Catalytic One-Step Deoxytrifluoromethylation of Alcohols

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Supporting Information – Experimental Details

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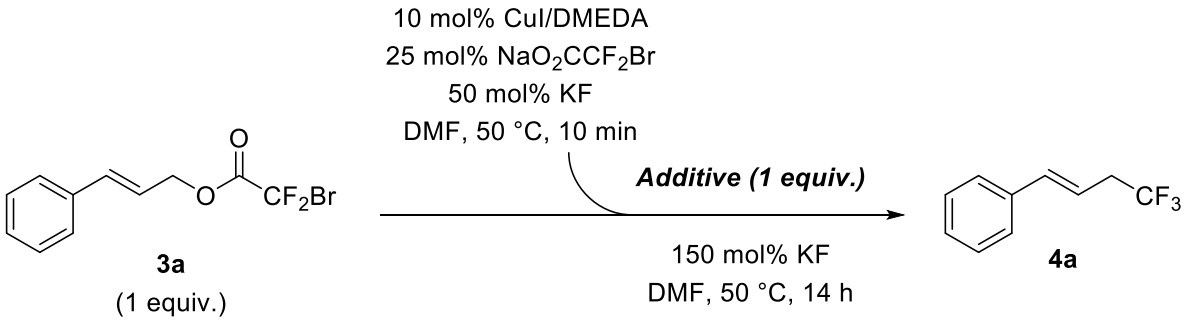
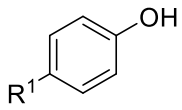
Additive Screening Experiment

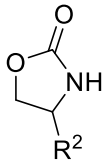
Table S1: Results of the Additive Screening to Identify Benign Leaving Groups



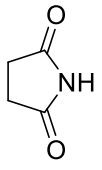
Additive	Yield
Control (no additive)	*75%*
MeONa	39%
H_2O	24%
MeOH	19%
^{i}PrOH	31%
CF_3CH_2OH	58%
$(CF_3)_2CHOH$	33%
EtSH	14%
PhSH	11%
$MsNH_2$	35%
Ts(Ph)NH	44%



R^1	Yield
H	59%
OMe	34%
F	41%
CN	36%
NO_2	25%



R^2	Yield
Ph	43%
Bn	45%
^{t}Bu	49%



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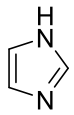

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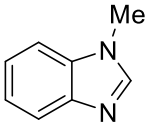

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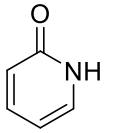

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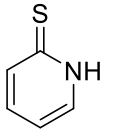
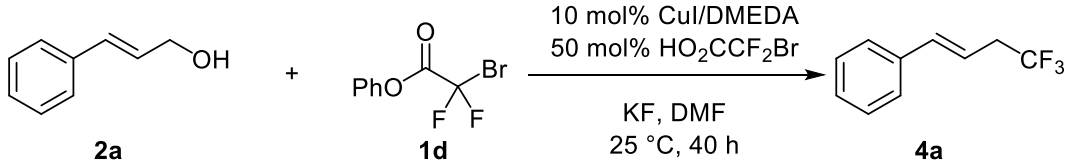


31%

Stability of the Phenyl Bromodifluoroacetate (1d)

The stability of phenyl bromodifluoroacetate (**1d**) was tested by storing it in 1-dram vials sealed with a PTFE-lined screw cap under three distinct conditions, namely 1) on the bench, 2) in a desiccator, and 3) in the freezer. The stability of the compound was evaluated by ^{1}H- and ^{19}F-NMR analysis (Figure S1 and S2), as well as the deoxytrifluoromethylation reaction of cinnamyl alcohol (**2a**) (Scheme S1). The compound was stable in all situations and showed no signs of decomposition by NMR. The reaction yields decreased as the reagent aged. However, the reaction yields were still satisfactory even after 6–8 months. During this work, the only decomposition pathway observed was the hydrolysis of the compound not properly protected against residual moisture. No light sensitivity was observed.



2a **1d** 2 equiv. **4a**

	Storage Condition		
Period	*Bench*	*Desiccator*	*Freezer*
Fresh reagent			*86*
37 days	86	82	
97 days	75	70	
183 days			73
242 days			67

[a] ^{19}F-NMR Yields.

Scheme S1: Phenyl bromodifluoroacetate (**1d**) provided satisfactory yields of trifluoromethyl compound **4a** after extended storage on the bench, in the desiccator, or in the freezer.

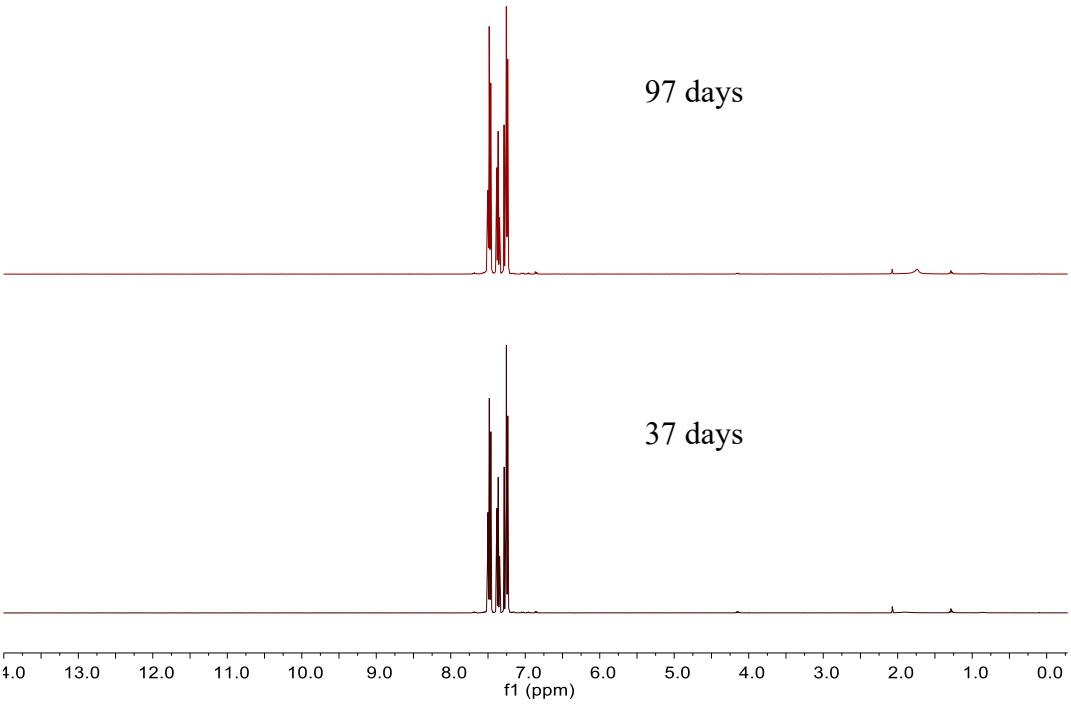


Figure S1: Representative ^{1}H-NMR spectra of phenyl bromodifluoroacetate (**1d**) obtained during the study of its stability. The spectra showed are from the sample stored on the bench.

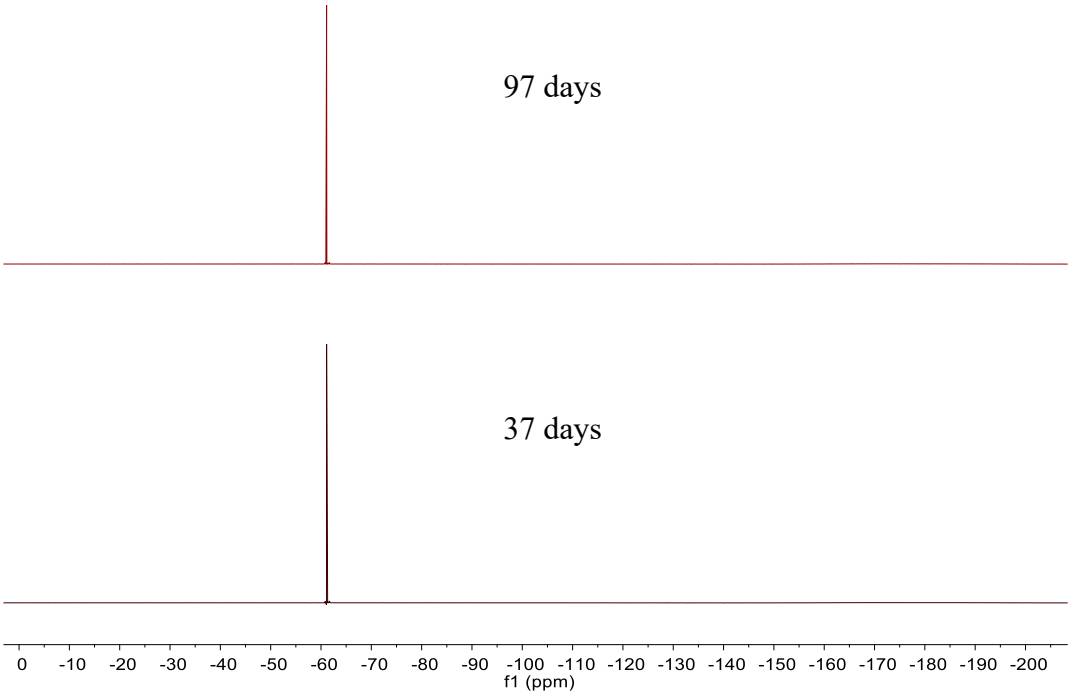


Figure S2: Representative ^{19}F-NMR spectra of phenyl bromodifluoroacetate (**1d**) obtained during the study of its stability. The spectra showed are from the sample stored on the bench.

Mechanistic Experiments (Scheme 2)

To better understand the reaction pathway, some experiments were done to probe the mechanism of the reaction. Specifically, the stability of phenyl bromodifluoroacetate (**1d**) under reaction conditions, the kinetic profile of the first hours of reaction, and a stepwise addition to study the formation of the intermediate ester.

Study of the Formation of Putative "Active Ester Intermediate" *In Situ*

KF facilitated the fast formation of the putative bromodifluoroacetate ester intermediate, as shown by stepwise addition of KF and bromodifluoroacetic acid to a DMF solution of cinnamyl alcohol **2a** and phenyl bromodifluoroacetate (**1d**). The key role of KF was both in the presence and absence of bromodifluoroacetic acid.

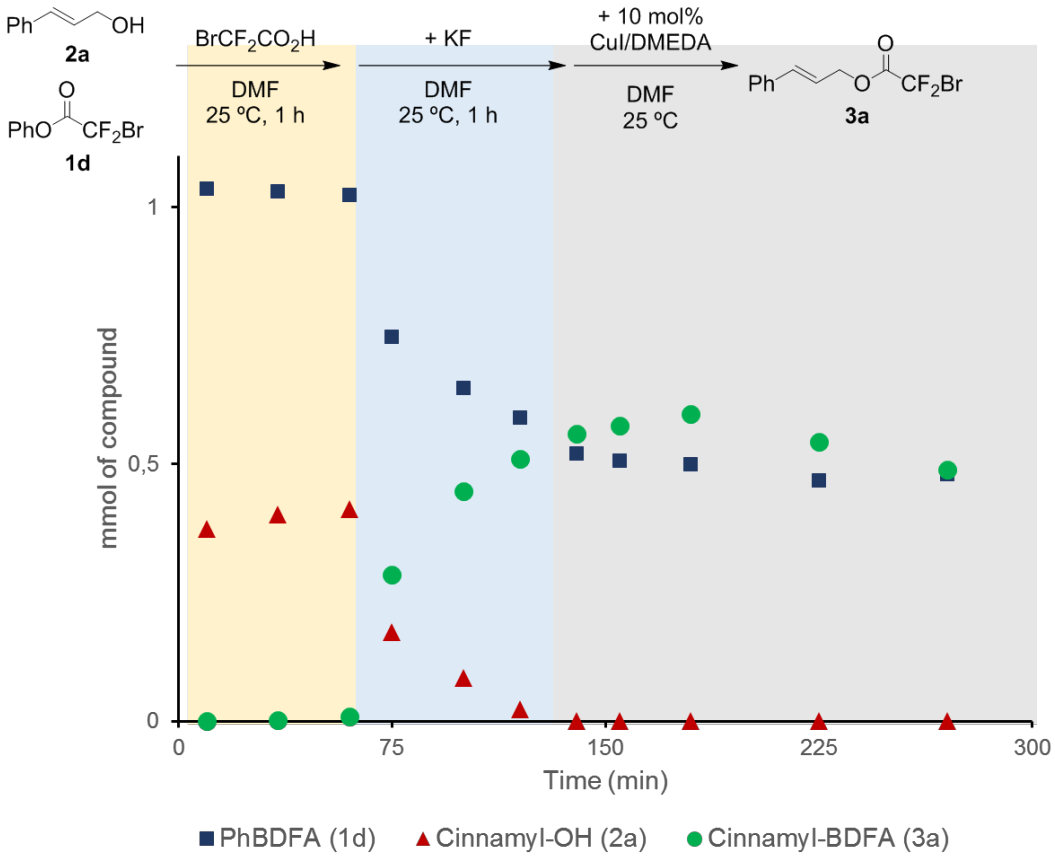


Figure S3: Cinnamyl Bromodifluoroacetate (**3a**) Formation Upon Stepwise Addition of KF and Bromodifluoroacetic Acid.

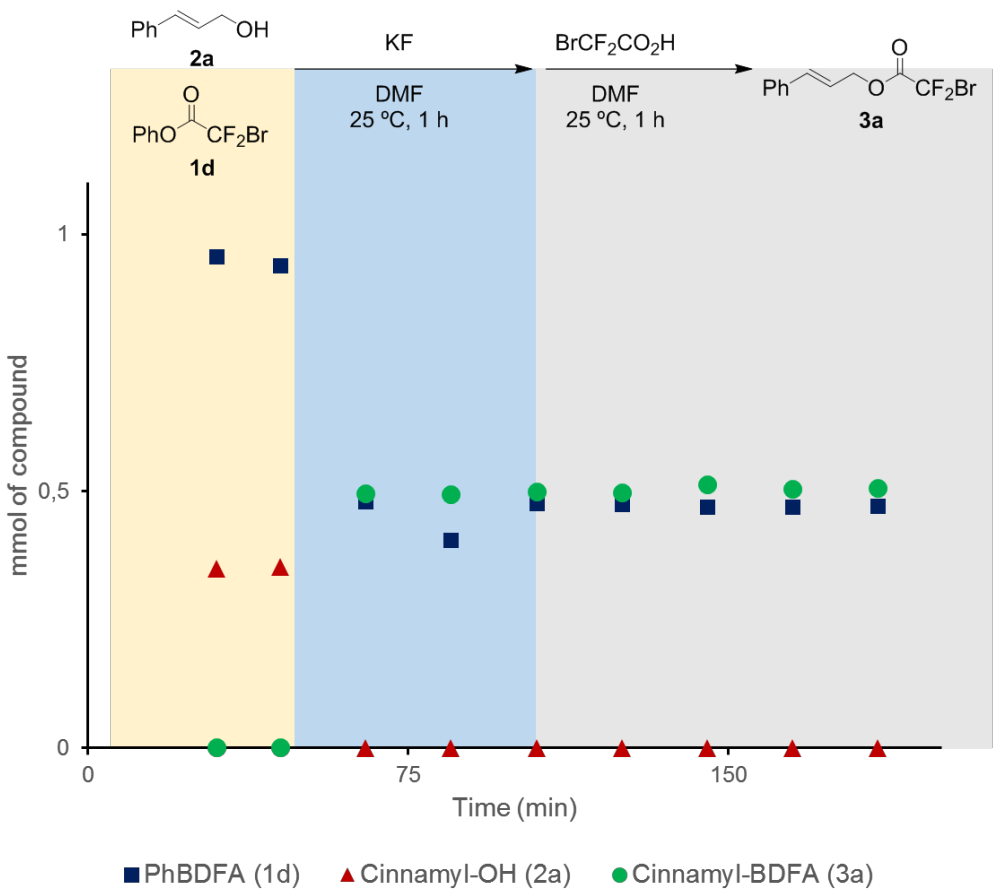


Figure S4: Cinnamyl Bromodifluoroacetate (**3a**) Formation Upon Stepwise Addition of KF and Bromodifluoroacetic Acid.

Time-Course Analysis of the Reaction

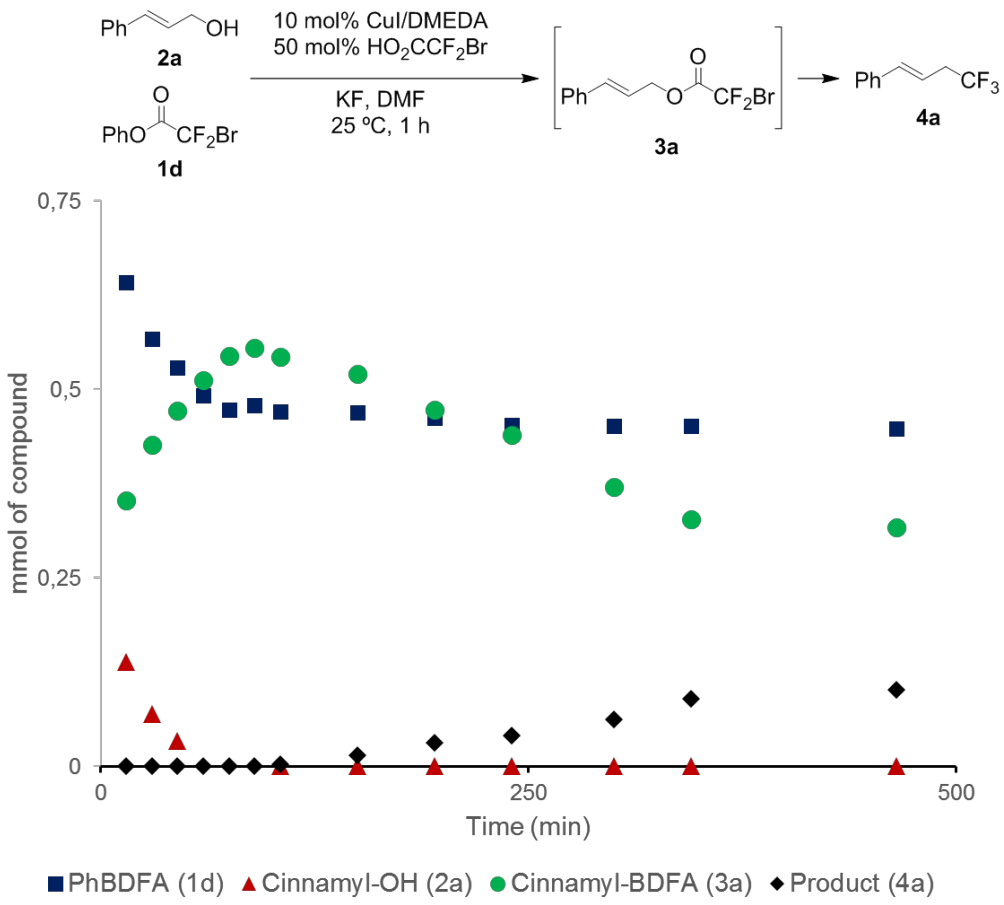
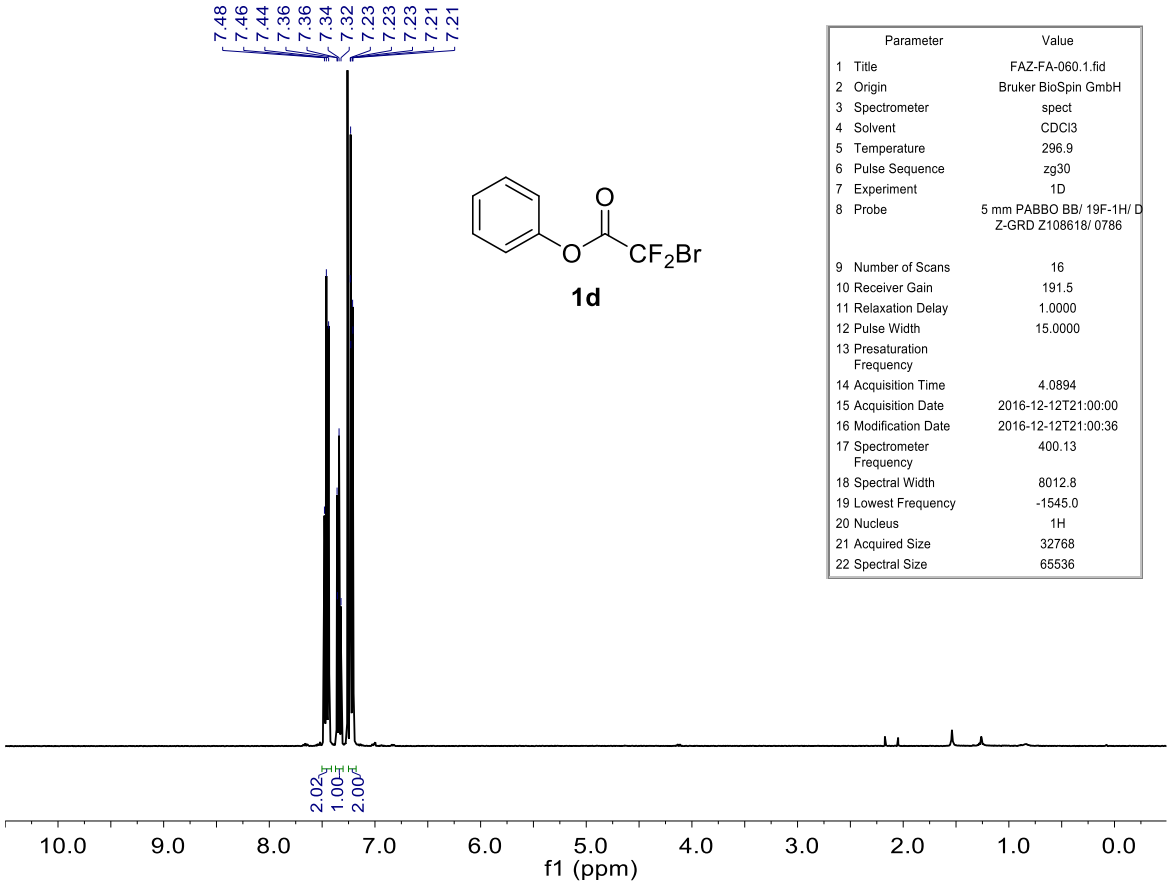


