Supporting Information for

Four-Component Acyloxytrifluoromethylation of Arylalkenes Mediated by Photoredox Catalyst

Xiaocong Zhou,[a,b] Guijie Li,*[,a] Zongzhou Shao,[a] Kun Fang,[a] Hongjun Gao,[b] Yuanqiang Li[b] and Yuanbin She*[,b]

[a] College of Chemical Engineering, Zhejiang University of Technology, Hangzhou, Zhejiang 310014, P.R. China

[b] Zhejiang Jiuzhou Pharmaceutical Technology Co., Ltd. Hangzhou, Zhejiang 310051, P.R. China

E-mail: guijieli@zjut.edu.cn; sheyb@zjut.edu.cn

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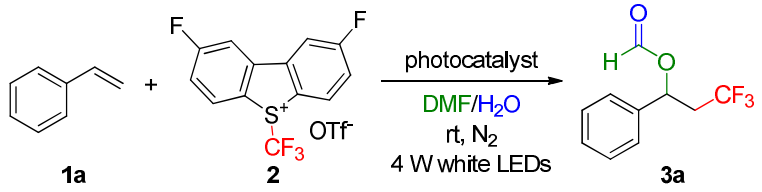
General Information. ^{1}H, ^{13}C, and ^{19}F NMR spectra were measured on a 400, 100, and 376 MHz spectrometers in $CDCl_3$ or DMSO-d_6, respectively. If $CDCl_3$ used as solvent, ^{1}H NMR spectra were recorded with residual $CDCl_3$ (δ = 7.26 ppm) as internal reference; If DMSO-d_6 used as solvent, ^{1}H NMR spectra were recorded with residual H_2O (δ = 3.33 ppm) as internal reference; ^{13}C NMR spectra were recorded with $CDCl_3$ (δ = 77.00 ppm) as internal reference; ^{19}F chemical shifts were given as δ in ppm downfield from $CFCl_3$. The following abbreviations (or combinations thereof) were used to explain the ^{1}H, ^{13}C, and ^{19}F NMR ultiplicities: s = singlet, d = doublet, t = triplet, q = quartet, p = quintet, m = multiplet, br = broad. All of the new compounds were analyzed for HRMS on an EI-TOF mass spectrometer using electrospray ionization in positive ion mode. The detection of compound **5** was analyzed for HRMS on an accurate mass Q TOF LC/MS. Unless otherwise noted, all reagents and substrates were obtained commercially and used without further purification.

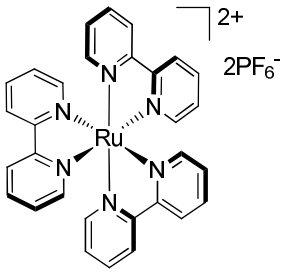
Table S1. Screening of Additives and Photocatalysts



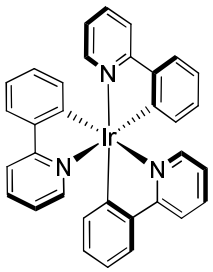
1a **2** **3a**

Entry	Photocatalyst	Additive (2.0 equiv)	Yield[a]
1	$Ru(bpy)_3(PF_6)_2$	K_2HPO_4	10
2	$Ru(bpy)_3(PF_6)_2$	$NaHCO_3$	14
3	$Ru(bpy)_3(PF_6)_2$	K_2CO_3	N.D
4	*fac*-$Ir(ppy)_3$	---	21
5	$[Ir(ppy)_2(bpy)]PF_6$	---	8
6	$[Ir(ppy)_2(dtbbpy)]PF_6$	---	18
7	$Ir[dFppy]_2(dtbbpy)PF_6$	---	11

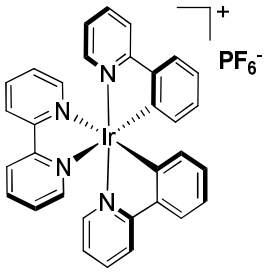
[a]The yields were determined by ^{19}F NMR spectroscopies of crude reaction mixtures with 1-chloro-4-(trifluoromethyl)benzene as an internal standard.



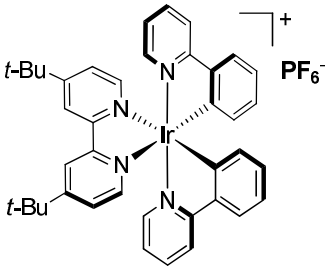
$Ru(bpy)_3(PF_6)_2$



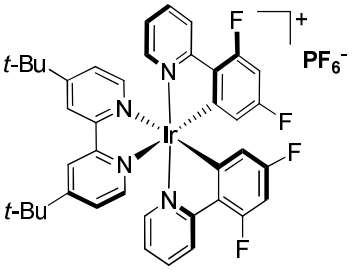
***fac*-$Ir(ppy)_3$**



$[Ir(ppy)_2(bpy)]PF_6$



$[Ir(ppy)_2(dtbbpy)]PF_6$

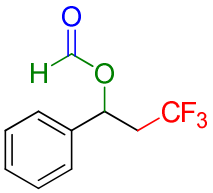


$Ir[dFppy]_2(dtbbpy)PF_6$

General Procedure for the Reaction of Arylalkenes and Umemoto Reagent

A 10 mL Schlenk tube equipped with a magnetic stir bar was charged with arylalkene **1** (1.2 equiv), Umemoto reagent **2** (1.0 equiv), DMF or DMA (5.0 mL/mmol **2**), H_2O (1.0 equiv) and $Ru(bpy)_3(PF_6)_2$ (0.5 mol %). The mixture was evacuated and back-filled with nitrogen three times. The tube was irradiated for 6 h by a 4 W white LED lamp placed at a distance of 1-2 cm. After that, 20 mL of water was added to the reaction mixture, which was then extracted with ethyl acetate (50 mL×3). The combined organic phases were washed with water, dried over $MgSO_4$ and concentrated in vacuum. The residue was purified by silica gel column chromatography to give the corresponding product **3** or **4**.

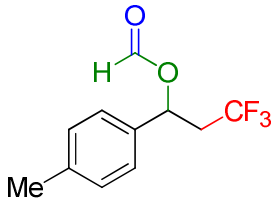
*3,3,3-Trifluoro-1-phenylpropyl formate (**3a**)*



3a

Following the general procedure, styrene **1a** (125 mg, 1.2 mmol, 1.2 equiv), **2** (438 mg, 1.0 mmol, 1.0 equiv), DMF (5.0 mL), H_2O (18 uL, 1.0 mmol, 1.0 equiv) and $Ru(bpy)_3(PF_6)_2$ (4.3 mg, 0.005 mmol, 0.5 mol %) irradiated by 4 W white LEDs for 6.0 h. After purification by silica gel column chromatography using 0-5 % ethyl acetate in hexanes as the eluent, the title compound was obtained as a colorless oil (161.2 mg, 74%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.51-2.63 (m, 1H), 2.80-2.93 (m, 1H), 6.22 (dd, J = 9.6, 3.6 Hz, 1H), 7.33-7.41 (m, 5H), 8.07 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 40.24 (q, J = 27.7 Hz), 69.07 (q, J = 3.3 Hz), 125.00 (q, J = 275.7 Hz), 126.35, 128.88, 128.97, 137.90, 159.36; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -64.14 (s, 3F); HRMS (EI): m/z calcd for $C_{10}H_9F_3O_2$ $[M]^+$ 218.0555, found 218.0558.

*3,3,3-Trifluoro-1-(p-tolyl)propyl formate (**3b**)*

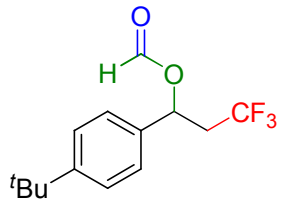


3b

Following the general procedure, 1-methyl-4-vinylbenzene **1b** (142 mg, 1.2 mmol, 1.2 equiv), **2** (438 mg, 1.0 mmol, 1.0 equiv), DMF (5.0 mL), H_2O (18 uL, 1.0 mmol, 1.0 equiv) and $Ru(bpy)_3(PF_6)_2$ (4.3

mg, 0.005 mmol, 0.5 mol %) irradiated by 4 W white LEDs for 6.0 h. After purification by silica gel column chromatography using 0-5 % ethyl acetate in hexanes as the eluent, the title compound was obtained as a colorless oil (194.1 mg, 84%). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 2.30 (s, 3H), 2.83-2.97 (m, 1H), 3.05-3.19 (m, 1 H), 6.09 (dd, J = 3.6, 9.2 Hz, 1H), 7.21 (d, J = 8.0 Hz, 2H), 7.34 (d, J = 8.0 Hz, 2H), 8.30 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 20.89, 40.00 (q, J = 28.0 Hz), 68.89 (q, J = 3.0 Hz), 125.08 (q, J = 276.0 Hz), 126.29, 129.43, 134.95, 138.82, 159.36; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -64.13 (s, 3F); HRMS (EI): m/z calcd for $C_{11}H_{11}F_3O_2$ $[M]^+$ 232.0711, found 232.0714.

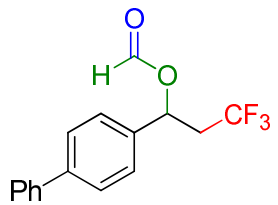
*1-(4-Tert-butylphenyl)-3,3,3-trifluoropropyl formate (**3c**)*



3c

Following the general procedure, 1-*tert*-butyl-4-vinylbenzene **1c** (384 mg, 2.4 mmol, 1.2 equiv), **2** (876 mg, 2.0 mmol, 1.0 equiv), DMF (10.0 mL), H_2O (36 uL, 2.0 mmol, 1.0 equiv) and $Ru(bpy)_3(PF_6)_2$ (8.6 mg, 0.01 mmol, 0.5 mol %) irradiated by 4 W white LEDs for 6.0 h. After purification by silica gel column chromatography using 0-5 % ethyl acetate in hexanes as the eluent, the title compound was obtained as a colorless oil (473.6 mg, 86%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.31 (s, 9H), 2.49-2.61 (m, 1H), 2.80-2.93 (m, 1H), 6.21 (dd, J = 9.4, 3.4 Hz, 1H), 7.30 (d, J = 8.4 Hz, 2H), 7.40 (d, J = 8.4 Hz, 2H), 8.06 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 31.18, 34.60, 40.16 (q, J = 28.3 Hz), 68.85 (q, J = 3.3 Hz), 125.11 (q, J = 276.0 Hz), 125.80, 126.14, 134.87, 152.09, 159.44; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -64.21 (s, 3F); HRMS (EI): m/z calcd for $C_{14}H_{17}F_3O_2$ $[M]^+$ 274.1181, found 274.1184.

*1-(Biphenyl-4-yl)-3,3,3-trifluoropropyl formate (**3d**)*

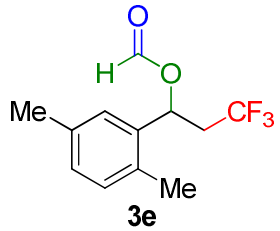


3d

Following the general procedure, 4-vinylbiphenyl **1d** (432 mg, 2.4 mmol, 1.2 equiv), **2** (876 mg, 2.0 mmol, 1.0 equiv), DMF (10.0 mL), H_2O (36 uL, 2.0 mmol, 1.0 equiv) and $Ru(bpy)_3(PF_6)_2$ (8.6 mg, 0.01 mmol, 0.5 mol %) irradiated by 4 W white LEDs for 6.0 h. After purification by silica gel column chromatography using 0-5 % ethyl acetate in hexanes as the eluent, the title compound was

obtained as a white solid (534.1 mg, 91%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.55-2.67 (m, 1H), 2.84-2.98 (m, 1H), 6.27 (dd, *J* = 9.4, 3.8 Hz 1H), 7.37 (t, *J* = 7.2 Hz 1H), 7.43-7.47 (m, 4H), 7.57-7.62 (m, 4H), 8.10 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 40.18 (q, *J* = 28.3 Hz), 68.88 (q, *J* = 3.3 Hz), 125.02 (q, *J* = 276.0 Hz), 126.84, 127.09, 127.61, 127.64, , 128.82, 136.74, 140.20, 141.96, 159.44; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -64.07 (s, 3F); HRMS (EI): m/z calcd for $C_{16}H_{13}F_3O_2$ $[M]^+$ 294.0868, found 294.0865.

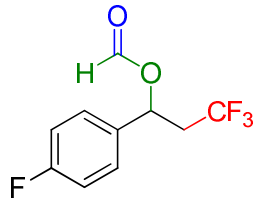
*1-(2,5-Dimethylphenyl)-3,3,3-trifluoropropyl formate (**3e**)*



3e

Following the general procedure, 1,4-dimethyl-2-vinylbenzene **1e** (317 mg, 2.4 mmol, 1.2 equiv), **2** (876 mg, 2.0 mmol, 1.0 equiv), DMF (10.0 mL), H_2O (36 uL, 2.0 mmol, 1.0 equiv) and $Ru(bpy)_3(PF_6)_2$ (8.6 mg, 0.01 mmol, 0.5 mol %) irradiated by 4 W white LEDs for 6.0 h. After purification by silica gel column chromatography using 0-5 % ethyl acetate in hexanes as the eluent, the title compound was obtained as a colorless oil (325.8 mg, 66%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.32 (s, 3H), 2.39 (s, 3H), 2.42-2.49 (m, 1H), 2.74-2.87 (m, 1H), 6.39 (dd, *J* = 9.4, 3.0 Hz, 1H), 7.02-7.07 (m, 2H), 7.15 (s, 1H), 8.06 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 18.23, 20.84, 39.81 (q, *J* = 28.3 Hz), 65.94 (q, *J* = 2.7 Hz), 125.16 (q, *J* = 275.7 Hz), 126.12, 129.36, 130.66, 131.55, 136.12, 136.31, 159.35; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -64.60 (s, 3F); HRMS (EI): m/z calcd for $C_{12}H_{13}F_3O_2$ $[M]^+$ 246.0868, found 246.0860.

*3,3,3-Trifluoro-1-(4-fluorophenyl)propyl formate (**3f**)*

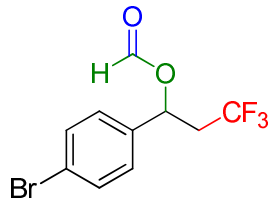


3f

Following the general procedure, 1-fluoro-4-vinylbenzene **1f** (144 mg, 1.2 mmol, 1.2 equiv), **2** (438 mg, 1.0 mmol, 1.0 equiv), DMF (5.0 mL), H_2O (18 uL, 1.0 mmol, 1.0 equiv) and $Ru(bpy)_3(PF_6)_2$ (4.3 mg, 0.005 mmol, 0.5 mol %) irradiated by 4 W white LEDs for 6.0 h. After purification by silica gel column chromatography using 0-5 % ethyl acetate in hexanes as the eluent, the title compound was obtained as a colorless oil (181.2 mg, 77%). ^{1}H NMR (400 MHz, $CDCl_3$): δ =2.49-2.61 (m, 1H),

2.78-2.92 (m, 1H), 6.19 (dd, *J* = 9.2, 4.0 Hz, 1H), 7.05-7.10 (m, 2H), 7.35-7.38 (m, 2H), 8.05 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 40.09 (q, *J* = 27.6 Hz), 68.40 (q, *J* = 3.0 Hz), 115.85 (q, *J* = 18.0 Hz), 124.96 (q, *J* = 275.7 Hz), 128.36 (d, *J* = 8.0 Hz), 133.82 (d, *J* = 3.0 Hz), 159.28, 162.83 (d, *J* = 249.5 Hz); ^{19}F NMR (376 MHz, $CDCl_3$): δ = -112.40 (s, 1F), -64.14 (s, 3F); HRMS (EI): m/z calcd for $C_{10}H_8F_4O_2$ $[M]^+$ 236.0460, found 236.0462.

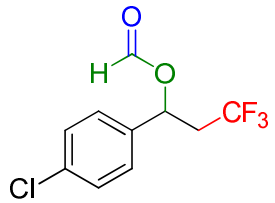
*1-(4-Bromophenyl)-3,3,3-trifluoropropyl formate (**3g**)*



3g

Following the general procedure, 1-bromo-4-vinylbenzene **1g** (220 mg, 1.2 mmol, 1.2 equiv), **2** (438 mg, 1.0 mmol, 1.0 equiv), DMF (5.0 mL), H_2O (18 uL, 1.0 mmol, 1.0 equiv) and $Ru(bpy)_3(PF_6)_2$ (4.3 mg, 0.005 mmol, 0.5 mol %) irradiated by 4 W white LEDs for 6.0 h. After purification by silica gel column chromatography using 0-5 % ethyl acetate in hexanes as the eluent, the title compound was obtained as a colorless oil (242.8 mg, 82%). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 2.88-3.01 (m, 1H), 3.07-3.21 (m, 1H), 6.11 (dd, *J* = 9.2, 4.0 Hz, 1H), 7.44 (d, *J* = 8.4 Hz, 2H), 7.61 (d, *J* = 8.4 Hz, 2H), 8.32 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 39.99 (q, *J* = 27.7 Hz), 68.43 (q, *J* = 3.0 Hz), 122.99, 124.83 (q, *J* = 275.7 Hz), 128.07, 132.04, 136.85, 159.19; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -64.01 (s, 3F); HRMS (EI): m/z calcd for $C_{10}H_8BrF_3O_2$ $[M]^+$ 295.9660, found 295.9656.

*1-(4-Chlorophenyl)-3,3,3-trifluoropropyl formate (**3h**)*

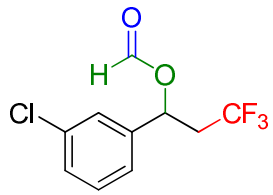


3h

Following the general procedure, 1-chloro-4-vinylbenzene **1h** (166 mg, 1.2 mmol, 1.2 equiv), **2** (438 mg, 1.0 mmol, 1.0 equiv), DMF (5.0 mL), H_2O (18 uL, 1.0 mmol, 1.0 equiv) and $Ru(bpy)_3(PF_6)_2$ (4.3 mg, 0.005 mmol, 0.5 mol %) irradiated by 4 W white LEDs for 6.0 h. After purification by silica gel column chromatography using 0-5 % ethyl acetate in hexanes as the eluent, the title compound was obtained as a colorless oil (194.0 mg, 77%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.48-2.61 (m, 1H), 2.77-2.91 (m, 1H), 6.17 (dd, *J* = 9.0, 4.2 Hz, 1H), 7.31 (d, *J* = 8.4 Hz, 2H), 7.37 (d, *J* = 8.4 Hz, 2H), 8.05

(s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 39.93 (q, J = 28.7 Hz), 68.34 (q, J = 3.0 Hz), 124.88 (q, J = 275.0 Hz), 127.77, 129.01, 134.76, 136.36, 159.21; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -64.02 (s, 3F); HRMS (EI): m/z calcd for $C_{10}H_8ClF_3O_2$ $[M]^+$ 252.0165, found 252.0174.

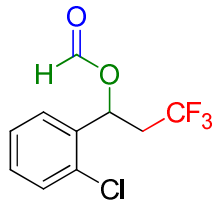
*1-(3-Chlorophenyl)-3,3,3-trifluoropropyl formate (**3i**)*



3i

Following the general procedure, 1-chloro-3-vinylbenzene **1i** (333 mg, 2.4 mmol, 1.2 equiv), **2** (876 mg, 2.0 mmol, 1.0 equiv), DMF (10.0 mL), H_2O (36 uL, 2.0 mmol, 1.0 equiv) and $Ru(bpy)_3(PF_6)_2$ (8.6 mg, 0.01 mmol, 0.5 mol %) irradiated by 4 W white LEDs for 6.0 h. After purification by silica gel column chromatography using 0-5 % ethyl acetate in hexanes as the eluent, the title compound was obtained as a colorless oil (258.0 mg, 51%). ^{1}H NMR (400 MHz, DMSO-d_6): δ = 2.92-3.04 (m, 1H), 3.10-3.24 (m, 1H), 6.13 (dd, J = 9.2, 3.2 Hz, 1H), 7.45 (bs, 3H), 7.59 (s, 1H), 8.34 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 40.03 (q, J = 28.7 Hz), 68.24 (q, J = 3.3 Hz), 124.53, 124.86 (q, J = 276.3 Hz), 126.43, 129.07, 130.16, 134.74, 139.85, 159.12; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -64.07 (s, 3F); HRMS (EI): m/z calcd for $C_{10}H_8ClF_3O_2$ $[M]^+$ 252.0165, found 252.0172.

*1-(2-Chlorophenyl)-3,3,3-trifluoropropyl formate (**3j**)*

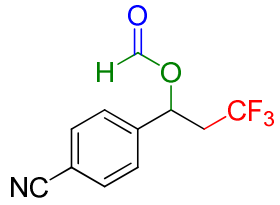


3j

Following the general procedure, 1-chloro-2-vinylbenzene **1j** (333 mg, 2.4 mmol, 1.2 equiv), **2** (876 mg, 2.0 mmol, 1.0 equiv), DMF (10.0 mL), H_2O (36 uL, 2.0 mmol, 1.0 equiv) and $Ru(bpy)_3(PF_6)_2$ (8.6 mg, 0.01 mmol, 0.5 mol %) irradiated by 4 W white LEDs for 6.0 h. After purification by silica gel column chromatography using 0-5 % ethyl acetate in hexanes as the eluent, the title compound was obtained as a colorless oil (247.1 mg, 49%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.60-2.78 (m, 2H), 6.59 (dd, J = 9.2, 2.8 Hz, 1H), 7.27-7.34 (m, 2H), 7.39-7.45 (m, 2H), 8.12 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 38.95 (q, J = 28.0 Hz), 66.02 (q, J = 3.0 Hz), 124.98 (q, J = 276.3 Hz), 126.80, 127.40,

129.82, 129.85, 131.61, 135.68, 158.98; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -64.23 (s, 3F); HRMS (EI): m/z calcd for $C_{10}H_8ClF_3O_2$ $[M]^+$ 252.0165, found 252.0179.

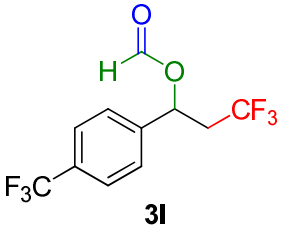
*1-(4-Cyanophenyl)-3,3,3-trifluoropropyl formate (**3k**)*



3k

Following the general procedure, 4-vinylbenzonitrile **1k** (310 mg, 2.4 mmol, 1.2 equiv), **2** (876 mg, 2.0 mmol, 1.0 equiv), DMF (10.0 mL), H_2O (36 uL, 2.0 mmol, 1.0 equiv) and $Ru(bpy)_3(PF_6)_2$ (8.6 mg, 0.01 mmol, 0.5 mol %) irradiated by 4 W white LEDs for 6.0 h. After purification by silica gel column chromatography using 5-15 % ethyl acetate in hexanes as the eluent, the title compound was obtained as a colorless oil (267.4 mg, 55%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.51-2.63 (m, 1H), 2.78-2.91 (m, 1H), 6.21 (q, *J* = 8.8, 4.4 Hz, 1H), 7.50 (d, *J* = 8.4 Hz, 2H), 7.70 (d, *J* = 8.4 Hz, 2H), 8.08 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 39.81 (q, *J* = 28.7 Hz), 68.22 (q, *J* = 3.0 Hz), 112.81, 118.00, 124.64 (q, *J* = 275.7 Hz), 127.02, 132.63, 142.66, 159.03; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -63.86 (s, 3F); HRMS (EI): m/z calcd for $C_{11}H_8F_3NO_2$ $[M]^+$ 243.0507, found 243.0509

*3,3,3-Trifluoro-1-(4-(trifluoromethyl)phenyl)propyl formate (**3l**)*

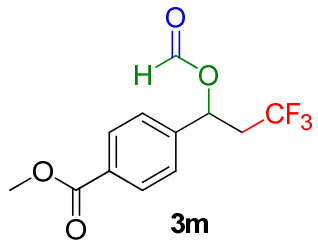


3l

Following the general procedure, 1-(trifluoromethyl)-4-vinylbenzene **1l** (413 mg, 2.4 mmol, 1.2 equiv), **2** (876 mg, 2.0 mmol, 1.0 equiv), DMF (10.0 mL), H_2O (36 uL, 2.0 mmol, 1.0 equiv) and $Ru(bpy)_3(PF_6)_2$ (8.6 mg, 0.01 mmol, 0.5 mol %) irradiated by 4 W white LEDs for 6.0 h. After purification by silica gel column chromatography using 0-5 % ethyl acetate in hexanes as the eluent, the title compound was obtained as a colorless oil (310.0 mg, 54%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.51-2.64 (m, 1H), 2.79-2.93 (m, 1H), 6.24 (q, J = 8.8, 3.6 Hz, 1H), 7.51 (d, *J* = 7.6 Hz, 2H), 7.66 (d, *J* = 8.0 Hz, 2H), 8.08 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 40.16 (q, *J* = 28.7 Hz), 68.49 (q, *J* = 3.3 Hz), 123.77 (q, *J* = 270.3 Hz), 124.85 (q, *J* = 275.7 Hz), 125.97 (q, *J* = 4.0 Hz), 126.78, 131.23 (q, *J* = 32.7 Hz), 141.76, 159.17; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -63.99 (s, 3F), -62.84 (s, 3F); HRMS (EI): m/z

calcd for $C_{11}H_8F_6O_2$ $[M]^+$ 286.0428, found 286.0426

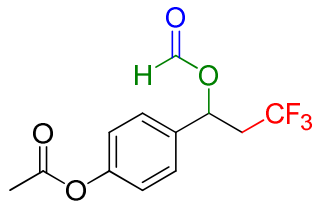
*Methyl 4-(3,3,3-trifluoro-1-(formyloxy)propyl)benzoate (**3m**)*



3m

Following the general procedure, methyl 4-vinylbenzoate **1m** (389 mg, 2.4 mmol, 1.2 equiv), **2** (876 mg, 2.0 mmol, 1.0 equiv), DMF (10.0 mL), H_2O (36 uL, 2.0 mmol, 1.0 equiv) and $Ru(bpy)_3(PF_6)_2$ (8.6 mg, 0.01 mmol, 0.5 mol %) irradiated by 4 W white LEDs for 6.0 h. After purification by silica gel column chromatography using 5-20 % ethyl acetate in hexanes as the eluent, the title compound was obtained as a colorless oil (285.5 mg, 52%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.51-2.63 (m, 1H), 2.79-2.92 (m, 1H), 3.92 (s, 3H), 6.24 (dd, *J* = 8.8, 3.6 Hz, 1H), 7.45 (d, *J* = 8.0 Hz, 2H), 8.06 (d, *J* = 8.4 Hz, 2H), 8.08 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 39.99 (q, *J* = 28.7 Hz), 52.11, 68.52 (q, *J* = 3.3 Hz), 124.82 (q, *J* = 276.0 Hz), 126.24, 130.10, 130.66, 142.51, 159.16, 166.23; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -63.99 (s, 3F); HRMS (EI): m/z calcd for $C_{12}H_{11}F_3O_4$ $[M]^+$ 276.0609, found 276.0609.

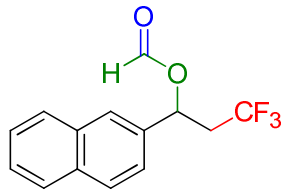
*4-(3,3,3-Trifluoro-1-(formyloxy)propyl)phenyl acetate (**3n**)*



3n

Following the general procedure, 4-vinylphenyl acetate **1n** (389 mg, 2.4 mmol, 1.2 equiv), **2** (876 mg, 2.0 mmol, 1.0 equiv), DMF (10.0 mL), H_2O (36 uL, 2.0 mmol, 1.0 equiv) and $Ru(bpy)_3(PF_6)_2$ (8.6 mg, 0.01 mmol, 0.5 mol %) irradiated by 4 W white LEDs for 6.0 h. After purification by silica gel column chromatography using 0-5 % ethyl acetate in hexanes as the eluent, the title compound was obtained as a white solid (418.1 mg, 76%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.30 (s, 3H), 2.49-2.61 (m, 1H), 2.78-2.92 (m, 1H), 6.22 (dd, *J* = 9.2, 3.2 Hz, 1H), 7.12 (d, *J* = 8.4 Hz, 2H), 7.39 (d, *J* = 8.4 Hz, 2H), 8.05 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 20.81, 39.96 (q, *J* = 28.3 Hz), 68.27 (q, *J* = 3.3 Hz), 121.99, 124.91 (q, *J* = 275.7 Hz), 127.53, 135.28, 150.86, 159.24, 169.09; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -64.15 (s, 3F); HRMS (EI): m/z calcd for $C_{12}H_{11}F_3O_4$ $[M]^+$ 276.0609, found 276.0617.

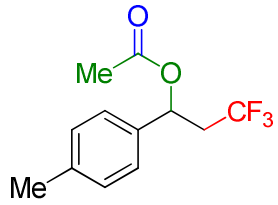
*3,3,3-Trifluoro-1-(naphthalen-2-yl)propyl formate (**3o**)*



3o

Following the general procedure, 2-vinylnaphthalene **1o** (370 mg, 2.4 mmol, 1.2 equiv), **2** (876 mg, 2.0 mmol, 1.0 equiv), DMF (10.0 mL), H_2O (36 uL, 2.0 mmol, 1.0 equiv) and $Ru(bpy)_3(PF_6)_2$ (8.6 mg, 0.01 mmol, 0.5 mol %) irradiated by 4 W white LEDs for 6.0 h. After purification by silica gel column chromatography using 0-5 % ethyl acetate in hexanes as the eluent, the title compound was obtained as a colorless oil (333.5 mg, 62%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.60-2.72 (m, 1H), 2.89-3.03 (m, 1H), 6.39 (dd, *J* = 9.2, 3.6 Hz, 1H), 7.46-7.54 (m, 3H), 7.84-7.90 (m, 4H), 8.11 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 40.10 (q, *J* = 28.3 Hz), 69.17 (q, *J* = 3.0 Hz), 123.35 125.08 (q, *J* = 275.7 Hz), 125.96, 126.60, 126.67, 127.67, 128.04, 128.91, 132.95, 133.29, 135.06, 159.38; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -64.05 (s, 3F); HRMS (EI): m/z calcd for $C_{14}H_{11}F_3O_2$ $[M]^+$ 268.0711, found 268.0714.

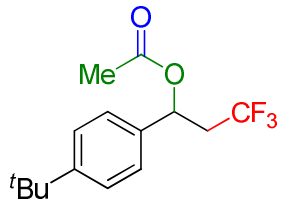
*1-(4-Tert-butylphenyl)-3,3,3-trifluoropropyl acetate (**4b**)*



4b

Following the general procedure, 1-methyl-4-vinylbenzene **1b** (283 mg, 2.4 mmol, 1.2 equiv), **2** (876 mg, 2.0 mmol, 1.0 equiv), DMA (10.0 mL), H_2O (36 uL, 2.0 mmol, 1.0 equiv) and $Ru(bpy)_3(PF_6)_2$ (8.6 mg, 0.01 mmol, 0.5 mol %) irradiated by 4 W white LEDs for 6.0 h. After purification by silica gel column chromatography using 0-5 % ethyl acetate in hexanes as the eluent, the title compound was obtained as a white solid (310 mg, 63%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 2.07 (s, 3H), 2.35 (s, 3H), 2.45-2.57 (m, 1H), 2.73-2.86 (m, 1H), 6.08 (dd, *J* = 9.4, 3.8 Hz, 1H), 7.18 (d, *J* = 8.0 Hz, 2H), 7.25 (d, *J* = 8.0 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 20.70, 20.92, 40.14 (q, *J* = 28.0 Hz), 69.14 (q, *J* = 3.0 Hz), 125.22 (q, *J* = 275.5 Hz), 126.22, 129.36, 135.66, 138.48, 169.39; **^{19}F NMR** (376 MHz, $CDCl_3$): δ = -64.16 (s, 3F); **HRMS (EI)**: m/z calcd for $C_{12}H_{13}F_3O_2$ $[M]^+$ 246.0868, found 246.0847.

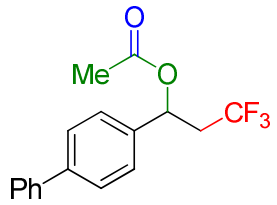
*1-(4-Tert-butylphenyl)-3,3,3-trifluoropropyl acetate (**4c**)*



4c

Following the general procedure, 1-tert-butyl-4-vinylbenzene **1c** (384 mg, 2.4 mmol, 1.2 equiv), **2** (876 mg, 2.0 mmol, 1.0 equiv), DMA (10.0 mL), H_2O (36 uL, 2.0 mmol, 1.0 equiv) and $Ru(bpy)_3(PF_6)_2$ (8.6 mg, 0.01 mmol, 0.5 mol %) irradiated by 4 W white LEDs for 6.0 h. After purification by silica gel column chromatography using 0-5 % ethyl acetate in hexanes as the eluent, the title compound was obtained as a colorless oil (354.2 mg, 61%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.31 (s, 3H) , 2.07 (s, 3H) , 2.44-2.57 (m, 1H) , 2.73-2.87 (m, 1H), 6.10 (dd, J = 9.6, 3.6 Hz, 1H), 7.28 (d, J = 8.0 Hz, 2H), 7.39 (d, J = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 20.74, 31.13, 34.49, 40.17 (q, J = 28.0 Hz), 69.02 (q, J = 3.3 Hz), 125.26 (q, J = 275.7 Hz), 125.63, 126.01, 135.60, 151.63, 169.42; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -64.24 (s, 3F); HRMS (EI): m/z calcd for $C_{15}H_{19}F_3O_2$ $[M]^+$ 288.1337, found 288.1339.

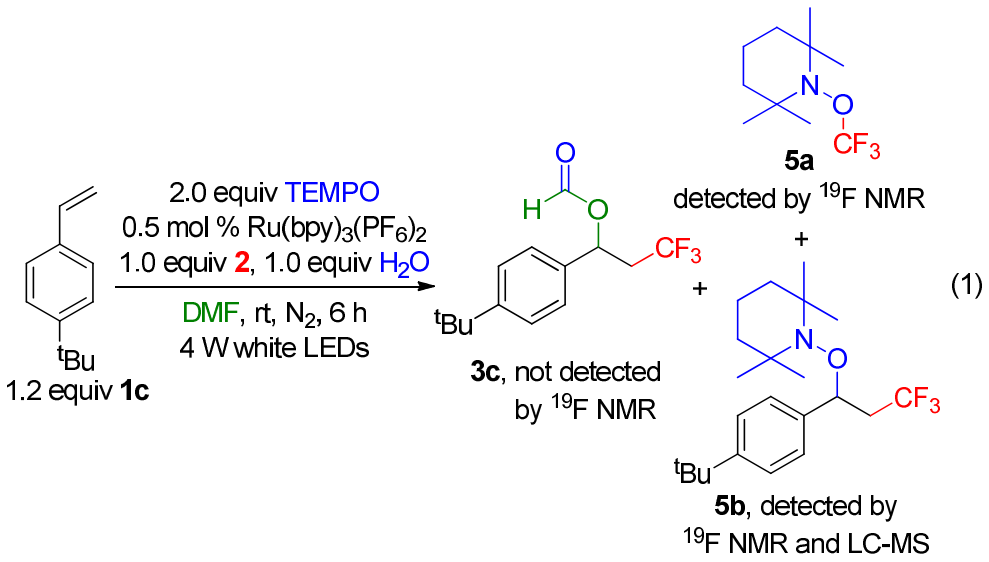
*1-(Biphenyl-4-yl)-3,3,3-trifluoropropyl acetate (**4d**)*



4d

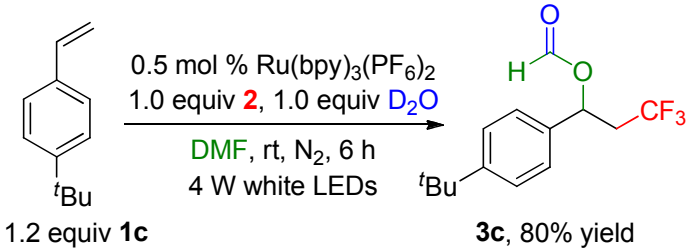
Following the general procedure, 4-vinylbiphenyl **1d** (216 mg, 1.2 mmol, 1.2 equiv), **2** (438 mg, 1.0 mmol, 1.0 equiv), DMA (5.0 mL), H_2O (18 uL, 1.0 mmol, 1.0 equiv) and $Ru(bpy)_3(PF_6)_2$ (4.3 mg, 0.005 mmol, 0.5 mol %) irradiated by 4 W white LEDs for 6.0 h. After purification by silica gel column chromatography using 0-5 % ethyl acetate in hexanes as the eluent, the title compound was obtained as a white solid (201.0 mg, 66%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.11 (s, 3H), 2.50-2.63 (m, 1H), 2.78-2.92 (m, 1H), 6.16 (dd, J = 9.4, 3.8 Hz, 1H), 7.34-7.38 (m, 1H), 7.42-7.47 (m, 4H), 7.56-7.67 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 20.94, 40.29 (q, J = 28.0 Hz), 69.15 (q, J = 3.0 Hz), 125.20 (q, J = 275.7 Hz), 126.76, 127.09, 127.54, 127.56, 128.81, 137.52, 140.36, 141.70, 169.57; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -64.11 (s, 3F); HRMS (EI): m/z calcd for $C_{17}H_{15}F_3O_2$ $[M]^+$ 308.1024, found 308.0998.

Control Experiments (Scheme 2, eq 1)



A 10 mL Schlenk tube equipped with a magnetic stir bar was charged with 1-*tert*-butyl-4-vinylbenzene **1c** (384 mg, 2.4 mmol, 1.2 equiv), **2** (876 mg, 2.0 mmol, 1.0 equiv), DMF (10.0 mL), H_2O (36 uL, 2.0 mmol, 1.0 equiv), $Ru(bpy)_3(PF_6)_2$ (8.6 mg, 0.01 mmol, 0.5 mol %) and TEMPO (625 mg, 4.0 mmol, 2.0 equiv). The mixture was evacuated and back-filled with nitrogen three times. The tube was irradiated for 6 h by a 4 W white LED lamp placed at a distance of 1-2 cm. After that, the reaction mixture was analyzed by *in suit* ^{19}F NMR and LC-MS. No peak of **3c** was found in suit 19F NMR spectrum, however, as expected, both peaks of product **5a** and **5b** were found in suit 19F NMR spectrum. **5b** was also detected (See supporting information), HRMS (ESI): m/z calcd for $C_{22}H_{38}F_3N_2O$ $[M+NH_4]^+$ 403.2931, found 403.2935.

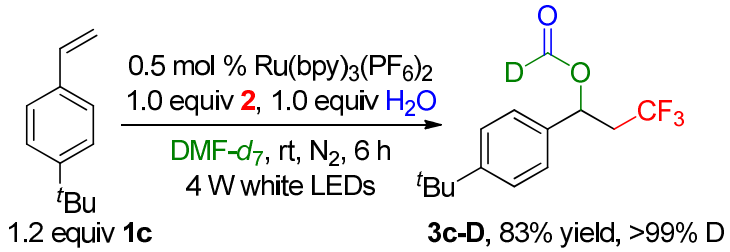
D-Labeling Experiment (Scheme 2, eq 2)



A 20 mL Schlenk tube equipped with a magnetic stir bar was charged with 1-*tert*-butyl-4-vinylbenzene **1c** (384 mg, 2.4 mmol, 1.2 equiv), **2** (876 mg, 2.0 mmol, 1.0 equiv), DMF (10.0 mL), D_2O (36 uL, 2.0 mmol, 1.0 equiv, 99.9% D, d: 1.107) and $Ru(bpy)_3(PF_6)_2$ (8.6 mg, 0.01 mmol, 0.5 mol %) irradiated by 4 W white LEDs for 6.0 h. After that, 40 mL of water was added to the reaction mixture, which was then extracted with ethyl acetate (100 mL×3). The combined

organic phases were washed with water, dried over $MgSO_4$ and concentrated in vacuum. The residue was purified by silica gel column chromatography using 0-5% ethyl acetate in hexanes as the eluent, the no deuterated product **3c** was obtained as a colorless oil (436.7 mg, 80%). The product was confirmed by ^{1}H NMR.

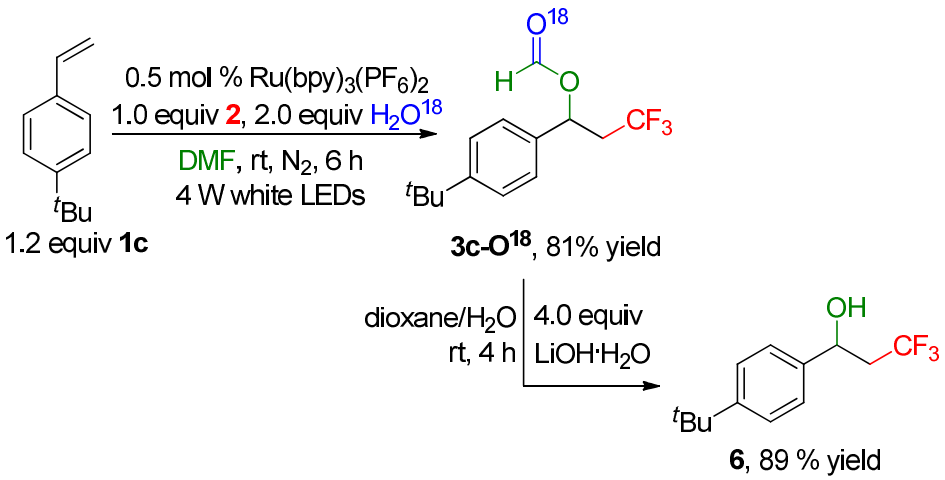
D-Labeling Experiment (Scheme 2, eq 3)



1.2 equiv **1c** — **3c-D**, 83% yield, >99% D

A 10 mL Schlenk tube equipped with a magnetic stir bar was charged with 1-*tert*-butyl-4-vinylbenzene **1c** (192 mg, 1.2 mmol, 1.2 equiv), **2** (438 mg, 1.0 mmol, 1.0 equiv), DMF-d_7 (5.0 mL, 99.5% D), H_2O (18 uL, 1.0 mmol, 1.0 equiv) and $Ru(bpy)_3(PF_6)_2$ (4.3 mg, 0.005 mmol, 0.5 mol %) irradiated by 4 W white LEDs for 6.0 h. After that, 20 mL of water was added to the reaction mixture, which was then extracted with ethyl acetate (50 mL×3). The combined organic phases were washed with water, dried over $MgSO_4$ and concentrated in vacuum. The residue was purified by silica gel column chromatography using 0-5% ethyl acetate in hexanes as the eluent, the title deuterated product **3c-D** was obtained as a colorless oil (228.4 mg, 83%, >99% D). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.31 (s, 9H), 2.49-2.62 (m, 1H), 2.79-2.93 (m, 1H), 6.22 (dd, J = 9.2, 3.6 Hz, 1H), 7.30 (d, J = 8.4 Hz, 2H), 7.40 (d, J = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 31.15, 34.57, 40.13 (q, J = 28.0 Hz), 68.77 (q, J = 3.0 Hz), 125.13 (q, J = 275.7 Hz), 125.78, 126.13, 134.89, 152.07, 159.21 (t, J = 34.5 Hz); ^{19}F NMR (376 MHz, $CDCl_3$): δ = -64.21 (s, 3F); HRMS (EI): m/z calcd for $C_{14}H_{16}DF_3O_2$ $[M]^+$ 275.1243, found 275.1231.

