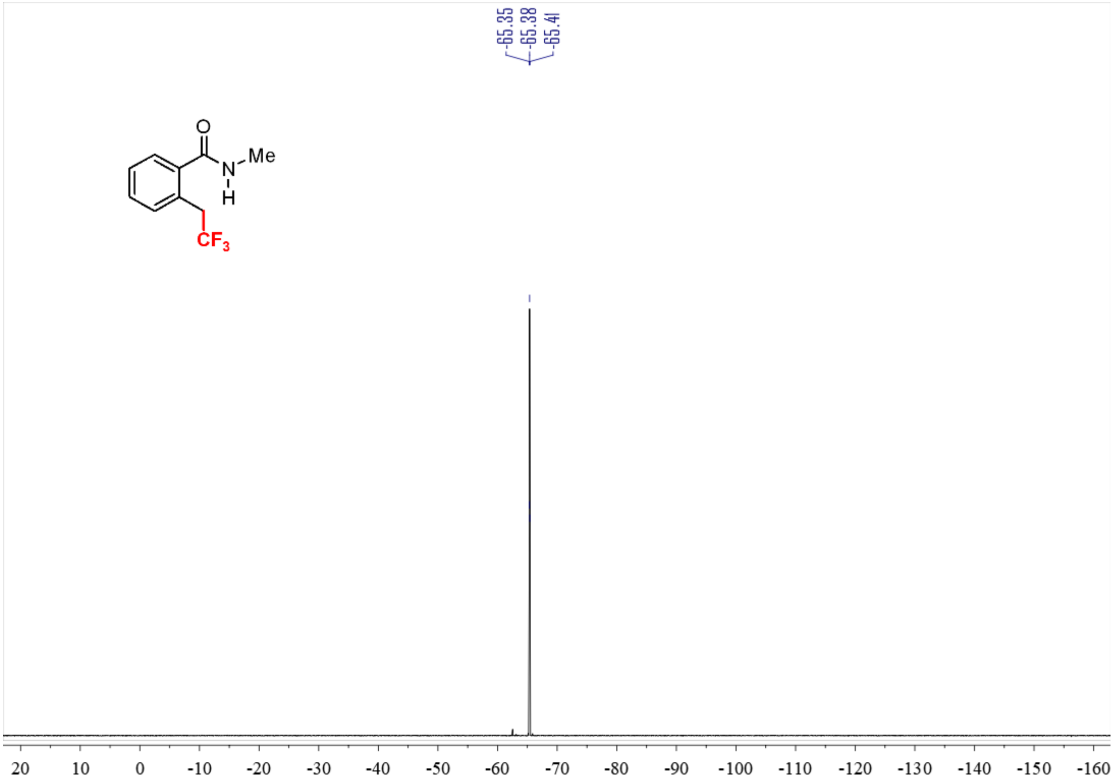
^{19}F NMR spectrum (375 MHz, CDCl₃, 23 ºC) of **3i**



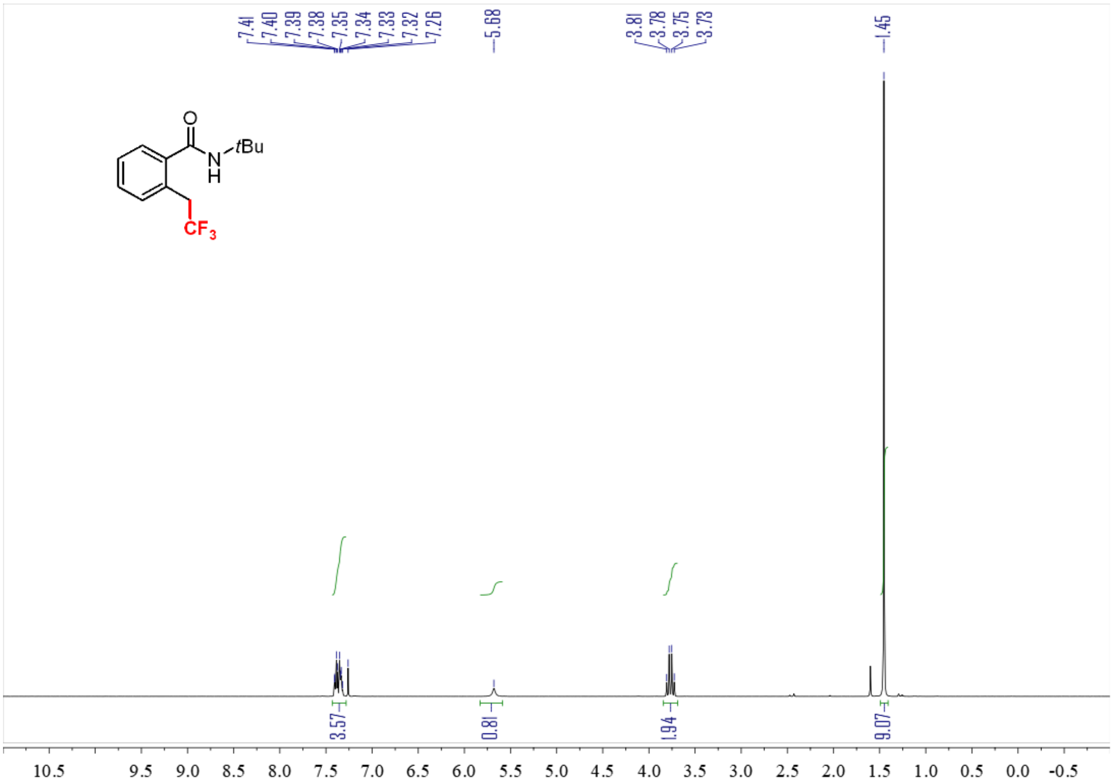
[1]H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of **3j**



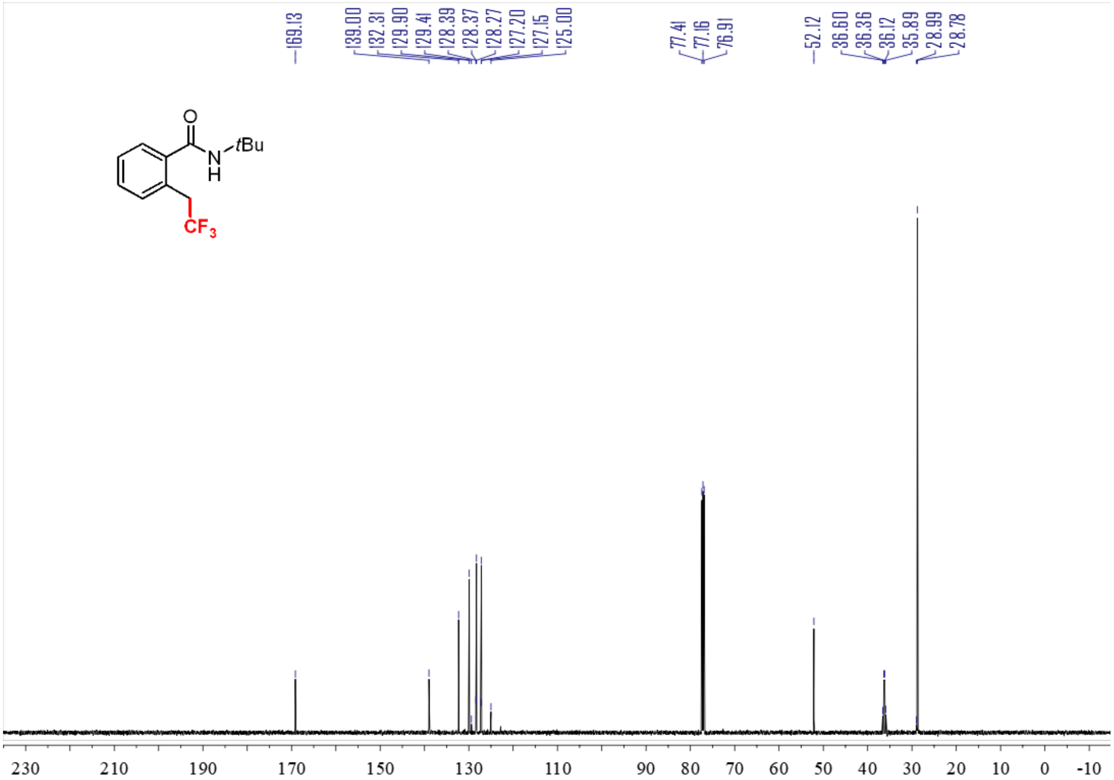
[13]C NMR spectrum (126 MHz, $CDCl_3$, 23 ºC) of **3j**



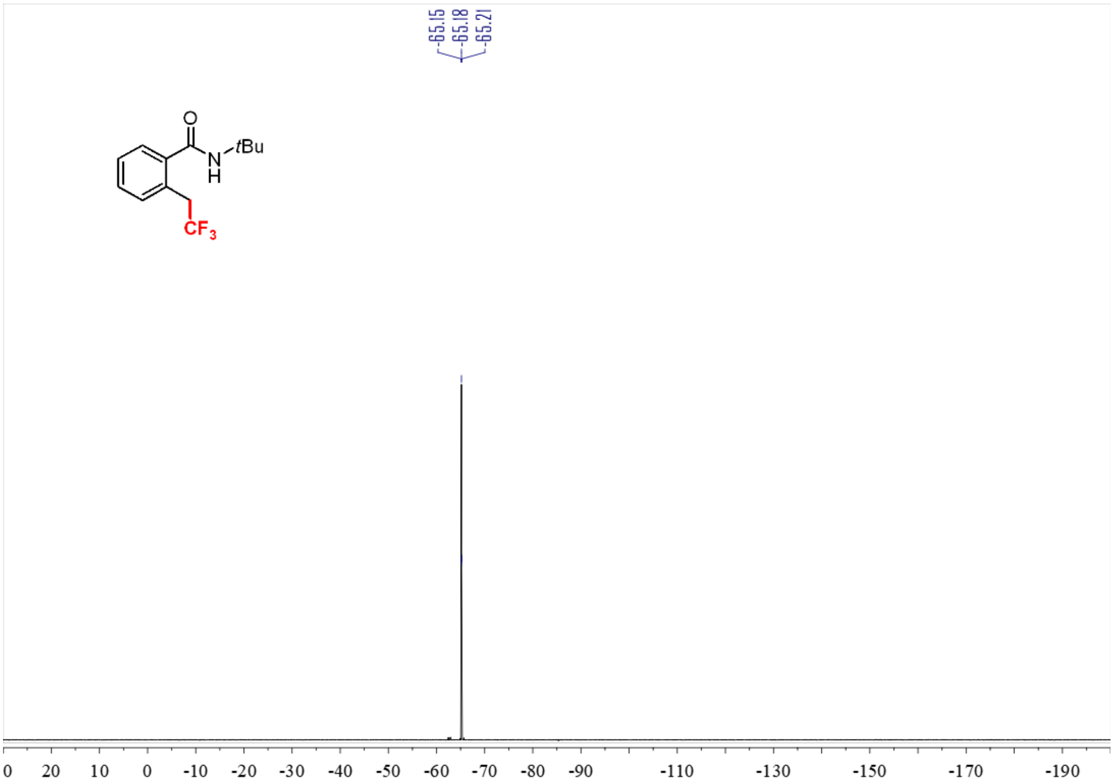
[19]F NMR spectrum (375 MHz, CDCl3, 23 ºC) of **3j**



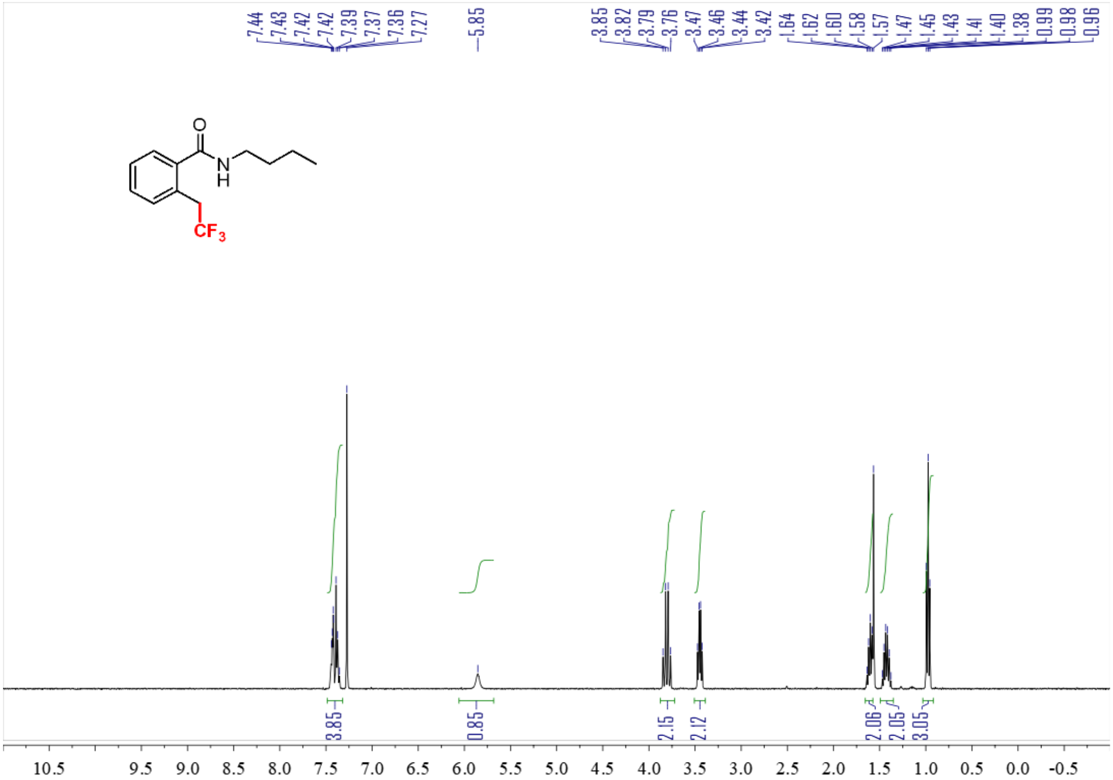
[1]H NMR spectrum (400 MHz, CDCl3, 23 ºC) of **3k**



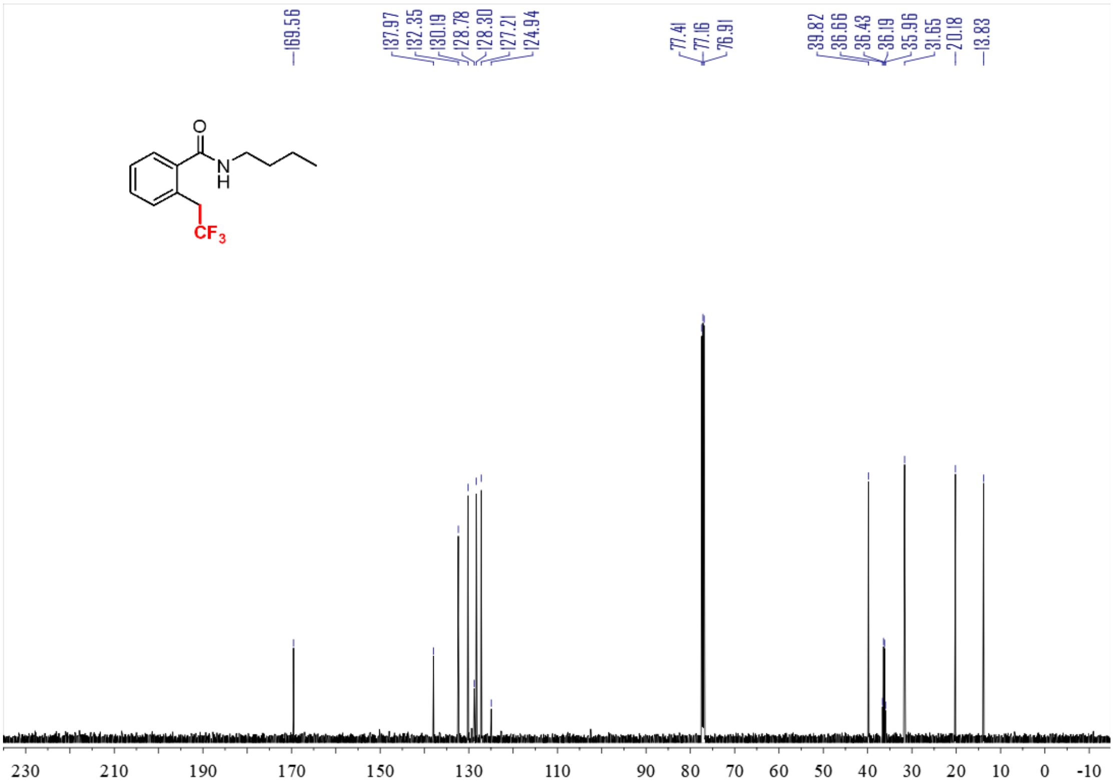
^{13}C NMR spectrum (126 MHz, CDCl3, 23 ºC) of **3k**



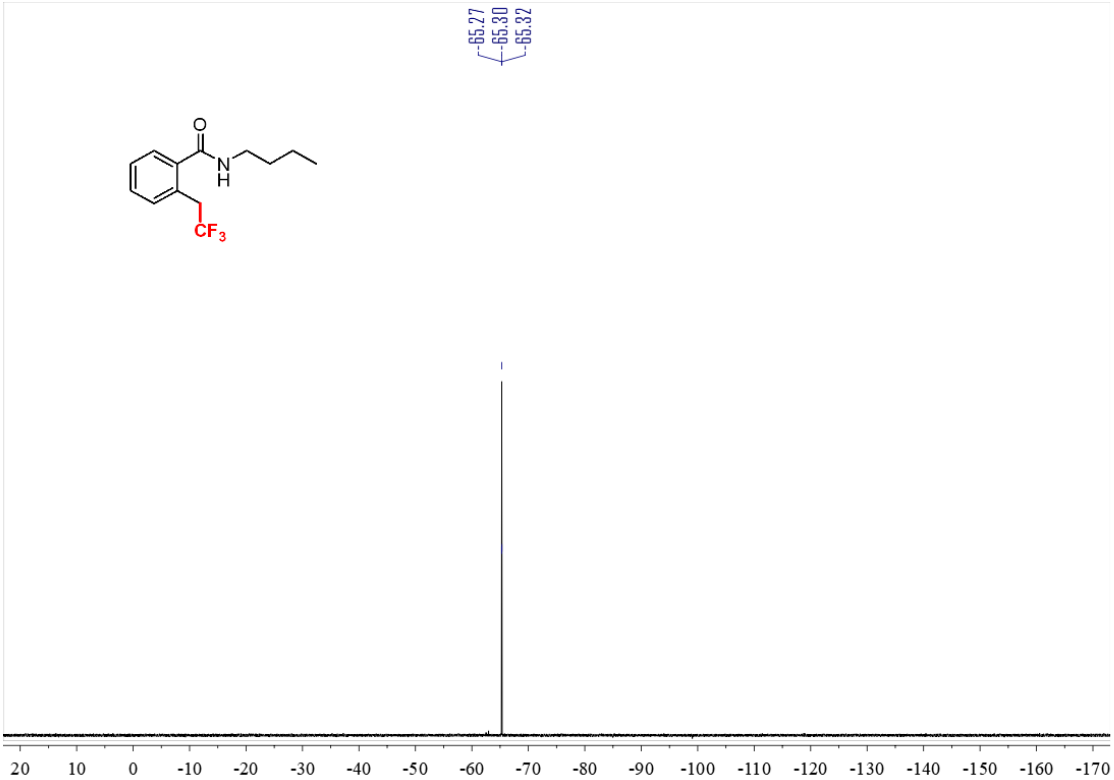
^{19}F NMR spectrum (375 MHz, CDCl3, 23 ºC) of **3k**



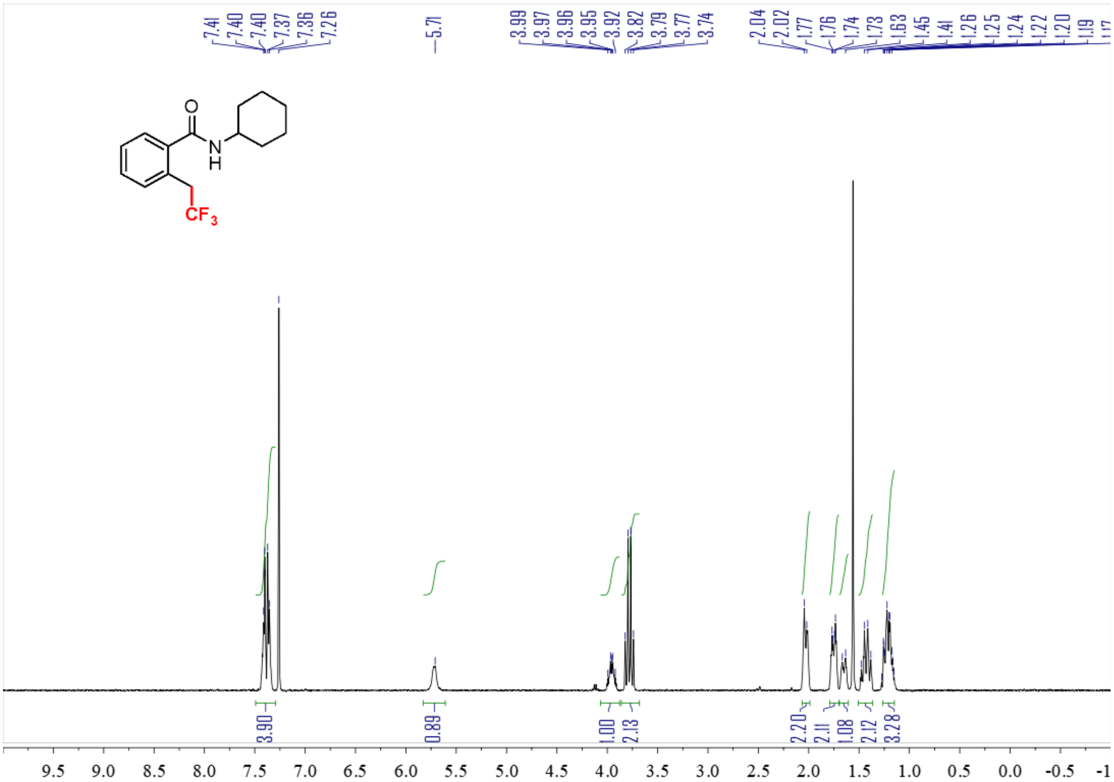
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of **3l**



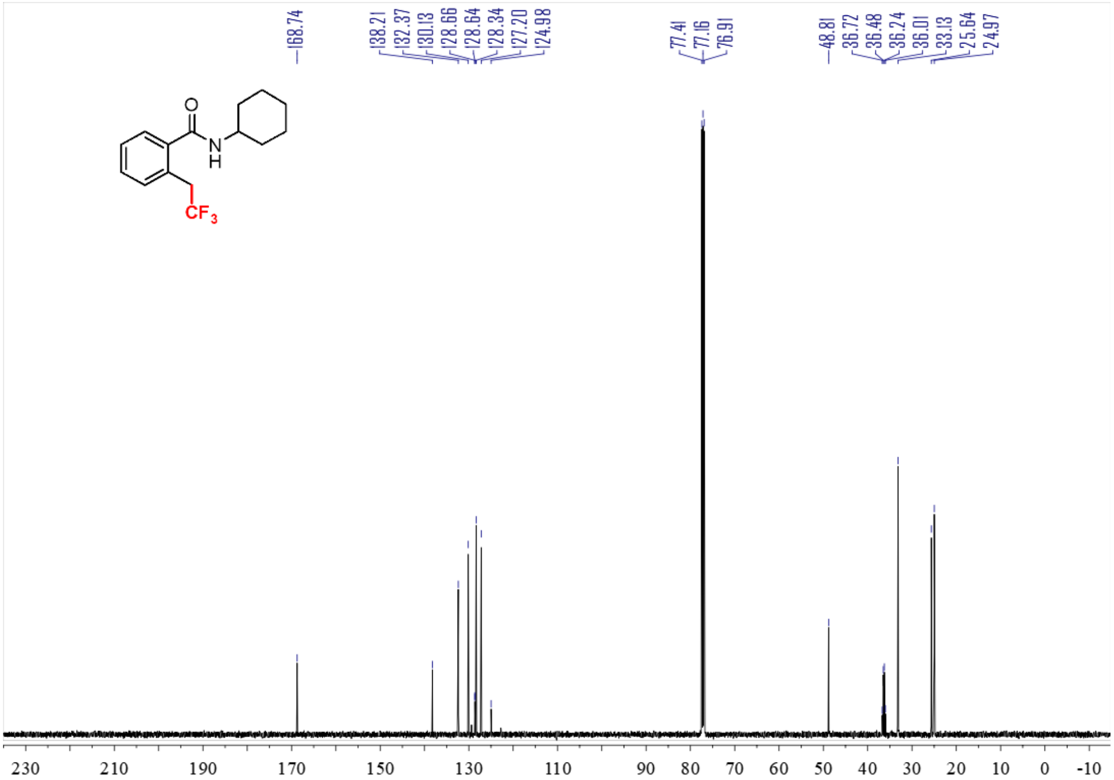
^{13}C NMR spectrum (126 MHz, $CDCl_3$, 23 ºC) of **3l**