Figure S5: Time Course Analysis of the Deoxytrifluorometylation of Alcohol **2a**

NMR Spectra

Bromodifluoroacetate Reagents



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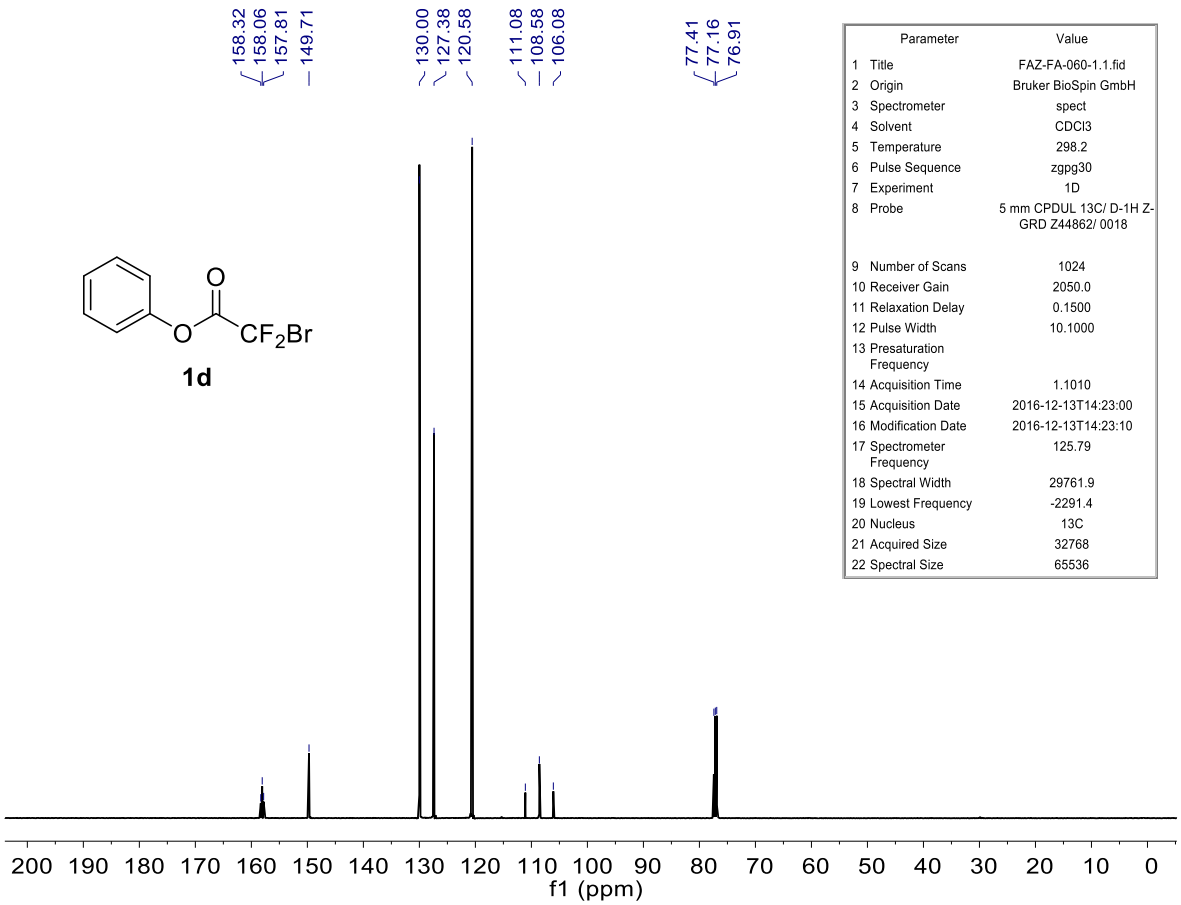

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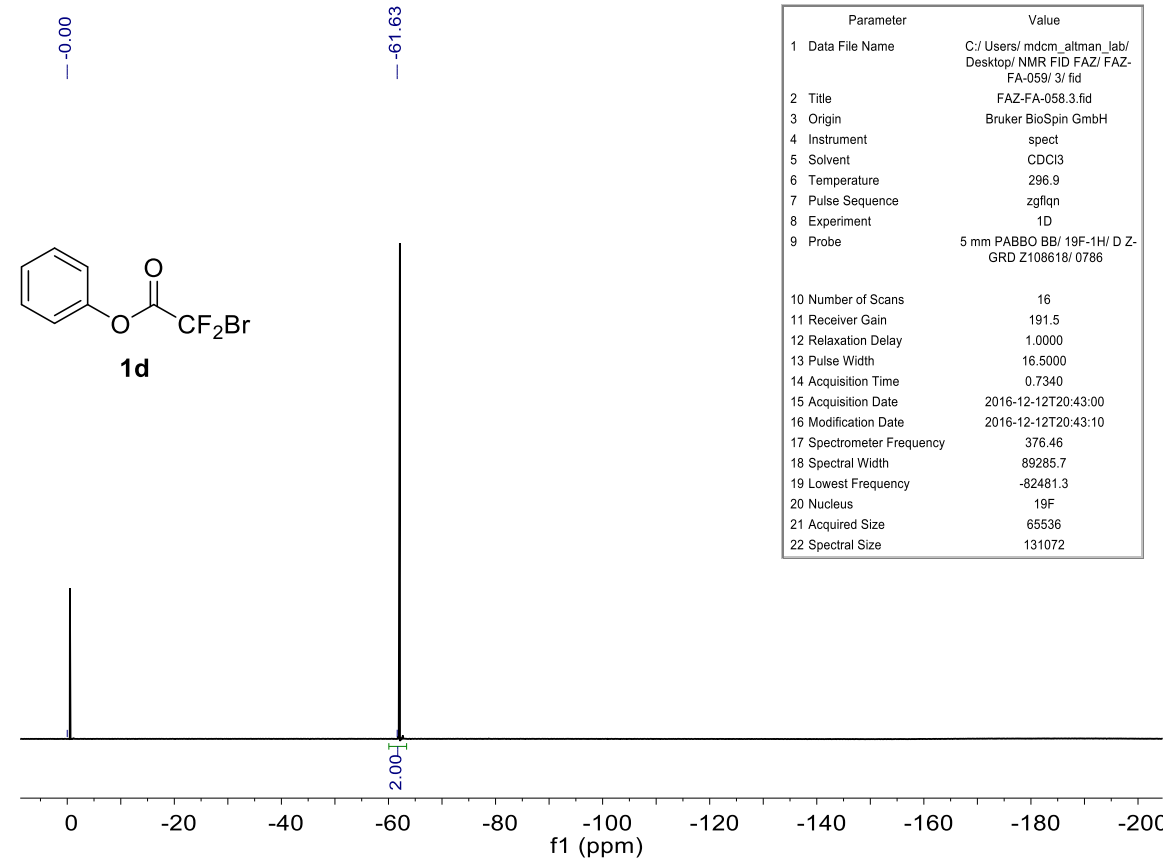

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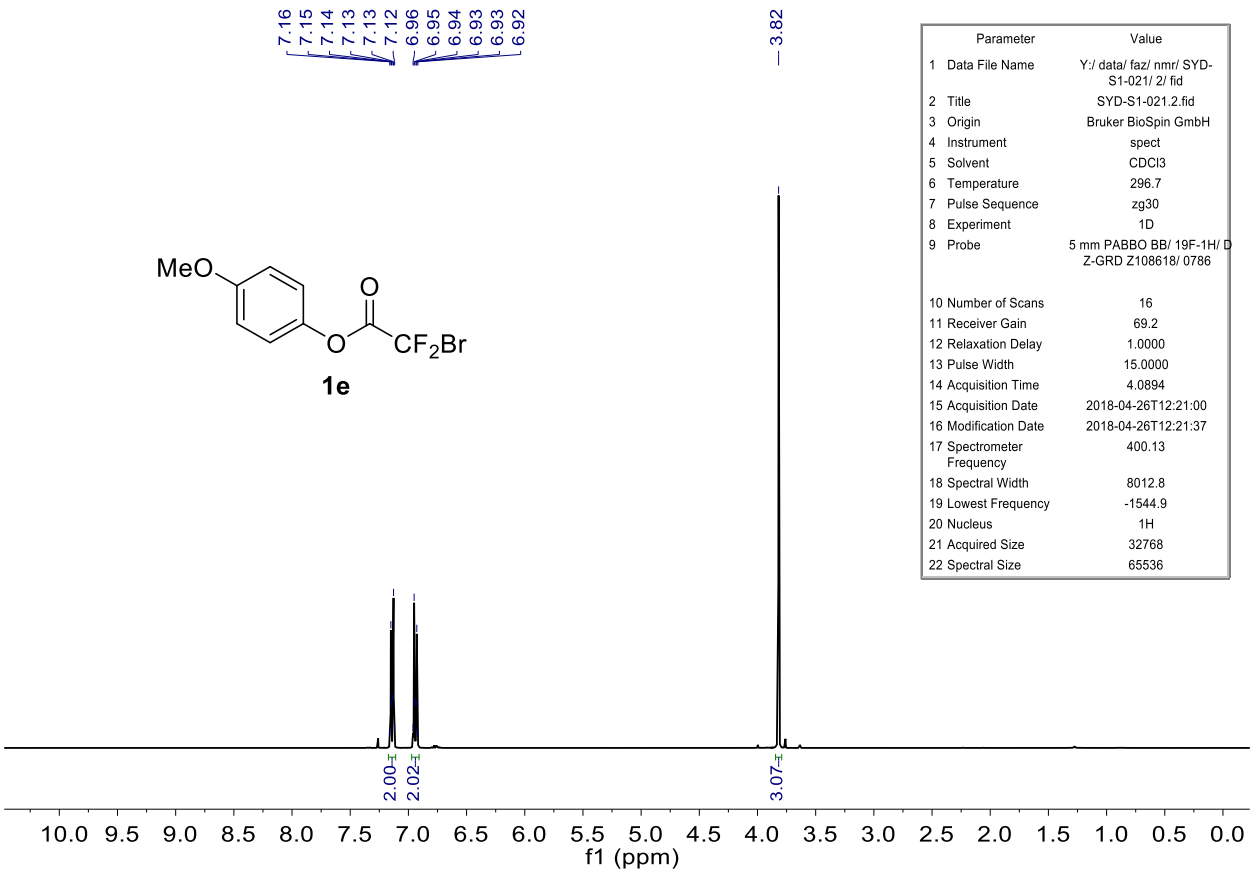

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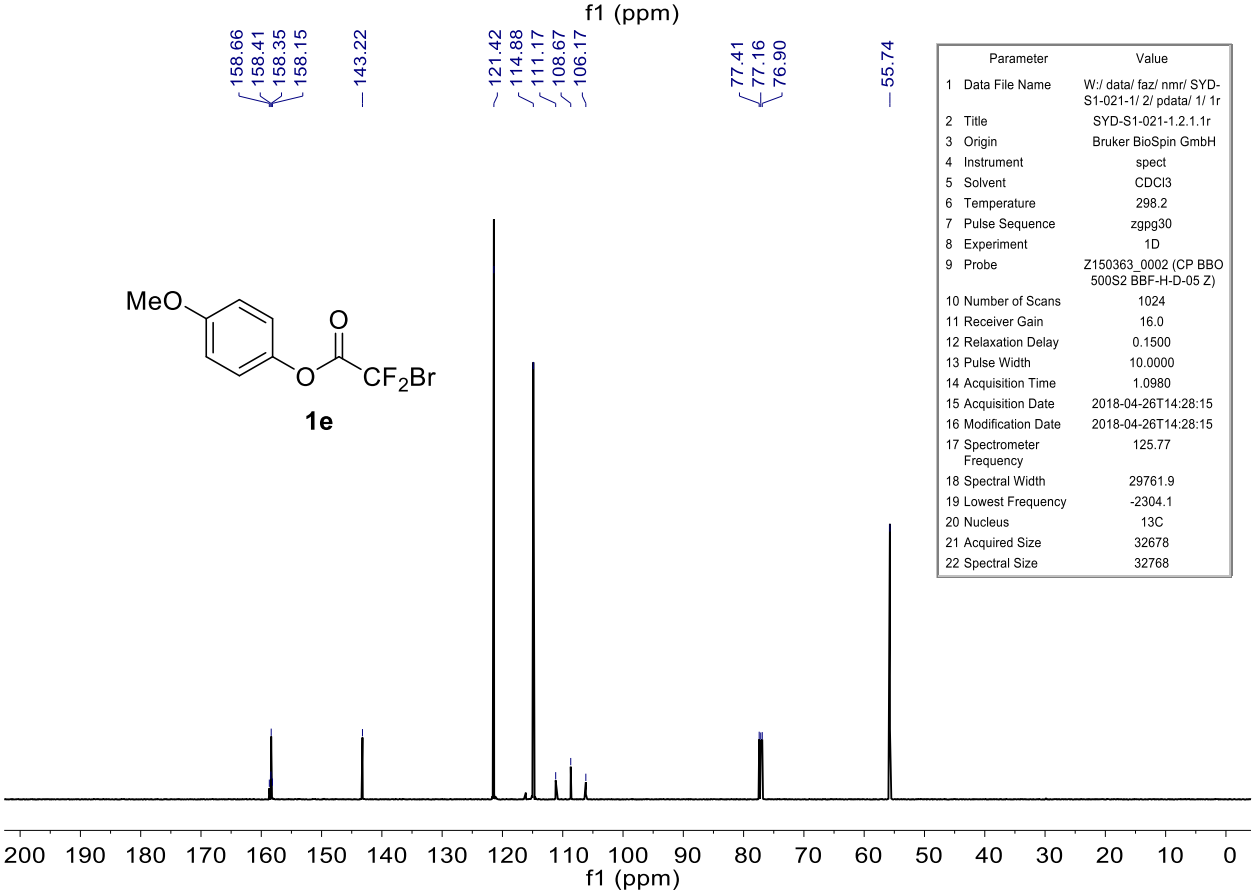

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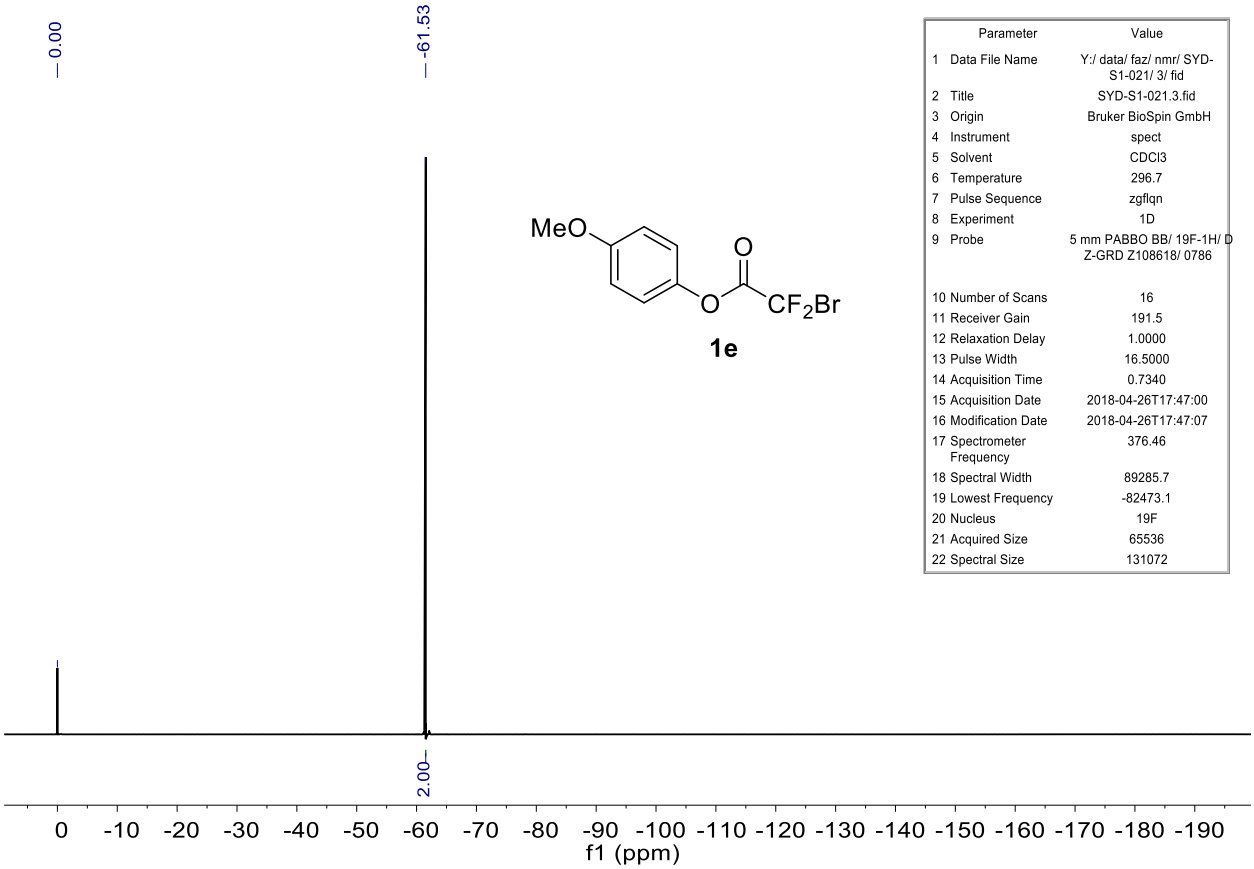

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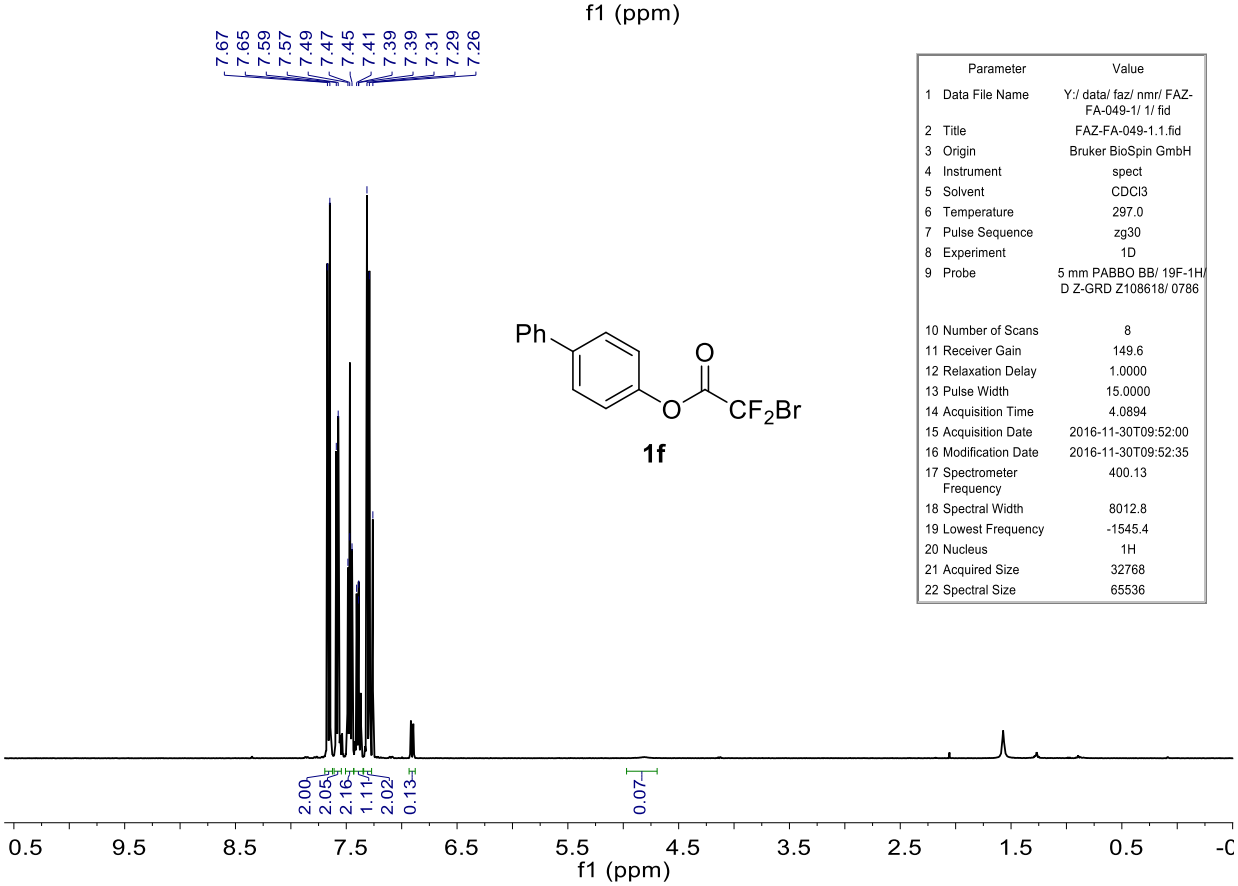