O^{18}-Labeling Experiment (Scheme 2, eqs 4 and 5)

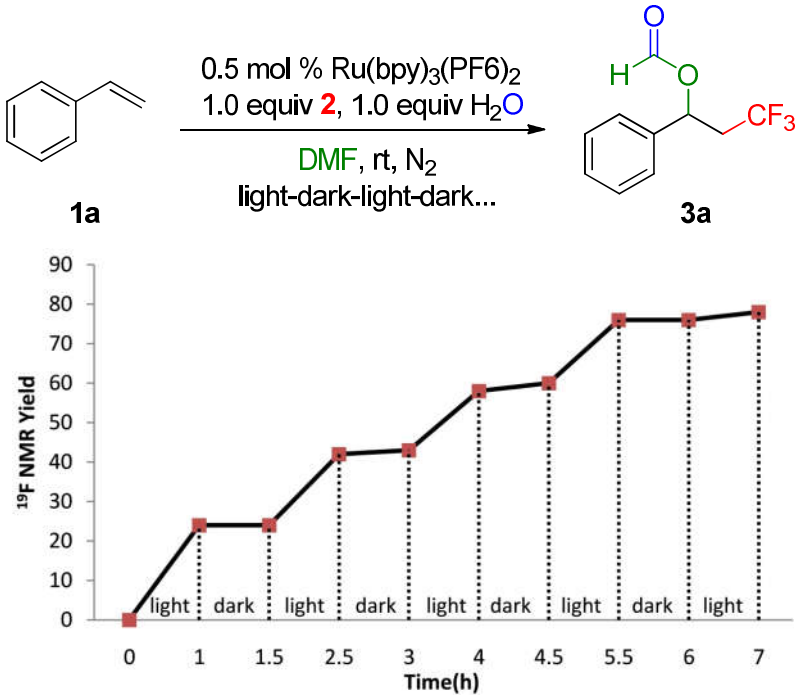


A 20 mL Schlenk tube equipped with a magnetic stir bar was charged with 1-tert-butyl-4-vinylbenzene **1c** (384 mg, 2.4 mmol, 1.2 equiv), **2** (876 mg, 2.0 mmol, 1.0 equiv), DMF (10.0 mL), H_2O^{18} (72 uL, 4.0 mmol, 2.0 equiv) and $Ru(bpy)_3(PF_6)_2$ (8.6 mg, 0.01 mmol, 0.5 mol %) irradiated by 4 W white LEDs for 6.0 h. After that, 40 mL of water was added to the reaction mixture, which was then extracted with ethyl acetate (100 mL×3). The combined organic phases were washed with water, dried over $MgSO_4$ and concentrated in vacuum. The residue was purified by silica gel column chromatography using 0-5 % ethyl acetate in hexanes as the eluent, the O^{18}-labeling product **3c-O^{18}** was obtained as a colorless oil (447.3 mg, 81%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.31 (s, 9H), 2.49-2.62 (m, 1H), 2.79-2.93 (m, 1H), 6.22 (dd, J = 9.6, 3.2 Hz, 1H), 7.30 (d, J = 8.4 Hz, 2H), 7.40 (d, J = 8.4 Hz, 2H), 8.06 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 31.16, 34.58, 40.15 (q, J = 28.3 Hz), 68.84 (q, J = 3.3 Hz), 125.12 (q, J = 275.7 Hz), 125.79, 126.14, 134.89, 152.08, 159.39; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -64.21 (s, 3F); HRMS (EI): m/z calcd for $C_{14}H_{17}F_3{}^{16}O^{18}O$ $[M]^+$ 276.1223, found 276.1210.

To a solution of **3c-O^{18}** (442.0mg, 1.6 mmol, 1.0 equiv) in dioxane (5 mL) and water (5 mL) was added lithium hydroxide monohydrate (268.5mg, 6.4 mmol, 4.0 equiv). The reaction mixture was stirred at room temperature for 4 hours. After removal of dioxane by evaporation under vacuum, the remaining aqueous phase was neutralized with 2N HCl and extracted with ethyl acetate (30 mL×3). The combined organic phases were washed with water, dried over $MgSO_4$ and concentrated in vacuum. The residue was purified by silica gel column chromatography using 5-10 % ethyl acetate in hexanes as the eluent, the title product 1-(4-(*tert*-butyl)phenyl)-3,3,3-trifluoropropyl formate (**6**) was obtained as a colorless oil (350.1 mg, 89%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.32 (s, 9H), 2.12 (s,

1H), 2.39-2.51 (m, 1H), 2.57-2.71 (m, 1H), 5.04-5.08 (m, 1H), 7.31 (d, *J* = 8.4 Hz, 2H), 7.41 (d, *J* = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 31.21, 34.50, 40.51 (q, *J* = 26.7 Hz), 68.41 (q, *J* = 3.0 Hz), 125.41, 125.63, 125.90 (q, *J* = 275.7 Hz), 139.40, 151.36; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -63.77 (s, 3F); HRMS (EI): m/z calcd for $C_{13}H_{17}F_3O$ $[M]^+$ 246.1232, found 276.1236.

Light-dark interval experiment (Scheme 3)



A 10 mL Schlenk tube equipped with a magnetic stir bar was charged with styrene **1a** (125 mg, 1.2 mmol, 1.2 equiv), Umemoto reagent **2** (438 mg, 1.0 mmol, 1.0 equiv), and $Ru(bpy)_3(PF_6)_2$ (4.3 mg, 0.005 mmol, 0.5 mol %). The mixture was evacuated and back-filled with nitrogen three times. Then DMF (5.0 mL), H_2O (18 uL, 1.0 mmol, 1.0 equiv) and 1-chloro-4-(trifluoromethyl)benzene (134 uL, 1.0 mmol, 1.0 equiv) was added to the tube *via* syringe. The tube was irradiated for by a 4 W white LED lamp placed at a distance of 1-2 cm. The yield was determined by ^{19}F NMR spectroscopies of an aliquot from the reaction mixture with 1-chloro-4-(trifluoromethyl)benzene as an internal standard.

Quantum Yield Measurement

The quantum yield (Φ) of the photochemical reaction was measured according to the procedure reported by Melchiorre's group (M. Silvi, C. Verrier, Y. P. Rey, L. Buzzetti and P. Melchiorre, *Nat.*

Chem., 2017, **9**, 868.) and Gong's group (X. Shen, Y. Li, Z. Wen, S, Cao, X. Hou and L. Gong, *Chem. Sci*., 2018, **9**, 4562).

A ferrioxalate actinometer solution was prepared according to the literature (S. L. Murov, Ed. *Handbook of Photochemistry,* Marcel Dekker, New York, 1973), and used for determination of photon flux of the light source. Under irradiation, the ferrioxalate actinometer solution undergoes decomposition from ferric ions to ferrous ions, which are complexed by 1,10-phenanthroline and monitored by UV/Vis absorbance at 510 nm. The moles of iron-phenanthroline complex formed are related to moles of photons absorbed.

Preparation of the stock solutions:

Potassium ferrioxalate solution: potassium ferrioxalate (294.8 mg) and sulfuric acid (139 μL) were added to a 50 mL volumetric flask, and filled to the mark with deionized water. Phenanthroline solution: 1,10-phenanthroline (100 mg) was added to a 50 mL volumetric flask, and filled to the mark with deionized water. Buffer solution: sodium acetate (2.47 g) and sulfuric acid (0.5 mL) were added to a 50 mL volumetric flask, and filled to the mark with deionized water. Model reaction solution: 1-*tert*-butyl-4-vinylbenzene **1c** (192 mg, 1.2 mmol), **2** (438 mg, 1.0 mmol), H_2O (18 uL, 1.0 mmol) and $Ru(bpy)_3(PF_6)_2$ (4.3 mg, 0.005 mmol, 0.5 mol %) were sequentially added to a 25 mL volumetric flask and filled to the mark with *N*,*N*-dimethylformamide. *Note: all the stock solutions were prepared and stored in the dark.*

Actinometry measurements:

The actinometer solution (potassium ferrioxalate in water, 1.0 mL) and the model reaction solution (**1c** with **2** catalyzed by $Ru(bpy)_3(PF_6)_2$ in DMF, 1.0 mL) were added to two identical Schlenk tubes (diameter = 12 mm) respectively. The Schlenk tubes were placed 2 cm away from the light source. They were irradiated together with a 4 W white LEDs Lamp without stirring. This procedure was repeated 4 times, quenching the two reactions after different time intervals: 45 sec, 60 sec, 75 sec, and 90 sec for the actinometry solution; 30 min, 60 min, 90 min, and 120 min for the model reaction. After irradiation, the actinometer solution was removed and placed in a 10 mL volumetric flask containing 1,10-phenanthroline solution (0.5 mL) and buffer solution (2 mL). This flask was filled to the mark with deionized water. The UV-Vis spectra of the complexed actinometer samples were recorded for each time interval. The absorbance of the complexed actinometer solution was monitored at 510 nm. (**Fig. S1**).

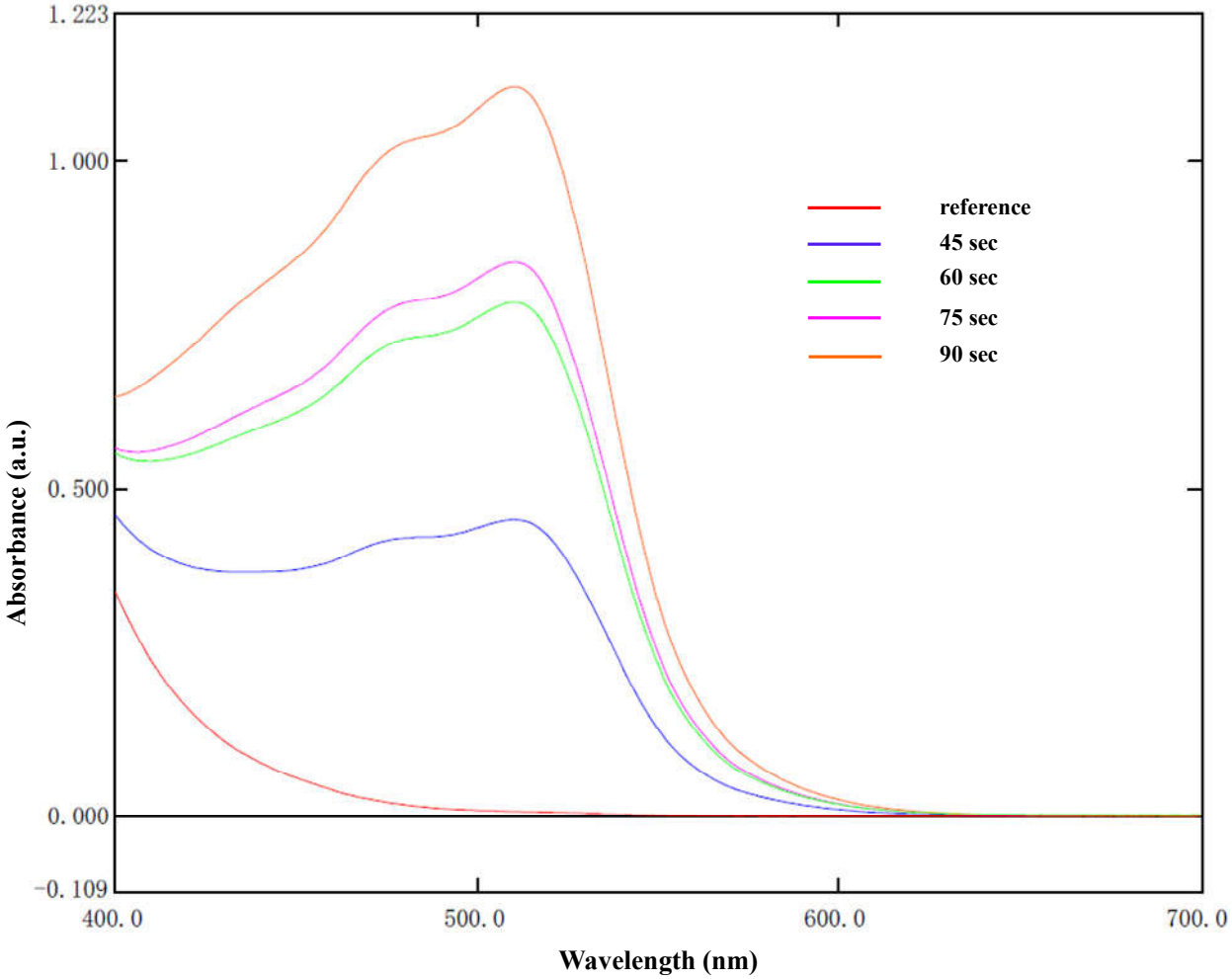


Fig. S1 UV - Vis spectra of the complexed actinometer samples at each time interval (45 sec, 60 sec, 75 sec, and 90 sec).

Calculation of photon flux of the light source:

Moles of Fe^{2+} formed for each sample is determined using Beers' Law (**Eq. 1**)

$$\text{Moles of Fe(II)} = \frac{V_1 \times V_3 \times \Delta A(510\ nm)}{10^3 \times V_2 \times l \times \varepsilon(510\ nm)} \qquad \textbf{(Eq. 1)}$$

V_1 is the irradiated volume (1.0 mL), V_2 is the aliquot of the irradiated solution taken for the determination of the ferrous ions (1.0 mL), V_3 is the final volume after complexation with phenanthroline (10 mL), *l* is the optical path-length of the irradiation cell (1.0 cm), ΔA(510 nm) is the optical difference in absorbance between the irradiated solution and the one stored in the dark, ε(510 nm) is the extinction coefficient the complex $Fe(phen)_3^{2+}$ at 510 nm (11100 L mol^{-}1 cm^{-}1). The moles of Fe^{2+} formed (x) are plotted as a function of time (t) **(Fig. S2)**.

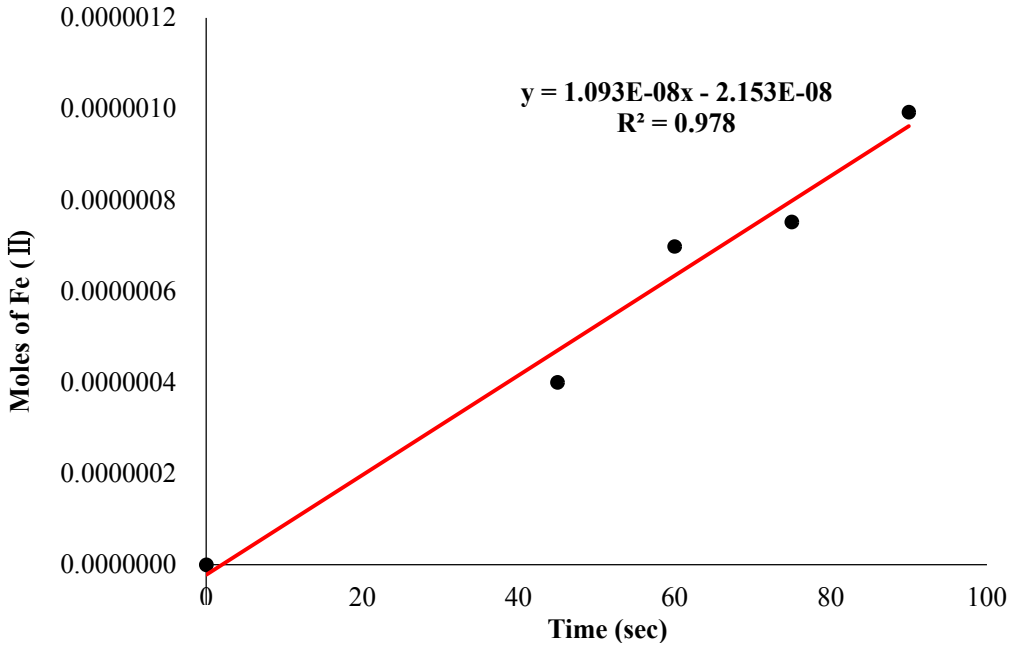


Fig. S2 The moles of Fe^{2+} formed (x) versus time (t).

The slope of this line was correlated to the moles of incident photons by unit of time ($q^0_{n,p}$) by the use of the following **Eq. 2**:

$$\Phi(\lambda) = \frac{\mathrm{dx/dt}}{\mathrm{q}^0_{n,p}[1-10^{-\mathrm{A}(\lambda)}]} \qquad \textbf{(Eq. 2)}$$

dx/dt is the rate of change of a measurable quantity (spectral or any other property), the quantum yield (Φ) for Fe^{2+} at 400 nm is 1.13 (C. G. Hatchard and C. A. Parker, *Proc. R. Soc. Lond. A* 1956, **235**, 518–536), $[1\text{-}10^{-A(\lambda)}]$ is the ratio of absorbed photons by the solution, and *A*(λ) is the absorbance of the actinometer at the wavelength used to carry out the experiments (400 nm). The absorbance at 400 nm *A*(400) was measured using a Shimadzu UV-2550 UV-Vis spectrophotometer in a 10 mm path quartz cuvette, obtaining an absorbance of 2.52.

Calculation of quantum yield of the photochemical reaction:

The moles of product **3c** formed for the model reaction were determined by ^{19}F NMR. The moles of product per unit of time are related to the number of photons absorbed. The photons absorbed are correlated to the number of incident photons by the use of **Eq. 2**. According to this, if we plot the moles of product (x) versus the moles of incident photons ($q^0_{n,p}$·dt), the slope is equal to: **Φ·(1-10$^{-A(\lambda)}$)**, where Φ is the quantum yield to be determined and *A*(400 nm) is the absorption of the reaction under study **(Fig. S3)**.

A(400 nm) was measured using a Shimadzu UV-2550 UV-Vis spectrophotometer in 10 mm path quartz. An absorbance of 1.61 was determined for the model reaction mixture.

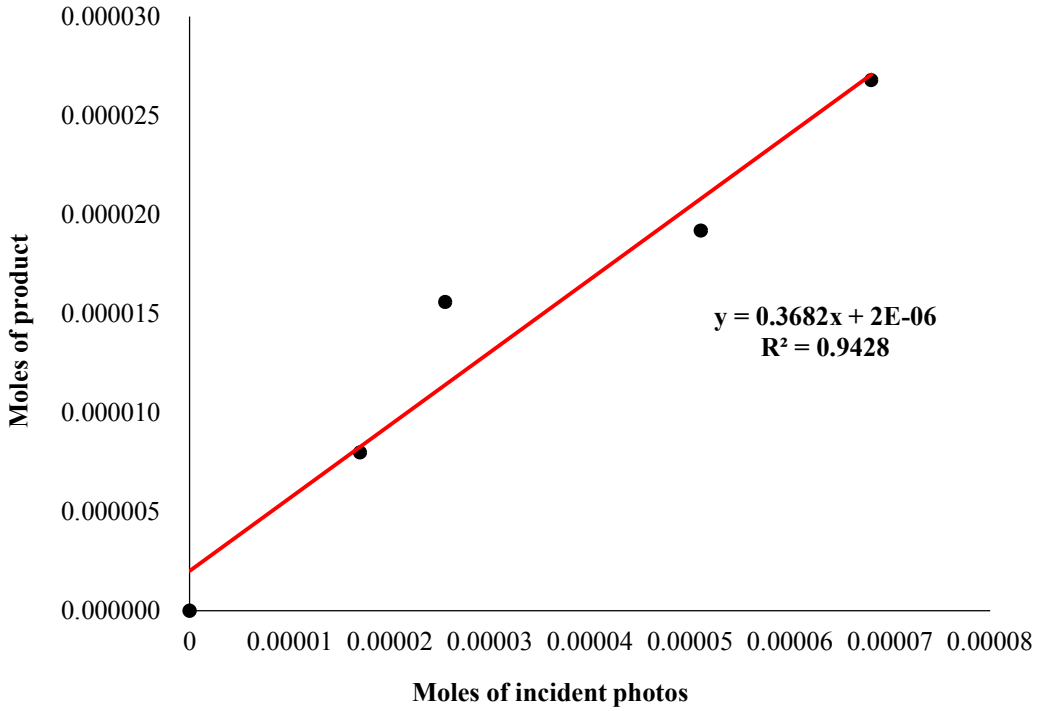
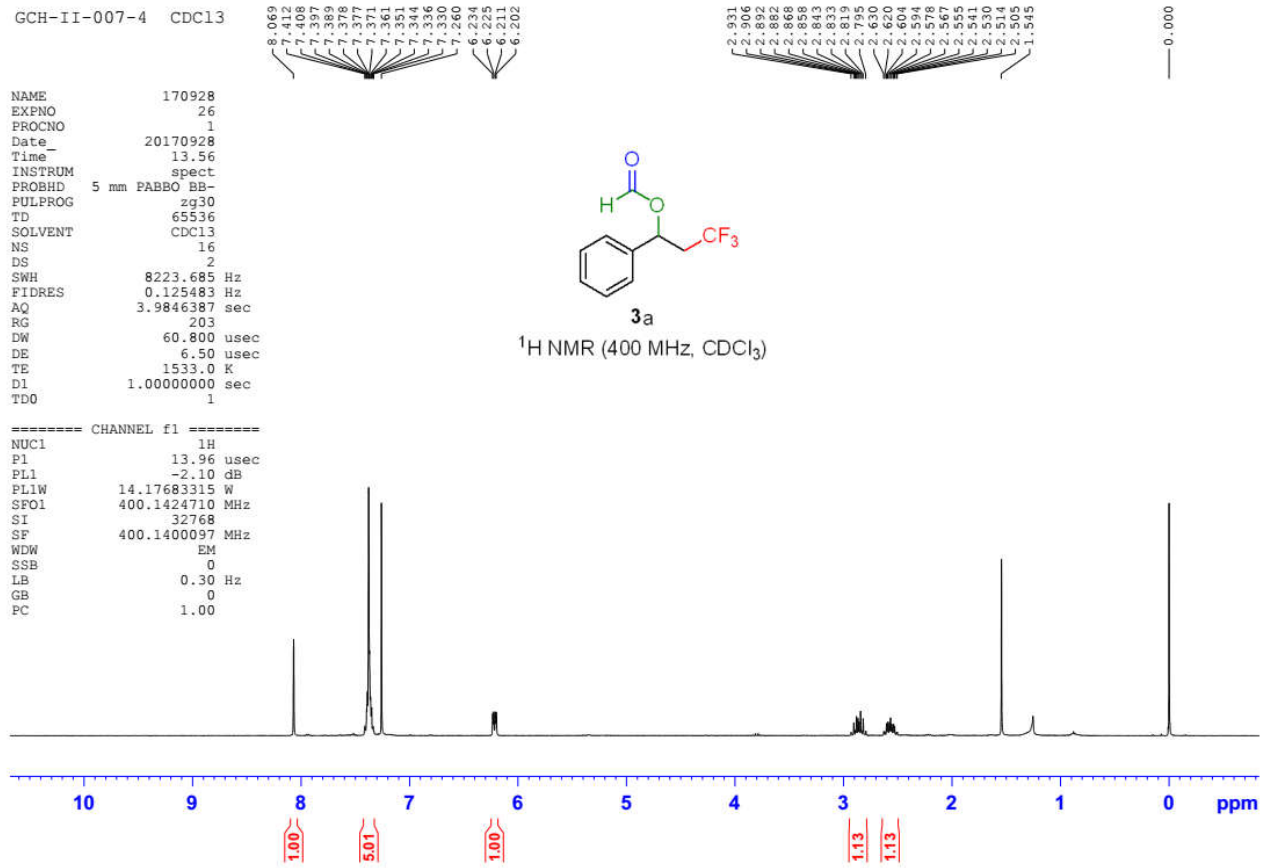


Fig. S3 The moles of product (x) versus the moles of incident photons ($q^0_{n,p}$·dt).

The quantum yield (Φ) of the photochemical reaction of **1c** with 2 catalyzed by $Ru(bpy)_3(PF_6)_2$ was calculated to be **0.39**.


GCH-II-007-4 CDCl3
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7.412
7.408
7.397
7.389
7.378
7.377
7.371
7.361
7.351
7.344
7.336
7.330
7.260
6.234
6.225
6.211
6.202
2.931
2.906
2.892
2.882
2.868
2.858
2.843
2.833
2.819
2.795
2.630
2.620
2.604
2.594
2.578
2.567
2.555
2.541
2.530
2.514
2.505
1.545
0.000
NAME 170928
EXPNO 26
PROCNO 1
Date_ 20170928
Time 13.56
INSTRUM spect
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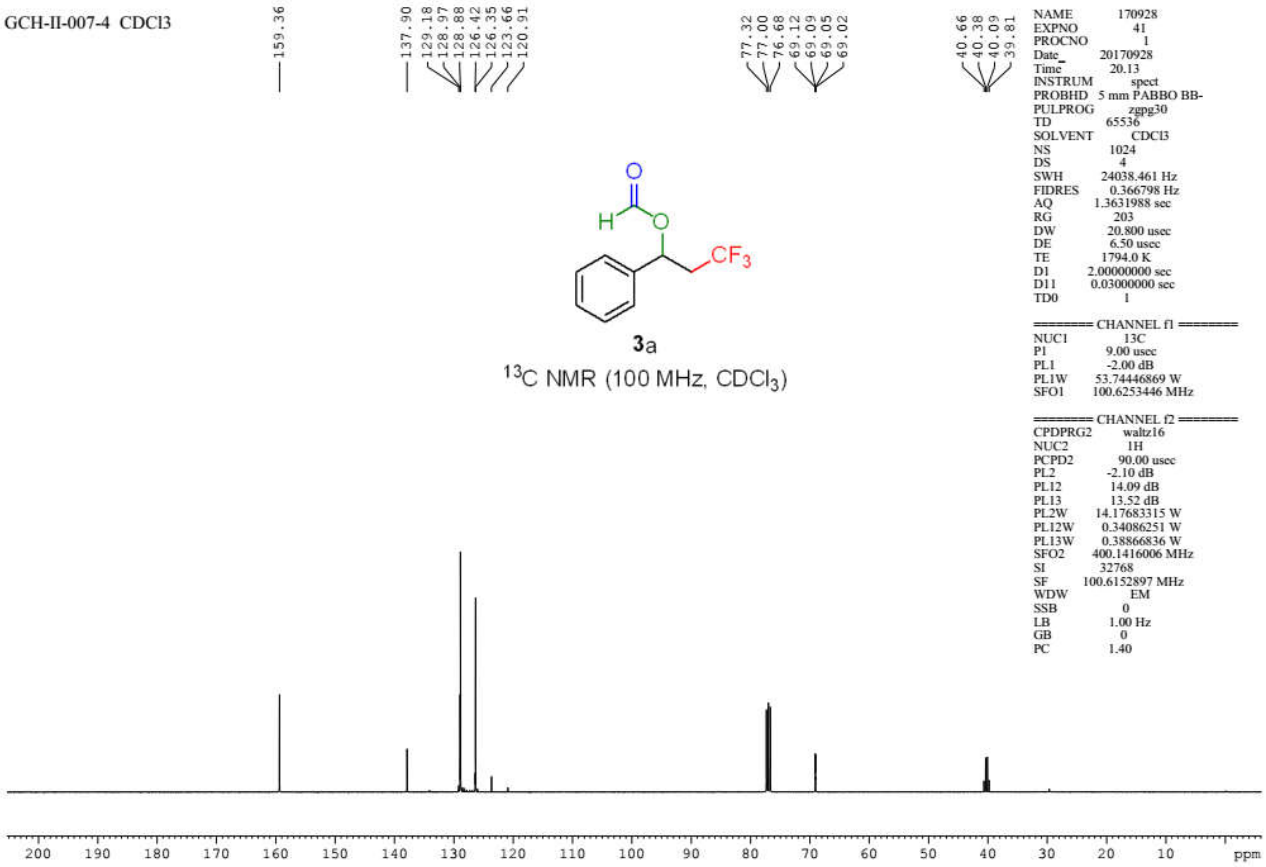
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 1533.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.96 usec
PL1 -2.10 dB
PL1W 14.17683315 W
SFO1 400.1424710 MHz
SI 32768
SF 400.1400097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
H
O
CF3
3a
1H NMR (400 MHz, CDCl3)
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
5.01
1.00
1.13
1.13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137.90
129.18
128.97
128.88
126.42
126.35
123.66
120.91
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77.00
76.68
69.12
69.09
69.05
69.02
40.66
40.38
40.09
39.81
NAME 170928
EXPNO 41
PROCNO 1
Date_ 20170928
Time 20.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 1794.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.00 usec
PL1 -2.00 dB
PL1W 53.74446869 W
SFO1 100.6253446 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.10 dB
PL12 14.09 dB
PL13 13.52 dB
PL2W 14.17683315 W
PL12W 0.34086251 W
PL13W 0.38866836 W
SFO2 400.1416006 MHz
SI 32768
SF 100.6152897 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
H
O
CF3
3a
13C NMR (100 MHz, CDCl3)
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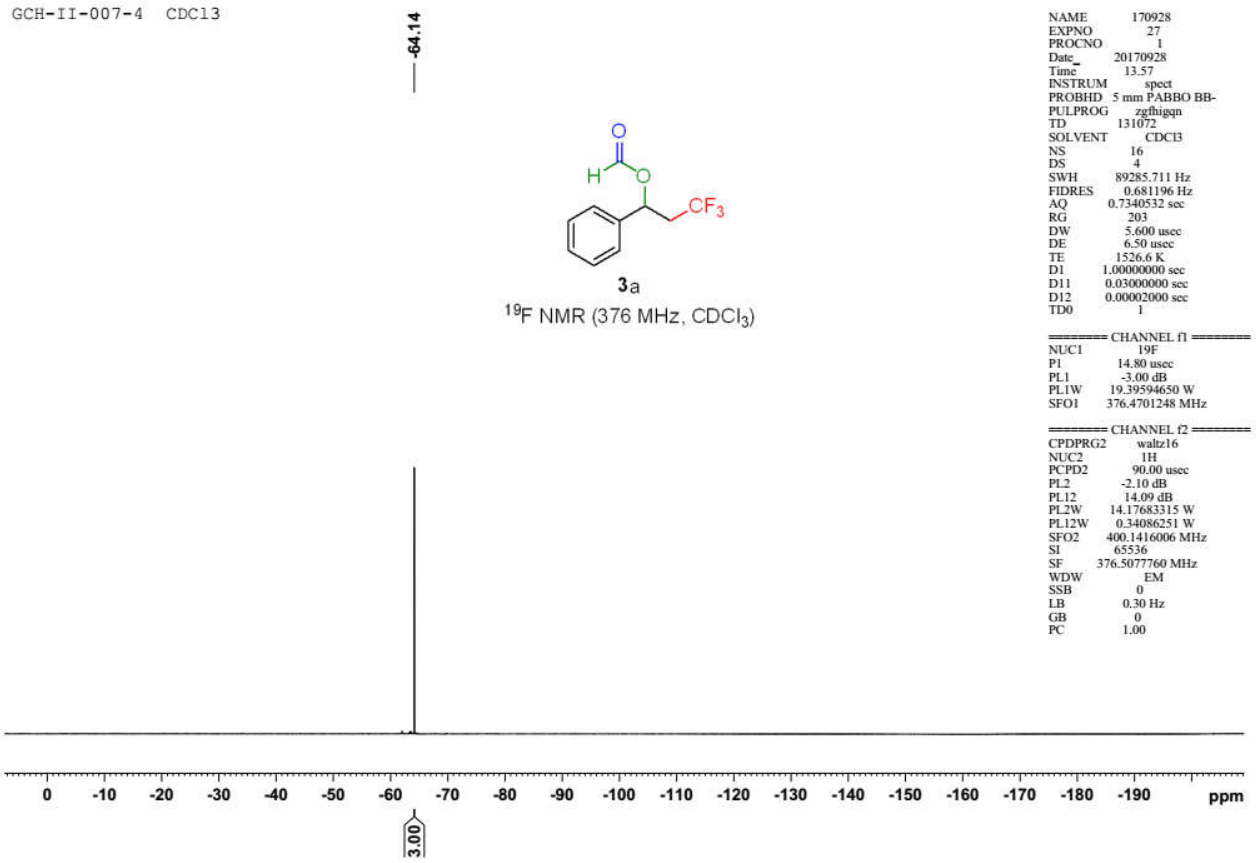
90
80
70
60
50
40
30
20
10
ppm



Monoisotopic Mass, Odd and Even Electron Ions
45 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
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default file
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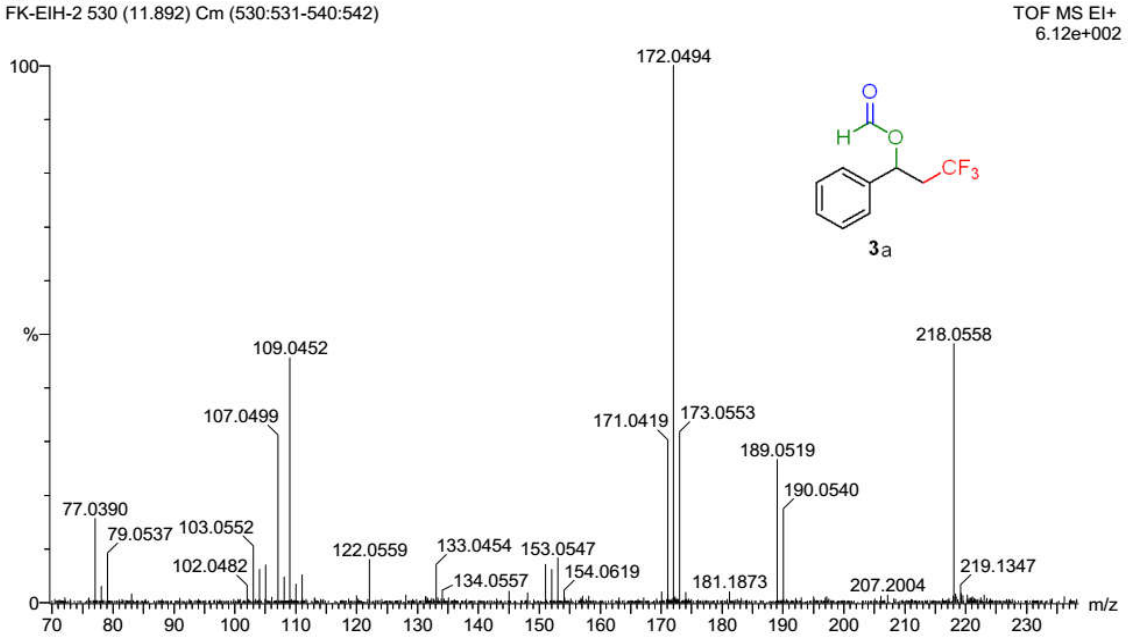

Minimum:				-1.5		
Maximum:		5.0	10.0	50.0		
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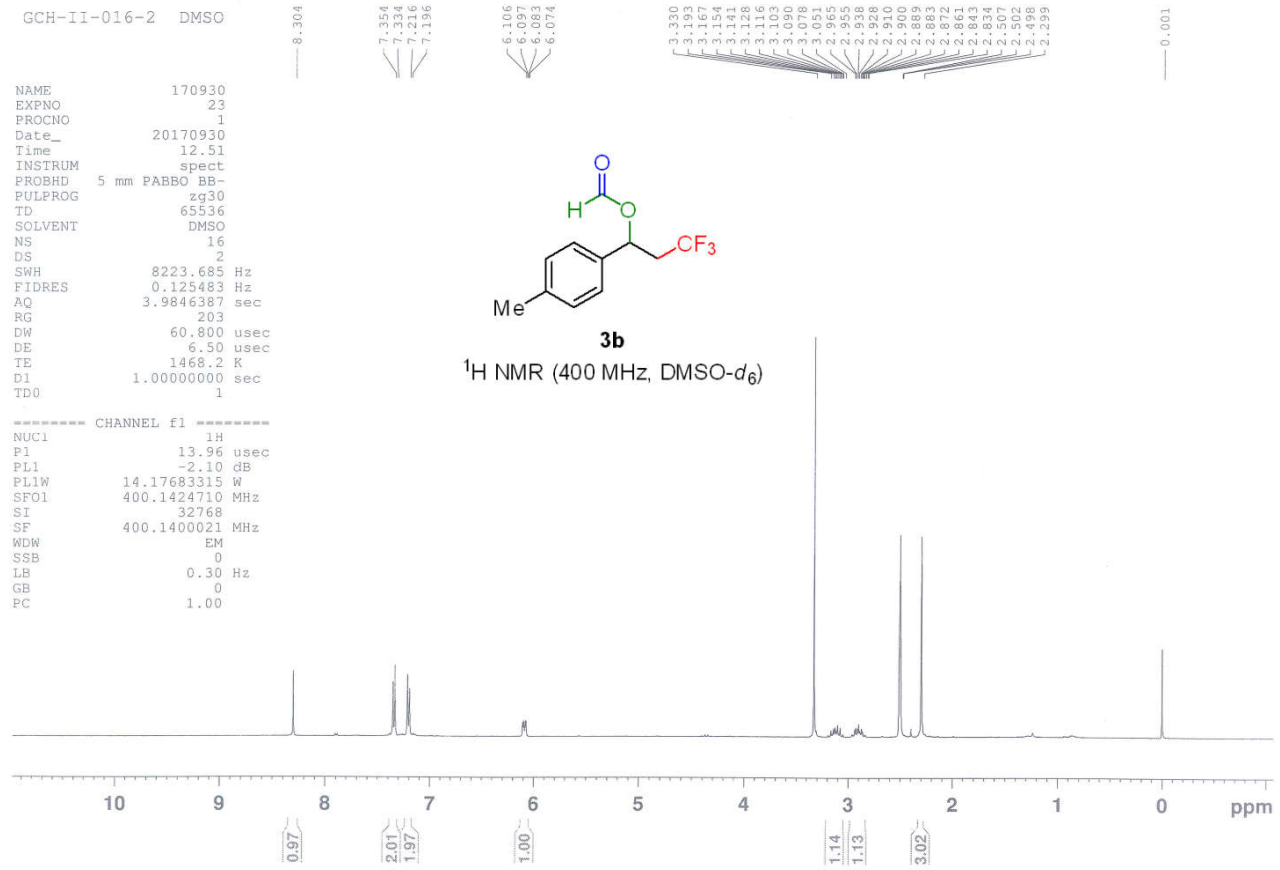
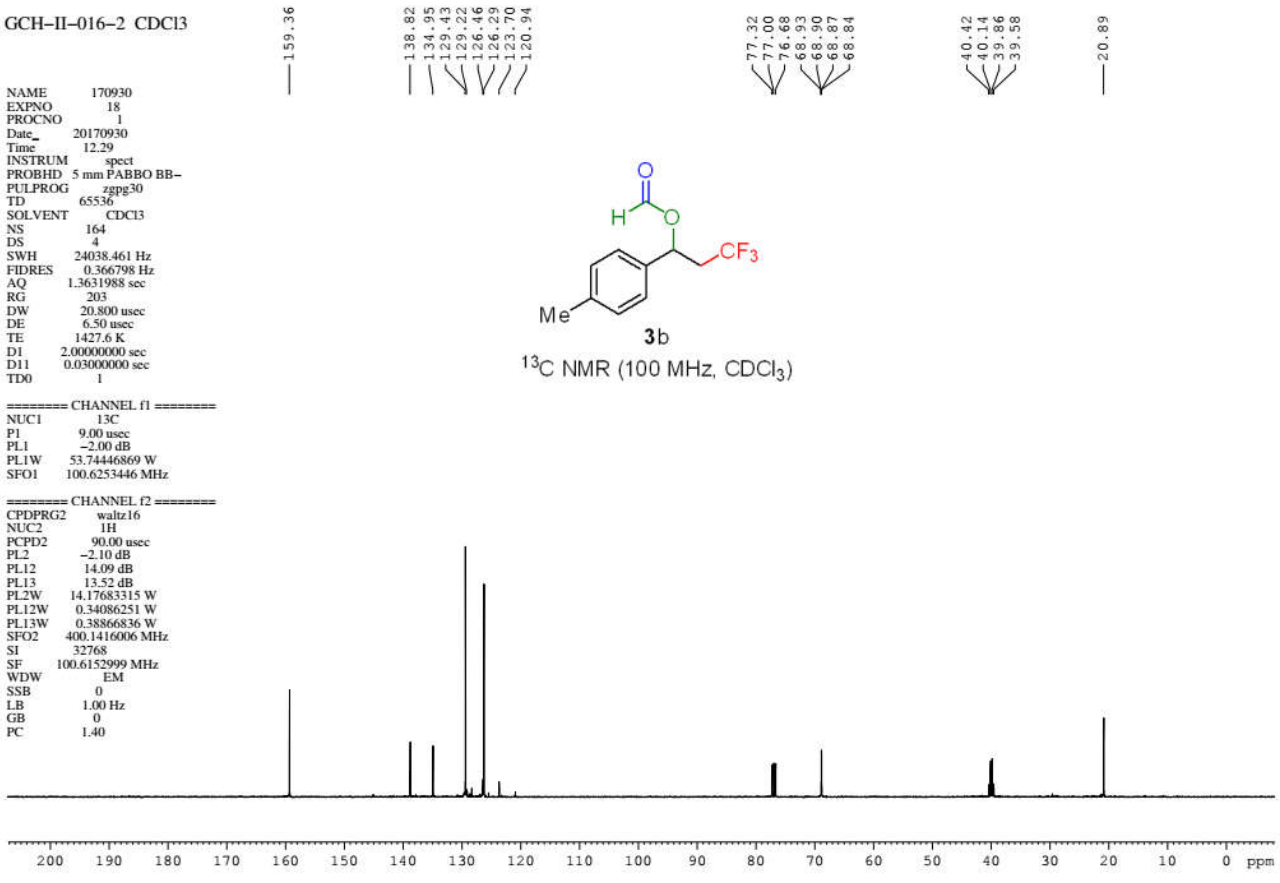


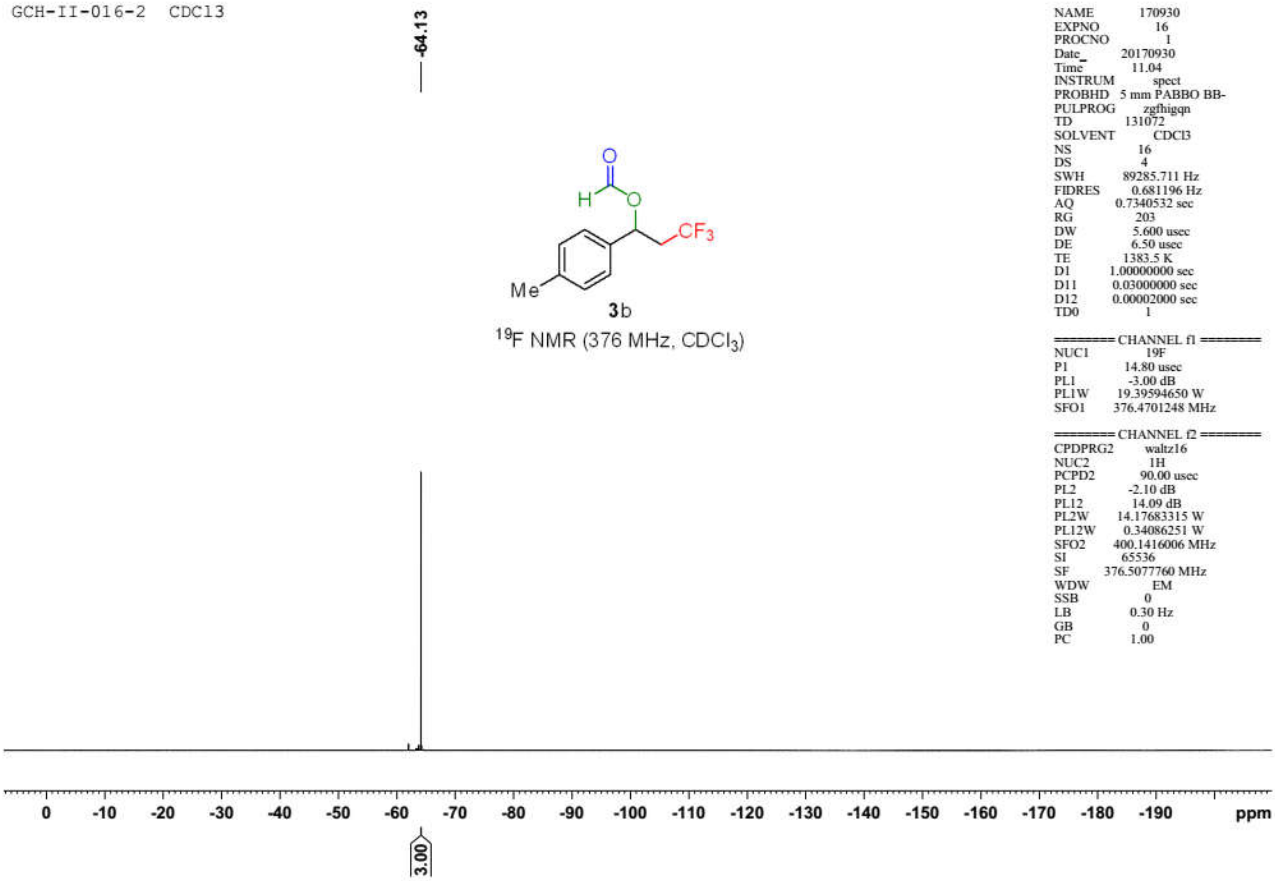
3b

^{1}H NMR (400 MHz, DMSO-d_6)