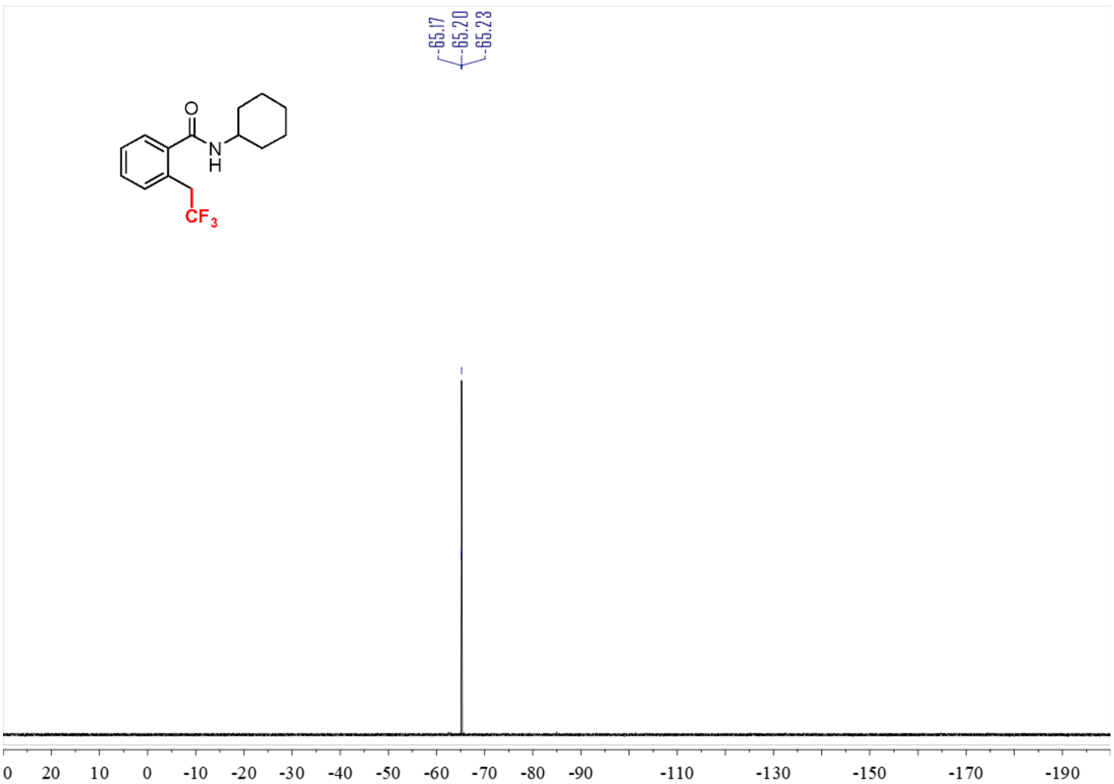
^{19}F NMR spectrum (375 MHz, $CDCl_3$, 23 ºC) of **3l**



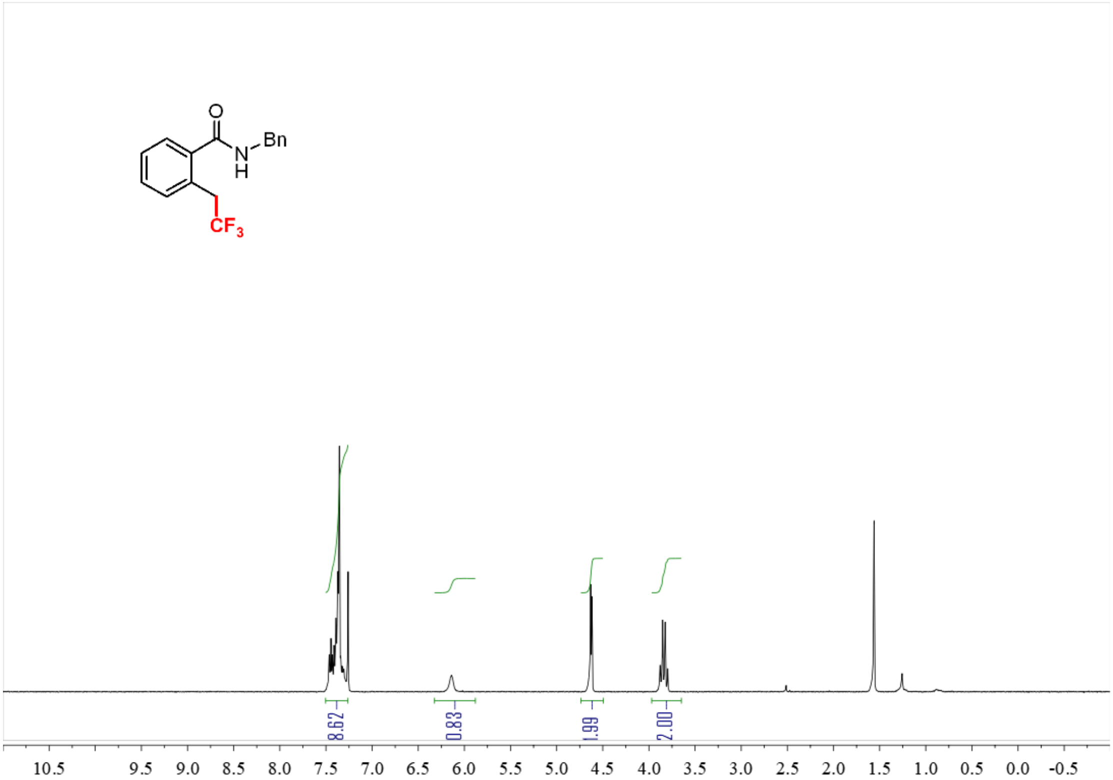
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of **3m**



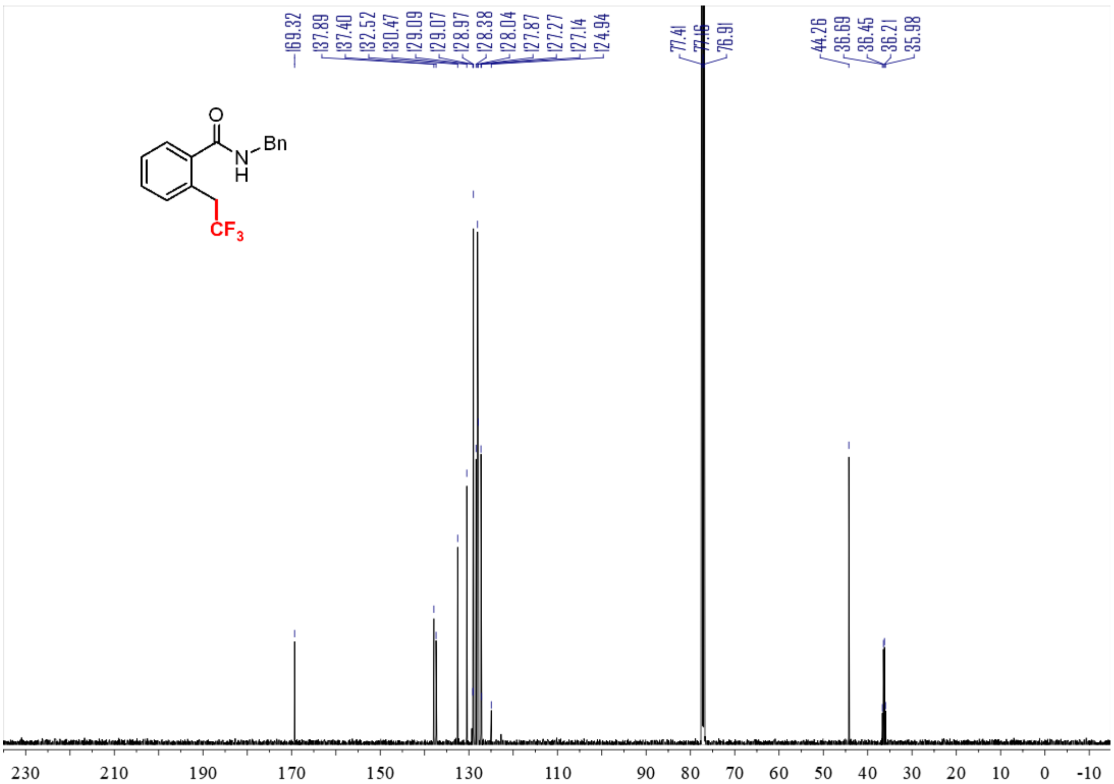
^{13}C NMR spectrum (126 MHz, $CDCl_3$, 23 °C) of **3m**



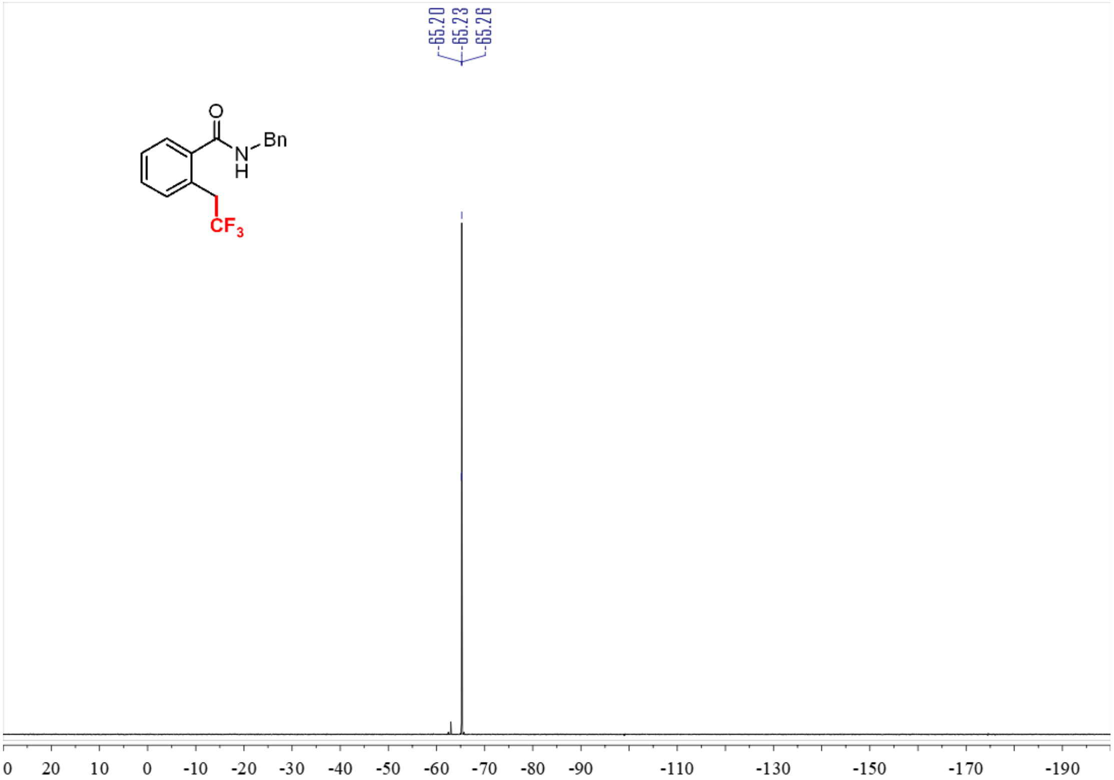
^{19}F NMR spectrum (375 MHz, $CDCl_3$, 23 °C) of **3m**



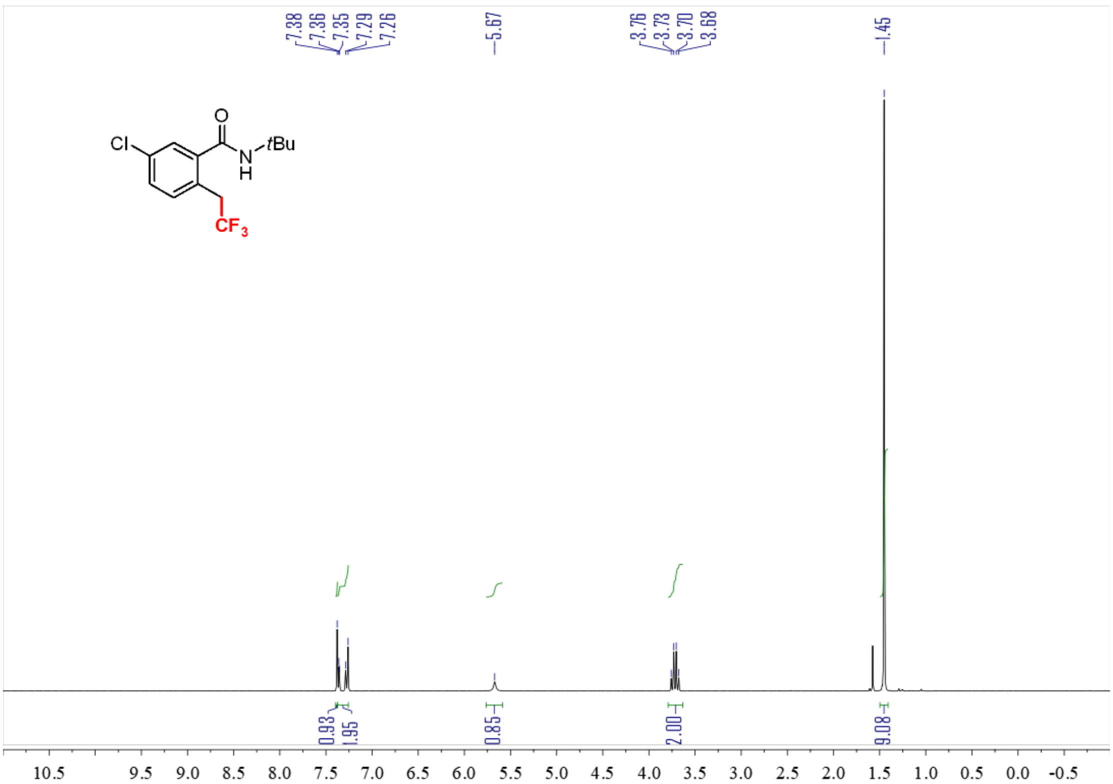
[1]H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of **3n**



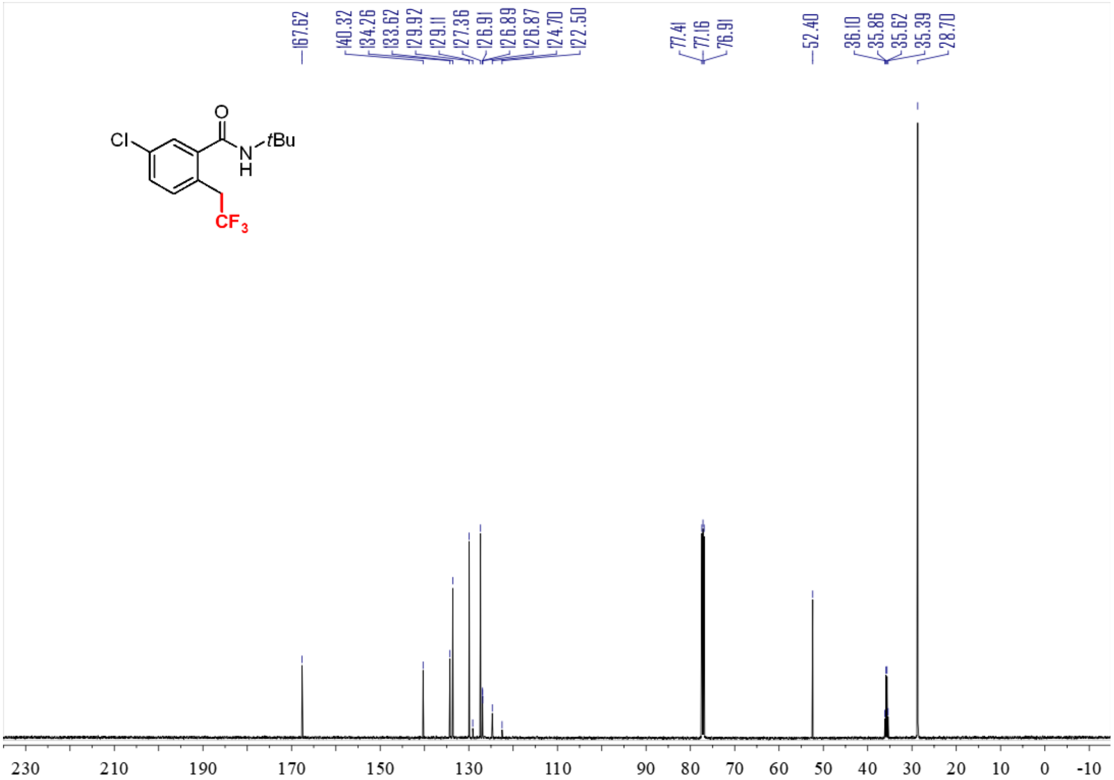
[13]C NMR spectrum (126 MHz, $CDCl_3$, 23 ºC) of **3n**



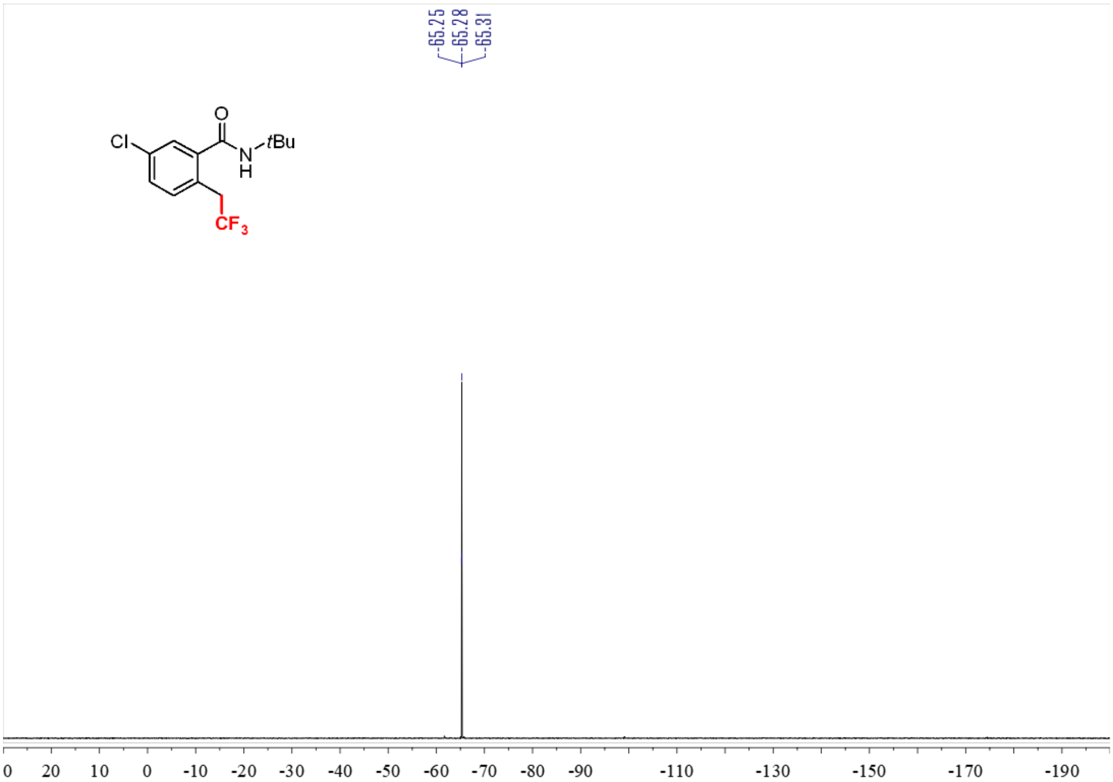
^{19}F NMR spectrum (375 MHz, $CDCl_3$, 23 ºC) of **3n**



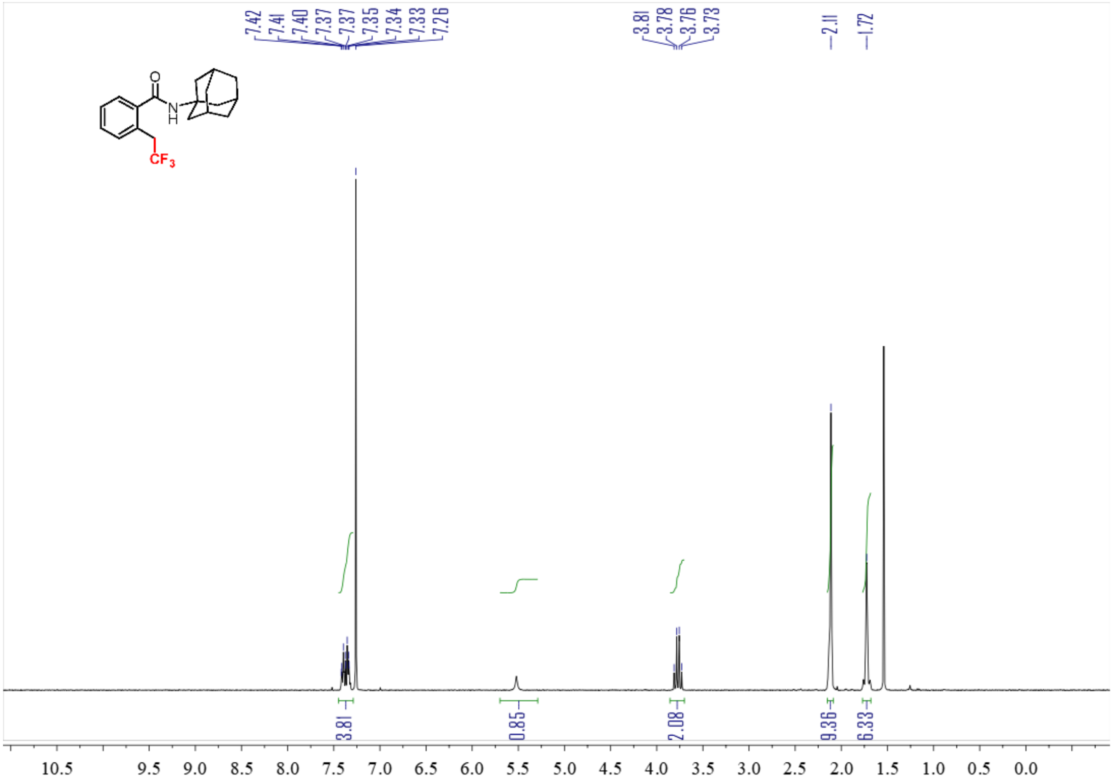
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of **3o**



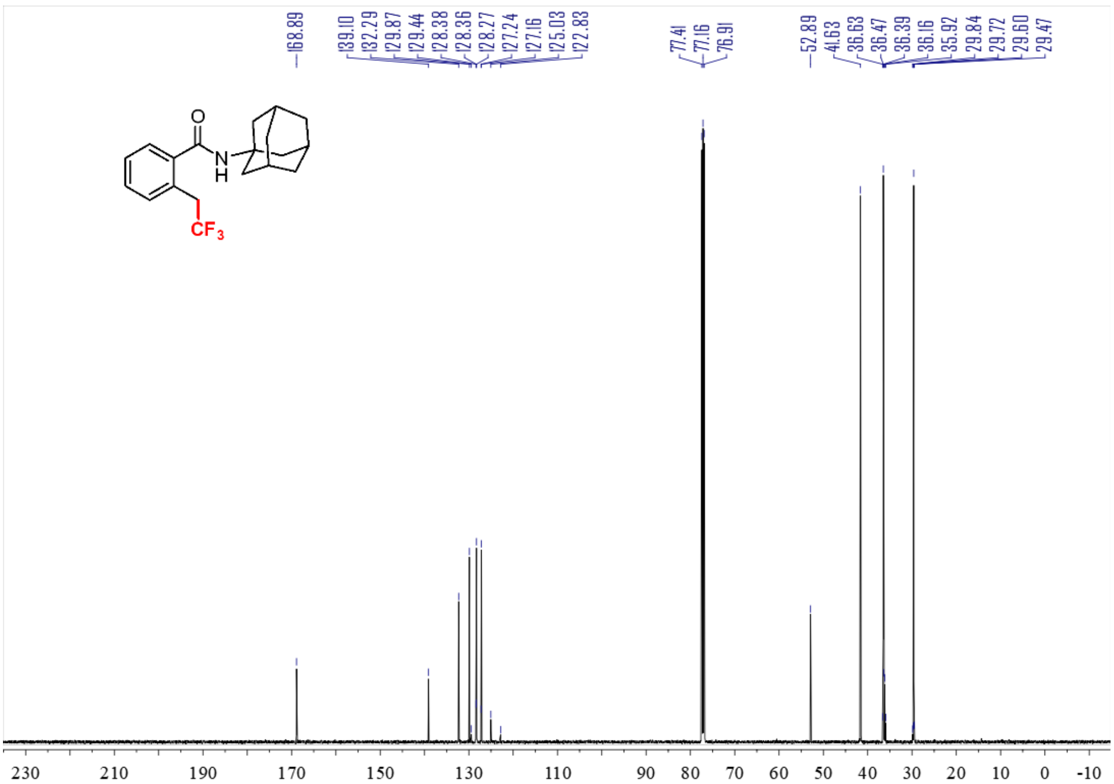
^{13}C NMR spectrum (126 MHz, CDCl₃, 23 ºC) of **3o**



