

Supporting Information

Ruthenium-catalyzed regioselective allylic amination of 2,3,3-trifluoroallylic carbonates

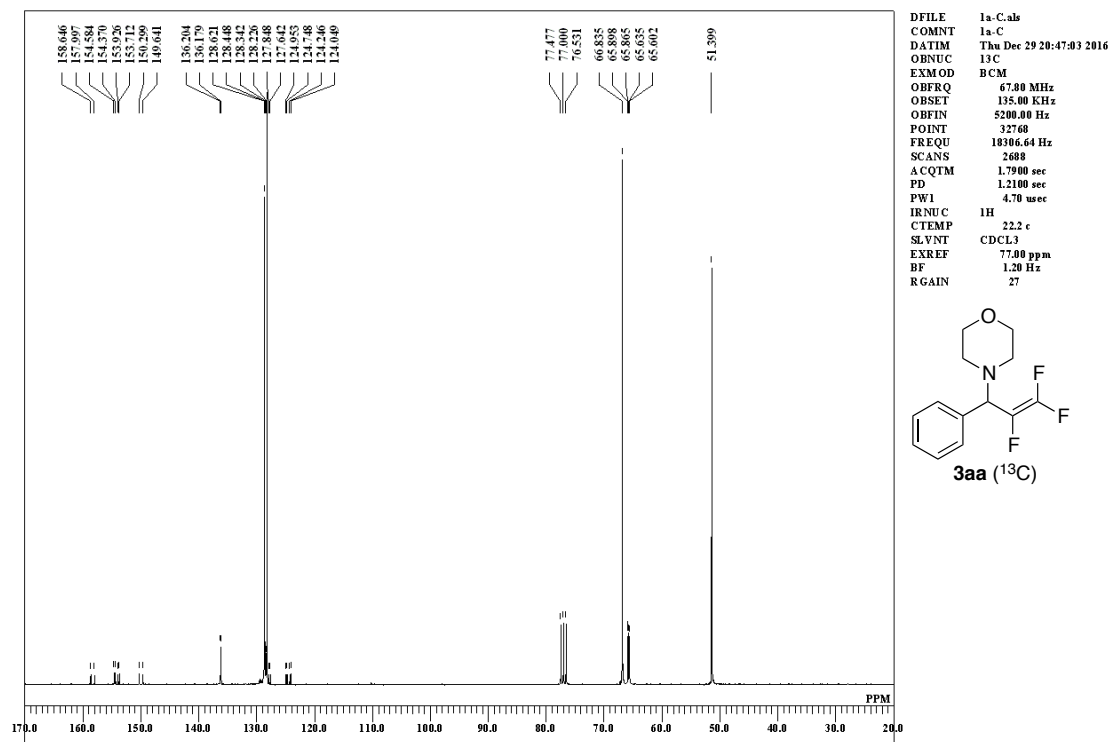
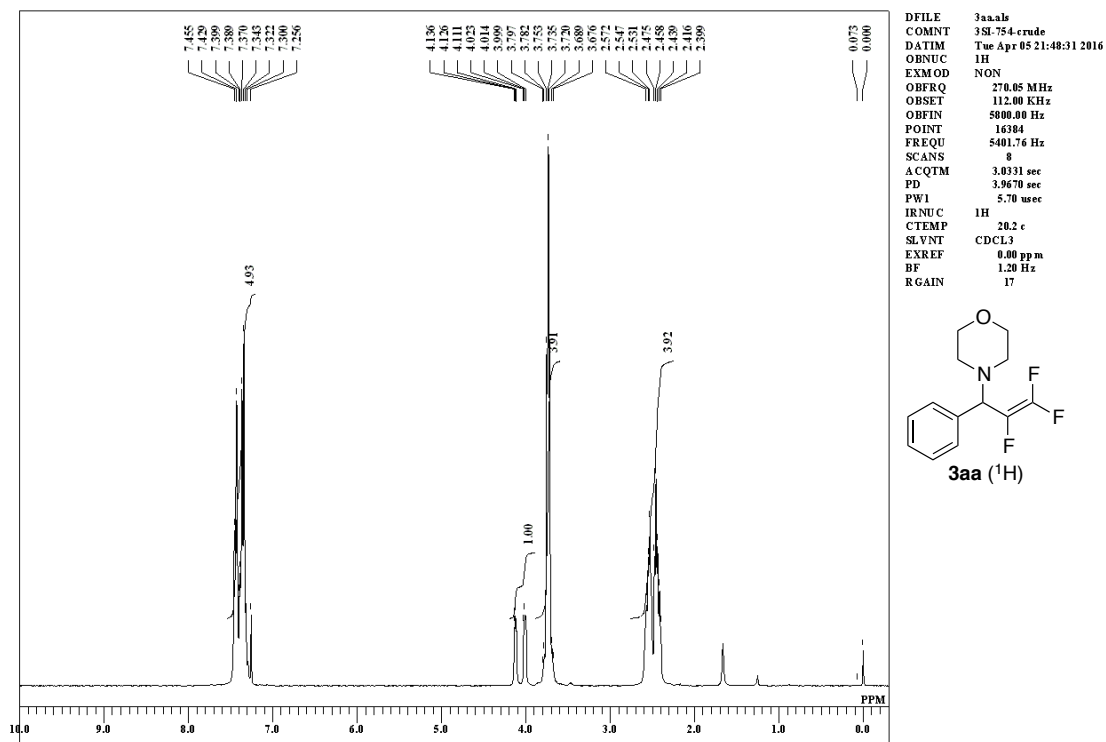
Shin-ichi Isobe, Shou Terasaki, Taisyun Hanakawa, Shota Mizuno and Motoi Kawatsura*

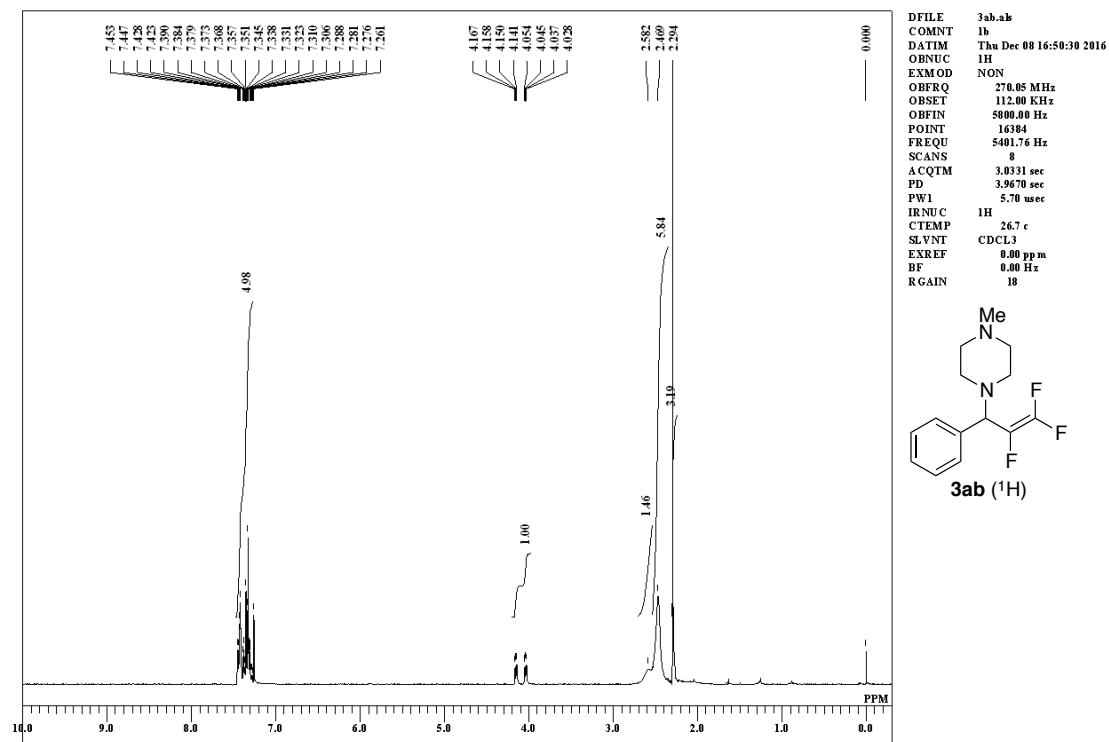
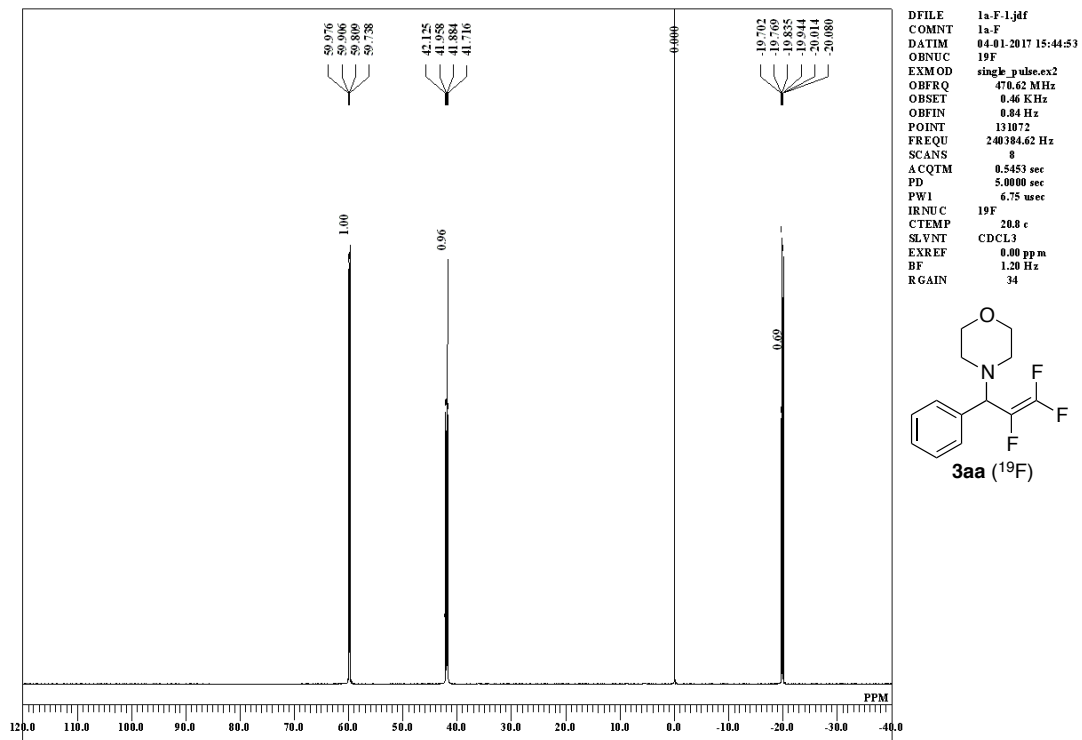
Department of Chemistry, College of Humanities & Sciences, Nihon University, Sakurajosui, Setagaya-ku, Tokyo 156-8550, Japan

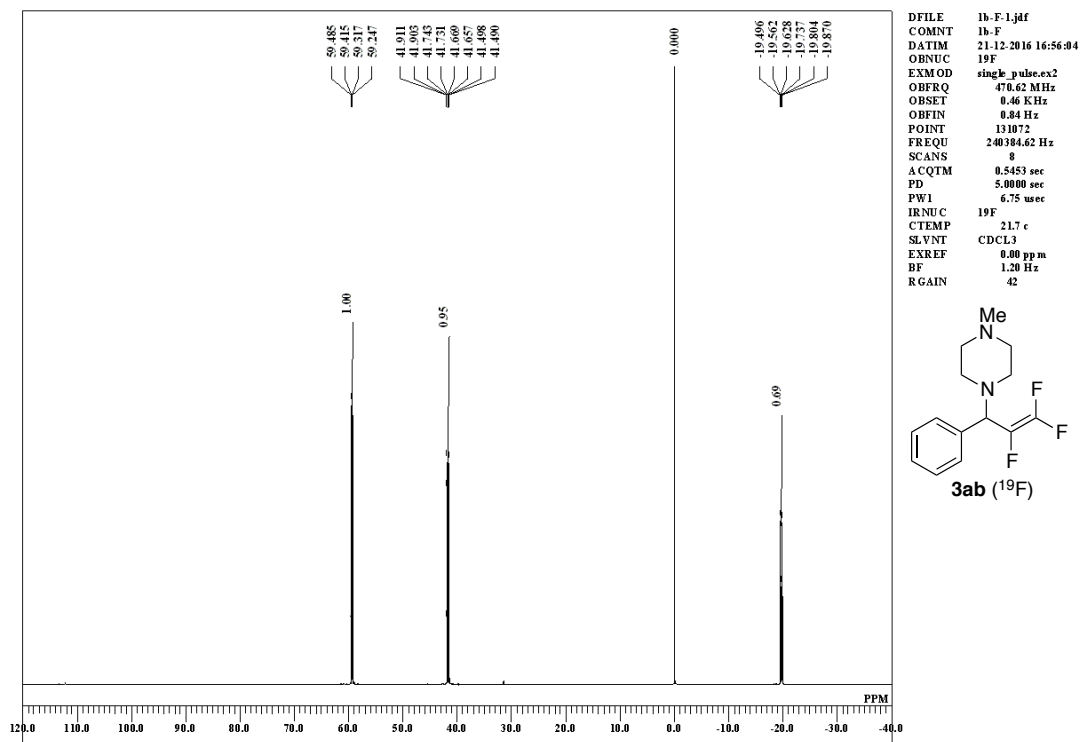
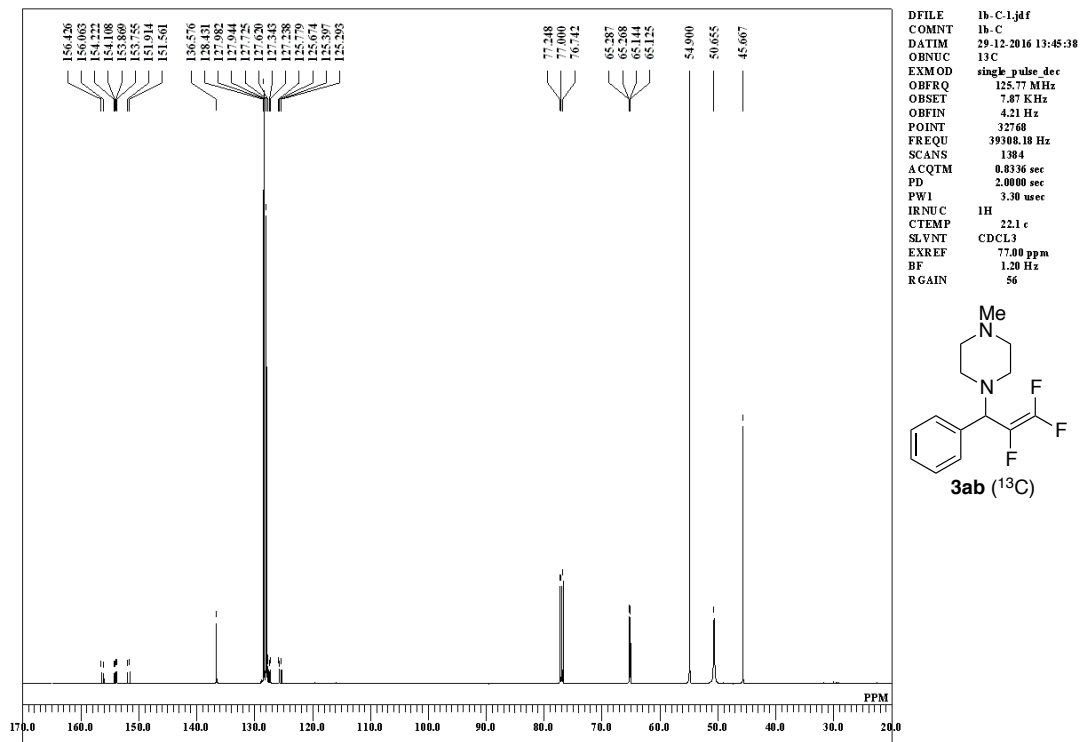
kawatsur@chs.nihon-u.ac.jp