3b

^{13}C NMR (100 MHz, $CDCl_3$)



Monoisotopic Mass, Odd and Even Electron Ions
29 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
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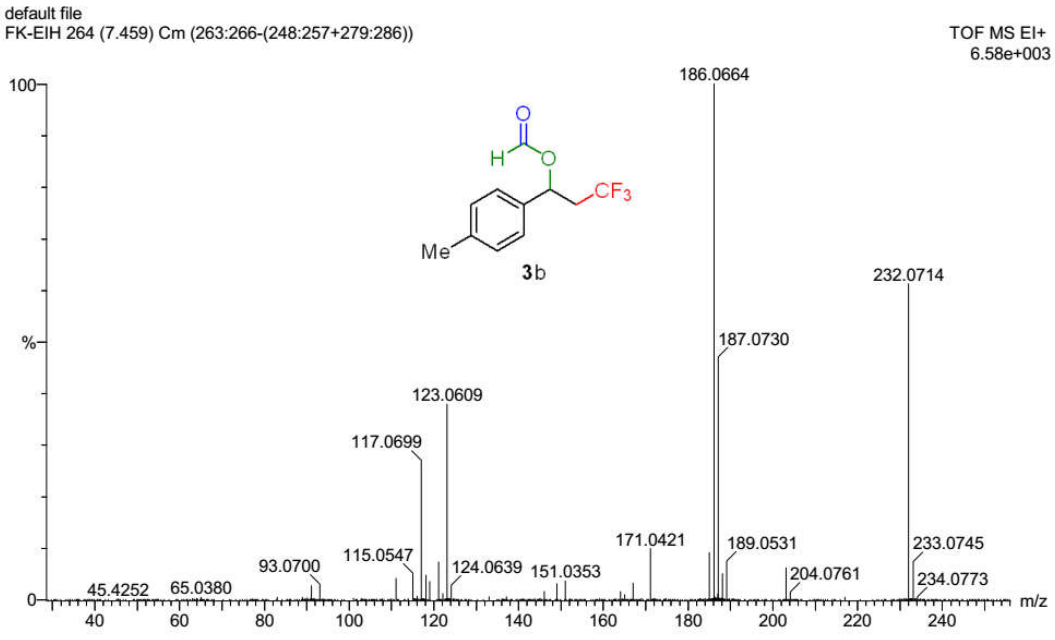

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Maximum:		5.0	10.0	50.0		
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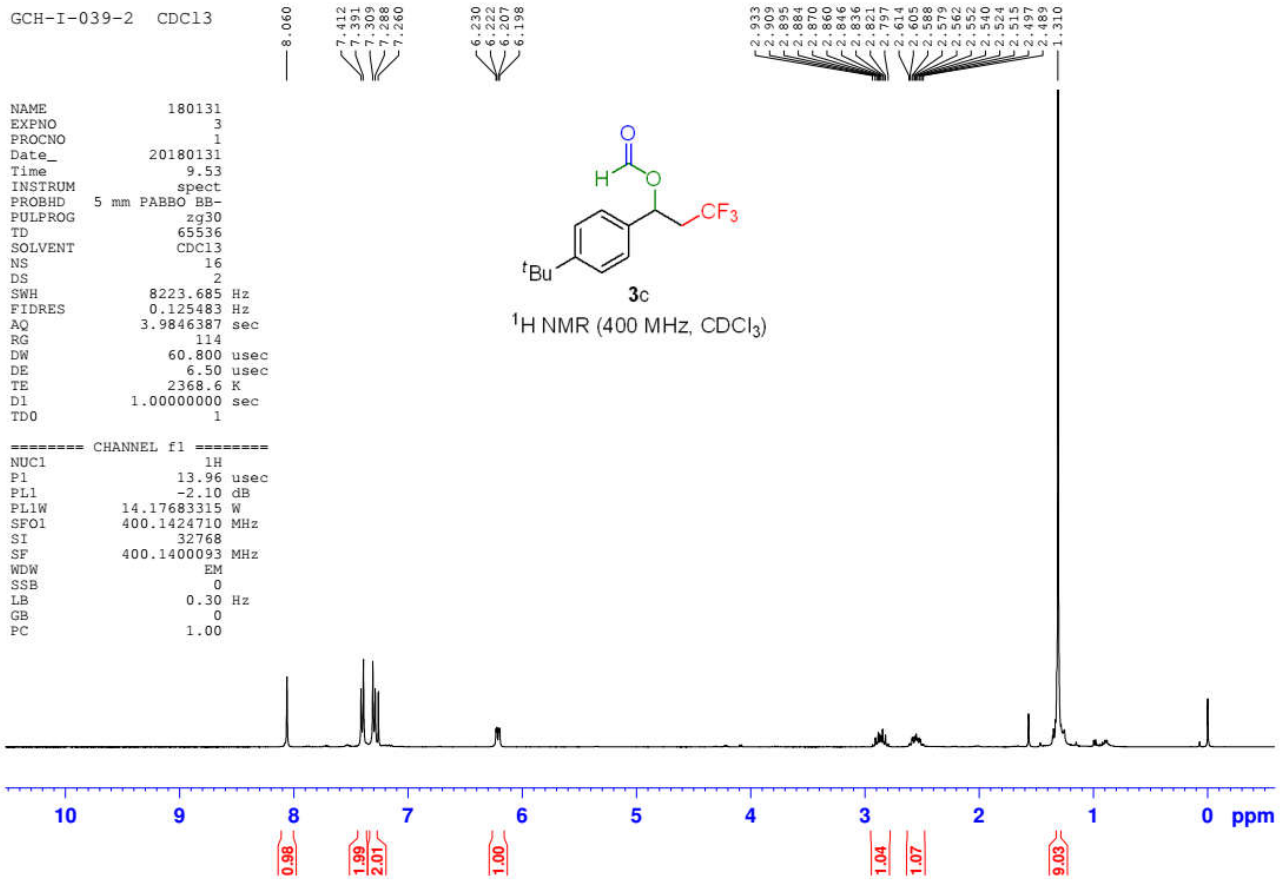
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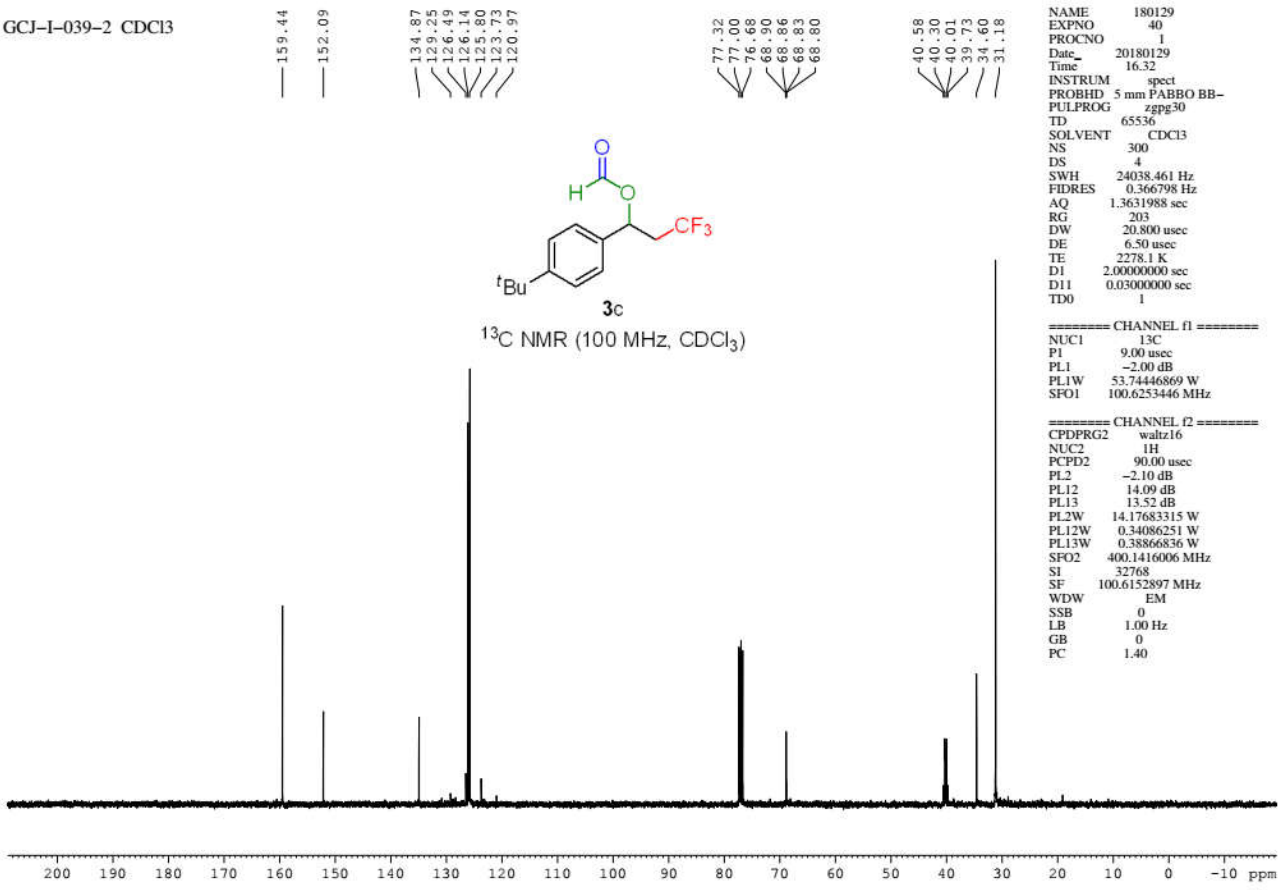
7.412
7.391
7.309
7.288
7.260
6.230
6.222
6.207
6.198
2.933
2.909
2.895
2.884
2.870
2.860
2.846
2.836
2.821
2.797
2.614
2.605
2.588
2.579
2.562
2.552
2.540
2.524
2.515
2.497
2.489
1.310
NAME 180131
EXPNO 3
PROCNO 1
Date_ 20180131
Time 9.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 114
DW 60.800 usec
DE 6.50 usec
TE 2368.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.96 usec
PL1 -2.10 dB
PL1W 14.17683315 W
SFO1 400.1424710 MHz
SI 32768
SF 400.1400093 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
H
O
CF3
tBu
3c
1H NMR (400 MHz, CDCl3)
10
9
8
7
6
5
4
3
2
1
0 ppm
0.98
1.99
2.01
1.00
1.04
1.07
9.03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152.09
134.87
129.25
126.49
126.14
125.80
123.73
120.97
77.32
77.00
76.68
68.90
68.86
68.83
68.80
40.58
40.30
40.01
39.73
34.60
31.18
NAME 180129
EXPNO 40
PROCNO 1
Date_ 20180129
Time 16.32
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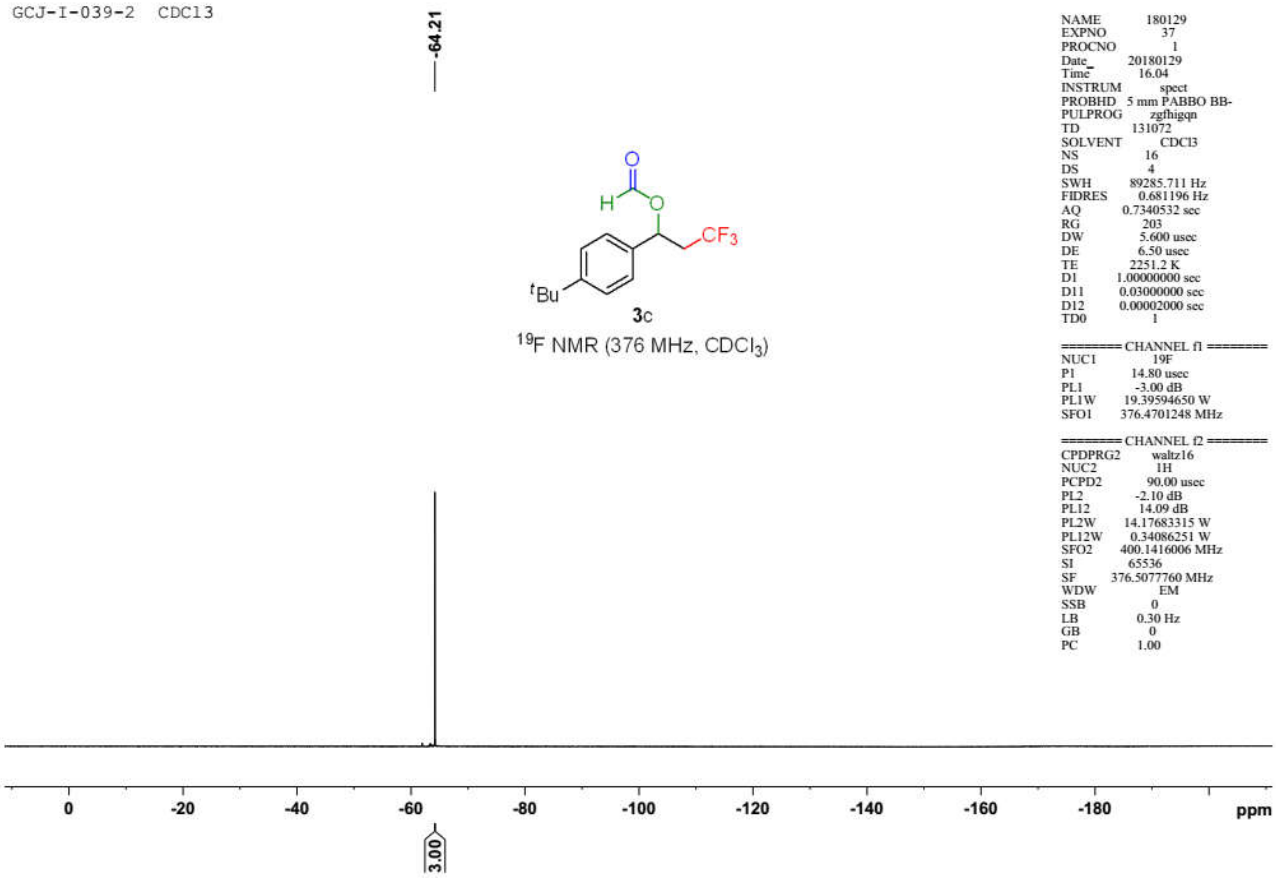
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 300
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 2278.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.00 usec
PL1 -2.00 dB
PL1W 53.74446869 W
SFO1 100.6253446 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.10 dB
PL12 14.09 dB
PL13 13.52 dB
PL2W 14.17683315 W
PL12W 0.34086251 W
PL13W 0.38866836 W
SFO2 400.1416006 MHz
SI 32768
SF 100.6152897 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
H
O
CF3
tBu
3c
13C NMR (100 MHz, CDCl3)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10 ppm



Monoisotopic Mass, Odd and Even Electron Ions
69 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
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default file
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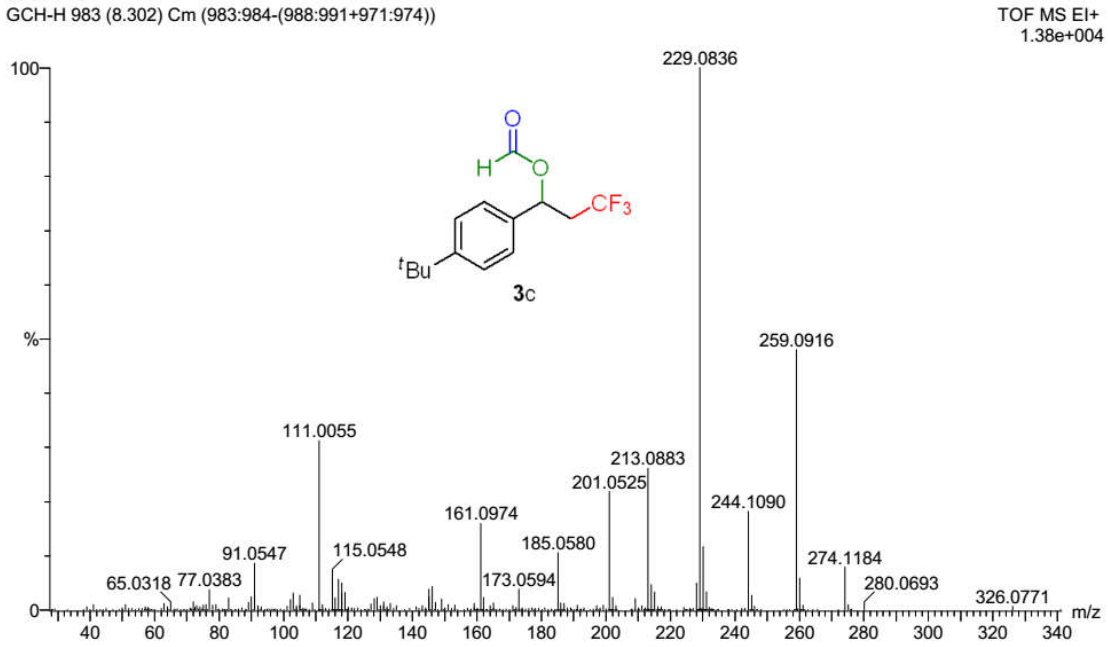

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Maximum:		5.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
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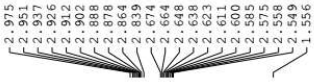
GCH-I-040-2 CDCl3



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PROCNO	1
Date_	20180131
Time	13.09
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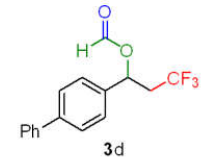
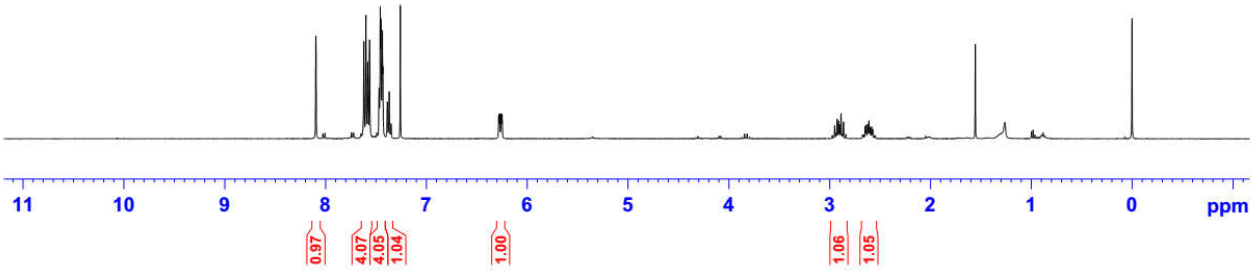
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	203
DW	60.800 usec
DE	6.50 usec
TE	2339.4 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.96 usec
PL1	-2.10 dB
PL1W	14.17683315 W
SFO1	400.1424710 MHz
SI	32768
SF	400.1400093 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



3d

^{1}H NMR (400 MHz, $CDCl_3$)



GCH-I-040-2 CDCl3

NAME	180131
EXPNO	19
PROCNO	1
Date_	20180131
Time	15.52
INSTRUM	spect
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PULPROG	zgpg30
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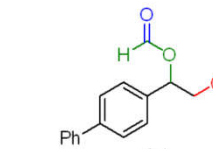
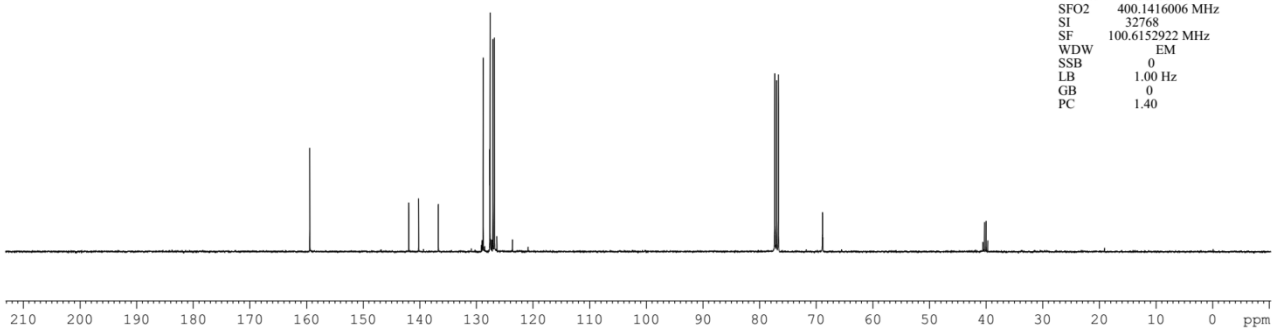
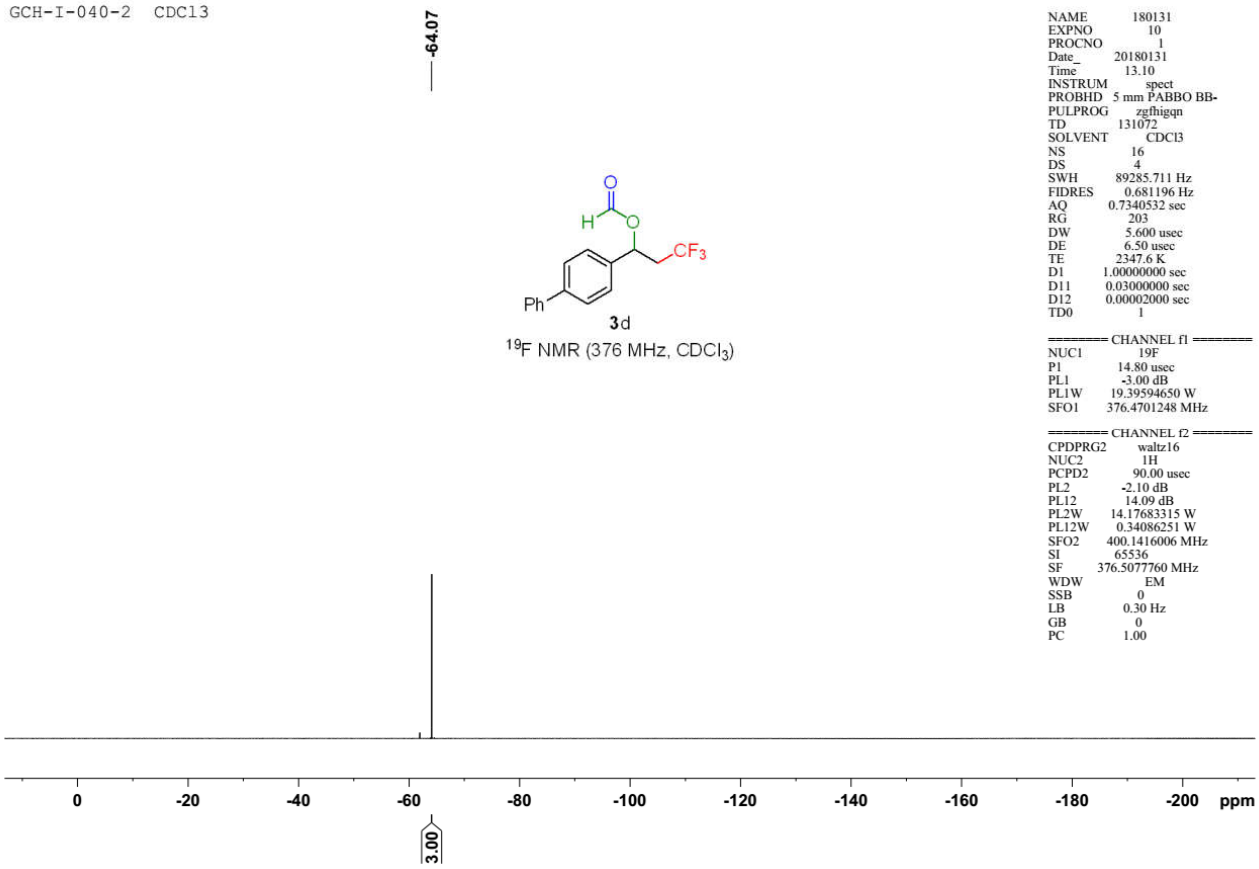
SOLVENT	CDCl3
NS	354
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	2517.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.00 usec
PL1	-2.00 dB
PL1W	53.74446869 W
SFO1	100.6253446 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.10 dB
PL12	14.09 dB
PL13	13.52 dB
PL2W	14.17683315 W
PL12W	0.34086251 W
PL13W	0.38866836 W
SFO2	400.1416006 MHz
SI	32768
SF	100.6152922 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



3d

^{13}C NMR (100 MHz, $CDCl_3$)





Monoisotopic Mass, Odd and Even Electron Ions
16 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
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default file
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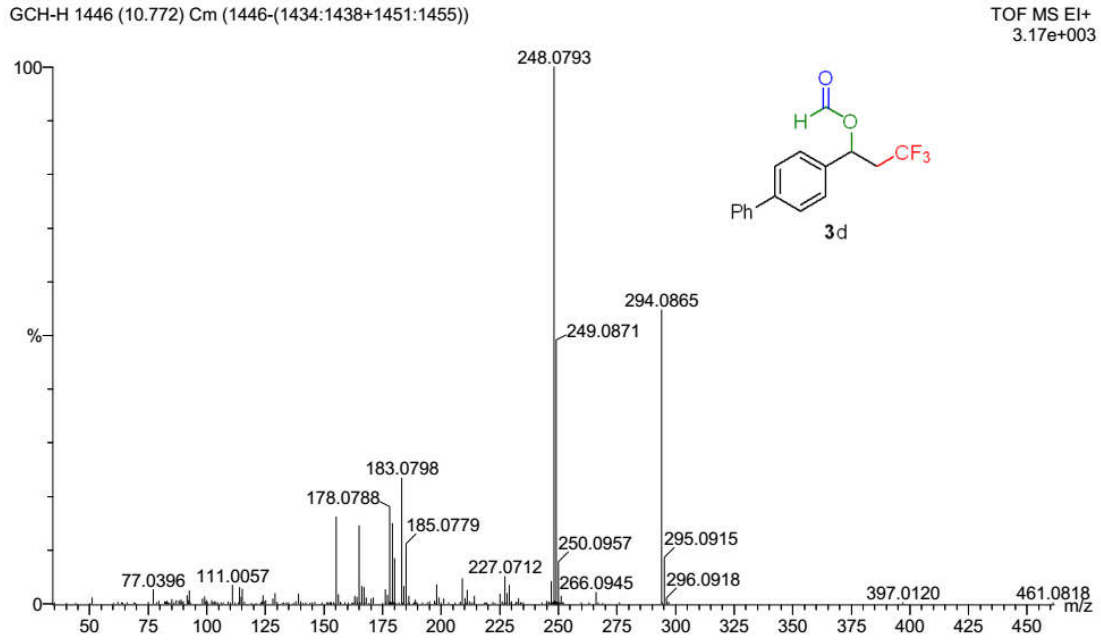
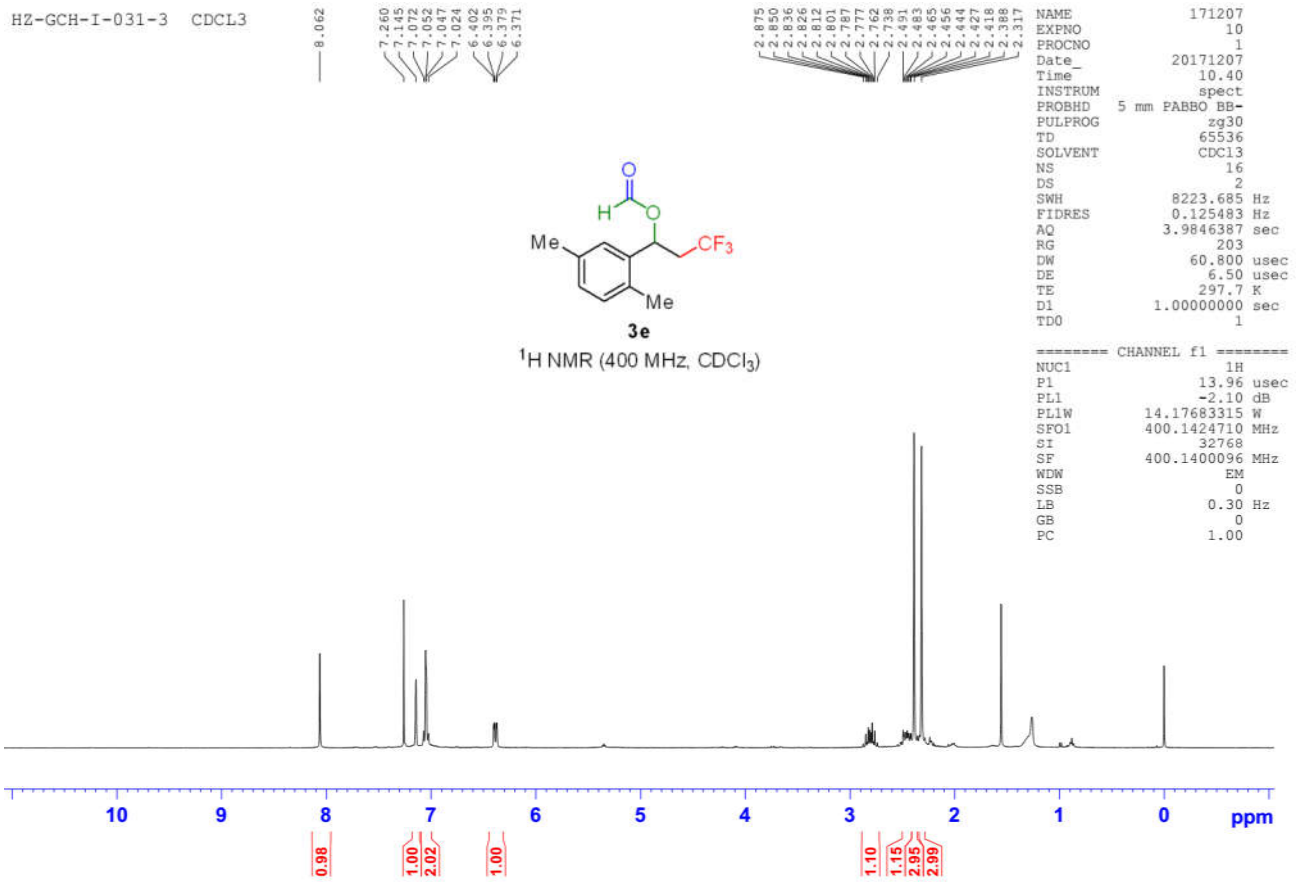


Minimum:				-1.5		
Maximum:		5.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
294.0865	294.0868	-0.3	-1.0	9.0	3.1	C16 H13 O2 F3

HZ-GCH-I-031-3 CDCL3



NAME 171207
EXPNO 10
PROCNO 1
Date_ 20171207
Time 10.40
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 297.7 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 13.96 usec
PL1 -2.10 dB
PL1W 14.17683315 W
SFO1 400.1424710 MHz
SI 32768
SF 400.1400096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

3e

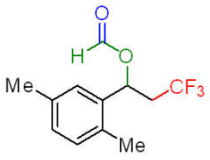
^{1}H NMR (400 MHz, $CDCl_3$)

HZ-GCH-I-031-3 CDCL3

NAME 171207
EXPNO 11
PROCNO 1
Date_ 20171207
Time 11.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 170
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 298.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

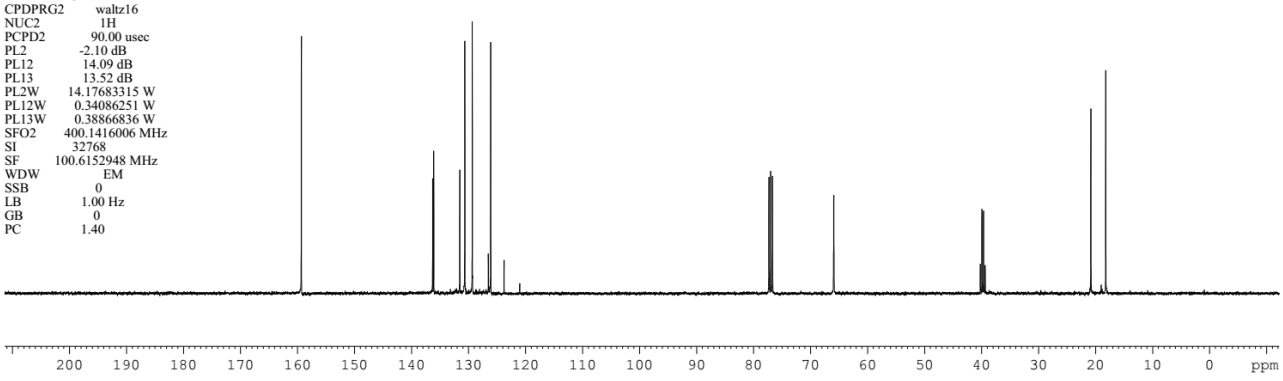
======== CHANNEL f1 ========
NUC1 13C
P1 9.00 usec
PL1 -2.00 dB
PL1W 53.74446869 W
SFO1 100.6253446 MHz

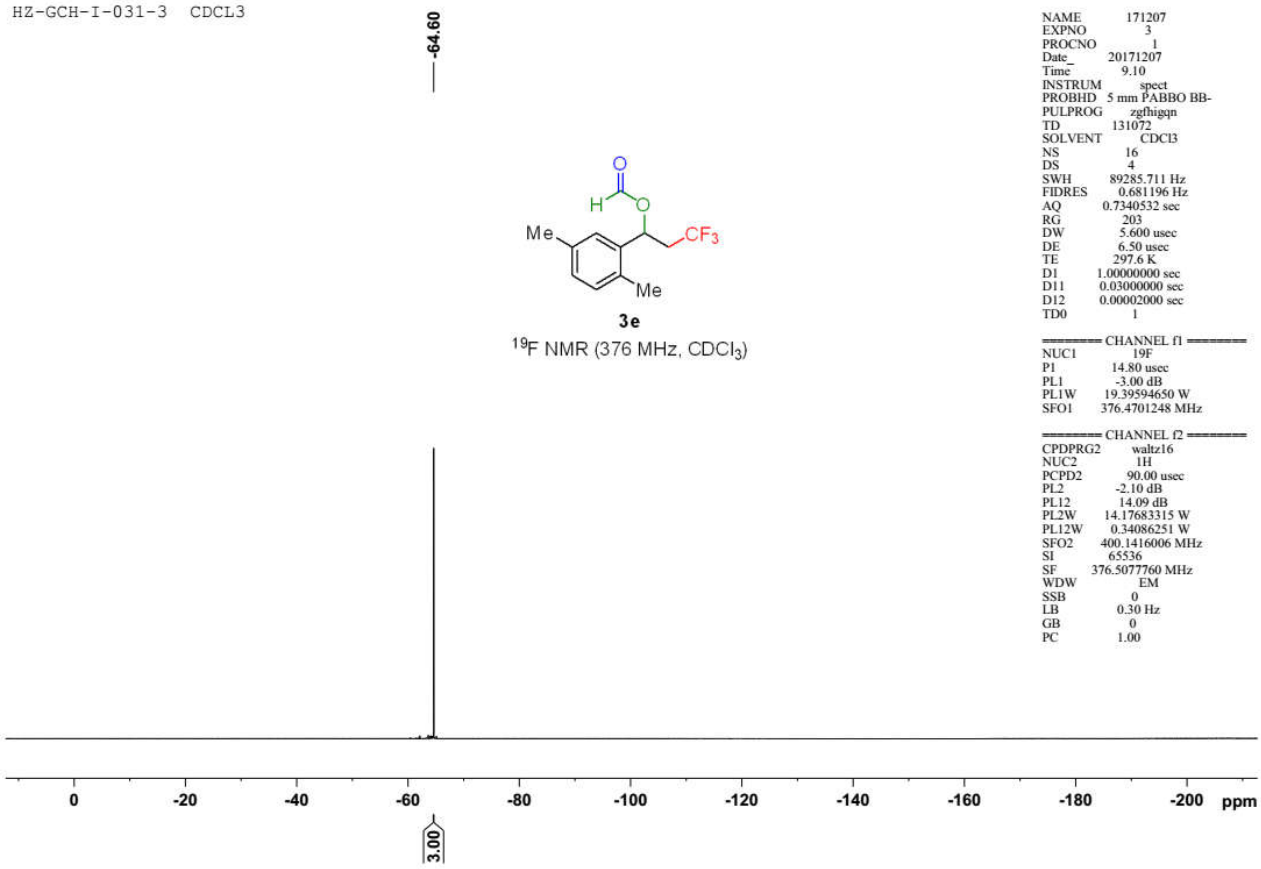
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.10 dB
PL12 14.09 dB
PL13 13.52 dB
PL2W 14.17683315 W
PL12W 0.34086251 W
PL13W 0.38866836 W
SFO2 400.1416006 MHz
SI 32768
SF 100.6152948 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



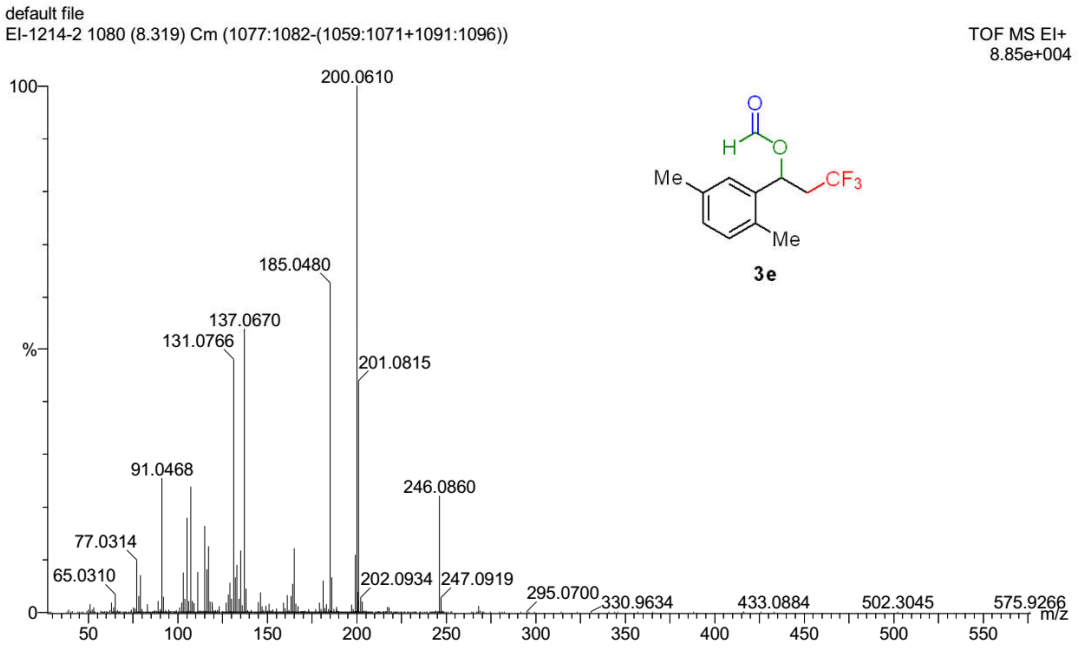
3e

^{13}C NMR (100 MHz, $CDCl_3$)



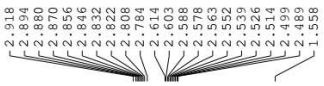


Monoisotopic Mass, Odd and Even Electron Ions
13 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-14 H: 0-14 O: 0-3 F: 0-3

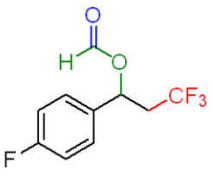


Minimum:				-1.5		
Maximum:		5.0	10.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
246.0860	246.0868	-0.8	-3.3	5.0	20.0	C12 H13 O2 F3