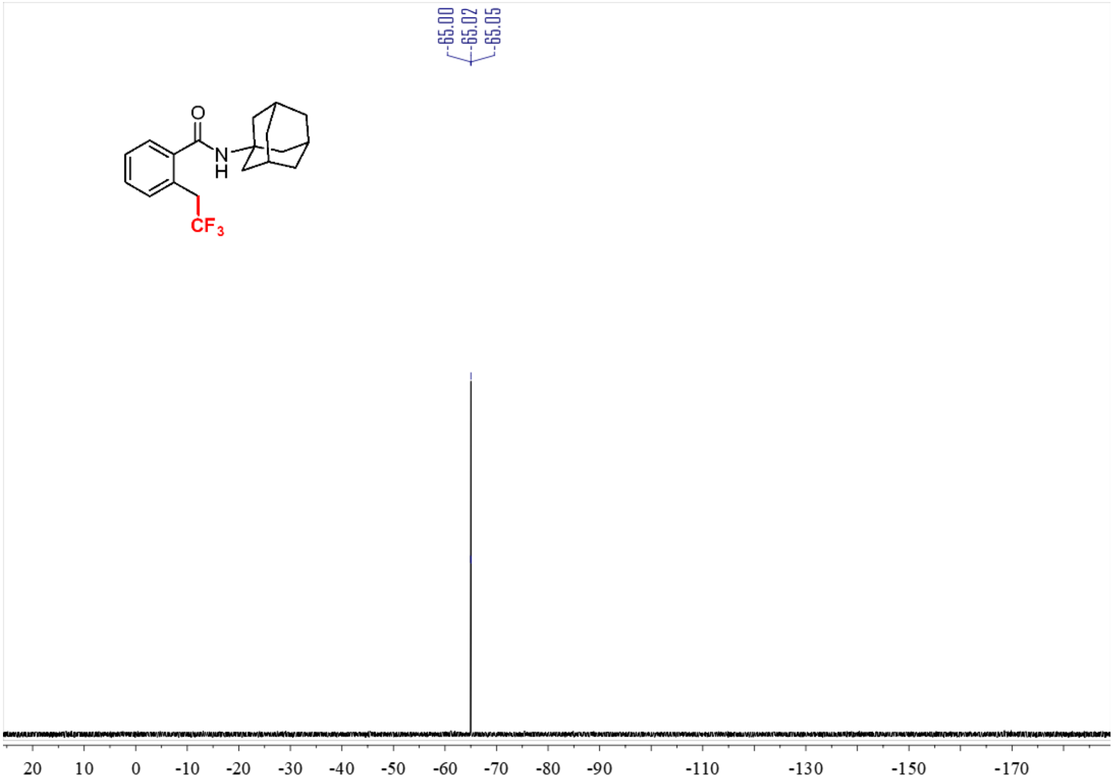
^{19}F NMR spectrum (375 MHz, CDCl₃, 23 ºC) of **3o**



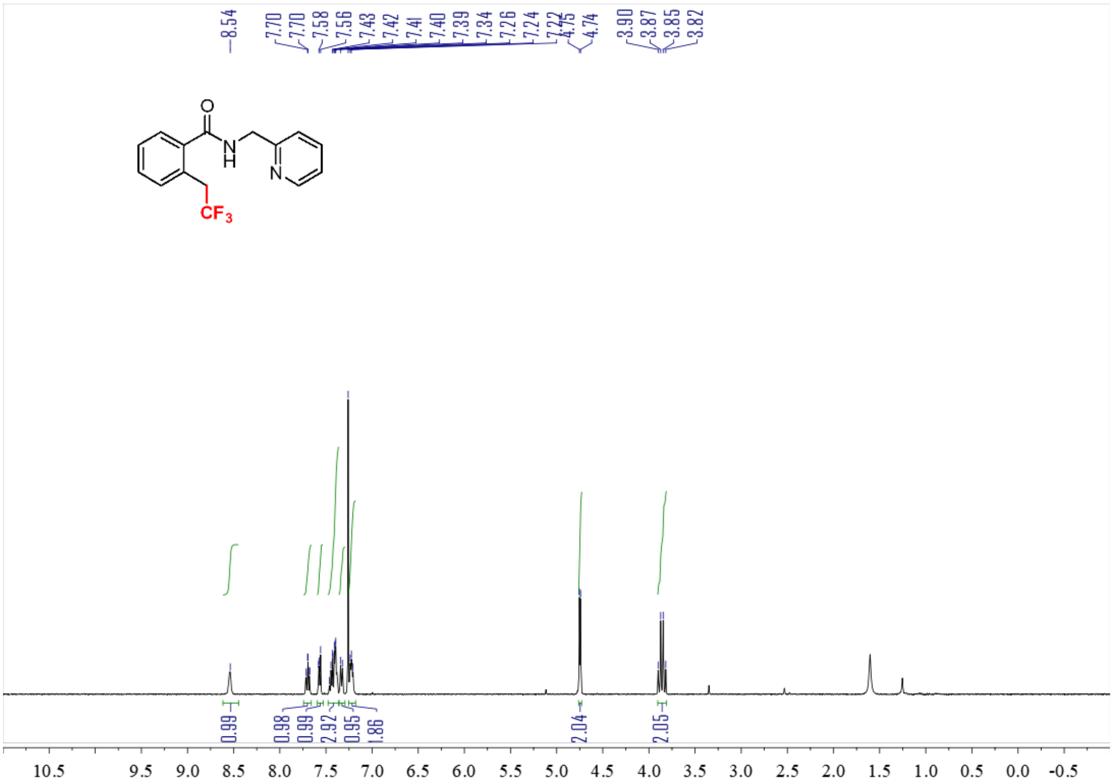
[1]H NMR spectrum (400 MHz, $CDCl_3$, 23 °C) of **3p**



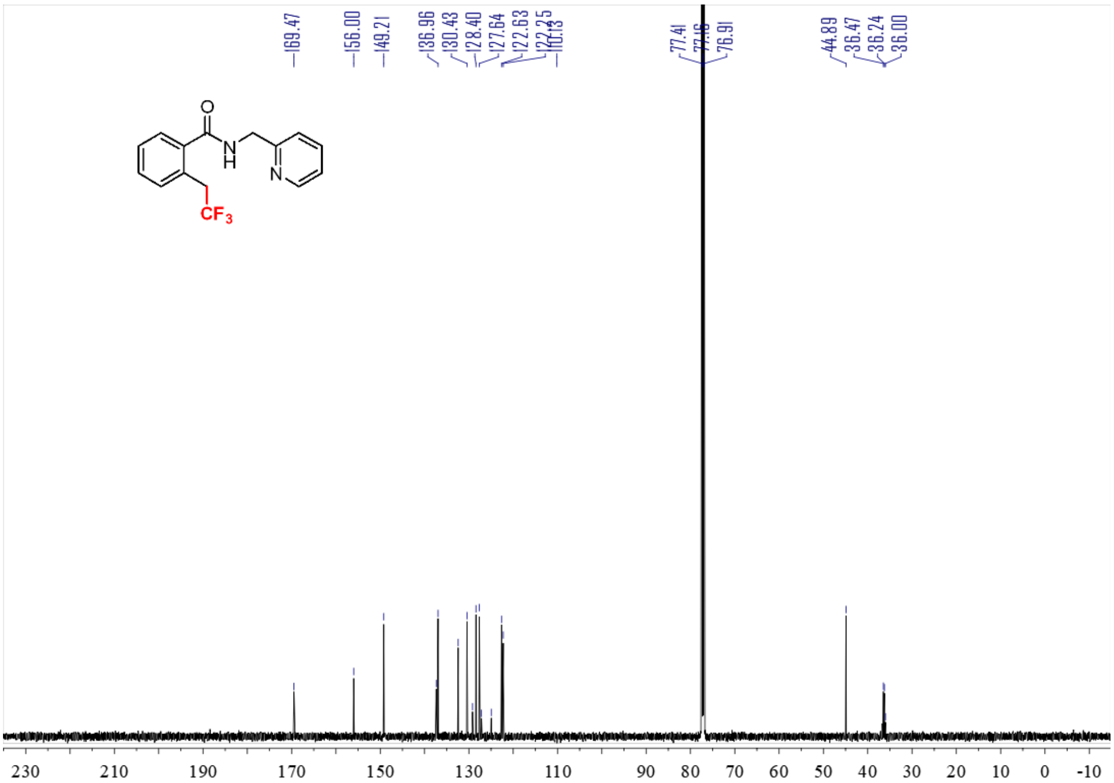
[13]C NMR spectrum (126 MHz, $CDCl_3$, 23 °C) of **3p**



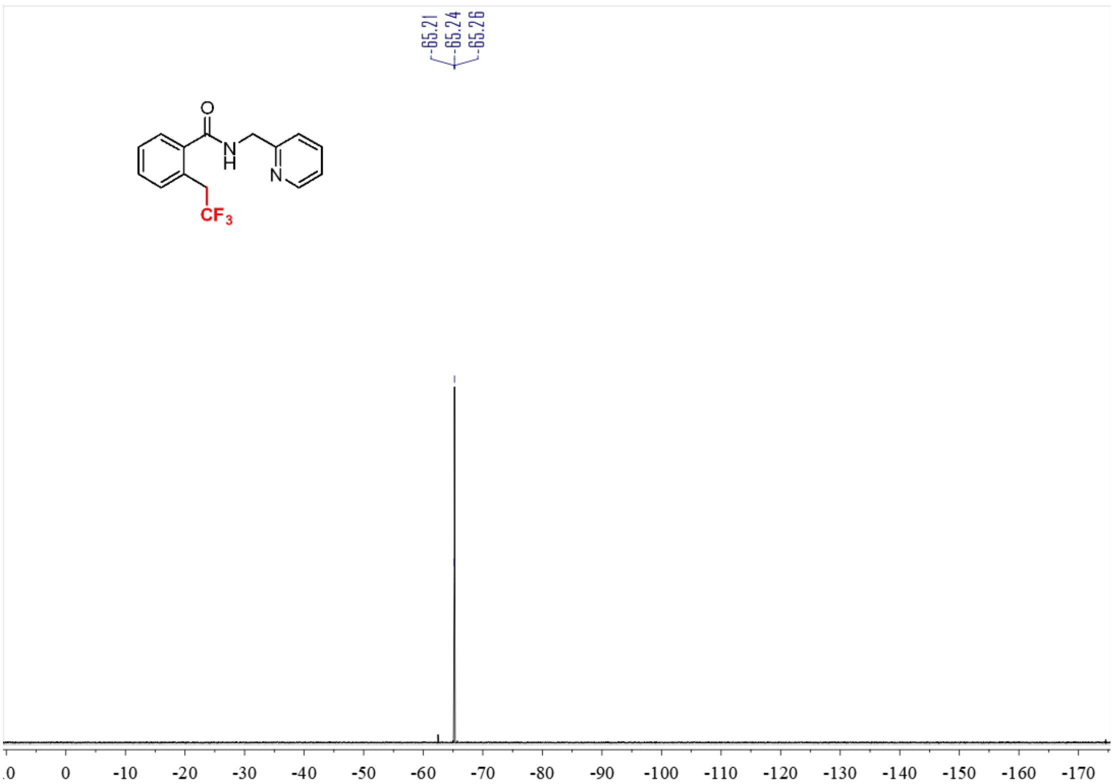
[19]F NMR spectrum (375 MHz, $CDCl_3$, 23 ºC) of **3p**



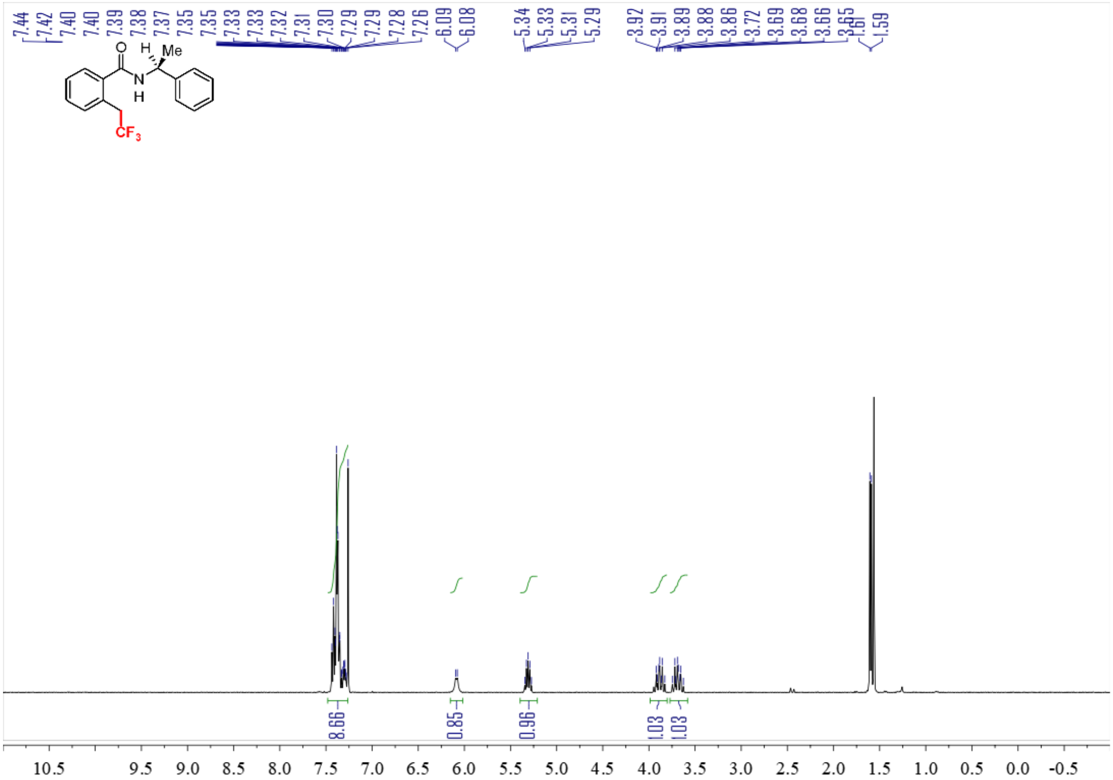
[1]H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of **3q**



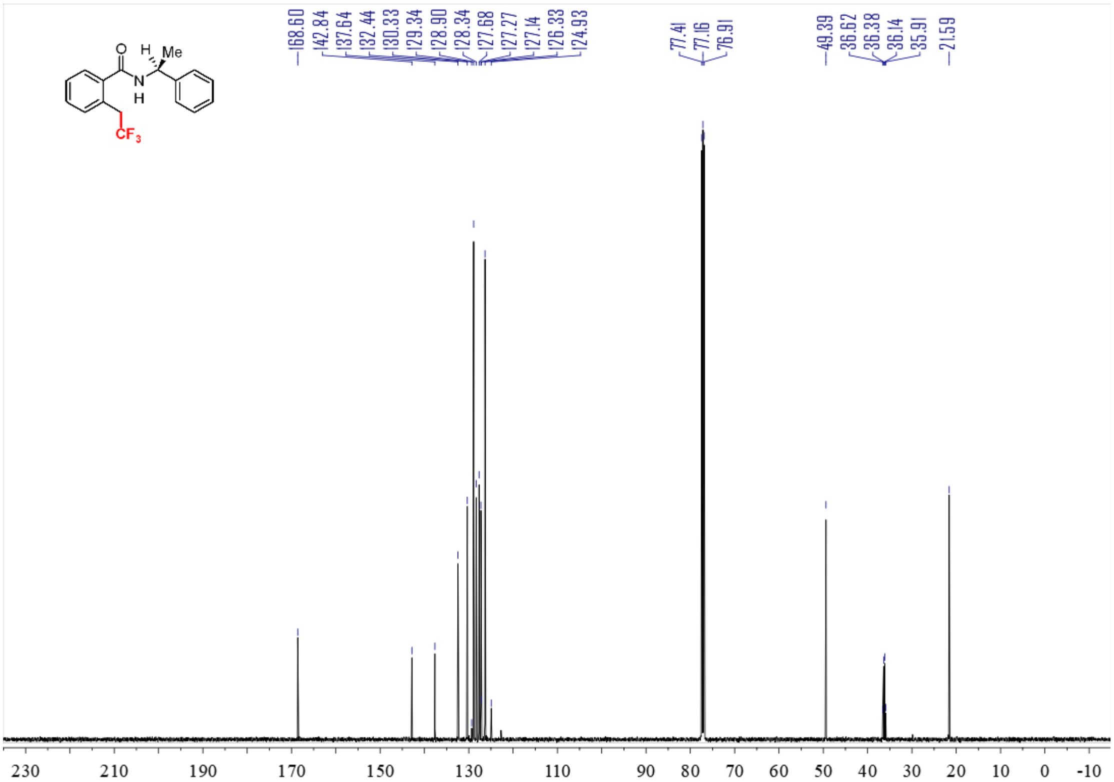
^{13}C NMR spectrum (126 MHz, CDCl₃, 23 ºC) of **3q**



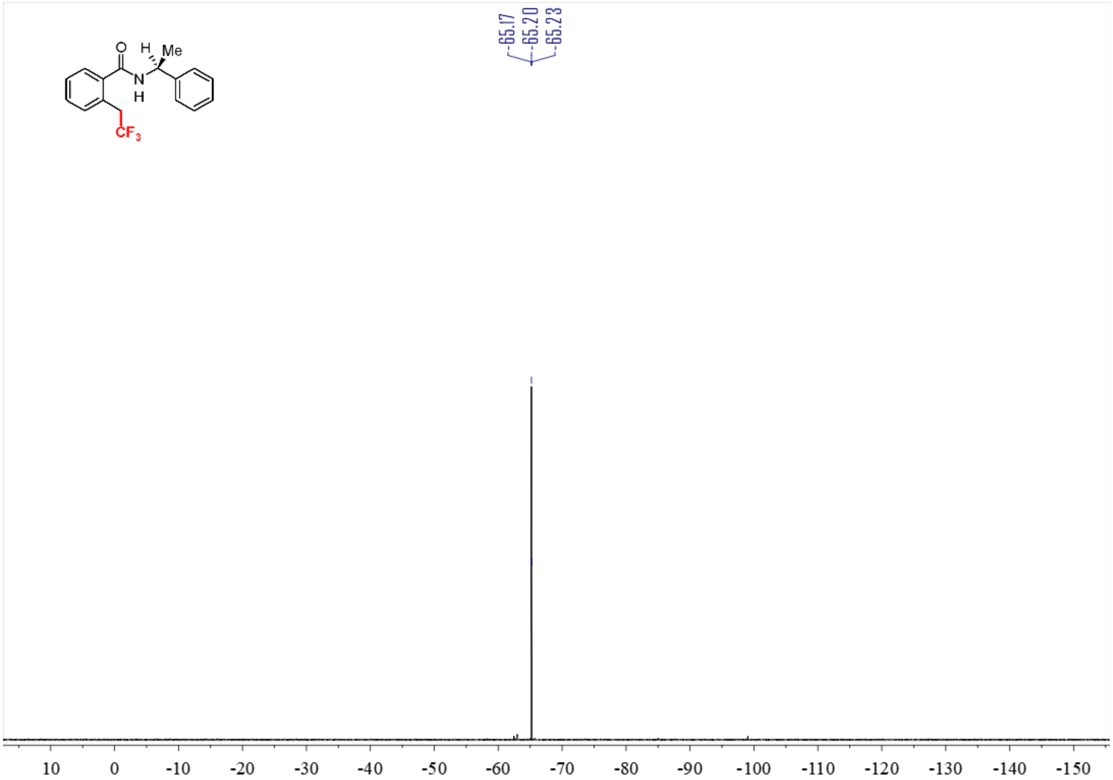
^{19}F NMR spectrum (375 MHz, CDCl₃, 23 ºC) of **3q**



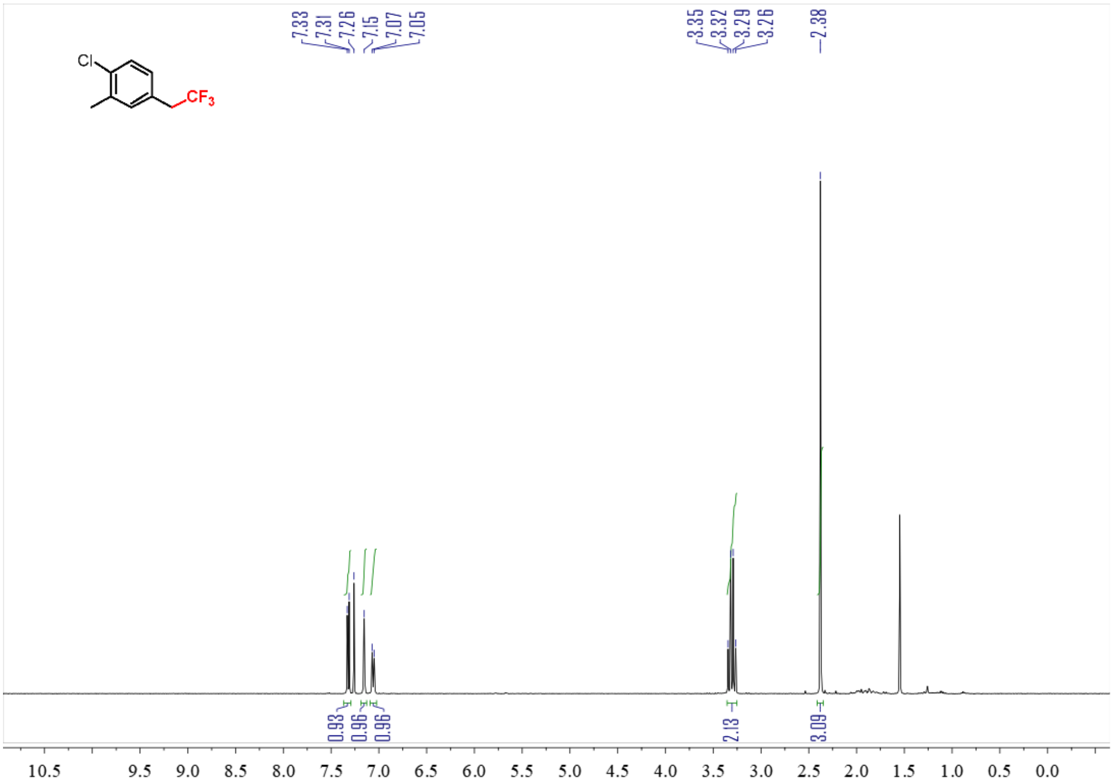
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of **3r**



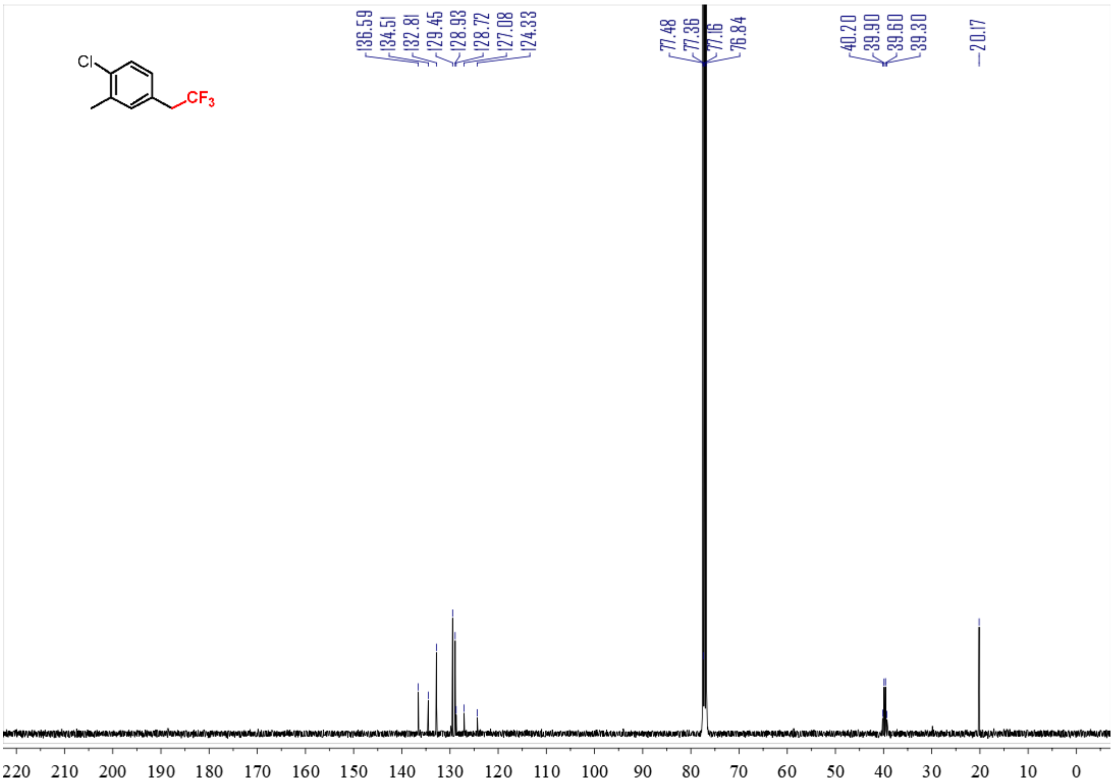
^{13}C NMR spectrum (126 MHz, $CDCl_3$, 23 ºC) of **3r**