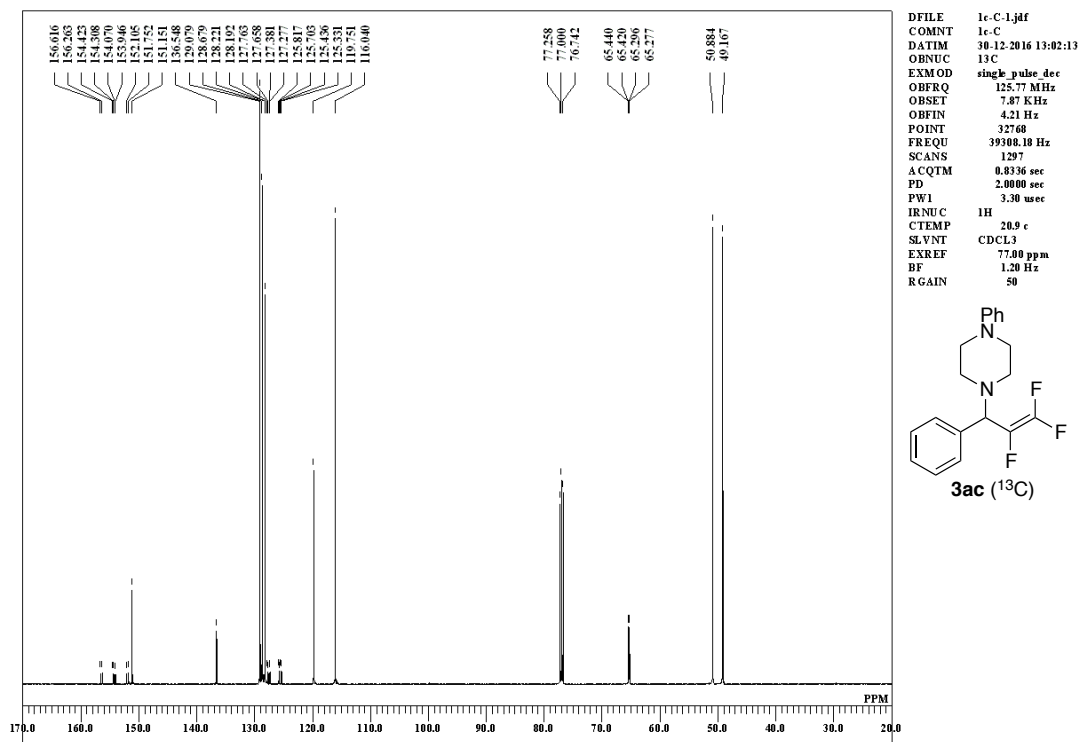
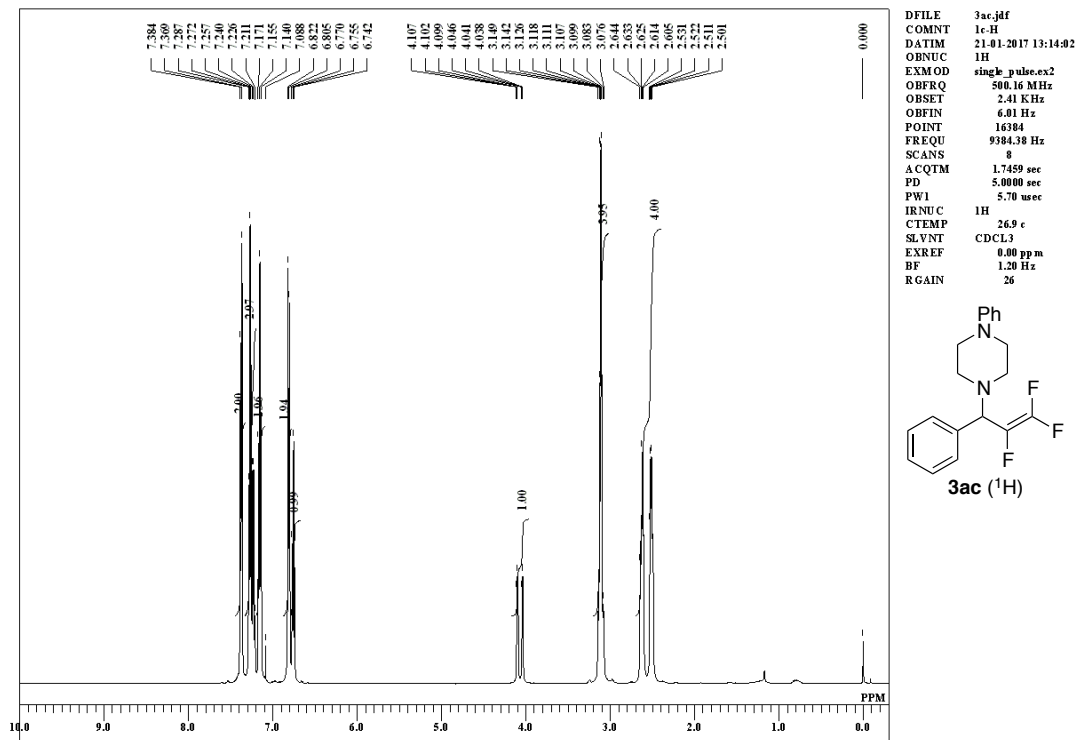
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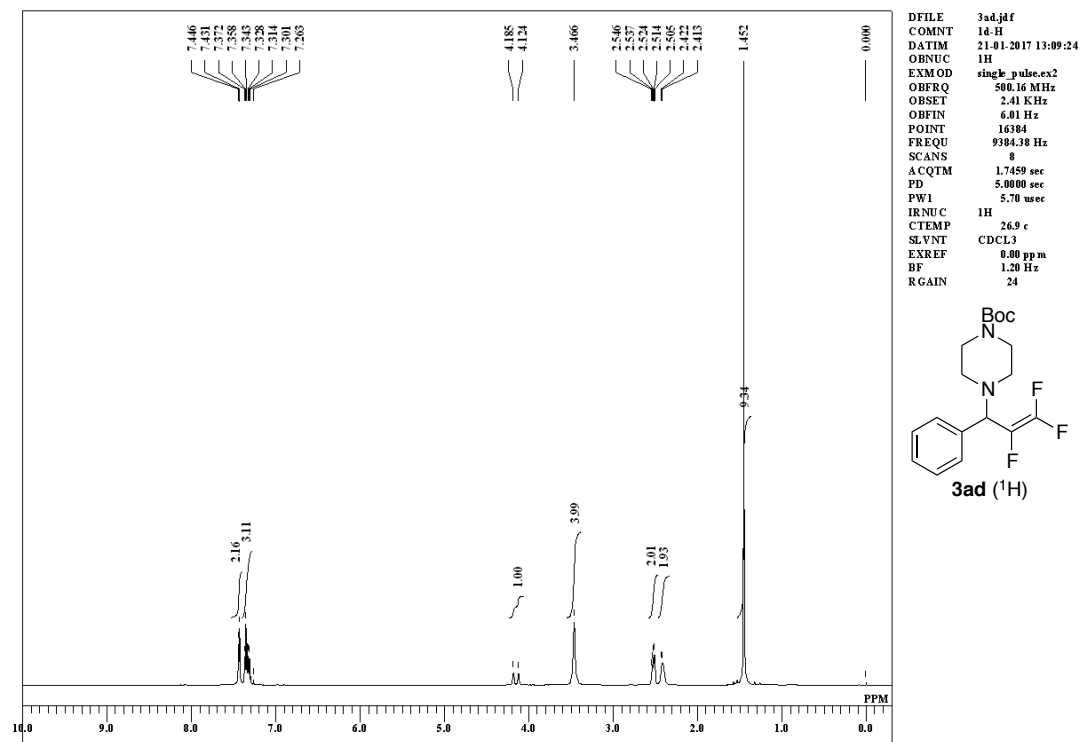
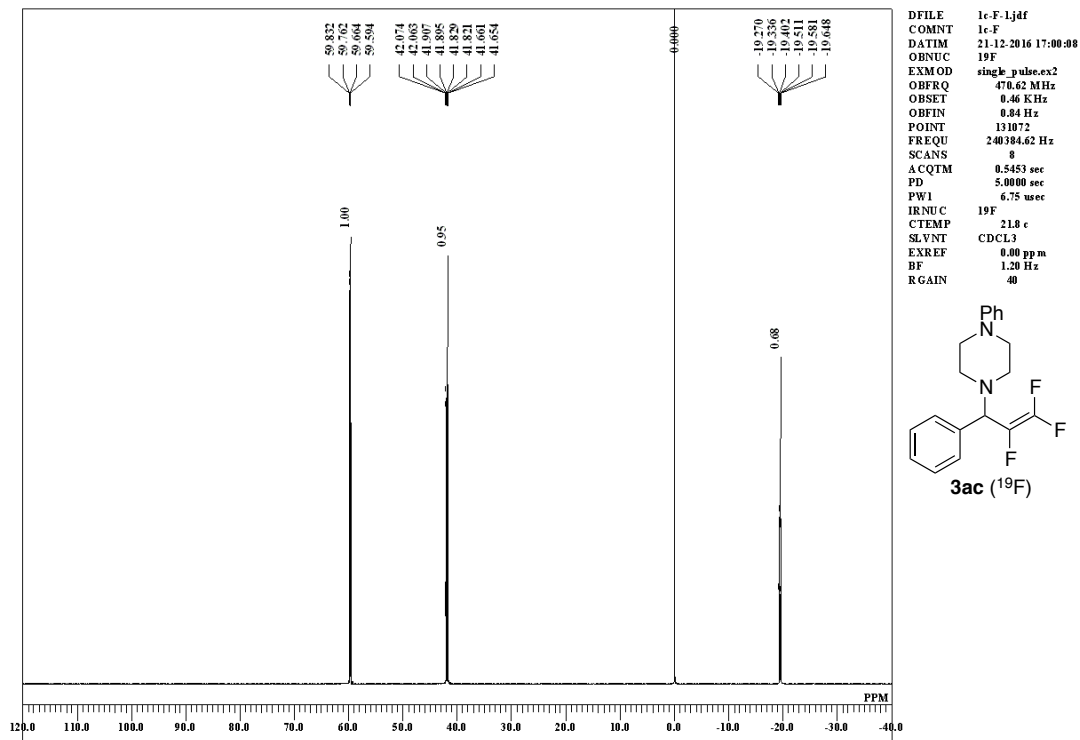
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| 1) ^1H , ^{13}C , and ^{19}F NMR spectra | S-2 |
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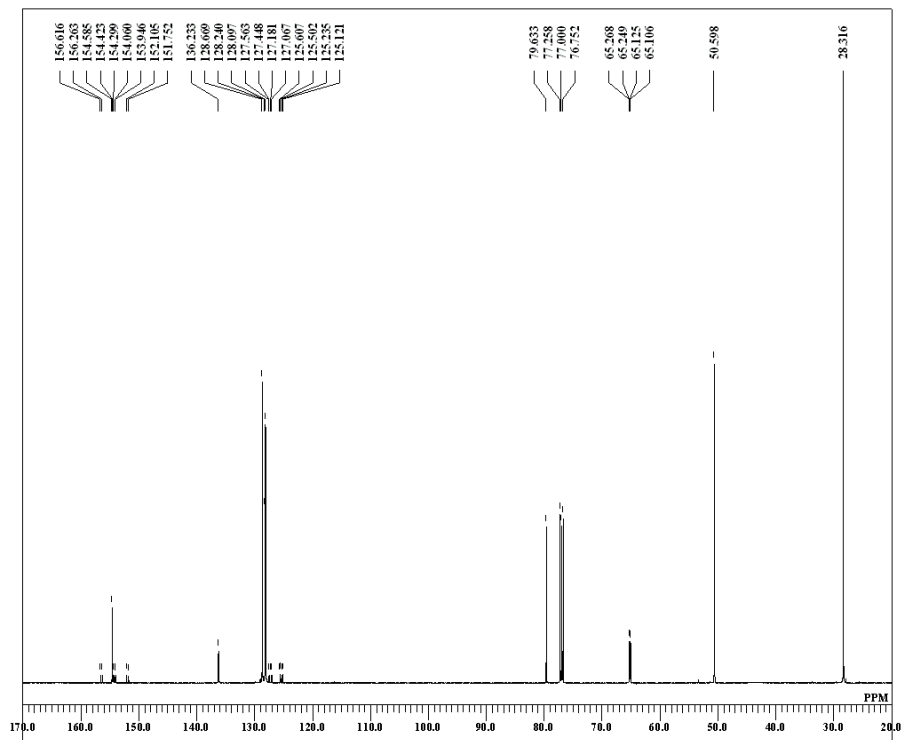




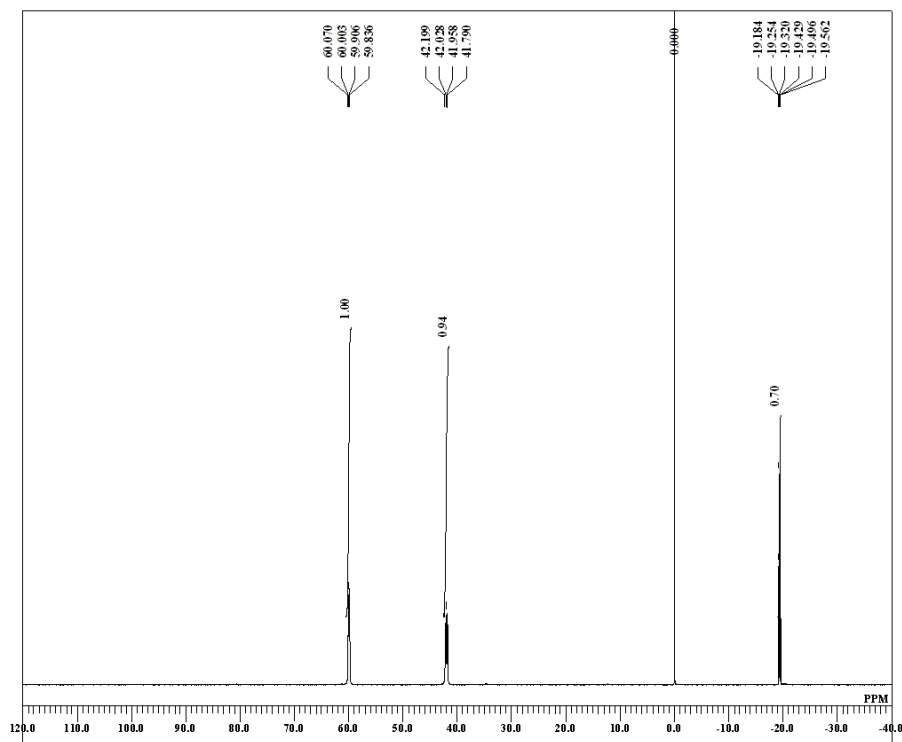
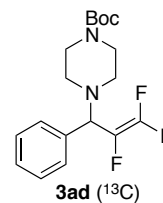




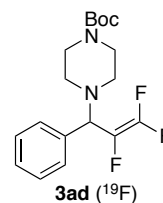


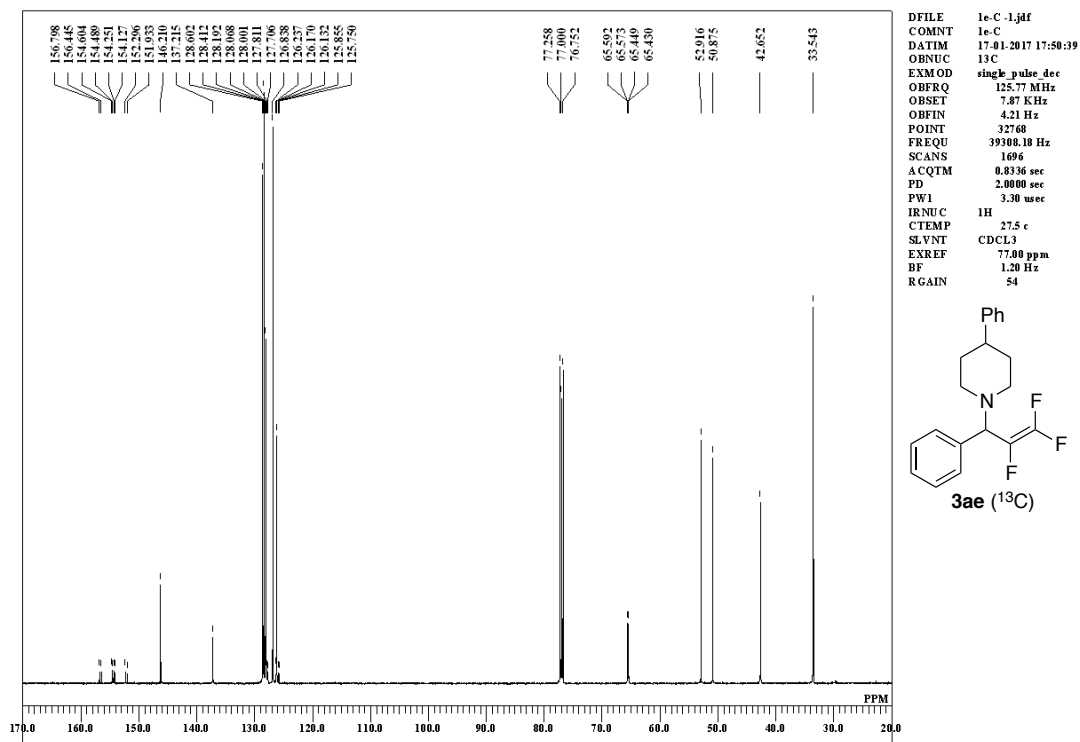
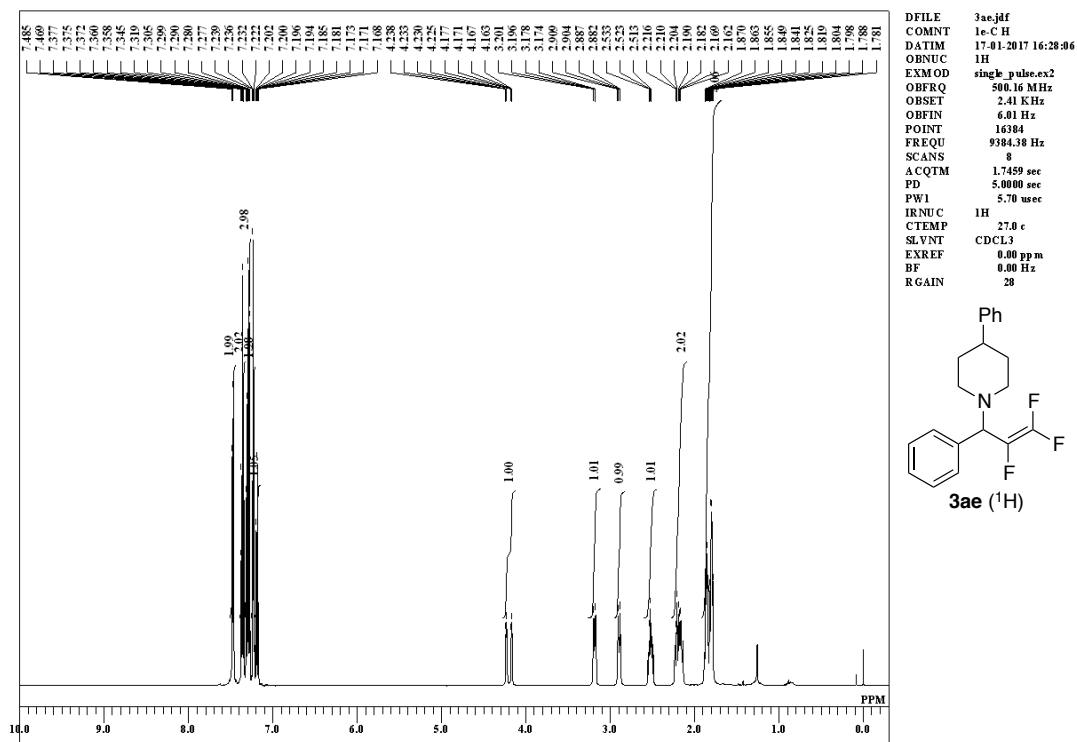


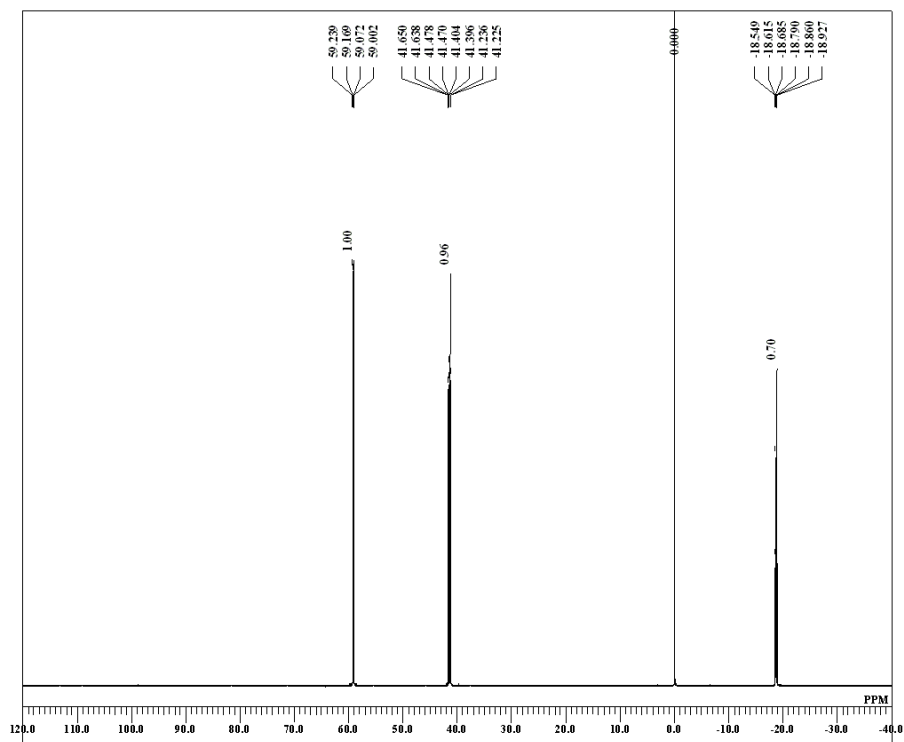
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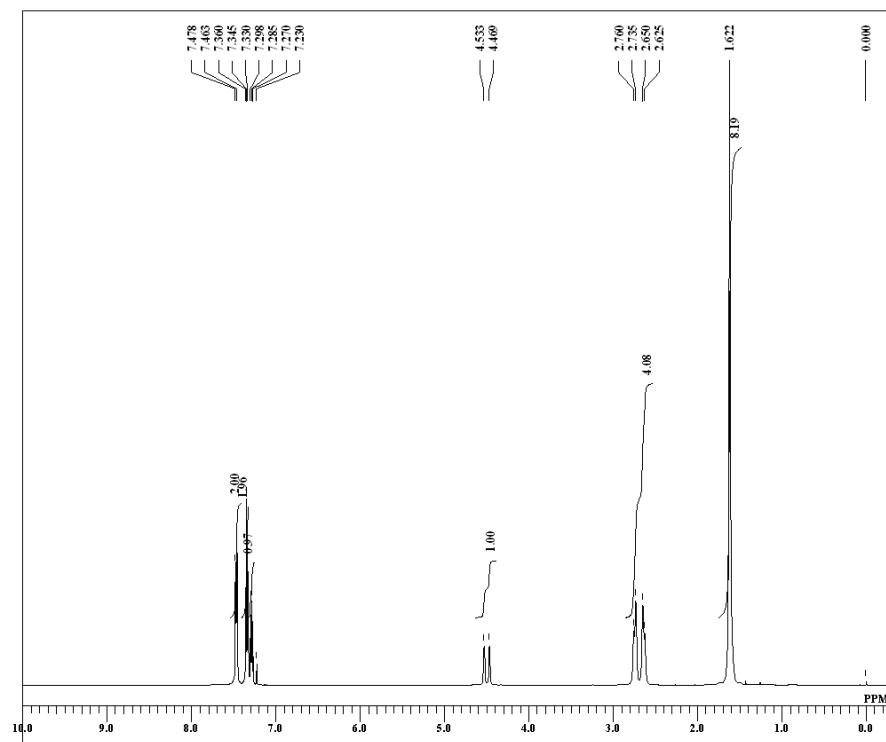
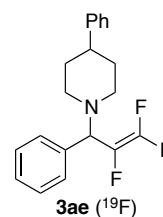
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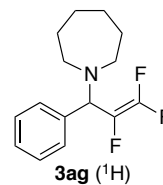