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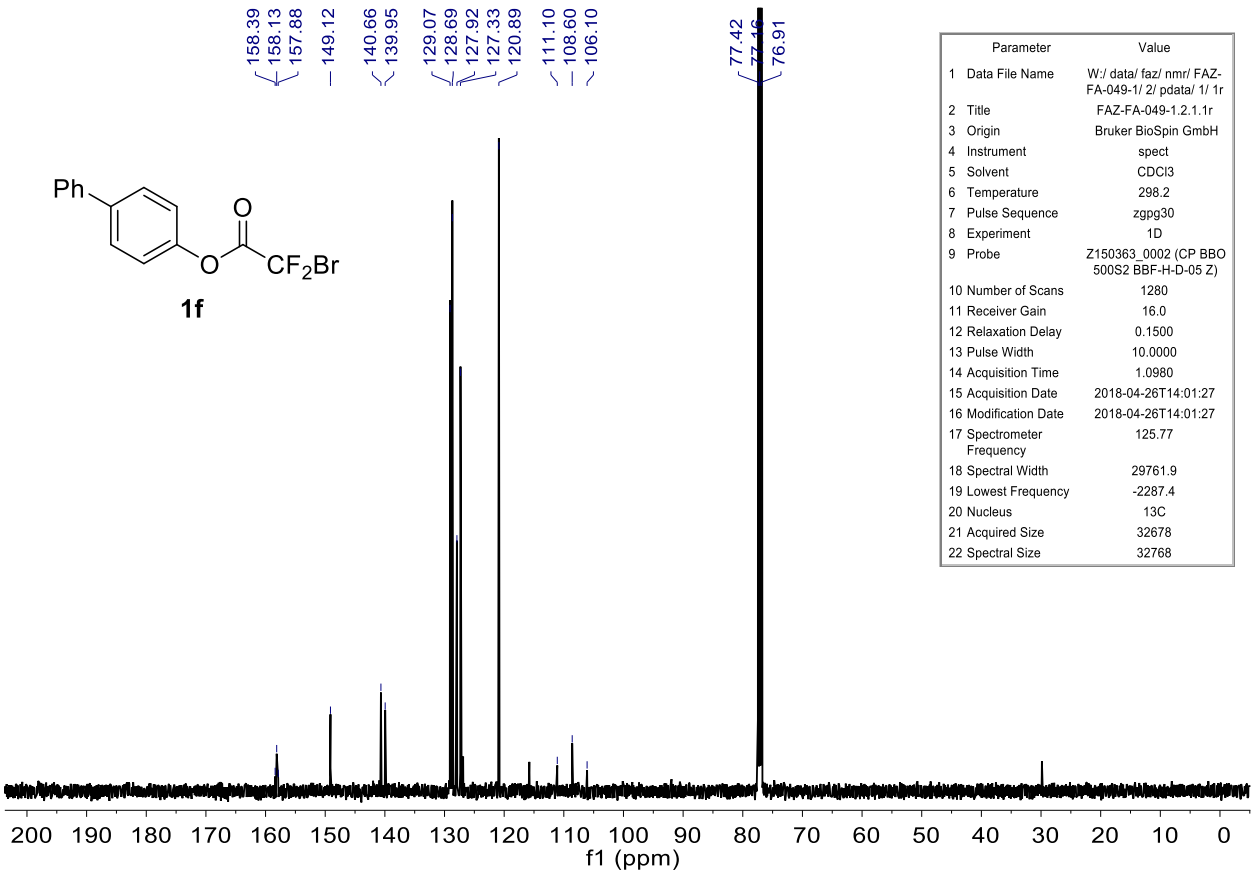

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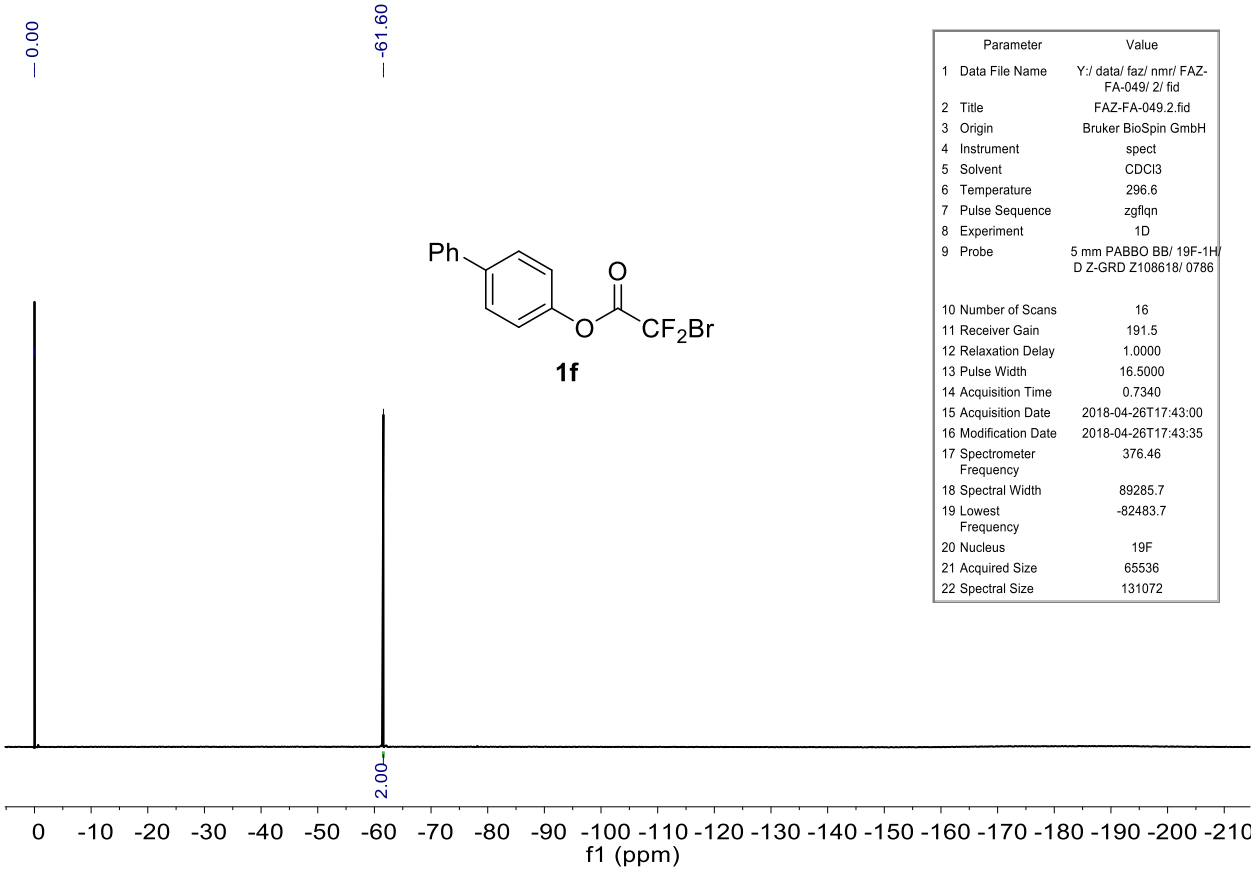

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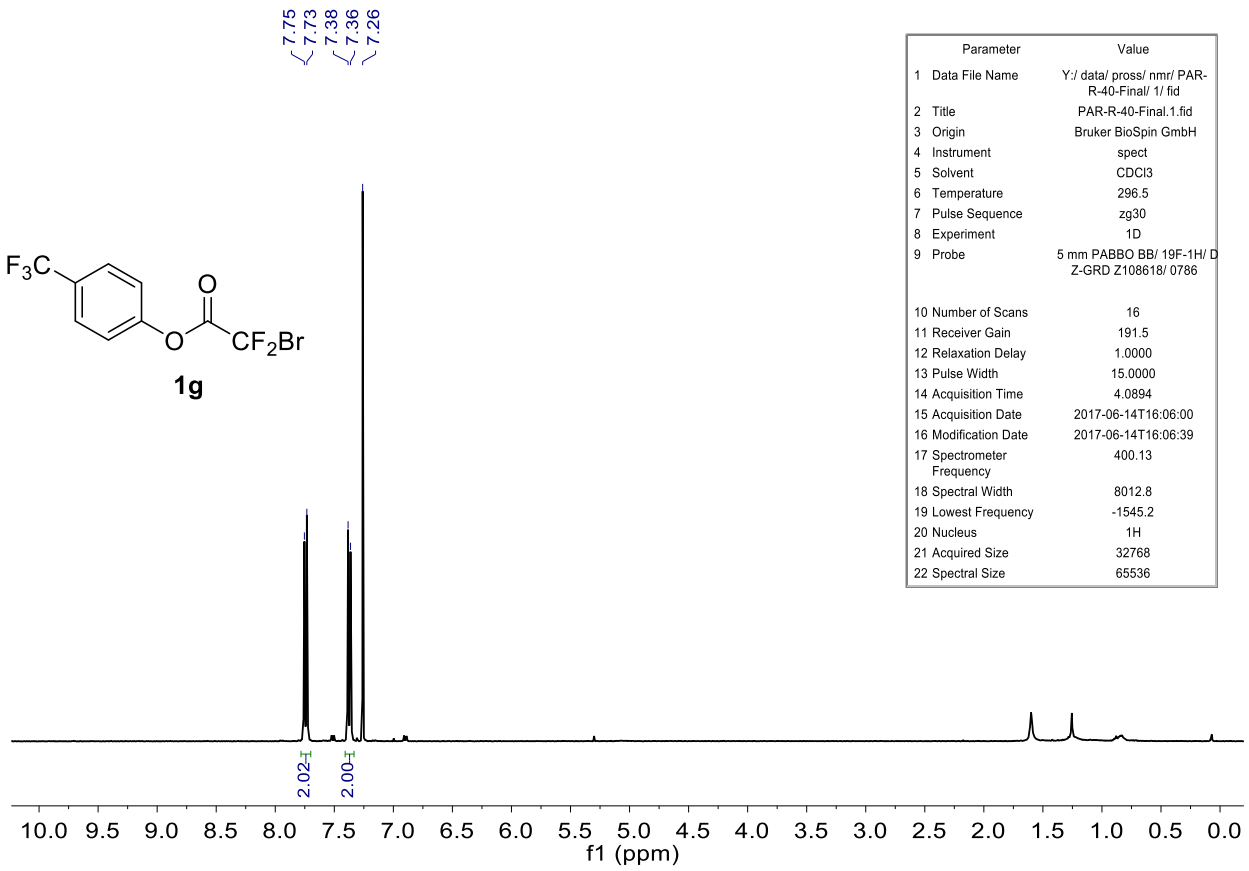

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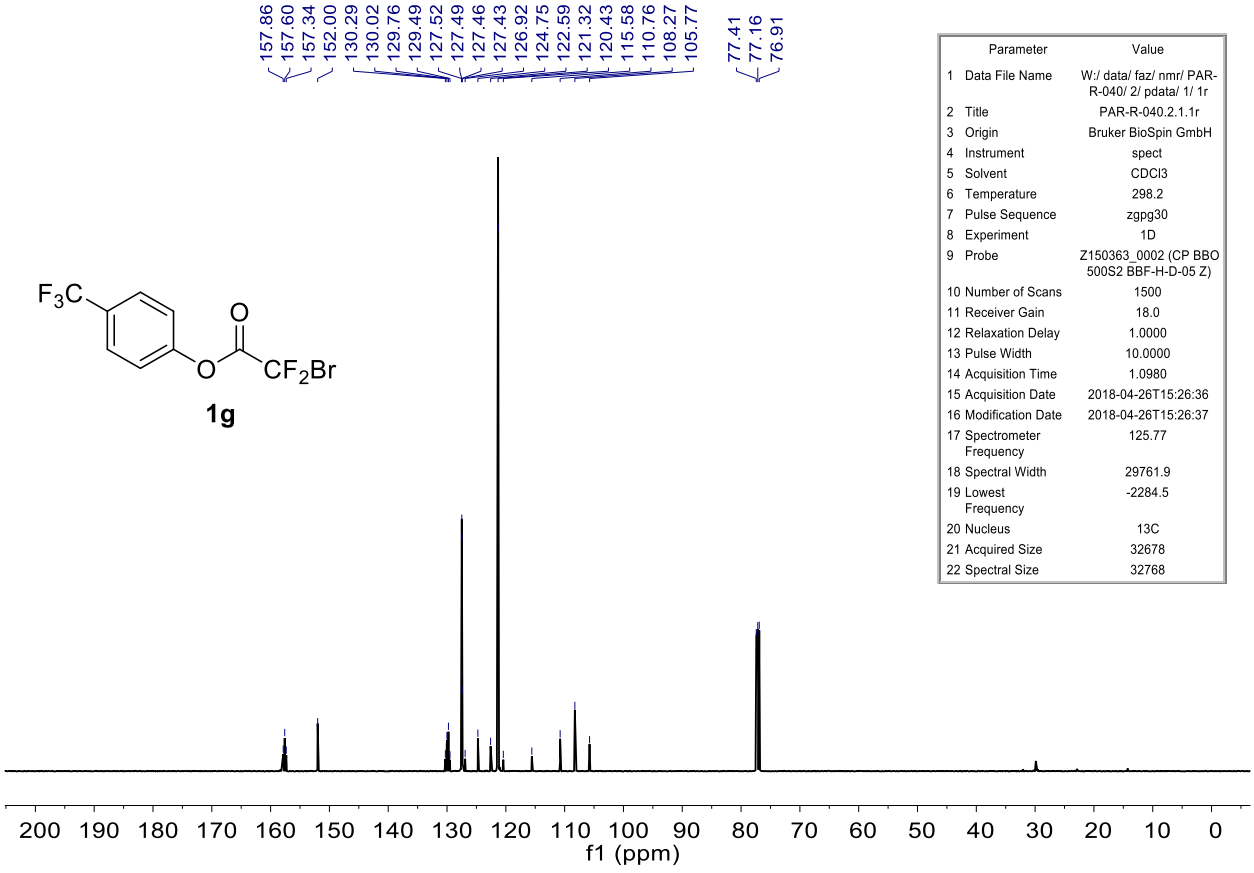

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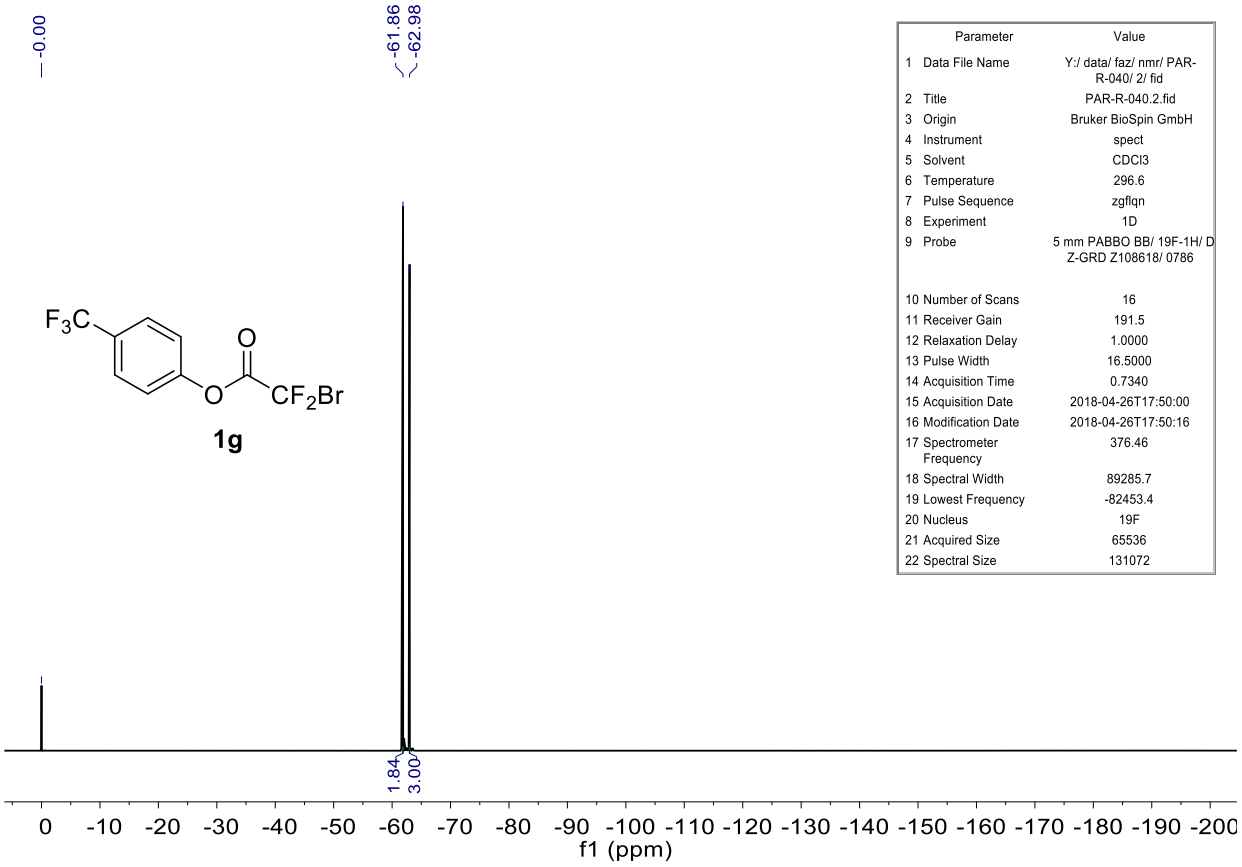

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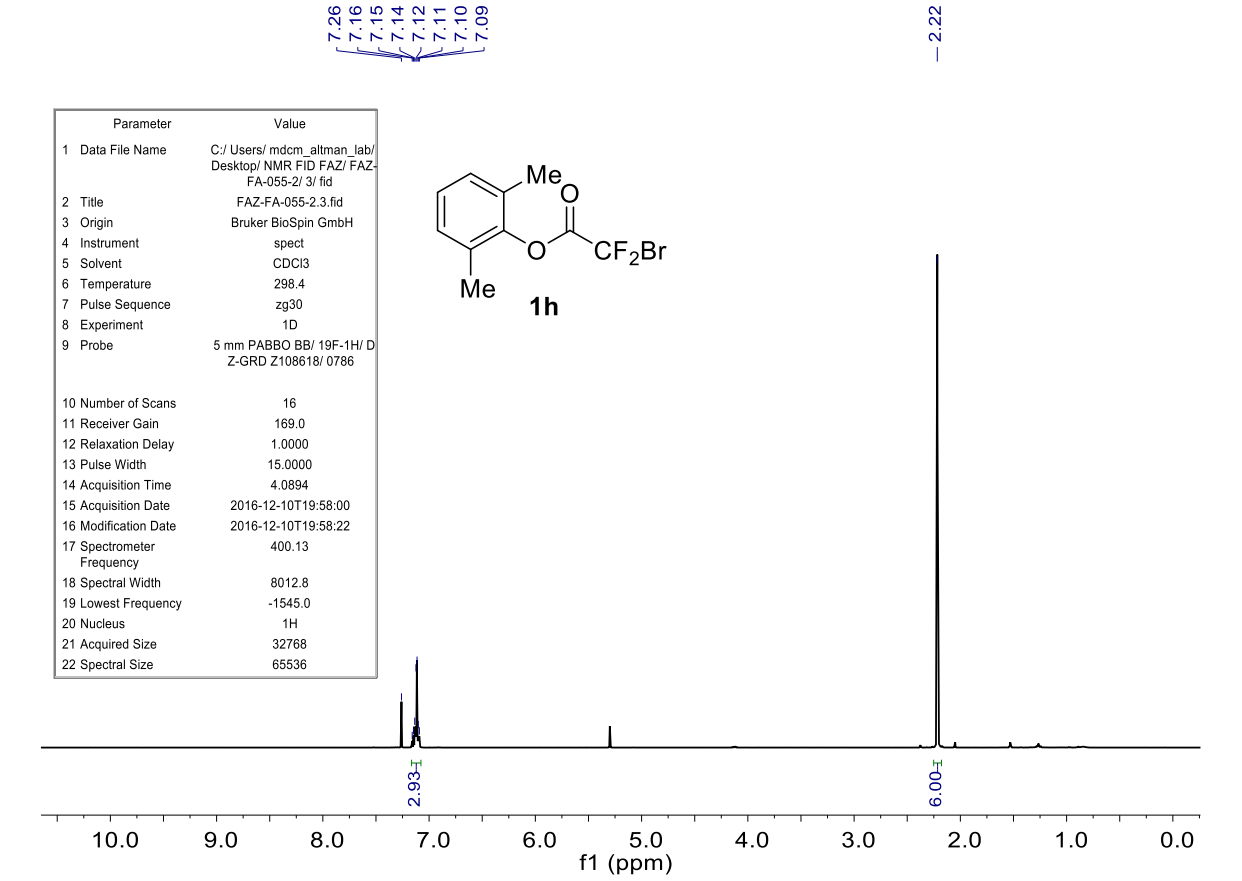
1g