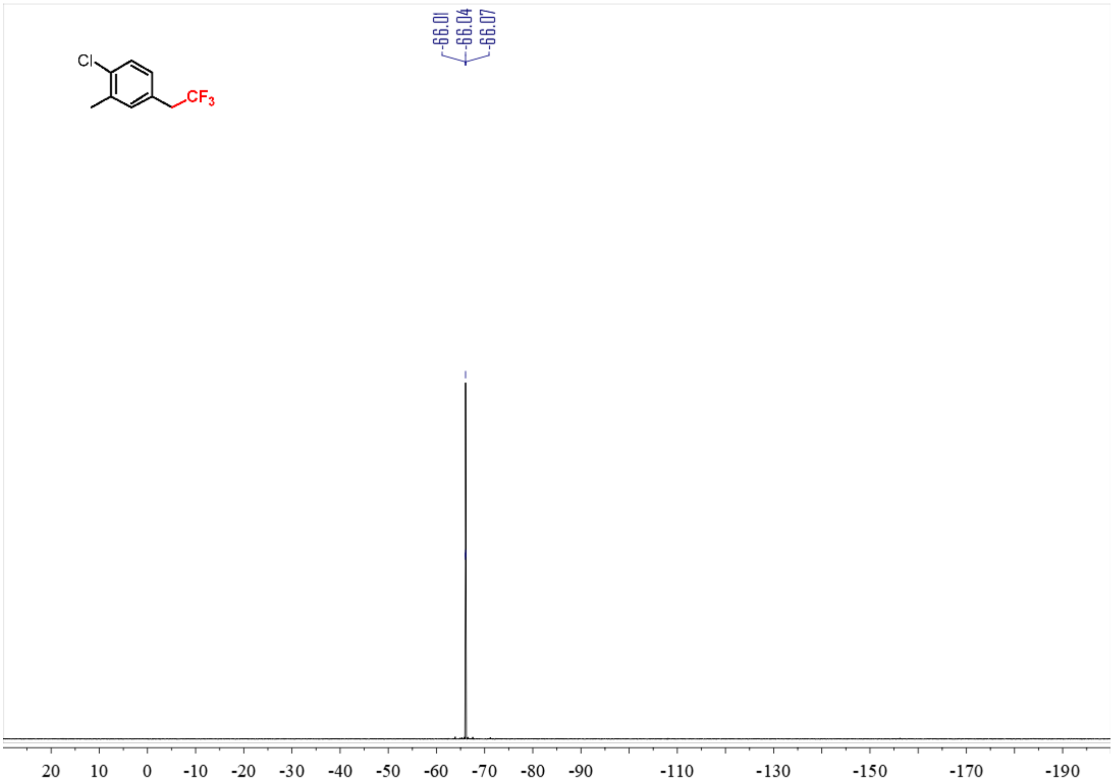
^{19}F NMR spectrum (375 MHz, $CDCl_3$, 23 ºC) of **3r**



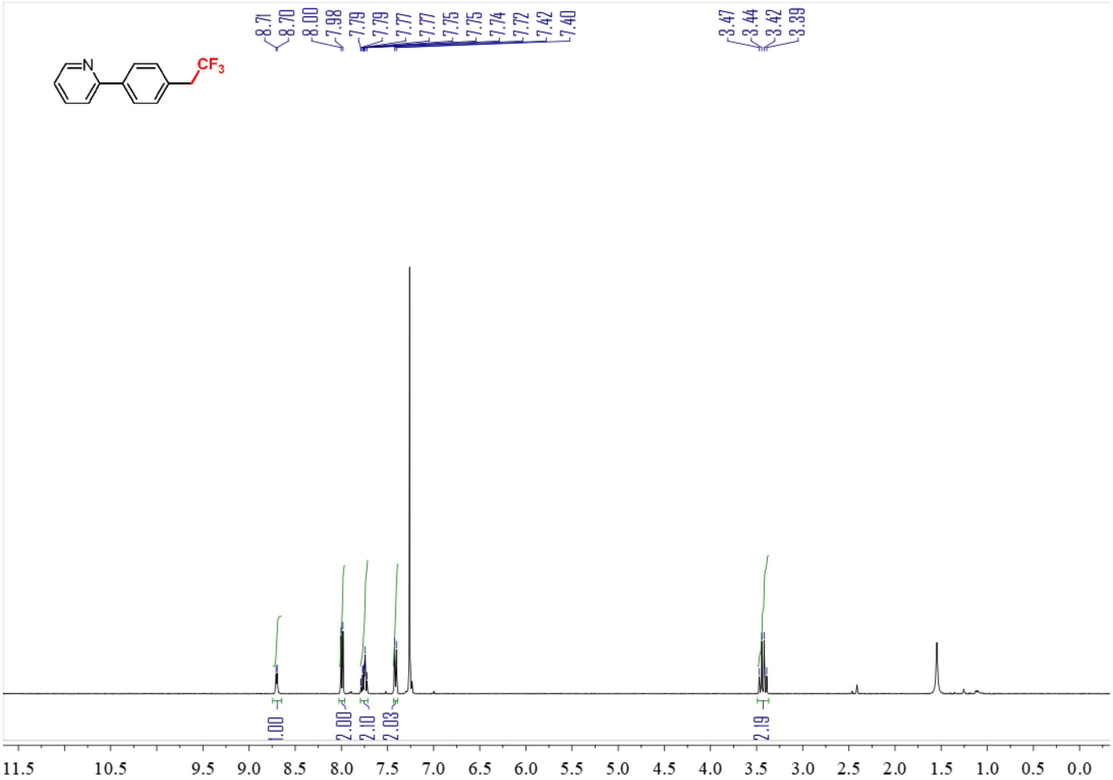
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of **3s**



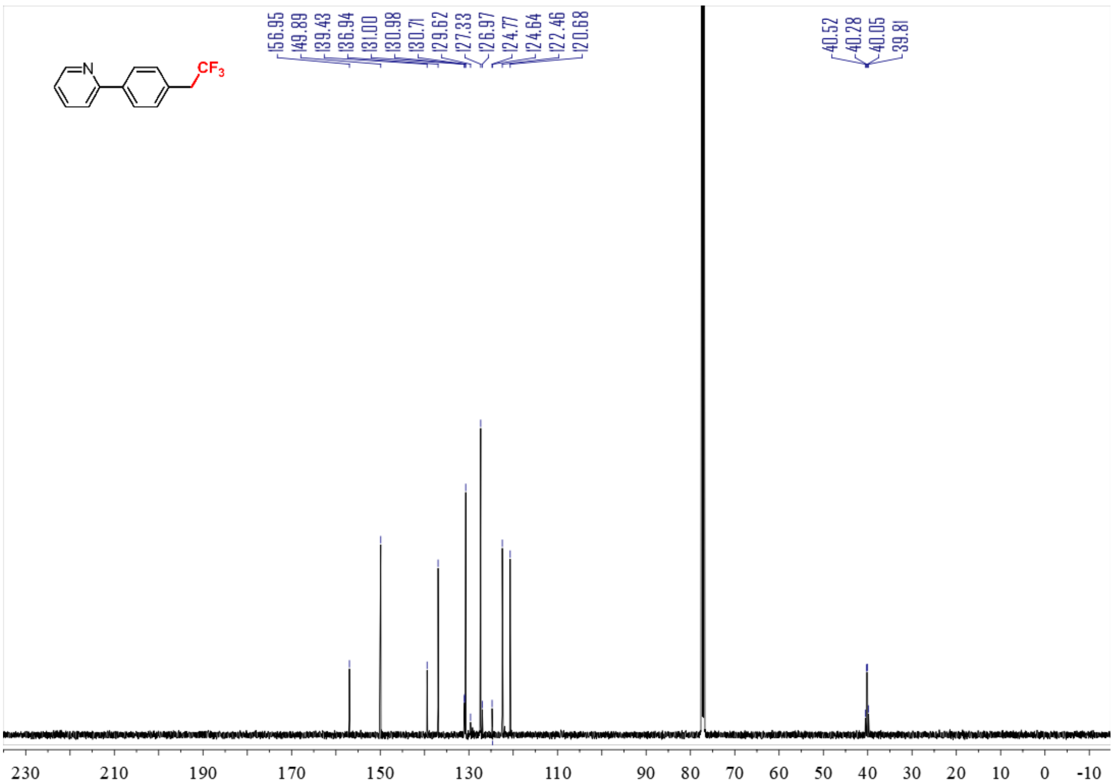
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 23 ºC) of **3s**



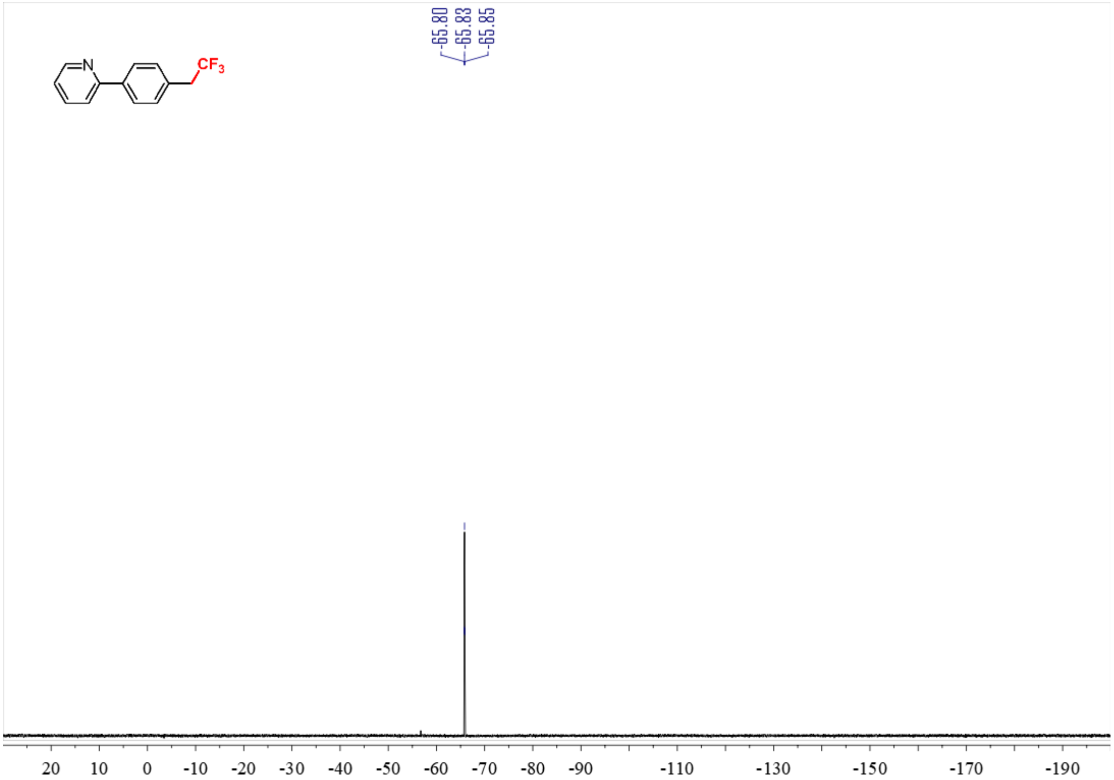
^{19}F NMR spectrum (375 MHz, $CDCl_3$, 23 ºC) of **3s**



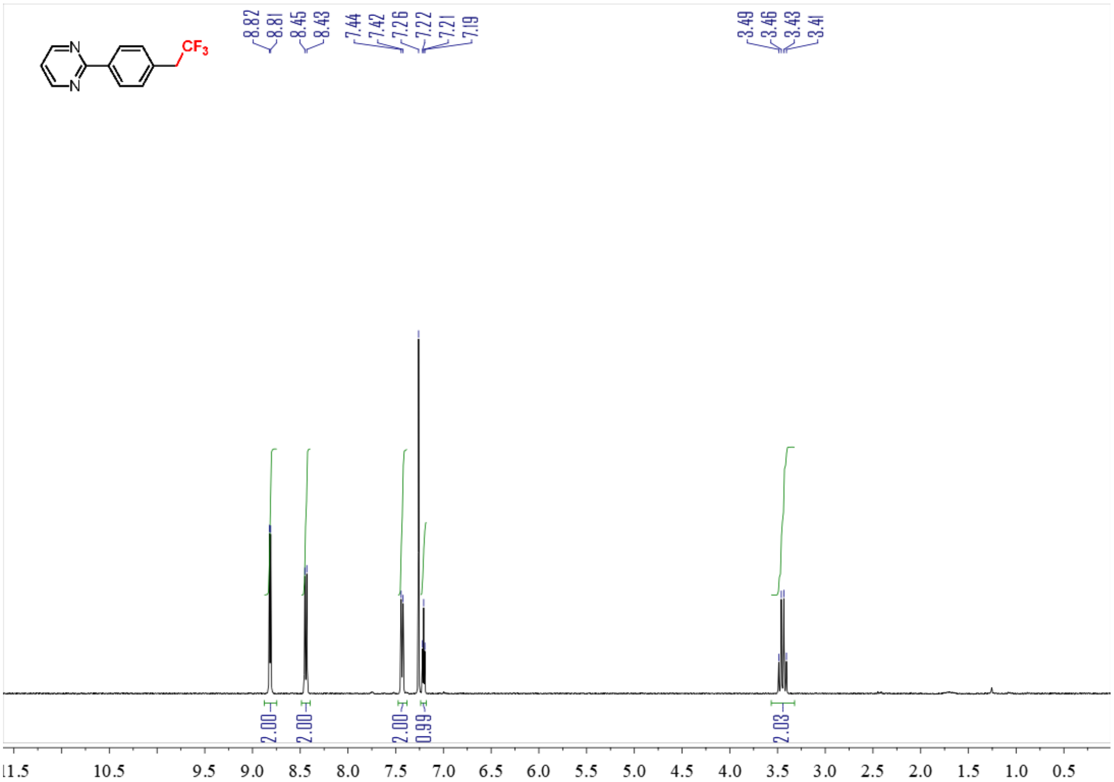
[1]H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of **3t**



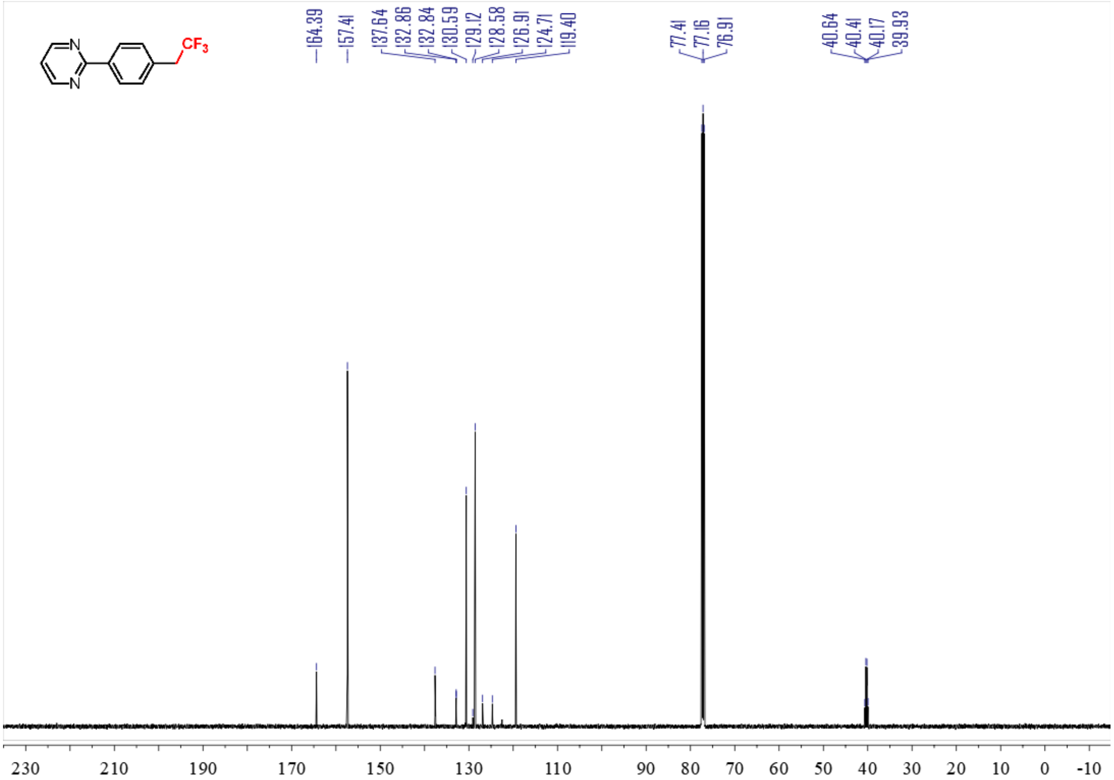
[13]C NMR spectrum (126 MHz, $CDCl_3$, 23 ºC) of **3t**



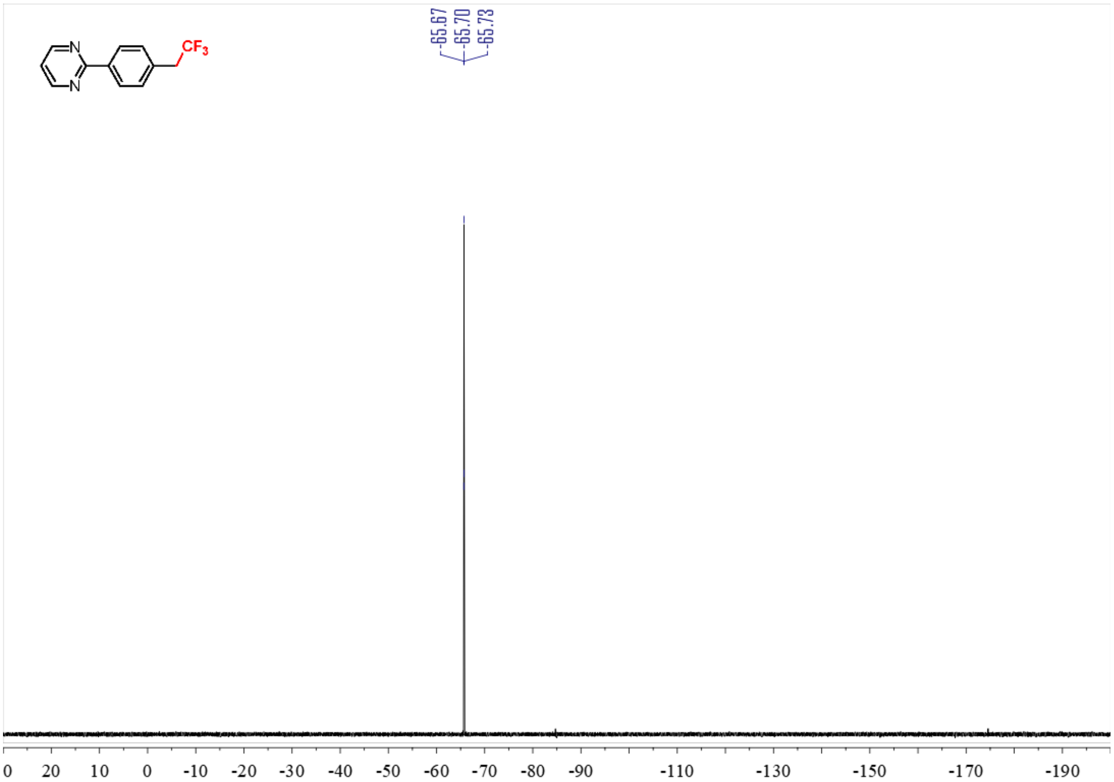
[19]F NMR spectrum (375 MHz, $CDCl_3$, 23 ºC) of **3t**



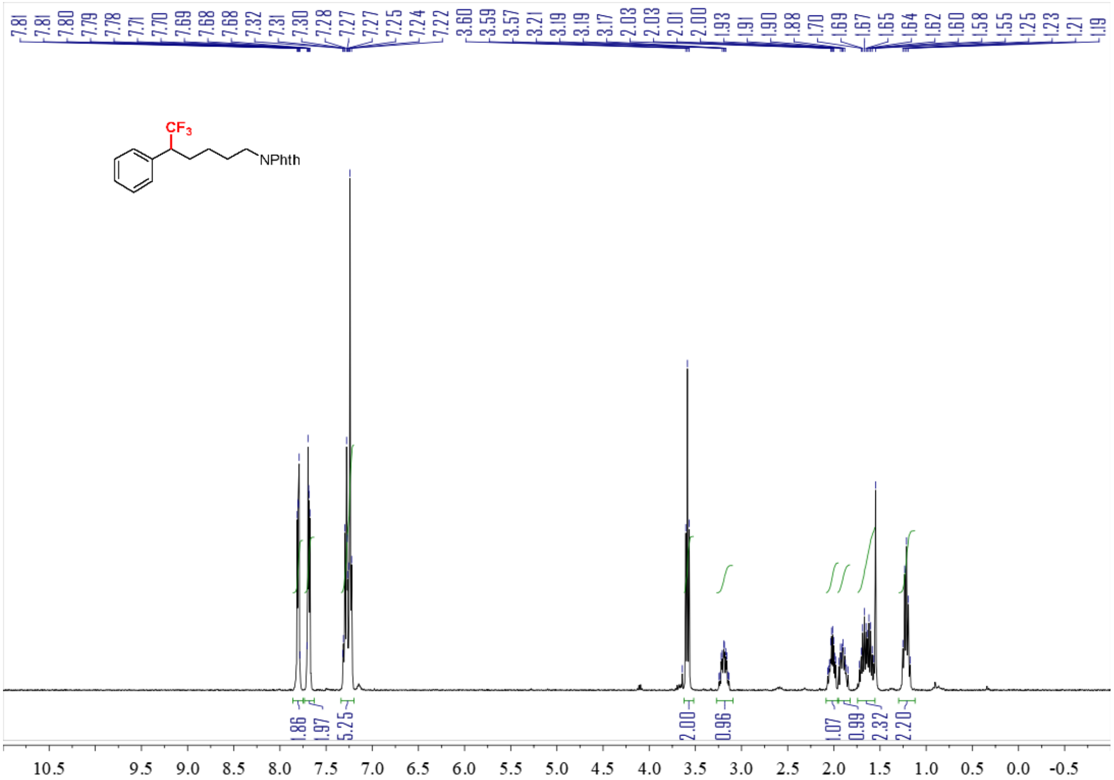
[1]H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of **3u**



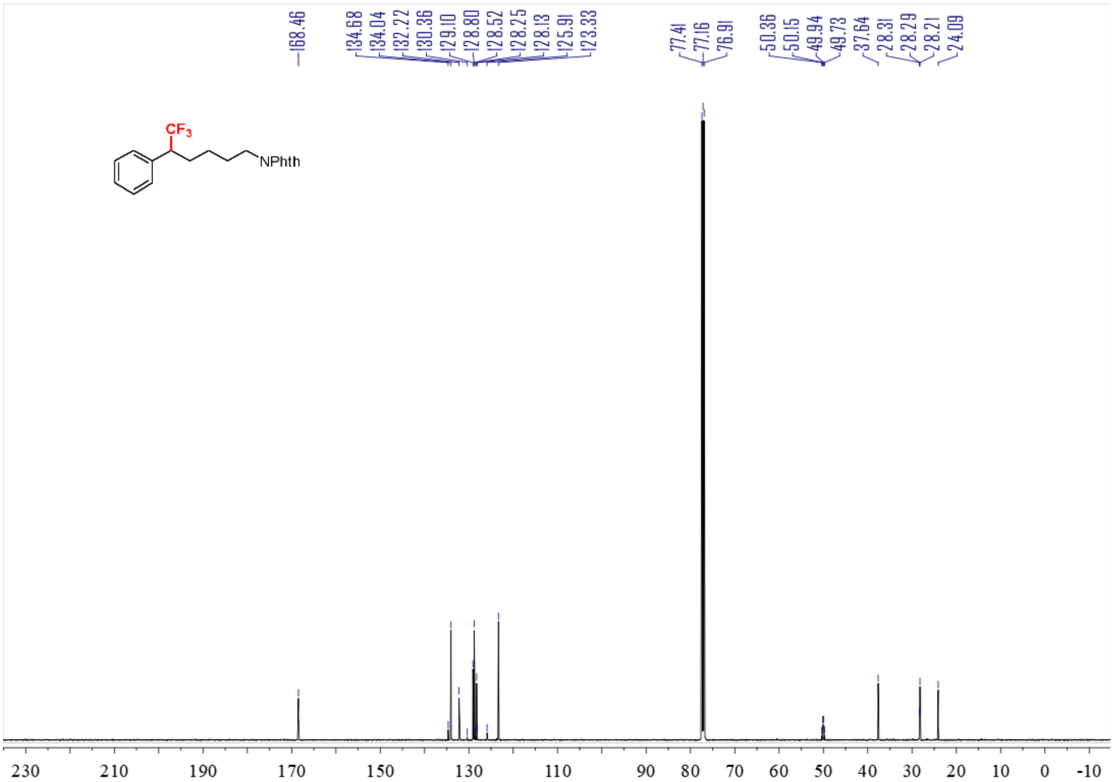
^{13}C NMR spectrum (126 MHz, $CDCl_3$, 23 ºC) of **3u**



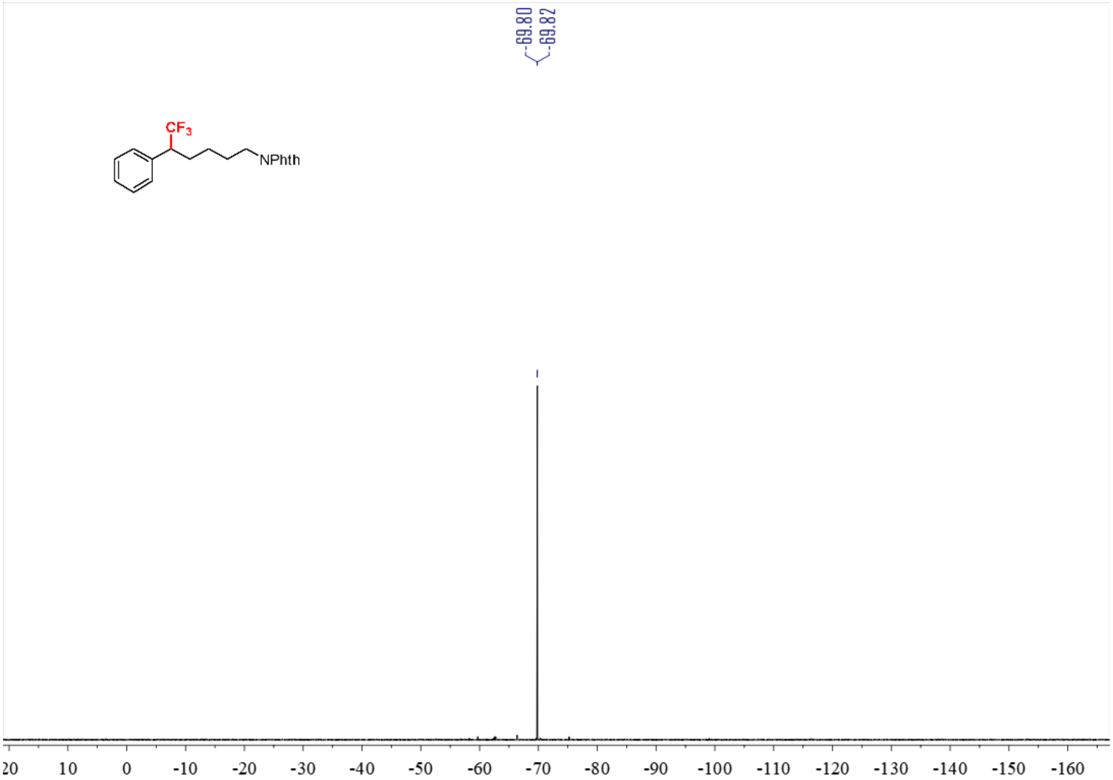
^{19}F NMR spectrum (375 MHz, $CDCl_3$, 23 ºC) of **3u**