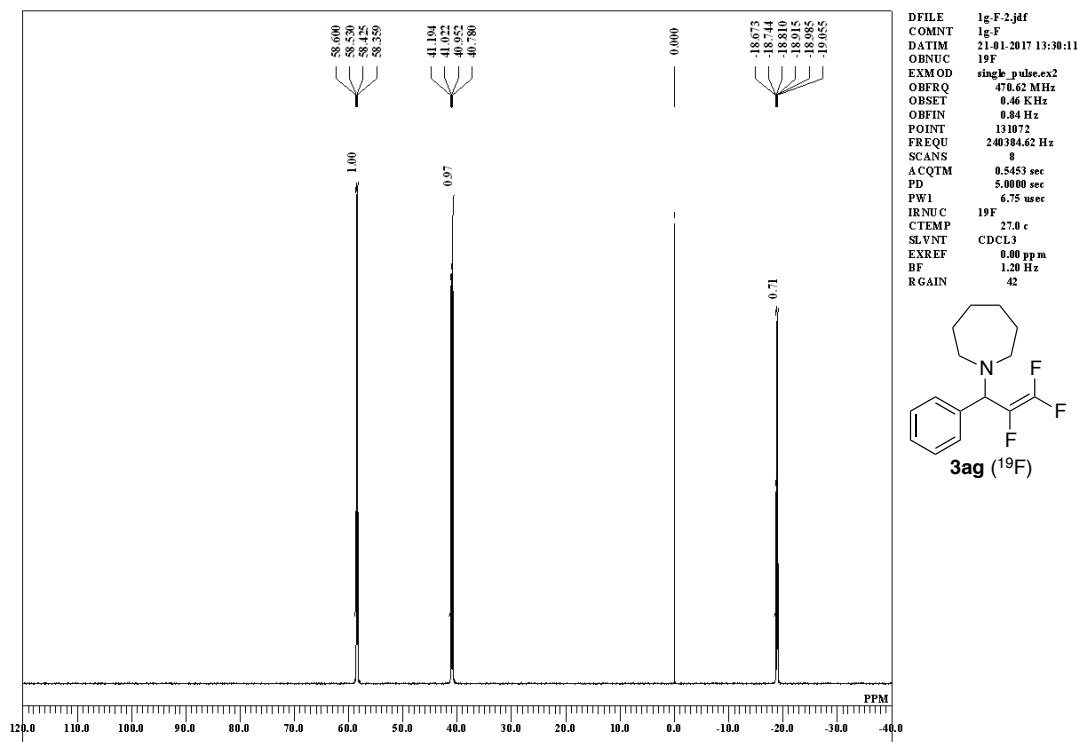
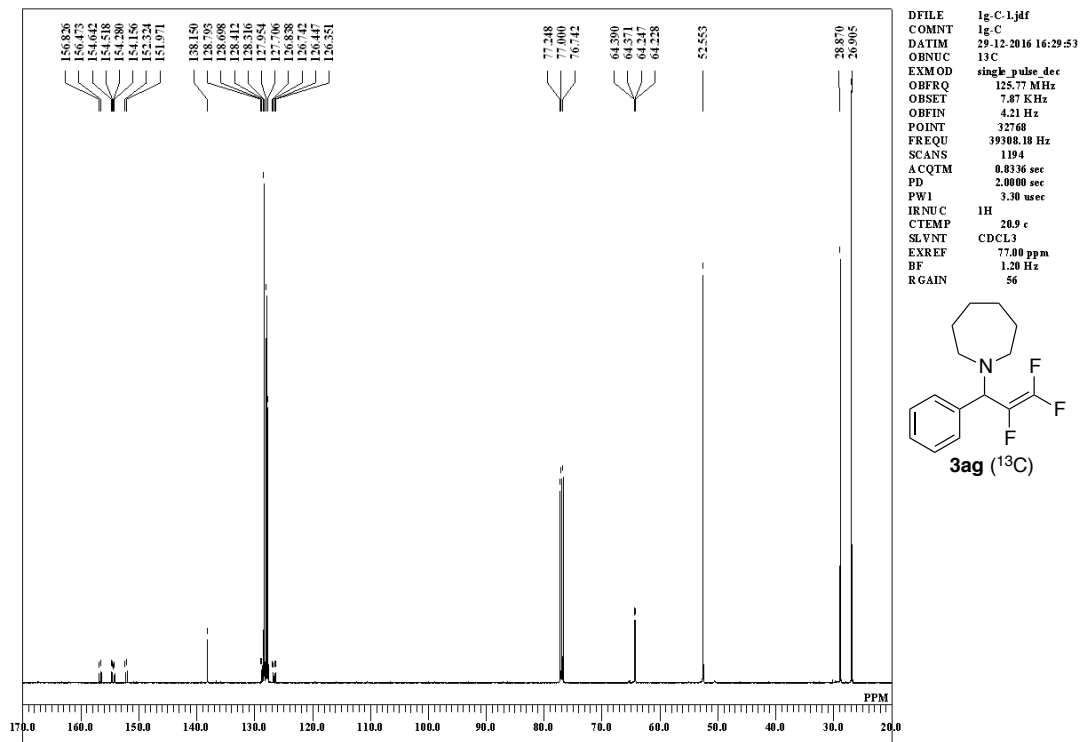


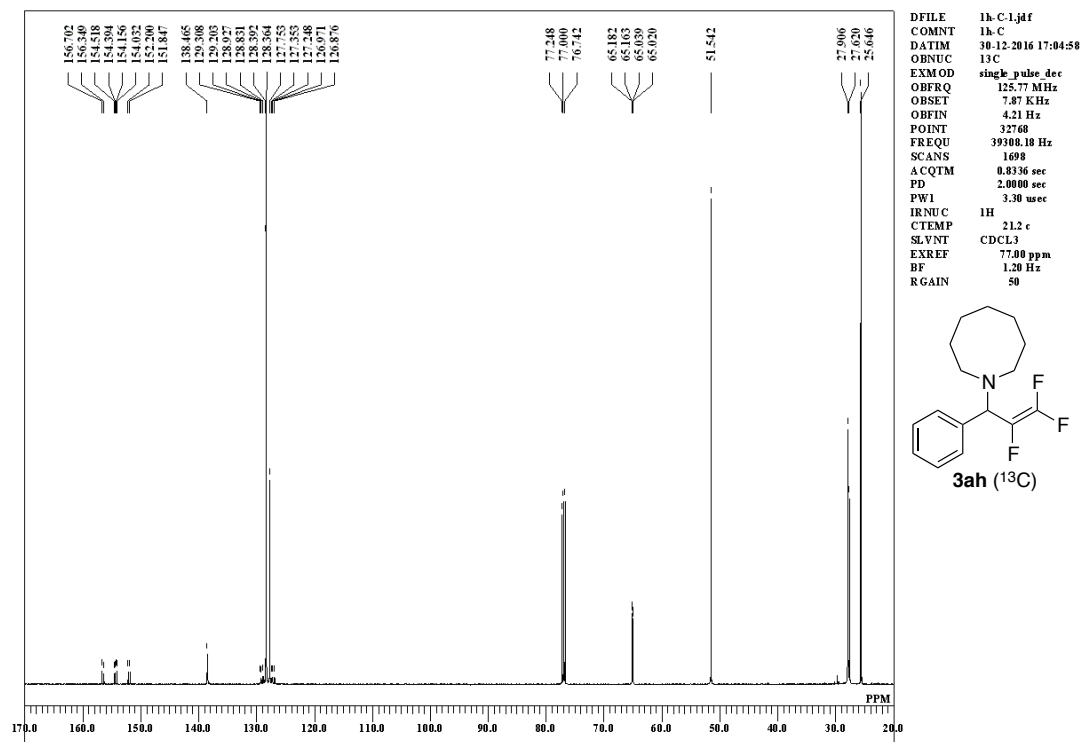
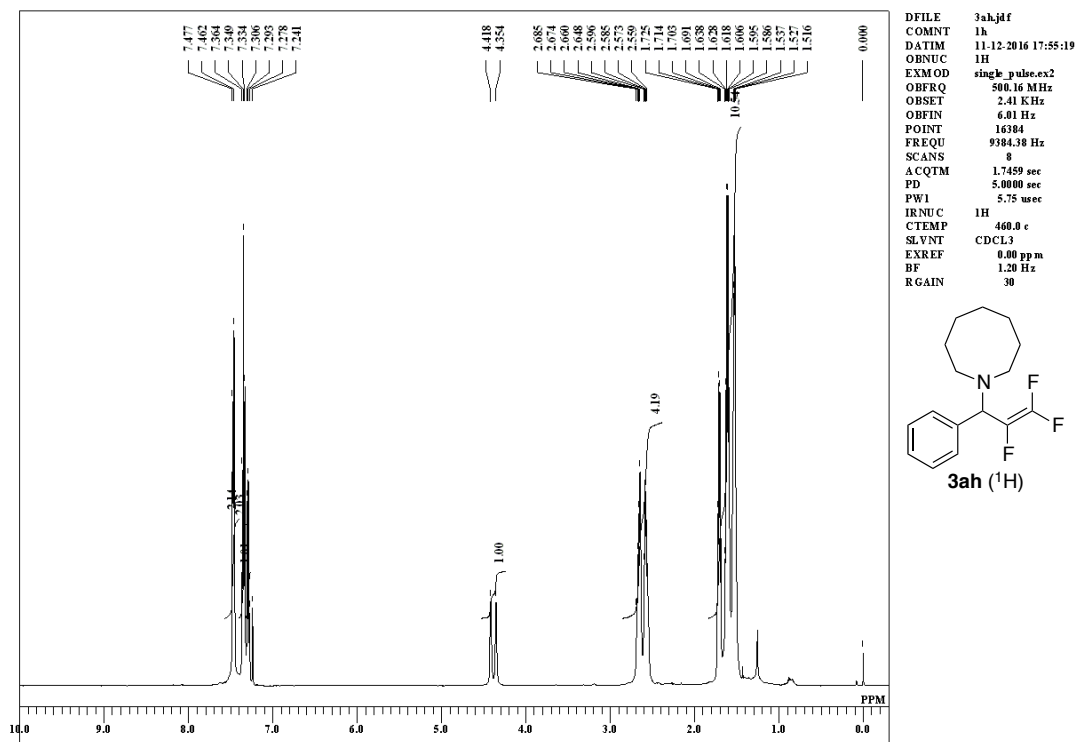
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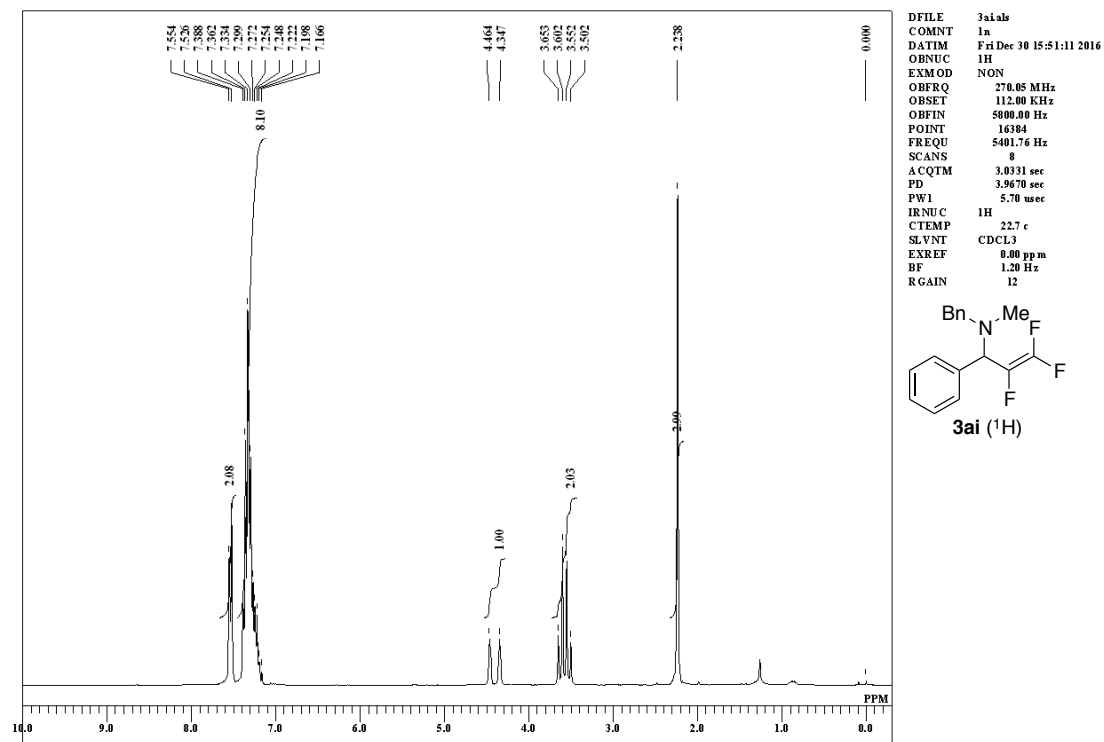
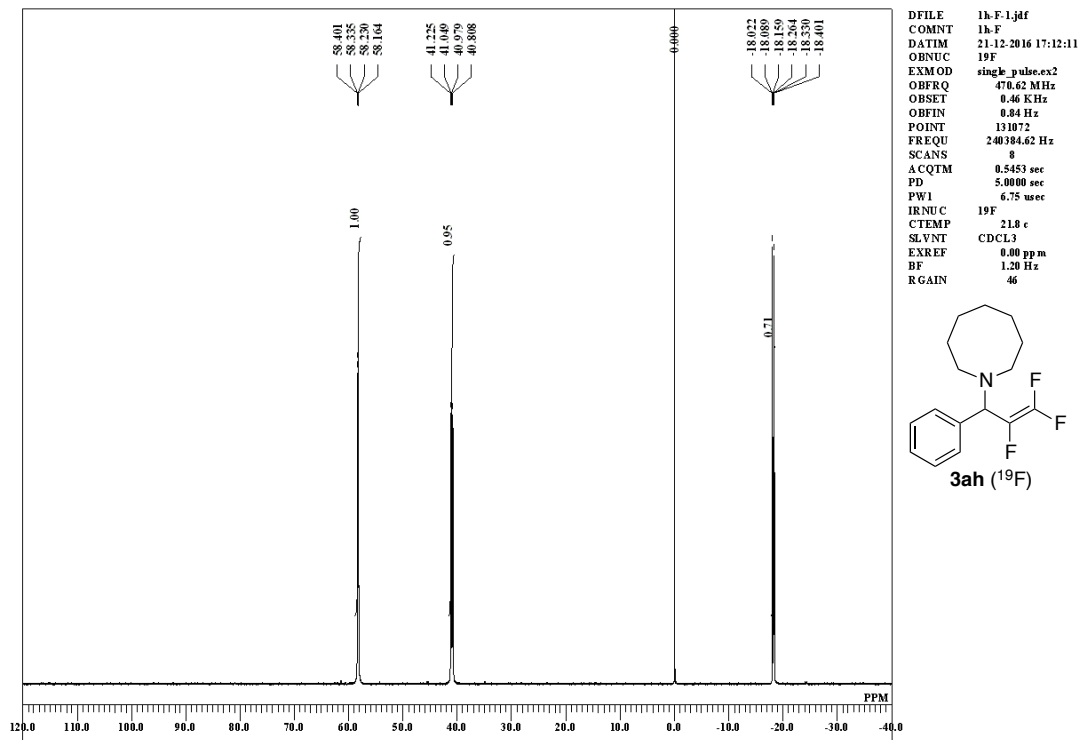