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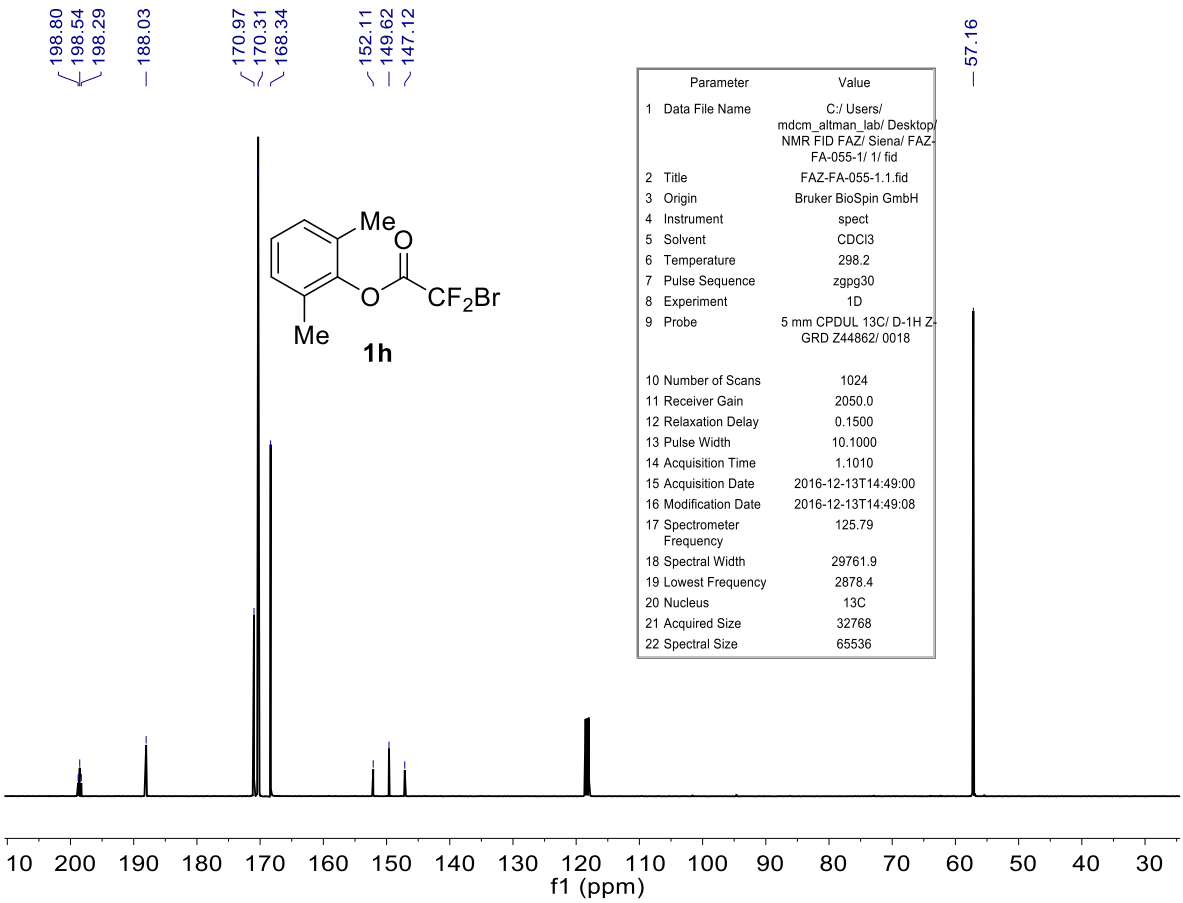
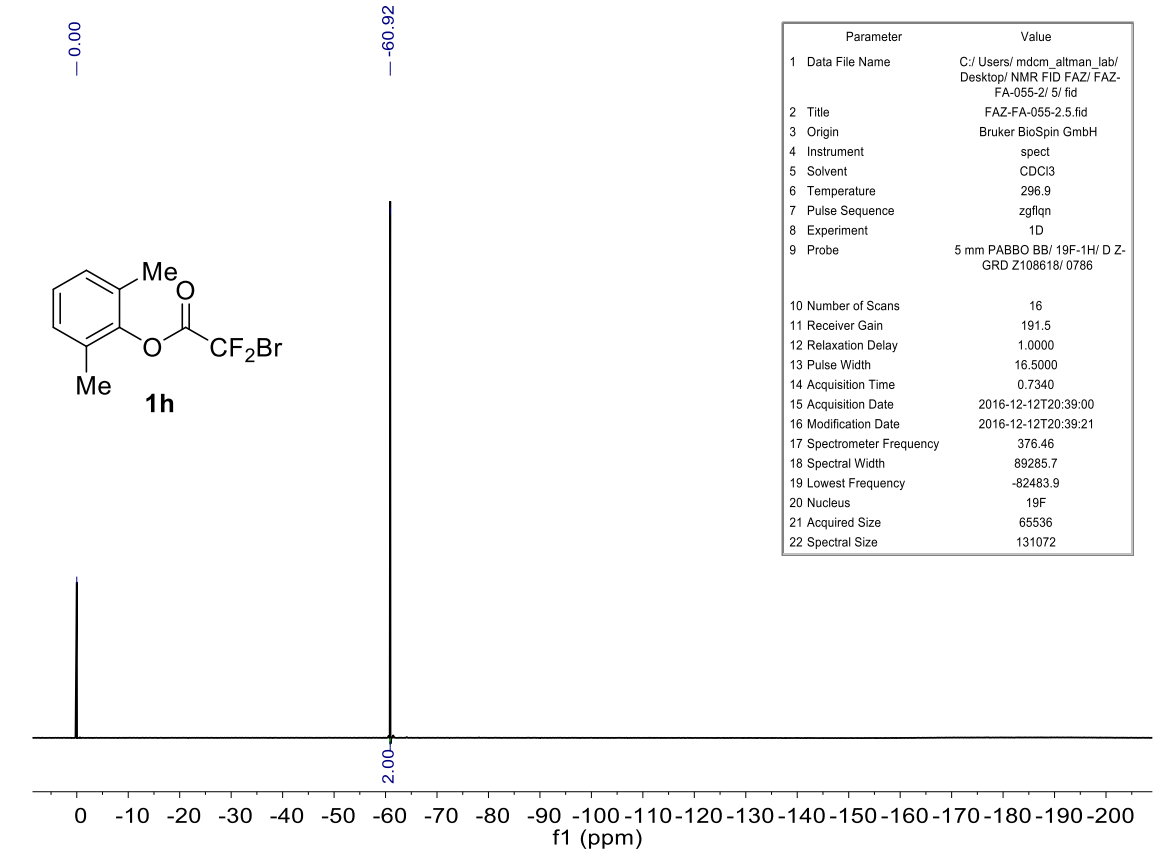
2	Title	FAZ-FA-055-2.3.fid
3	Origin	Bruker BioSpin GmbH
4	Instrument	spect
5	Solvent	CDCl3
6	Temperature	298.4
7	Pulse Sequence	zg30
8	Experiment	1D
9	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0786
10	Number of Scans	16
11	Receiver Gain	169.0
12	Relaxation Delay	1.0000
13	Pulse Width	15.0000
14	Acquisition Time	4.0894
15	Acquisition Date	2016-12-10T19:58:00
16	Modification Date	2016-12-10T19:58:22
17	Spectrometer Frequency	400.13
18	Spectral Width	8012.8
19	Lowest Frequency	-1545.0
20	Nucleus	1H
21	Acquired Size	32768
22	Spectral Size	65536

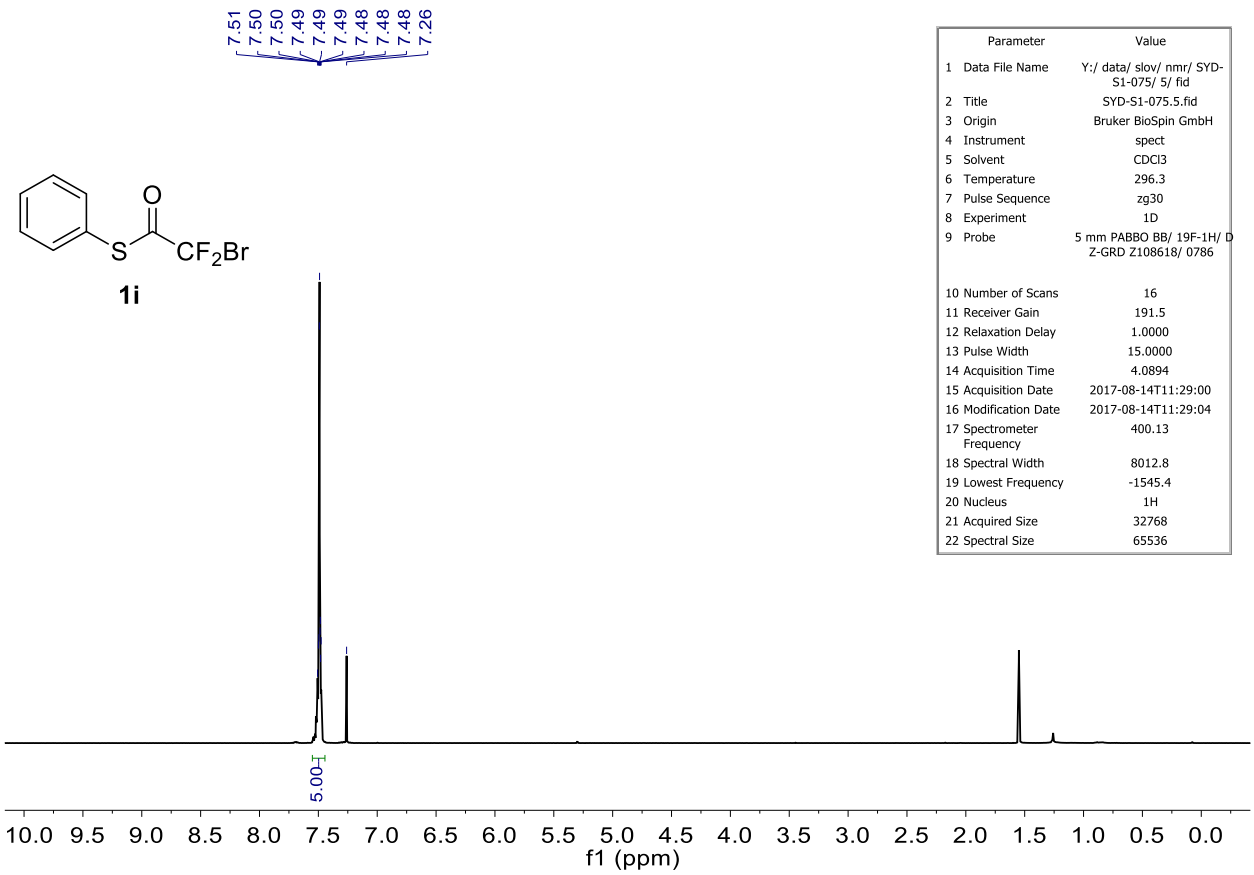
1h



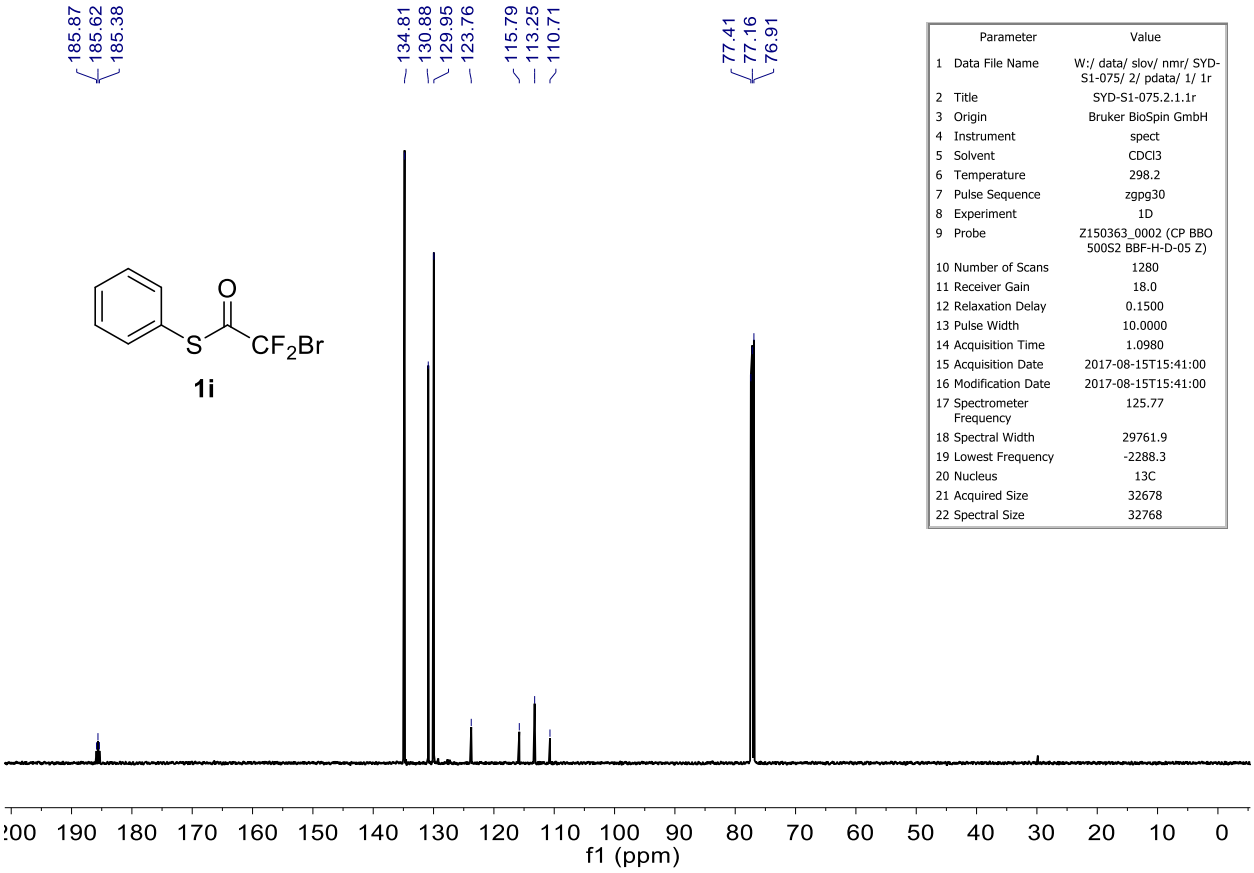
	Parameter	Value
1	Data File Name	C:/ Users/ mdcm_altman_lab/ Desktop/ NMR FID FAZ/ Siena/ FAZ-FA-055-1/ 1/ fid
2	Title	FAZ-FA-055-1.1.fid
3	Origin	Bruker BioSpin GmbH
4	Instrument	spect
5	Solvent	CDCl3
6	Temperature	298.2
7	Pulse Sequence	zgpg30
8	Experiment	1D
9	Probe	5 mm CPDUL 13C/ D-1H Z-GRD Z44862/ 0018
10	Number of Scans	1024
11	Receiver Gain	2050.0
12	Relaxation Delay	0.1500
13	Pulse Width	10.1000
14	Acquisition Time	1.1010
15	Acquisition Date	2016-12-13T14:49:00
16	Modification Date	2016-12-13T14:49:08
17	Spectrometer Frequency	125.79
18	Spectral Width	29761.9
19	Lowest Frequency	2878.4
20	Nucleus	13C
21	Acquired Size	32768
22	Spectral Size	65536



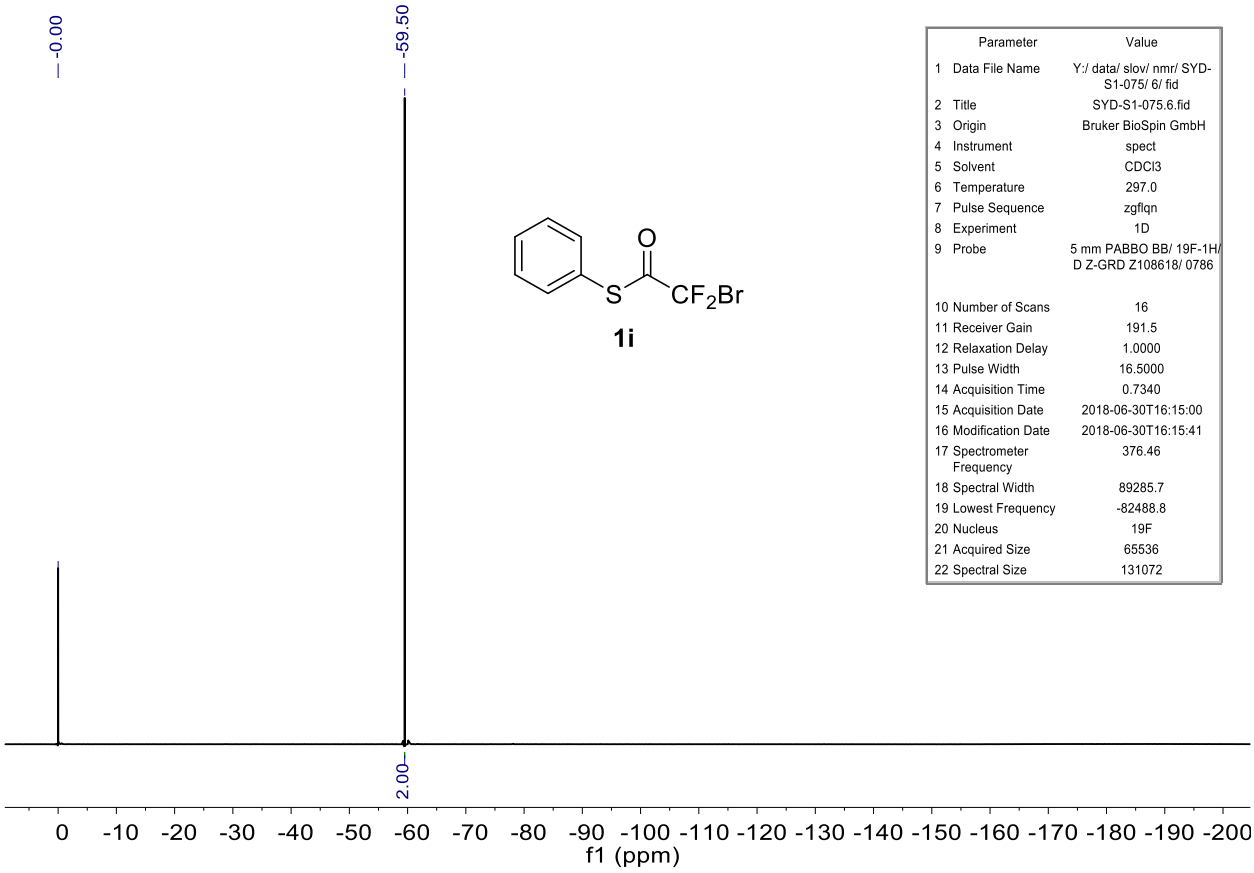
	Parameter	Value
1	Data File Name	C:/ Users/ mdcm_altman_lab/ Desktop/ NMR FID FAZ/ FAZ-FA-055-2/ 5/ fid
2	Title	FAZ-FA-055-2.5.fid
3	Origin	Bruker BioSpin GmbH
4	Instrument	spect
5	Solvent	CDCl3
6	Temperature	296.9
7	Pulse Sequence	zgflqn
8	Experiment	1D
9	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0786
10	Number of Scans	16
11	Receiver Gain	191.5
12	Relaxation Delay	1.0000
13	Pulse Width	16.5000
14	Acquisition Time	0.7340
15	Acquisition Date	2016-12-12T20:39:00
16	Modification Date	2016-12-12T20:39:21
17	Spectrometer Frequency	376.46
18	Spectral Width	89285.7
19	Lowest Frequency	-82483.9
20	Nucleus	19F
21	Acquired Size	65536
22	Spectral Size	131072



	Parameter	Value
1	Data File Name	Y:/ data/ slov/ nmr/ SYD-S1-075/ 5/ fid
2	Title	SYD-S1-075.5.fid
3	Origin	Bruker BioSpin GmbH
4	Instrument	spect
5	Solvent	CDCl3
6	Temperature	296.3
7	Pulse Sequence	zg30
8	Experiment	1D
9	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0786
10	Number of Scans	16
11	Receiver Gain	191.5
12	Relaxation Delay	1.0000
13	Pulse Width	15.0000
14	Acquisition Time	4.0894
15	Acquisition Date	2017-08-14T11:29:00
16	Modification Date	2017-08-14T11:29:04
17	Spectrometer Frequency	400.13
18	Spectral Width	8012.8
19	Lowest Frequency	-1545.4
20	Nucleus	1H
21	Acquired Size	32768
22	Spectral Size	65536

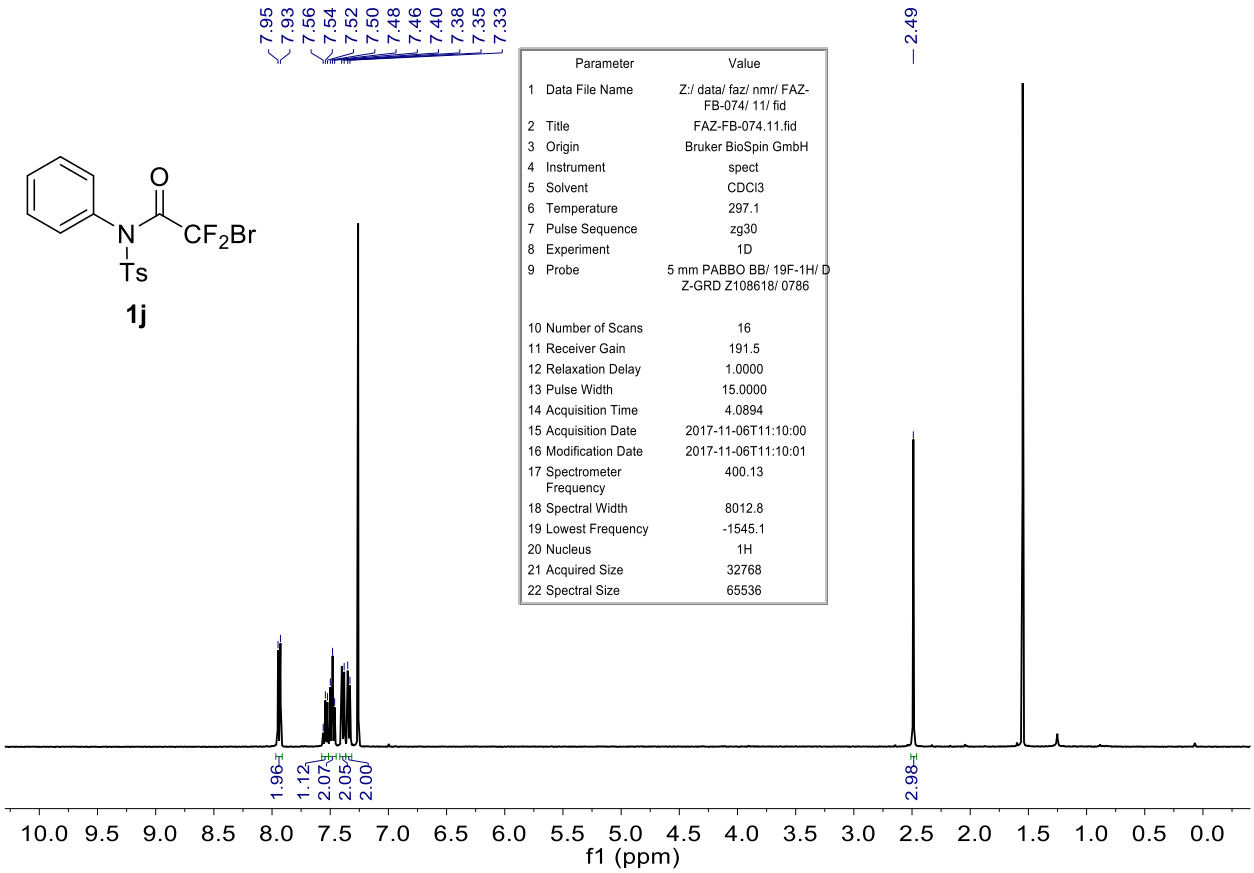


	Parameter	Value
1	Data File Name	W:/ data/ slov/ nmr/ SYD-S1-075/ 2/ pdata/ 1/ 1r
2	Title	SYD-S1-075.2.1.1r
3	Origin	Bruker BioSpin GmbH
4	Instrument	spect
5	Solvent	CDCl3
6	Temperature	298.2
7	Pulse Sequence	zgpg30
8	Experiment	1D
9	Probe	Z150363_0002 (CP BBO 500S2 BBF-H-D-05 Z)
10	Number of Scans	1280
11	Receiver Gain	18.0
12	Relaxation Delay	0.1500
13	Pulse Width	10.0000
14	Acquisition Time	1.0980
15	Acquisition Date	2017-08-15T15:41:00
16	Modification Date	2017-08-15T15:41:00
17	Spectrometer Frequency	125.77
18	Spectral Width	29761.9
19	Lowest Frequency	-2288.3
20	Nucleus	13C
21	Acquired Size	32678
22	Spectral Size	32768