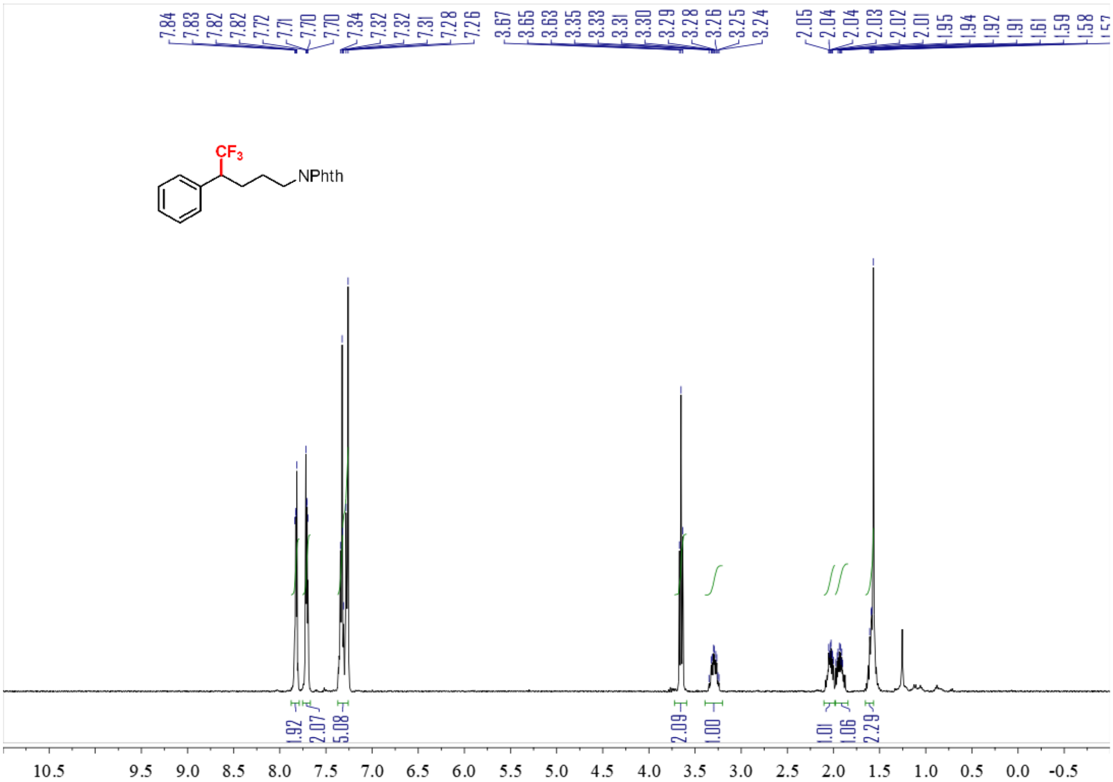
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 °C) of **3v**



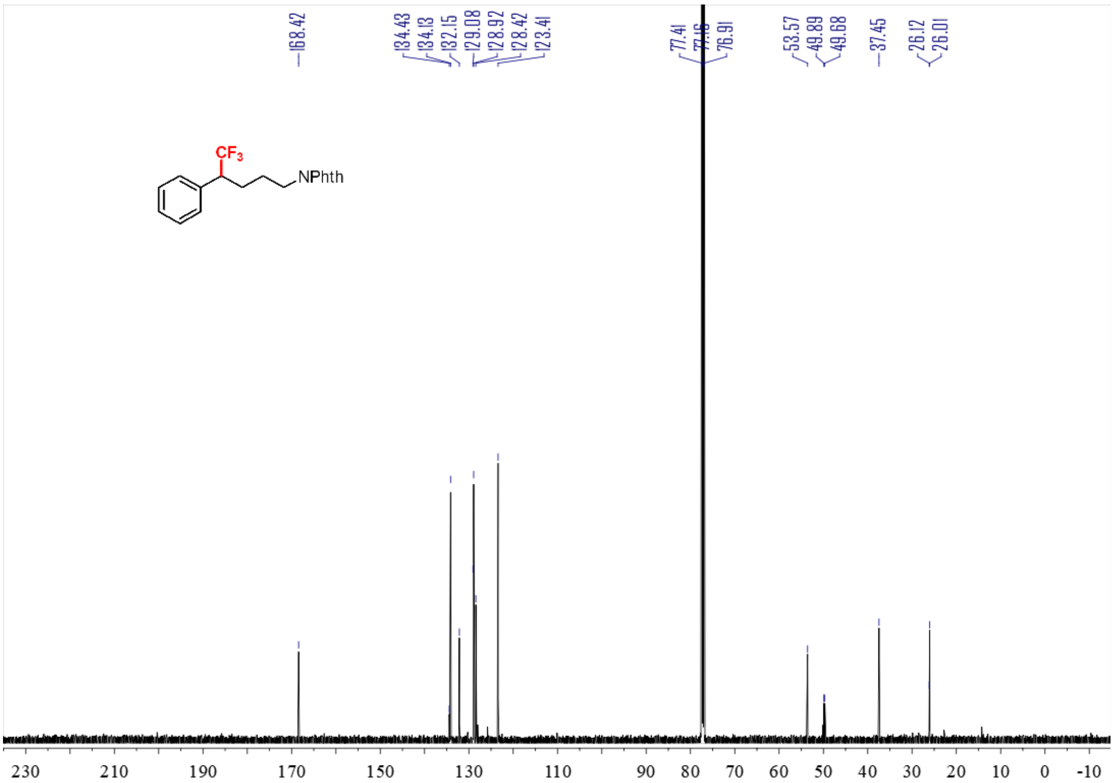
^{13}C NMR spectrum (126 MHz, $CDCl_3$, 23 °C) of **3v**



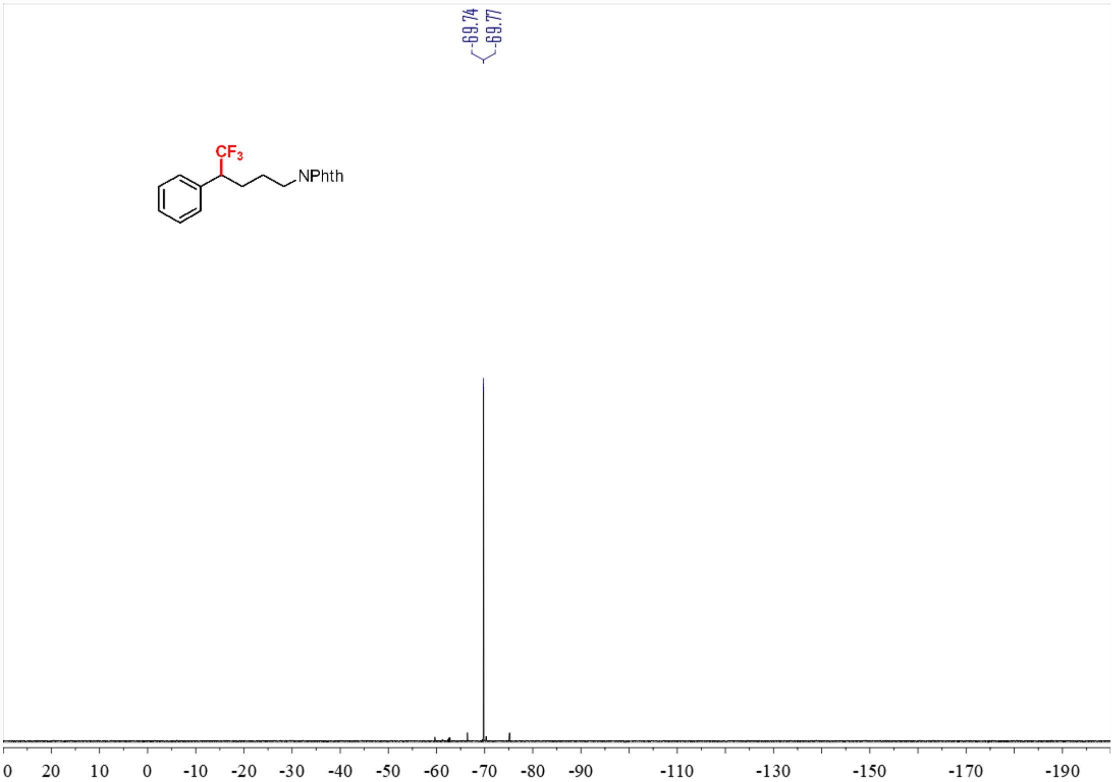
^{19}F NMR spectrum (375 MHz, $CDCl_3$, 23 ºC) of **3v**



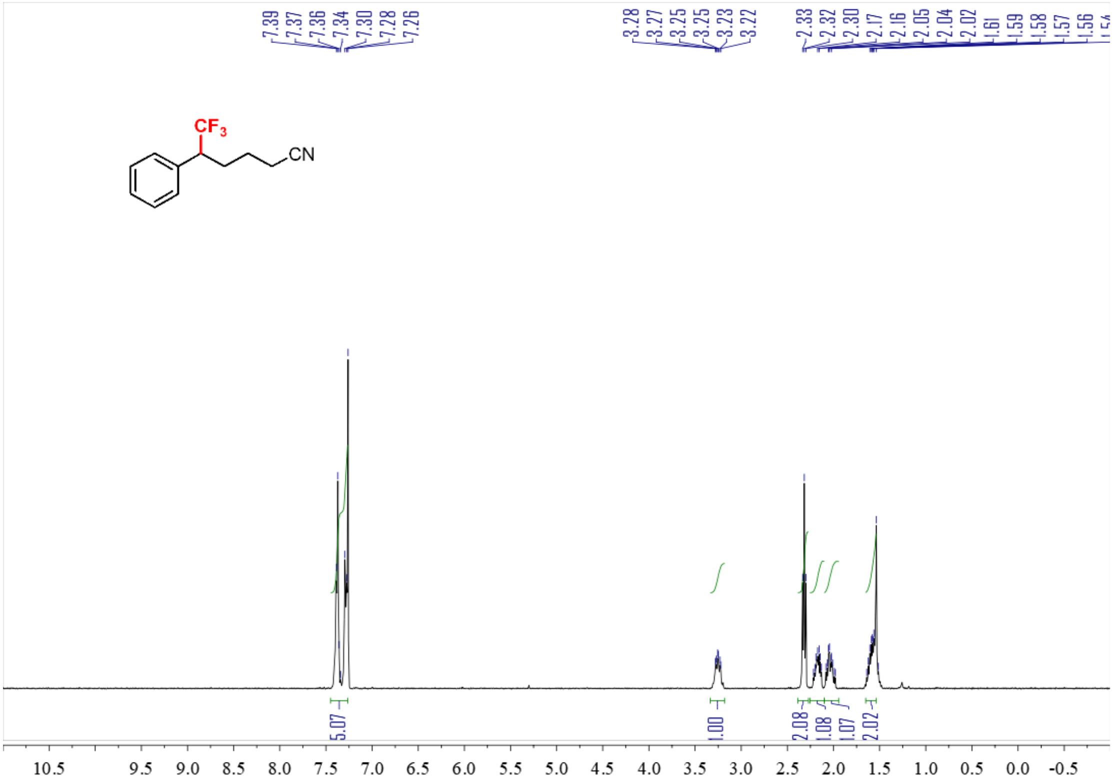
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of **3w**



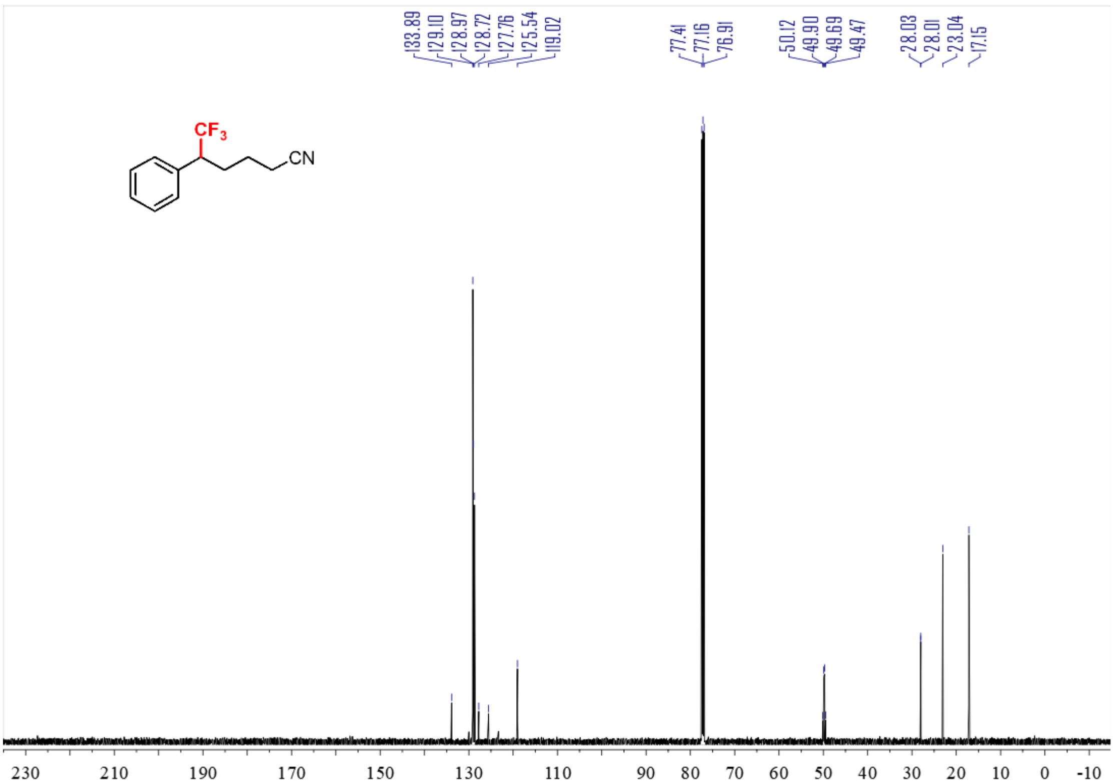
^{13}C NMR spectrum (126 MHz, $CDCl_3$, 23 ºC) of **3w**



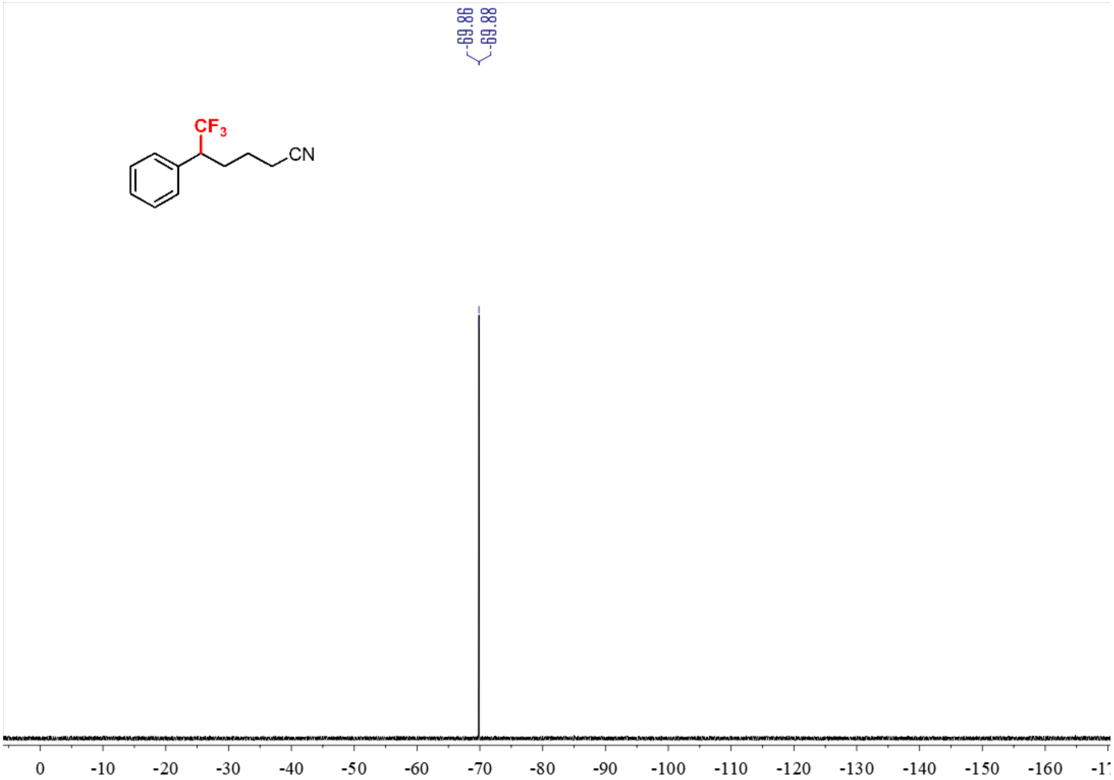
^{19}F NMR spectrum (375 MHz, $CDCl_3$, 23 ºC) of **3w**



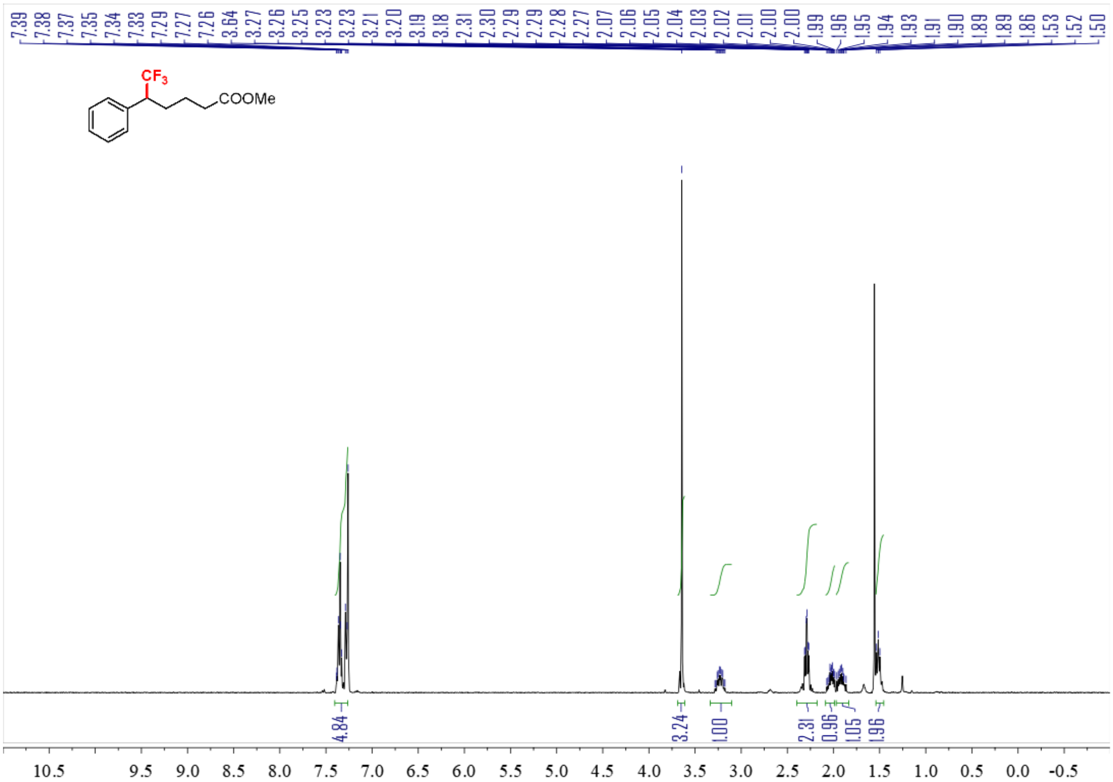
^{1}H NMR spectrum (400 MHz, CDCl3, 23 ºC) of **3x**



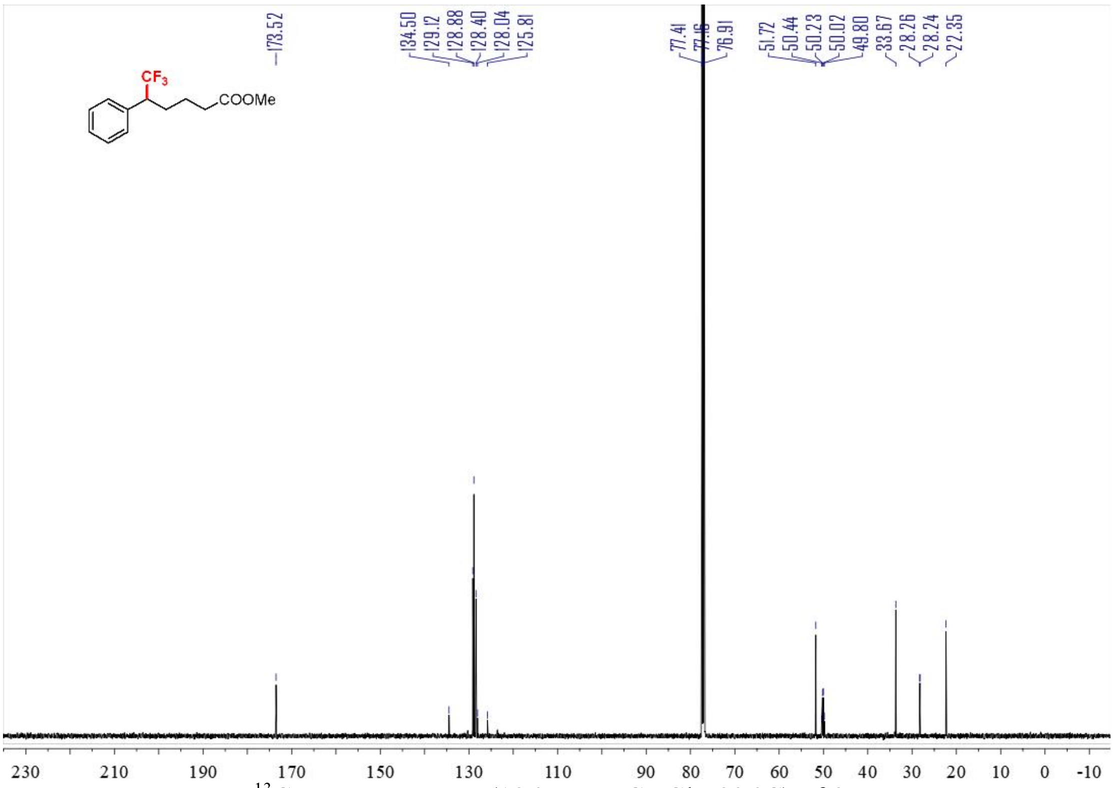
^{13}C NMR spectrum (126 MHz, CDCl3, 23 ºC) of **3x**



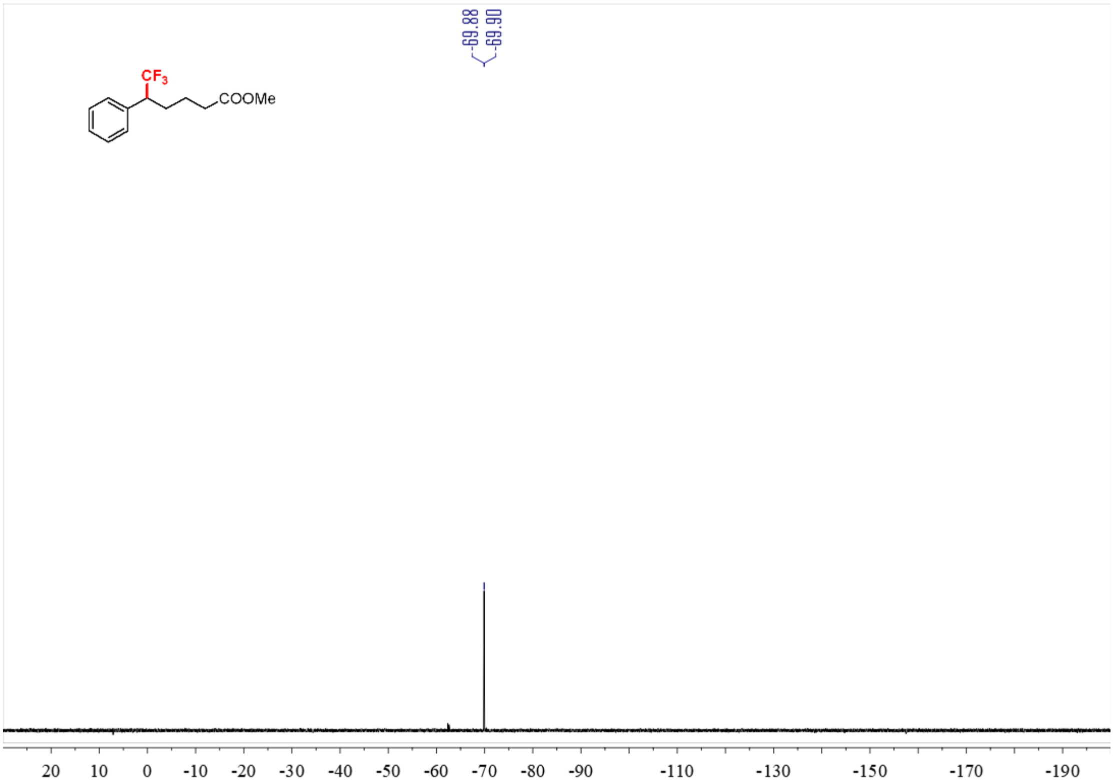
[19]F NMR spectrum (375 MHz, $CDCl_3$, 23 ºC) of **3x**