GCH-II-009-2 CDCl3

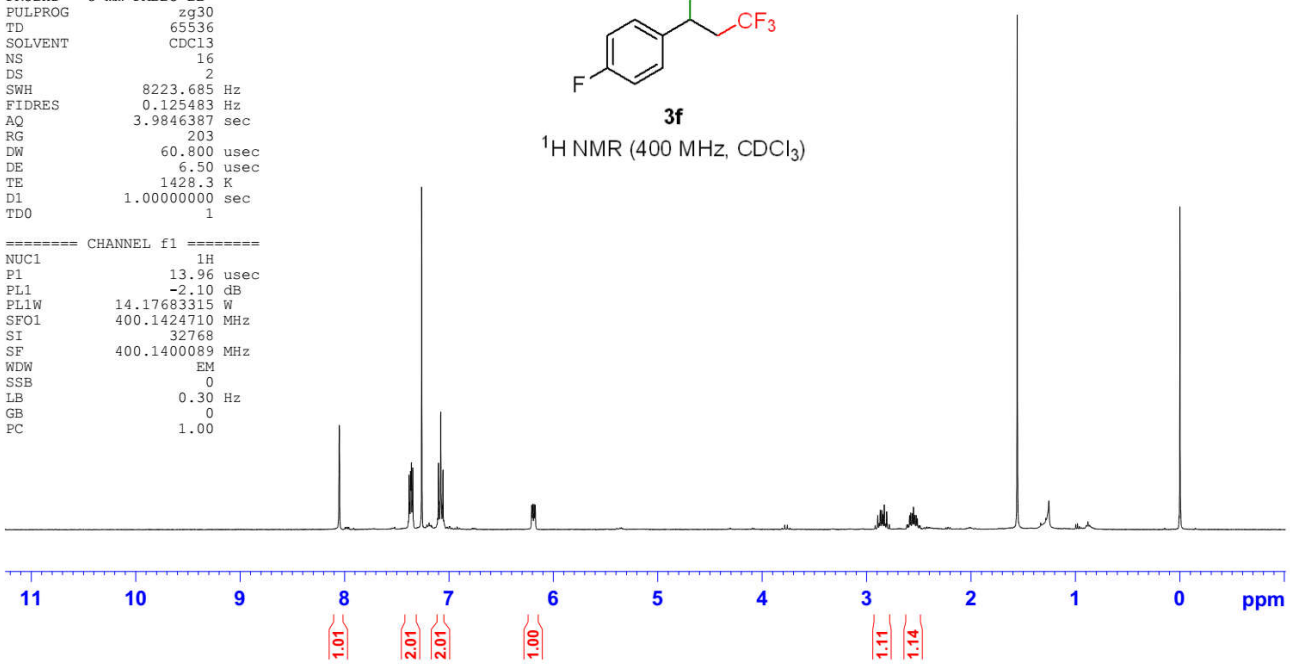



```
NAME              170930
EXPNO                 35
PROCNO                 1
Date_           20170930
Time               15.02
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9846387 sec
RG                   203
DW                60.800 usec
DE                 6.50 usec
TE                1428.3 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 13.96 usec
PL1                -2.10 dB
PL1W        14.17683315 W
SFO1        400.1424710 MHz
SI                 32768
SF          400.1400089 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

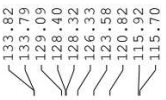


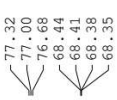
3f

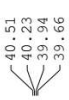
^{1}H NMR (400 MHz, $CDCl_3$)



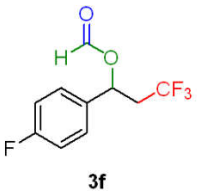
GCH-II-009-2 CDCl3





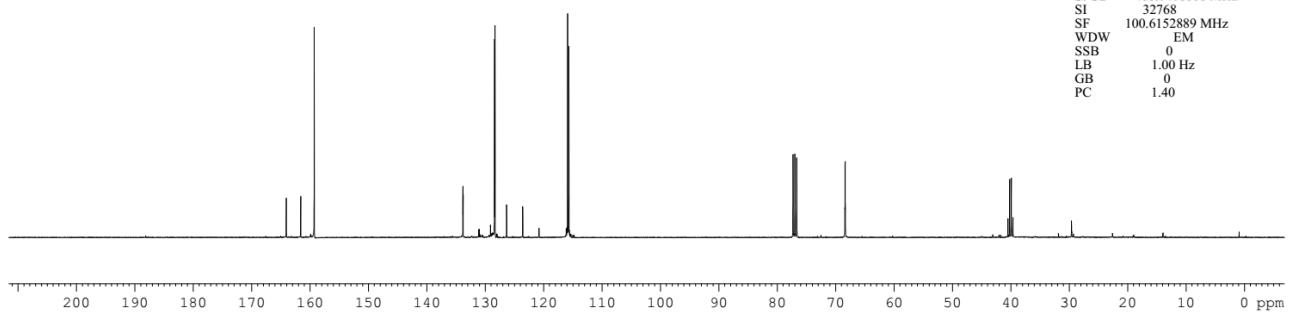


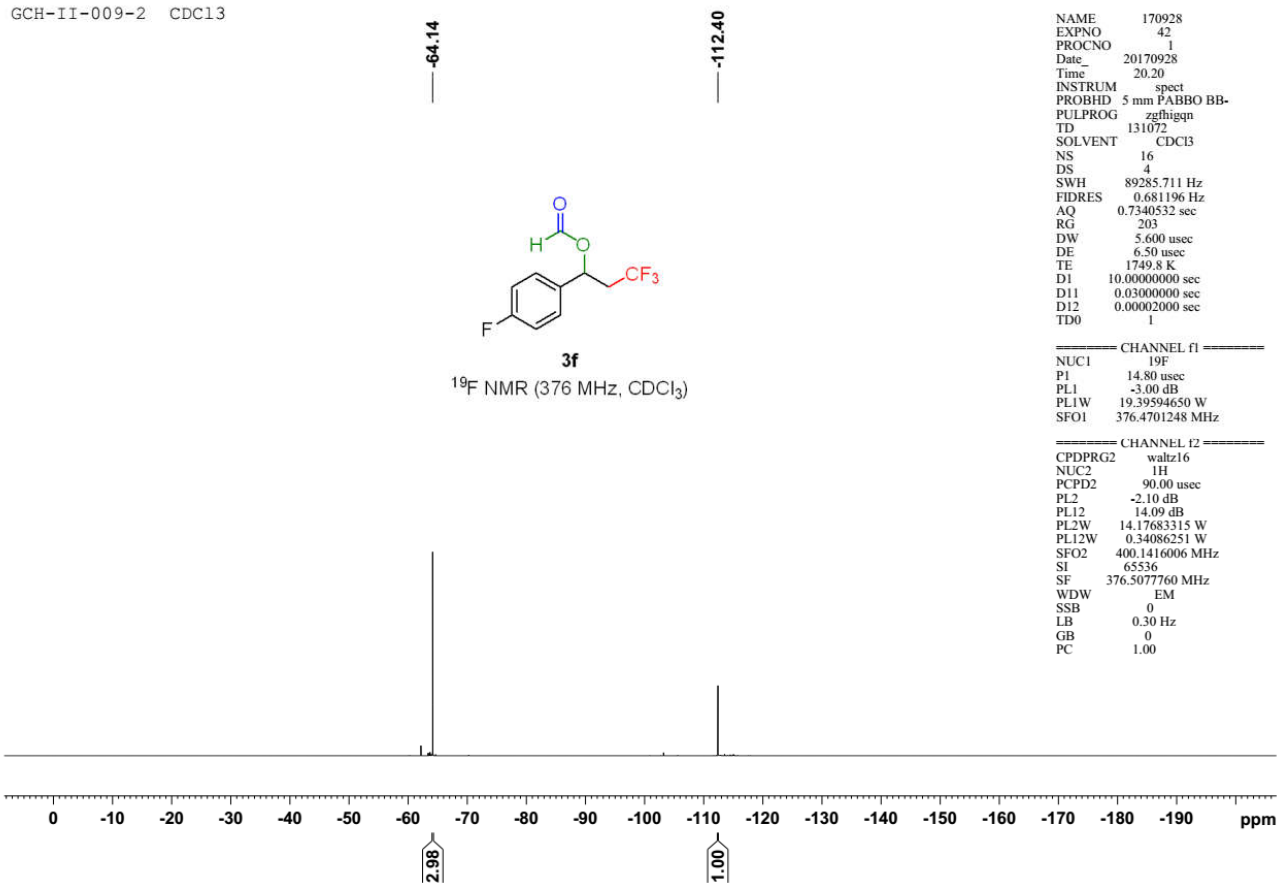

```
NAME              170928
EXPNO                 43
PROCNO                 1
Date_           20170928
Time               21.20
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631988 sec
RG                   203
DW                20.800 usec
DE                 6.50 usec
TE                1950.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.00 usec
PL1                -2.00 dB
PL1W       53.74446869 W
SFO1       100.6253446 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              90.00 usec
PL2                -2.10 dB
PL12               14.09 dB
PL13               13.52 dB
PL2W       14.17683315 W
PL12W       0.34086251 W
PL13W       0.38866836 W
SFO2       400.1416006 MHz
SI                 32768
SF         100.6152889 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40
```



3f

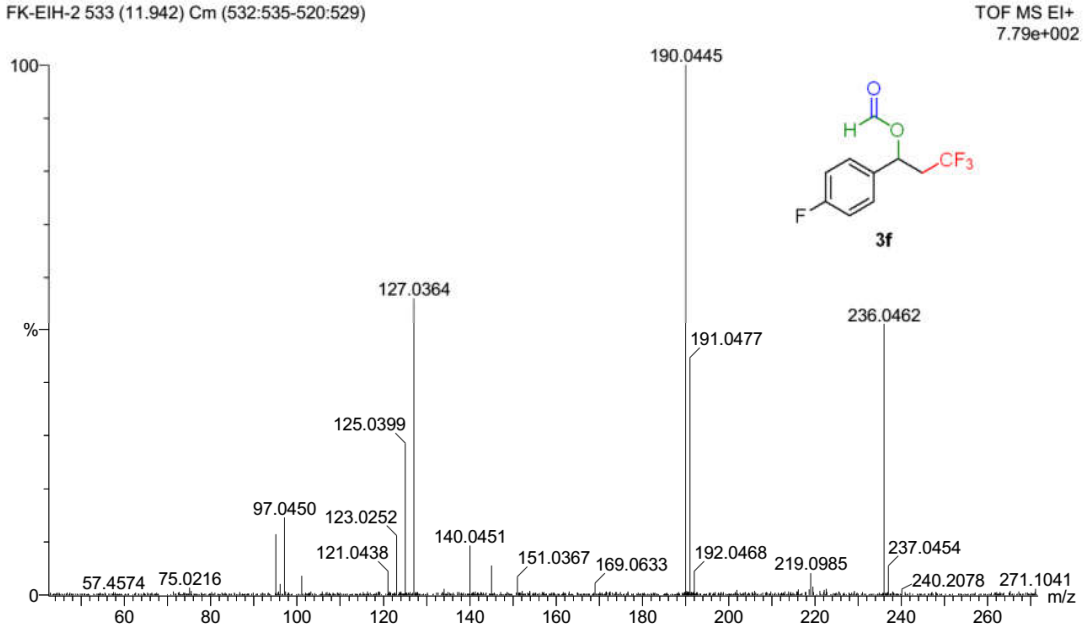
^{13}C NMR (100 MHz, $CDCl_3$)



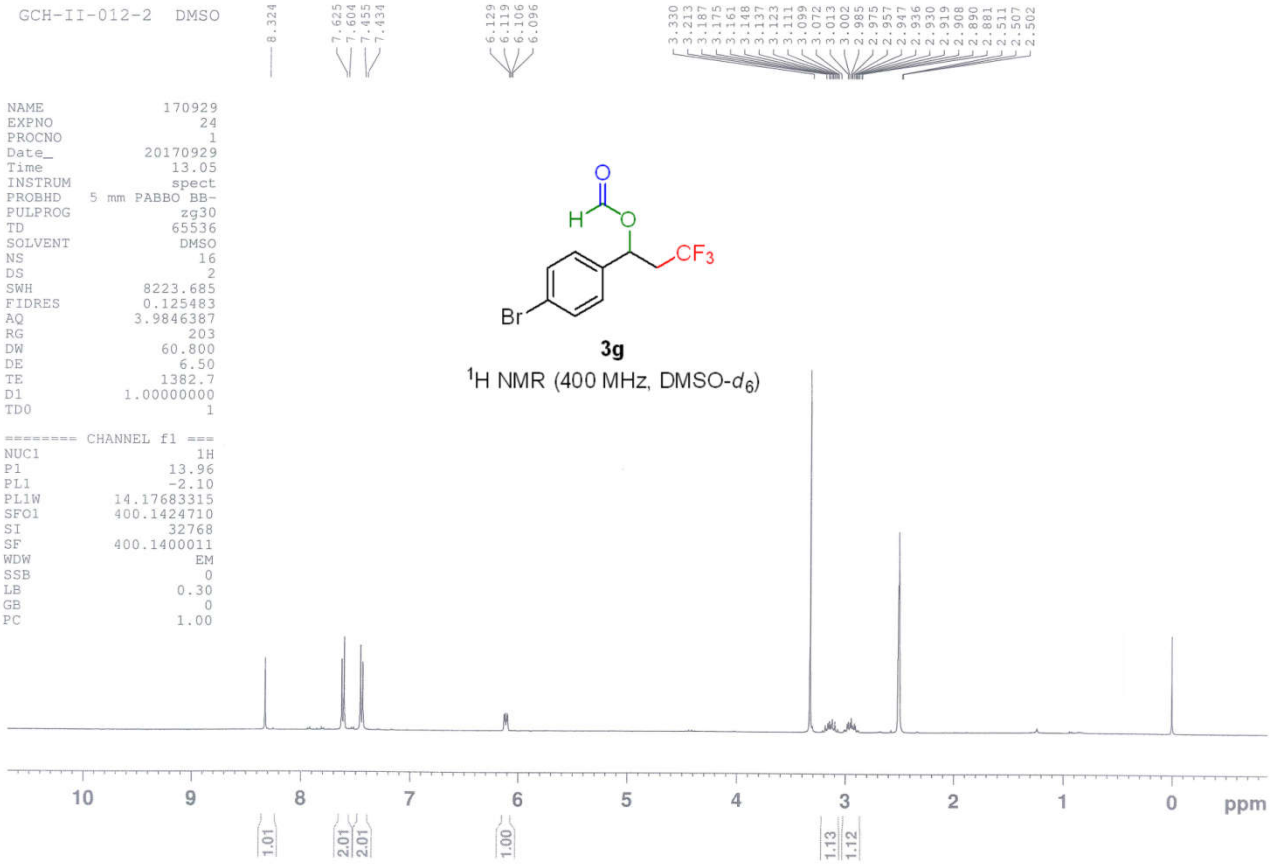


Monoisotopic Mass, Odd and Even Electron Ions
43 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-12 H: 0-12 O: 0-2 F: 0-4 Cl: 0-2

default file
FK-EIH-2 533 (11.942) Cm (532:535-520:529)

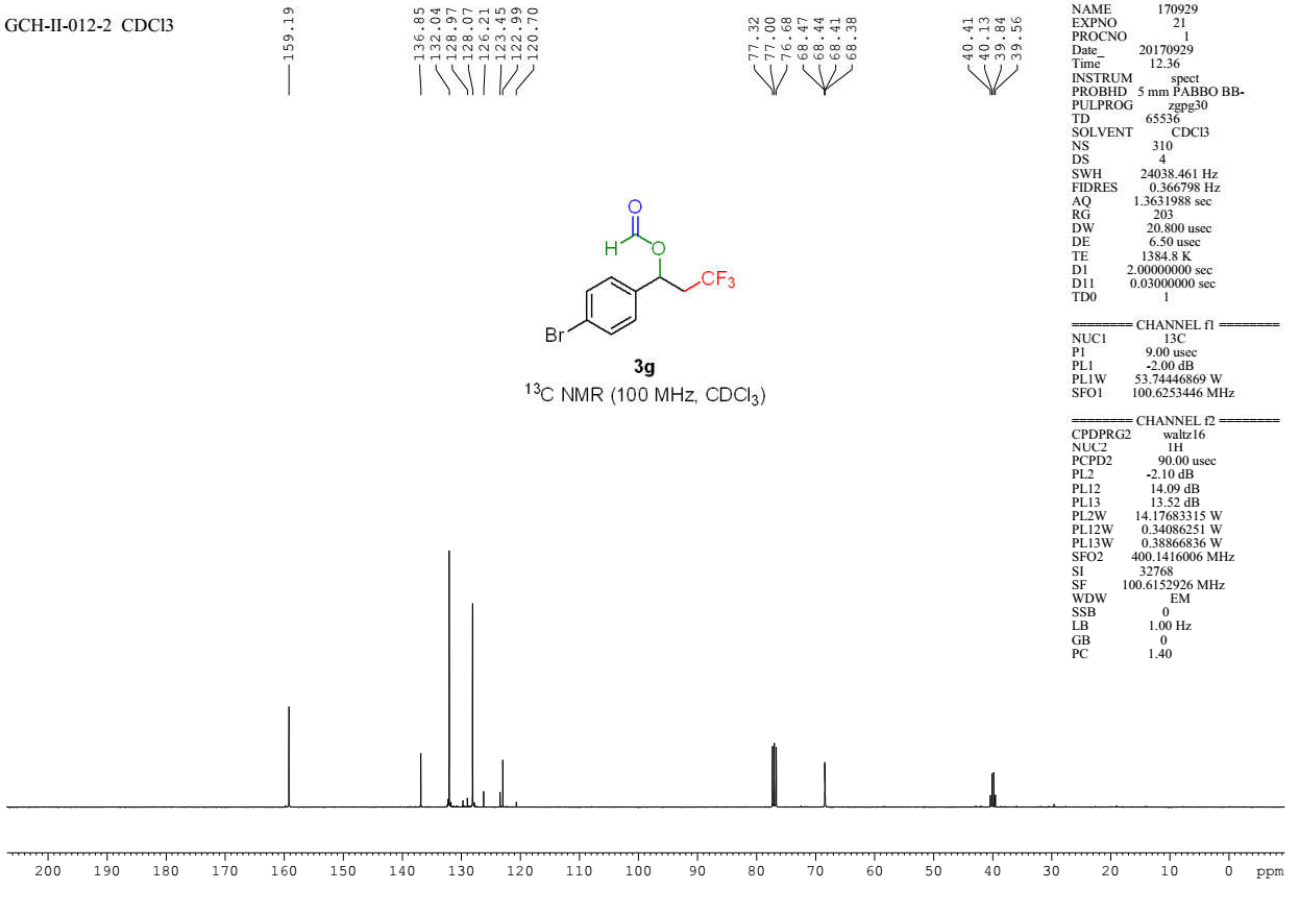


Minimum:				-1.5		
Maximum:		5.0	10.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
236.0462	236.0460	0.2	0.8	5.0	0.2	C10 H8 O2 F4



3g

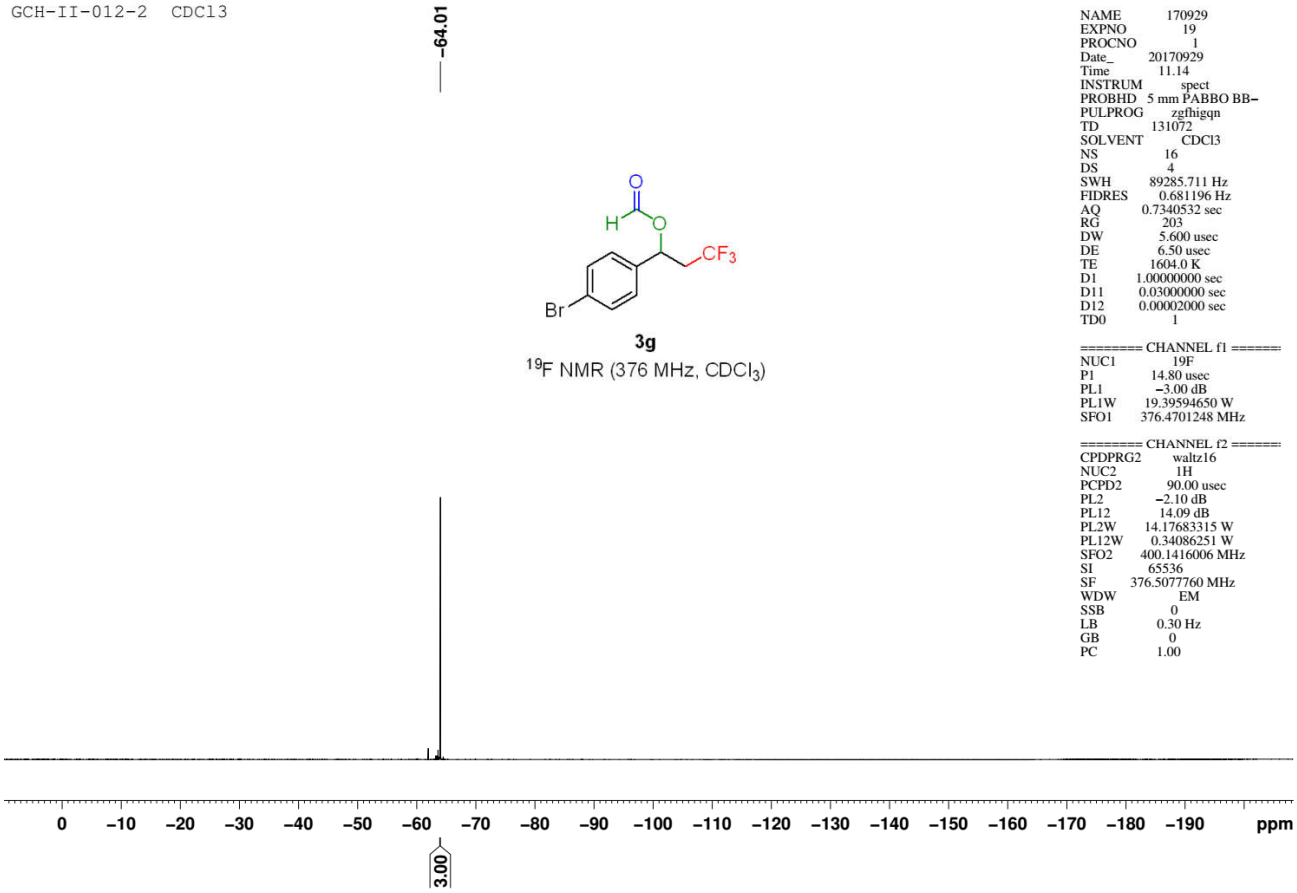
^{1}H NMR (400 MHz, DMSO-d_6)



3g

^{13}C NMR (100 MHz, $CDCl_3$)

GCH-II-012-2 CDCl3



3g

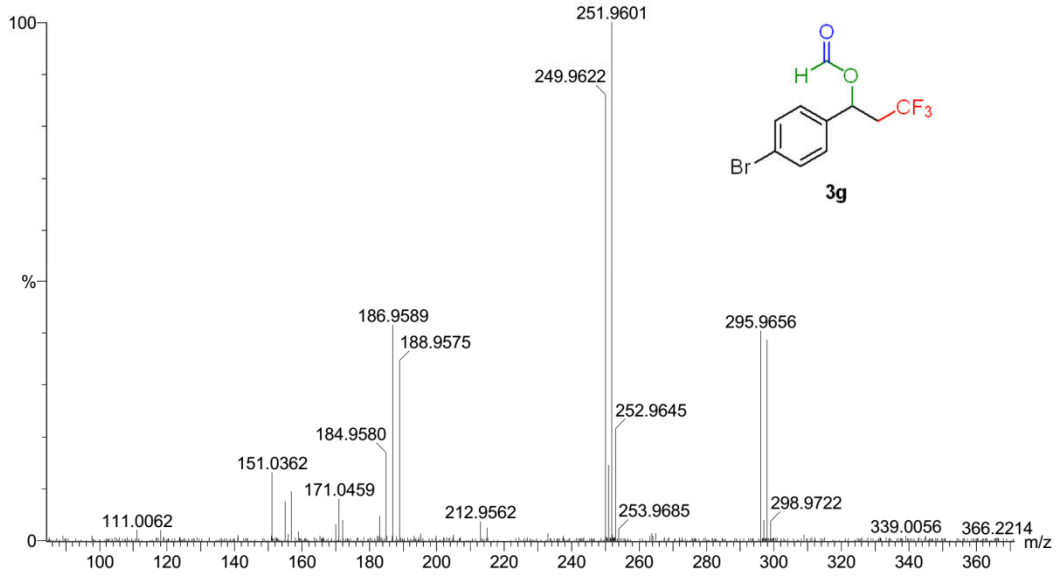
^{19}F NMR (376 MHz, $CDCl_3$)

```
NAME          170929
EXPNO             19
PROCNO             1
Date_       20170929
Time           11.14
INSTRUM         spect
PROBHD  5 mm PABBO BB-
PULPROG     zgfhigqn
TD           131072
SOLVENT         CDCl3
NS                16
DS                 4
SWH        89285.711 Hz
FIDRES       0.681196 Hz
AQ         0.7340532 sec
RG               203
DW           5.600 usec
DE           6.50 usec
TE           1604.0 K
D1        1.00000000 sec
D11       0.03000000 sec
D12       0.00002000 sec
TD0               1

======== CHANNEL f1 =======
NUC1             19F
P1           14.80 usec
PL1          -3.00 dB
PL1W      19.39594650 W
SFO1     376.4701248 MHz

======== CHANNEL f2 =======
CPDPRG2       waltz16
NUC2              1H
PCPD2        90.00 usec
PL2          -2.10 dB
PL12         14.09 dB
PL2W      14.17683315 W
PL12W      0.34086251 W
SFO2     400.1416006 MHz
SI            65536
SF       376.5077760 MHz
WDW              EM
SSB               0
LB            0.30 Hz
GB                0
PC             1.00
```

Monoisotopic Mass, Odd and Even Electron Ions
28 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-12 H: 0-12 O: 0-2 F: 0-4 Br: 0-1

default file
FK-EIH 339 (8.709) Cm (339:340-(329:333+349:354))

TOF MS EI+
3.98e+002

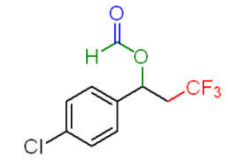


3g

Minimum:				-1.5		
Maximum:		5.0	10.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
295.9656	295.9660	-0.4	-1.4	5.0	0.2	C10 H8 O2 F3 Br

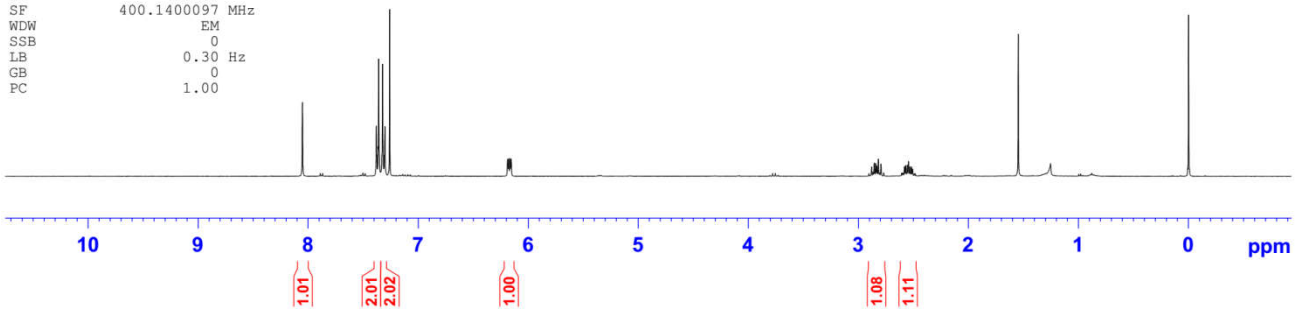
GCH-II-011-2 CDCl3


```
NAME              170929
EXPNO                  4
PROCNO                 1
Date_           20170929
Time                9.14
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9846387 sec
RG                   203
DW                60.800 usec
DE                 6.50 usec
TE                1812.5 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                13.96 usec
PL1                -2.10 dB
PL1W         14.17683315 W
SFO1         400.1424710 MHz
SI                 32768
SF           400.1400097 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



3h

^{1}H NMR (400 MHz, $CDCl_3$)

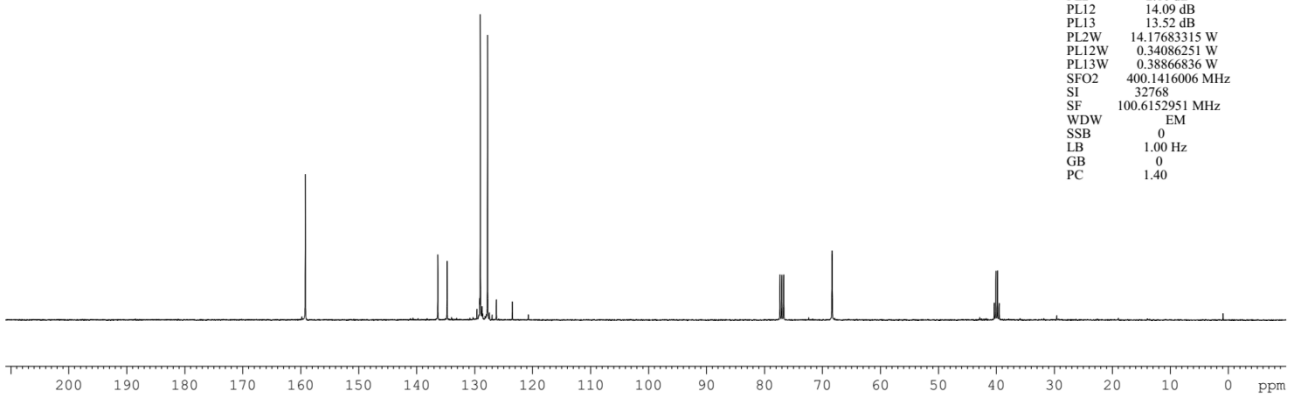


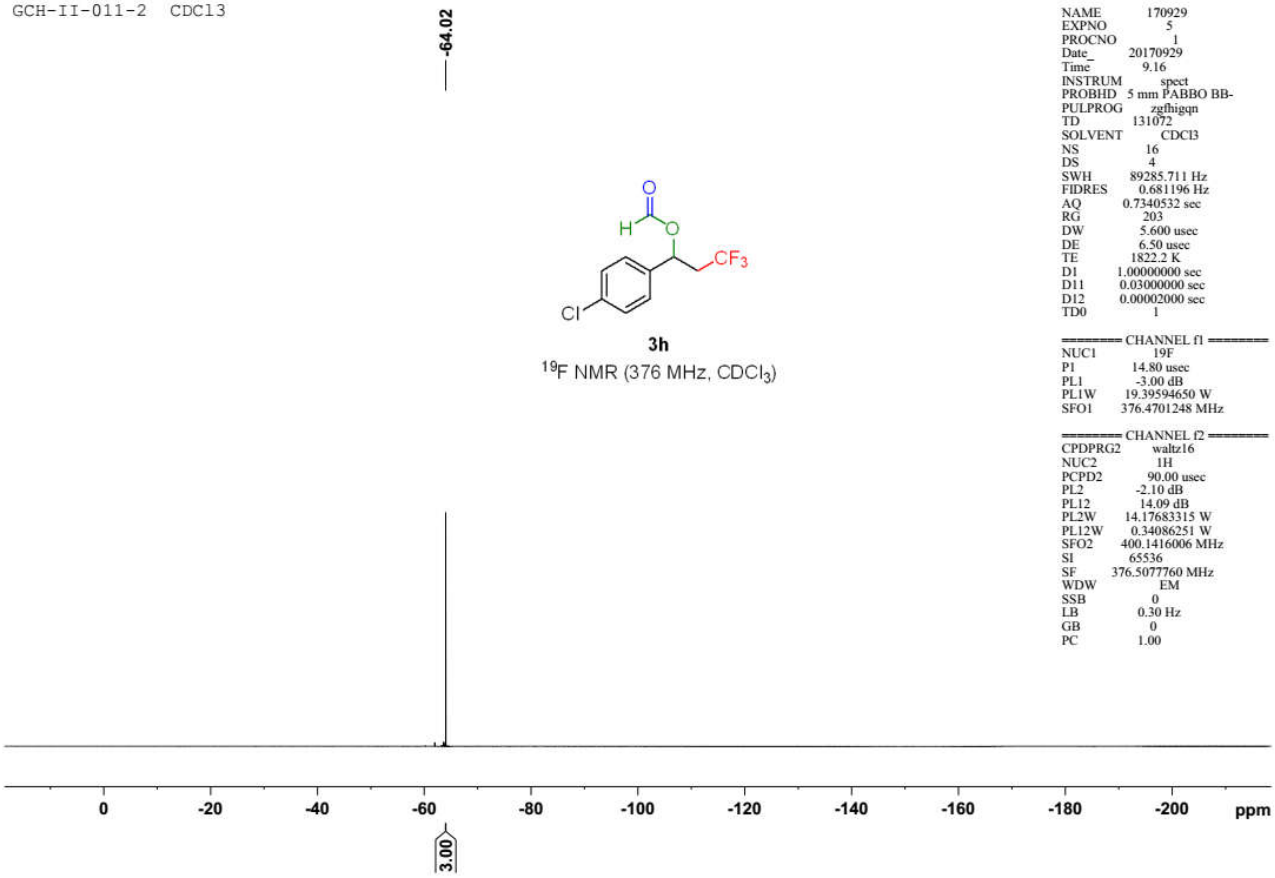
GCH-II-011-2 CDCl3


```
NAME          170930
EXPNO             36
PROCNO             1
Date_       20170930
Time           15.46
INSTRUM        spect
PROBHD  5 mm PABBO BB-
PULPROG       zgpg30
TD             65536
SOLVENT        CDCl3
NS               300
DS                 4
SWH        24038.461 Hz
FIDRES      0.366798 Hz
AQ          1.3631988 sec
RG               203
DW            20.800 usec
DE             6.50 usec
TE           1382.1 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                1

======== CHANNEL f1 ========
NUC1              13C
P1             9.00 usec
PL1           -2.00 dB
PL1W       53.74446869 W
SFO1       100.6253446 MHz

======== CHANNEL f2 ========
CPDPRG2       waltz16
NUC2              1H
PCPD2         90.00 usec
PL2           -2.10 dB
PL12          14.09 dB
PL13          13.52 dB
PL2W       14.17683315 W
PL12W       0.34086251 W
PL13W       0.38866836 W
SFO2       400.1416006 MHz
SI             32768
SF         100.6152951 MHz
WDW               EM
SSB                0
LB              1.00 Hz
GB                 0
PC              1.40
```

3h

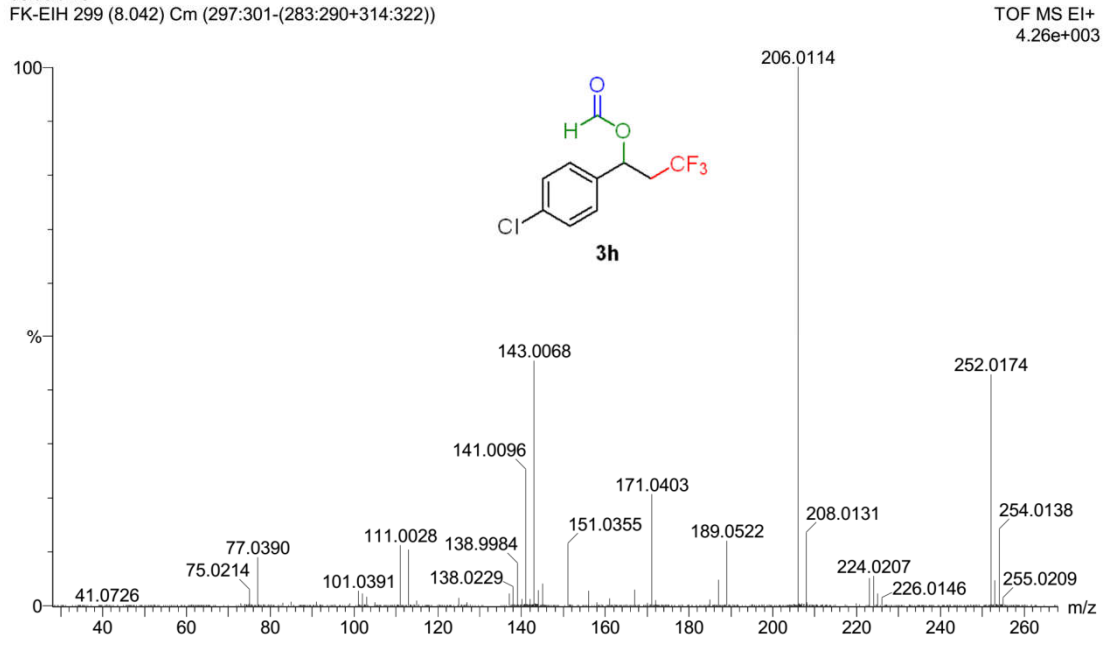
^{13}C NMR (100 MHz, $CDCl_3$)



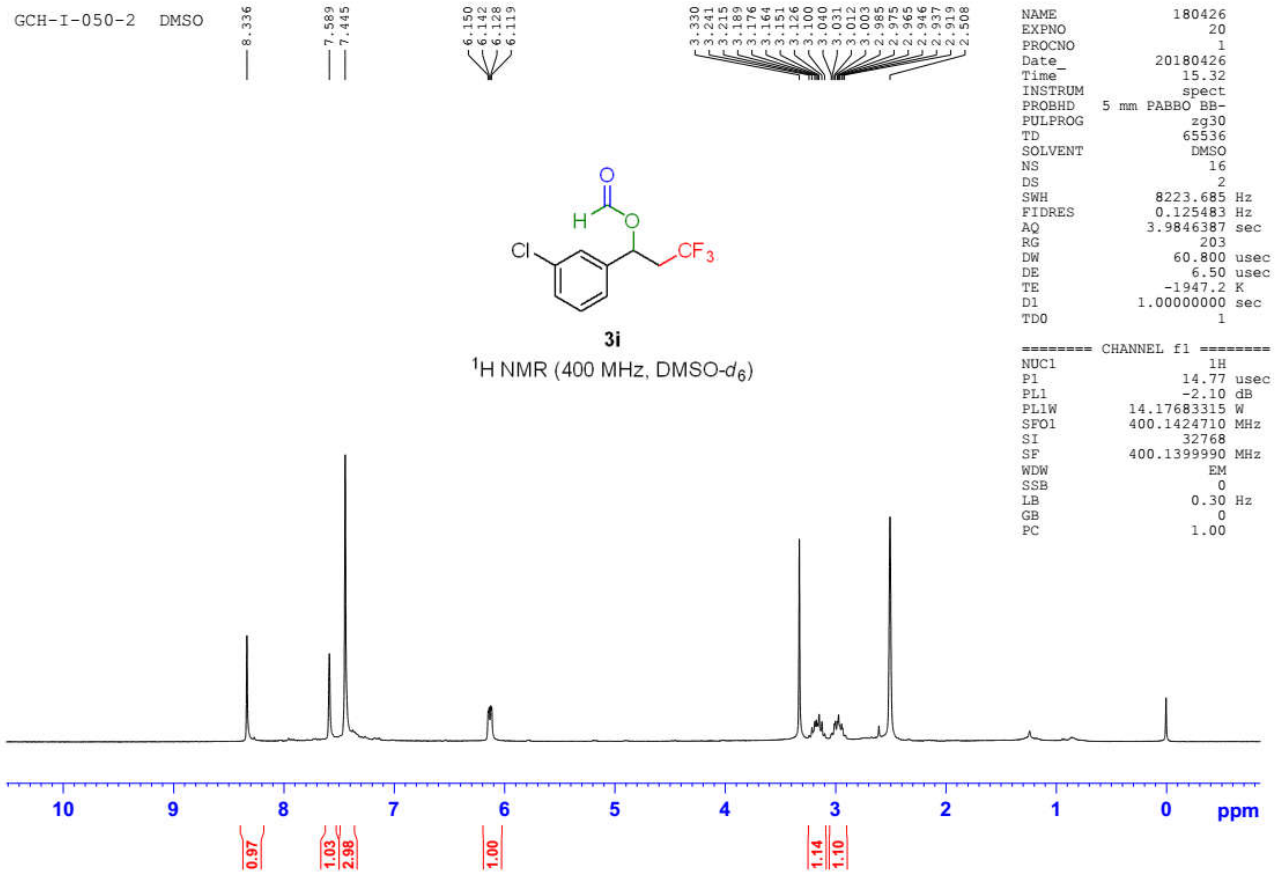


Monoisotopic Mass, Odd and Even Electron Ions
41 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-12 H: 0-12 O: 0-2 F: 0-4 Cl: 0-2

default file
FK-EIH 299 (8.042) Cm (297:301-(283:290+314:322))

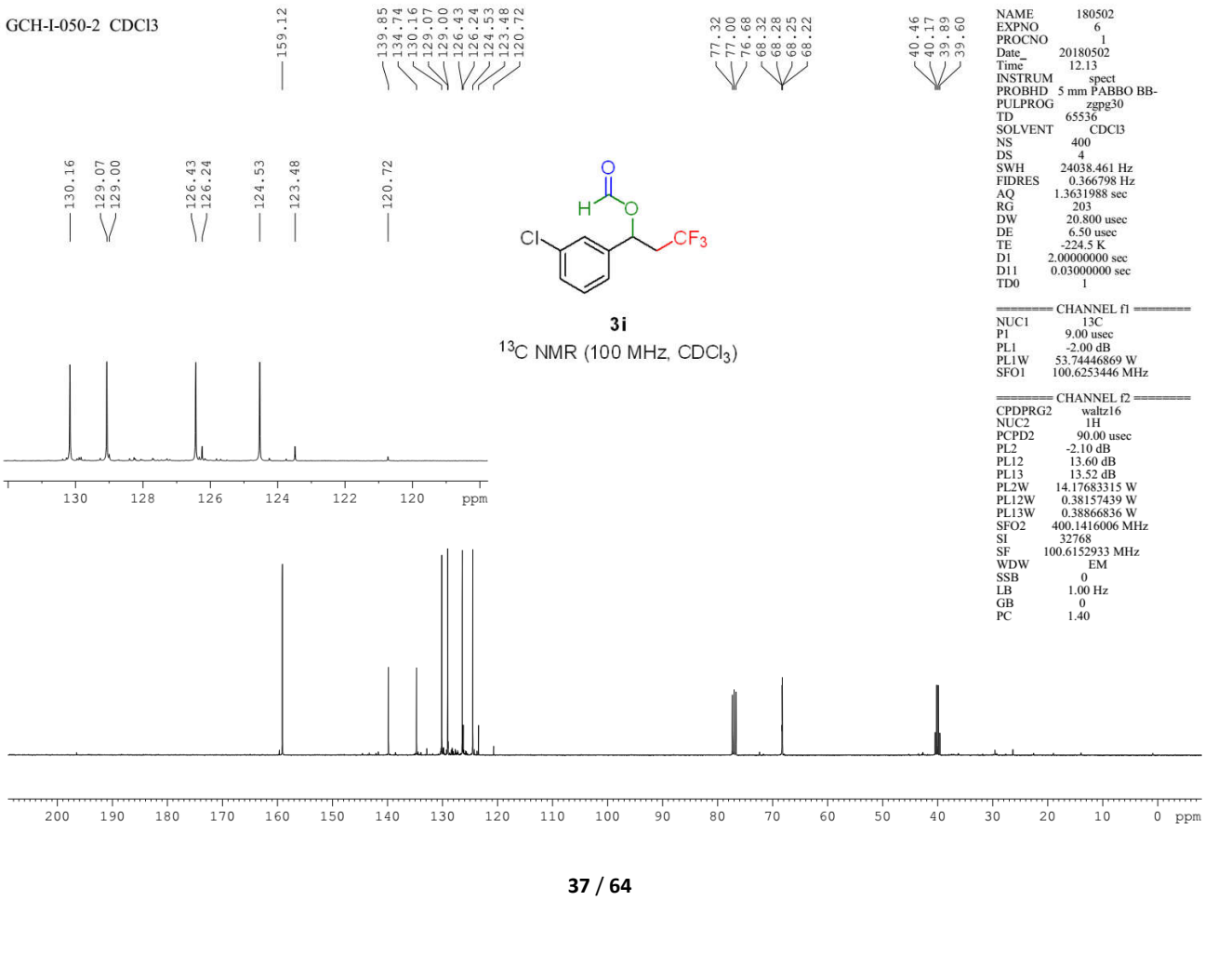


Minimum:				-1.5		
Maximum:		5.0	10.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
252.0174	252.0165	0.9	3.6	5.0	0.3	C10 H8 O2 F3 Cl