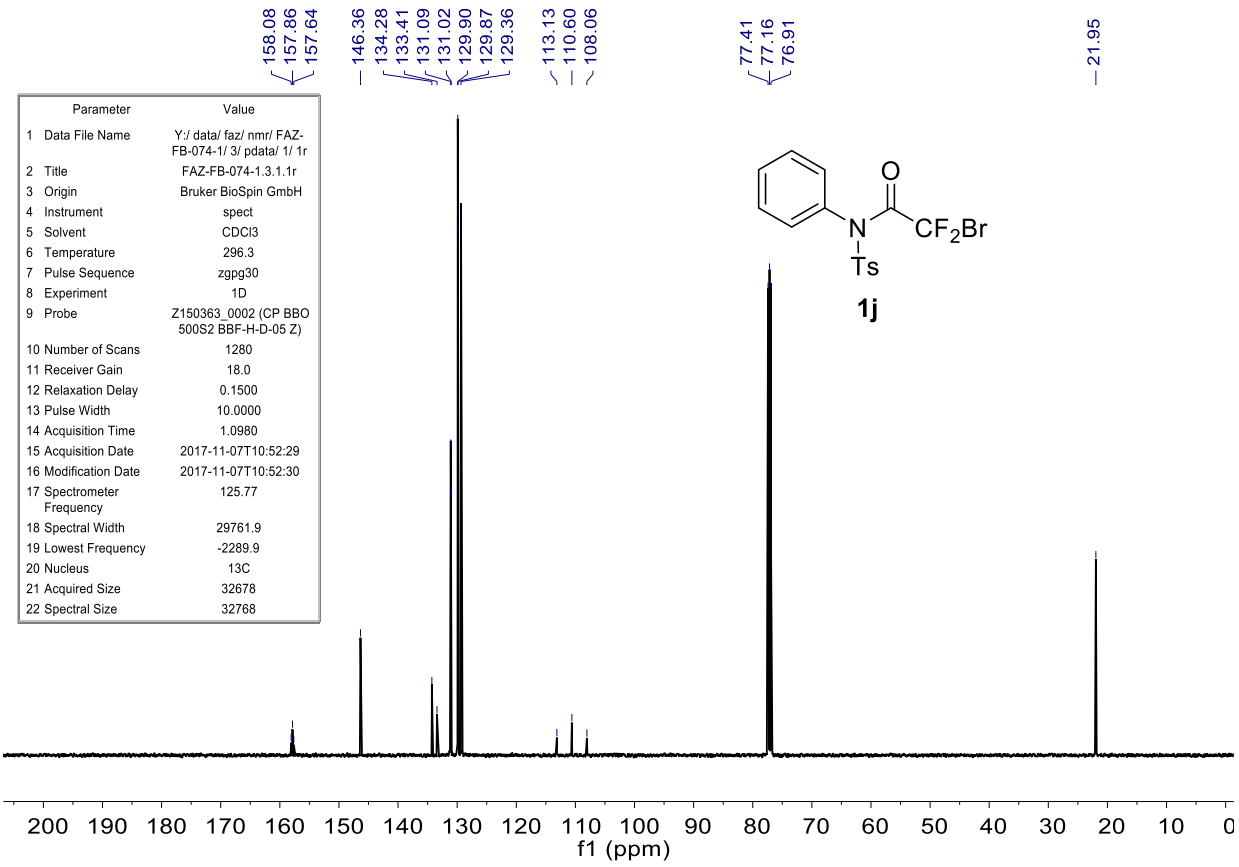
	Parameter	Value
1	Data File Name	Y:/ data/ slov/ nmr/ SYD-S1-075/ 6/ fid
2	Title	SYD-S1-075.6.fid
3	Origin	Bruker BioSpin GmbH
4	Instrument	spect
5	Solvent	CDCl3
6	Temperature	297.0
7	Pulse Sequence	zgflqn
8	Experiment	1D
9	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0786
10	Number of Scans	16
11	Receiver Gain	191.5
12	Relaxation Delay	1.0000
13	Pulse Width	16.5000
14	Acquisition Time	0.7340
15	Acquisition Date	2018-06-30T16:15:00
16	Modification Date	2018-06-30T16:15:41
17	Spectrometer Frequency	376.46
18	Spectral Width	89285.7
19	Lowest Frequency	-82488.8
20	Nucleus	19F
21	Acquired Size	65536
22	Spectral Size	131072

1i

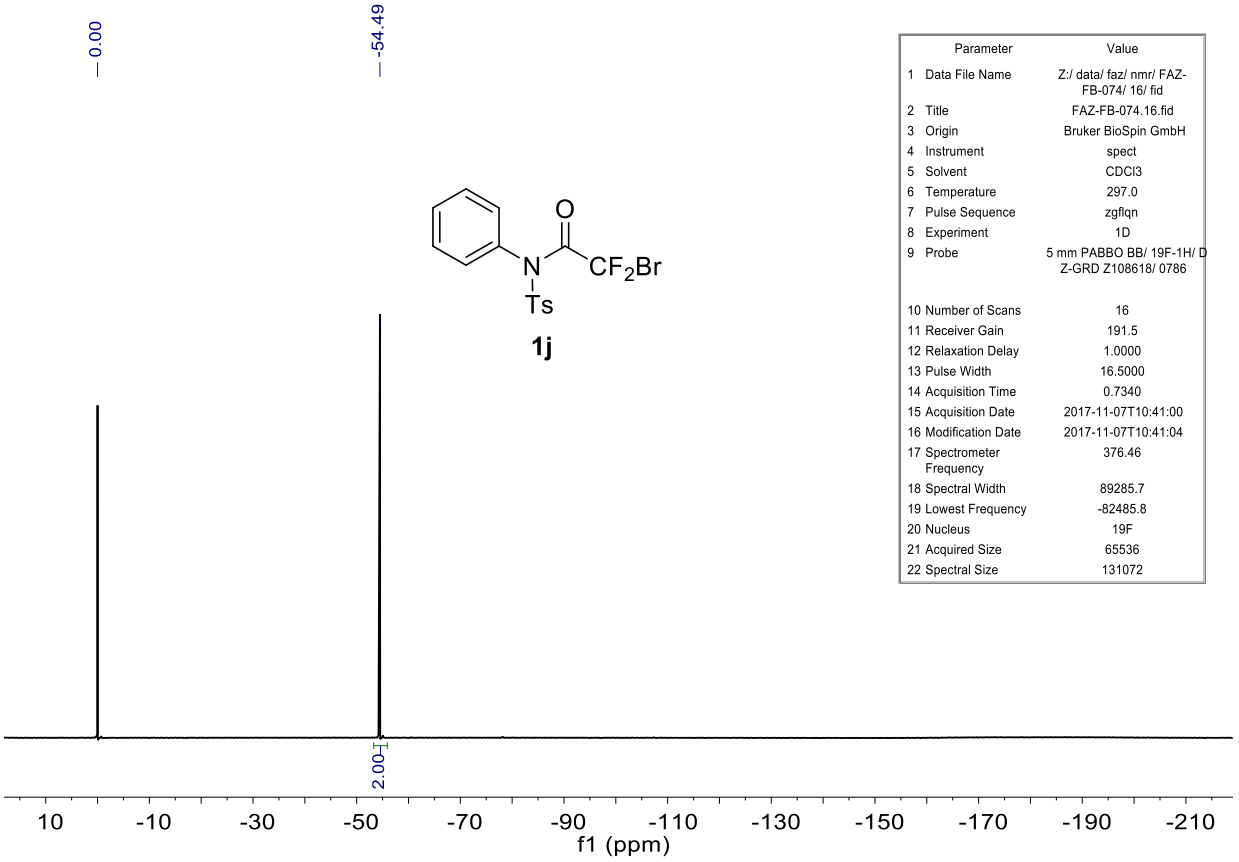


	Parameter	Value
1	Data File Name	Z:/ data/ faz/ nmr/ FAZ-FB-074/ 11/ fid
2	Title	FAZ-FB-074.11.fid
3	Origin	Bruker BioSpin GmbH
4	Instrument	spect
5	Solvent	CDCl3
6	Temperature	297.1
7	Pulse Sequence	zg30
8	Experiment	1D
9	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0786
10	Number of Scans	16
11	Receiver Gain	191.5
12	Relaxation Delay	1.0000
13	Pulse Width	15.0000
14	Acquisition Time	4.0894
15	Acquisition Date	2017-11-06T11:10:00
16	Modification Date	2017-11-06T11:10:01
17	Spectrometer Frequency	400.13
18	Spectral Width	8012.8
19	Lowest Frequency	-1545.1
20	Nucleus	1H
21	Acquired Size	32768
22	Spectral Size	65536

1j



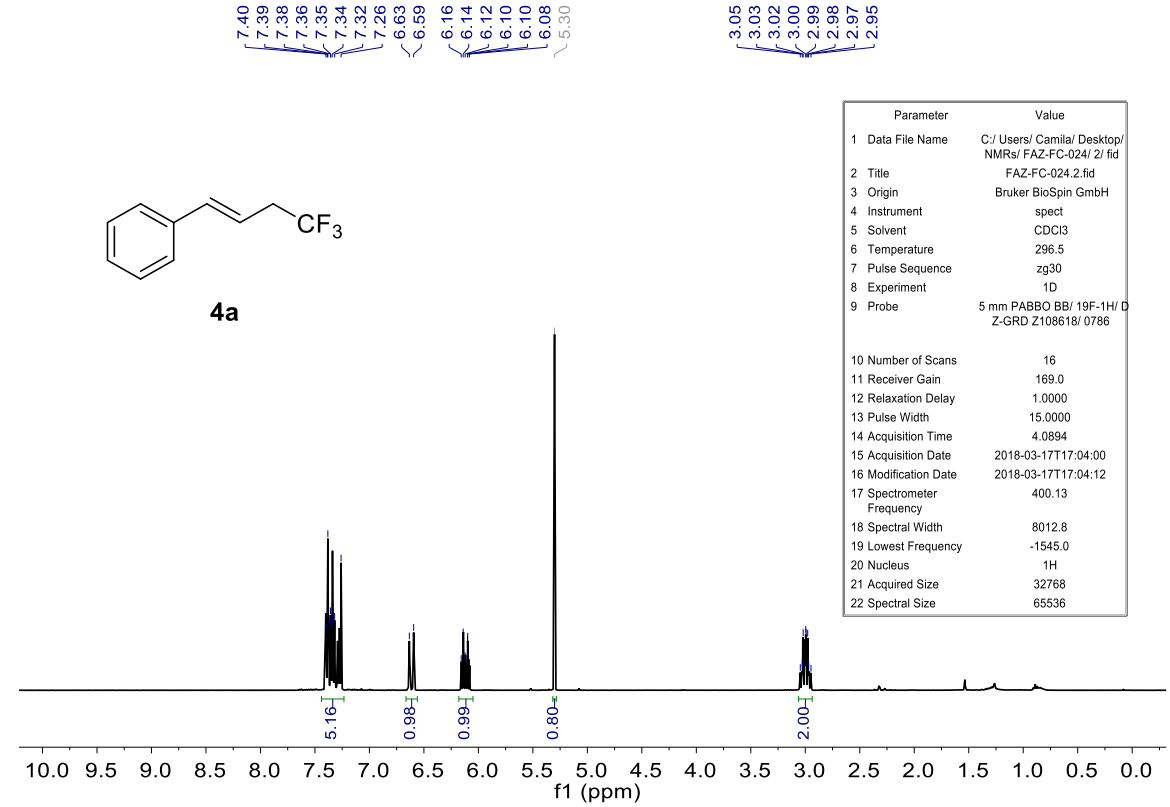
	Parameter	Value
1	Data File Name	Y:/ data/ faz/ nmr/ FAZ-FB-074-1/ 3/ pdata/ 1/ 1r
2	Title	FAZ-FB-074-1.3.1.1r
3	Origin	Bruker BioSpin GmbH
4	Instrument	spect
5	Solvent	CDCl3
6	Temperature	296.3
7	Pulse Sequence	zgpg30
8	Experiment	1D
9	Probe	Z150363_0002 (CP BBO 500S2 BBF-H-D-05 Z)
10	Number of Scans	1280
11	Receiver Gain	18.0
12	Relaxation Delay	0.1500
13	Pulse Width	10.0000
14	Acquisition Time	1.0980
15	Acquisition Date	2017-11-07T10:52:29
16	Modification Date	2017-11-07T10:52:30
17	Spectrometer Frequency	125.77
18	Spectral Width	29761.9
19	Lowest Frequency	-2289.9
20	Nucleus	13C
21	Acquired Size	32678
22	Spectral Size	32768

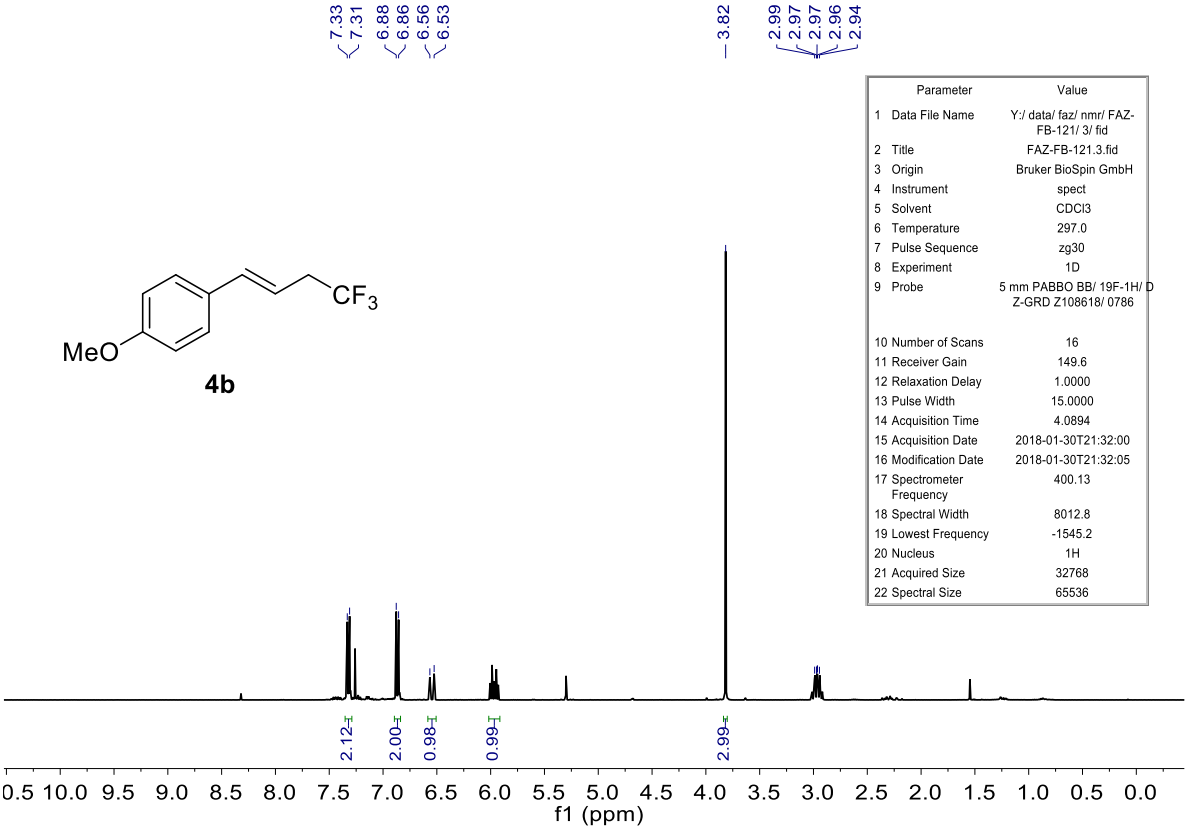


	Parameter	Value
1	Data File Name	Z:/ data/ faz/ nmr/ FAZ-FB-074/ 16/ fid
2	Title	FAZ-FB-074.16.fid
3	Origin	Bruker BioSpin GmbH
4	Instrument	spect
5	Solvent	CDCl3
6	Temperature	297.0
7	Pulse Sequence	zgflqn
8	Experiment	1D
9	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0786
10	Number of Scans	16
11	Receiver Gain	191.5
12	Relaxation Delay	1.0000
13	Pulse Width	16.5000
14	Acquisition Time	0.7340
15	Acquisition Date	2017-11-07T10:41:00
16	Modification Date	2017-11-07T10:41:04
17	Spectrometer Frequency	376.46
18	Spectral Width	89285.7
19	Lowest Frequency	-82485.8
20	Nucleus	19F
21	Acquired Size	65536
22	Spectral Size	131072

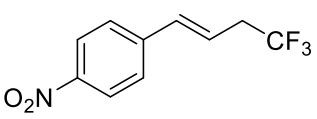
Reaction Scope

Allyl Trifluoromethanes (Table 2)



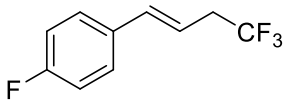


	Parameter	Value
1	Data File Name	Y:/ data/ faz/ nmr/ FAZ-FB-122/ 7/ fid
2	Title	FAZ-FB-122.7.fid
3	Origin	Bruker BioSpin GmbH
4	Instrument	spect
5	Solvent	CDCl3
6	Temperature	296.9
7	Pulse Sequence	zg30
8	Experiment	1D
9	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0786
10	Number of Scans	16
11	Receiver Gain	191.5
12	Relaxation Delay	1.0000
13	Pulse Width	15.0000
14	Acquisition Time	4.0894
15	Acquisition Date	2018-07-17T16:17:00
16	Modification Date	2018-07-17T16:17:44
17	Spectrometer Frequency	400.13
18	Spectral Width	8012.8
19	Lowest Frequency	-1545.4
20	Nucleus	1H
21	Acquired Size	32768
22	Spectral Size	65536