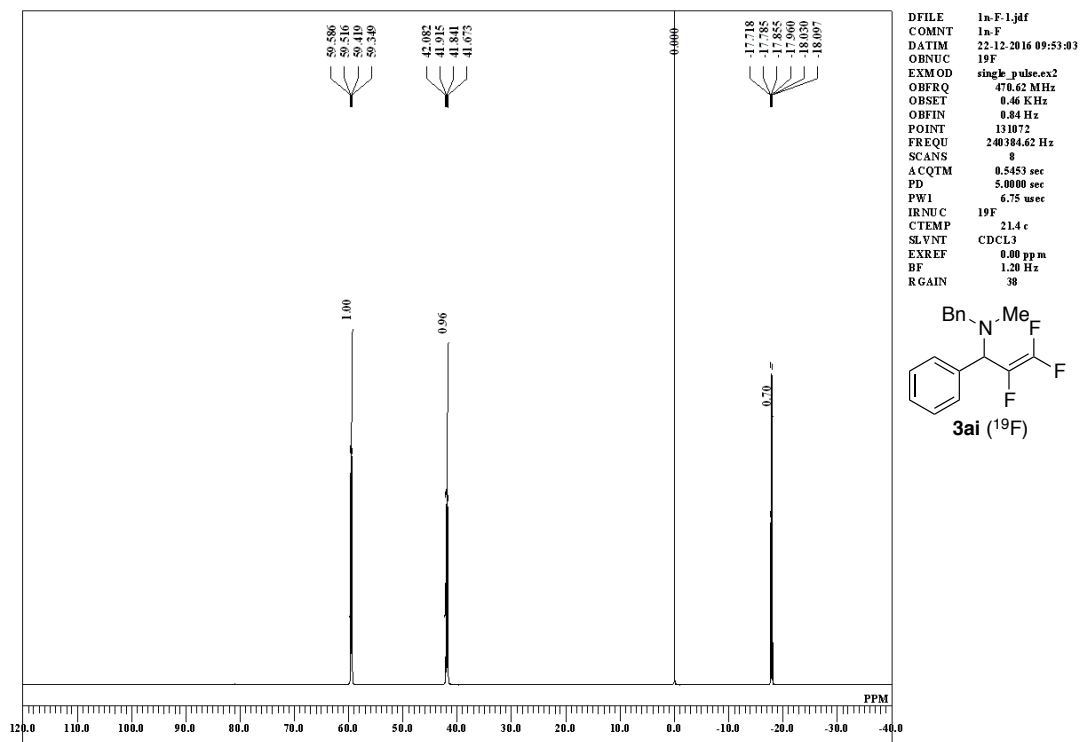
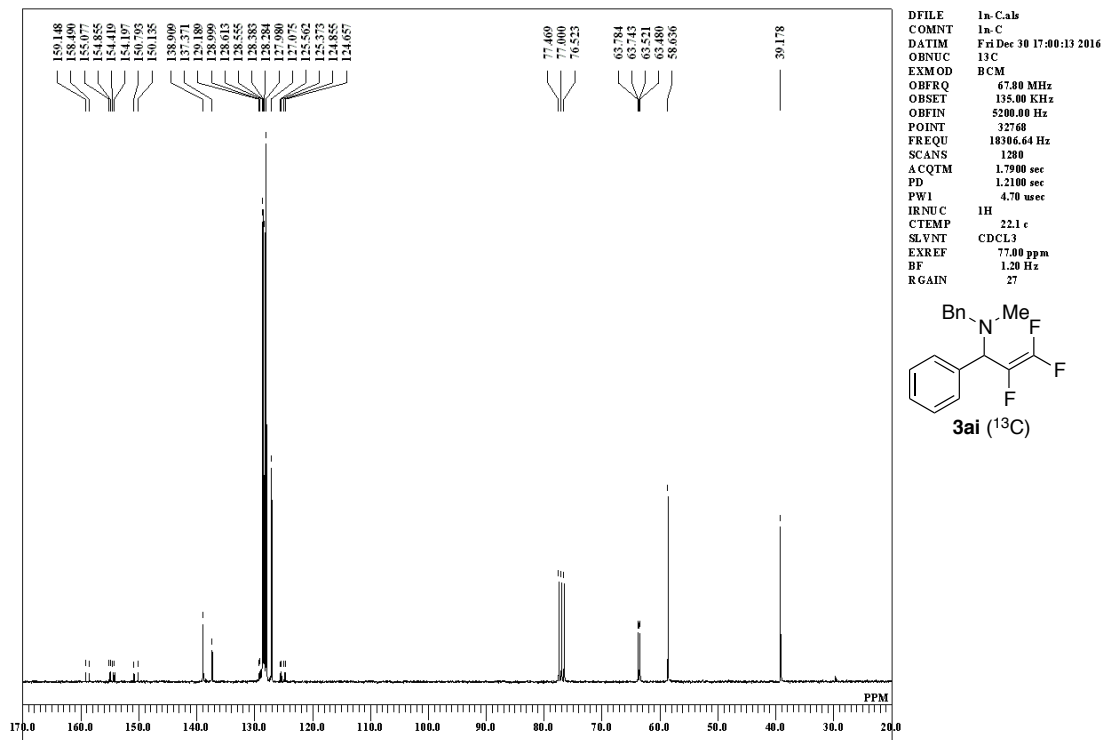
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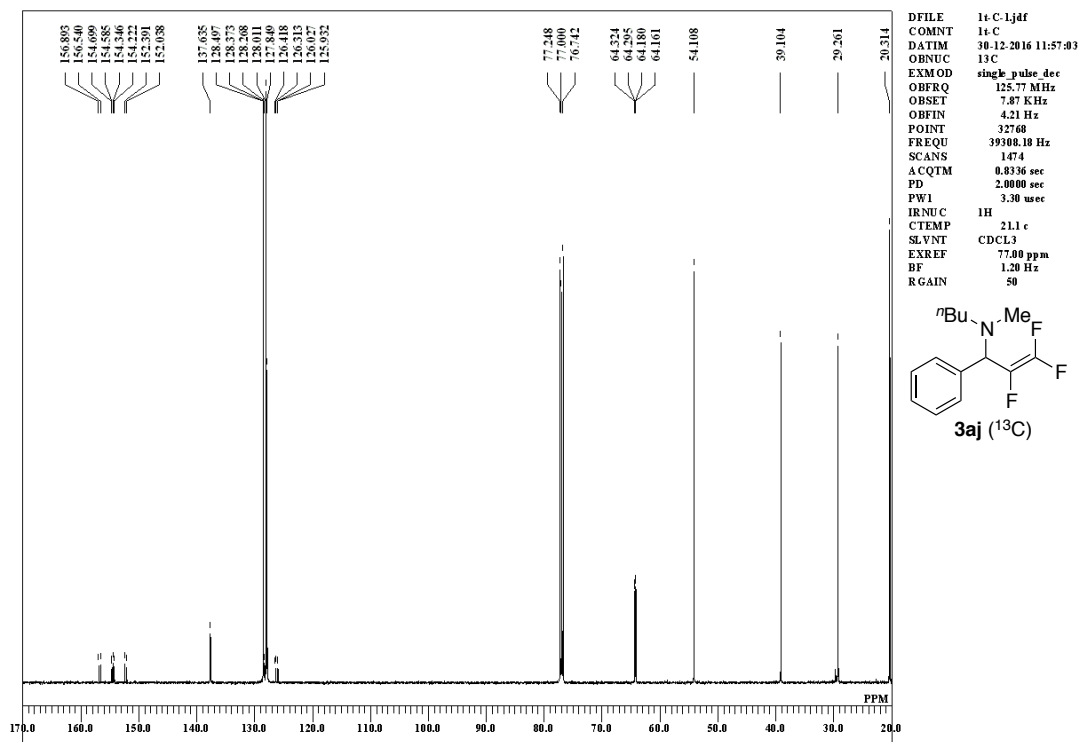
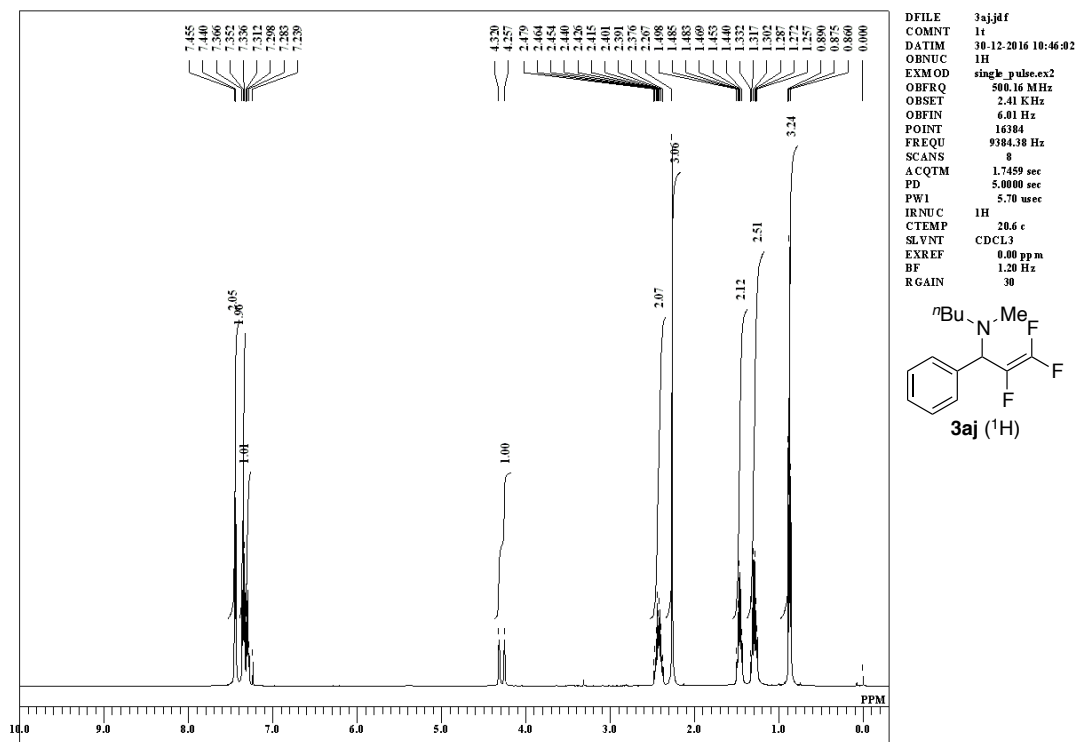


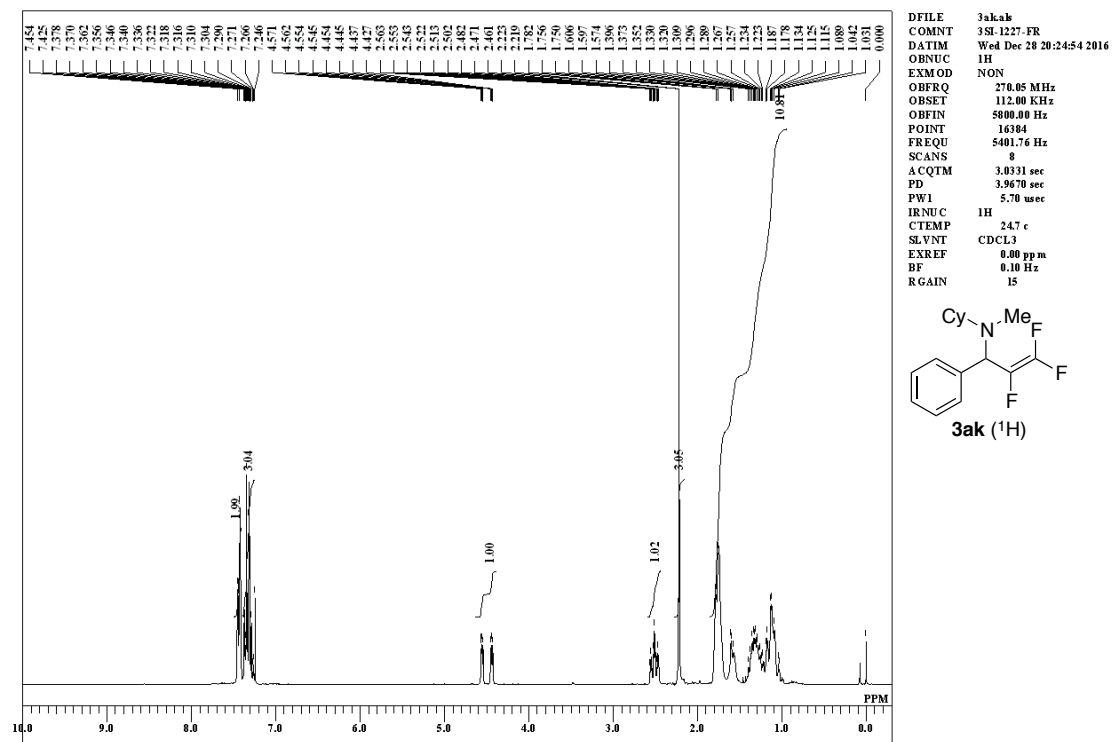
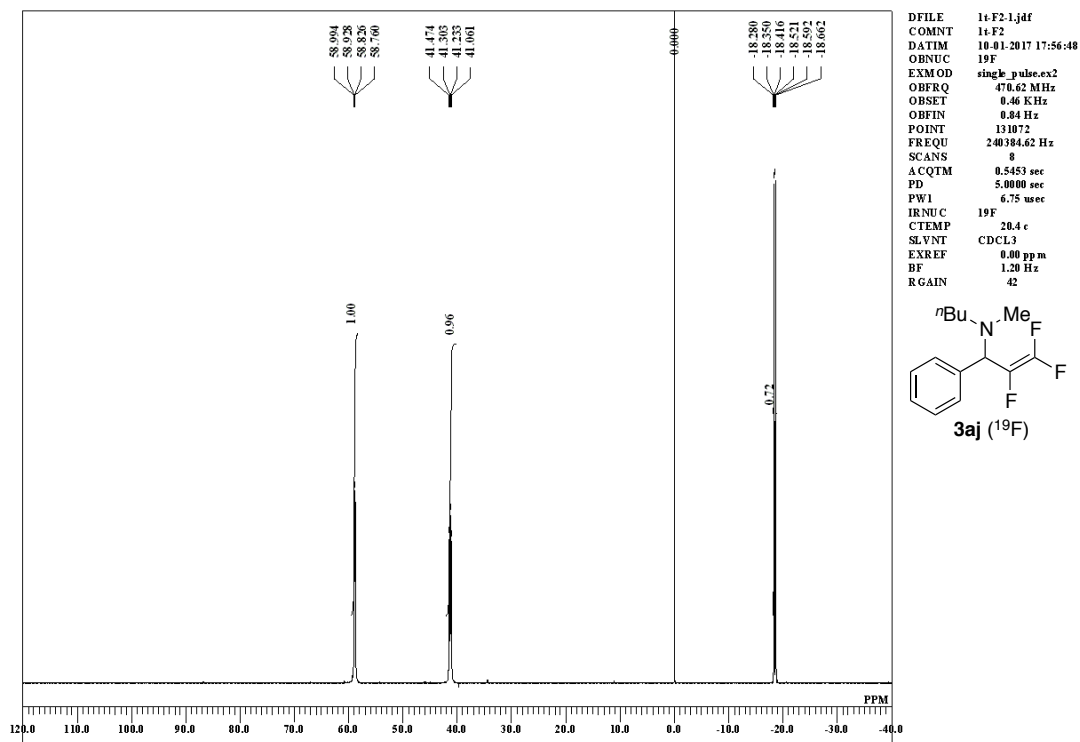


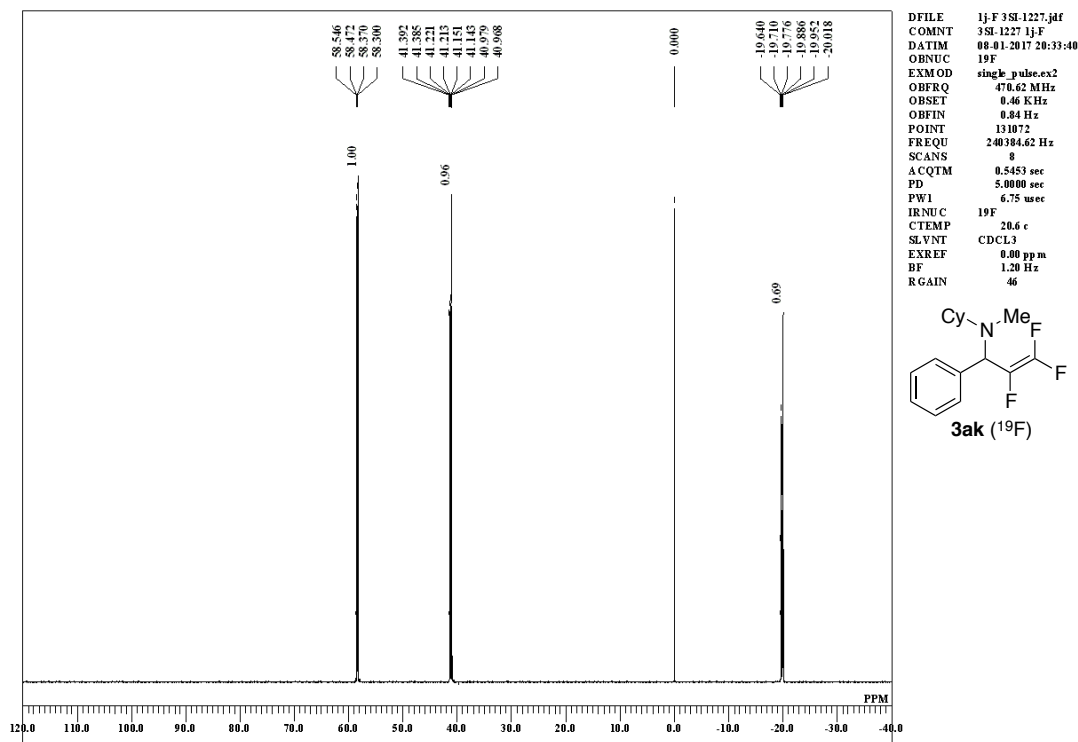
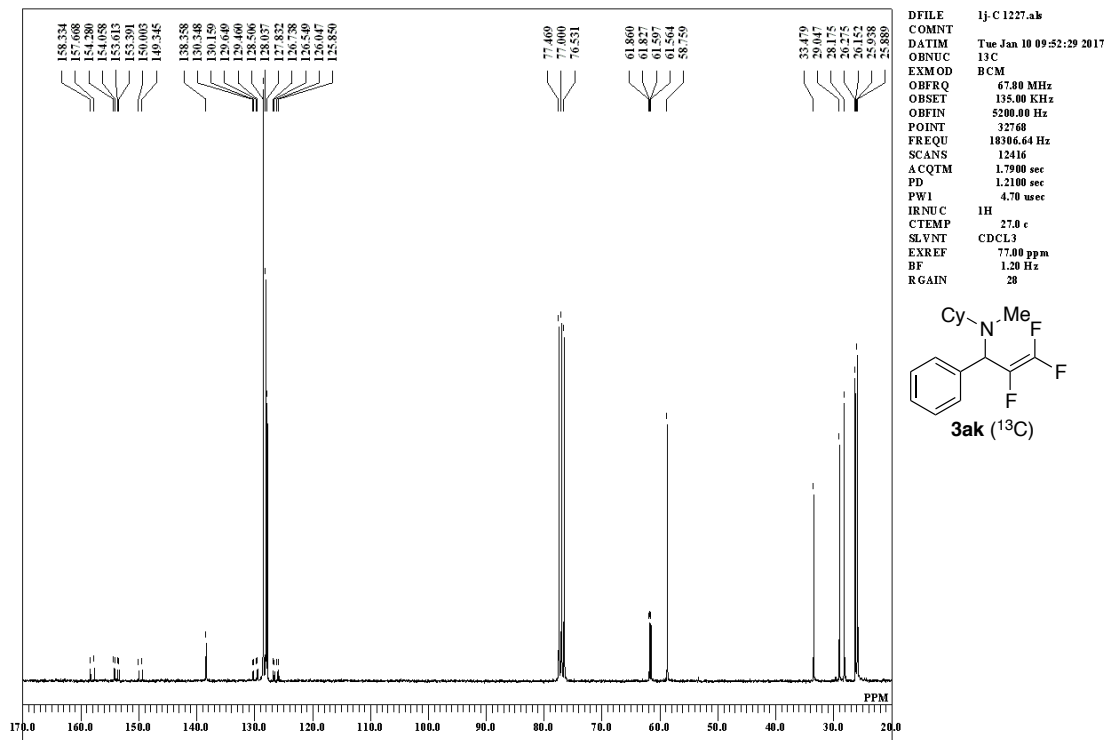