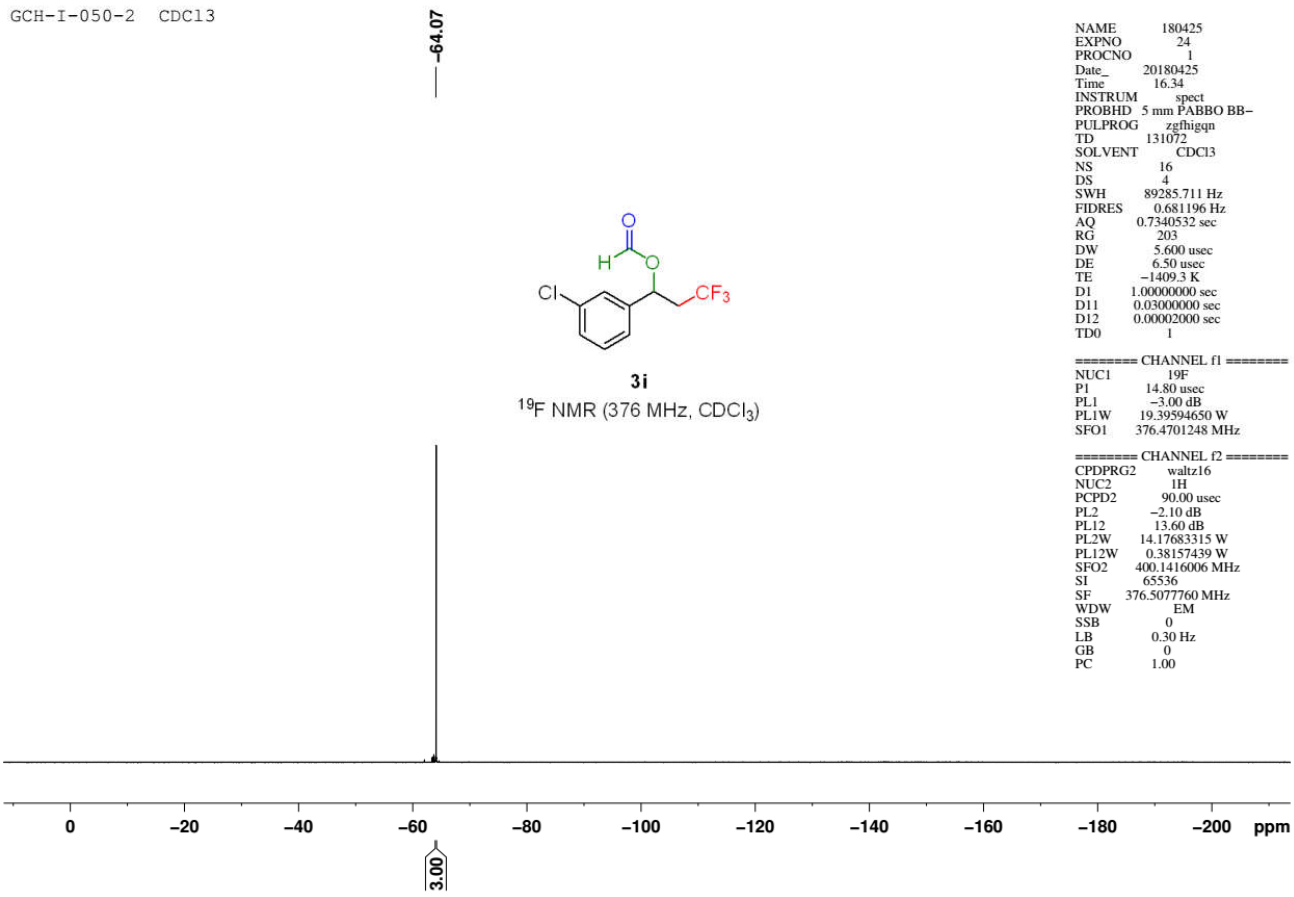
3i

^{1}H NMR (400 MHz, DMSO-d_6)



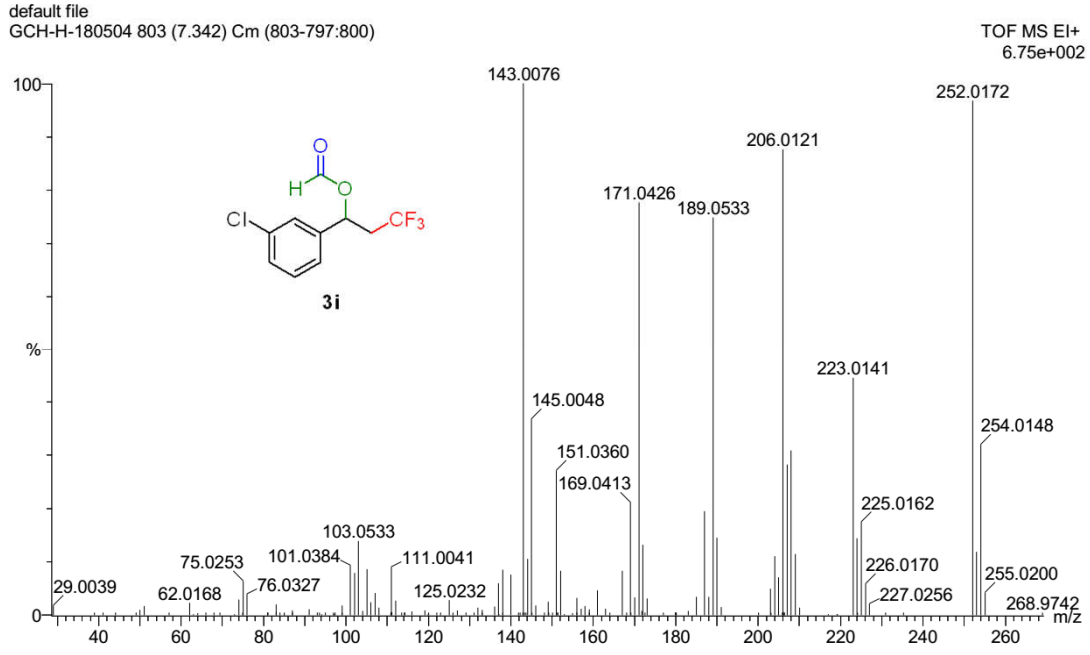
3i

^{13}C NMR (100 MHz, $CDCl_3$)



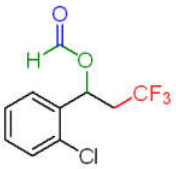
Monoisotopic Mass, Odd and Even Electron Ions
179 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 10-18 H: 0-60 O: 0-5 F: 0-3 Cl: 0-3

default file
GCH-H-180504 803 (7.342) Cm (803-797:800)



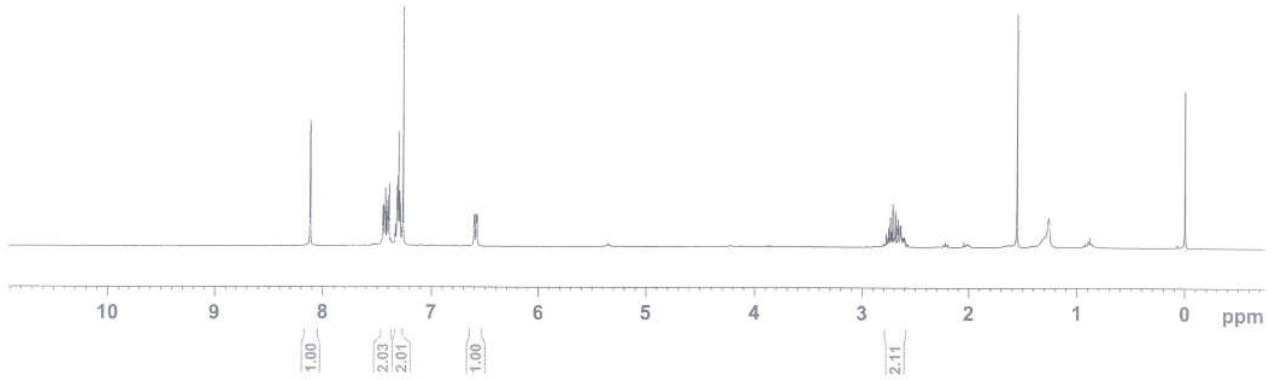
Minimum:				-1.5		
Maximum:		5.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
252.0172	252.0165	0.7	2.8	5.0	0.2	C10 H8 O2 F3 Cl

HZ-GCH-I-028-4 CDCl3

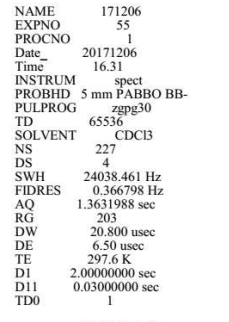


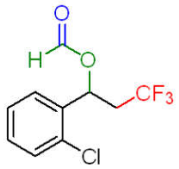
3j

^{1}H NMR (400 MHz, DMSO-d_6)



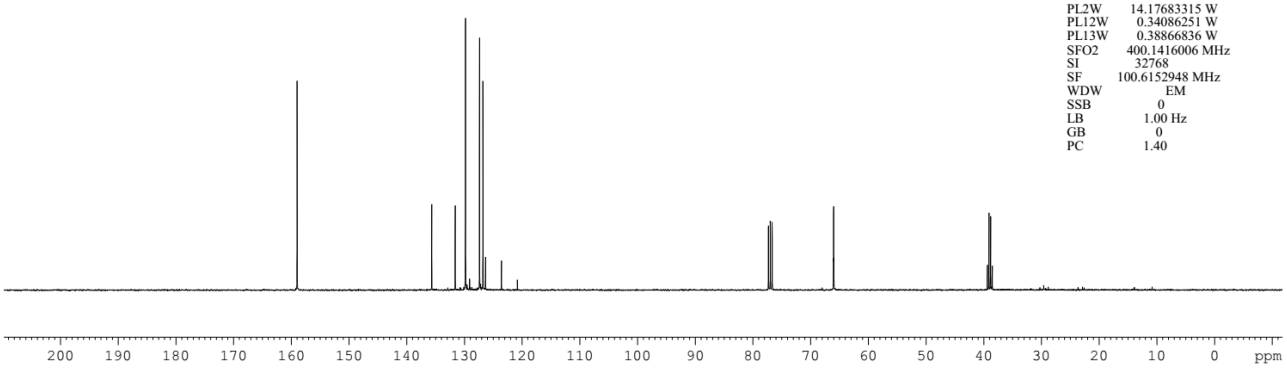
HZ-GCH-I-028-4 CDCl3

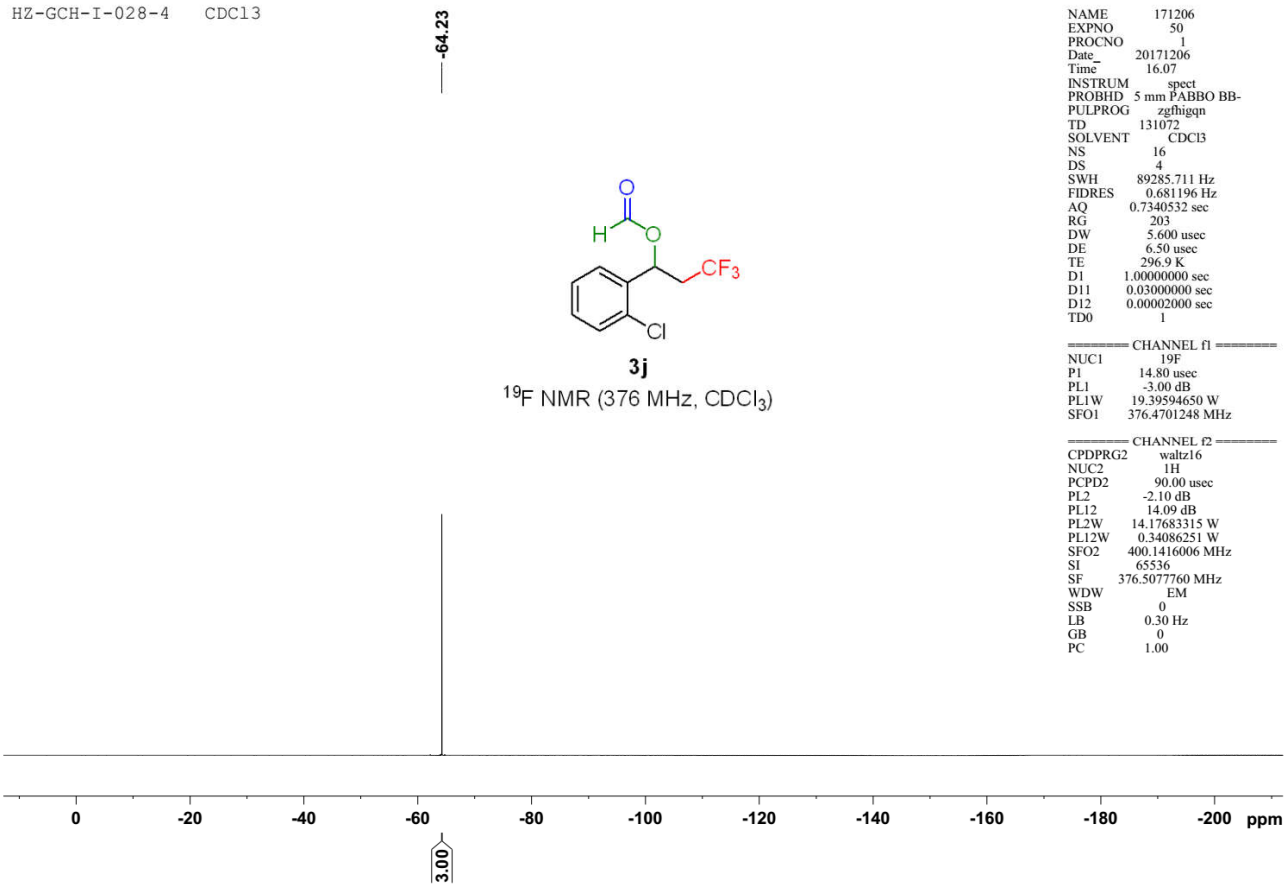




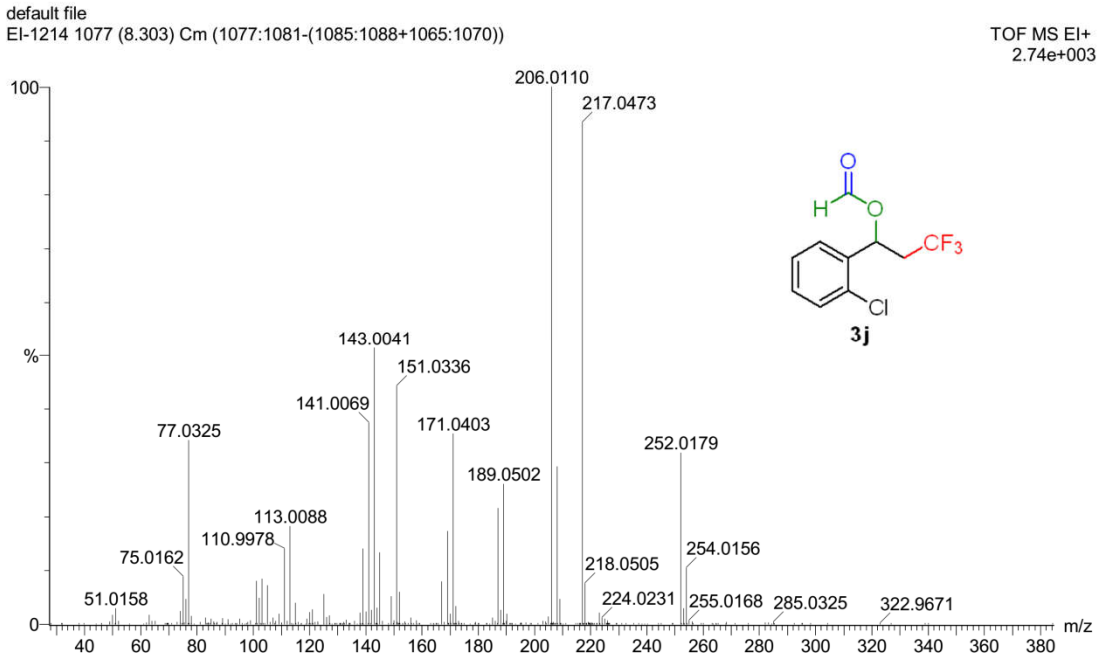
3j

^{13}C NMR (100 MHz, $CDCl_3$)



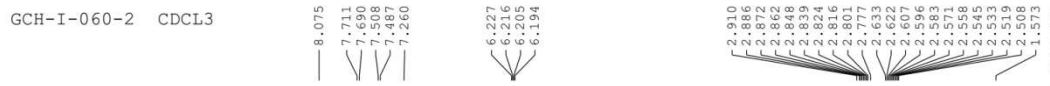


Monoisotopic Mass, Odd and Even Electron Ions
42 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-14 H: 0-12 O: 0-3 Cl: 0-2 F: 0-3



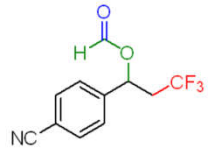
Minimum:				-1.5		
Maximum:		5.0	10.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
252.0179	252.0165	1.4	5.6	5.0	2.5	C10 H8 O2 Cl F3

GCH-I-060-2 CDCL3



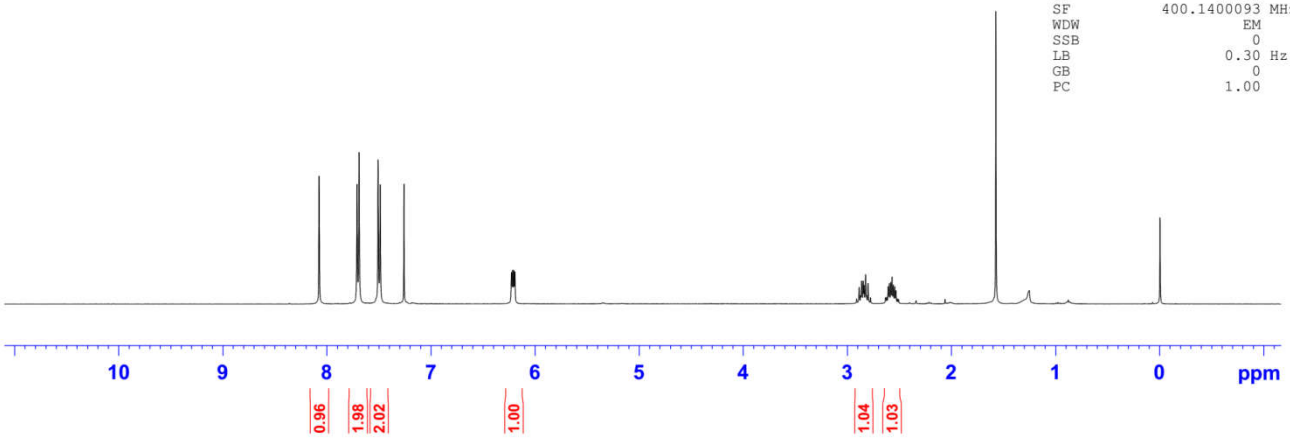
NAME	180528
EXPNO	5
PROCNO	1
Date_	20180528
Time	14.51
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	203
DW	60.800 use
DE	6.50 use
TE	297.4 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========	
NUC1	1H
P1	14.77 use
PL1	-2.10 dB
PL1W	14.17683315 W
SFO1	400.1424710 MHz
SI	32768
SF	400.1400093 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



3k

^{1}H NMR (400 MHz, $CDCl_3$)

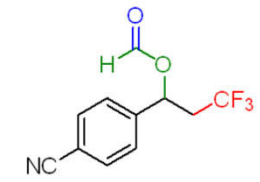


GCH-I-060-2 CDCL3

NAME	180528
EXPNO	6
PROCNO	1
Date_	20180528
Time	15.18
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	269
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	298.3 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1

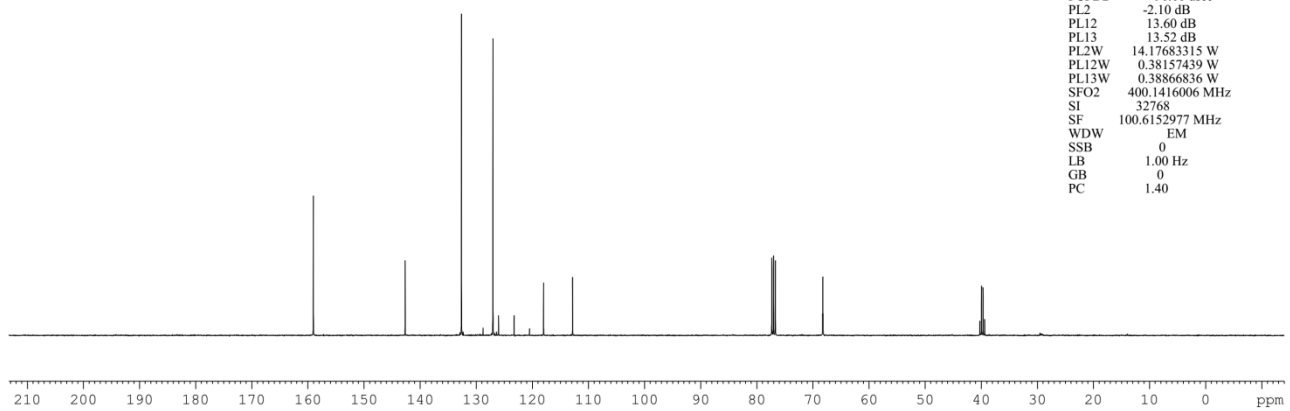
======== CHANNEL f1 ========	
NUC1	13C
P1	9.00 usec
PL1	-2.00 dB
PL1W	53.74446869 W
SFO1	100.6253446 MHz

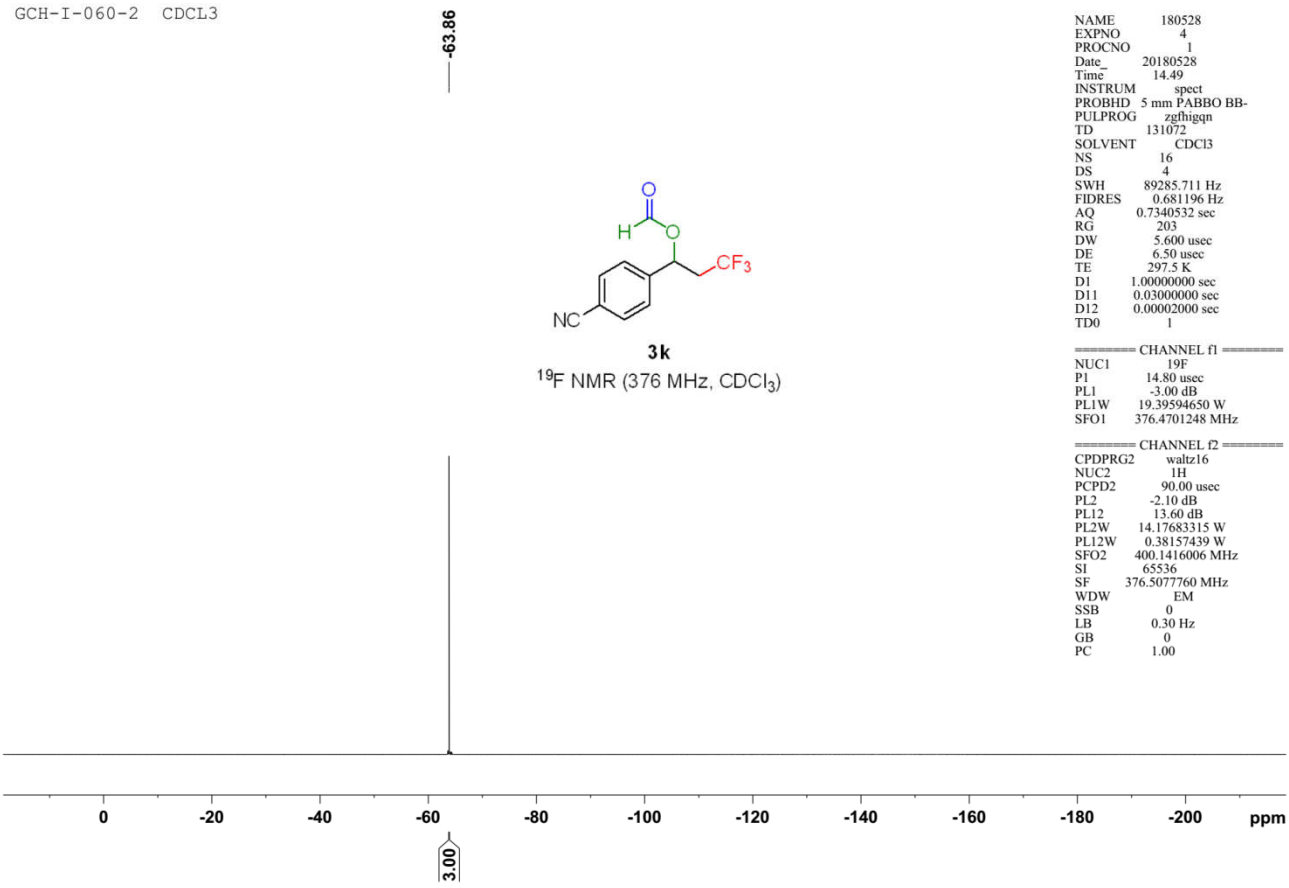
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.10 dB
PL12	13.60 dB
PL13	13.52 dB
PL2W	14.17683315 W
PL12W	0.38157439 W
PL13W	0.38866836 W
SFO2	400.1416006 MHz
SI	32768
SF	100.6152977 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



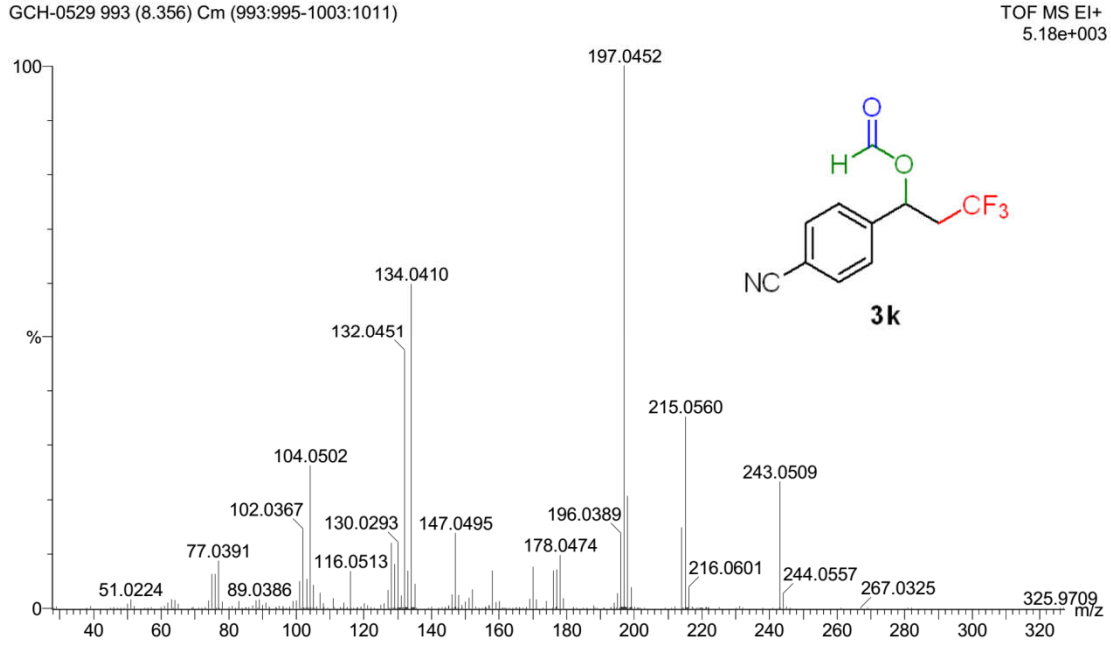
3k

^{13}C NMR (100 MHz, $CDCl_3$)





Monoisotopic Mass, Odd and Even Electron Ions
209 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 9-30 H: 0-60 N: 0-2 O: 0-4 F: 1-8
default file
GCH-0529 993 (8.356) Cm (993:995-1003:1011)



Minimum:				-1.5		
Maximum:		5.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
243.0509	243.0507	0.2	0.8	7.0	3.3	C11 H8 N O2 F3

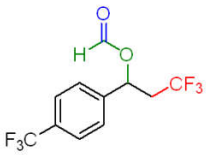
GCH-057-2 CDCl3

8.078 7.673 7.653 7.514 7.495 7.260 6.258 6.249 6.236 6.227 2.927 2.903 2.879 2.865 2.856 2.841 2.817 2.793 2.636 2.627 2.611 2.601 2.586 2.575 2.563 2.549 2.538 2.523 2.512 1.558

NAME	180507
EXPNO	10
PROCNO	1
Date_	20180507
Time	15.47
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	203
DW	60.800 usec
DE	6.50 usec
TE	-731.0 K
D1	1.00000000 sec
TD0	1

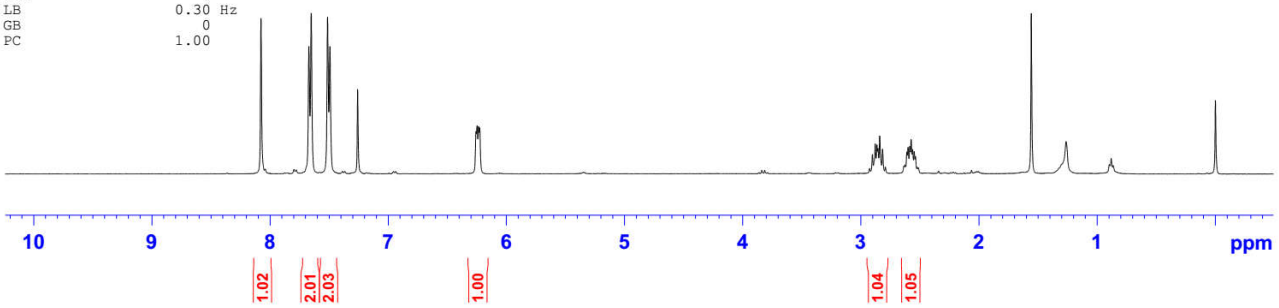
======== CHANNEL f1 ========

NUC1	1H
P1	14.77 usec
PL1	-2.10 dB
PL1W	14.17683315 W
SFO1	400.1424710 MHz
SI	32768
SF	400.1400094 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



3l

^{1}H NMR (400 MHz, $CDCl_3$)



HZ-ETA-XIII-057-2 CDCl3

159.17 141.76 131.72 131.39 131.07 130.74 128.99 127.82 126.78 126.23 126.03 125.99 125.95 125.91 125.12 123.47 122.41 120.72 119.71 77.32 77.00 76.68 68.53 68.50 68.47 68.43 40.59 40.30 40.02 39.73

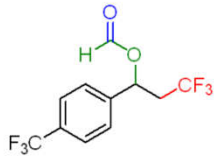
NAME	180507
EXPNO	11
PROCNO	1
Date_	20180507
Time	16.32
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	331
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	-1055.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1

======== CHANNEL f1 ========

NUC1	13C
P1	9.00 usec
PL1	-2.00 dB
PL1W	53.74446869 W
SFO1	100.6253446 MHz

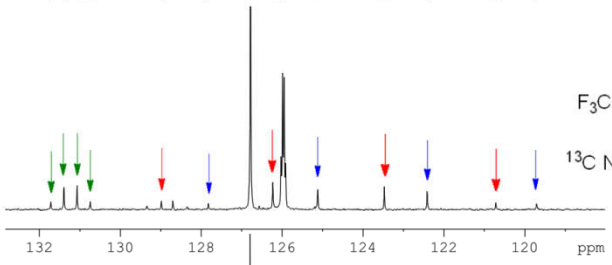
======== CHANNEL f2 ========

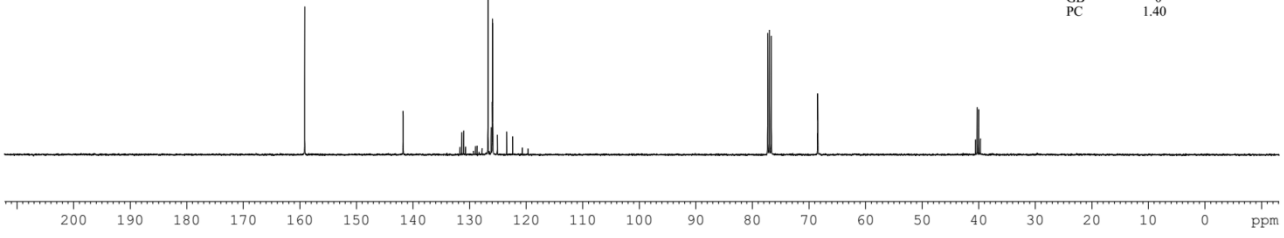
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.10 dB
PL12	13.60 dB
PL13	13.52 dB
PL2W	14.17683315 W
PL12W	0.38157439 W
PL13W	0.38866836 W
SFO2	400.1416006 MHz
SI	32768
SF	100.6152830 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



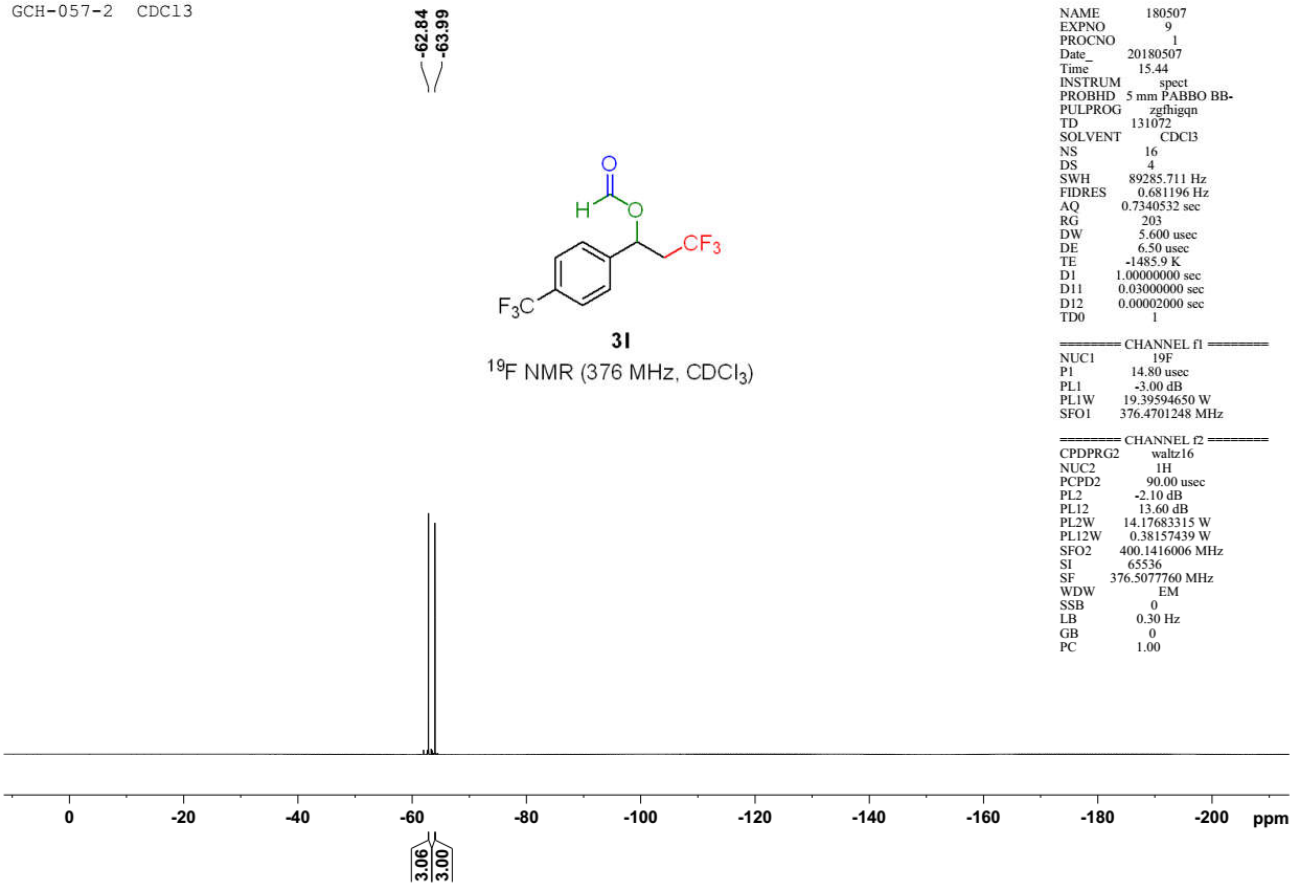
3l

^{13}C NMR (100 MHz, $CDCl_3$)





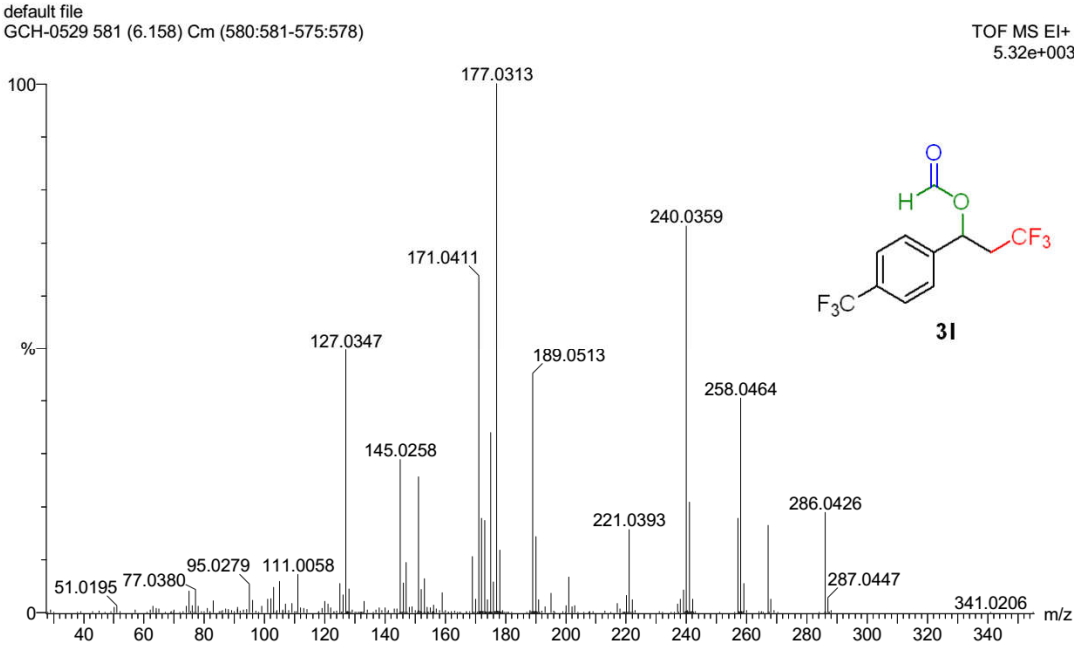
GCH-057-2 CDCl3



3l

^{19}F NMR (376 MHz, $CDCl_3$)

Monoisotopic Mass, Odd and Even Electron Ions
122 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 5-30 H: 0-60 O: 1-5 F: 0-8
default file
GCH-0529 581 (6.158) Cm (580:581-575:578)



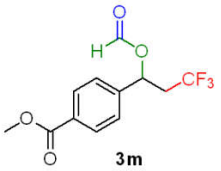
3l

Minimum:				-1.5		
Maximum:		5.0	1.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
286.0426	286.0428	-0.2	-0.7	5.0	1.4	C11 H8 O2 F6

GCH-I-036-4 CDCl3

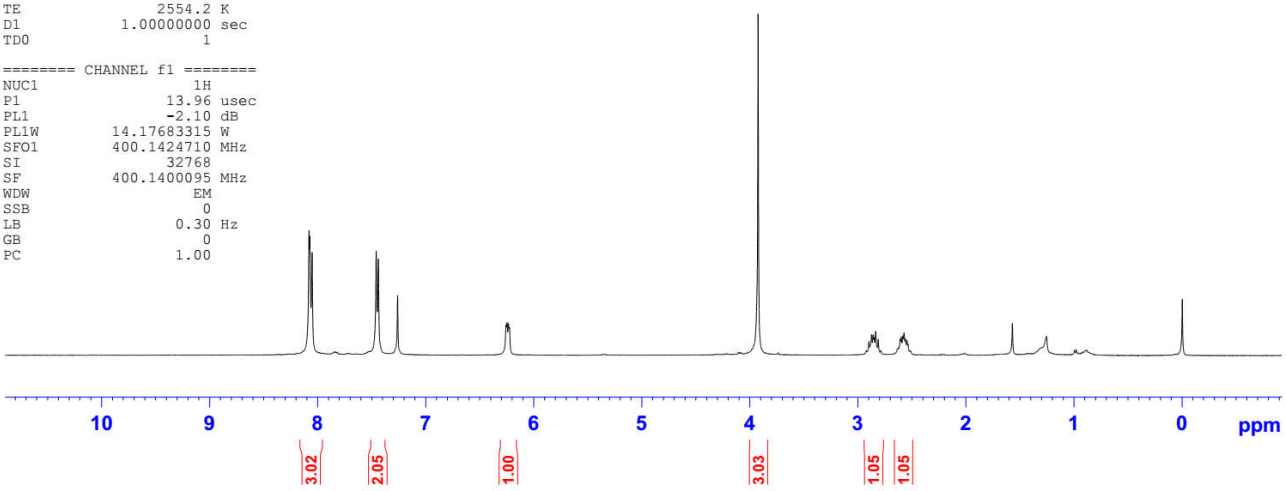
8.079 8.072 8.051 7.458 7.438 7.260 6.256 6.247 6.234 6.225 3.923 2.922 2.897 2.873 2.859 2.849 2.835 2.811 2.787 2.633 2.623 2.608 2.598 2.583 2.572 2.560 2.546 2.535 2.520 2.509 1.570

NAME	180123
EXPNO	13
PROCNO	1
Date_	20180123
Time	15.59
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	203
DW	60.800 usec
DE	6.50 usec
TE	2554.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.96 usec
PL1	-2.10 dB
PL1W	14.17683315 W
SFO1	400.1424710 MHz
SI	32768
SF	400.1400095 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



3m

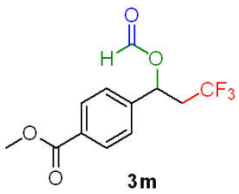
^{1}H NMR (400 MHz, $CDCl_3$)



GCH-I-036-4 CDCl3

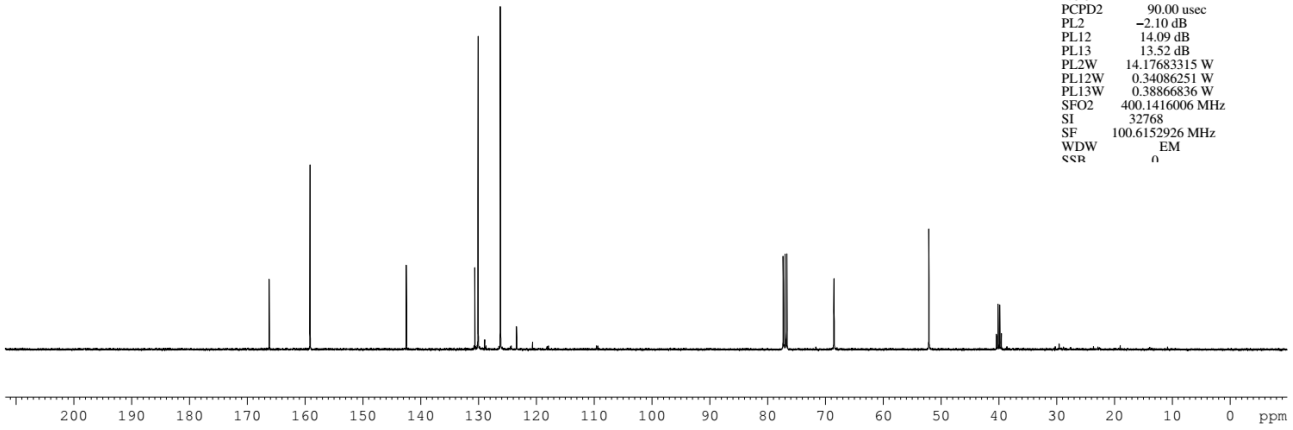
166.23 159.16 142.51 130.66 130.10 128.96 126.24 126.20 123.44 120.68 77.32 77.00 76.68 68.57 68.54 68.50 68.47 52.11 40.42 40.13 39.85 39.56