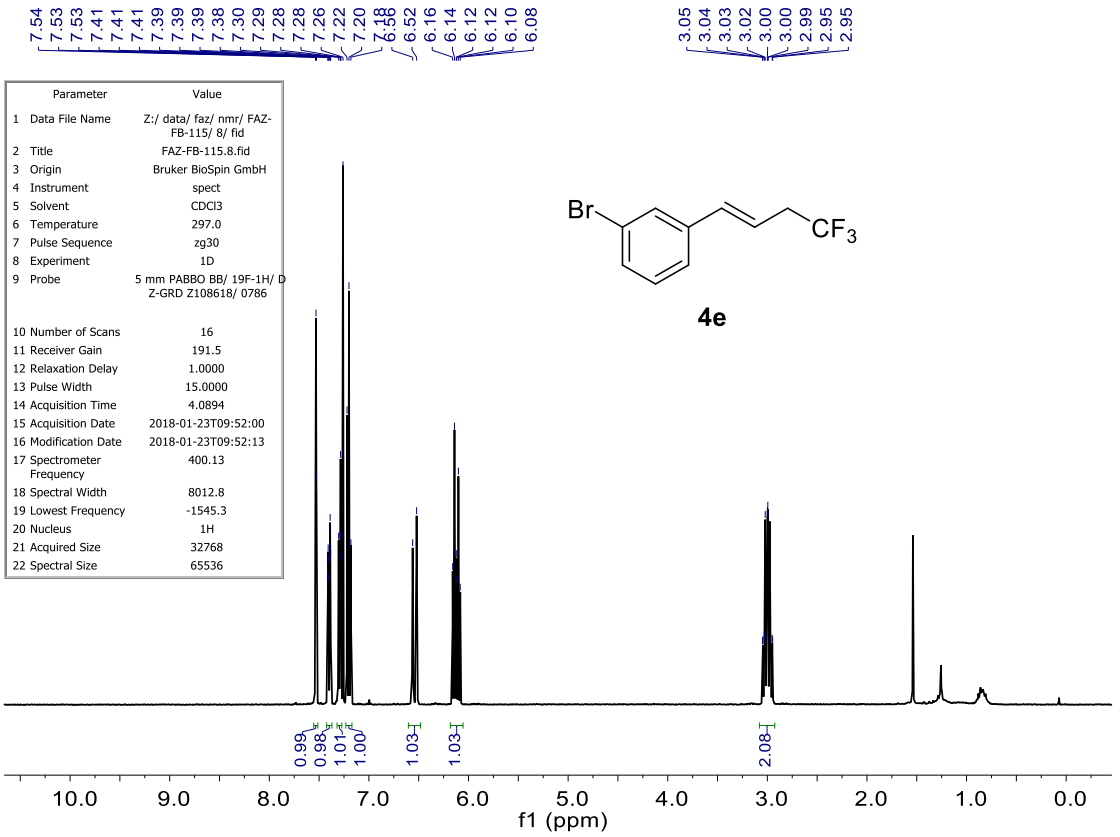


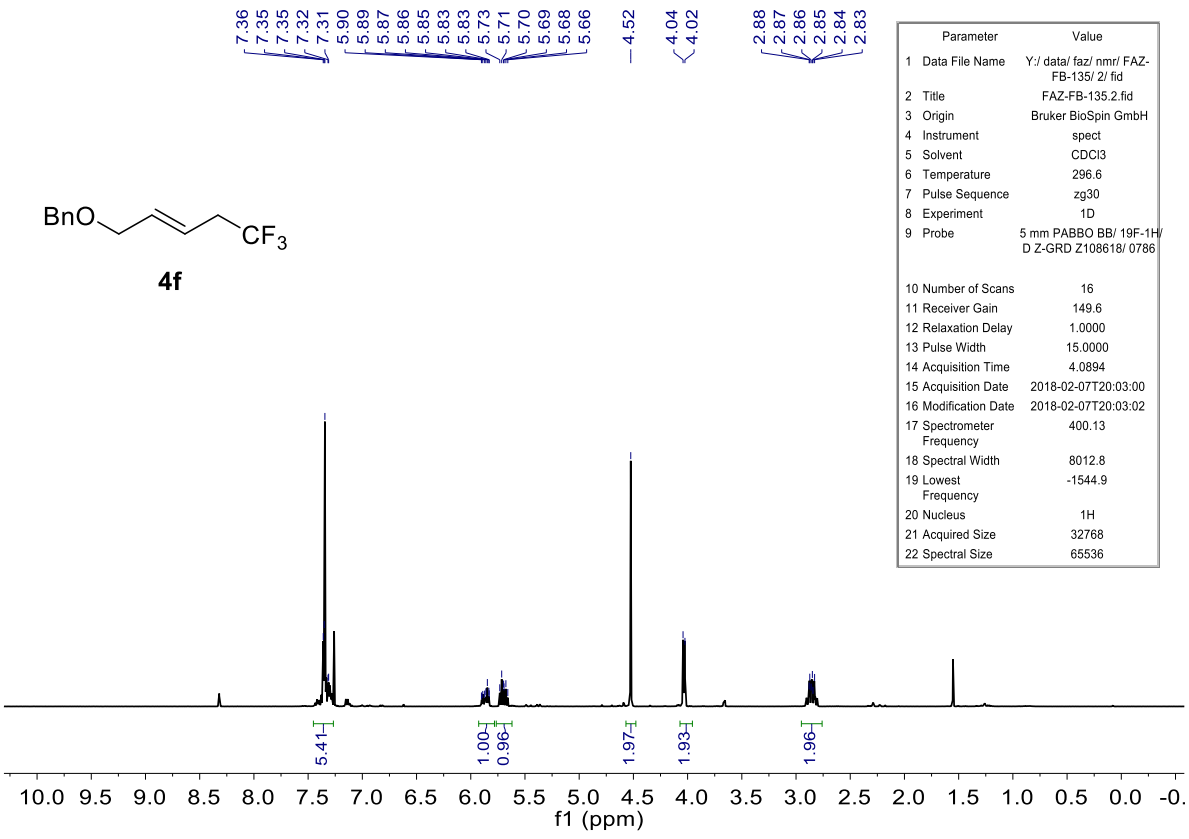
4c

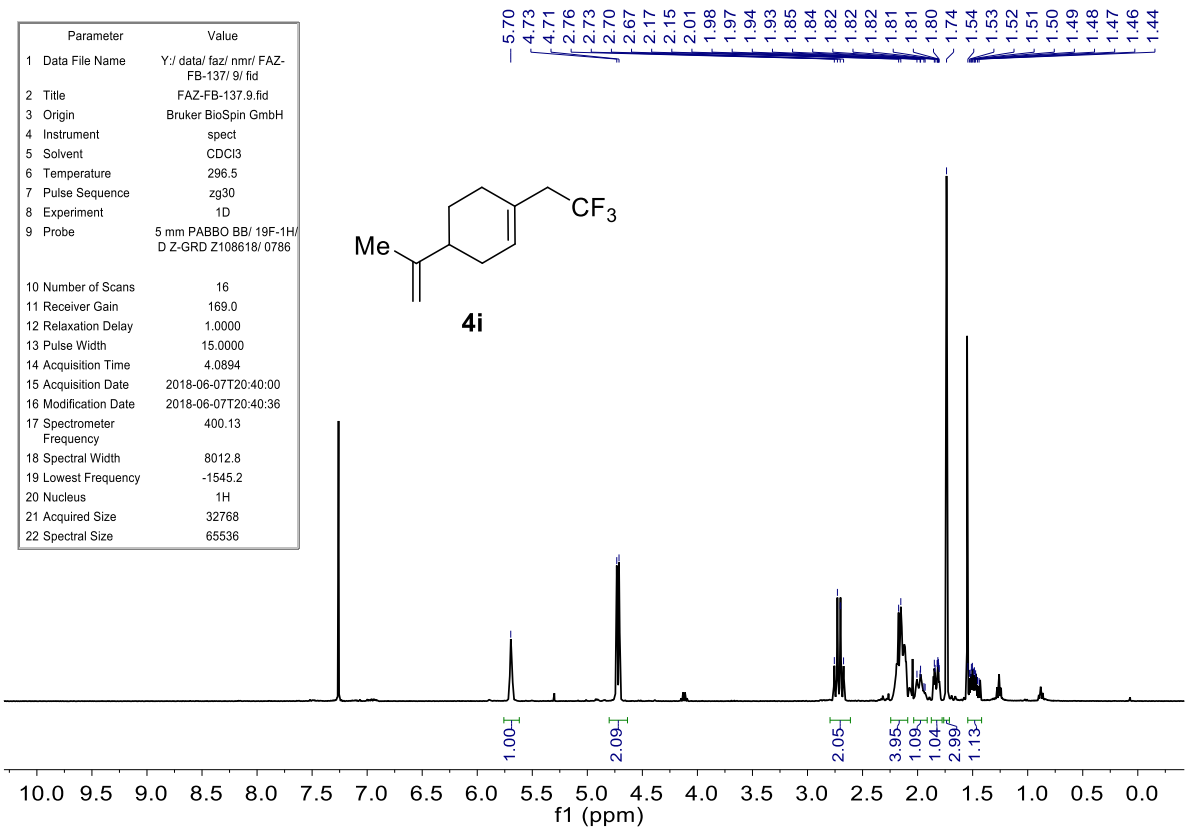
	Parameter	Value
1	Data File Name	Z:/ data/ faz/ nmr/ FAZ-FB-118/ 5/ fid
2	Title	FAZ-FB-118.5.fid
3	Origin	Bruker BioSpin GmbH
4	Instrument	spect
5	Solvent	CDCl3
6	Temperature	297.0
7	Pulse Sequence	zg30
8	Experiment	1D
9	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0786
10	Number of Scans	16
11	Receiver Gain	169.0
12	Relaxation Delay	1.0000
13	Pulse Width	15.0000
14	Acquisition Time	4.0894
15	Acquisition Date	2018-01-30T15:35:00
16	Modification Date	2018-01-30T15:35:17
17	Spectrometer Frequency	400.13
18	Spectral Width	8012.8
19	Lowest Frequency	-1545.3
20	Nucleus	1H
21	Acquired Size	32768
22	Spectral Size	65536



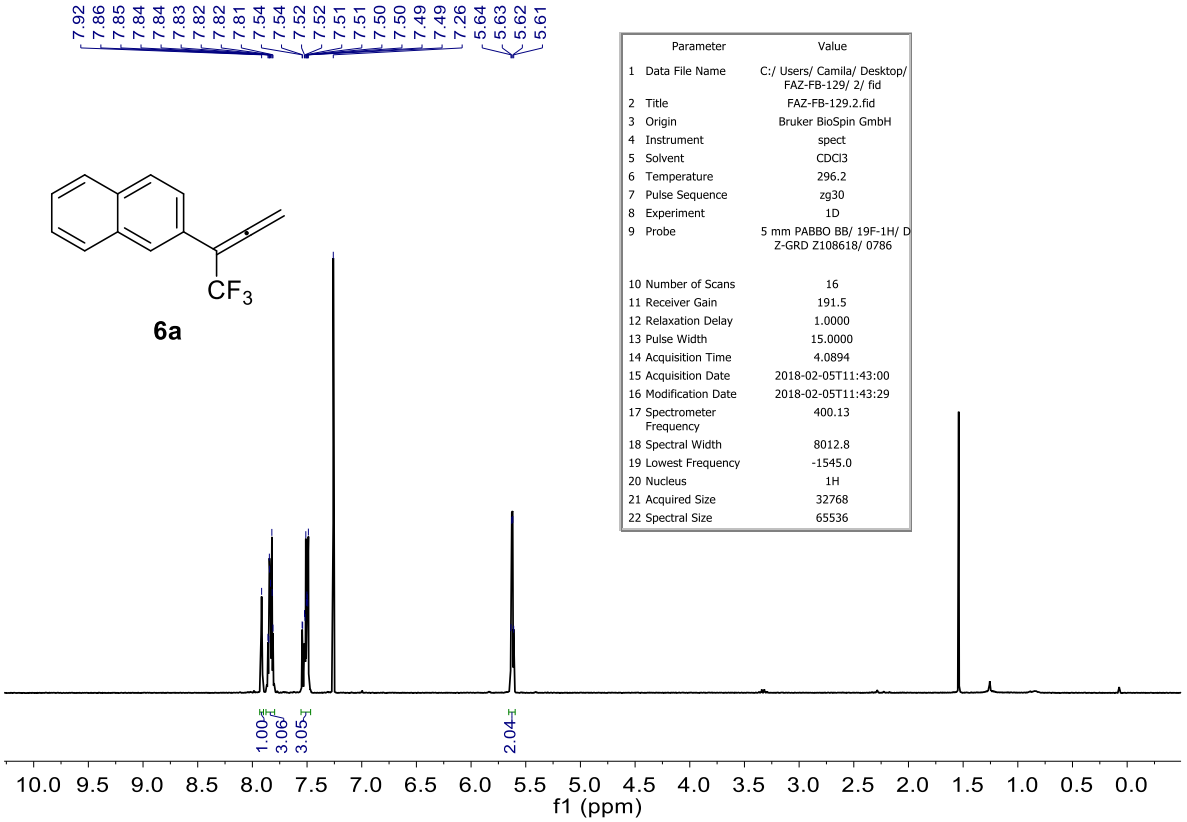
4d


7.54 7.53 7.53 7.41 7.41 7.41 7.39 7.39 7.39 7.38 7.30 7.29 7.28 7.28 7.26 7.22 7.20 7.18 6.56 6.52 6.16 6.14 6.12 6.12 6.10 6.08
3.05 3.04 3.03 3.02 3.00 3.00 2.99 2.95 2.95
Parameter Value
1 Data File Name Z:/ data/ faz/ nmr/ FAZ-FB-115/ 8/ fid
2 Title FAZ-FB-115.8.fid
3 Origin Bruker BioSpin GmbH
4 Instrument spect
5 Solvent CDCl3
6 Temperature 297.0
7 Pulse Sequence zg30
8 Experiment 1D
9 Probe 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0786
10 Number of Scans 16
11 Receiver Gain 191.5
12 Relaxation Delay 1.0000
13 Pulse Width 15.0000
14 Acquisition Time 4.0894
15 Acquisition Date 2018-01-23T09:52:00
16 Modification Date 2018-01-23T09:52:13
17 Spectrometer Frequency 400.13
18 Spectral Width 8012.8
19 Lowest Frequency -1545.3
20 Nucleus 1H
21 Acquired Size 32768
22 Spectral Size 65536
Br
CF3
4e
0.99 0.98 1.01 1.00 1.03 1.03 2.08
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)

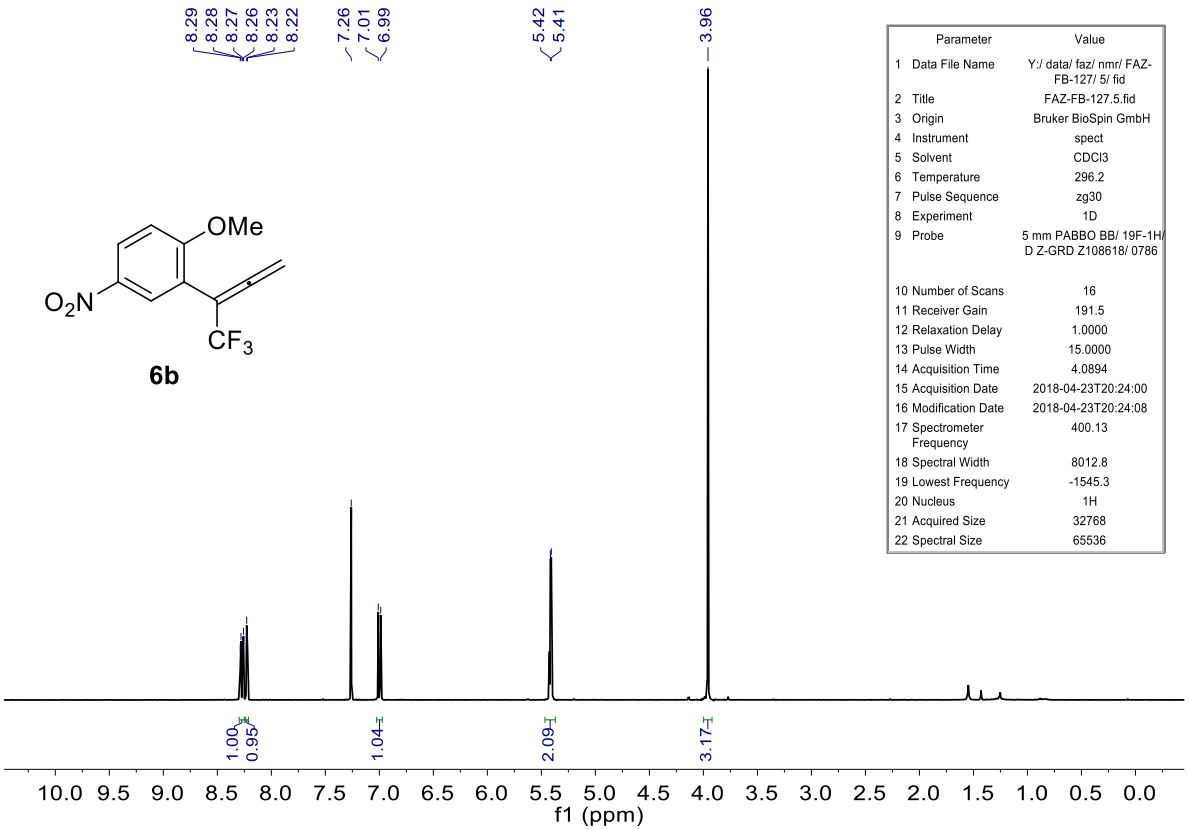

7.36 7.35 7.35 7.32 7.31 5.90 5.89 5.87 5.86 5.85 5.83 5.83 5.73 5.71 5.70 5.69 5.68 5.66 4.52 4.04 4.02 2.88 2.87 2.86 2.85 2.84 2.83
Parameter Value
1 Data File Name Y:/ data/ faz/ nmr/ FAZ-FB-135/ 2/ fid
2 Title FAZ-FB-135.2.fid
3 Origin Bruker BioSpin GmbH
4 Instrument spect
5 Solvent CDCl3
6 Temperature 296.6
7 Pulse Sequence zg30
8 Experiment 1D
9 Probe 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0786
10 Number of Scans 16
11 Receiver Gain 149.6
12 Relaxation Delay 1.0000
13 Pulse Width 15.0000
14 Acquisition Time 4.0894
15 Acquisition Date 2018-02-07T20:03:00
16 Modification Date 2018-02-07T20:03:02
17 Spectrometer Frequency 400.13
18 Spectral Width 8012.8
19 Lowest Frequency -1544.9
20 Nucleus 1H
21 Acquired Size 32768
22 Spectral Size 65536
BnO
CF3
4f
5.41 1.00 0.96 1.97 1.93 1.96
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)


Parameter Value
1 Data File Name Y:/ data/ faz/ nmr/ FAZ-FB-137/ 9/ fid
2 Title FAZ-FB-137.9.fid
3 Origin Bruker BioSpin GmbH
4 Instrument spect
5 Solvent CDCl3
6 Temperature 296.5
7 Pulse Sequence zg30
8 Experiment 1D
9 Probe 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0786
10 Number of Scans 16
11 Receiver Gain 169.0
12 Relaxation Delay 1.0000
13 Pulse Width 15.0000
14 Acquisition Time 4.0894
15 Acquisition Date 2018-06-07T20:40:00
16 Modification Date 2018-06-07T20:40:36
17 Spectrometer Frequency 400.13
18 Spectral Width 8012.8
19 Lowest Frequency -1545.2
20 Nucleus 1H
21 Acquired Size 32768
22 Spectral Size 65536
5.70 4.73 4.71 2.76 2.73 2.70 2.67 2.17 2.15 2.01 1.98 1.97 1.94 1.93 1.85 1.84 1.82 1.82 1.82 1.81 1.81 1.80 1.74 1.54 1.53 1.52 1.51 1.50 1.49 1.48 1.47 1.46 1.44
Me
CF3
4i
1.00 2.09 2.05 3.95 1.09 1.04 2.99 1.13
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

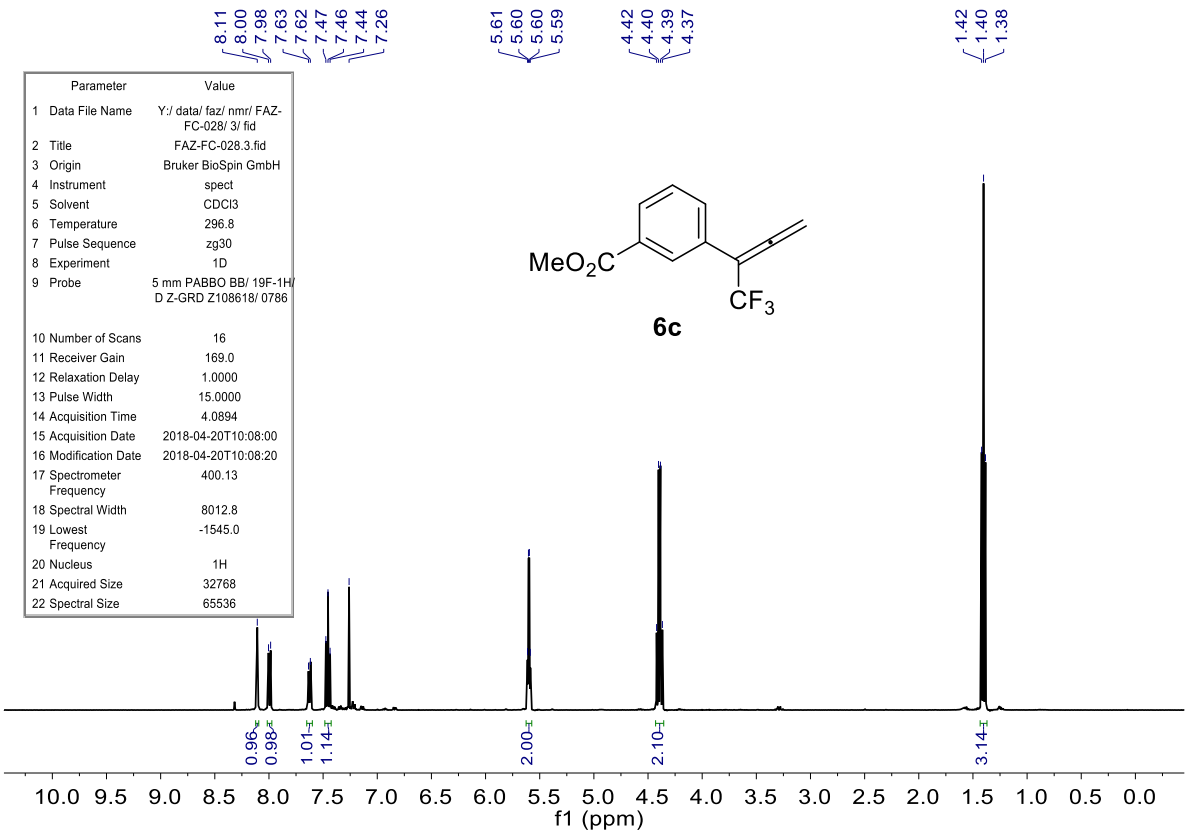
Allenyl Trifluoromethanes (Table 3)