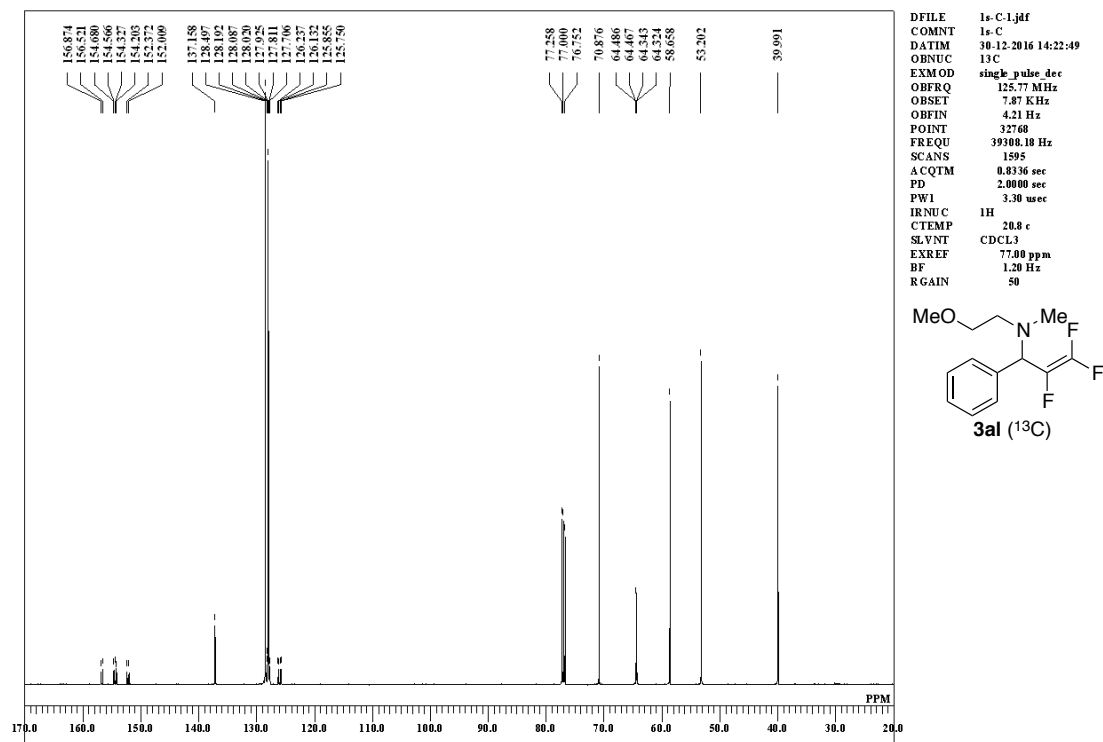
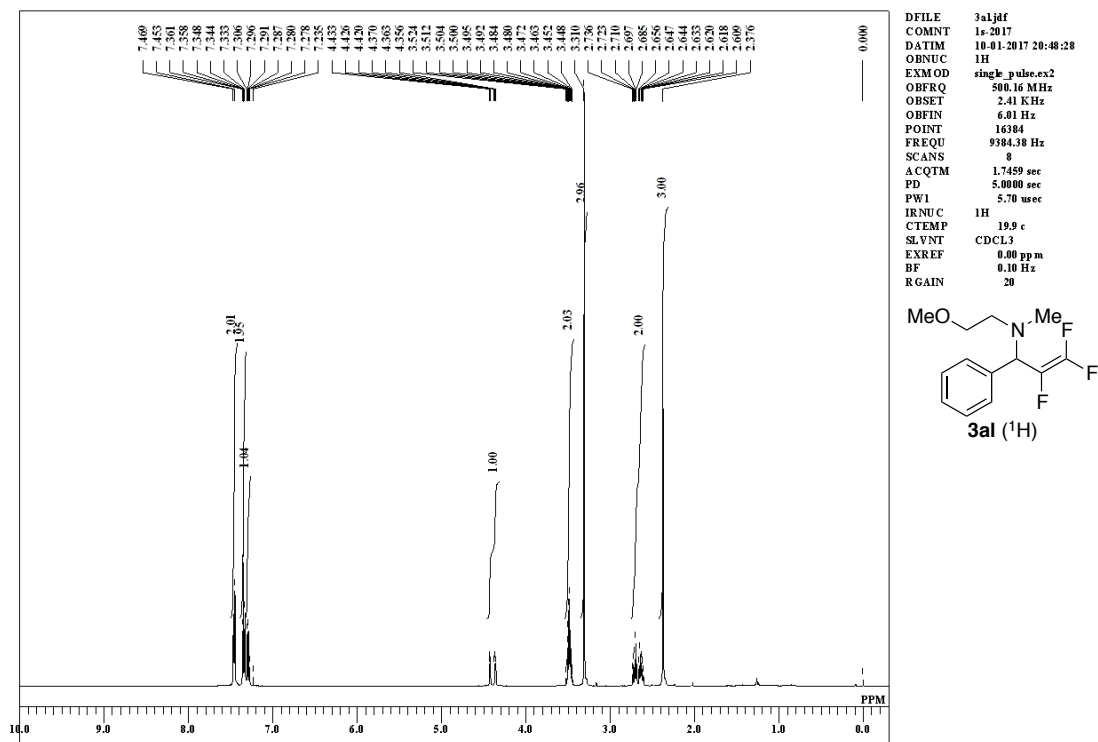


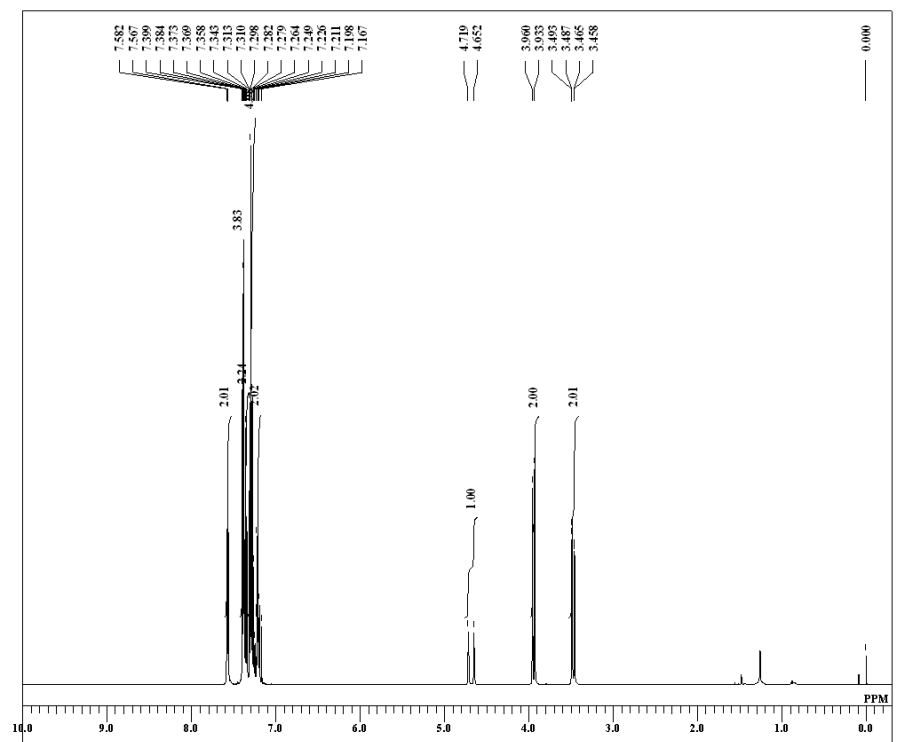
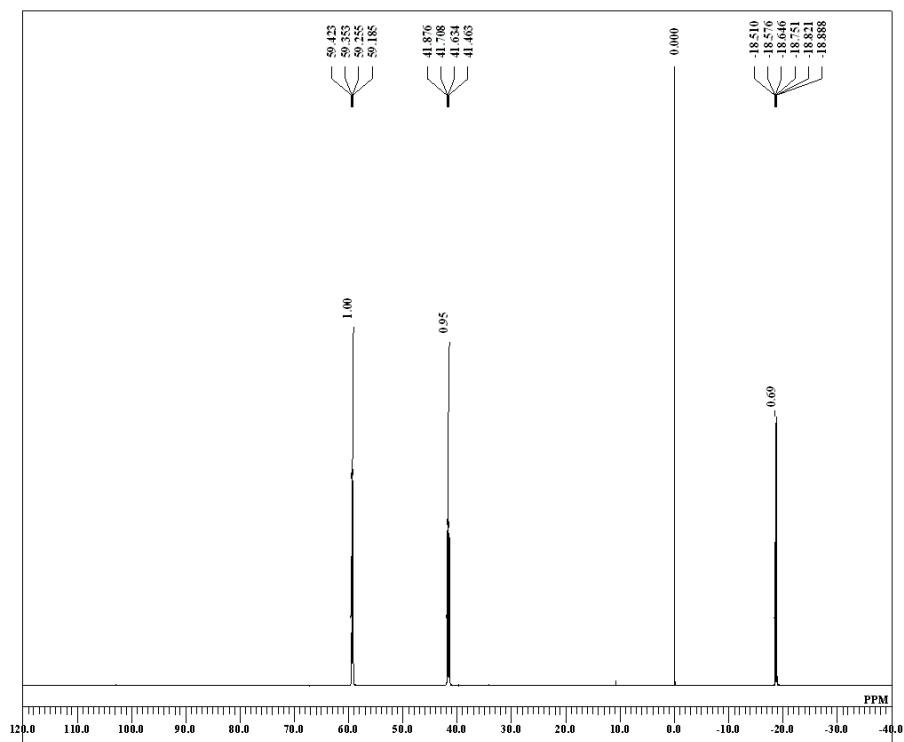


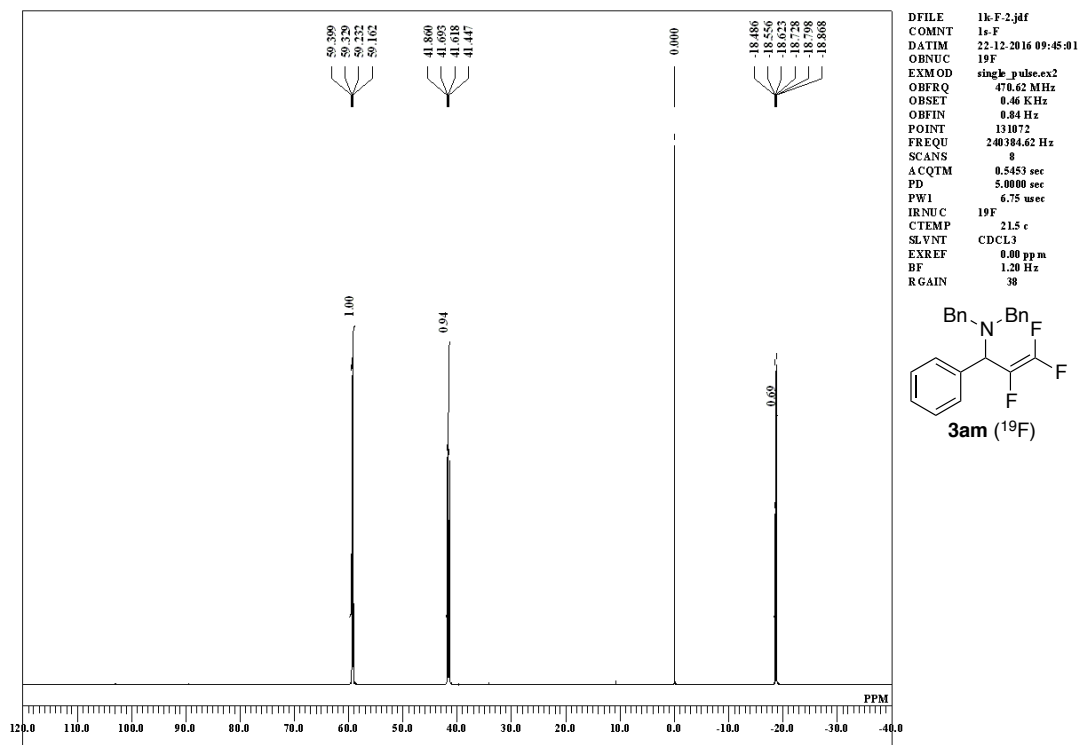
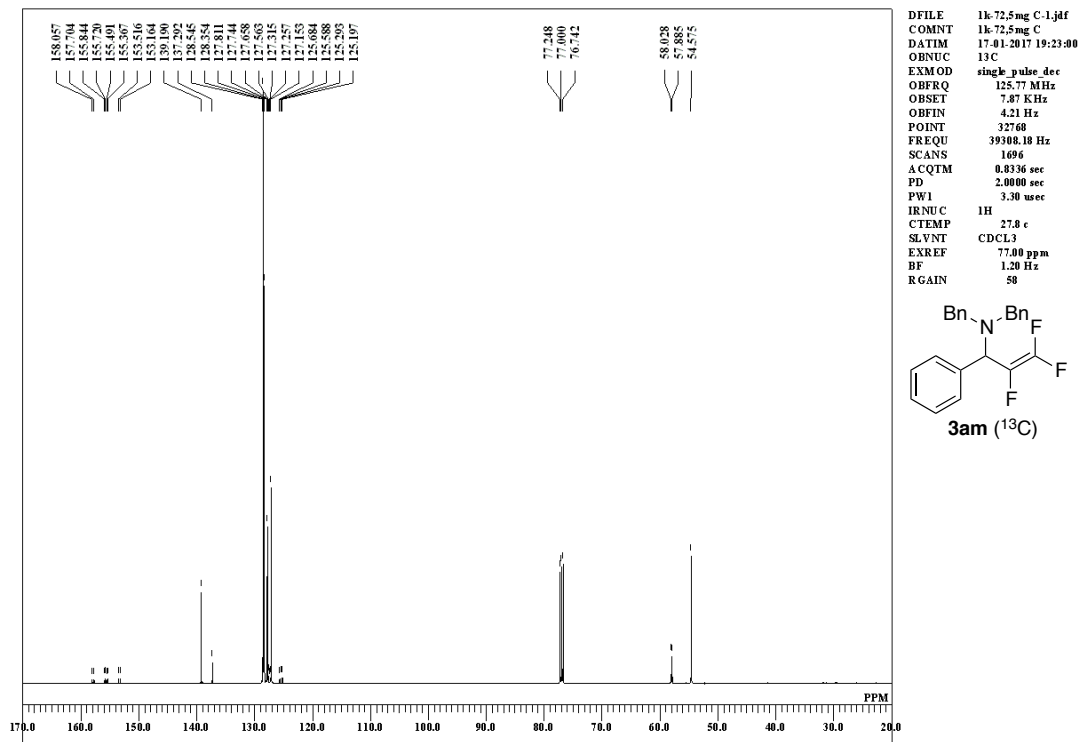


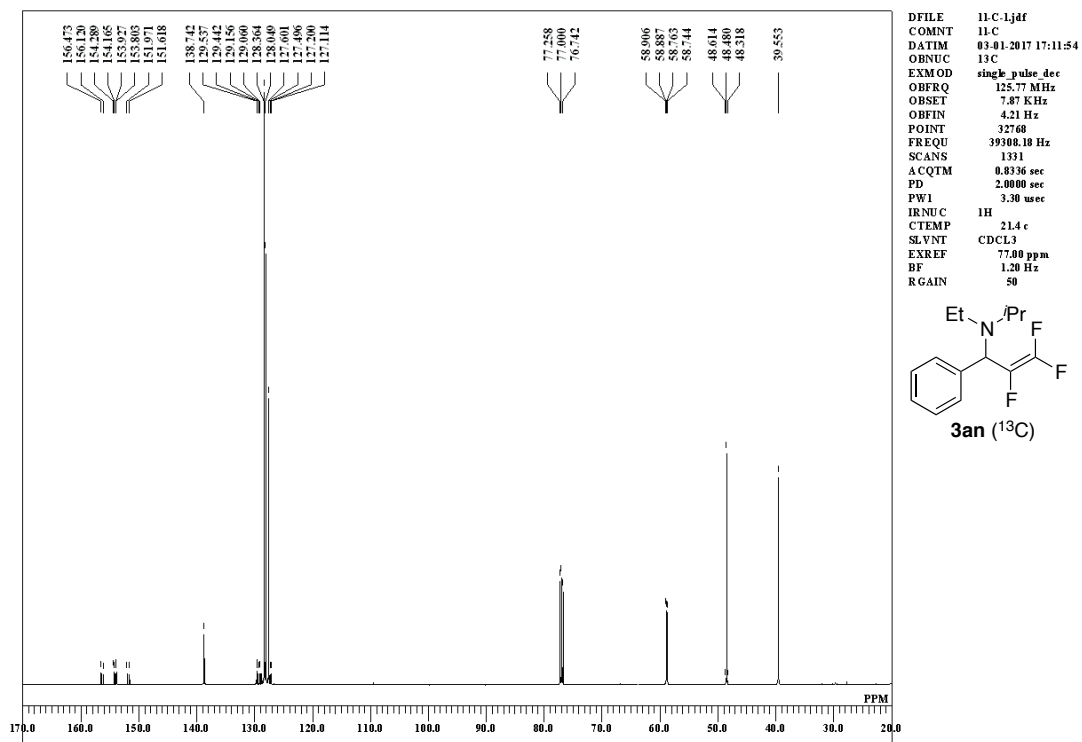
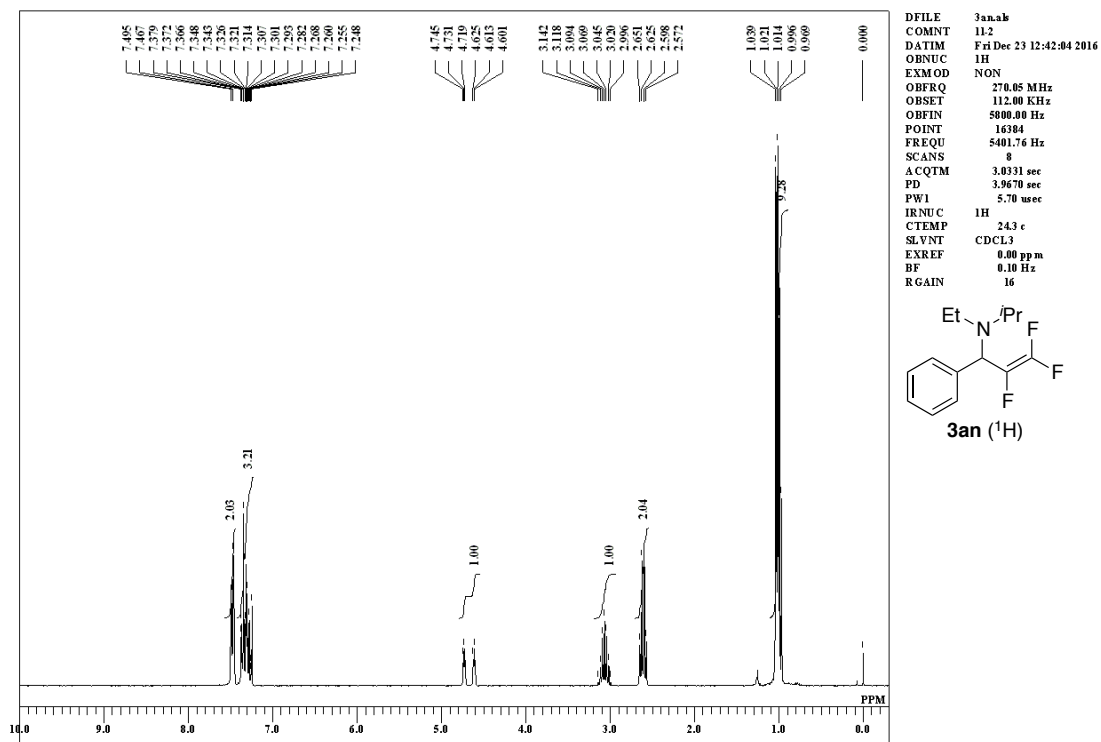