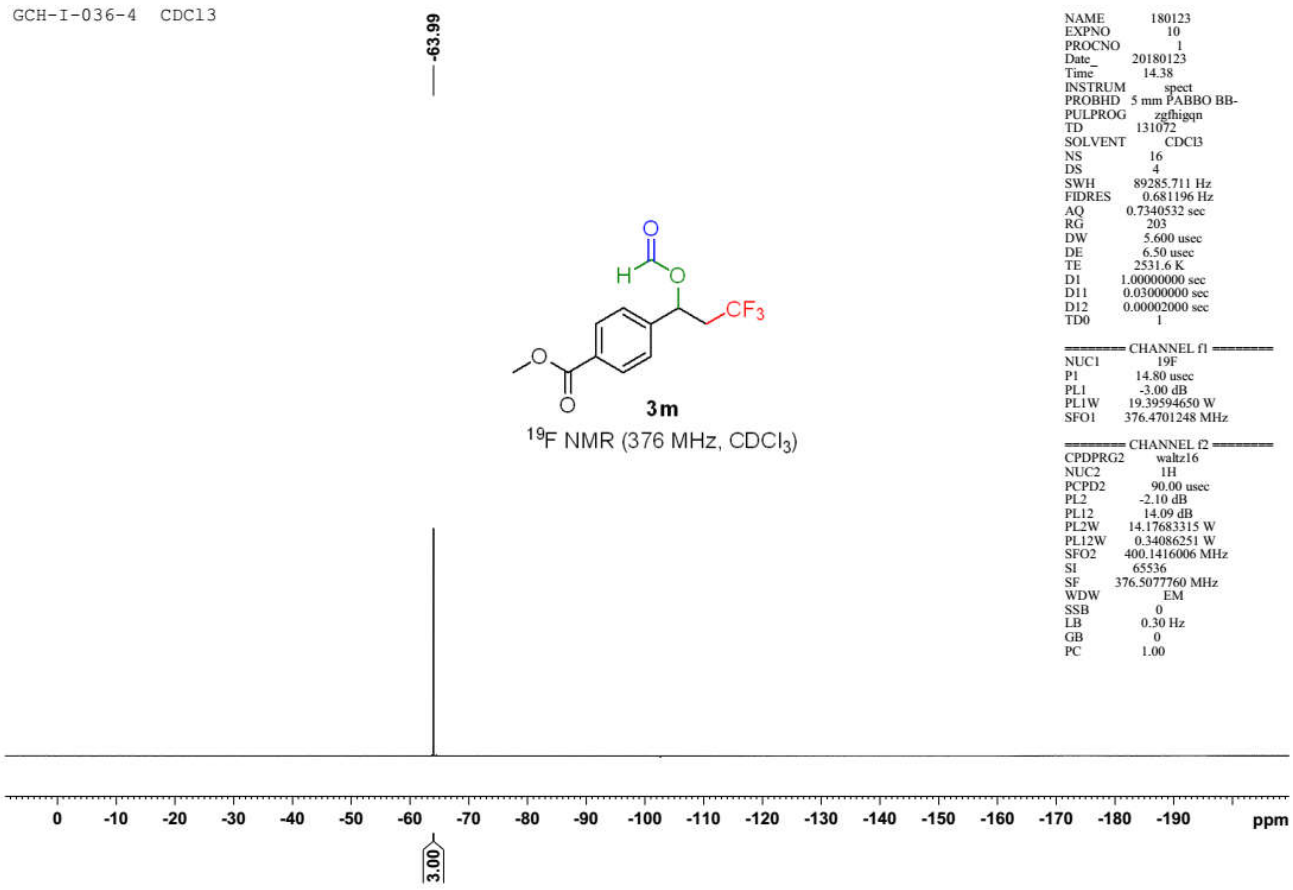
NAME	180123
EXPNO	16
PROCNO	1
Date_	20180123
Time	16.30
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	282
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	2509.9 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.00 usec
PL1	-2.00 dB
PL1W	53.74446869 W
SFO1	100.6253446 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.10 dB
PL12	14.09 dB
PL13	13.52 dB
PL2W	14.17683315 W
PL12W	0.34086251 W
PL13W	0.38866836 W
SFO2	400.1416006 MHz
SI	32768
SF	100.6152926 MHz
WDW	EM
SSB	0



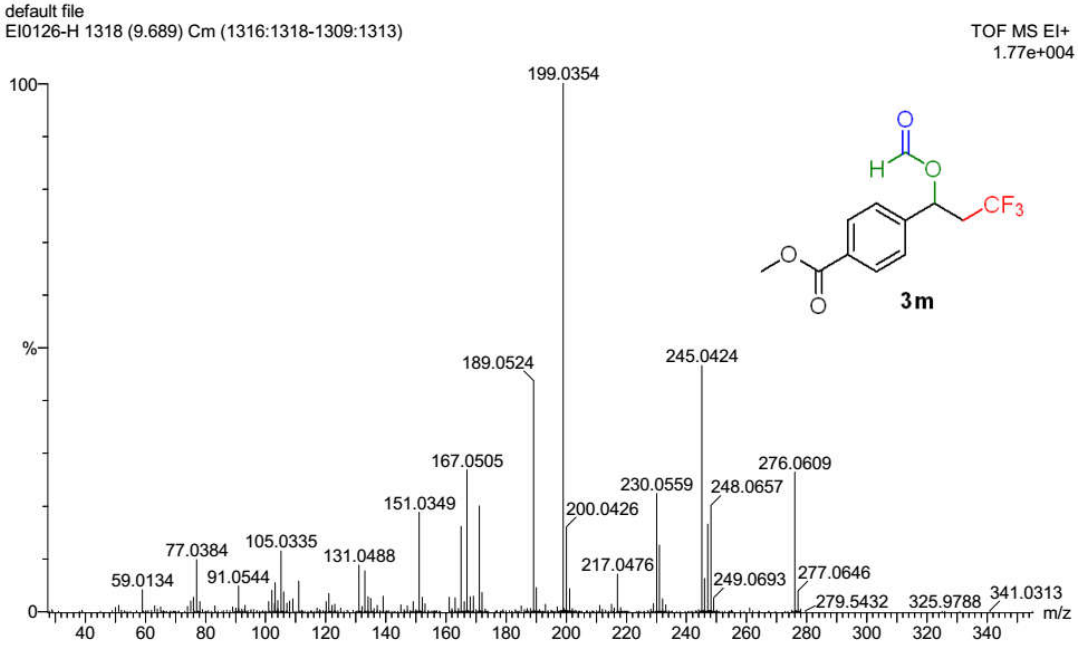
3m

^{13}C NMR (100 MHz, $CDCl_3$)



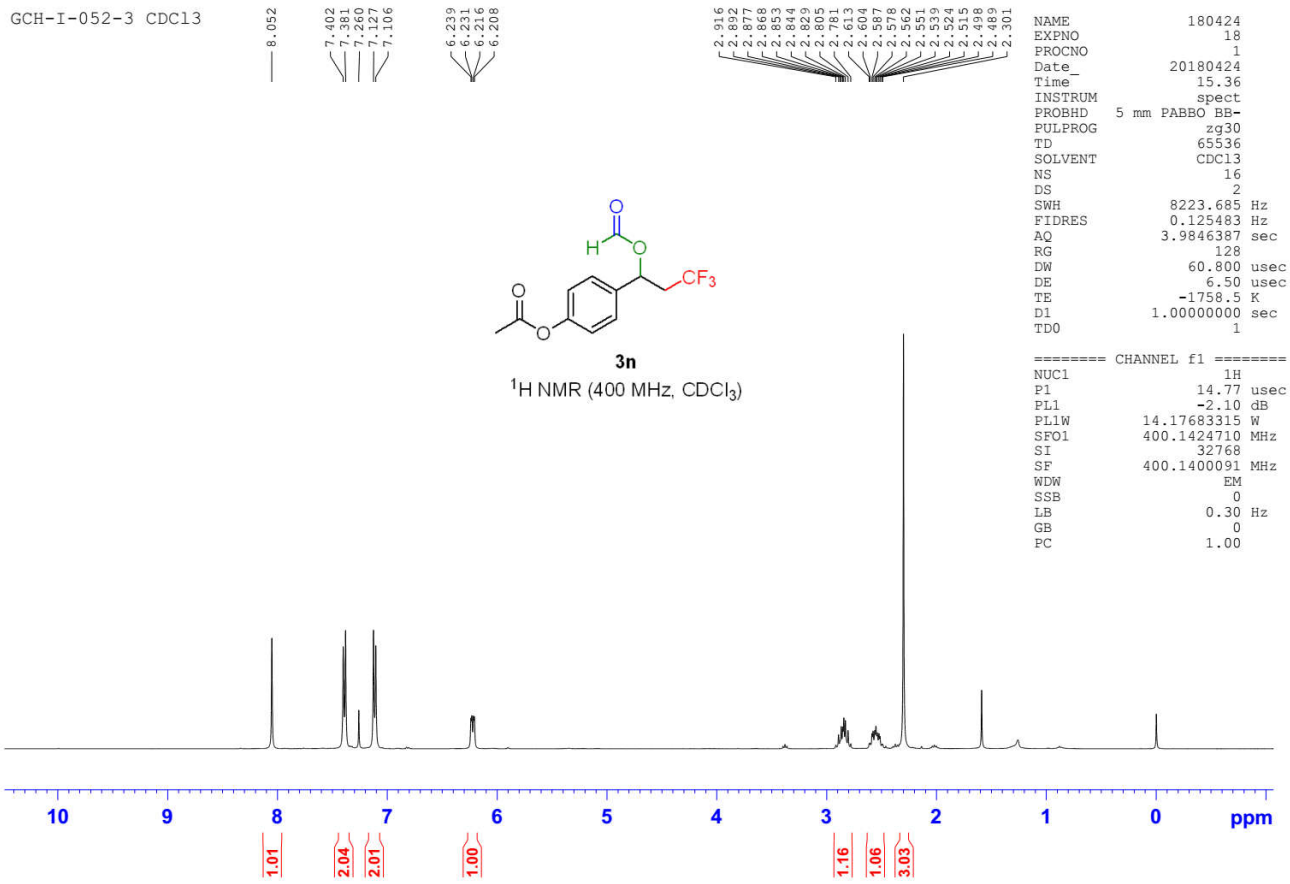


Monoisotopic Mass, Odd and Even Electron Ions
21 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-13 H: 0-16 O: 0-5 F: 0-3



Minimum:				-1.5		
Maximum:		5.0	10.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
276.0609	276.0609	0.0	0.0	6.0	0.6	C12 H11 O4 F3

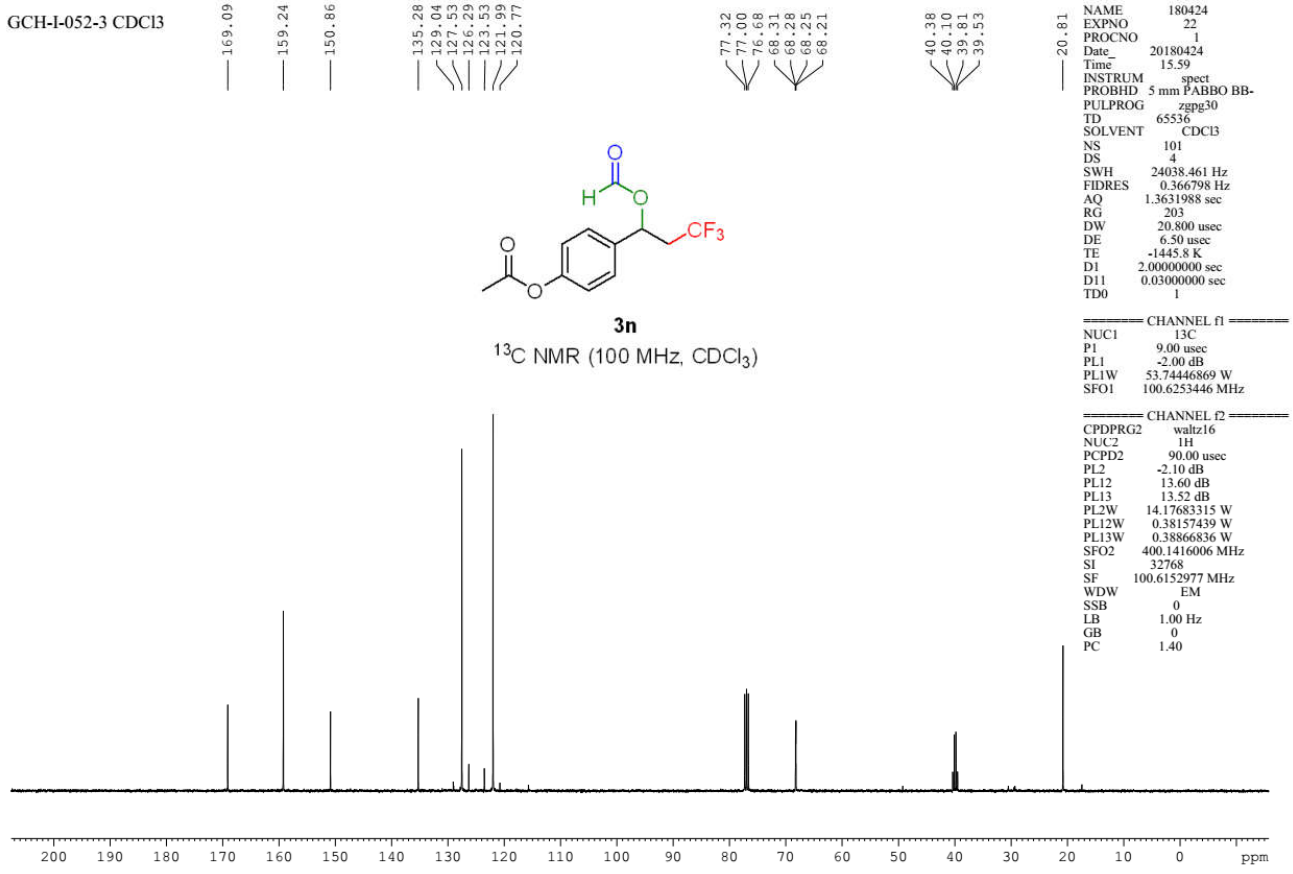
GCH-I-052-3 CDCl3



3n

^{1}H NMR (400 MHz, $CDCl_3$)

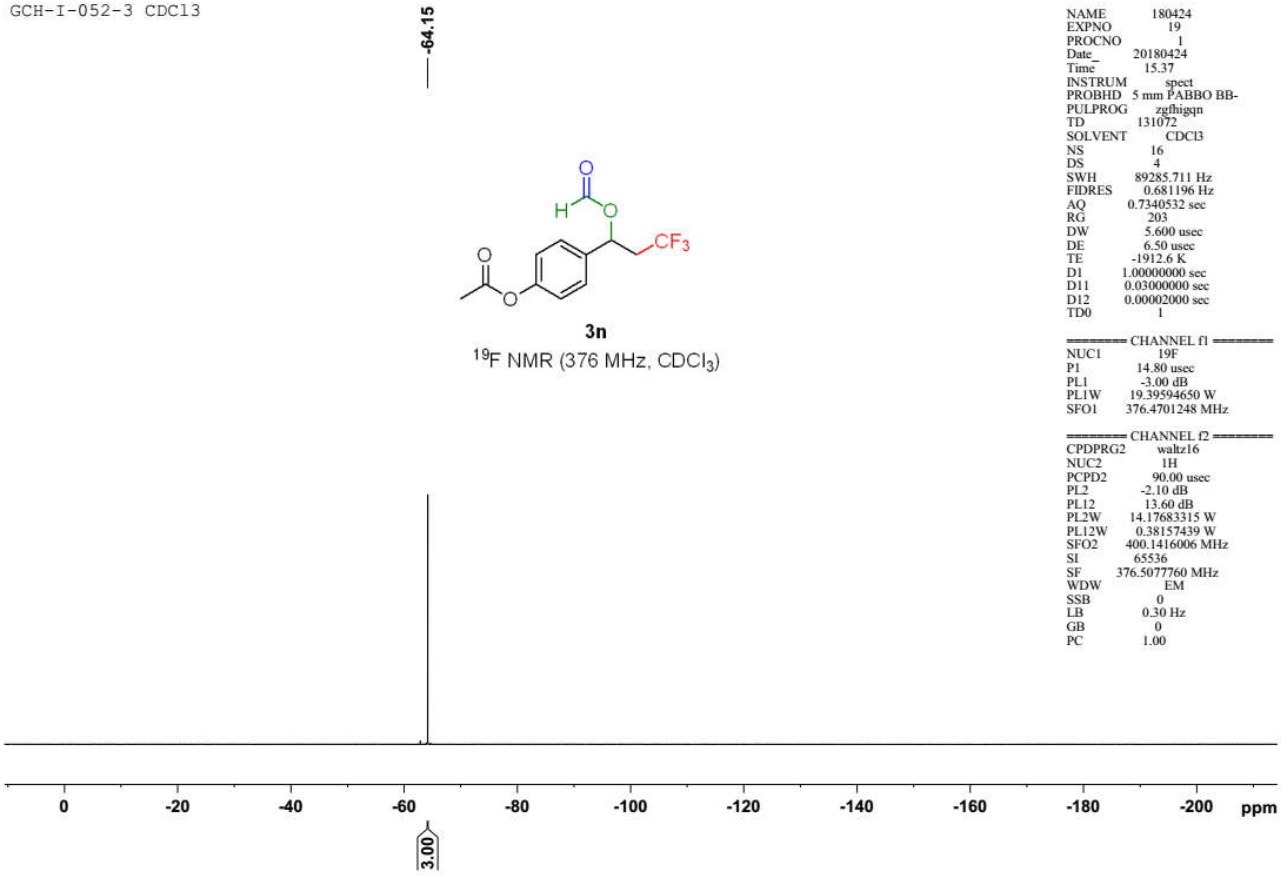
GCH-I-052-3 CDCl3



3n

^{13}C NMR (100 MHz, $CDCl_3$)

GCH-I-052-3 CDCl3



NAME 180424
EXPNO 19
PROCNO 1
Date_ 20180424
Time 15.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340532 sec
RG 203
DW 5.600 usec
DE 6.50 usec
TE -1912.6 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

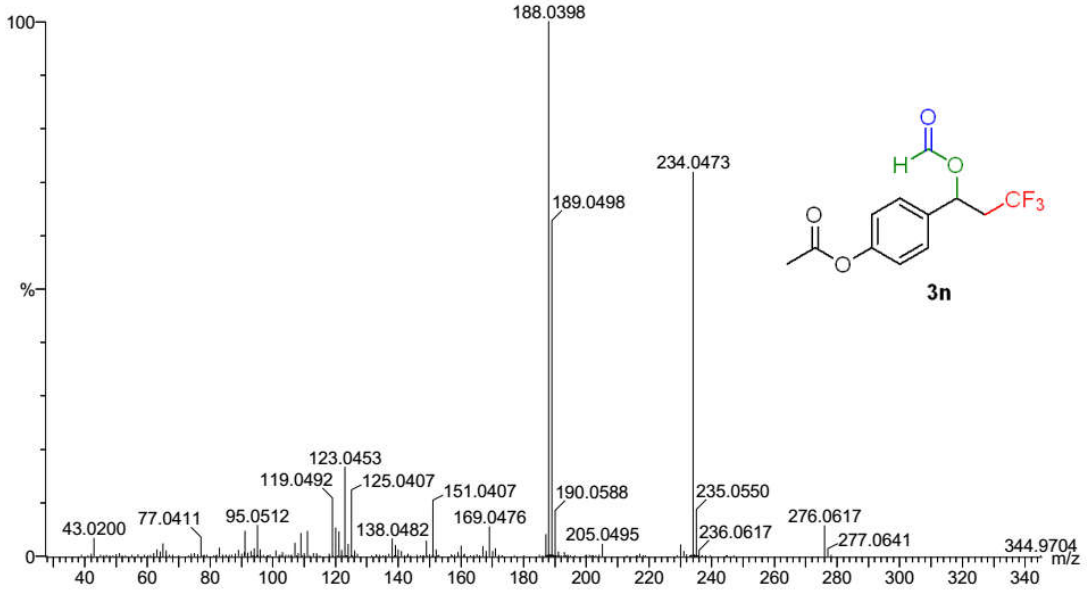
======== CHANNEL f1 ========
NUC1 19F
P1 14.80 usec
PL1 -3.00 dB
PL1W 19.39594650 W
SFO1 376.4701248 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.10 dB
PL12 13.60 dB
PL2W 14.17683315 W
PL12W 0.38157439 W
SFO2 400.1416006 MHz
SI 65536
SF 376.5077760 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Monoisotopic Mass, Odd and Even Electron Ions
66 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 10-18 H: 0-60 O: 0-5 F: 0-3

default file
GCH-H-180504 1055 (8.687) Cm (1055-1046:1052)

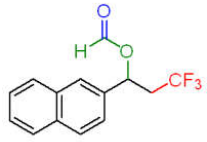
TOF MS EI+
8.79e+003



Minimum:				-1.5		
Maximum:		5.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
276.0617	276.0609	0.8	2.9	6.0	6.4	C12 H11 O4 F3

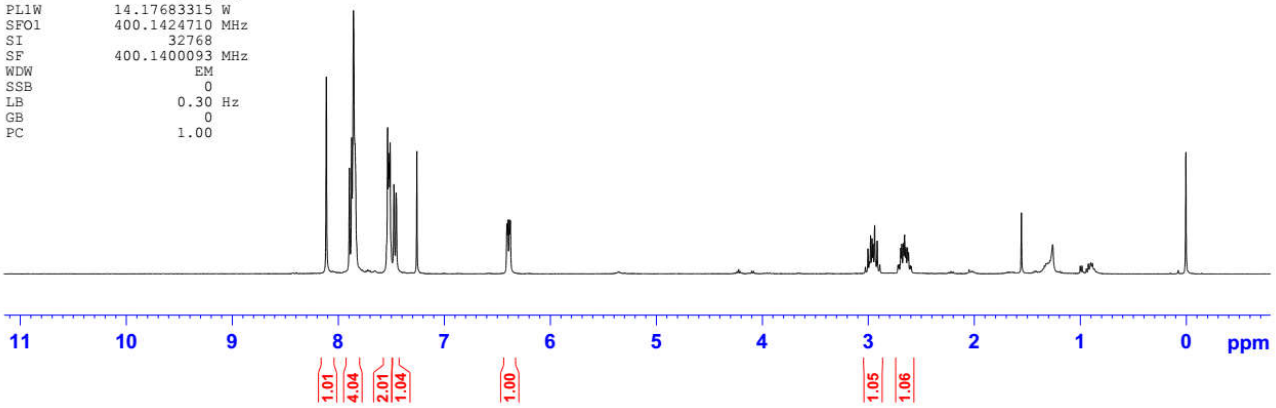
GCH-I-037-2 CDCl3


```
NAME              180119
EXPNO                 44
PROCNO                 1
Date_           20180119
Time               16.01
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9846387 sec
RG                   161
DW                60.800 usec
DE                 6.50 usec
TE                2807.6 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 13.96 usec
PL1                -2.10 dB
PL1W        14.17683315 W
SFO1        400.1424710 MHz
SI                 32768
SF          400.1400093 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



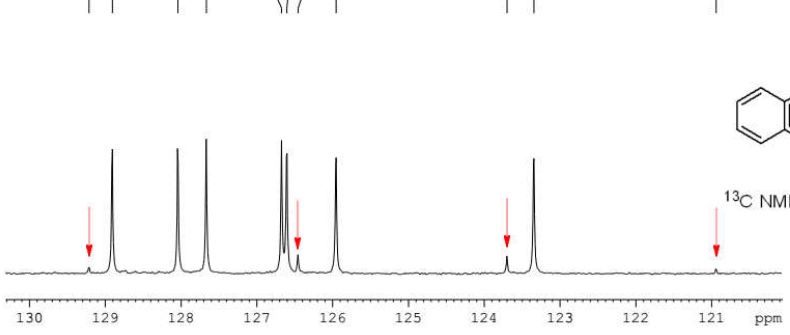
3o

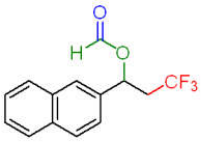
^{1}H NMR (400 MHz, $CDCl_3$)



GCH-I-037-2 CDCl3

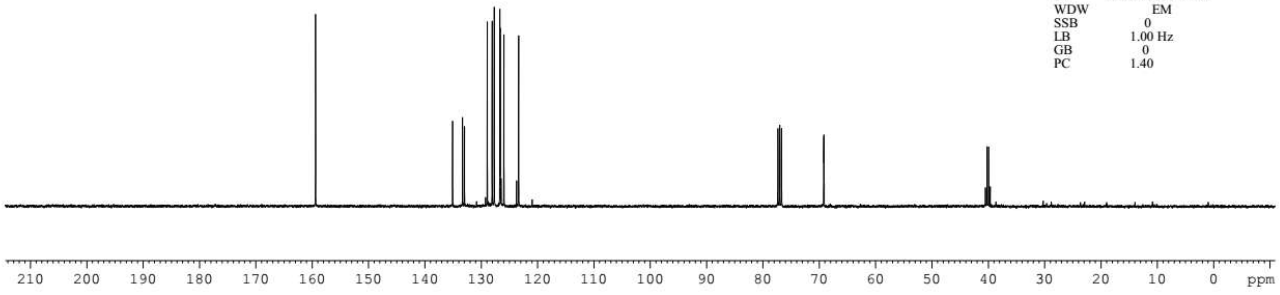

```
NAME              180119
EXPNO                 47
PROCNO                 1
Date_           20180119
Time               16.35
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   192
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631988 sec
RG                   203
DW                20.800 usec
DE                 6.50 usec
TE                3032.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.00 usec
PL1                -2.00 dB
PL1W        53.74446869 W
SFO1        100.6253446 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                 1H
PCPD2           90.00 usec
PL2                -2.10 dB
PL12               14.09 dB
PL13               13.52 dB
PL2W        14.17683315 W
PL12W        0.34086251 W
PL13W        0.38866836 W
SFO2        400.1416006 MHz
SI                 32768
SF          100.6153007 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```



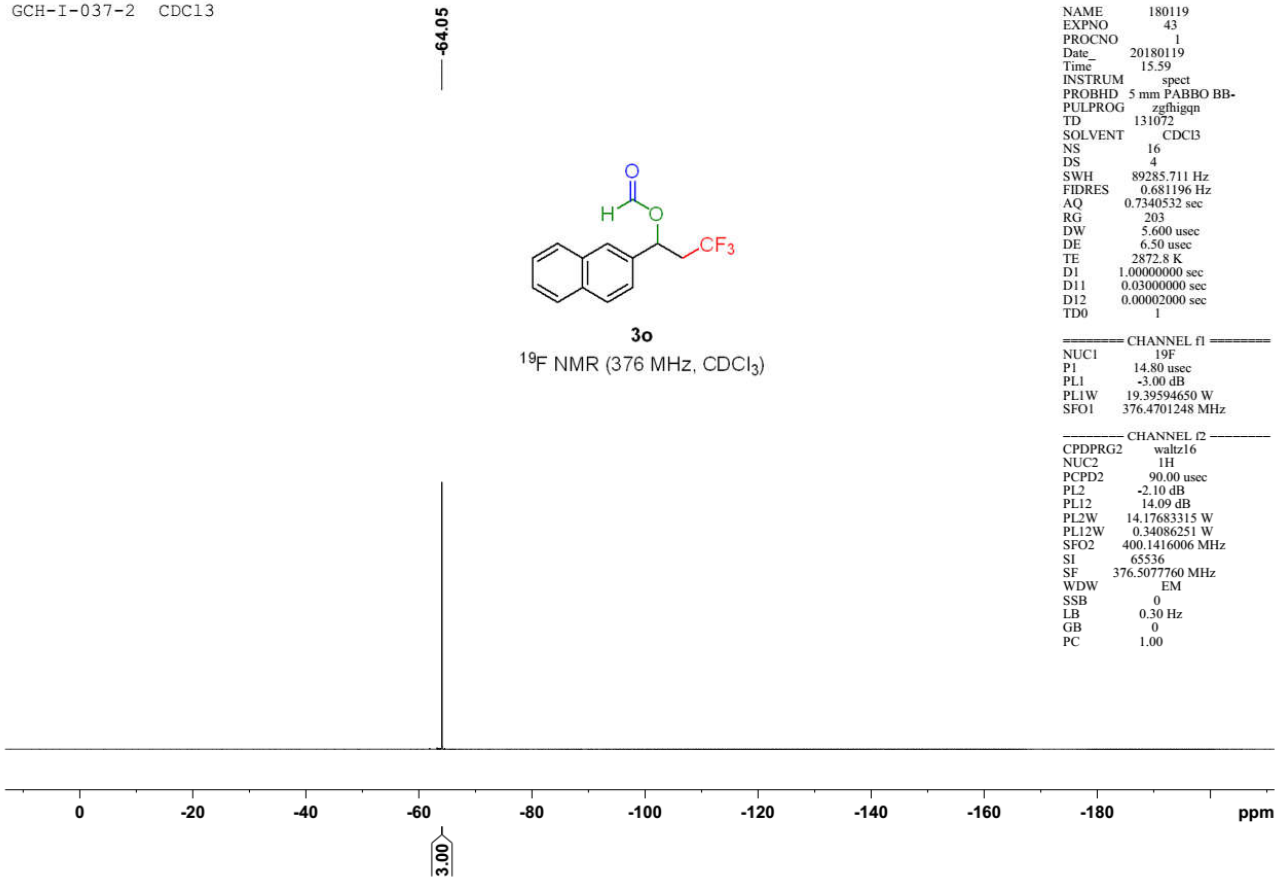


3o

^{13}C NMR (100 MHz, $CDCl_3$)

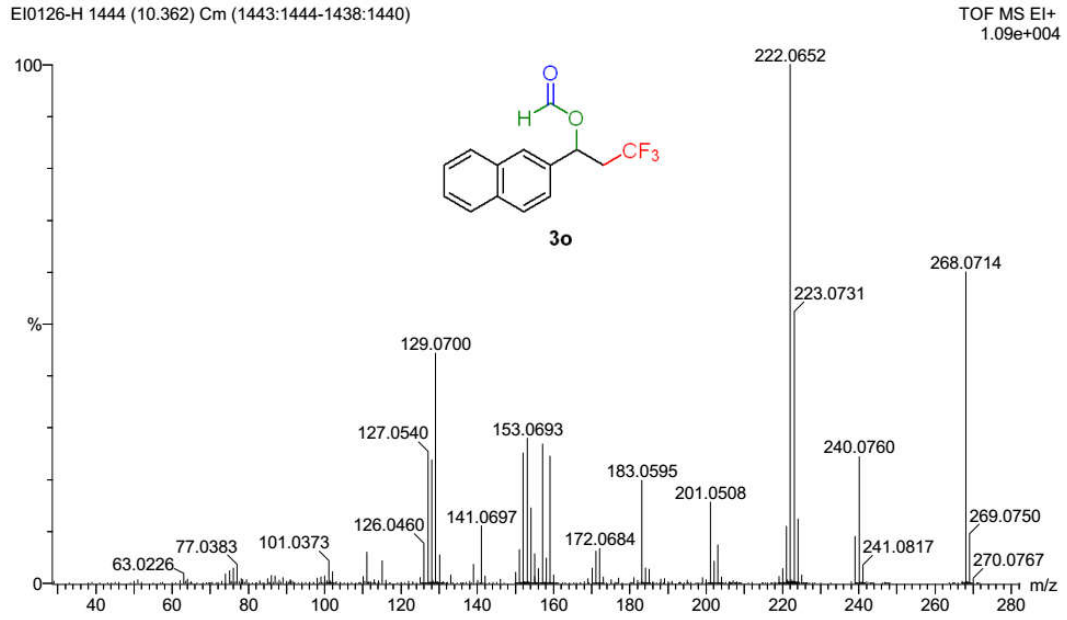


GCH-I-037-2 CDCl3



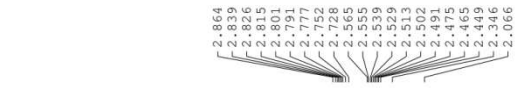
^{19}F NMR (376 MHz, $CDCl_3$)

Monoisotopic Mass, Odd and Even Electron Ions
22 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-15 H: 0-16 O: 0-5 F: 0-3
default file
EI0126-H 1444 (10.362) Cm (1443:1444-1438:1440)

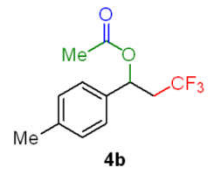


Minimum:				-1.5		
Maximum:		5.0	10.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
268.0714	268.0711	0.3	1.1	8.0	1.8	C14 H11 O2 F3

GCH-I-053-1 CDCl3

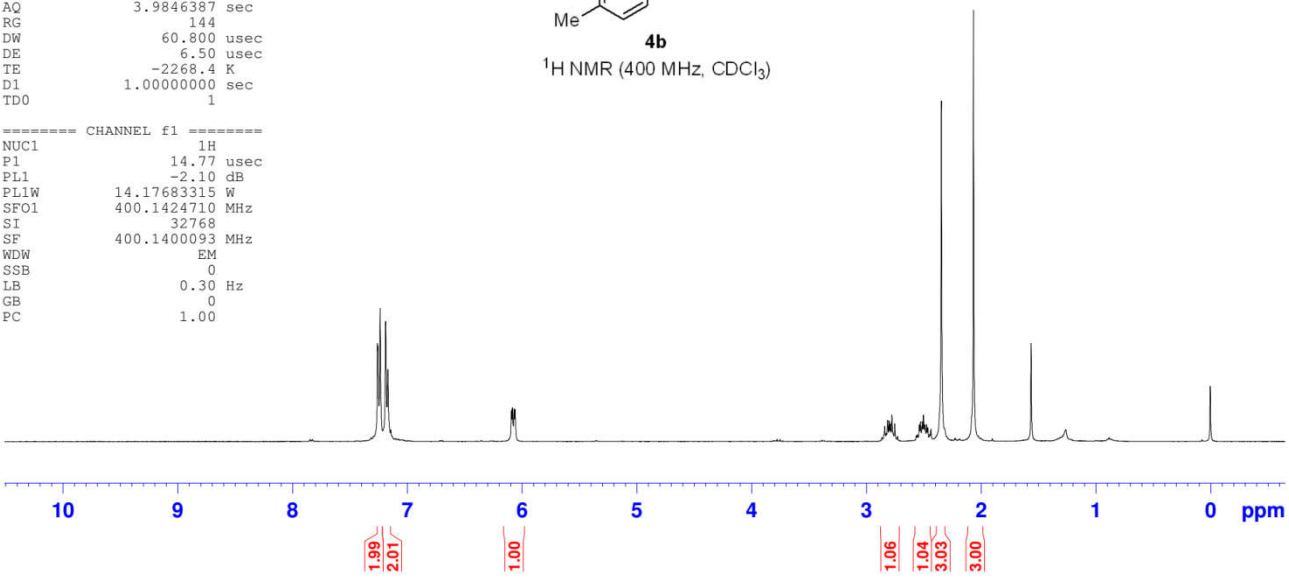


NAME	180502
EXPNO	2
PROCNO	1
Date_	20180502
Time	11.00
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	144
DW	60.800 usec
DE	6.50 usec
TE	-2268.4 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.77 usec
PL1	-2.10 dB
PL1W	14.17683315 W
SFO1	400.1424710 MHz
SI	32768
SF	400.1400093 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



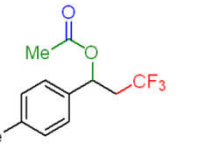
4b

^{1}H NMR (400 MHz, $CDCl_3$)



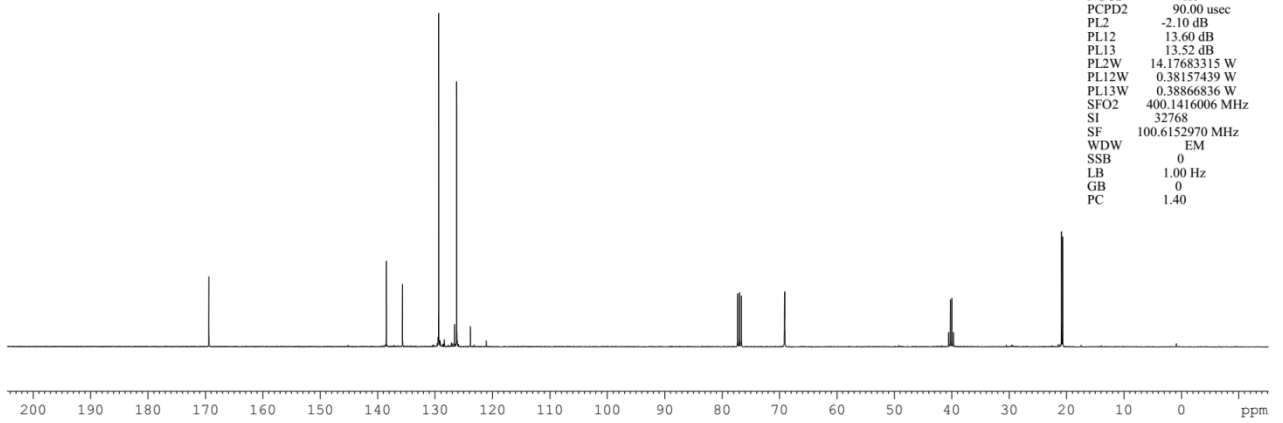
GCH-I-053-1 CDCl3

NAME	180502
EXPNO	5
PROCNO	1
Date_	20180502
Time	11.47
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	400
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	-1264.3 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.00 usec
PL1	-2.00 dB
PL1W	53.74446869 W
SFO1	100.6253446 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.10 dB
PL12	13.60 dB
PL13	13.52 dB
PL2W	14.17683315 W
PL12W	0.38157439 W
PL13W	0.38866836 W
SFO2	400.1416006 MHz
SI	32768
SF	100.6152970 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

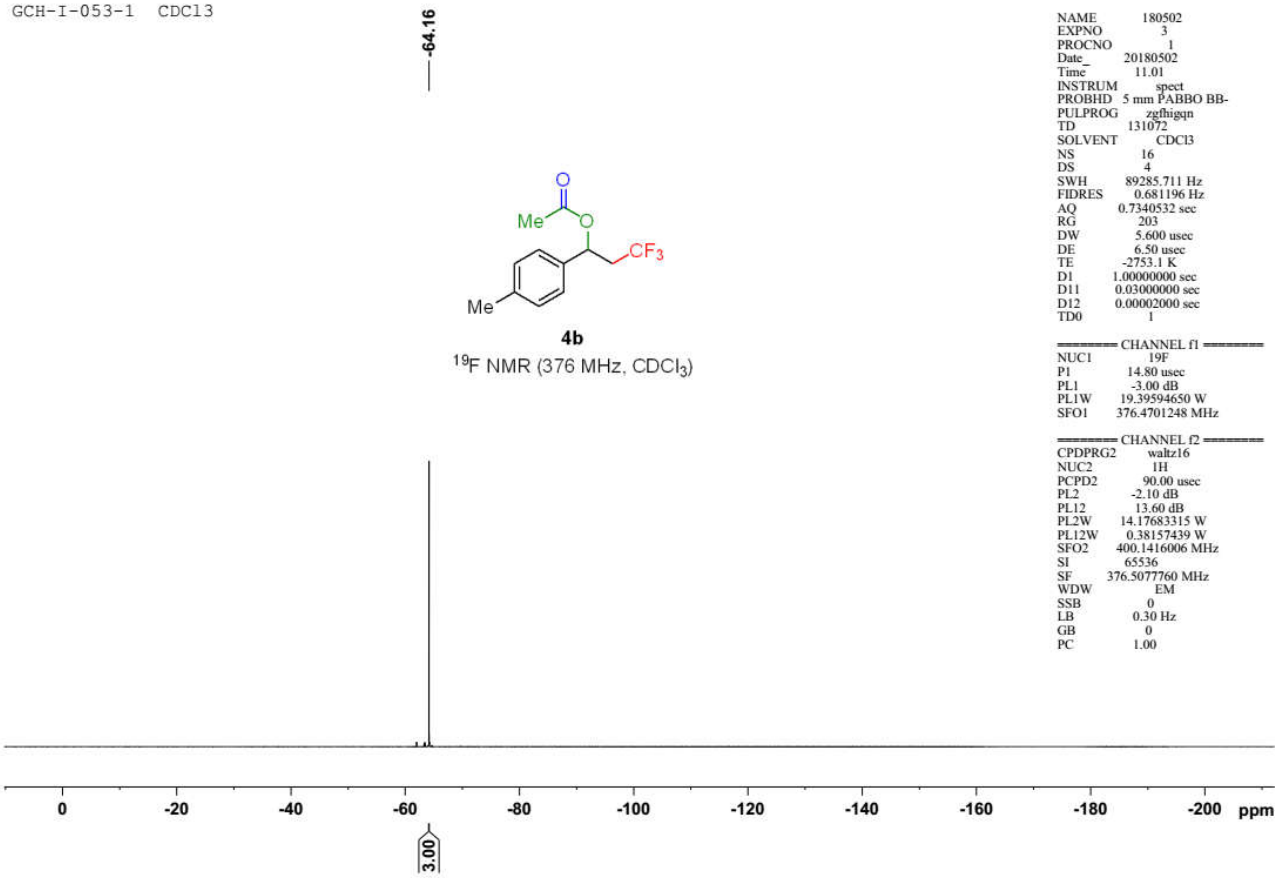


4b

^{13}C NMR (100 MHz, $CDCl_3$)



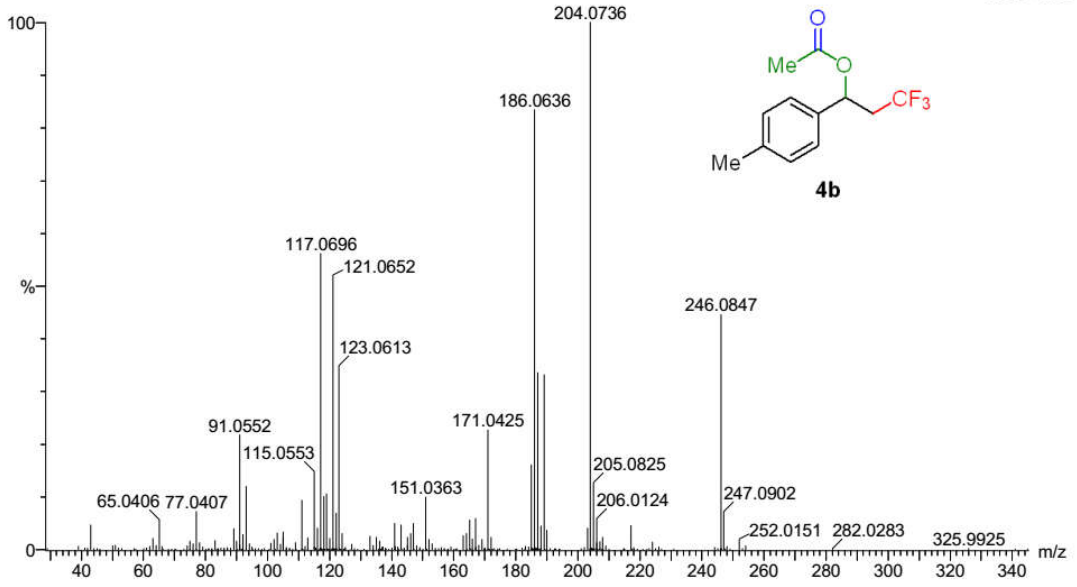
GCH-I-053-1 CDCl3




```
NAME          180502
EXPNO              3
PROCNO             1
Date_       20180502
Time           11.01
INSTRUM         spect
PROBHD  5 mm PABBO BB-
PULPROG       zgfhigqn
TD           131072
SOLVENT         CDCl3
NS                16
DS                 4
SWH        89285.711 Hz
FIDRES       0.681196 Hz
AQ          0.7340532 sec
RG                203
DW            5.600 usec
DE            6.50 usec
TE           -2753.1 K
D1         1.00000000 sec
D11        0.03000000 sec
D12        0.00002000 sec
TD0                1

======== CHANNEL f1 ========
NUC1             19F
P1           14.80 usec
PL1           -3.00 dB
PL1W      19.39594650 W
SFO1      376.4701248 MHz

======== CHANNEL f2 ========
CPDPRG2       waltz16
NUC2              1H
PCPD2        90.00 usec
PL2           -2.10 dB
PL12          13.60 dB
PL2W      14.17683315 W
PL12W      0.38157439 W
SFO2      400.1416006 MHz
SI             65536
SF        376.5077760 MHz
WDW              EM
SSB               0
LB             0.30 Hz
GB                0
PC             1.00
```