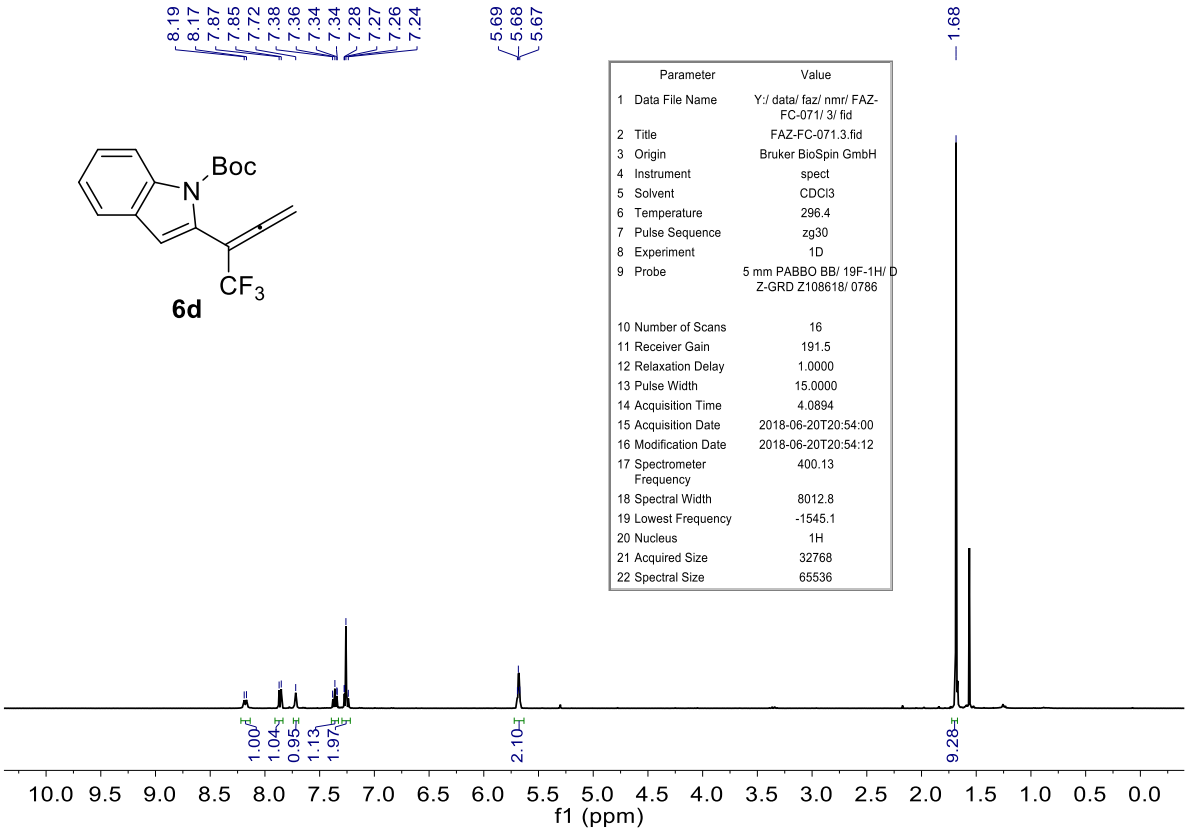
	Parameter	Value
1	Data File Name	C:/ Users/ Camila/ Desktop/ FAZ-FB-129/ 2/ fid
2	Title	FAZ-FB-129.2.fid
3	Origin	Bruker BioSpin GmbH
4	Instrument	spect
5	Solvent	CDCl3
6	Temperature	296.2
7	Pulse Sequence	zg30
8	Experiment	1D
9	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0786
10	Number of Scans	16
11	Receiver Gain	191.5
12	Relaxation Delay	1.0000
13	Pulse Width	15.0000
14	Acquisition Time	4.0894
15	Acquisition Date	2018-02-05T11:43:00
16	Modification Date	2018-02-05T11:43:29
17	Spectrometer Frequency	400.13
18	Spectral Width	8012.8
19	Lowest Frequency	-1545.0
20	Nucleus	1H
21	Acquired Size	32768
22	Spectral Size	65536



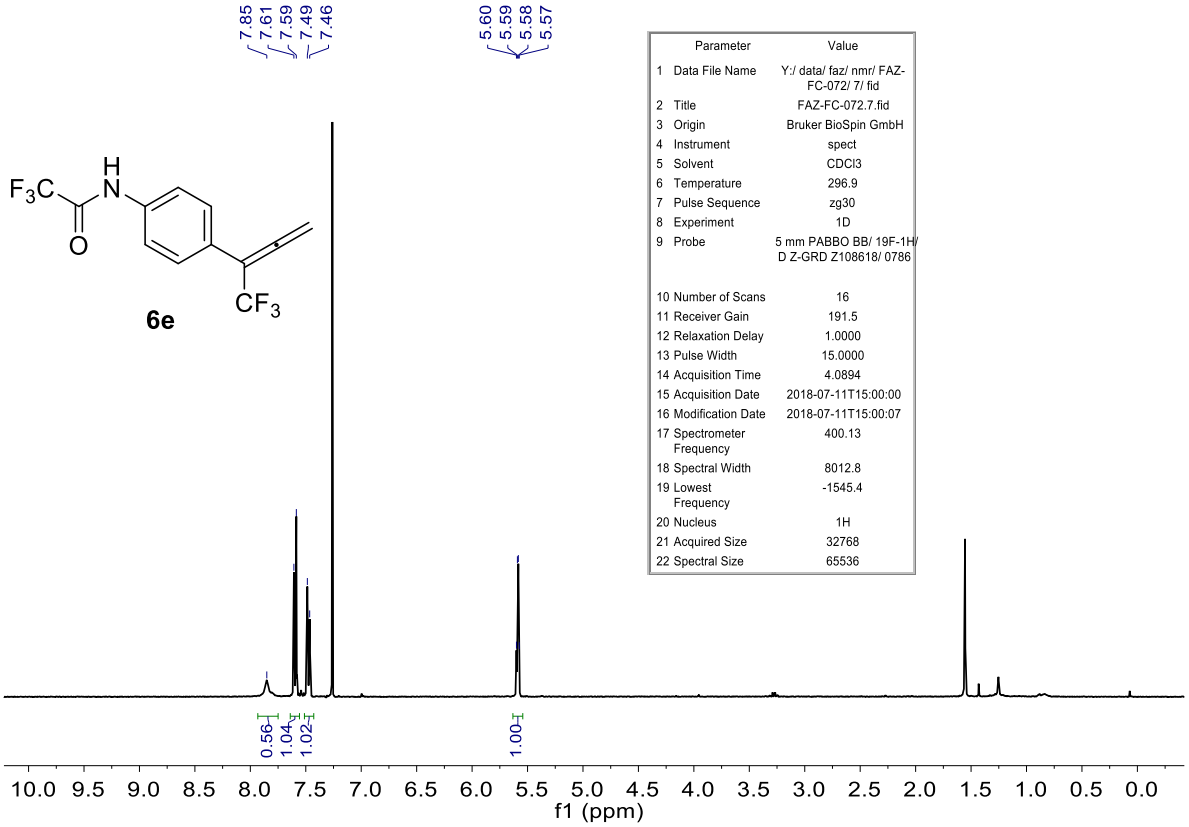
	Parameter	Value
1	Data File Name	Y:/ data/ faz/ nmr/ FAZ-FB-127/ 5/ fid
2	Title	FAZ-FB-127.5.fid
3	Origin	Bruker BioSpin GmbH
4	Instrument	spect
5	Solvent	CDCl3
6	Temperature	296.2
7	Pulse Sequence	zg30
8	Experiment	1D
9	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0786
10	Number of Scans	16
11	Receiver Gain	191.5
12	Relaxation Delay	1.0000
13	Pulse Width	15.0000
14	Acquisition Time	4.0894
15	Acquisition Date	2018-04-23T20:24:00
16	Modification Date	2018-04-23T20:24:08
17	Spectrometer Frequency	400.13
18	Spectral Width	8012.8
19	Lowest Frequency	-1545.3
20	Nucleus	1H
21	Acquired Size	32768
22	Spectral Size	65536



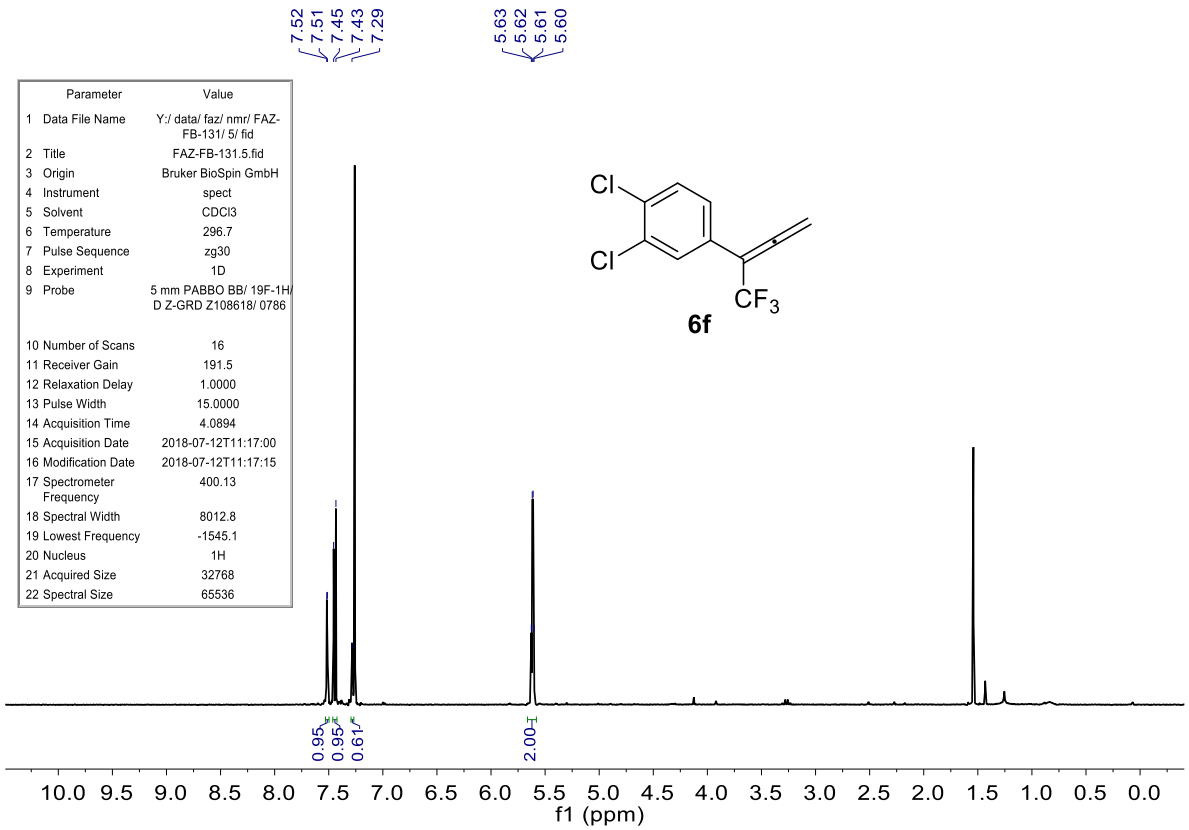
Parameter	Value
1 Data File Name	Y:/ data/ faz/ nmr/ FAZ-FC-028/ 3/ fid
2 Title	FAZ-FC-028.3.fid
3 Origin	Bruker BioSpin GmbH
4 Instrument	spect
5 Solvent	CDCl3
6 Temperature	296.8
7 Pulse Sequence	zg30
8 Experiment	1D
9 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0786
10 Number of Scans	16
11 Receiver Gain	169.0
12 Relaxation Delay	1.0000
13 Pulse Width	15.0000
14 Acquisition Time	4.0894
15 Acquisition Date	2018-04-20T10:08:00
16 Modification Date	2018-04-20T10:08:20
17 Spectrometer Frequency	400.13
18 Spectral Width	8012.8
19 Lowest Frequency	-1545.0
20 Nucleus	1H
21 Acquired Size	32768
22 Spectral Size	65536



Parameter	Value
1 Data File Name	Y:/ data/ faz/ nmr/ FAZ-FC-071/ 3/ fid
2 Title	FAZ-FC-071.3.fid
3 Origin	Bruker BioSpin GmbH
4 Instrument	spect
5 Solvent	CDCl3
6 Temperature	296.4
7 Pulse Sequence	zg30
8 Experiment	1D
9 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0786
10 Number of Scans	16
11 Receiver Gain	191.5
12 Relaxation Delay	1.0000
13 Pulse Width	15.0000
14 Acquisition Time	4.0894
15 Acquisition Date	2018-06-20T20:54:00
16 Modification Date	2018-06-20T20:54:12
17 Spectrometer Frequency	400.13
18 Spectral Width	8012.8
19 Lowest Frequency	-1545.1
20 Nucleus	1H
21 Acquired Size	32768
22 Spectral Size	65536

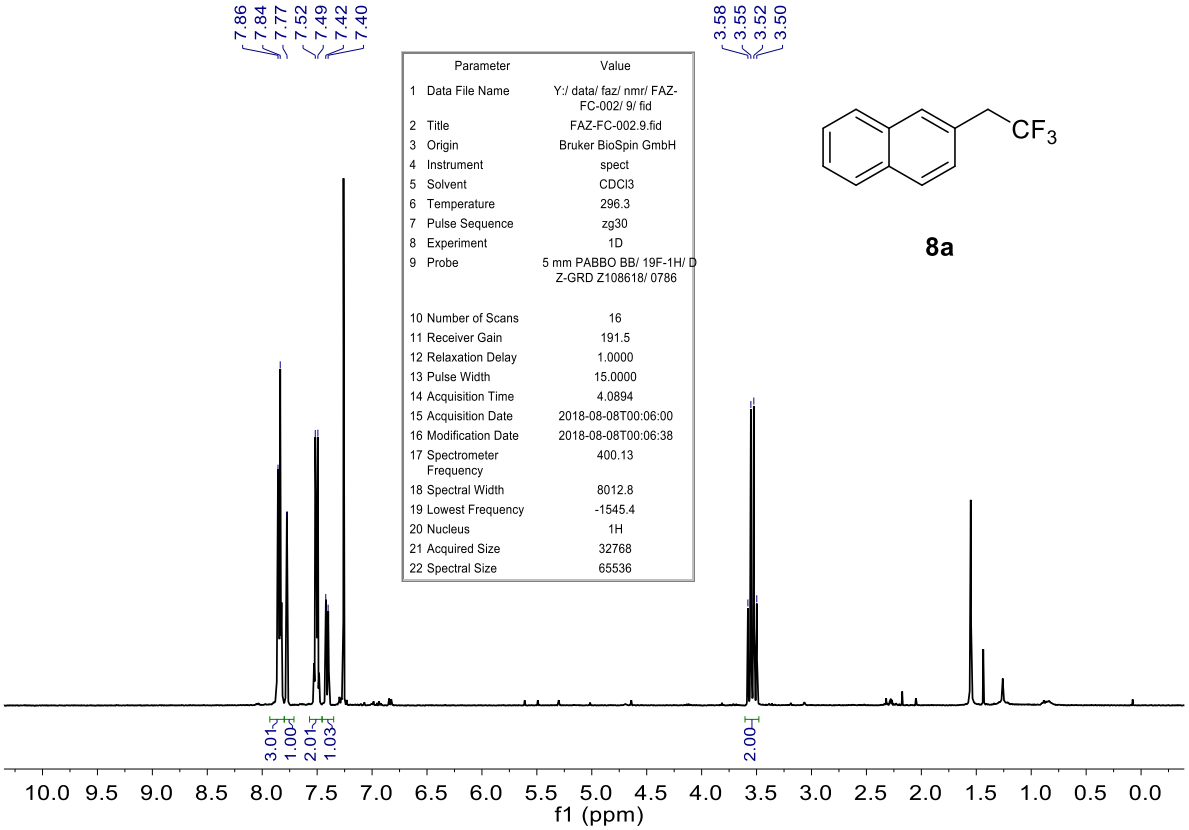


	Parameter	Value
1	Data File Name	Y:/ data/ faz/ nmr/ FAZ-FC-072/ 7/ fid
2	Title	FAZ-FC-072.7.fid
3	Origin	Bruker BioSpin GmbH
4	Instrument	spect
5	Solvent	CDCl3
6	Temperature	296.9
7	Pulse Sequence	zg30
8	Experiment	1D
9	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0786
10	Number of Scans	16
11	Receiver Gain	191.5
12	Relaxation Delay	1.0000
13	Pulse Width	15.0000
14	Acquisition Time	4.0894
15	Acquisition Date	2018-07-11T15:00:00
16	Modification Date	2018-07-11T15:00:07
17	Spectrometer Frequency	400.13
18	Spectral Width	8012.8
19	Lowest Frequency	-1545.4
20	Nucleus	1H
21	Acquired Size	32768
22	Spectral Size	65536

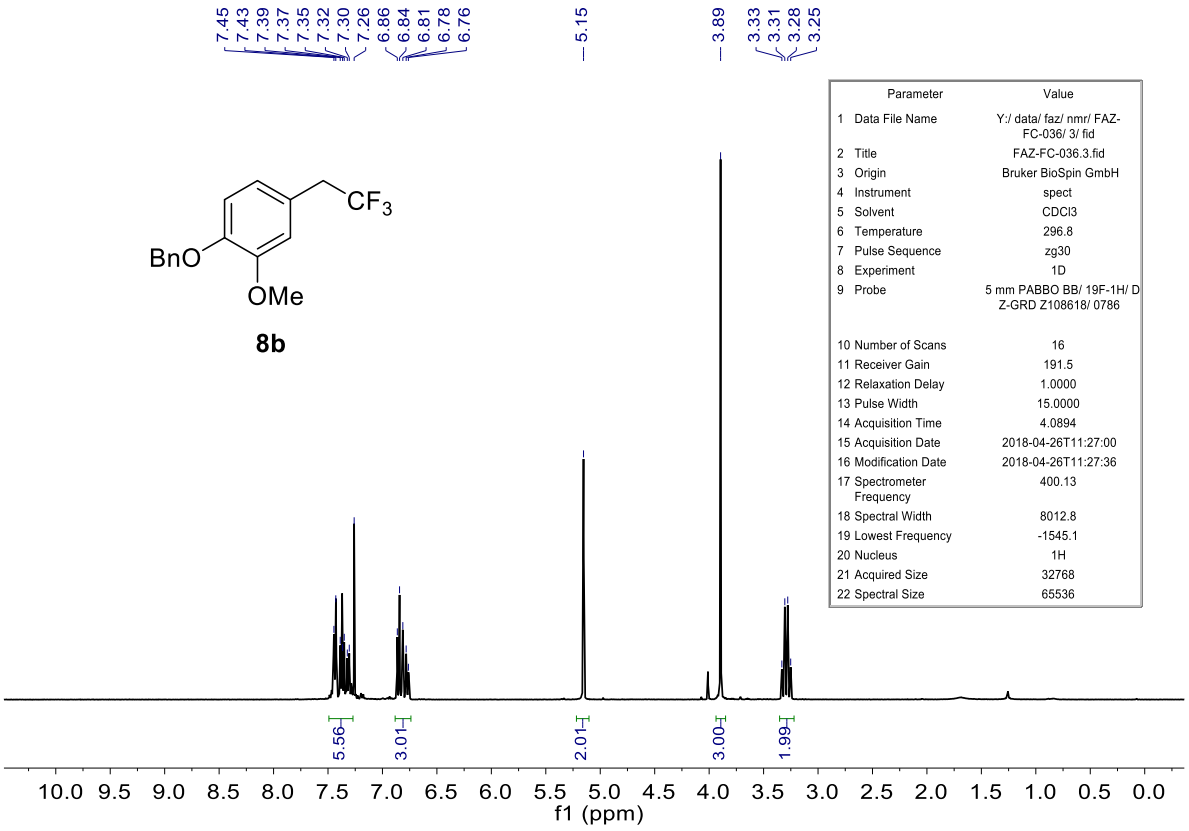


	Parameter	Value
1	Data File Name	Y:/ data/ faz/ nmr/ FAZ-FB-131/ 5/ fid
2	Title	FAZ-FB-131.5.fid
3	Origin	Bruker BioSpin GmbH
4	Instrument	spect
5	Solvent	CDCl3
6	Temperature	296.7
7	Pulse Sequence	zg30
8	Experiment	1D
9	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0786
10	Number of Scans	16
11	Receiver Gain	191.5
12	Relaxation Delay	1.0000
13	Pulse Width	15.0000
14	Acquisition Time	4.0894
15	Acquisition Date	2018-07-12T11:17:00
16	Modification Date	2018-07-12T11:17:15
17	Spectrometer Frequency	400.13
18	Spectral Width	8012.8
19	Lowest Frequency	-1545.1
20	Nucleus	1H
21	Acquired Size	32768
22	Spectral Size	65536

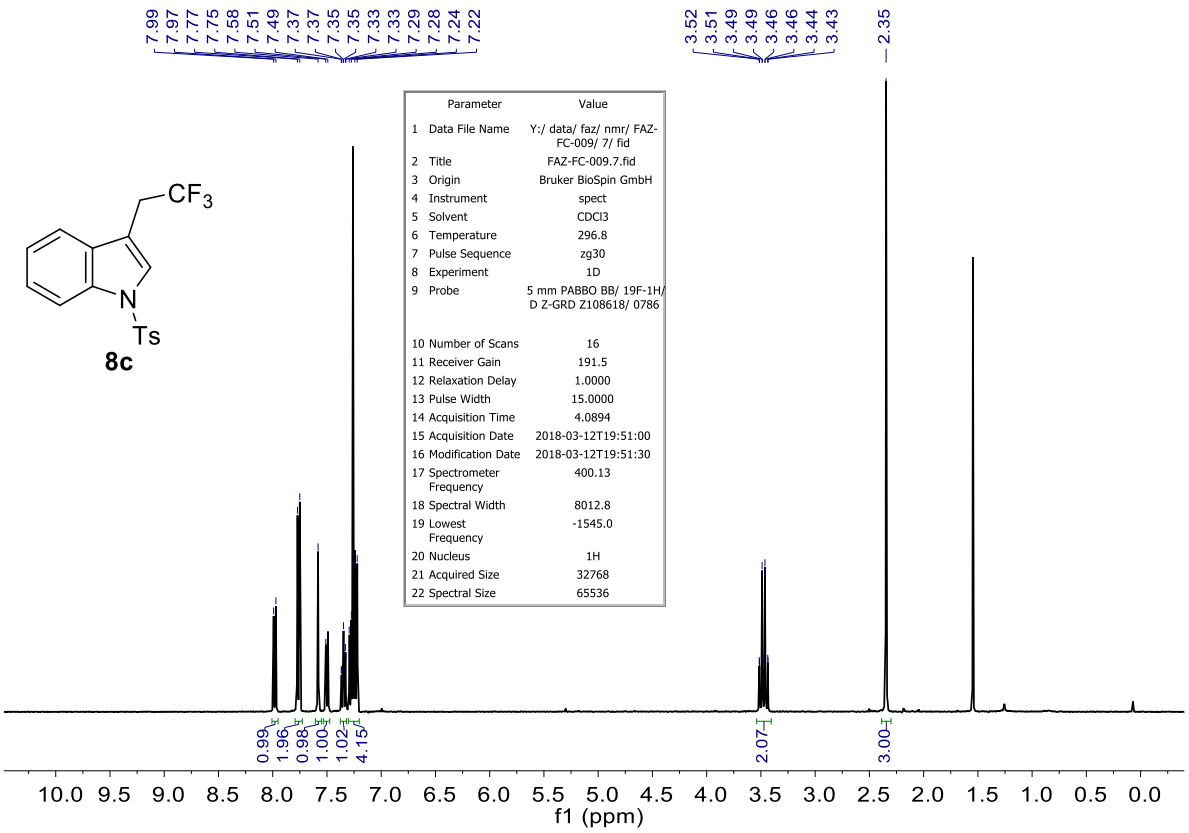
Benzyl Trifluoromethanes (Table 4)