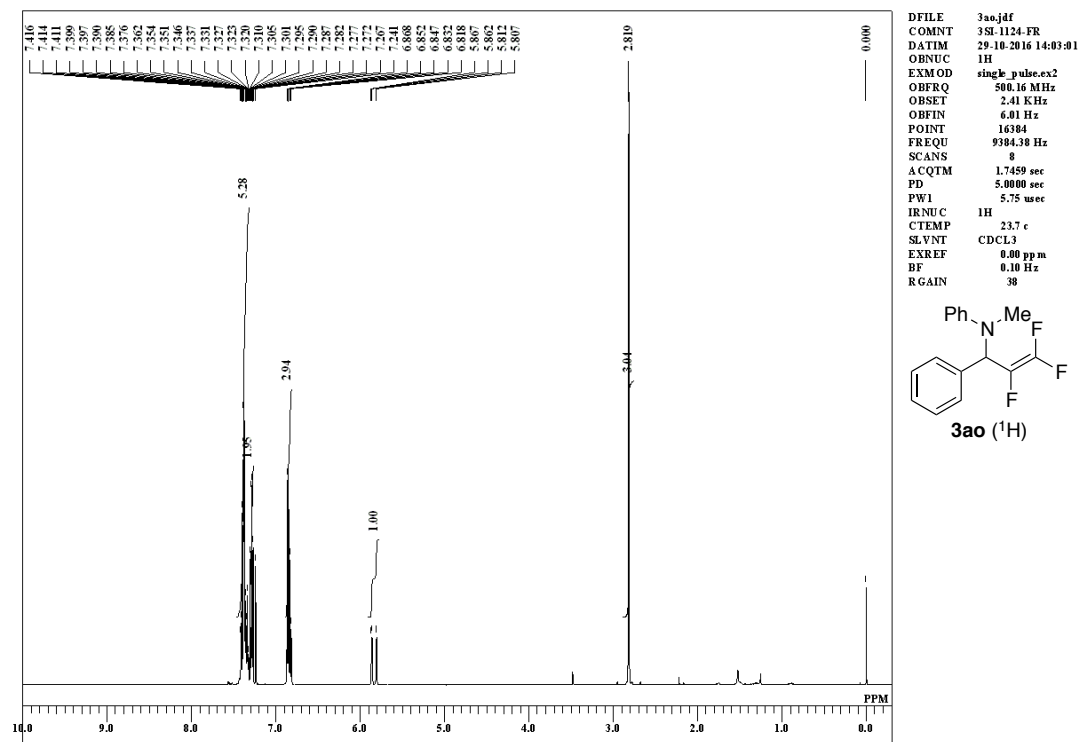
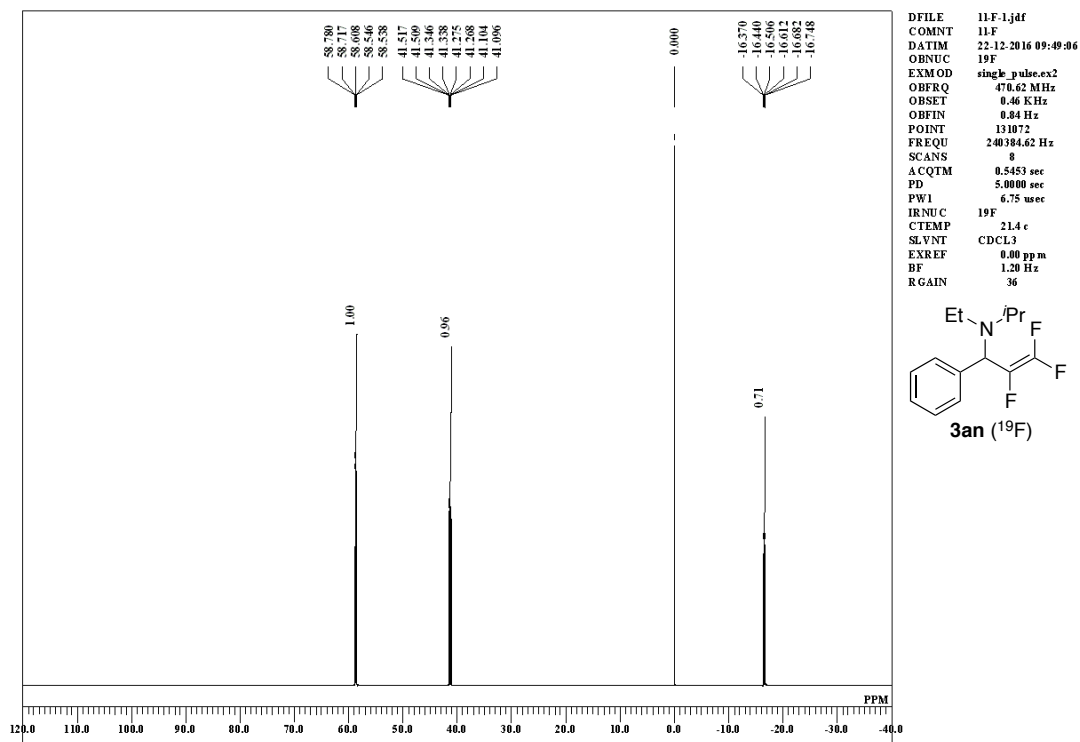


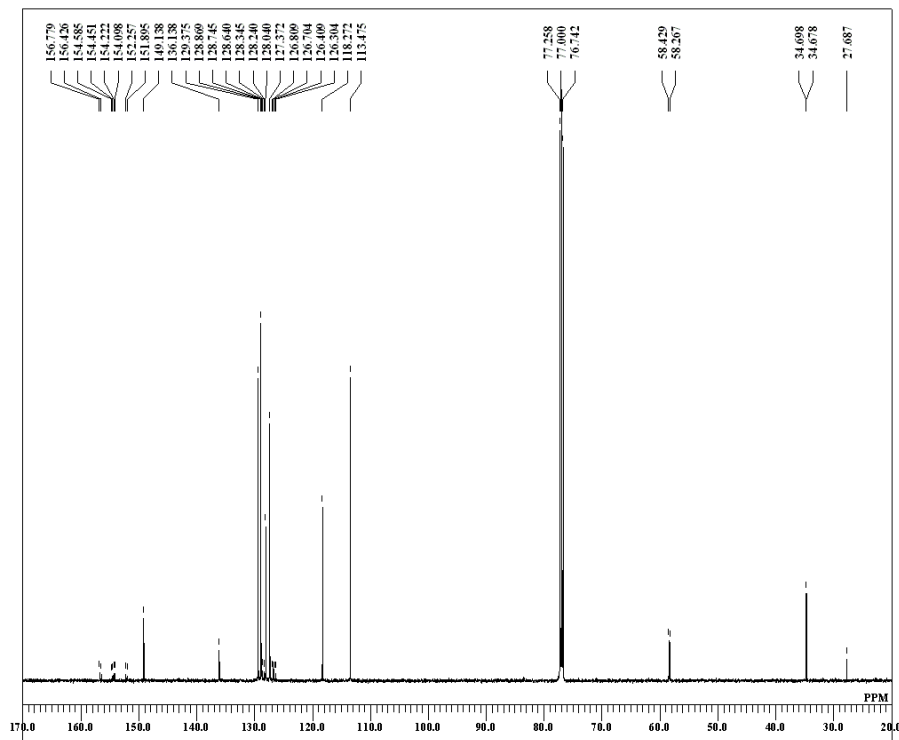




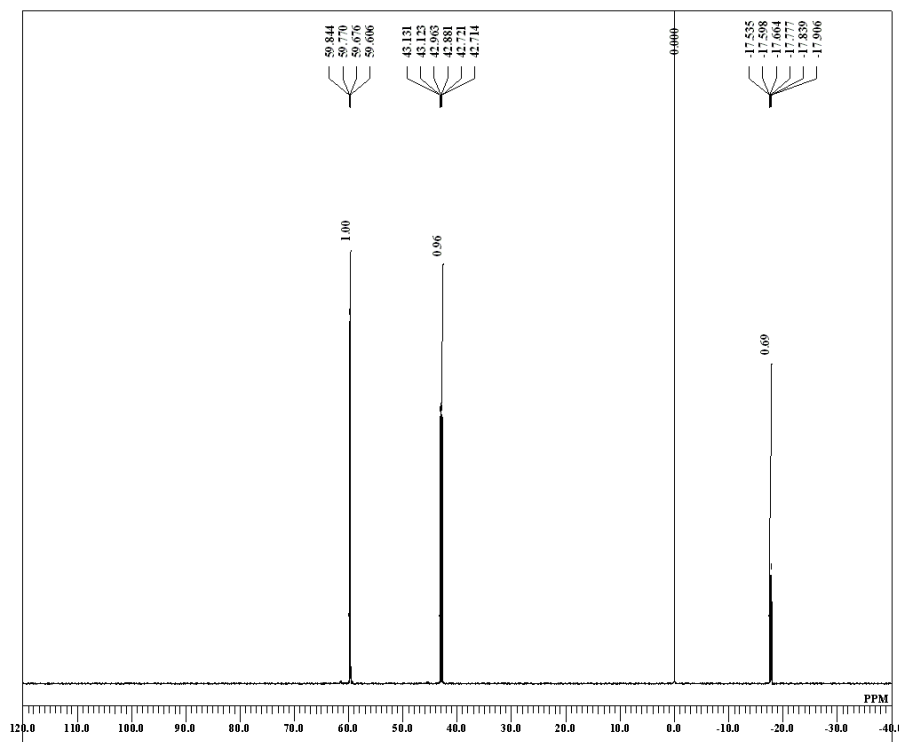
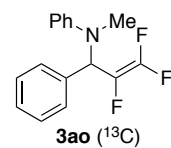




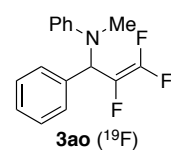


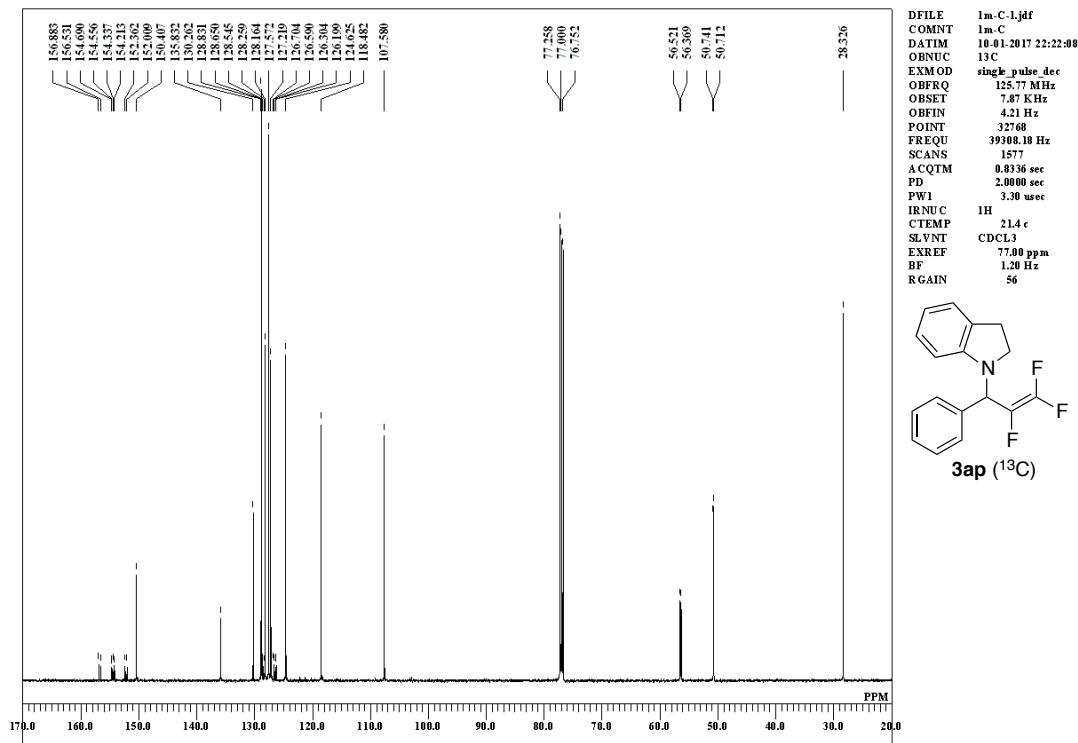
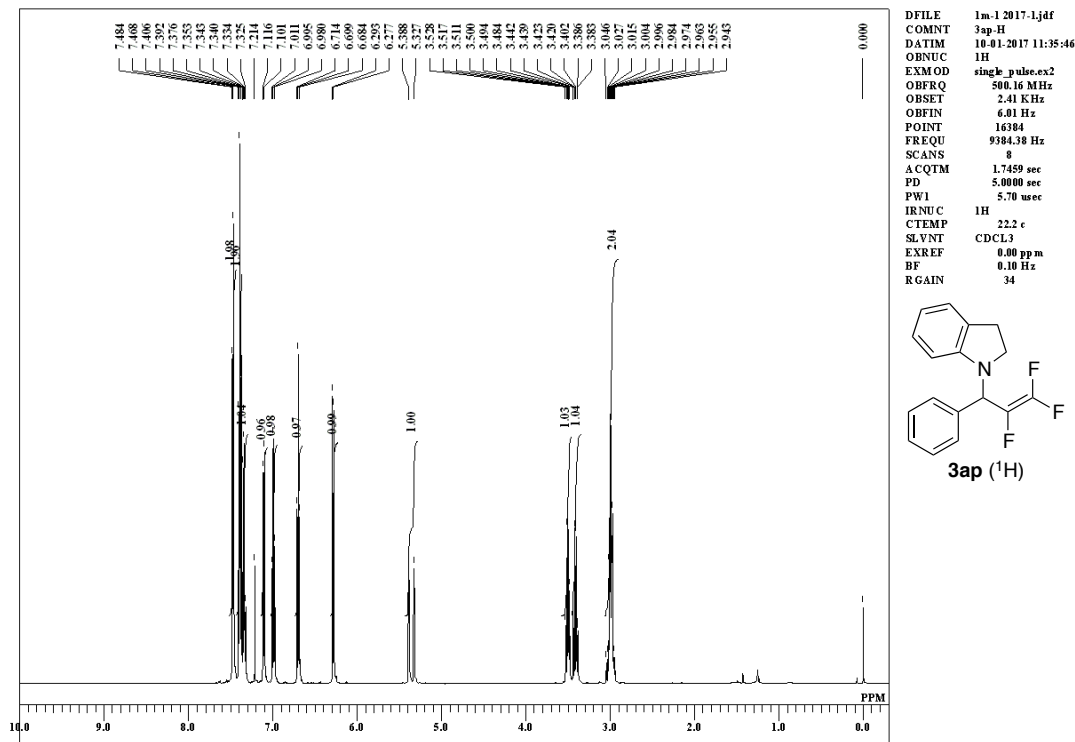