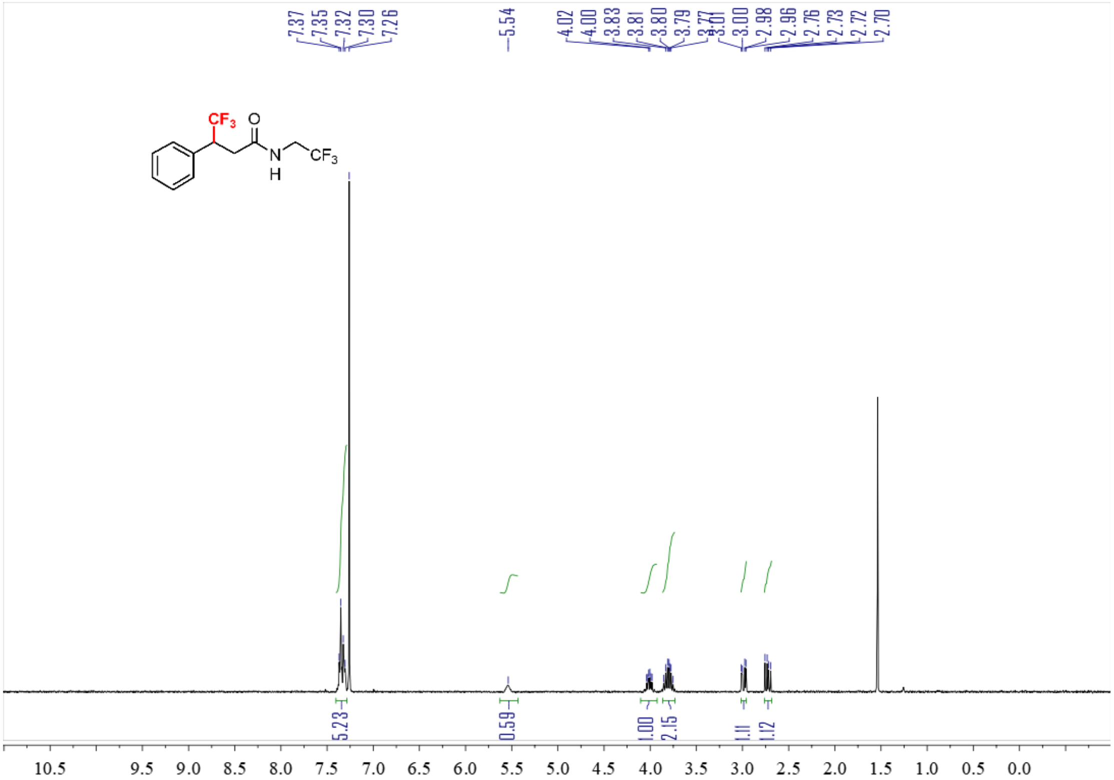
[1]H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of **3y**



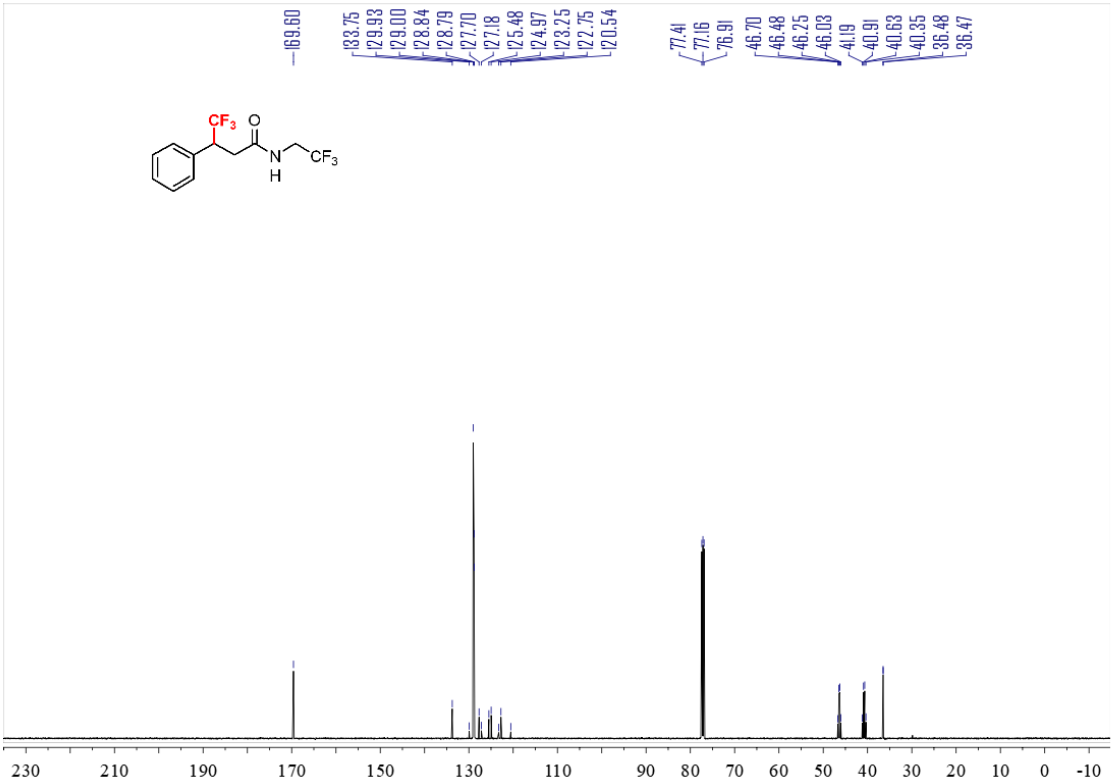
^{13}C NMR spectrum (126 MHz, $CDCl_3$, 23 ºC) of **3y**



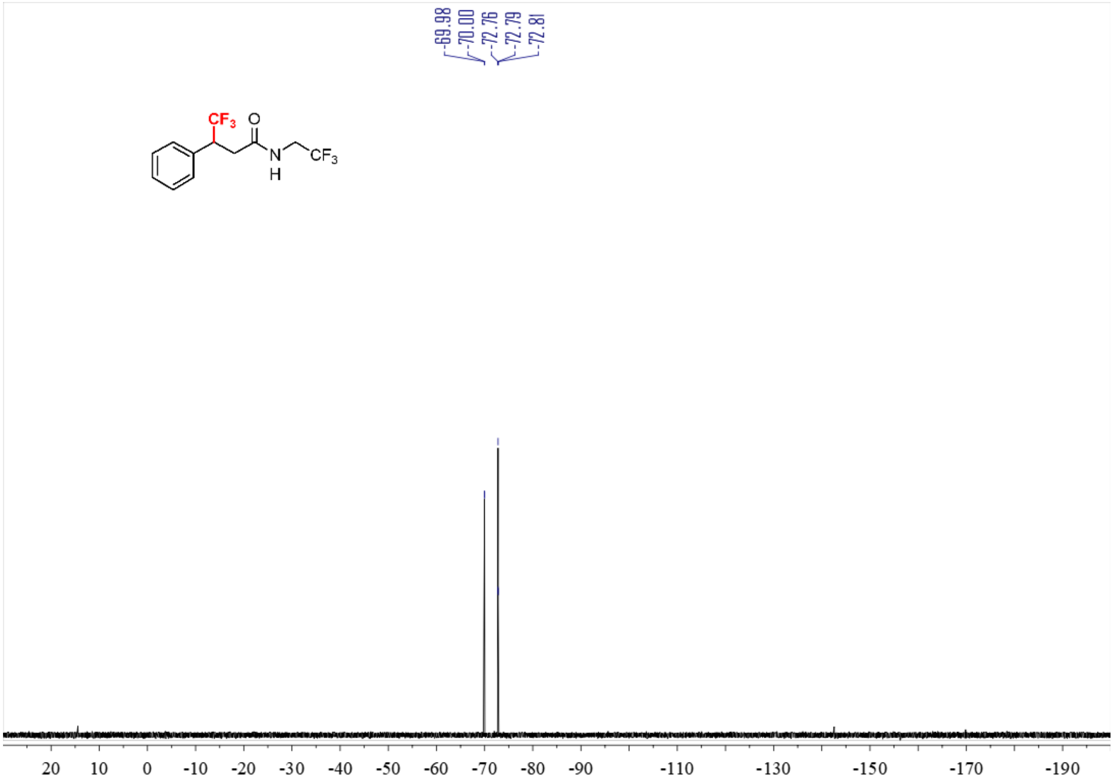
^{19}F NMR spectrum (375 MHz, $CDCl_3$, 23 ºC) of **3y**



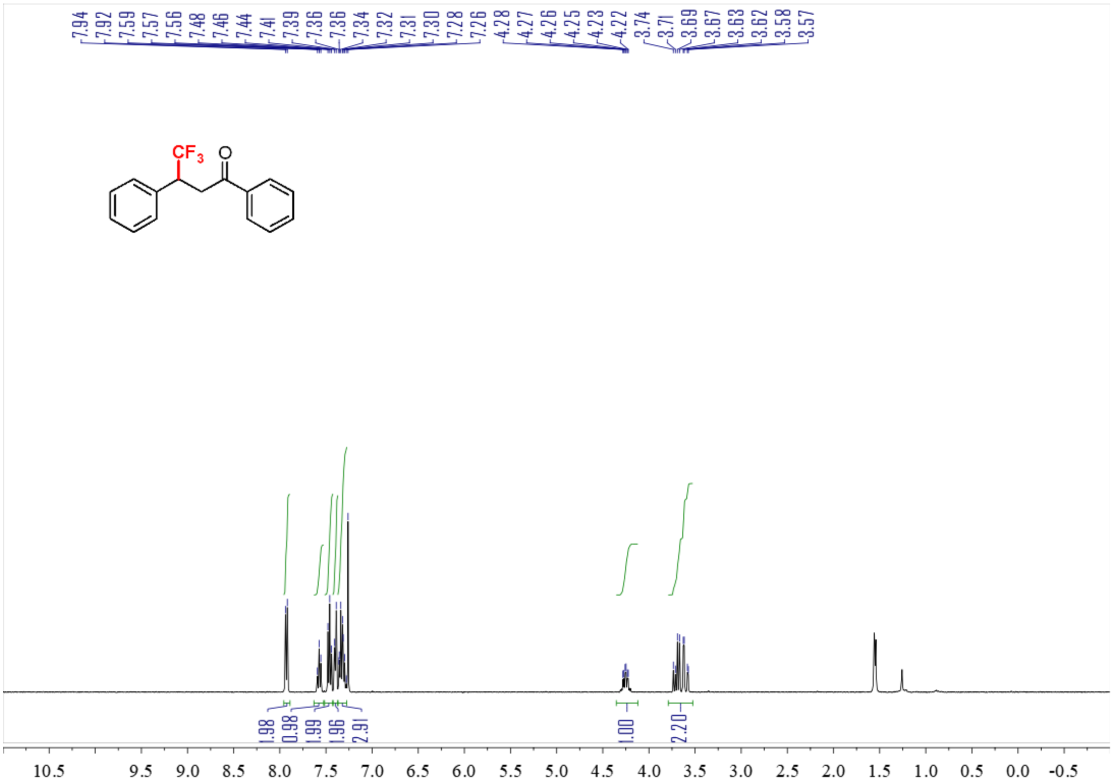
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of **3z**



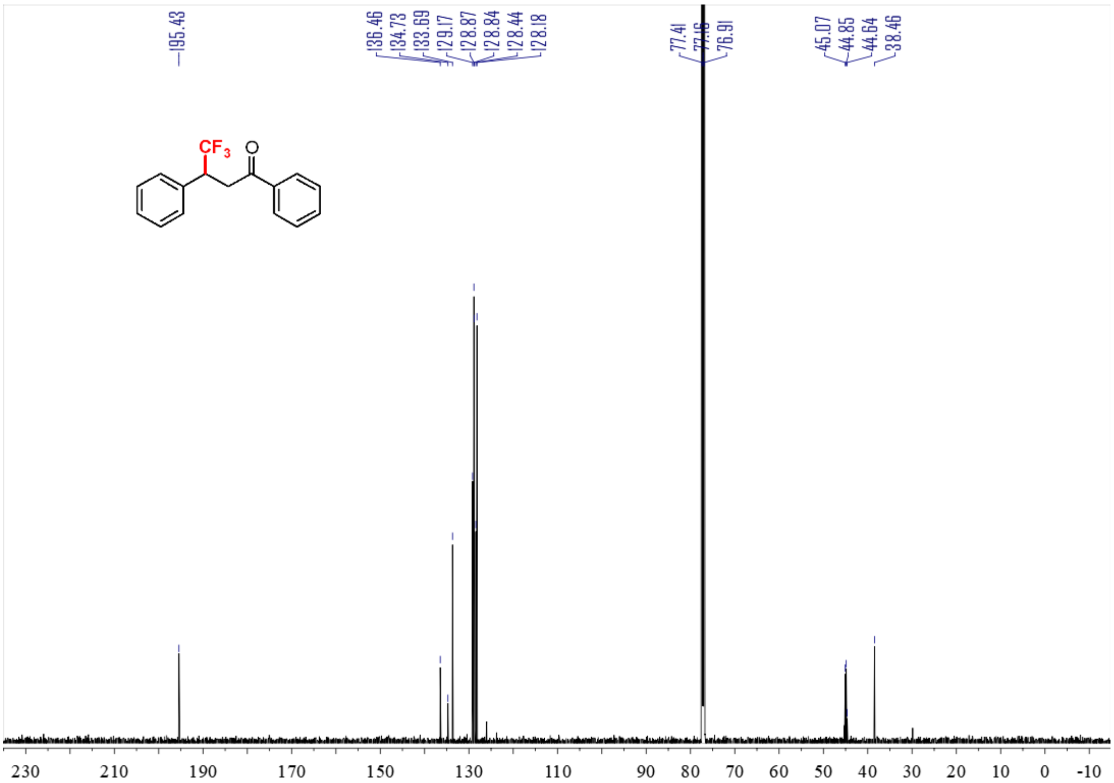
^{13}C NMR spectrum (126 MHz, $CDCl_3$, 23 ºC) of **3z**



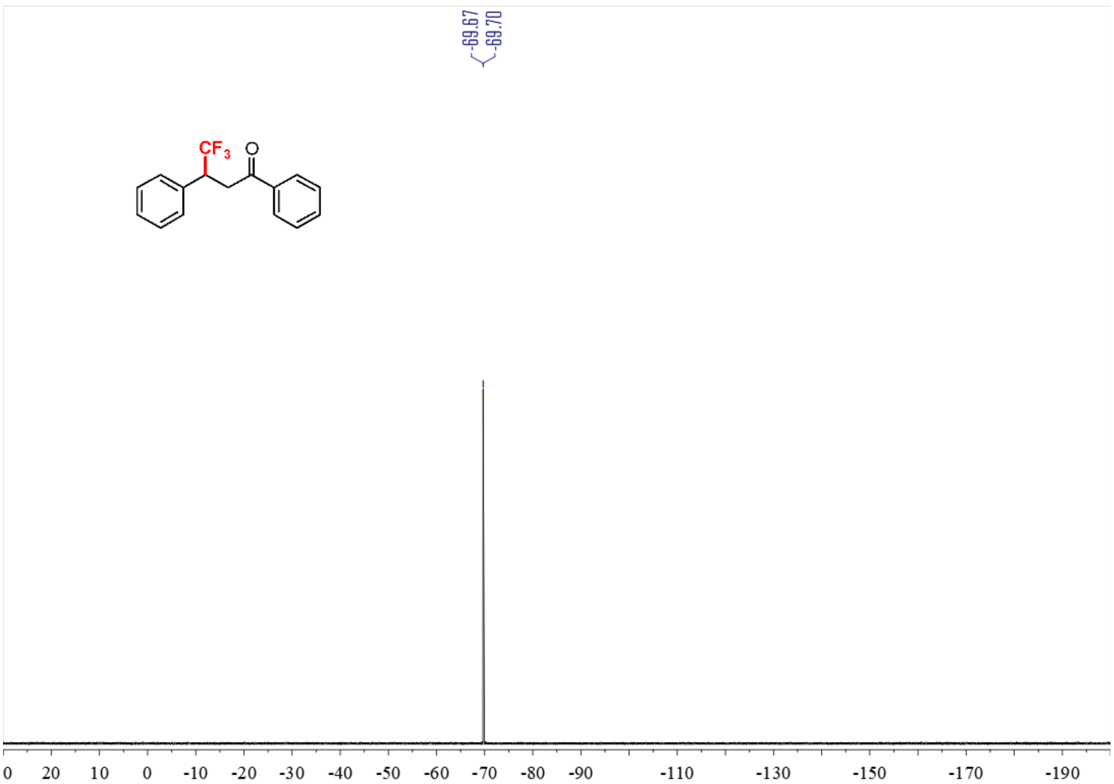
[19]F NMR spectrum (375 MHz, CDCl3, 23 ºC) of **3y**



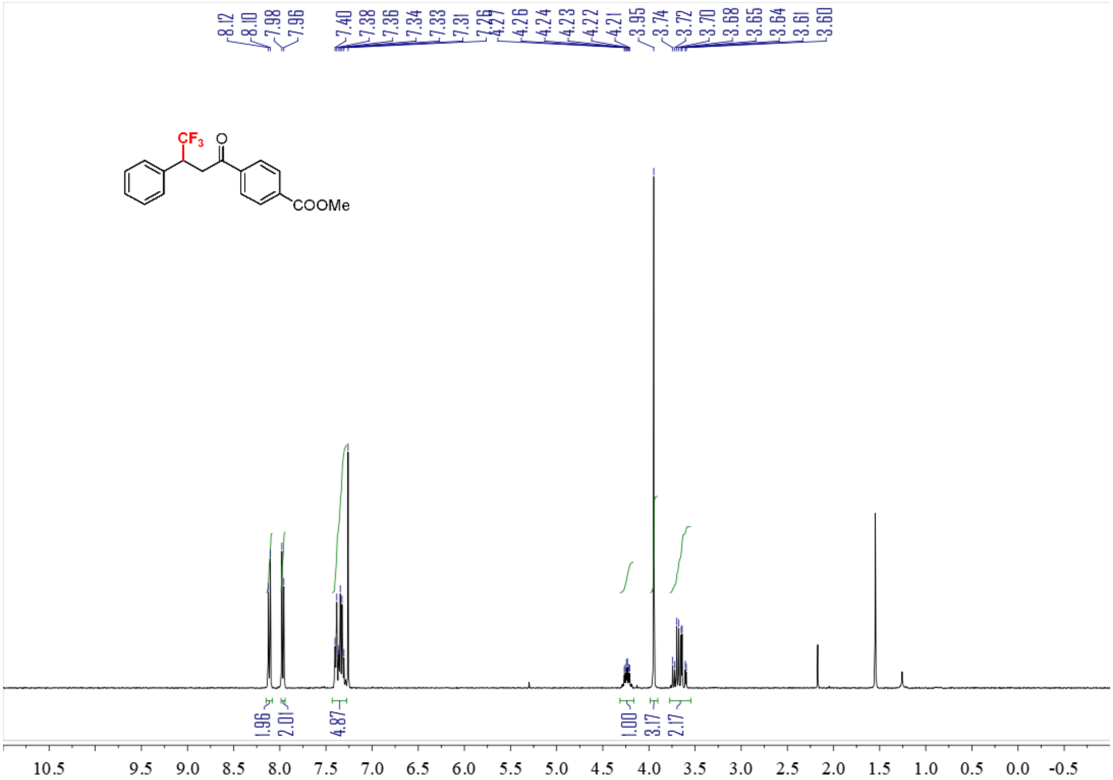
[1]H NMR spectrum (400 MHz, CDCl3, 23 ºC) of **3aa**



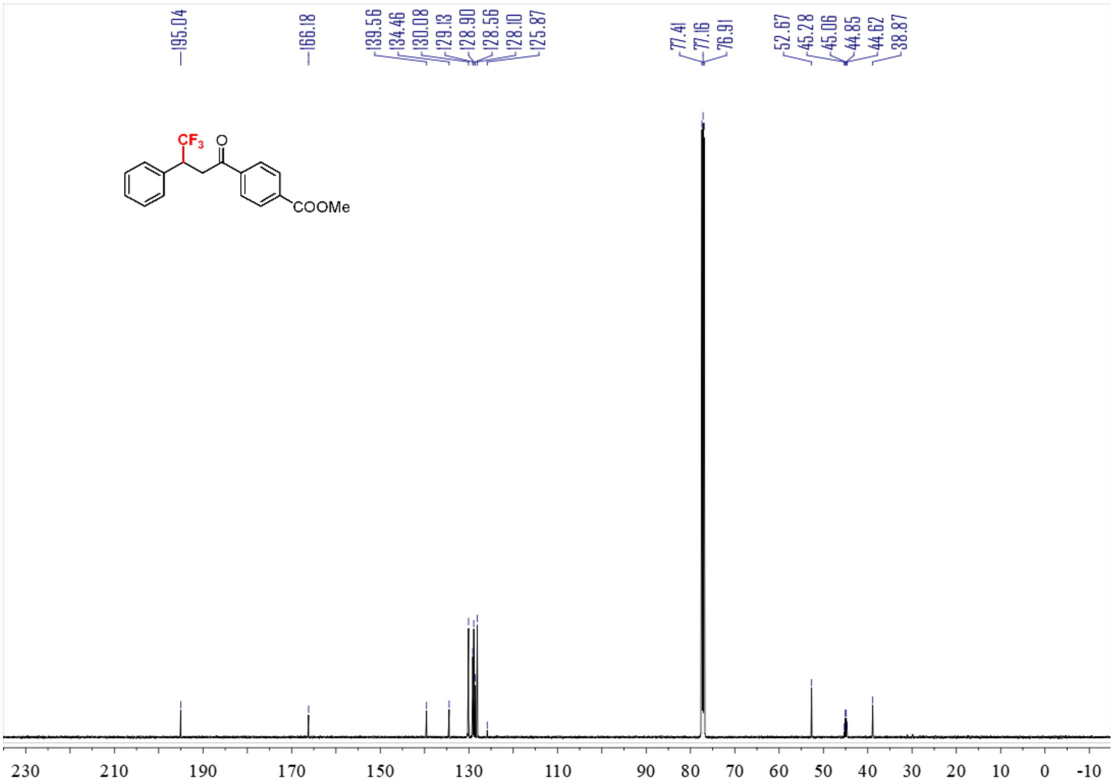
^{13}C NMR spectrum (126 MHz, $CDCl_3$, 23 ºC) of **3aa**



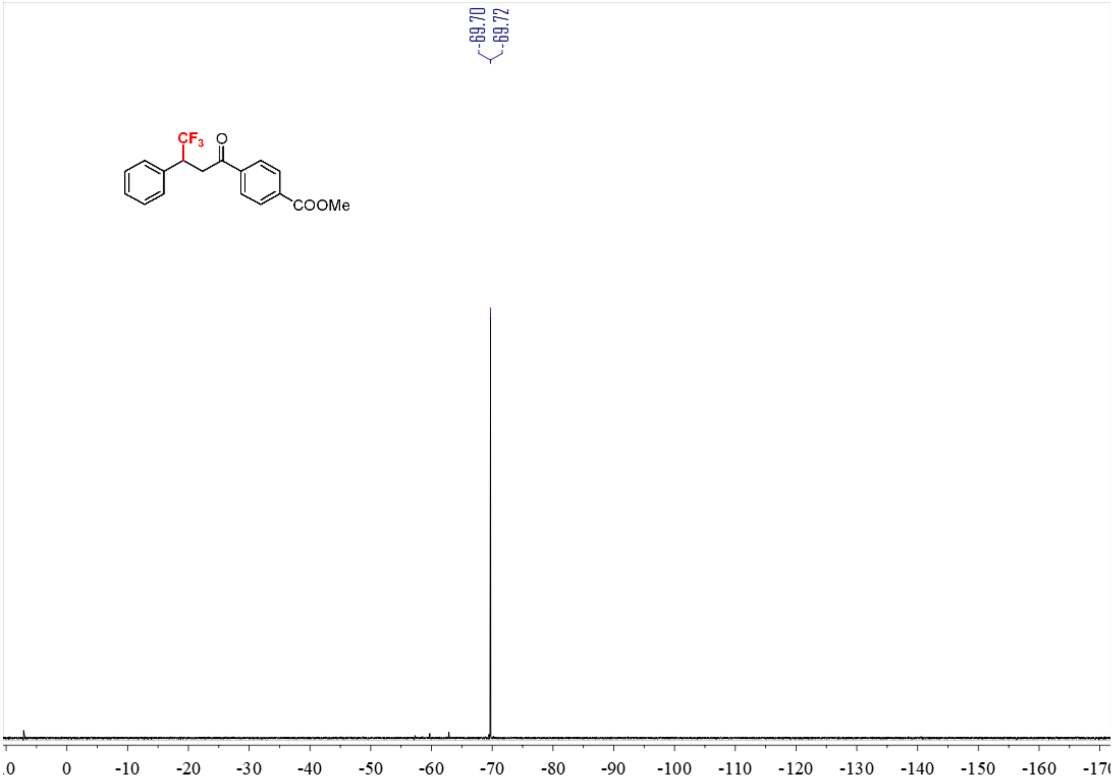
^{19}F NMR spectrum (375 MHz, $CDCl_3$, 23 ºC) of **3aa**