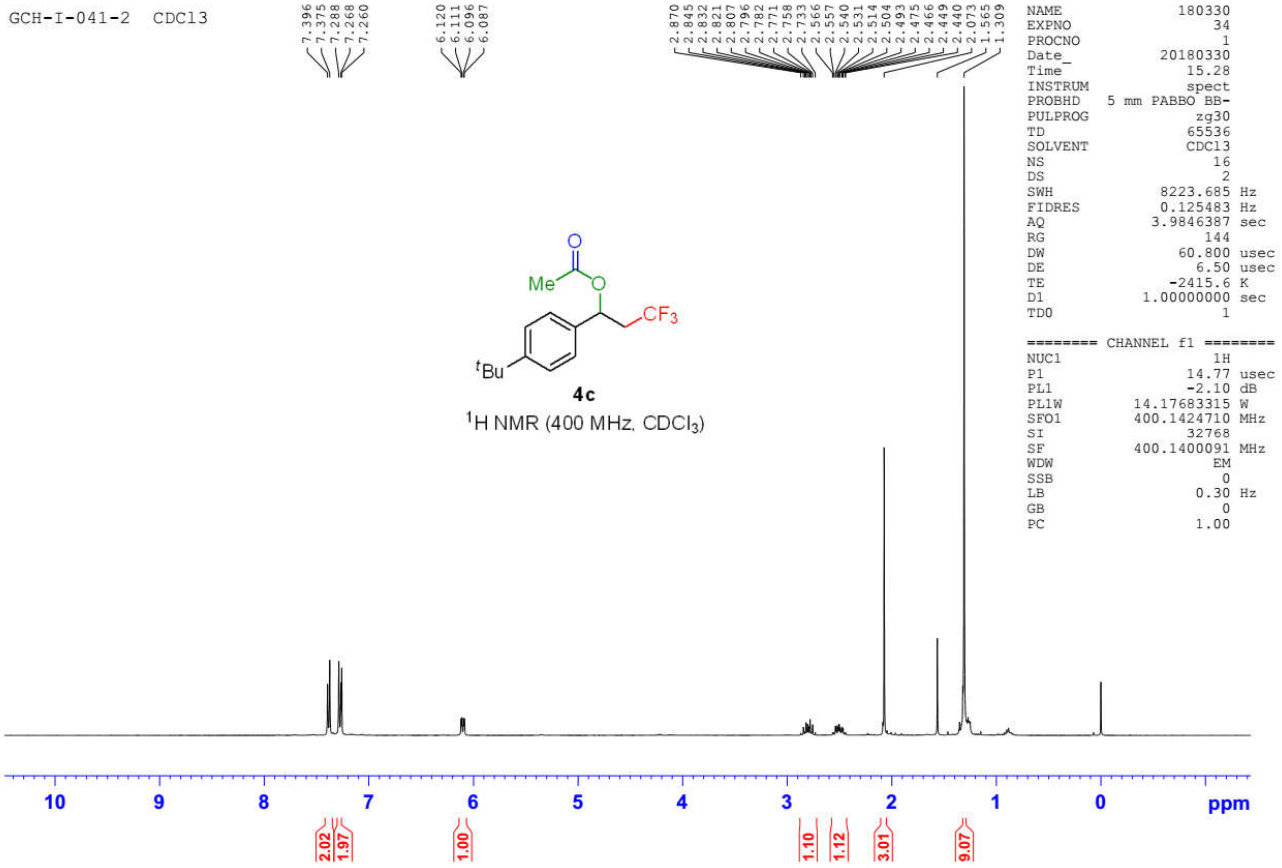
Monoisotopic Mass, Odd and Even Electron Ions
40 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 10-13 H: 0-60 O: 0-5 F: 0-3
default file
GCH-H-180504 788 (7.262) Cm (787:788-780:783)

TOF MS EI+
6.66e+003



Minimum:				-1.5		
Maximum:		5.0	10.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
246.0847	246.0868	-2.1	-8.5	5.0	4.5	C12 H13 O2 F3

GCH-I-041-2 CDCl3



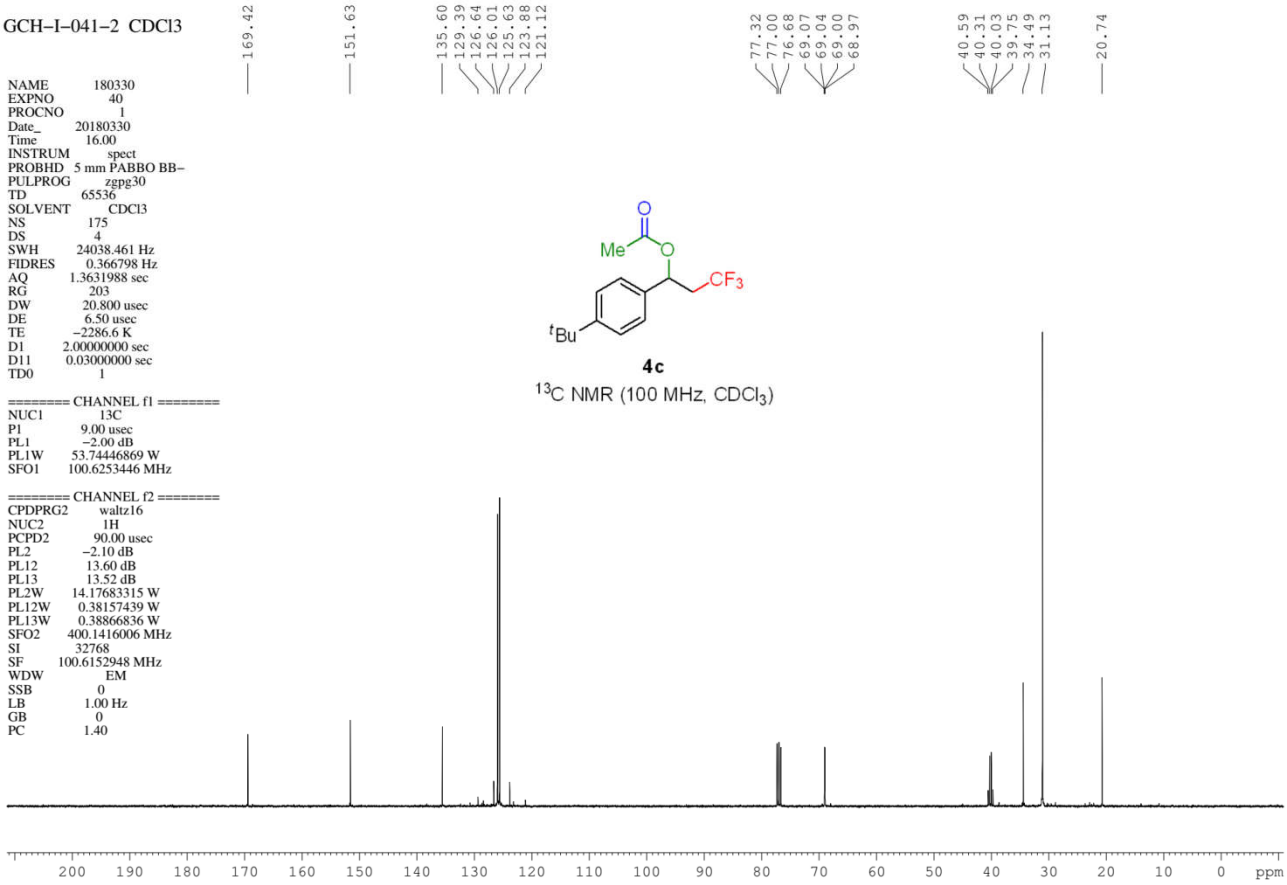
NAME 180330
EXPNO 34
PROCNO 1
Date_ 20180330
Time 15.28
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 144
DW 60.800 usec
DE 6.50 usec
TE -2415.6 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.77 usec
PL1 -2.10 dB
PL1W 14.17683315 W
SFO1 400.1424710 MHz
SI 32768
SF 400.1400091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

4c

^{1}H NMR (400 MHz, $CDCl_3$)

GCH-I-041-2 CDCl3



NAME 180330
EXPNO 40
PROCNO 1
Date_ 20180330
Time 16.00
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 175
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE -2286.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

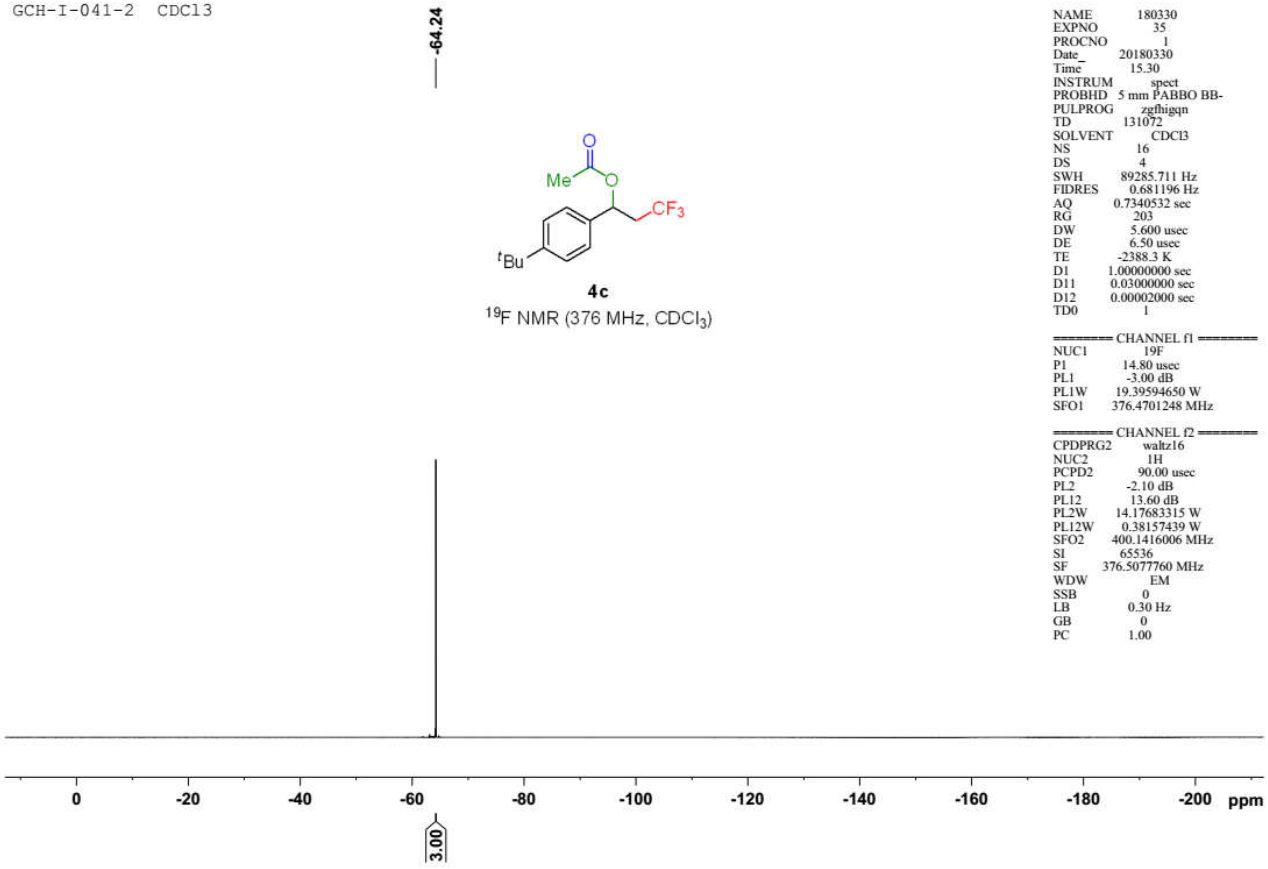
======== CHANNEL f1 ========
NUC1 13C
P1 9.00 usec
PL1 -2.00 dB
PL1W 53.74446869 W
SFO1 100.6253446 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.10 dB
PL12 13.60 dB
PL13 13.52 dB
PL2W 14.17683315 W
PL12W 0.38157439 W
PL13W 0.38866836 W
SFO2 400.1416006 MHz
SI 32768
SF 100.6152948 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

4c

^{13}C NMR (100 MHz, $CDCl_3$)

GCH-I-041-2 CDCl3



NAME	180330
EXPNO	35
PROCNO	1
Date_	20180330
Time	15.30
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgfhigqn
TD	131072
SOLVENT	CDCl3
NS	16
DS	4
SWH	89285.711 Hz
FIDRES	0.681196 Hz
AQ	0.7340532 sec
RG	203
DW	5.600 usec
DE	6.50 usec
TE	-2388.3 K
D1	1.00000000 sec
D11	0.03000000 sec
D12	0.00002000 sec
TD0	1

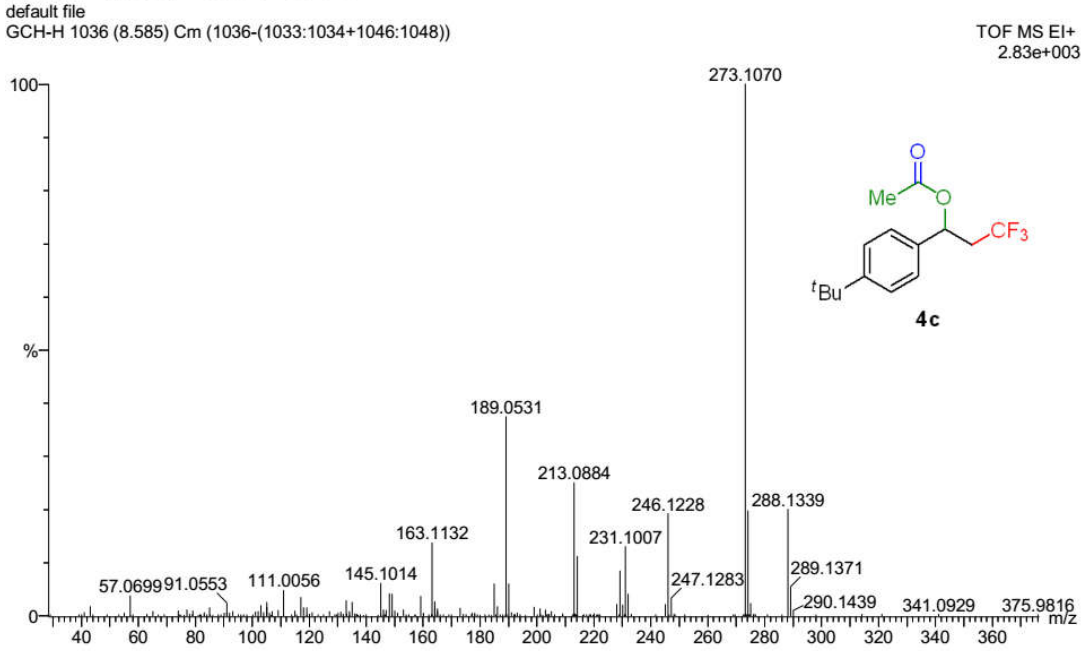
======== CHANNEL f1 ========

NUC1	19F
P1	14.80 usec
PL1	-3.00 dB
PL1W	19.39594650 W
SFO1	376.4701248 MHz

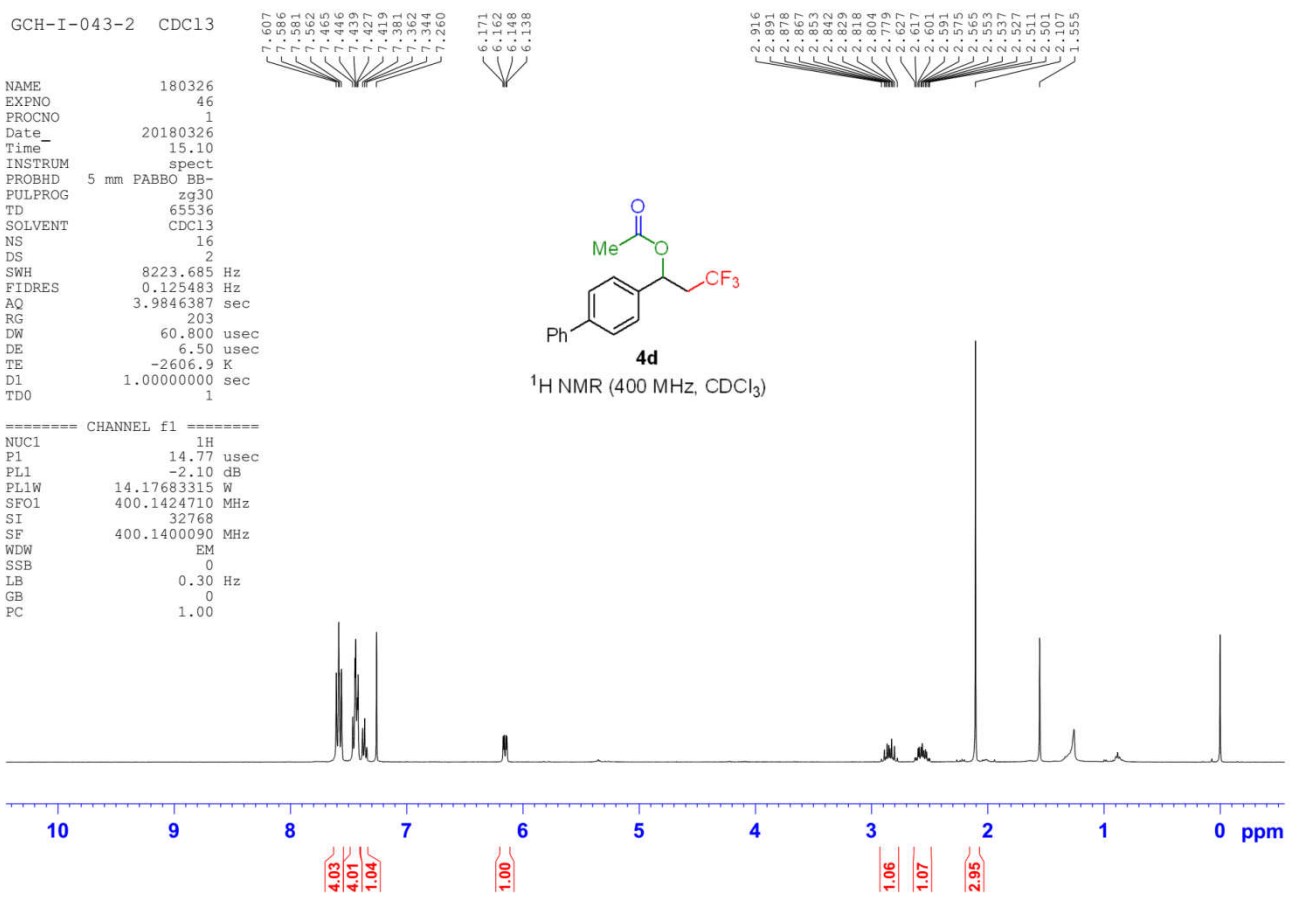
======== CHANNEL f2 ========

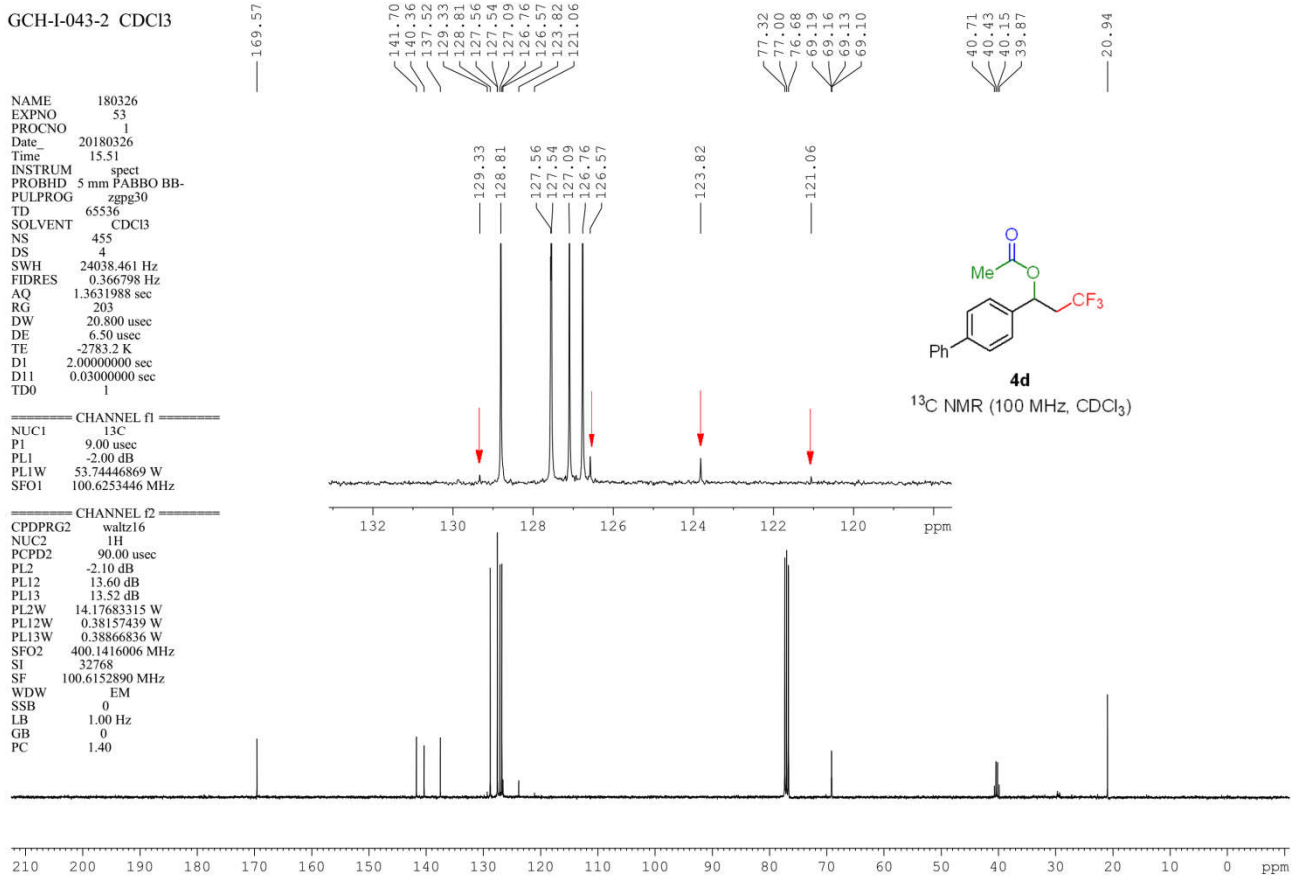
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.10 dB
PL12	13.60 dB
PL2W	14.17683315 W
PL12W	0.38157439 W
SFO2	400.1416006 MHz
SI	65536
SF	376.5077760 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

Monoisotopic Mass, Odd and Even Electron Ions
17 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-50 O: 0-4 F: 3-3
default file
GCH-H 1036 (8.585) Cm (1036-(1033:1034+1046:1048))

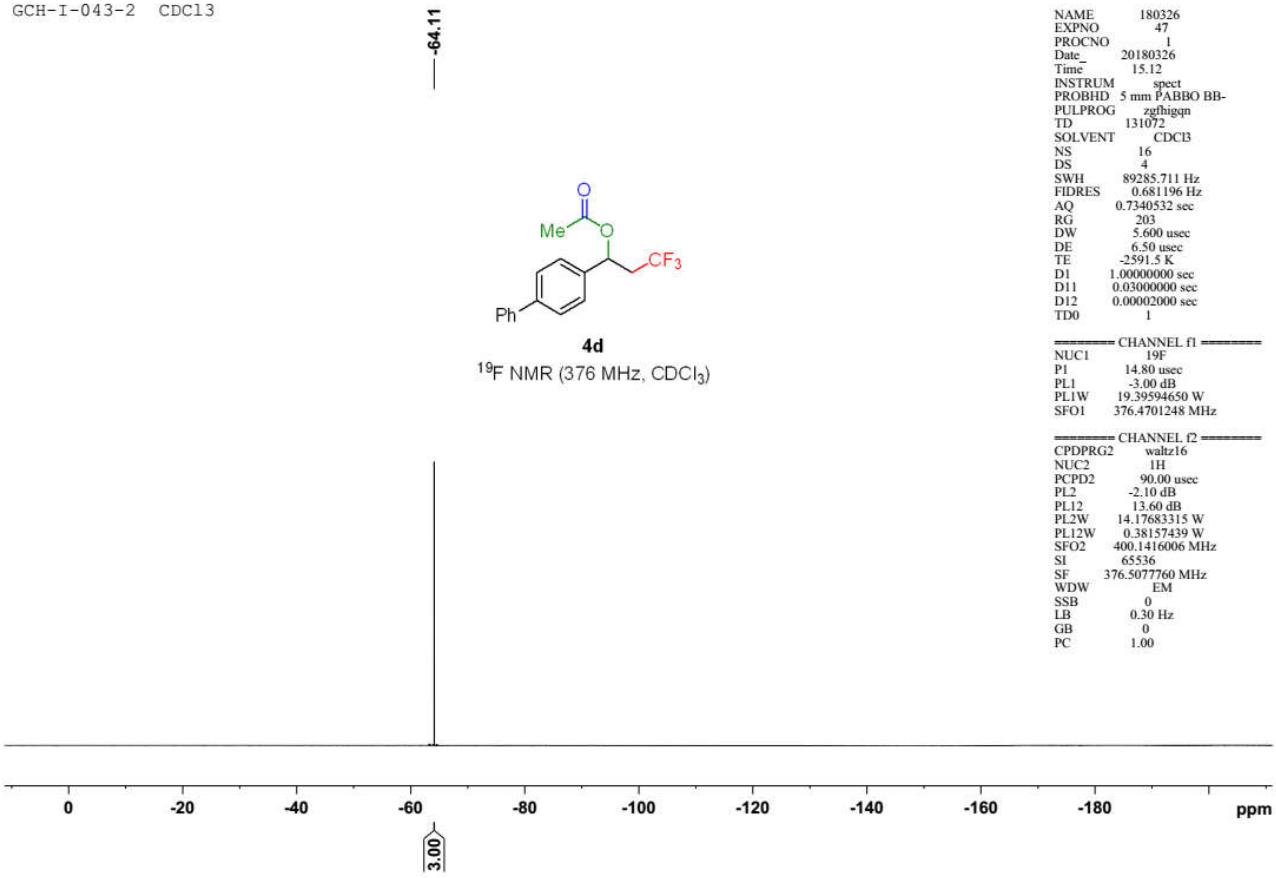


Minimum:				-1.5		
Maximum:		5.0	10.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
288.1339	288.1337	0.2	0.7	5.0	11.9	C15 H19 O2 F3


GCH-I-043-2 CDCl3
7.607
7.586
7.581
7.562
7.465
7.446
7.439
7.427
7.419
7.381
7.362
7.344
7.260
6.171
6.162
6.148
6.138
2.916
2.891
2.878
2.867
2.853
2.842
2.829
2.818
2.804
2.779
2.627
2.617
2.601
2.591
2.575
2.565
2.553
2.537
2.527
2.511
2.501
2.107
1.555
NAME 180326
EXPNO 46
PROCNO 1
Date_ 20180326
Time 15.10
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE -2606.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.77 usec
PL1 -2.10 dB
PL1W 14.17683315 W
SFO1 400.1424710 MHz
SI 32768
SF 400.1400090 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Me
O
O
CF3
Ph
4d
1H NMR (400 MHz, CDCl3)
10 9 8 7 6 5 4 3 2 1 0 ppm
4.03
4.01
1.04
1.00
1.06
1.07
2.95


GCH-I-043-2 CDCl3
169.57
141.70
140.36
137.52
129.33
128.81
127.56
127.54
127.09
126.76
126.57
123.82
121.06
77.32
77.00
76.68
69.19
69.16
69.13
69.10
40.71
40.43
40.15
39.87
20.94
NAME 180326
EXPNO 53
PROCNO 1
Date_ 20180326
Time 15.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 455
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE -2783.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.00 usec
PL1 -2.00 dB
PL1W 53.74446869 W
SFO1 100.6253446 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.10 dB
PL12 13.60 dB
PL13 13.52 dB
PL2W 14.17683315 W
PL12W 0.38157439 W
PL13W 0.38866836 W
SFO2 400.1416006 MHz
SI 32768
SF 100.6152890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
129.33
128.81
127.56
127.54
127.09
126.76
126.57
123.82
121.06
132 130 128 126 124 122 120 ppm
Me
O
O
CF3
Ph
4d
13C NMR (100 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

GCH-I-043-2 CDCl3

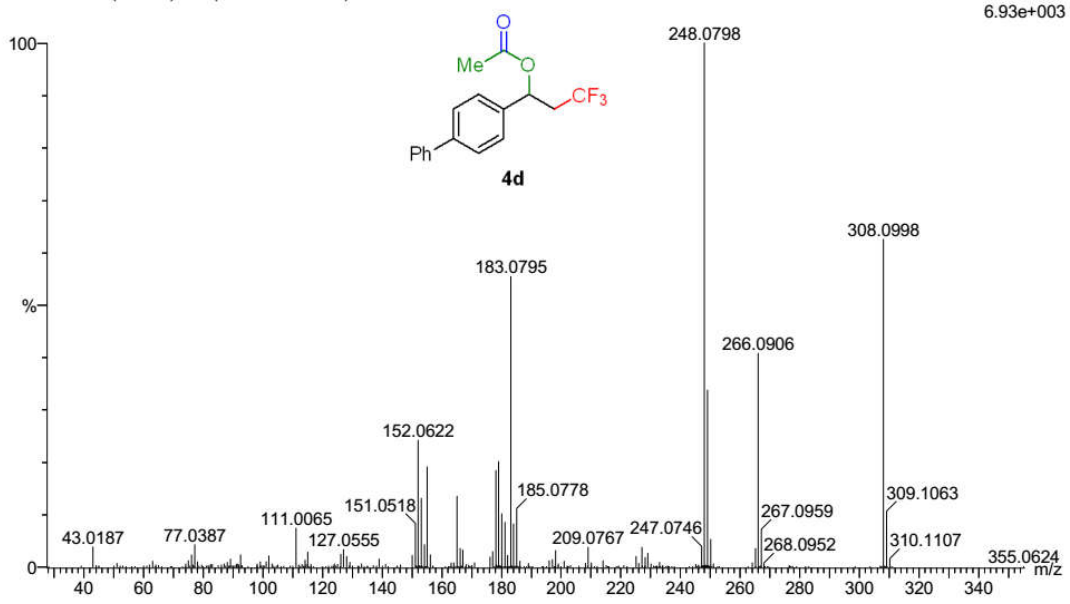


NAME	180326
EXPNO	47
PROCNO	1
Date_	20180326
Time	15.12
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgfhigqn
TD	131072
SOLVENT	CDCl3
NS	16
DS	4
SWH	89285.711 Hz
FIDRES	0.681196 Hz
AQ	0.7340532 sec
RG	203
DW	5.600 usec
DE	6.50 usec
TE	-2591.5 K
D1	1.00000000 sec
D11	0.03000000 sec
D12	0.00002000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	19F
P1	14.80 usec
PL1	-3.00 dB
PL1W	19.39594650 W
SFO1	376.4701248 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.10 dB
PL12	13.60 dB
PL2W	14.17683315 W
PL12W	0.38157439 W
SFO2	400.1416006 MHz
SI	65536
SF	376.5077760 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

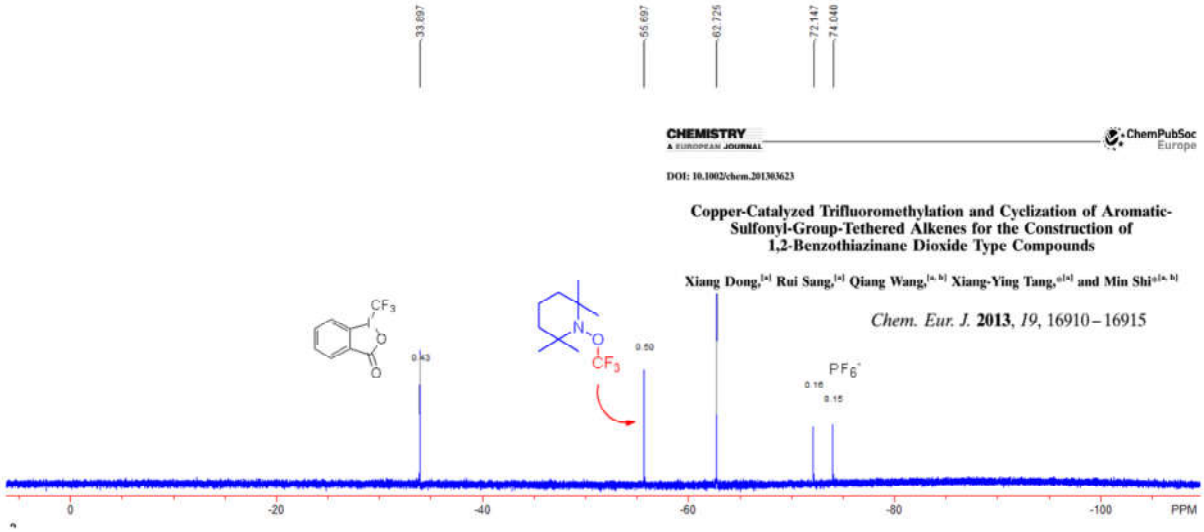
Monoisotopic Mass, Odd and Even Electron Ions
18 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-30 H: 0-50 O: 0-4 F: 3-3

default file
GCH-H 1490 (11.007) Cm (1490-1485:1487)

TOF MS EI+
6.93e+003



Minimum:				-1.5		
Maximum:		5.0	10.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
308.0998	308.1024	-2.6	-8.4	9.0	7.9	C17 H15 O2 F3

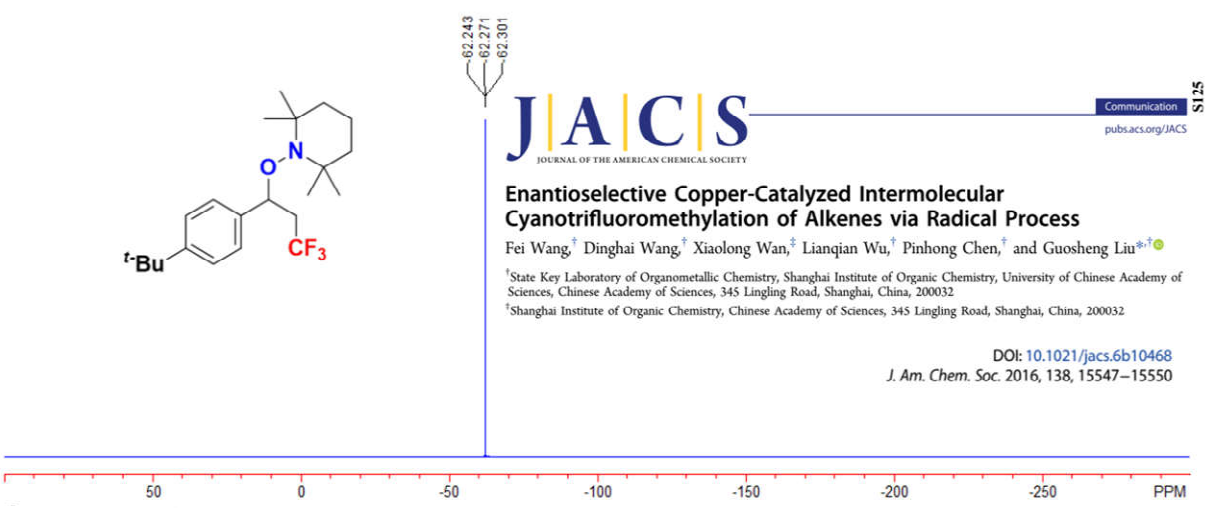


CHEMISTRY
A EUROPEAN JOURNAL
ChemPubSoc Europe
DOI: 10.1002/chem.201303623

Copper-Catalyzed Trifluoromethylation and Cyclization of Aromatic-Sulfonyl-Group-Tethered Alkenes for the Construction of 1,2-Benzothiazinane Dioxide Type Compounds

Xiang Dong,[a] Rui Sang,[a] Qiang Wang,[a, b] Xiang-Ying Tang,*[a] and Min Shi*[a, b]

Chem. Eur. J. **2013**, *19*, 16910 – 16915



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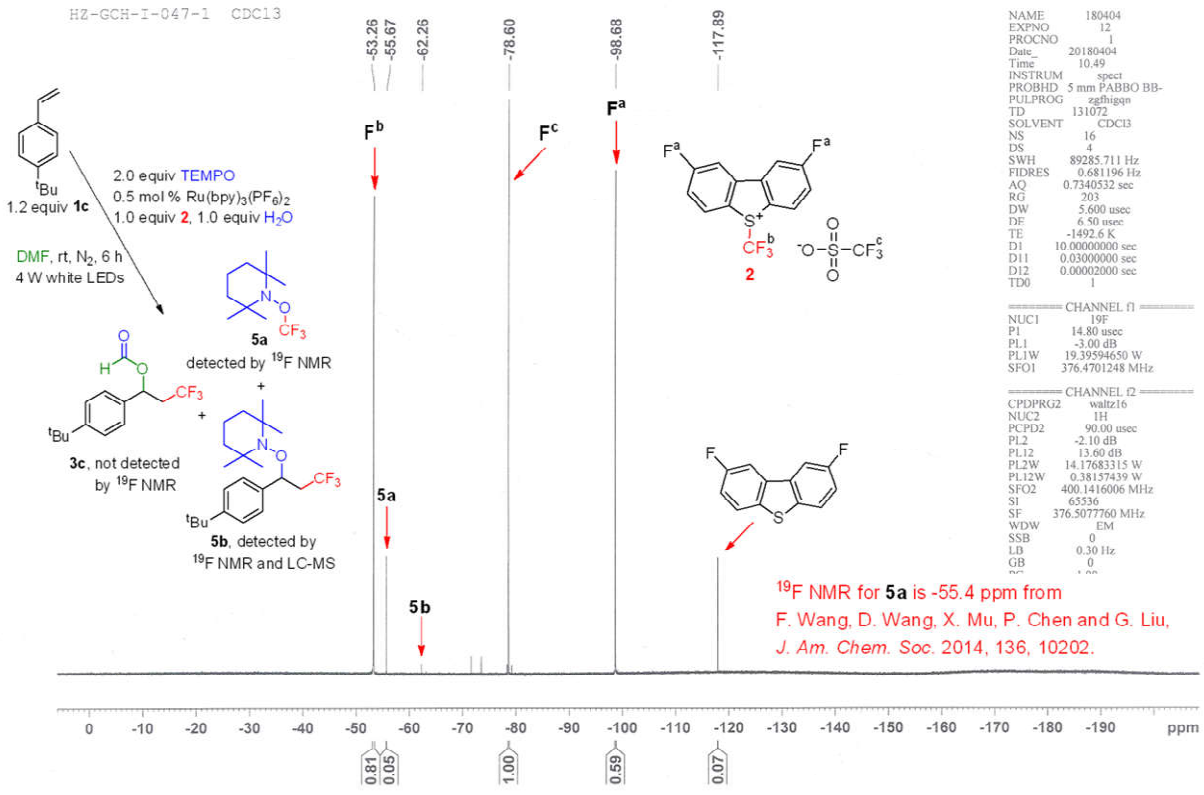
Enantioselective Copper-Catalyzed Intermolecular Cyanotrifluoromethylation of Alkenes via Radical Process

Fei Wang,[†] Dinghai Wang,[†] Xiaolong Wan,[‡] Lianqian Wu,[†] Pinhong Chen,[†] and Guosheng Liu*[,†]

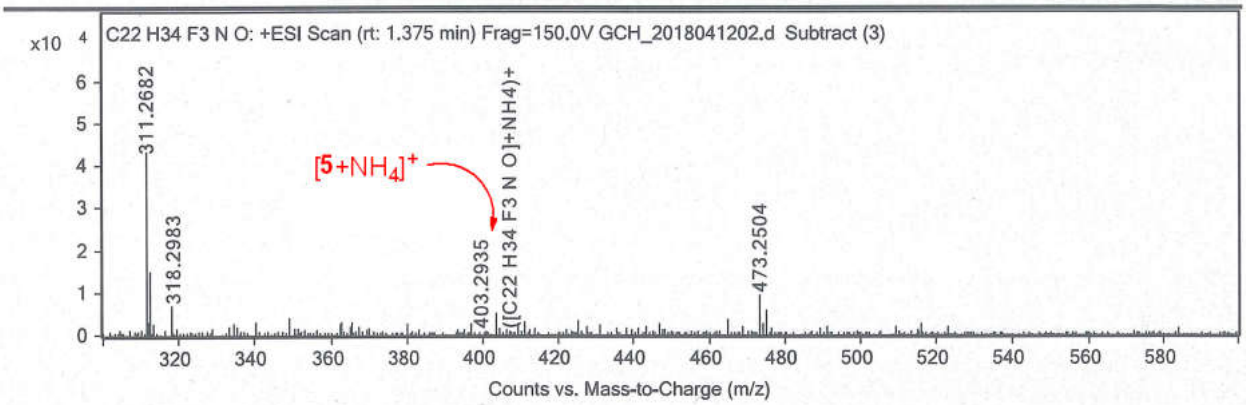
[†]State Key Laboratory of Organometallic Chemistry, Shanghai Institute of Organic Chemistry, University of Chinese Academy of Sciences, Chinese Academy of Sciences, 345 Lingling Road, Shanghai, China, 200032

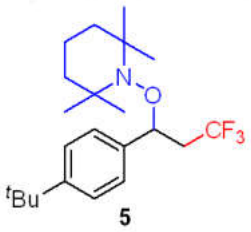
[‡]Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, 345 Lingling Road, Shanghai, China, 200032