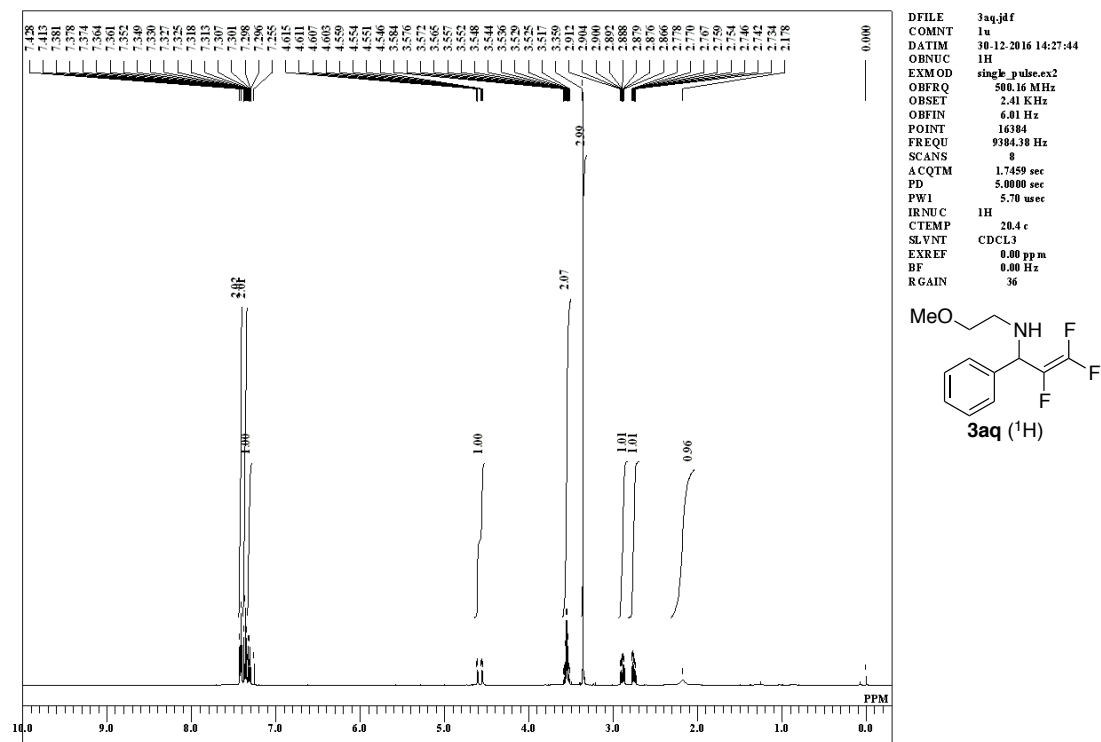
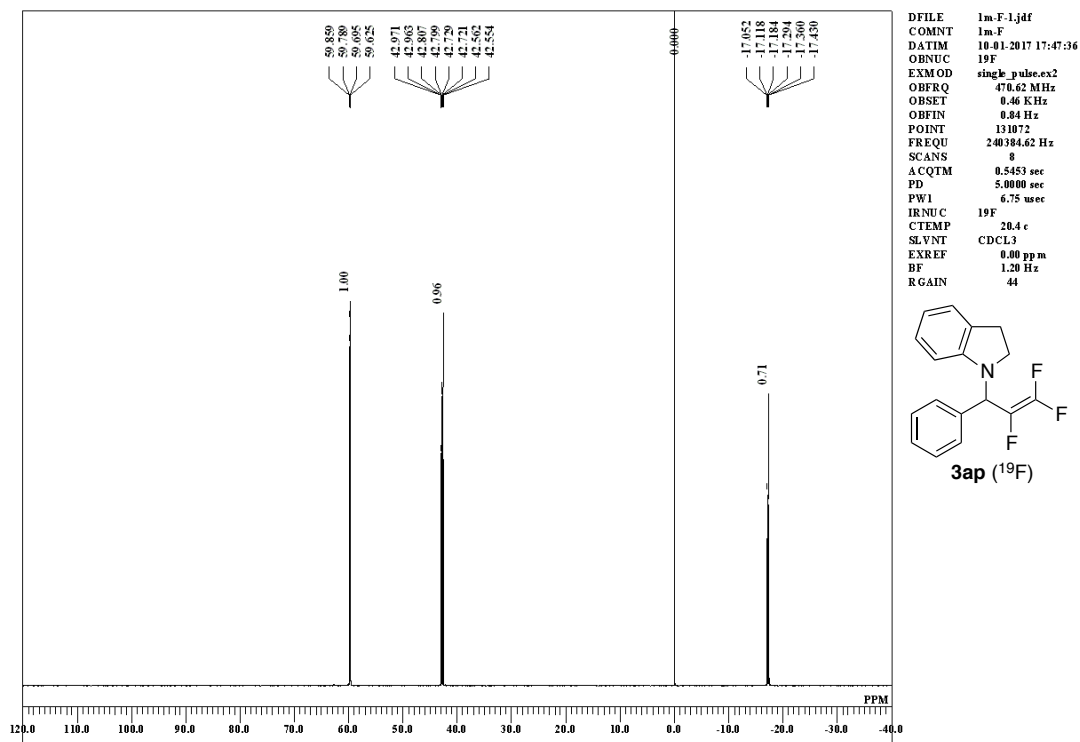
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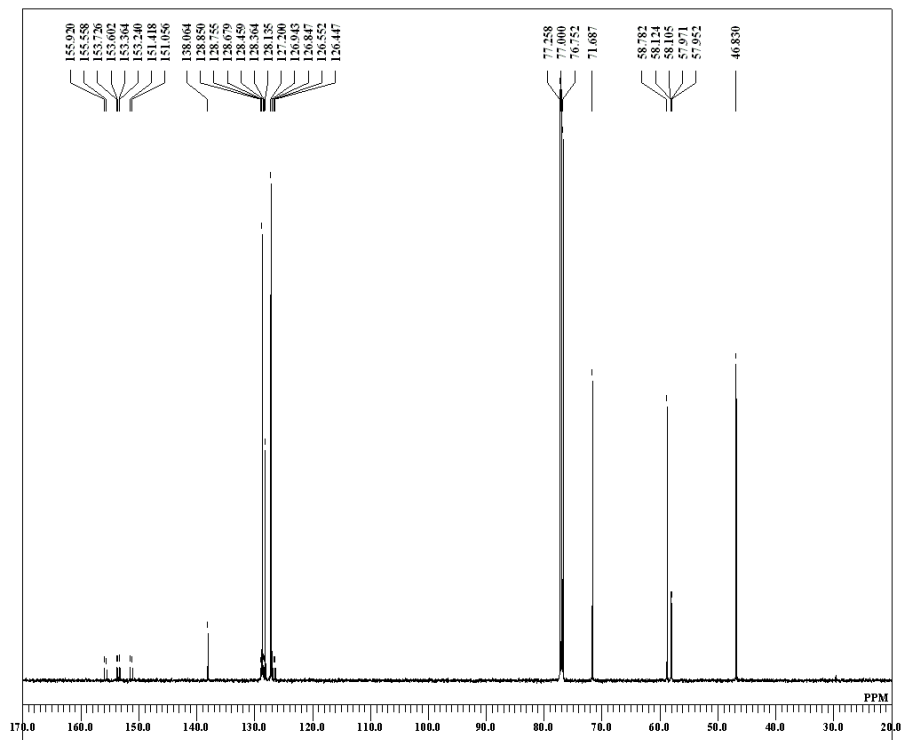


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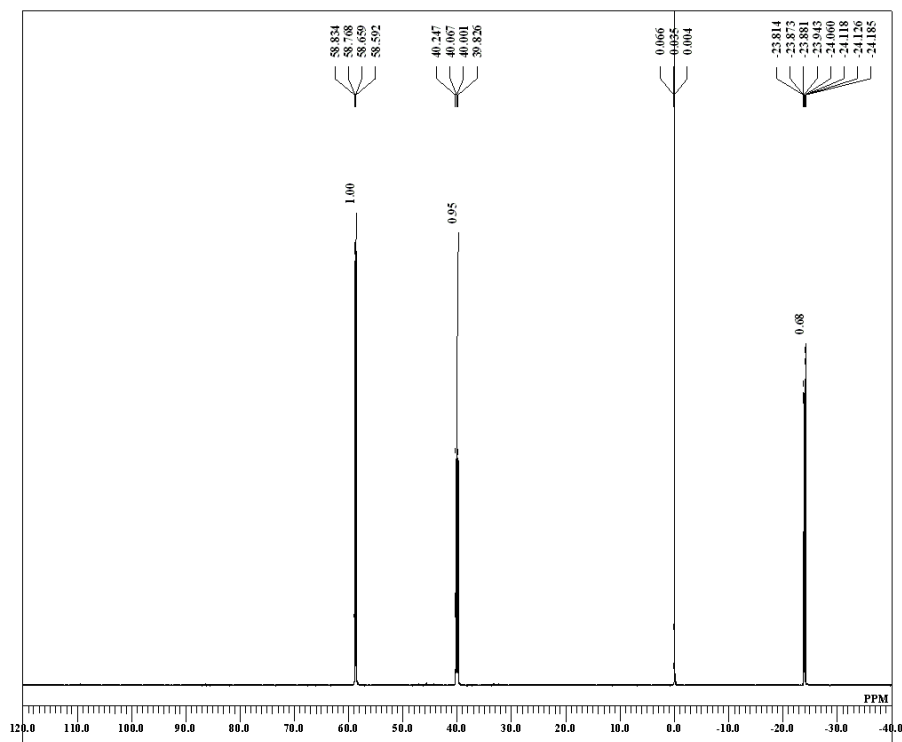
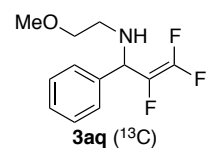




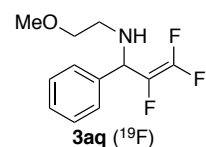


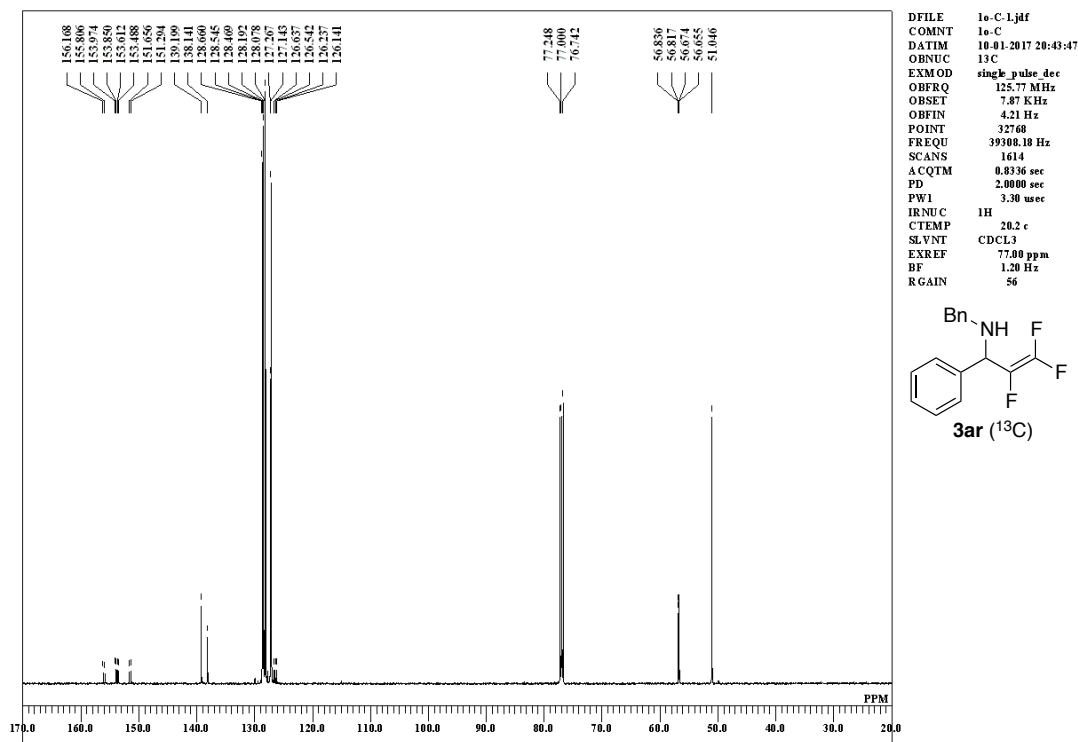
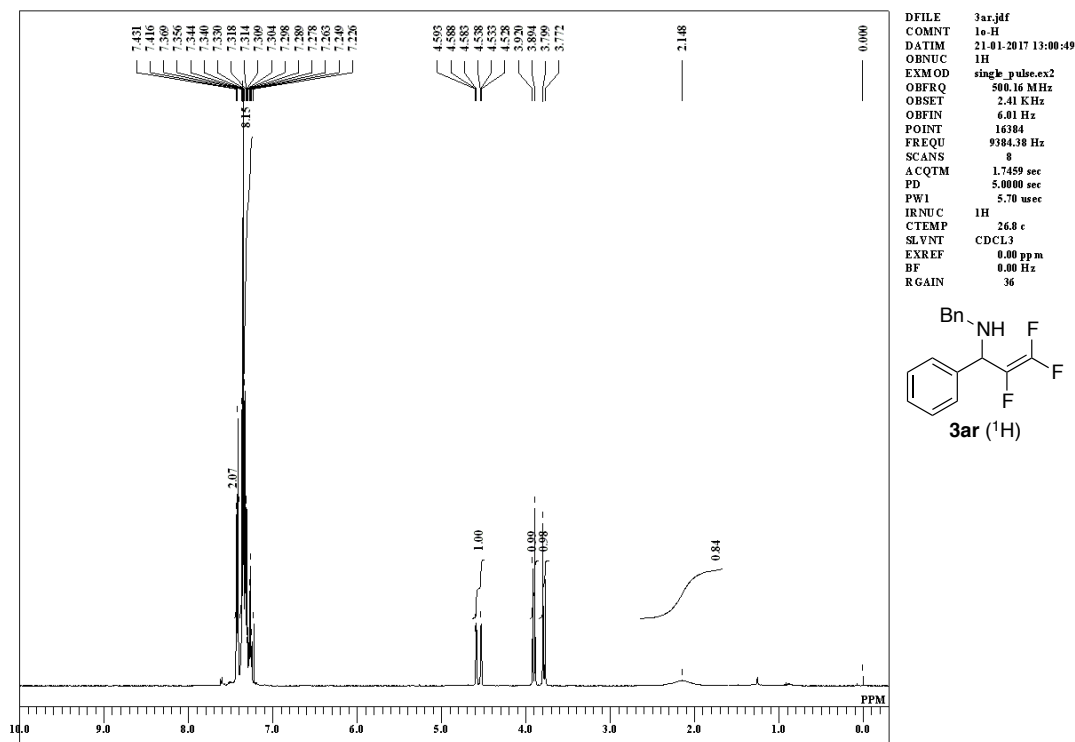


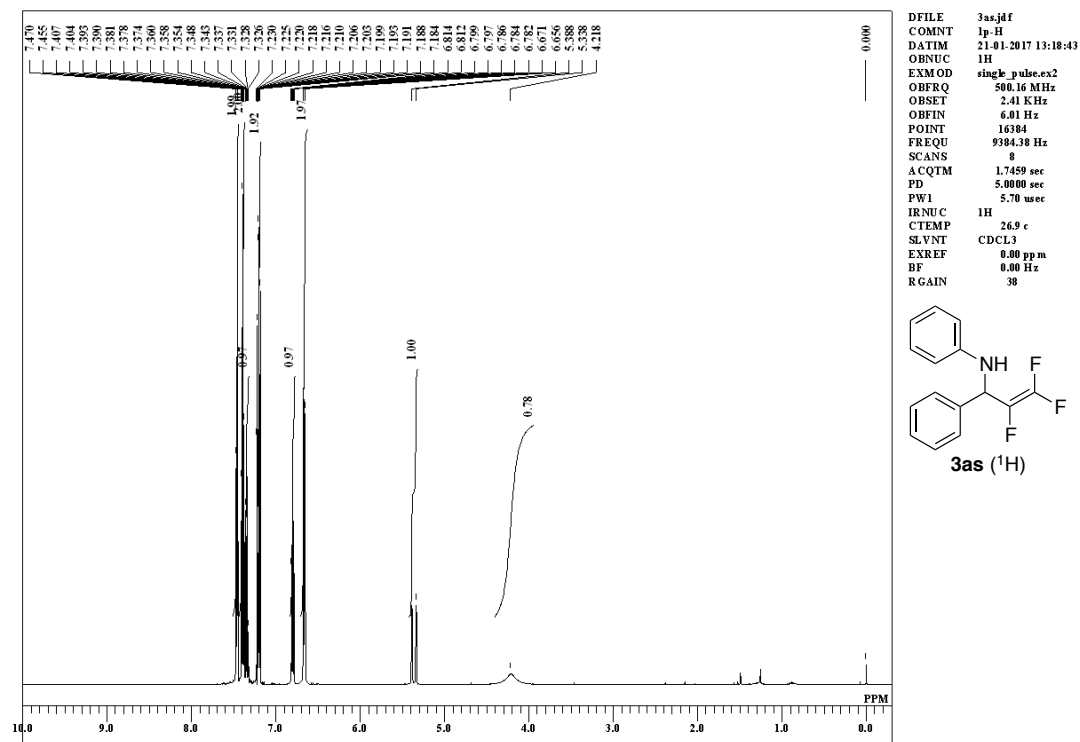
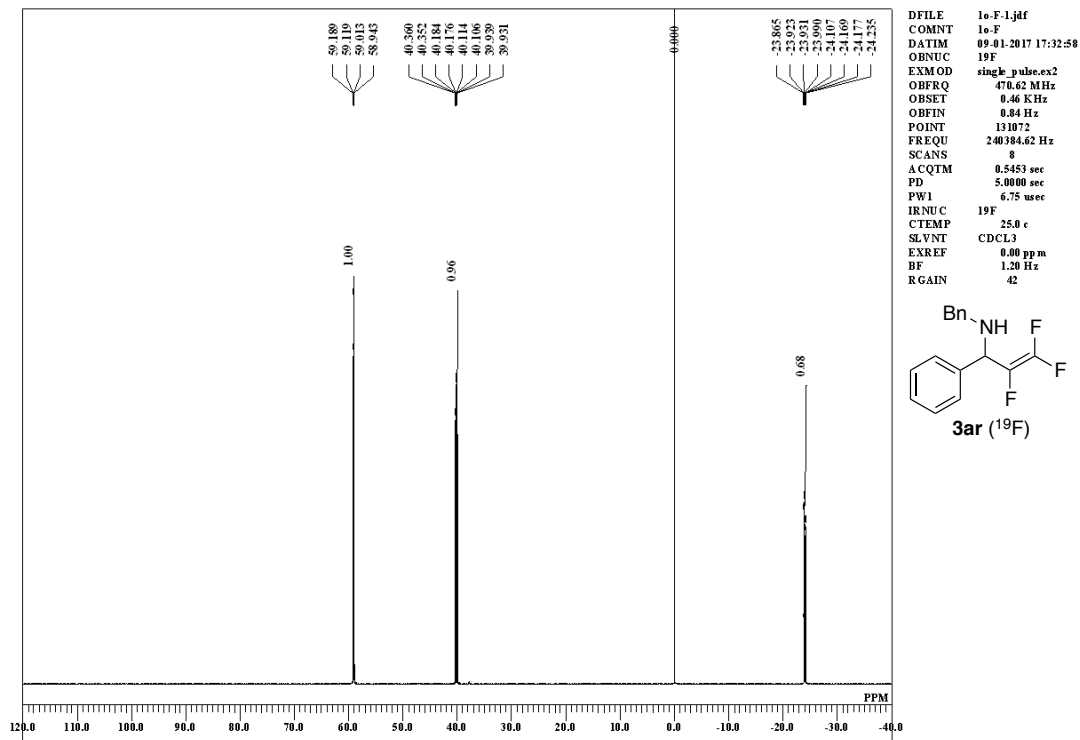
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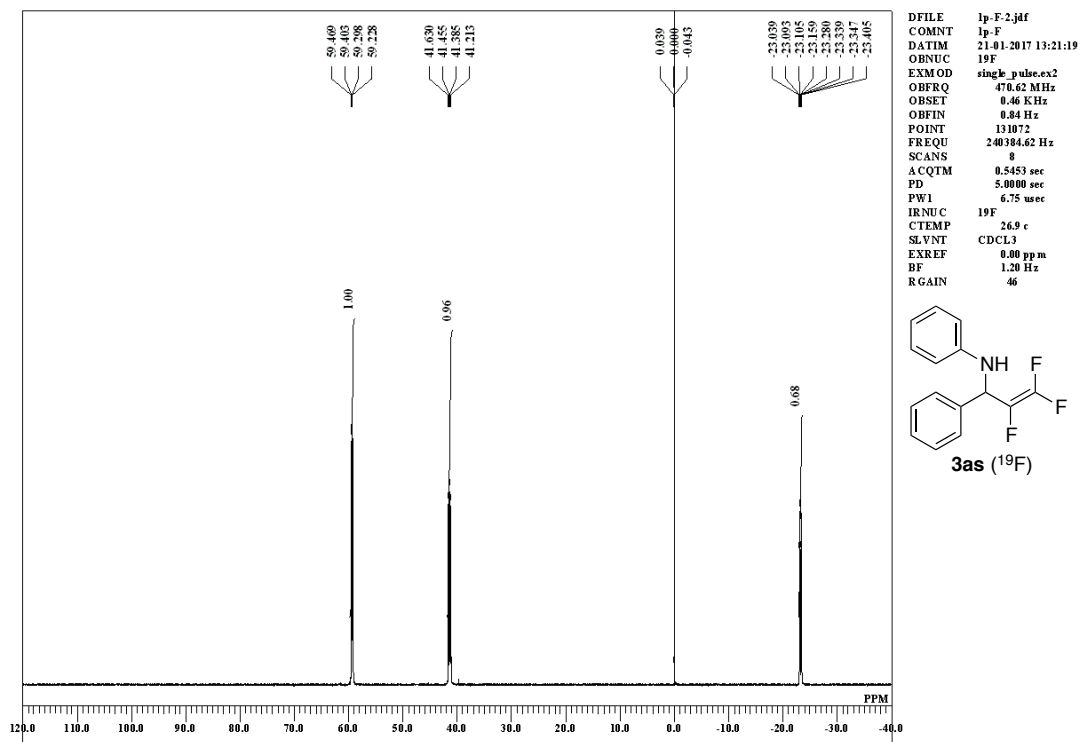
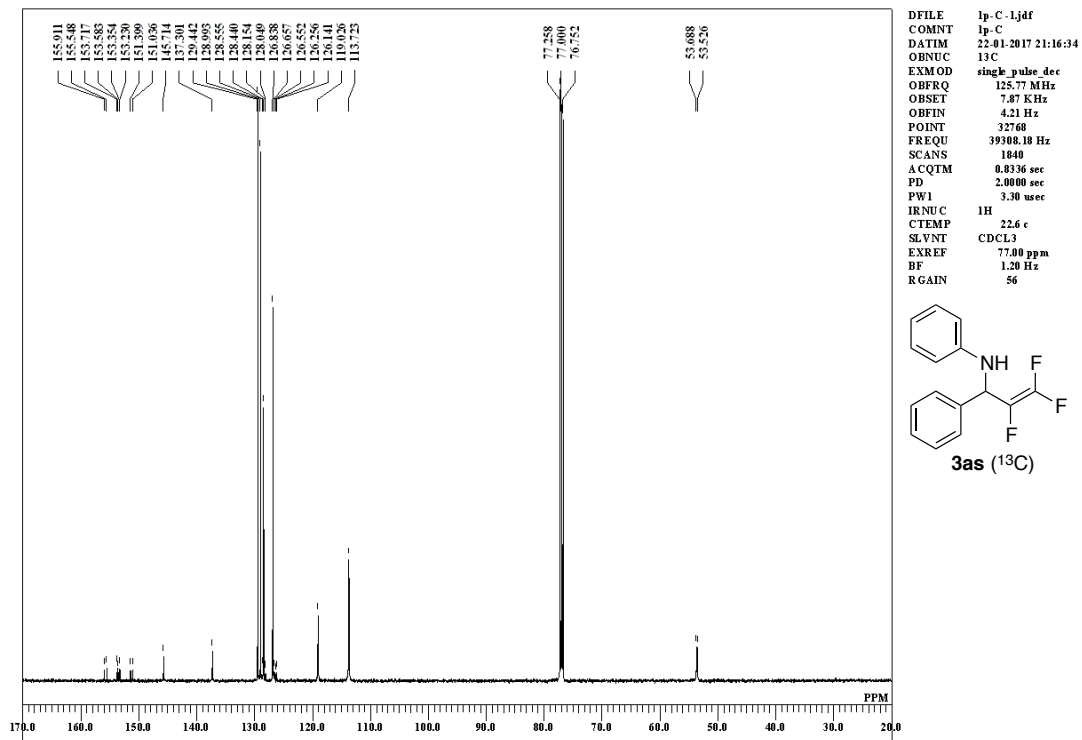