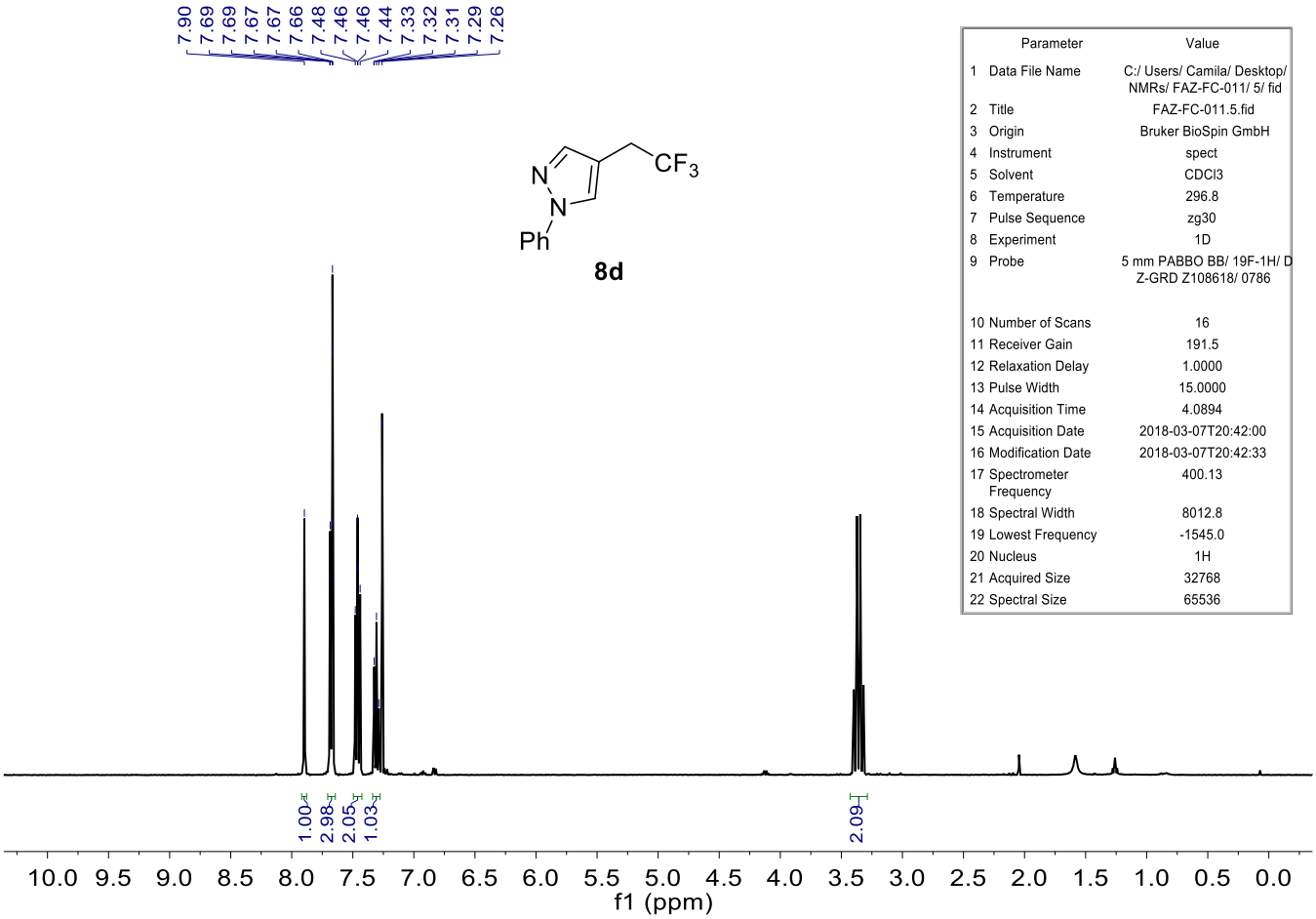


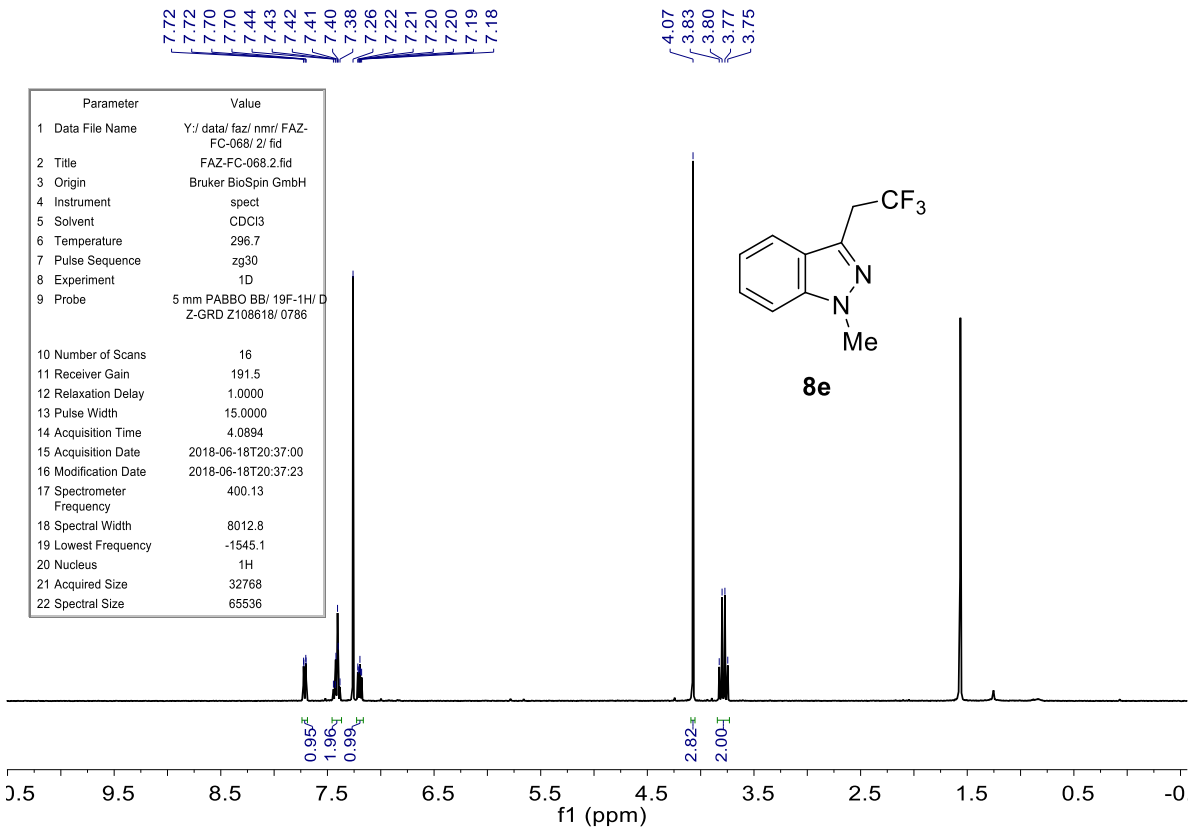
Parameter	Value
1 Data File Name	Y:/ data/ faz/ nmr/ FAZ-FC-002/ 9/ fid
2 Title	FAZ-FC-002.9.fid
3 Origin	Bruker BioSpin GmbH
4 Instrument	spect
5 Solvent	CDCl3
6 Temperature	296.3
7 Pulse Sequence	zg30
8 Experiment	1D
9 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0786
10 Number of Scans	16
11 Receiver Gain	191.5
12 Relaxation Delay	1.0000
13 Pulse Width	15.0000
14 Acquisition Time	4.0894
15 Acquisition Date	2018-08-08T00:06:00
16 Modification Date	2018-08-08T00:06:38
17 Spectrometer Frequency	400.13
18 Spectral Width	8012.8
19 Lowest Frequency	-1545.4
20 Nucleus	1H
21 Acquired Size	32768
22 Spectral Size	65536

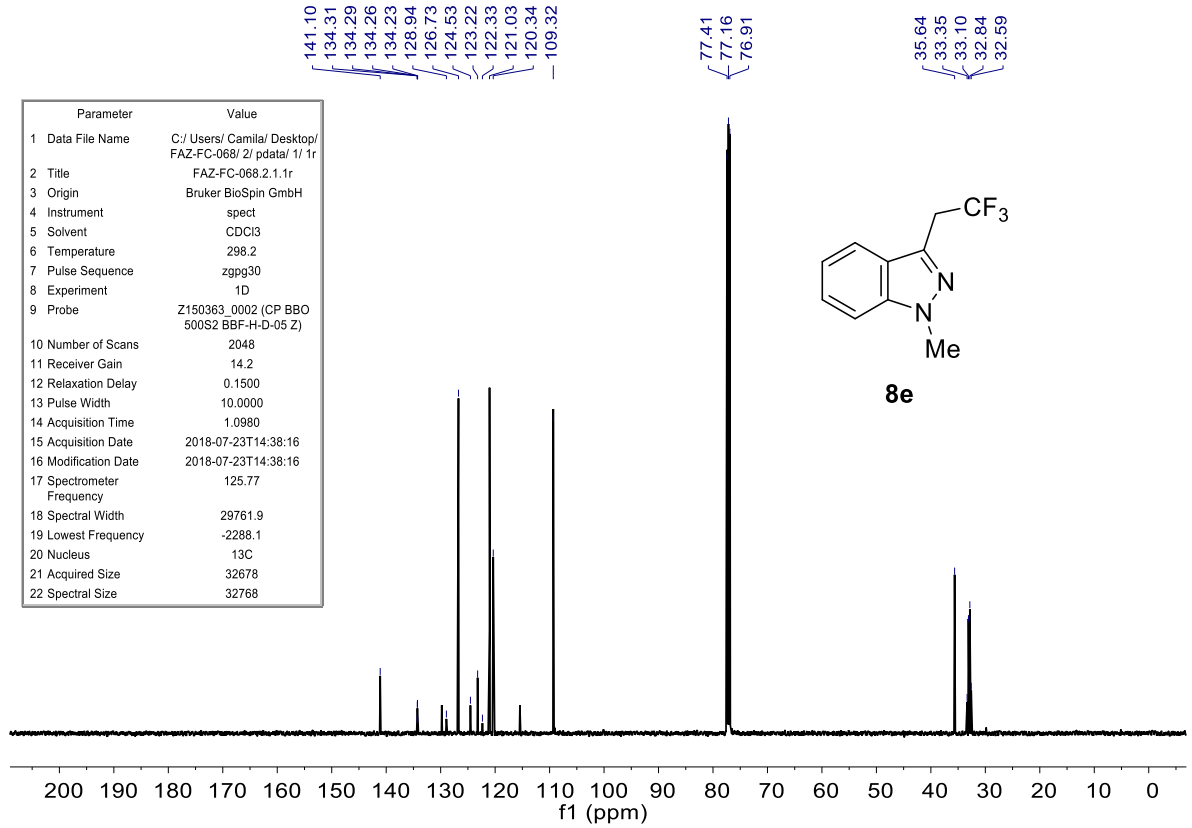


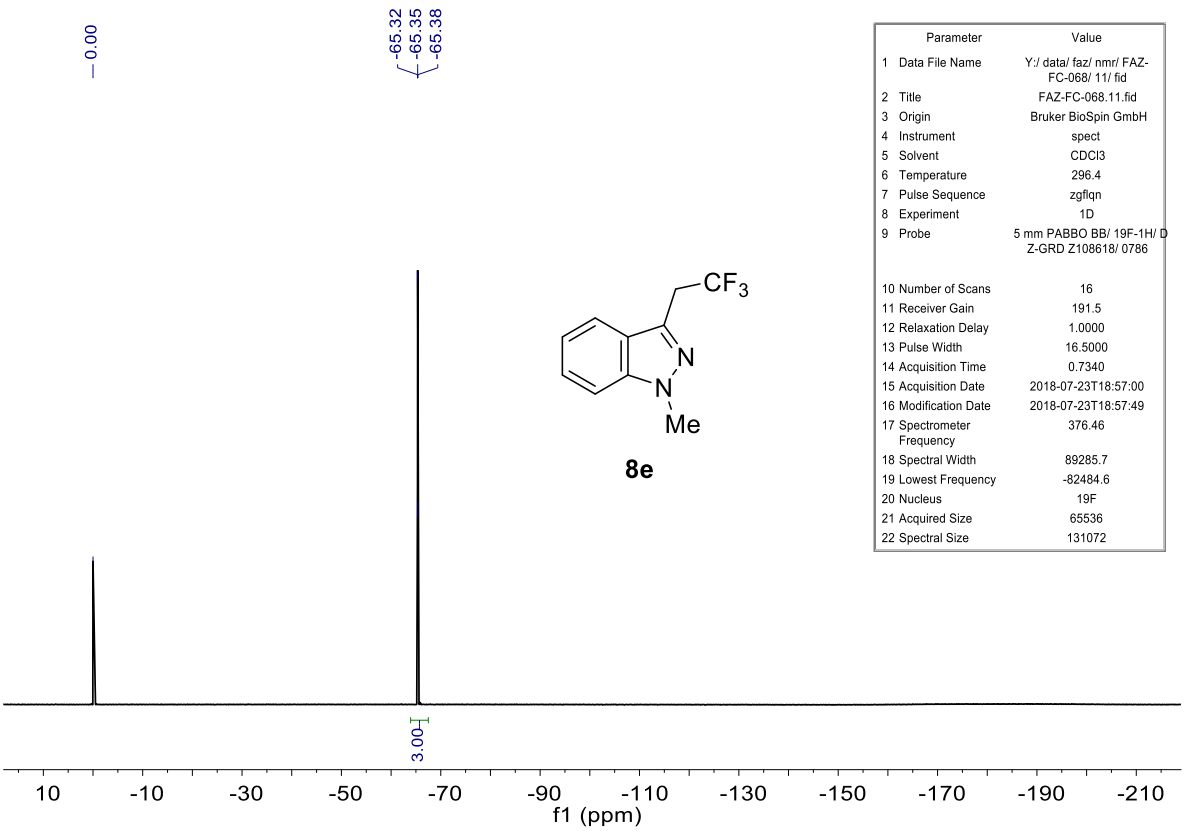
Parameter	Value
1 Data File Name	Y:/ data/ faz/ nmr/ FAZ-FC-036/ 3/ fid
2 Title	FAZ-FC-036.3.fid
3 Origin	Bruker BioSpin GmbH
4 Instrument	spect
5 Solvent	CDCl3
6 Temperature	296.8
7 Pulse Sequence	zg30
8 Experiment	1D
9 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0786
10 Number of Scans	16
11 Receiver Gain	191.5
12 Relaxation Delay	1.0000
13 Pulse Width	15.0000
14 Acquisition Time	4.0894
15 Acquisition Date	2018-04-26T11:27:00
16 Modification Date	2018-04-26T11:27:36
17 Spectrometer Frequency	400.13
18 Spectral Width	8012.8
19 Lowest Frequency	-1545.1
20 Nucleus	1H
21 Acquired Size	32768
22 Spectral Size	65536


7.99
7.97
7.77
7.75
7.58
7.51
7.49
7.37
7.37
7.35
7.35
7.33
7.33
7.29
7.28
7.24
7.22
3.52
3.51
3.49
3.49
3.46
3.46
3.44
3.43
2.35
CF3
N
Ts
8c
Parameter Value
1 Data File Name Y:/ data/ faz/ nmr/ FAZ-FC-009/ 7/ fid
2 Title FAZ-FC-009.7.fid
3 Origin Bruker BioSpin GmbH
4 Instrument spect
5 Solvent CDCl3
6 Temperature 296.8
7 Pulse Sequence zg30
8 Experiment 1D
9 Probe 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0786
10 Number of Scans 16
11 Receiver Gain 191.5
12 Relaxation Delay 1.0000
13 Pulse Width 15.0000
14 Acquisition Time 4.0894
15 Acquisition Date 2018-03-12T19:51:00
16 Modification Date 2018-03-12T19:51:30
17 Spectrometer Frequency 400.13
18 Spectral Width 8012.8
19 Lowest Frequency -1545.0
20 Nucleus 1H
21 Acquired Size 32768
22 Spectral Size 65536
0.99
1.96
0.98
1.00
1.02
4.15
2.07
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


7.90
7.69
7.69
7.67
7.67
7.66
7.48
7.46
7.46
7.44
7.33
7.32
7.31
7.29
7.26
N
N
Ph
CF3
8d
Parameter Value
1 Data File Name C:/ Users/ Camila/ Desktop/ NMRs/ FAZ-FC-011/ 5/ fid
2 Title FAZ-FC-011.5.fid
3 Origin Bruker BioSpin GmbH
4 Instrument spect
5 Solvent CDCl3
6 Temperature 296.8
7 Pulse Sequence zg30
8 Experiment 1D
9 Probe 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0786
10 Number of Scans 16
11 Receiver Gain 191.5
12 Relaxation Delay 1.0000
13 Pulse Width 15.0000
14 Acquisition Time 4.0894
15 Acquisition Date 2018-03-07T20:42:00
16 Modification Date 2018-03-07T20:42:33
17 Spectrometer Frequency 400.13
18 Spectral Width 8012.8
19 Lowest Frequency -1545.0
20 Nucleus 1H
21 Acquired Size 32768
22 Spectral Size 65536
1.00
2.98
2.05
1.03
2.09
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


7.72
7.72
7.70
7.70
7.44
7.43
7.42
7.41
7.40
7.38
7.26
7.22
7.21
7.20
7.20
7.19
7.18
4.07
3.83
3.80
3.77
3.75
Parameter Value
1 Data File Name Y:/ data/ faz/ nmr/ FAZ-FC-068/ 2/ fid
2 Title FAZ-FC-068.2.fid
3 Origin Bruker BioSpin GmbH
4 Instrument spect
5 Solvent CDCl3
6 Temperature 296.7
7 Pulse Sequence zg30
8 Experiment 1D
9 Probe 5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0786
10 Number of Scans 16
11 Receiver Gain 191.5
12 Relaxation Delay 1.0000
13 Pulse Width 15.0000
14 Acquisition Time 4.0894
15 Acquisition Date 2018-06-18T20:37:00
16 Modification Date 2018-06-18T20:37:23
17 Spectrometer Frequency 400.13
18 Spectral Width 8012.8
19 Lowest Frequency -1545.1
20 Nucleus 1H
21 Acquired Size 32768
22 Spectral Size 65536
CF3
N
N
Me
8e
0.95
1.96
0.99
2.82
2.00
f1 (ppm)


141.10
134.31
134.29
134.26
134.23
128.94
126.73
124.53
123.22
122.33
121.03
120.34
109.32
77.41
77.16
76.91
35.64
33.35
33.10
32.84
32.59
Parameter Value
1 Data File Name C:/ Users/ Camila/ Desktop/ FAZ-FC-068/ 2/ pdata/ 1/ 1r
2 Title FAZ-FC-068.2.1.1r
3 Origin Bruker BioSpin GmbH
4 Instrument spect
5 Solvent CDCl3
6 Temperature 298.2
7 Pulse Sequence zgpg30
8 Experiment 1D
9 Probe Z150363_0002 (CP BBO 500S2 BBF-H-D-05 Z)
10 Number of Scans 2048
11 Receiver Gain 14.2
12 Relaxation Delay 0.1500
13 Pulse Width 10.0000
14 Acquisition Time 1.0980
15 Acquisition Date 2018-07-23T14:38:16
16 Modification Date 2018-07-23T14:38:16
17 Spectrometer Frequency 125.77
18 Spectral Width 29761.9
19 Lowest Frequency -2288.1
20 Nucleus 13C
21 Acquired Size 32678
22 Spectral Size 32768
CF3
N
N
Me
8e
f1 (ppm)



	Parameter	Value
1	Data File Name	Y:/ data/ faz/ nmr/ FAZ-FC-068/ 11/ fid
2	Title	FAZ-FC-068.11.fid
3	Origin	Bruker BioSpin GmbH
4	Instrument	spect
5	Solvent	CDCl3
6	Temperature	296.4
7	Pulse Sequence	zgflqn
8	Experiment	1D
9	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0786
10	Number of Scans	16
11	Receiver Gain	191.5
12	Relaxation Delay	1.0000
13	Pulse Width	16.5000
14	Acquisition Time	0.7340
15	Acquisition Date	2018-07-23T18:57:00
16	Modification Date	2018-07-23T18:57:49
17	Spectrometer Frequency	376.46
18	Spectral Width	89285.7
19	Lowest Frequency	-82484.6
20	Nucleus	19F
21	Acquired Size	65536
22	Spectral Size	131072

Synthetic Applications (Scheme 1)