DOI: 10.1021/jacs.6b10468
J. Am. Chem. Soc. 2016, 138, 15547–15550



Qualitative Analysis Report



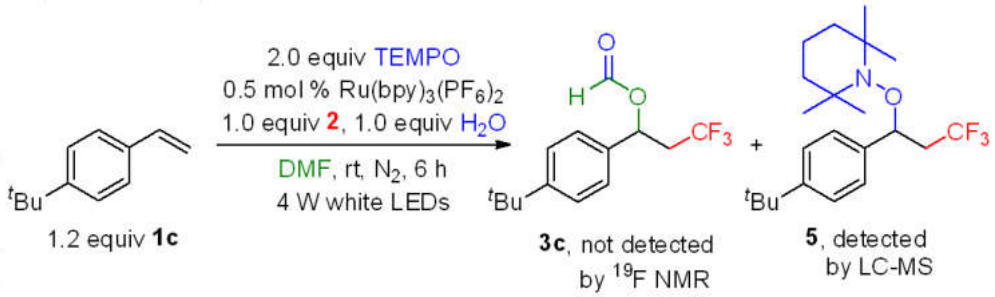


5

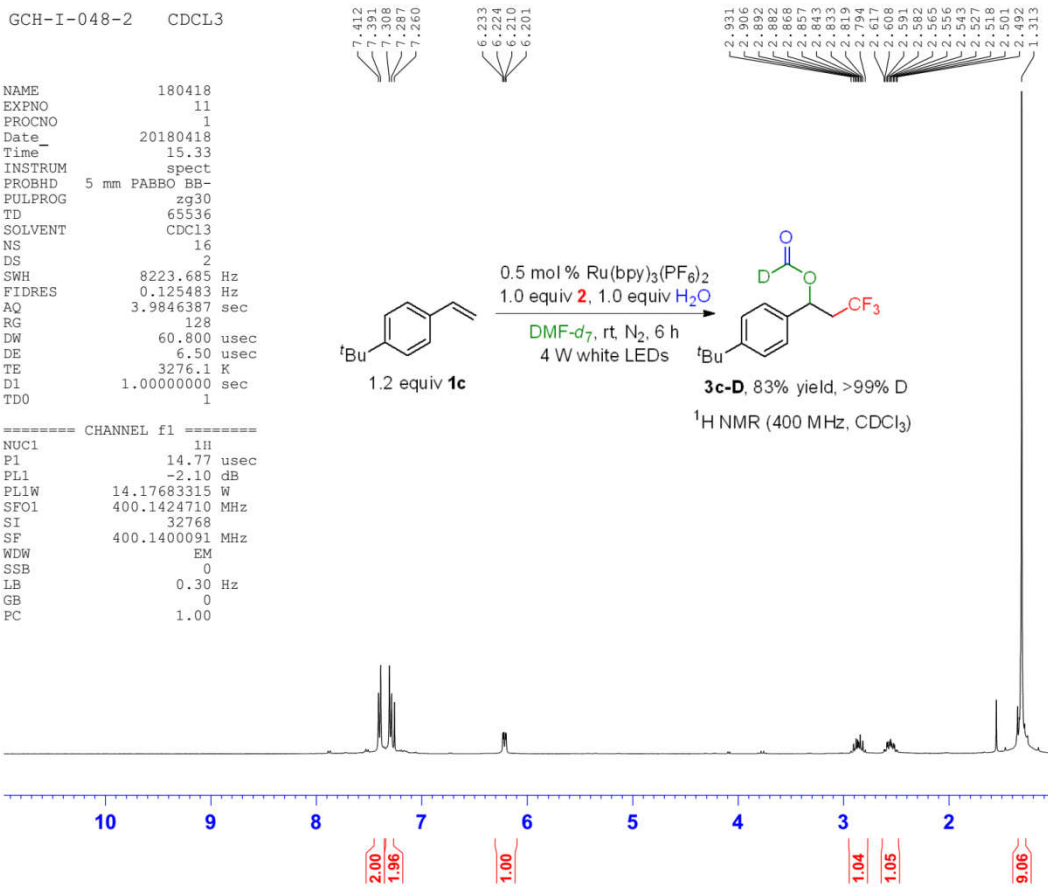
Chemical Formula: $C_{22}H_{34}F_3NO$
Exact Mass: 385.2592

$[\mathbf{5}+NH_4]^+$

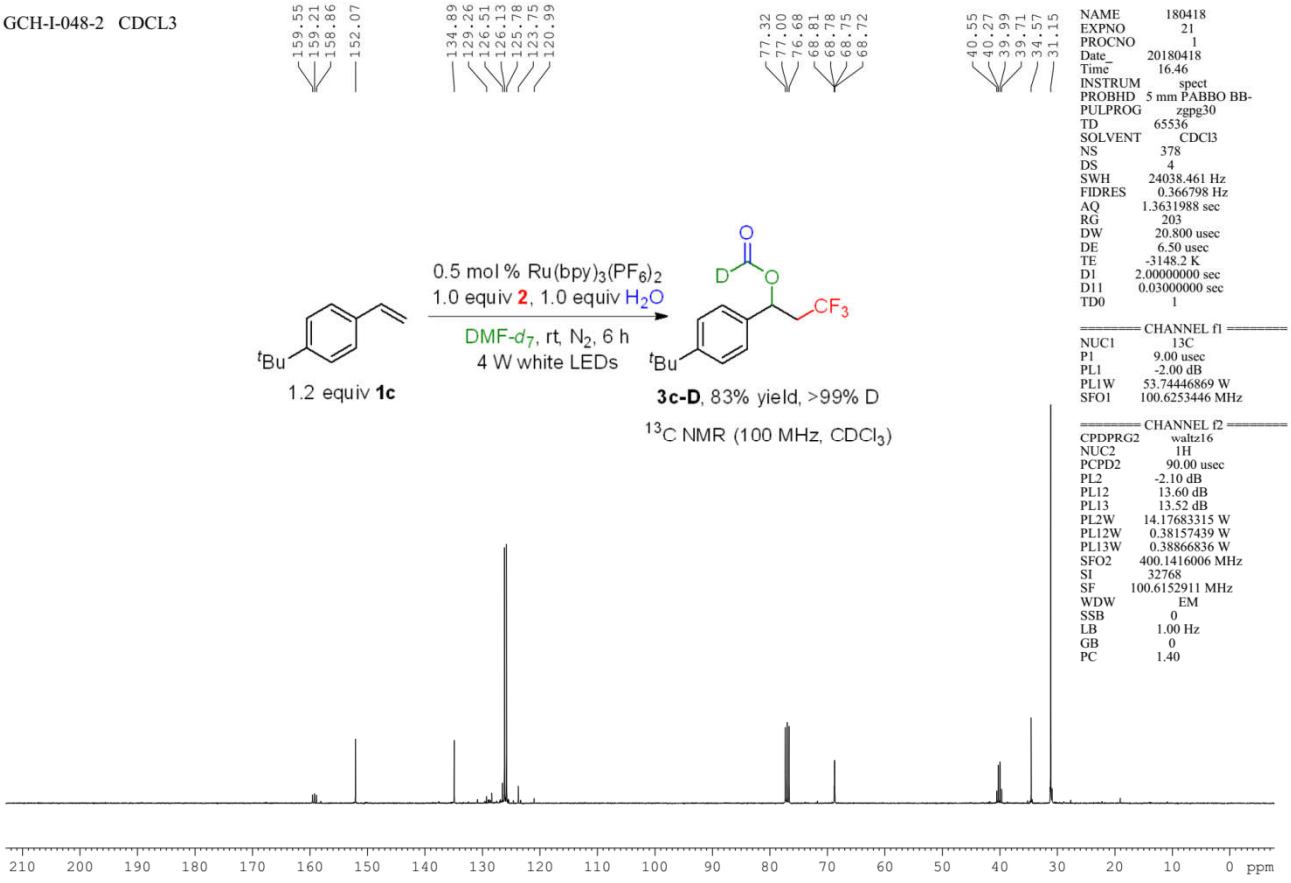
Chemical Formula: $C_{22}H_{38}F_3N_2O$
Exact Mass: 403.2931

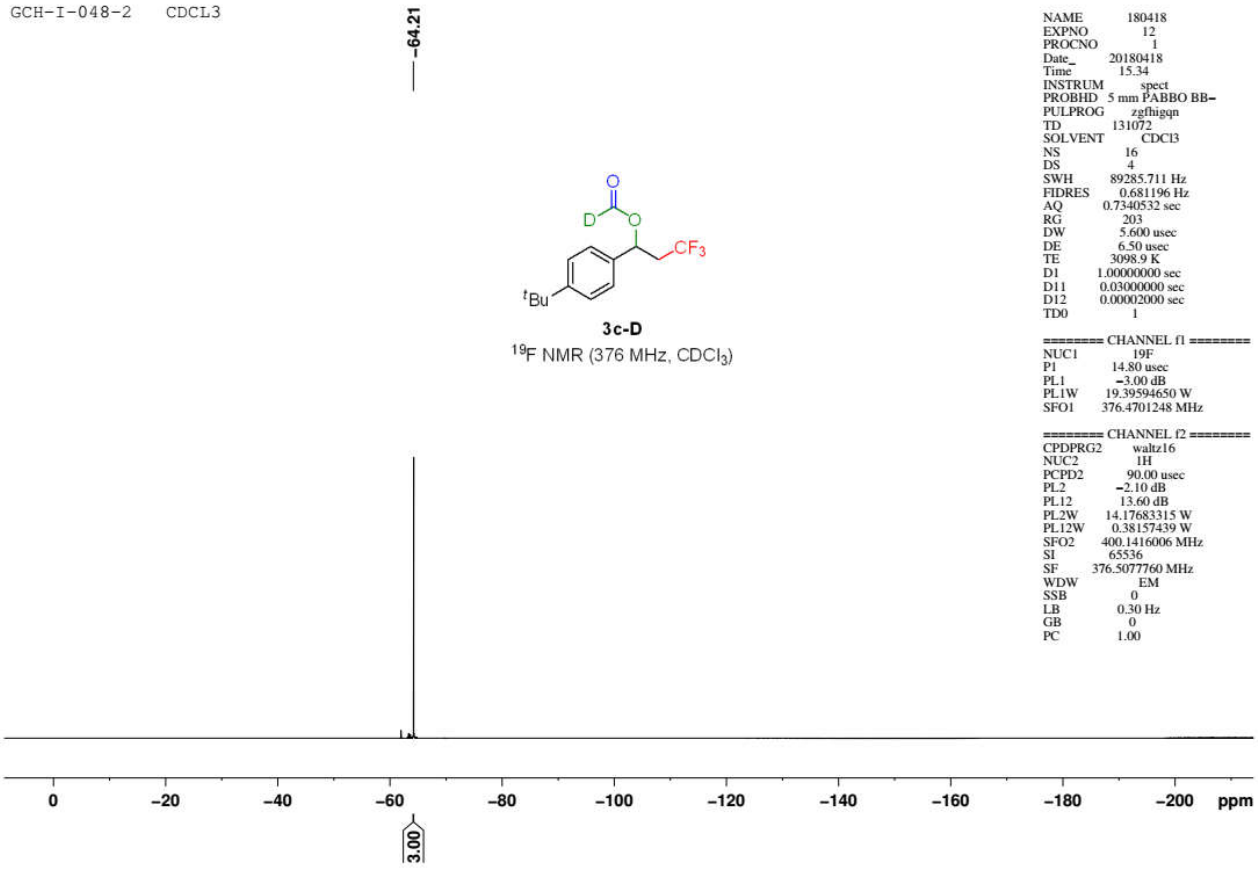


GCH-I-048-2 CDCL3



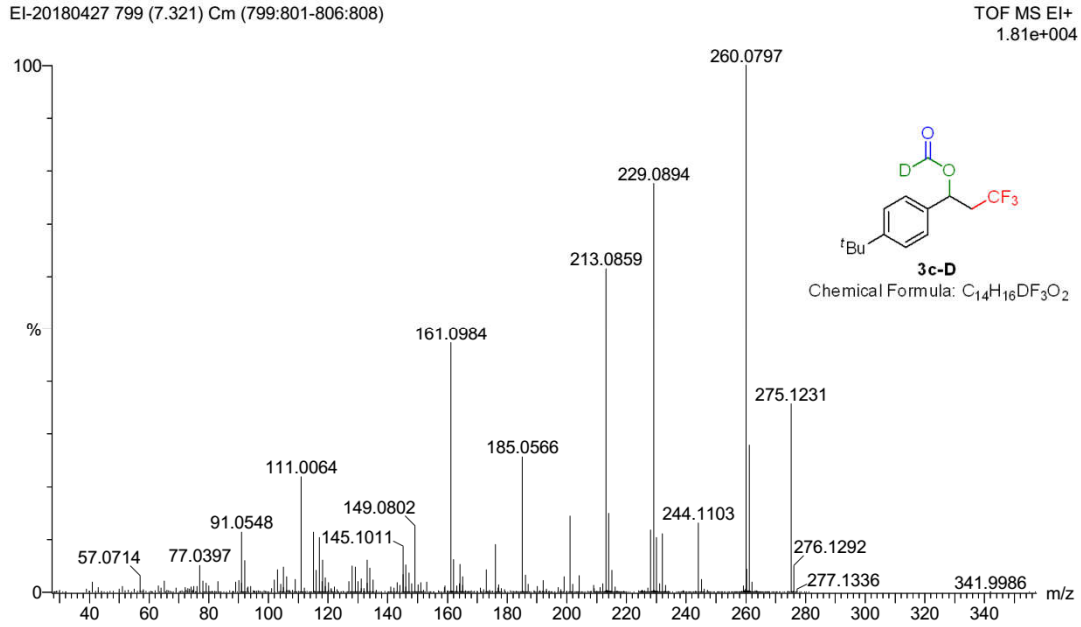
GCH-I-048-2 CDCL3



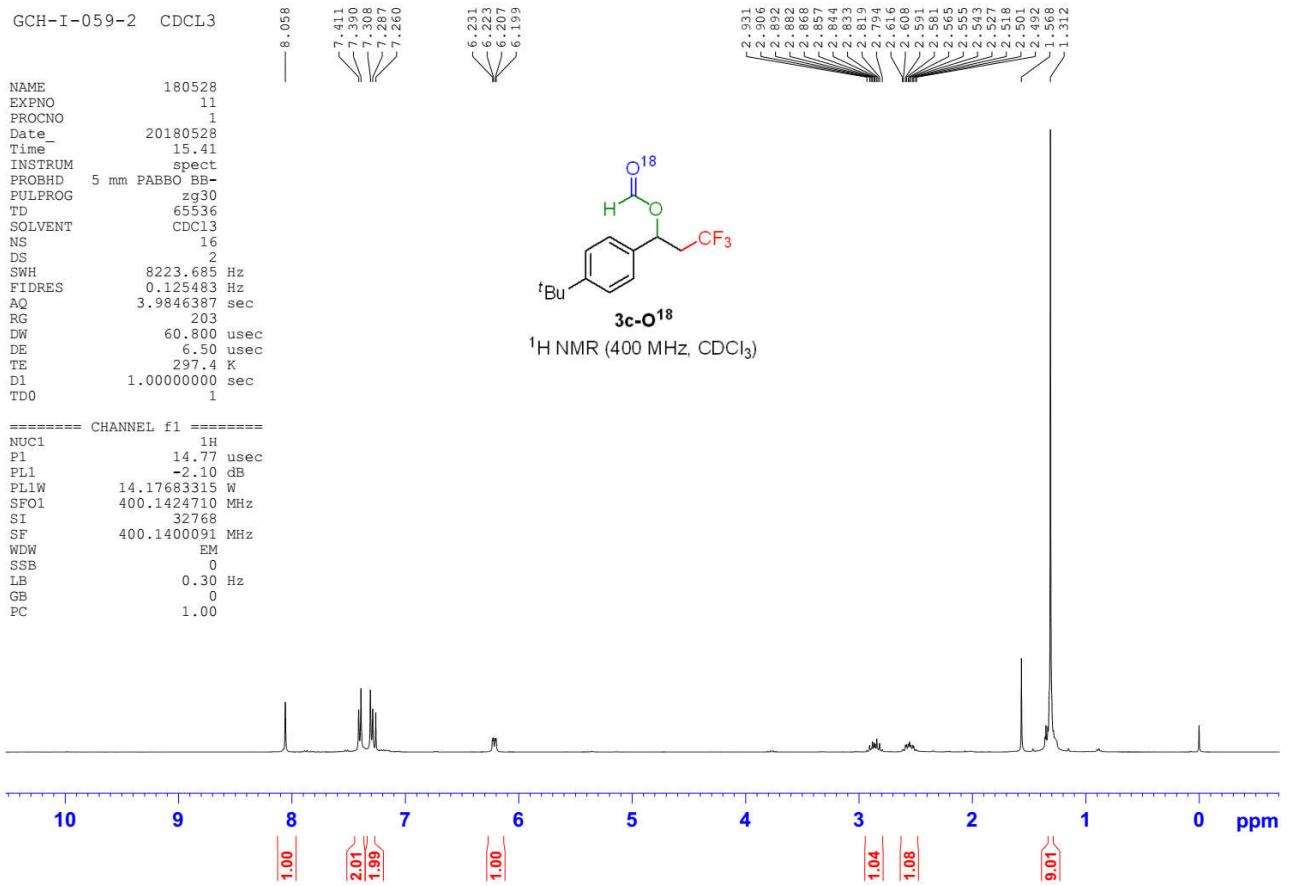


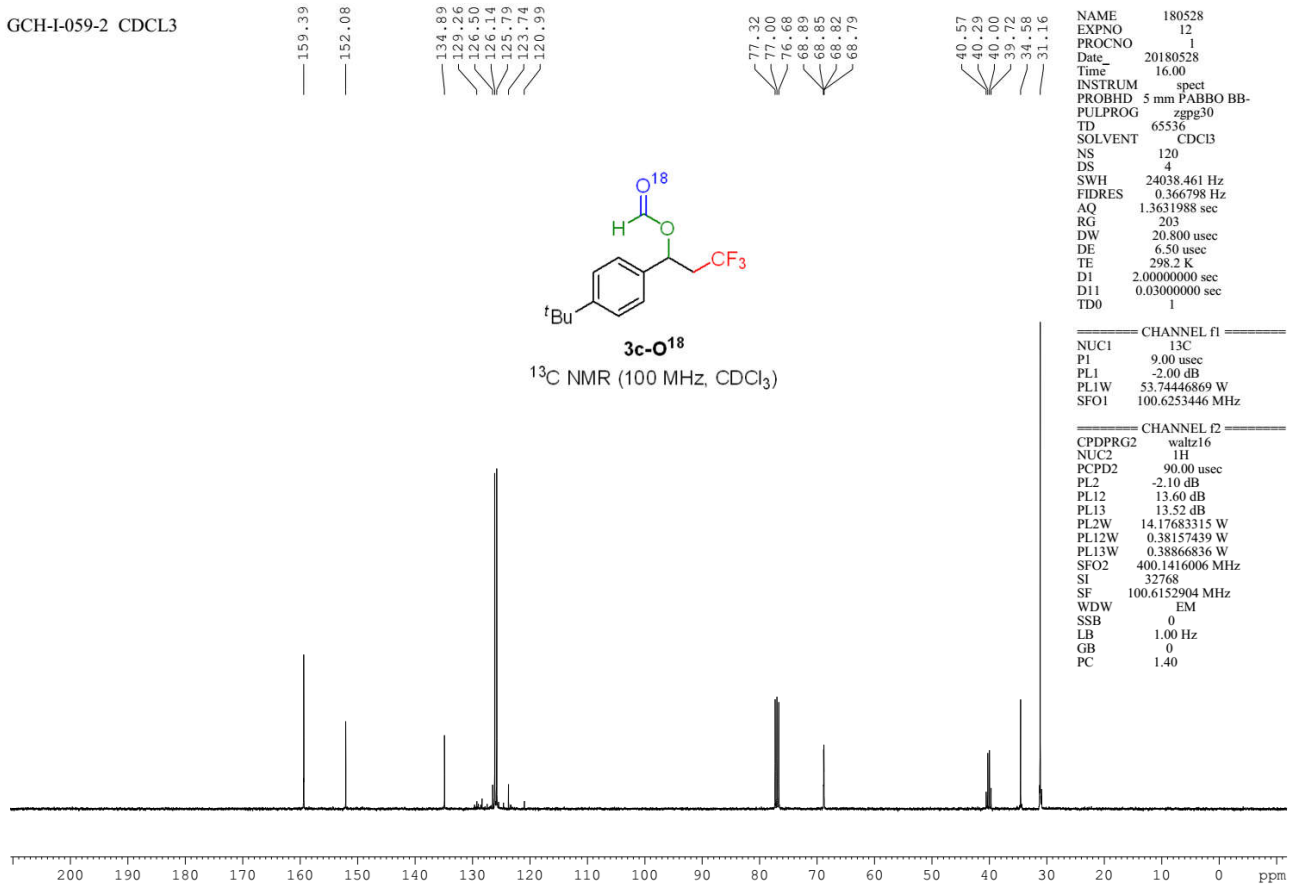
Monoisotopic Mass, Odd and Even Electron Ions
979 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 12-15 1H: 0-60 2H: 0-1 B: 0-1 O: 0-2 F: 0-3

default file
EI-20180427 799 (7.321) Cm (799:801-806:808)

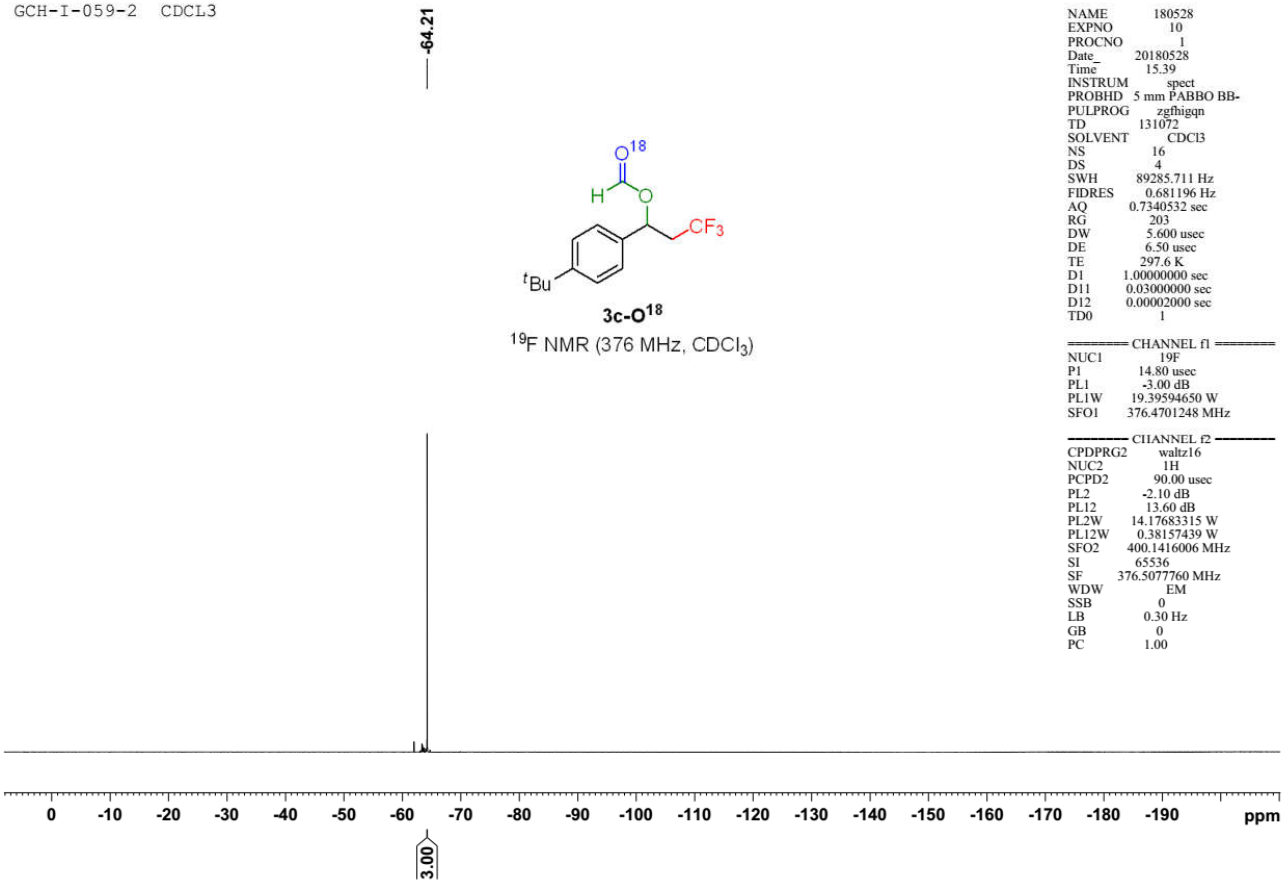


Minimum:				-1.5		
Maximum:		5.0	10.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
275.1231	275.1243	-1.2	-4.4	5.0	37.5	C14 1H16 2H O2 F3


GCH-I-059-2 CDCL3
8.058
7.411
7.390
7.308
7.287
7.260
6.231
6.223
6.207
6.199
2.931
2.906
2.892
2.882
2.868
2.857
2.844
2.833
2.819
2.794
2.616
2.608
2.591
2.581
2.565
2.555
2.543
2.527
2.518
2.501
2.492
1.568
1.312
NAME 180528
EXPNO 11
PROCNO 1
Date_ 20180528
Time 15.41
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 297.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.77 usec
PL1 -2.10 dB
PL1W 14.17683315 W
SFO1 400.1424710 MHz
SI 32768
SF 400.1400091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O18
H
O
CF3
tBu
3c-O18
1H NMR (400 MHz, CDCl3)
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
2.01
1.99
1.00
1.04
1.08
9.01


GCH-I-059-2 CDCL3
159.39
152.08
134.89
129.26
126.50
126.14
125.79
123.74
120.99
77.32
77.00
76.68
68.89
68.85
68.82
68.79
40.57
40.29
40.00
39.72
34.58
31.16
NAME 180528
EXPNO 12
PROCNO 1
Date_ 20180528
Time 16.00
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 120
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.00 usec
PL1 -2.00 dB
PL1W 53.74446869 W
SFO1 100.6253446 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.10 dB
PL12 13.60 dB
PL13 13.52 dB
PL2W 14.17683315 W
PL12W 0.38157439 W
PL13W 0.38866836 W
SFO2 400.1416006 MHz
SI 32768
SF 100.6152904 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O18
H
O
CF3
tBu
3c-O18
13C NMR (100 MHz, CDCl3)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

GCH-I-059-2 CDCL3



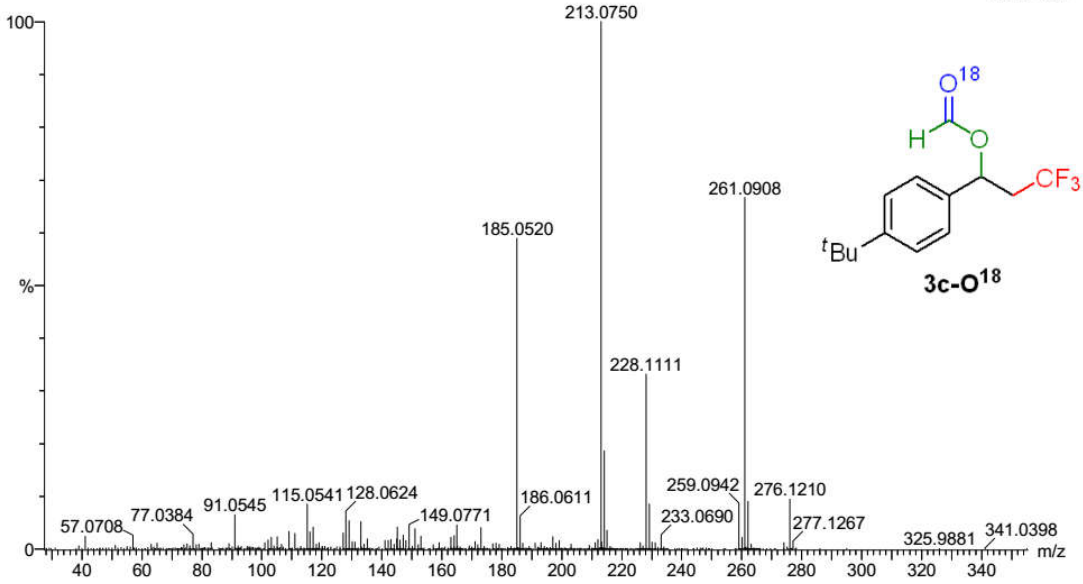
3c-O^{18}

^{19}F NMR (376 MHz, $CDCl_3$)

NAME	180528
EXPNO	10
PROCNO	1
Date_	20180528
Time	15.39
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgfhigqn
TD	131072
SOLVENT	CDCl3
NS	16
DS	4
SWH	89285.711 Hz
FIDRES	0.681196 Hz
AQ	0.7340532 sec
RG	203
DW	5.600 usec
DE	6.50 usec
TE	297.6 K
D1	1.00000000 sec
D11	0.03000000 sec
D12	0.00002000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	19F
P1	14.80 usec
PL1	-3.00 dB
PL1W	19.39594650 W
SFO1	376.4701248 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.10 dB
PL12	13.60 dB
PL2W	14.17683315 W
PL12W	0.38157439 W
SFO2	400.1416006 MHz
SI	65536
SF	376.5077760 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

Monoisotopic Mass, Odd and Even Electron Ions
243 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 12-30 H: 0-60 16O: 1-2 17O: 0-2 18O: 0-2 F: 1-8
default file
GCH-0529 981 (8.292) Cm (978:981-962:973)

TOF MS EI+
3.92e+004

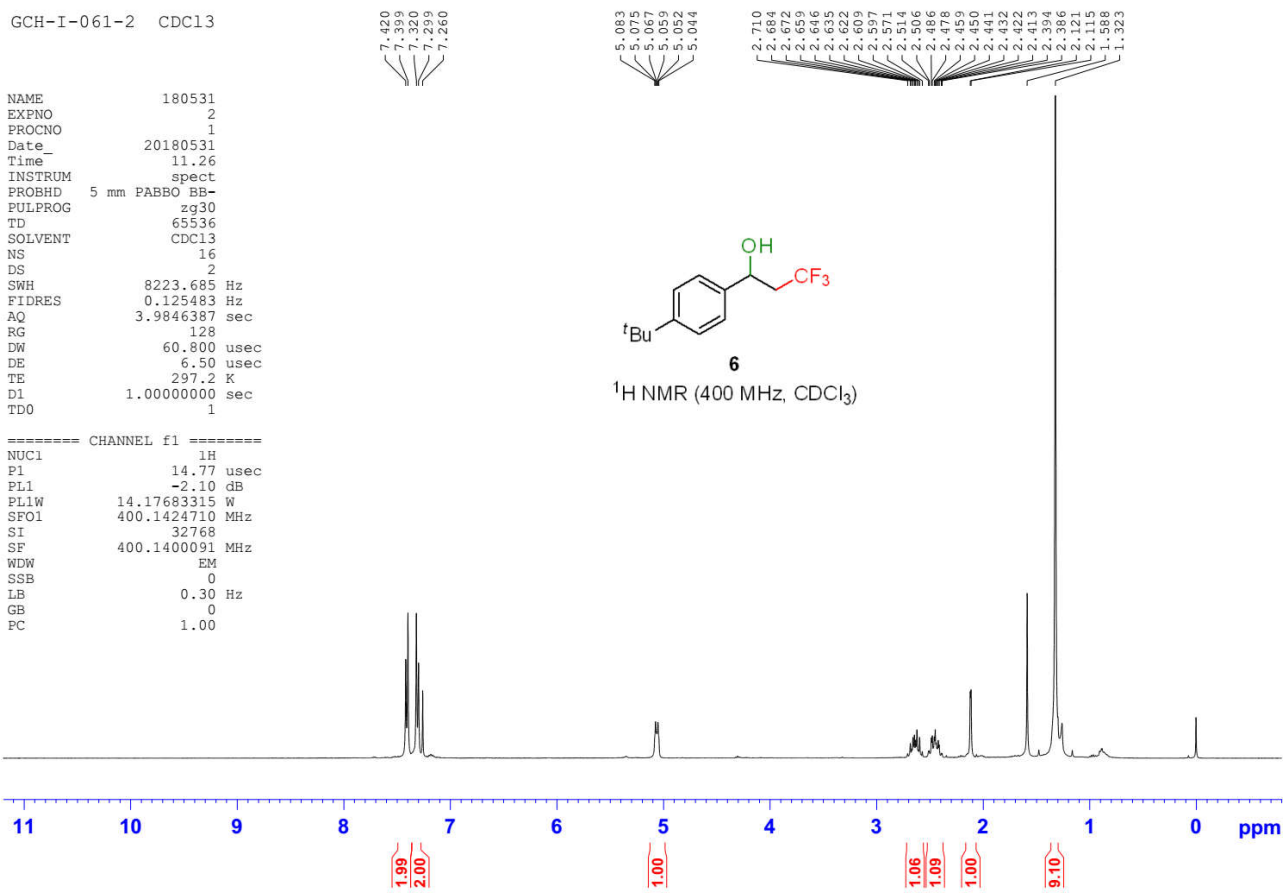


3c-O^{18}

Minimum:				-1.5		
Maximum:		5.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
276.1210	276.1223	-1.3	-4.7	5.0	63.3	C14 H17 160 180 F3

GCH-I-061-2 CDCl3

NAME	180531
EXPNO	2
PROCNO	1
Date_	20180531
Time	11.26
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	128
DW	60.800 usec
DE	6.50 usec
TE	297.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.77 usec
PL1	-2.10 dB
PL1W	14.17683315 W
SFO1	400.1424710 MHz
SI	32768
SF	400.1400091 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

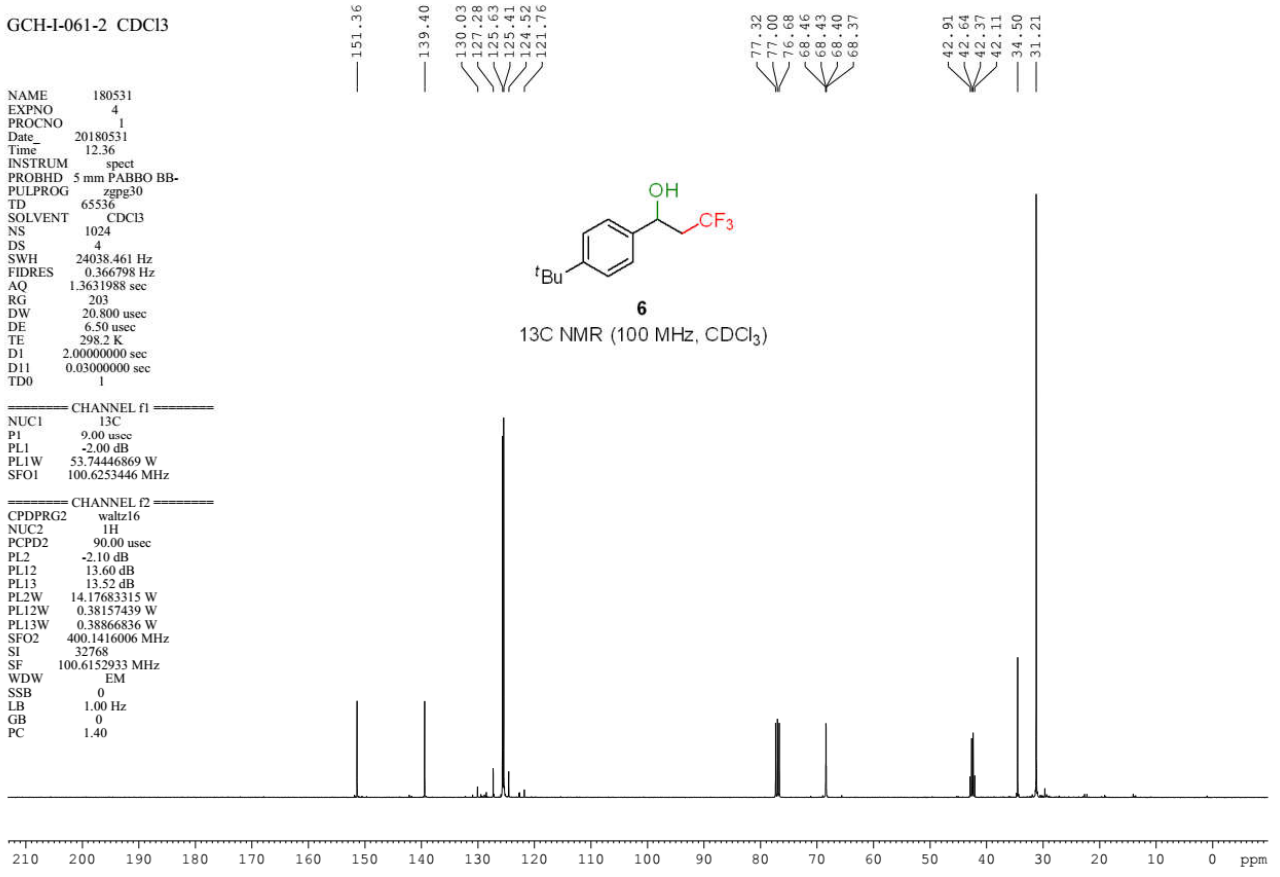


6

^{1}H NMR (400 MHz, $CDCl_3$)

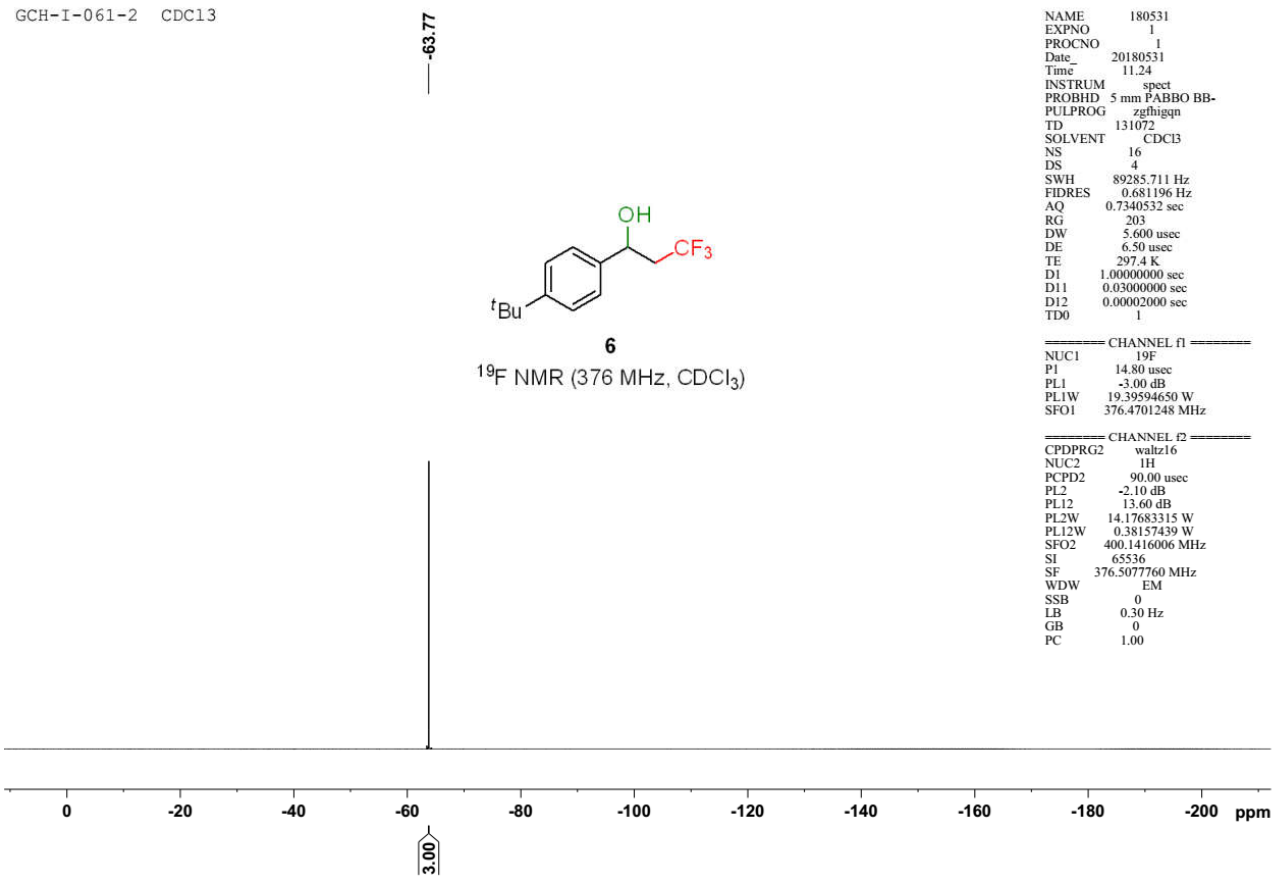
GCH-I-061-2 CDCl3

NAME	180531
EXPNO	4
PROCNO	1
Date_	20180531
Time	12.36
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	203
DW	20.800 usec
DE	6.50 usec
TE	298.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.00 usec
PL1	-2.00 dB
PL1W	53.74446869 W
SFO1	100.6253446 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.10 dB
PL12	13.60 dB
PL13	13.52 dB
PL2W	14.17683315 W
PL12W	0.38157439 W
PL13W	0.38866836 W
SFO2	400.1416006 MHz
SI	32768
SF	100.6152933 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

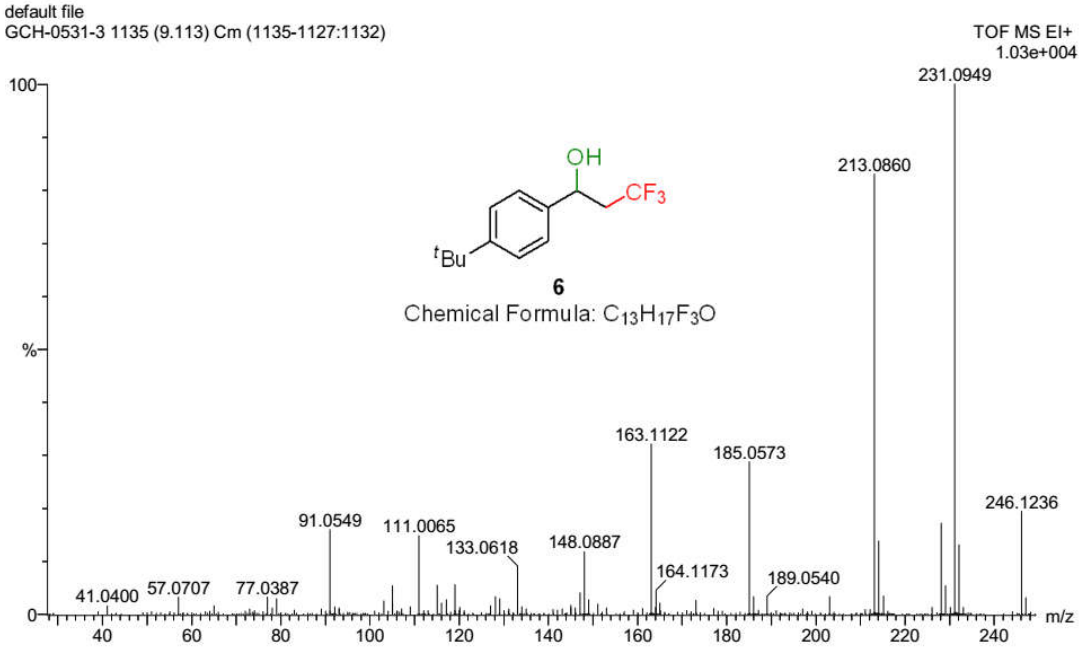


6

13C NMR (100 MHz, $CDCl_3$)



Monoisotopic Mass, Odd and Even Electron Ions
88 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 5-30 H: 0-60 O: 0-4 F: 1-8
default file
GCH-0531-3 1135 (9.113) Cm (1135-1127:1132)



Minimum:				-1.5		
Maximum:		5.0	2.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
246.1236	246.1232	0.4	1.6	4.0	1.1	C13 H17 O F3