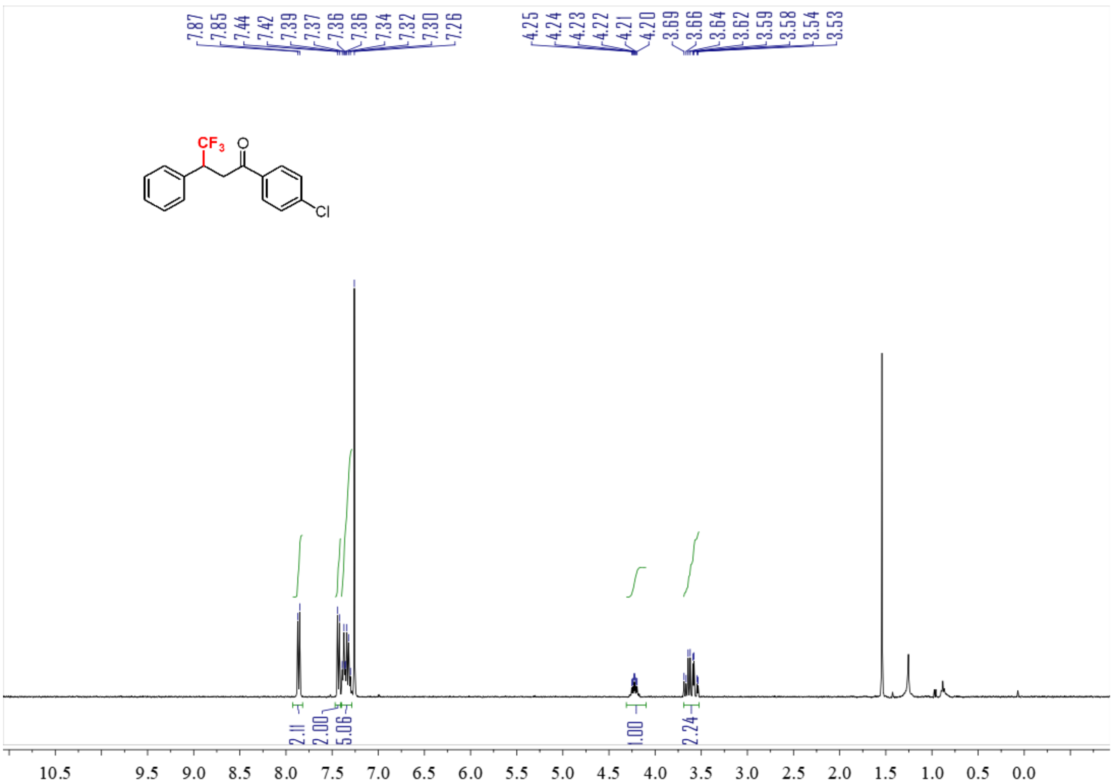
^{1}H NMR spectrum (400 MHz, CDCl$_3$, 23 ºC) of **3bb**



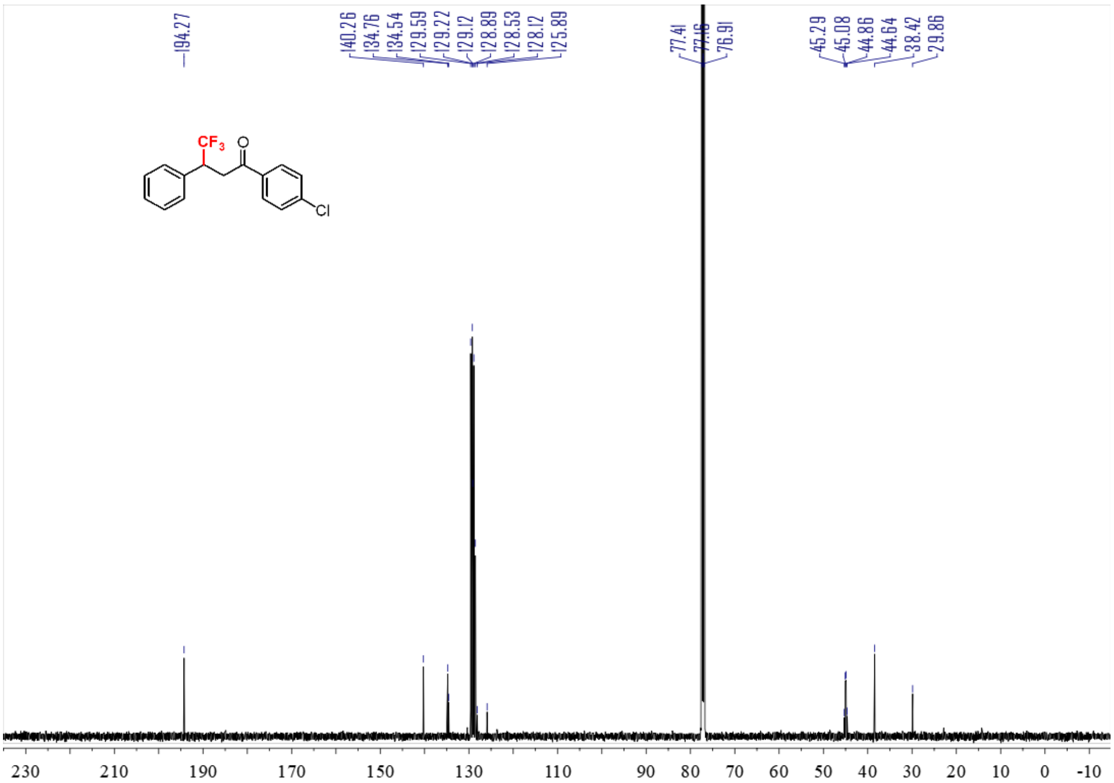
^{13}C NMR spectrum (126 MHz, CDCl$_3$, 23 ºC) of **3bb**



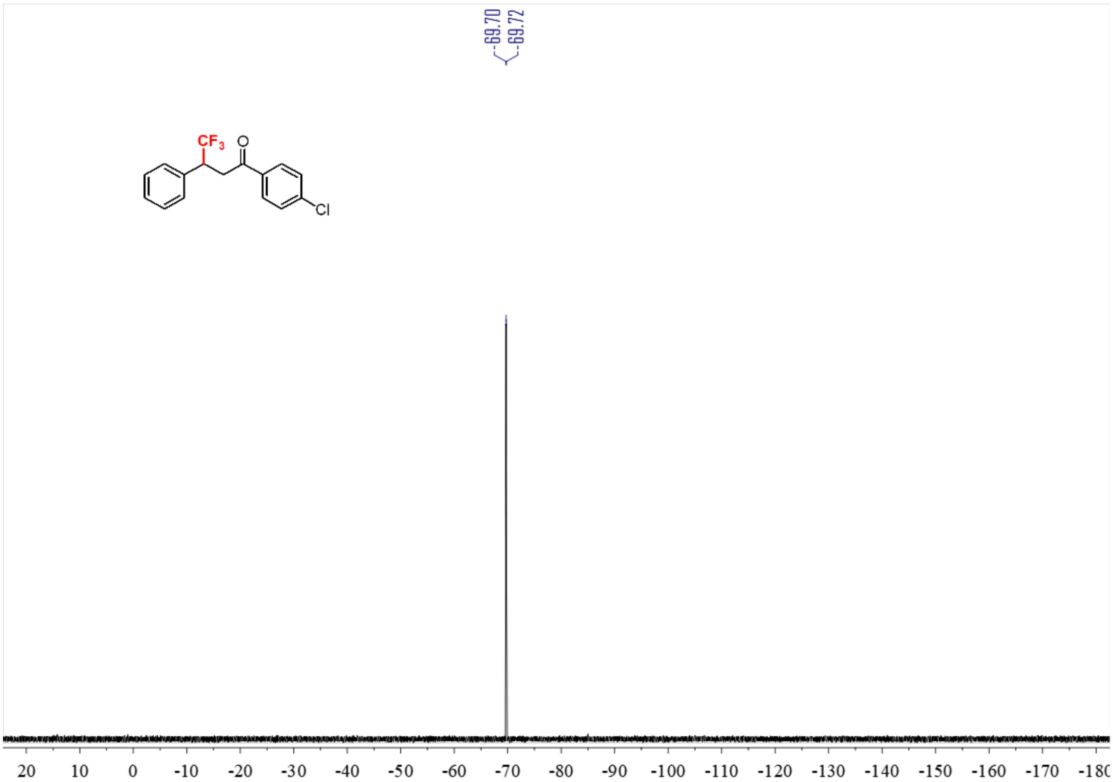
^{19}F NMR spectrum (375 MHz, CDCl$_3$, 23 ºC) of **3bb**



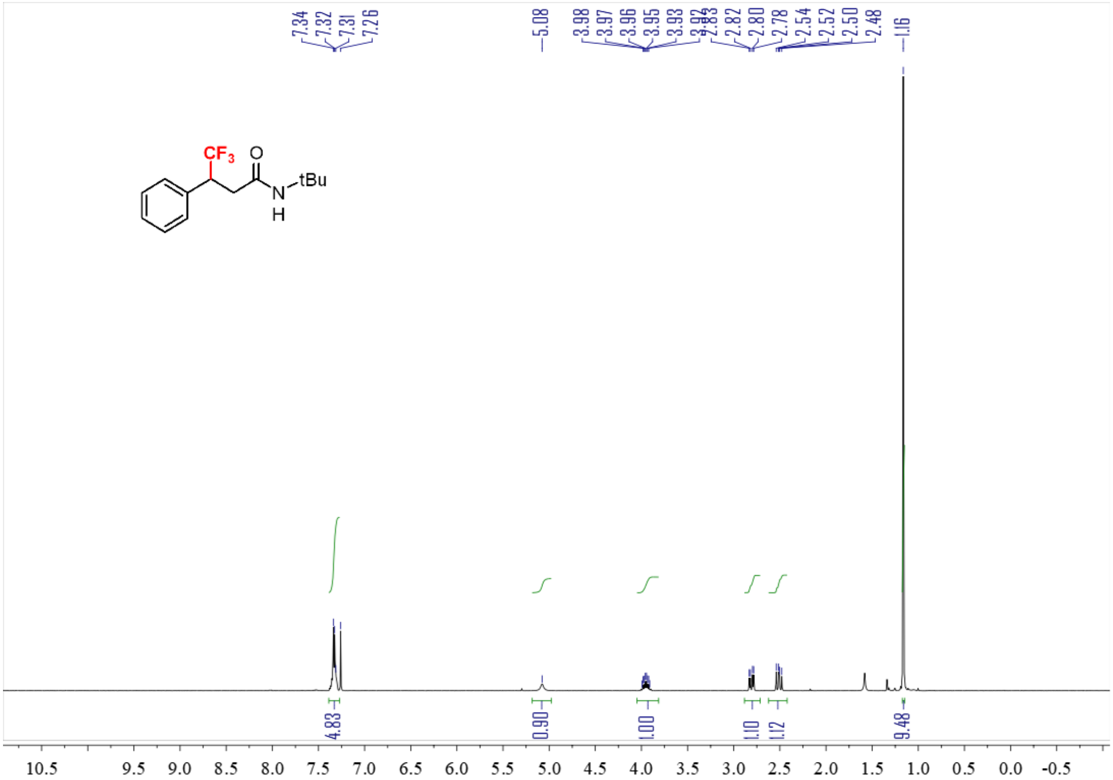
^{1}H NMR spectrum (400 MHz, CDCl$_3$, 23 ºC) of **3cc**



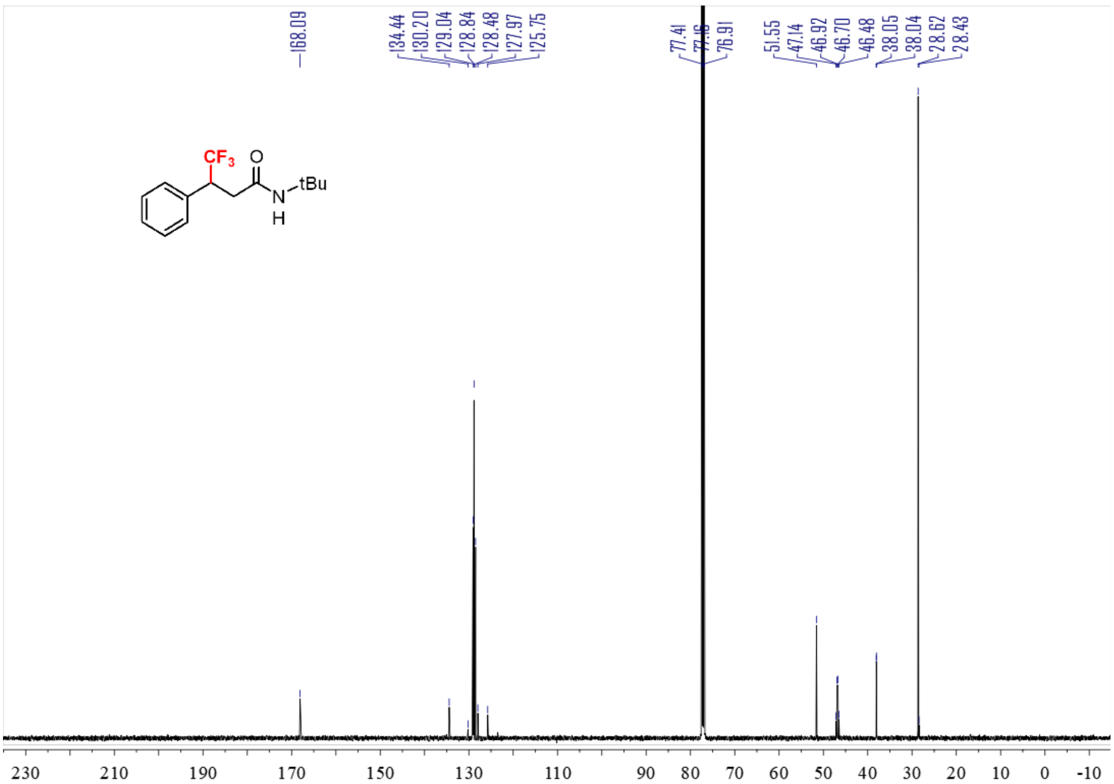
^{13}C NMR spectrum (126 MHz, $CDCl_3$, 23 ºC) of **3cc**



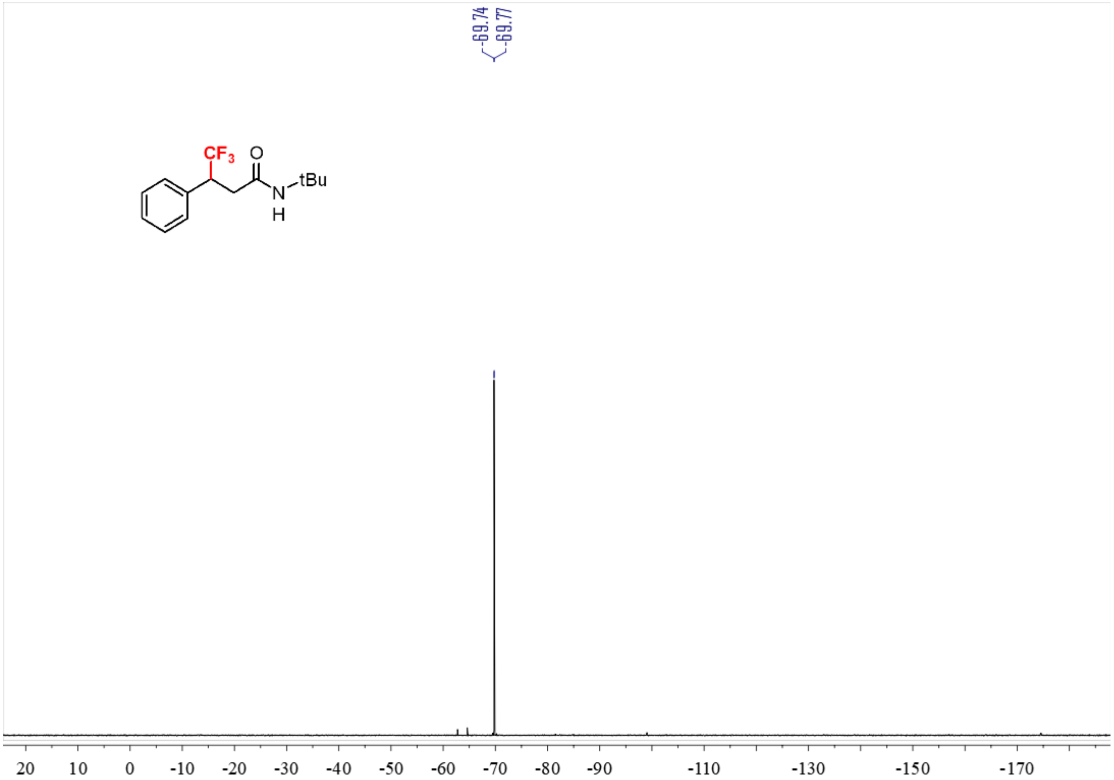
^{19}F NMR spectrum (375 MHz, $CDCl_3$, 23 ºC) of **3cc**



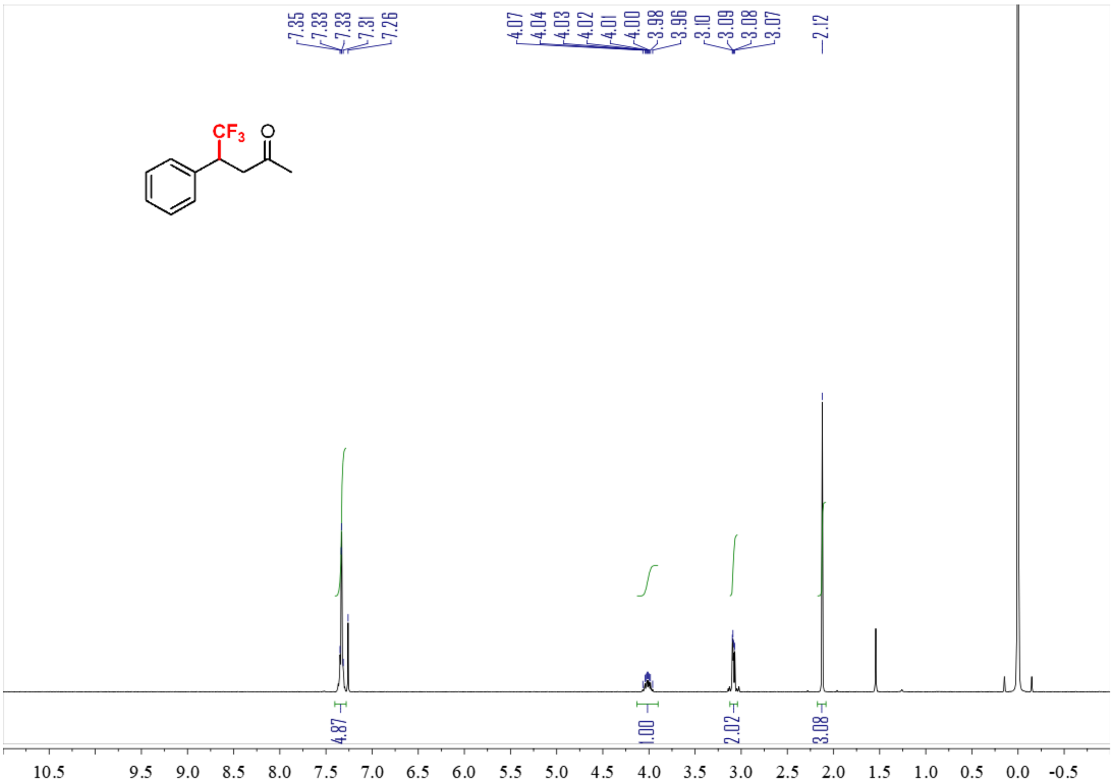
[1]H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of **3dd**



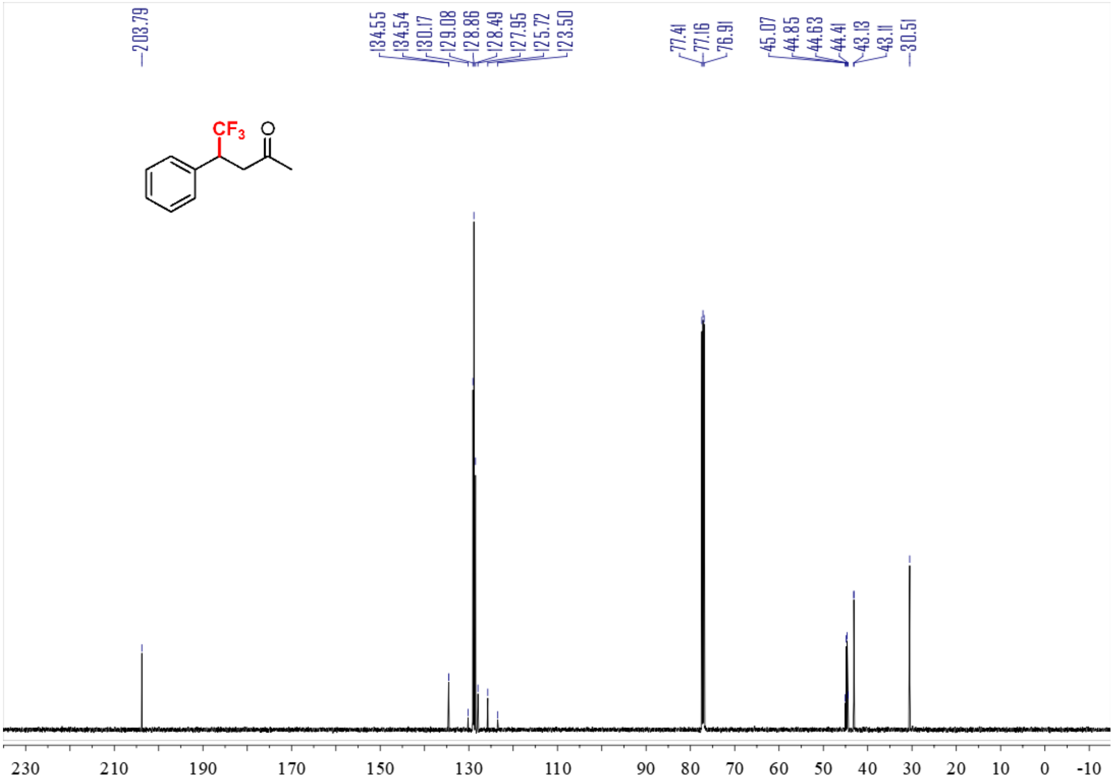
[13]C NMR spectrum (126 MHz, $CDCl_3$, 23 ºC) of **3dd**



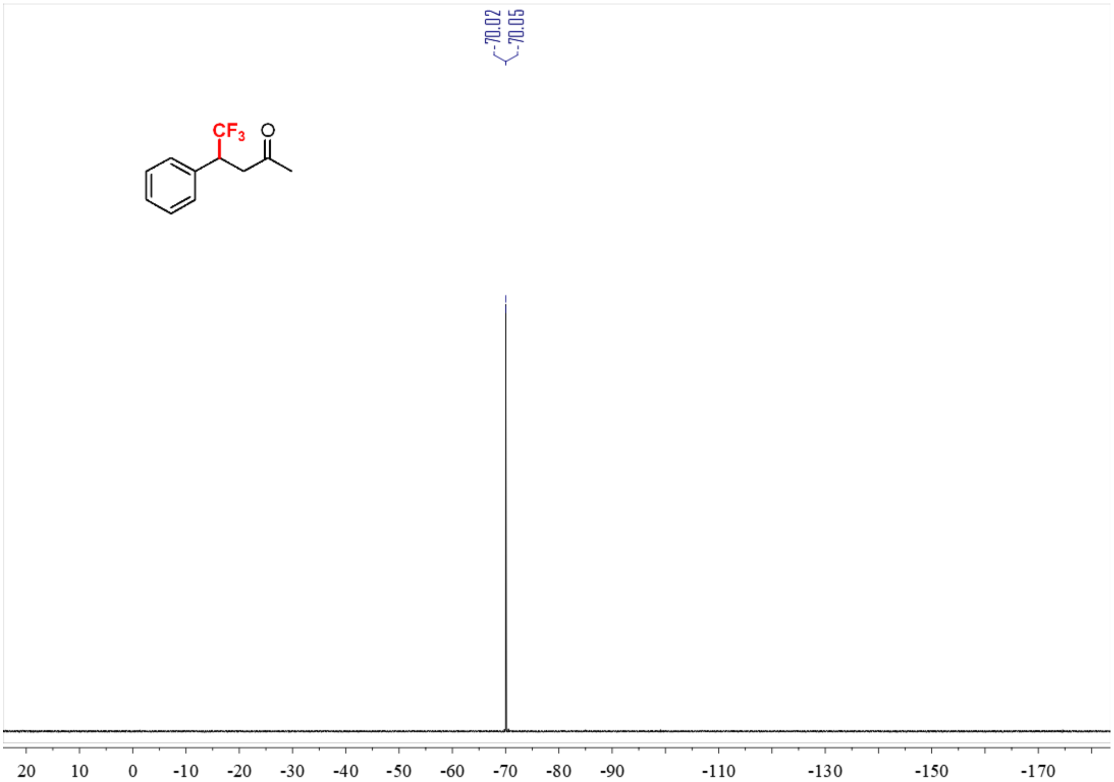
[19]F NMR spectrum (375 MHz, CDCl3, 23 ºC) of **3dd**



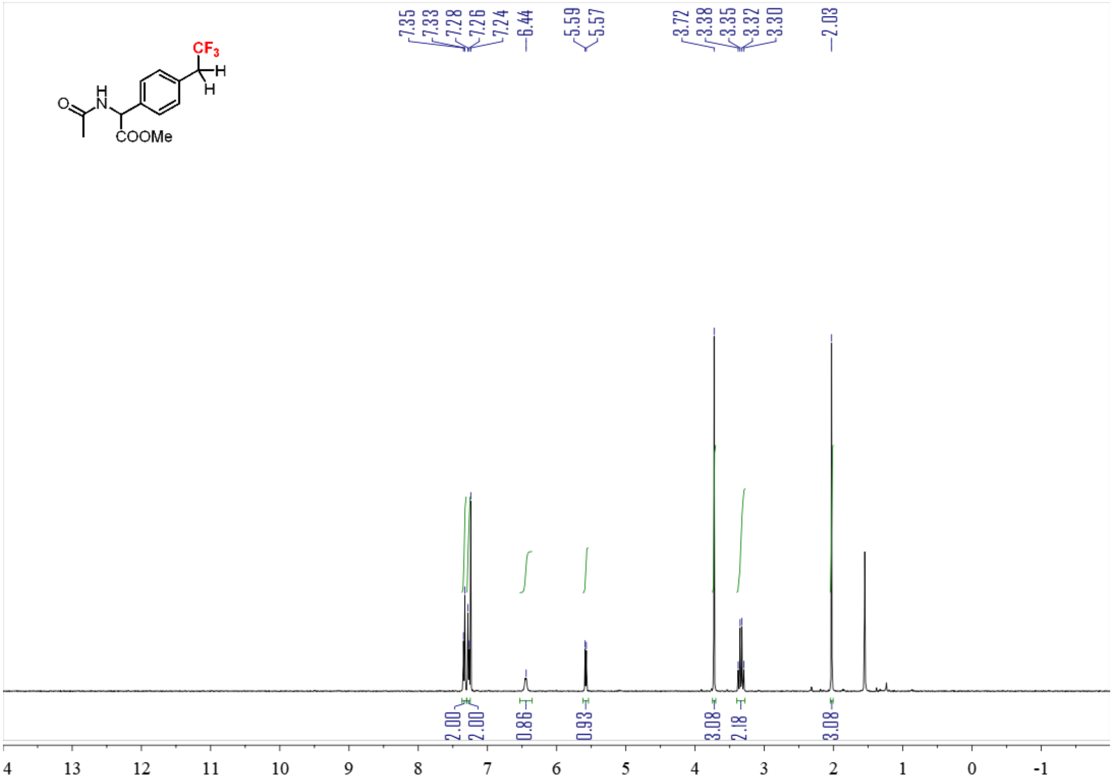
[1]H NMR spectrum (400 MHz, CDCl3, 23 ºC) of **3ee**



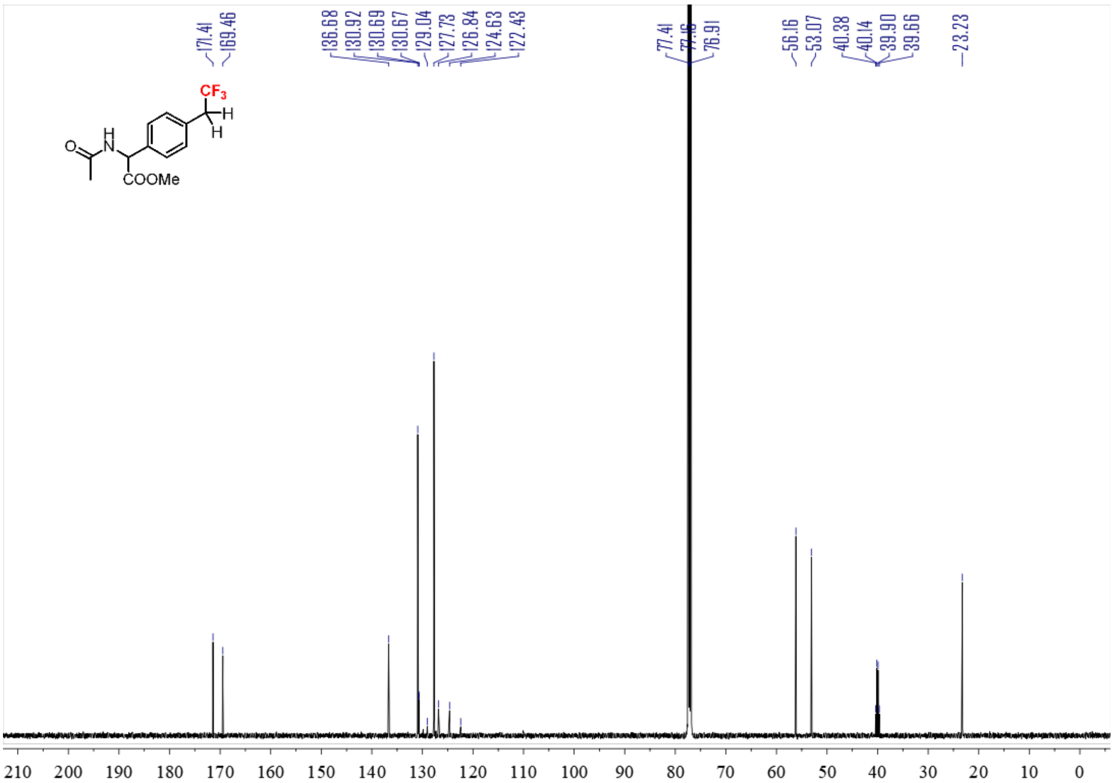
^{13}C NMR spectrum (126 MHz, $CDCl_3$, 23 °C) of **3ee**



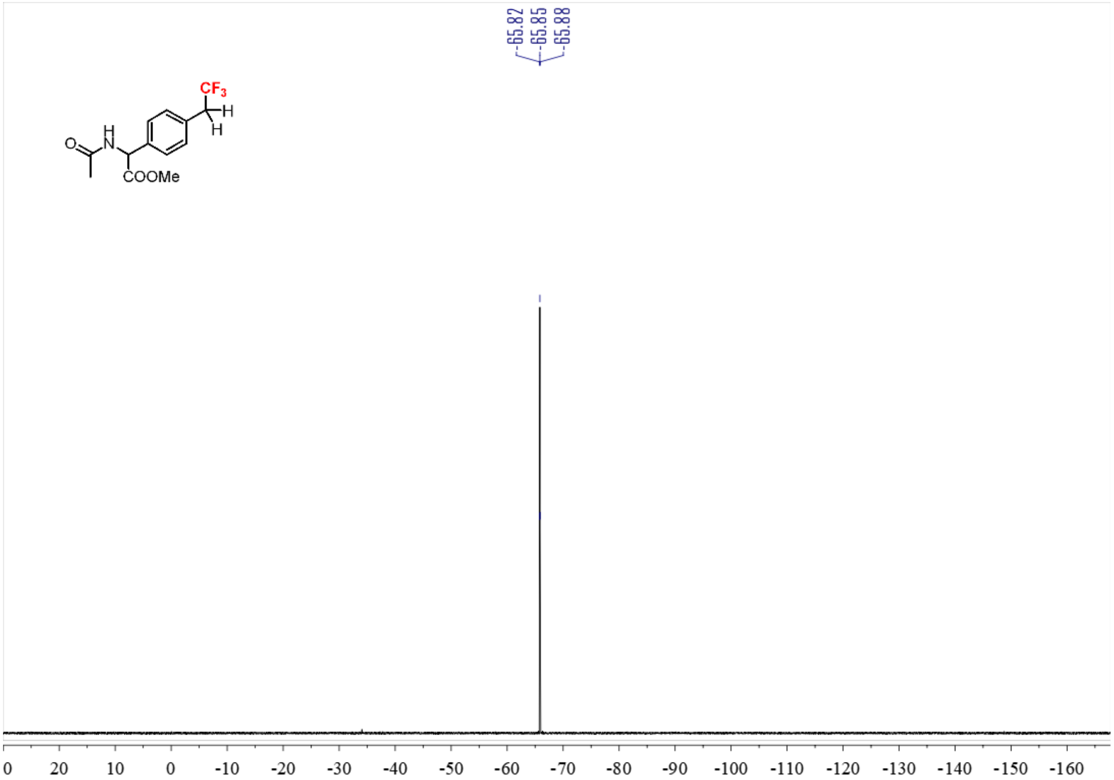
^{19}F NMR spectrum (375 MHz, $CDCl_3$, 23 °C) of **3ee**



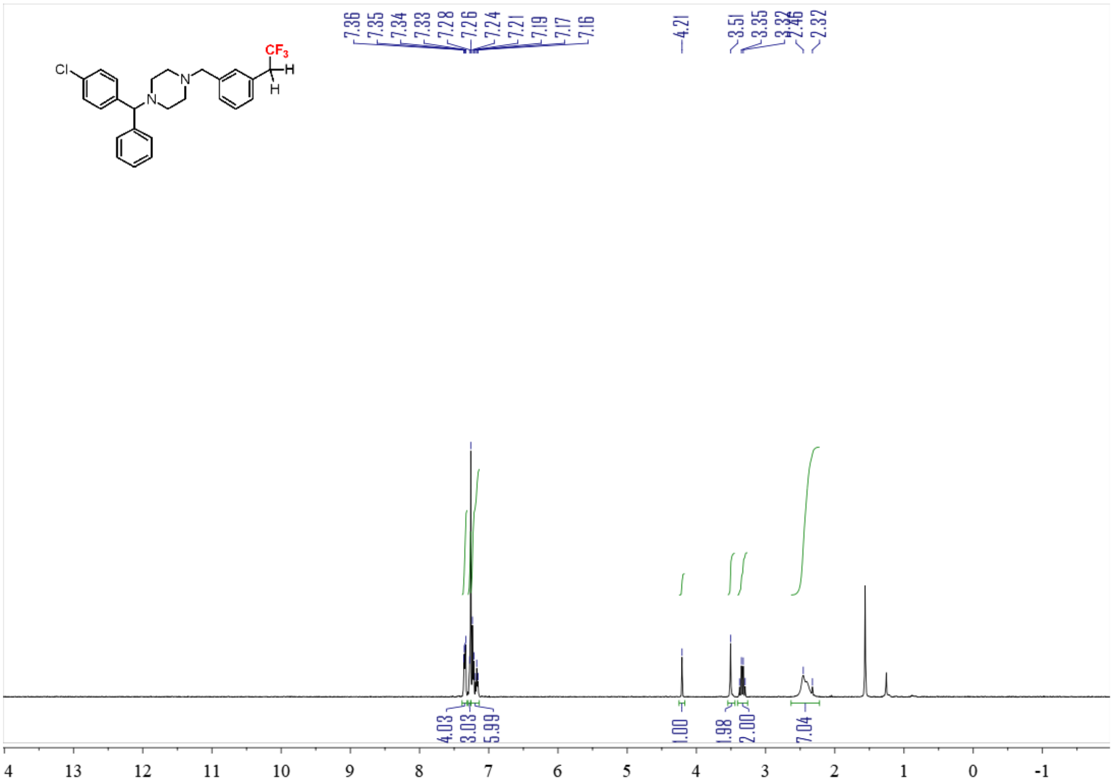
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of **7**



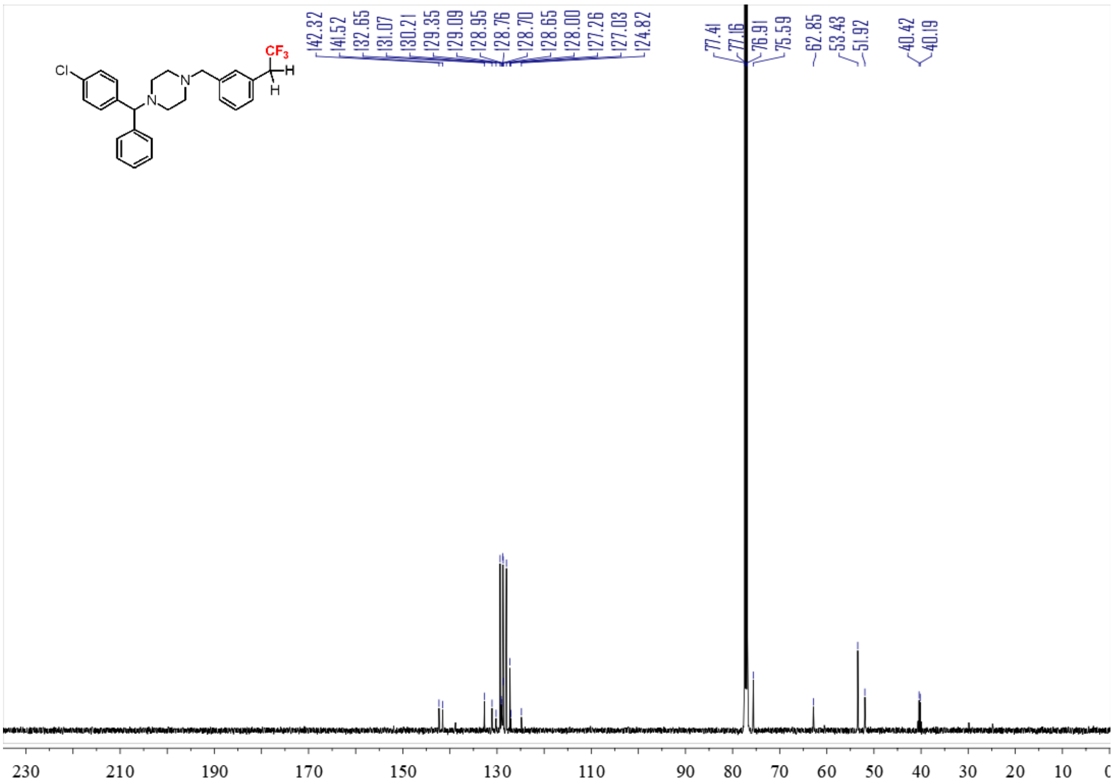
^{13}C NMR spectrum (126 MHz, $CDCl_3$, 23 ºC) of **7**



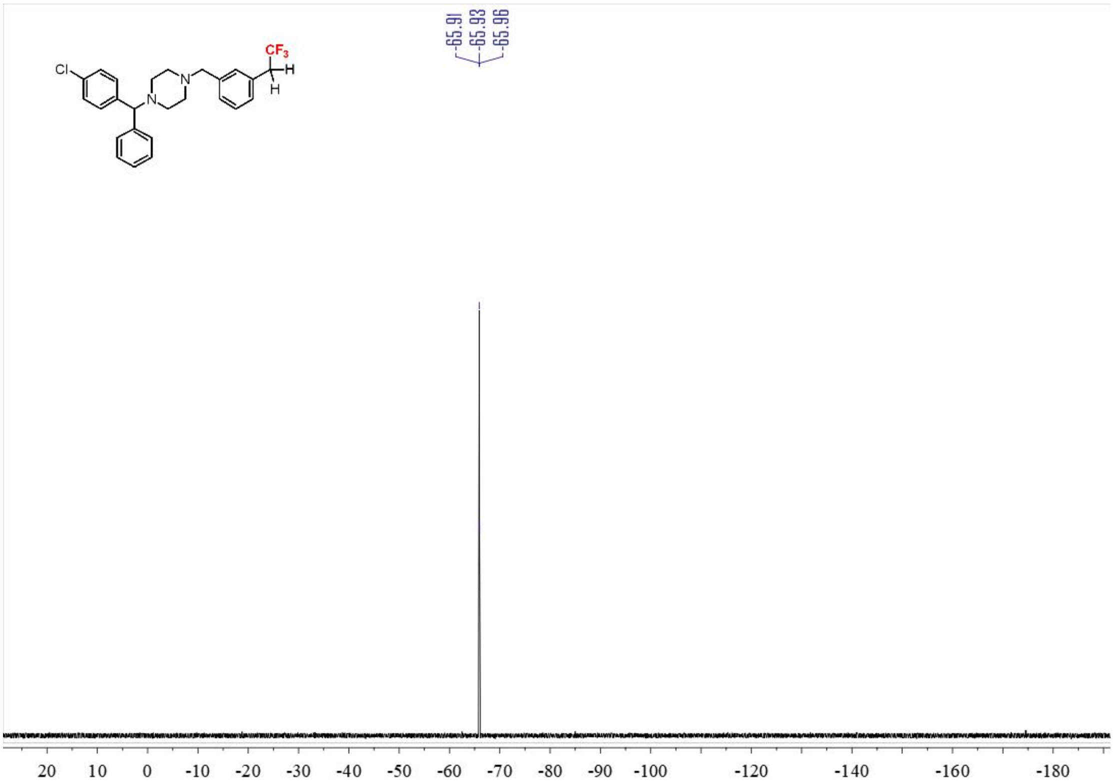
^{19}F NMR spectrum (375 MHz, $CDCl_3$, 23 ºC) of **7**



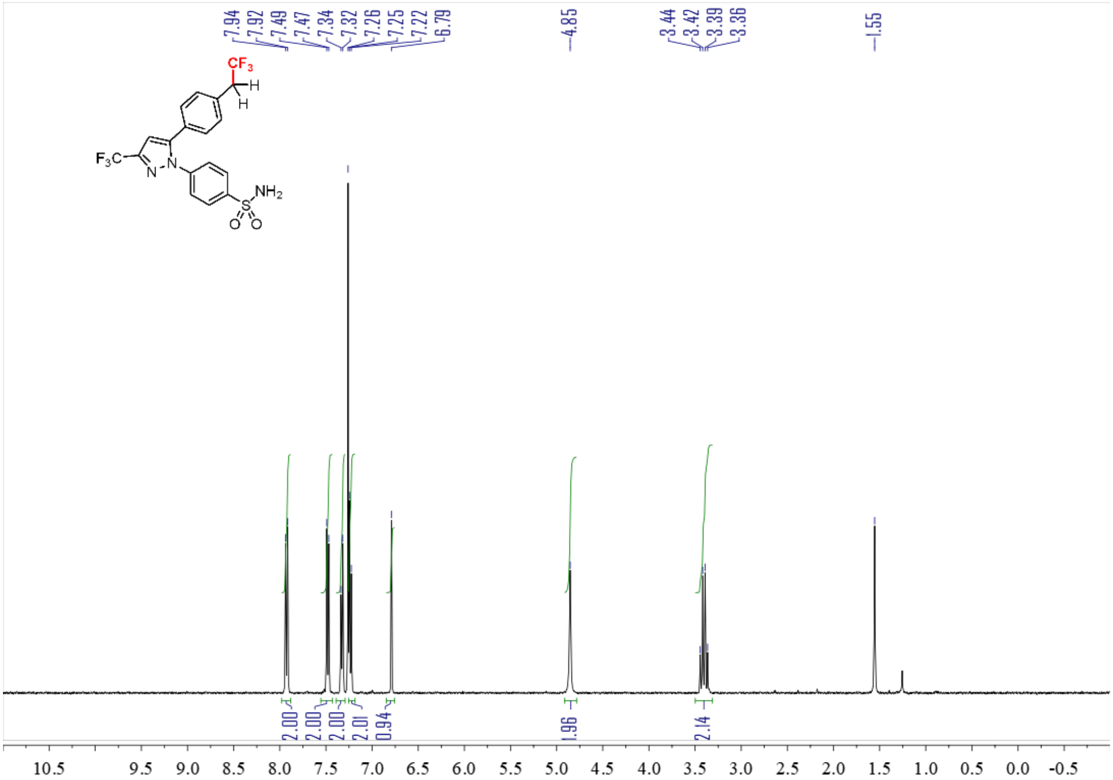
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of **8**



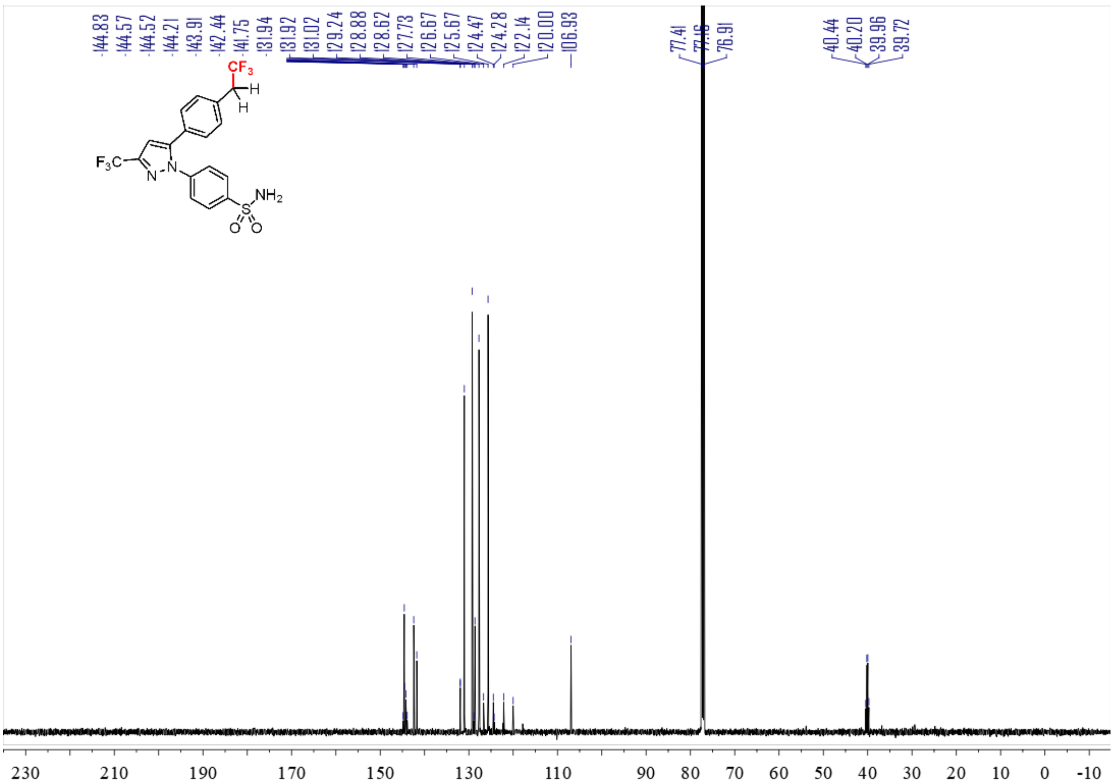
^{13}C NMR spectrum (126 MHz, $CDCl_3$, 23 ºC) of **8**



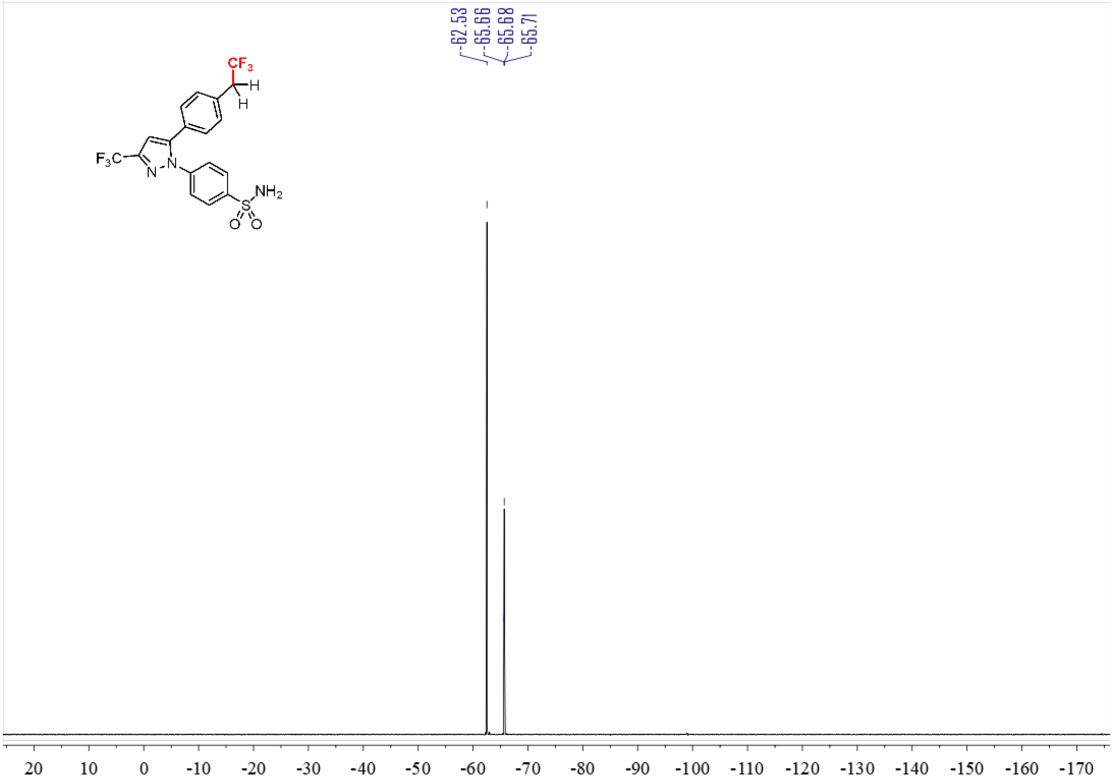
^{19}F NMR spectrum (375 MHz, $CDCl_3$, 23 ºC) of **8**



^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of **9**



^{13}C NMR spectrum (126 MHz, $CDCl_3$, 23 °C) of **9**



^{19}F NMR spectrum (375 MHz, $CDCl_3$, 23 ºC) of **9**