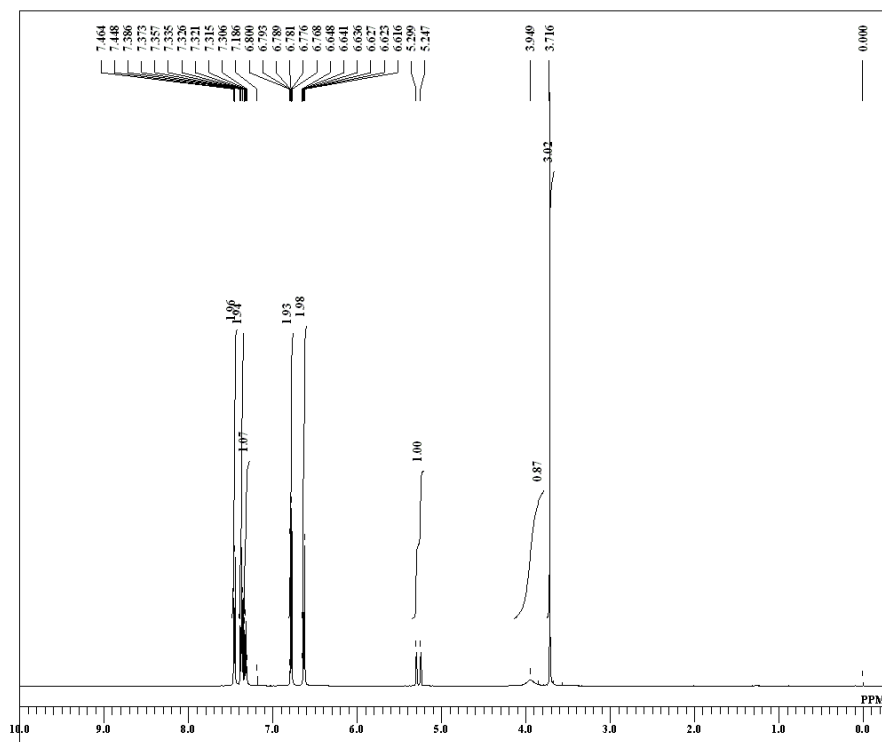
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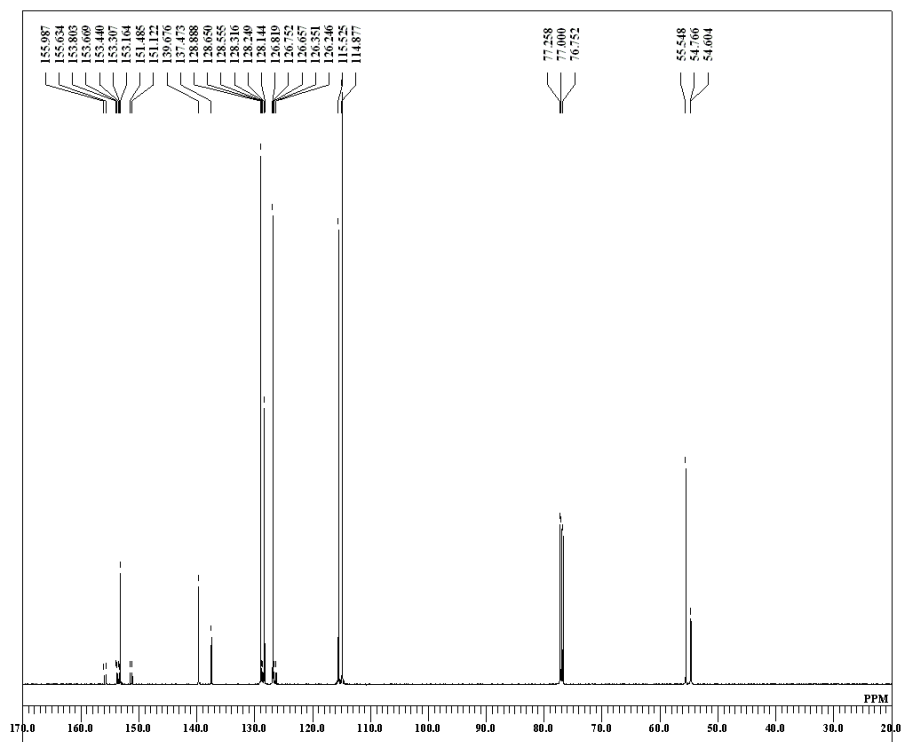
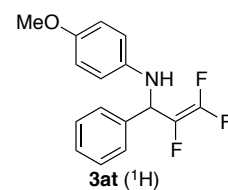




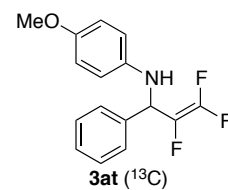


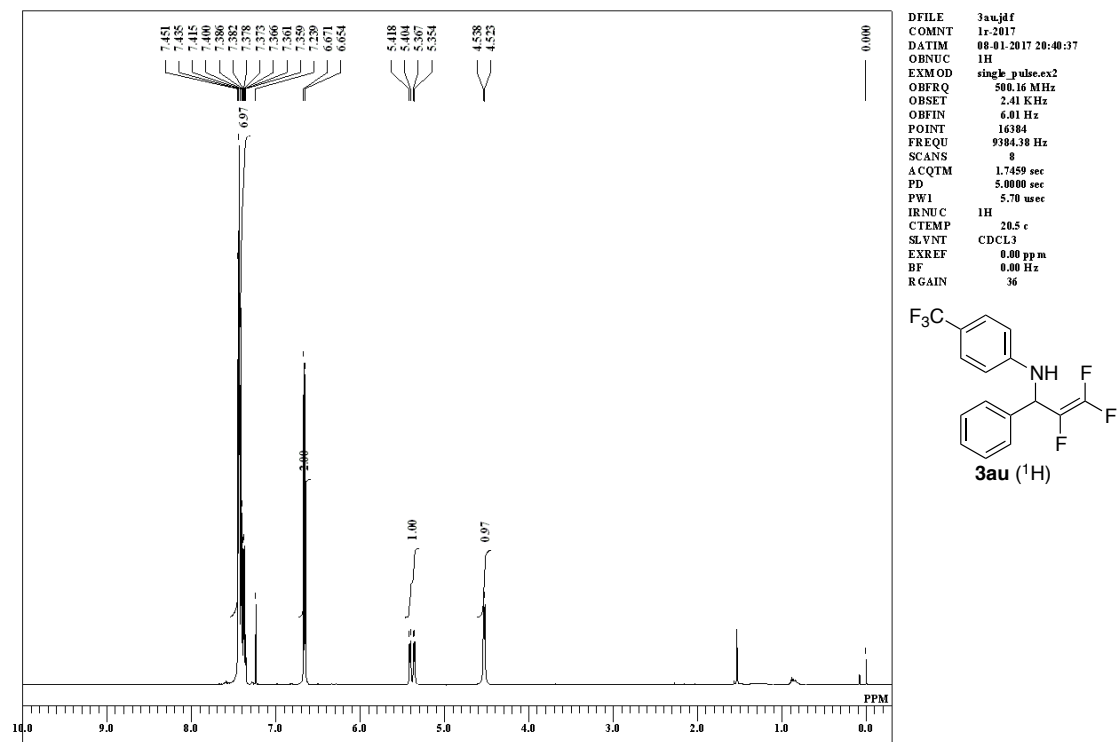
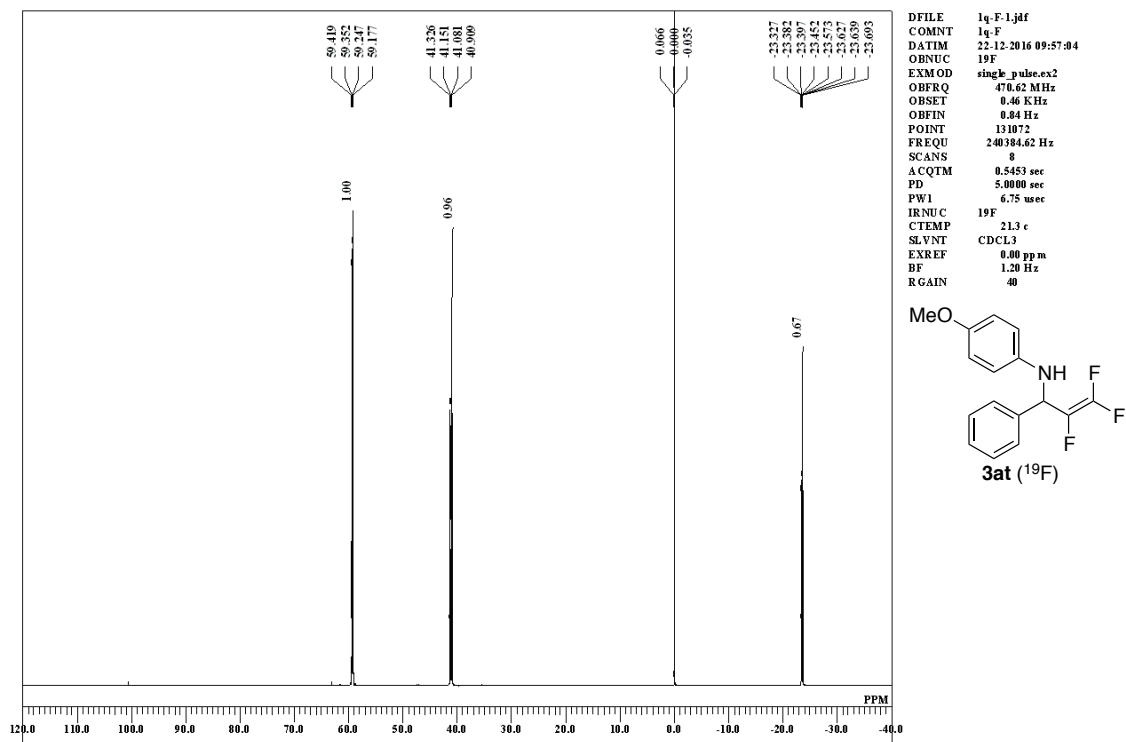


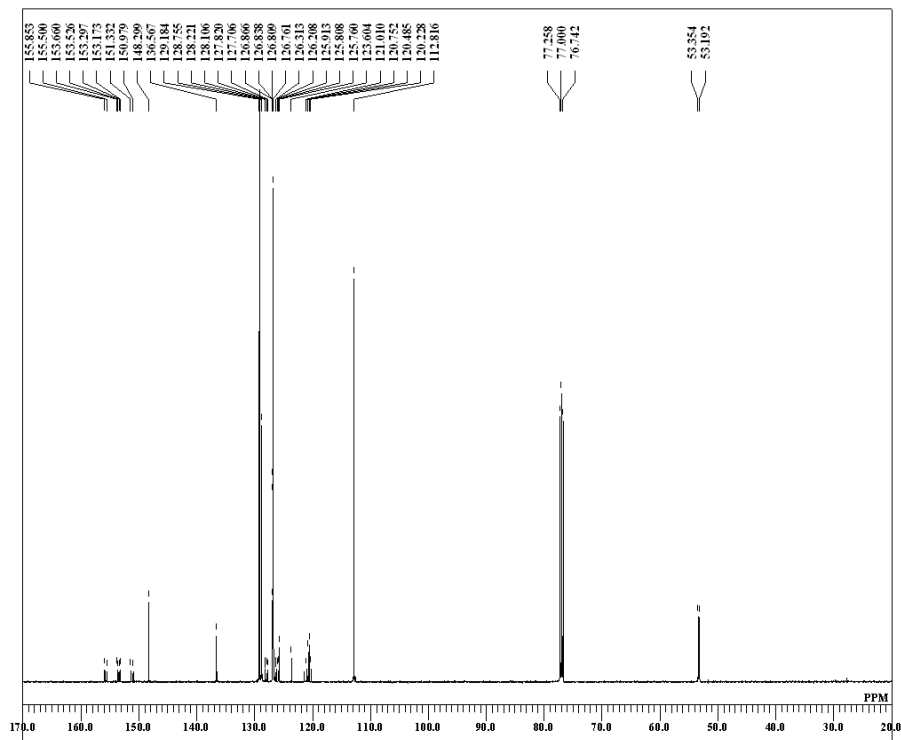
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 SCANS 8
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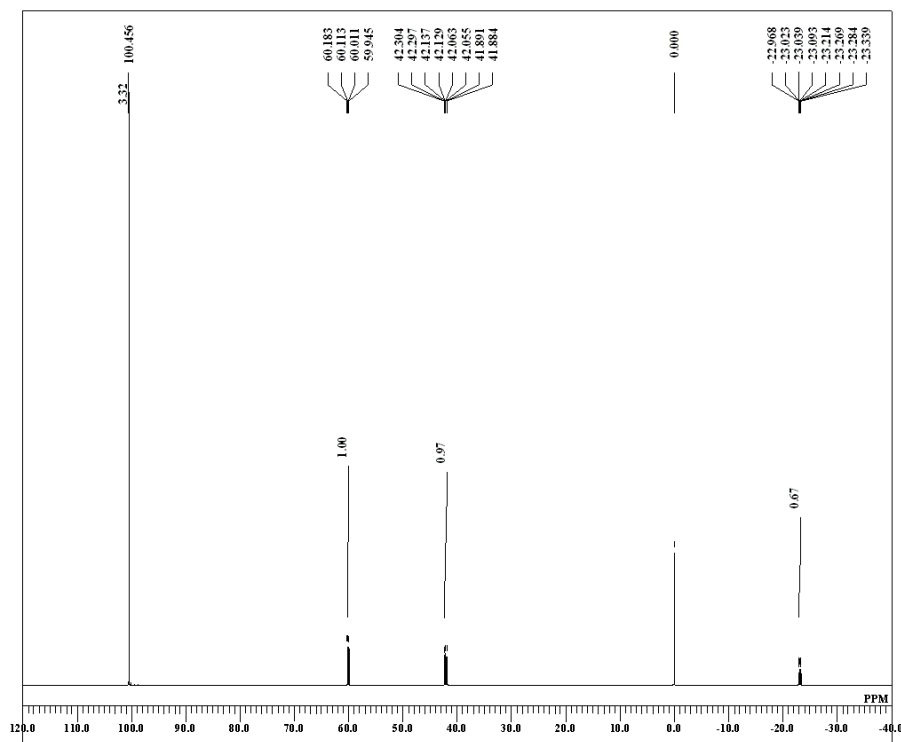
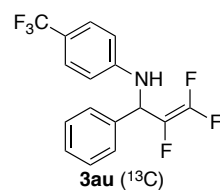
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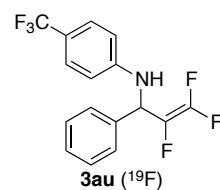


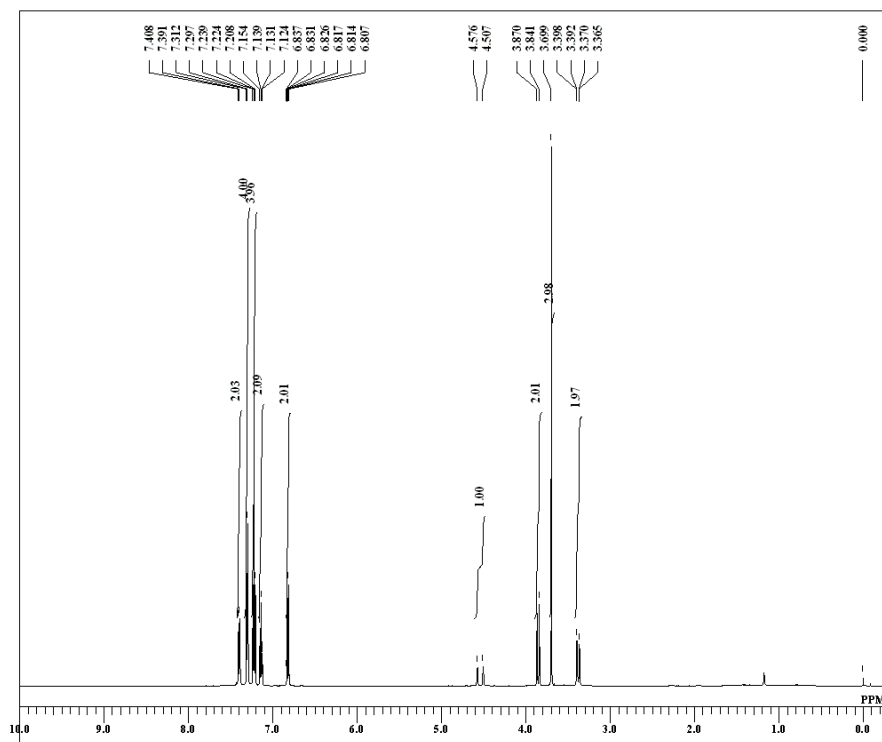


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 PD 2.0000 sec
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 BF 1.20 Hz
 RGAIN 50

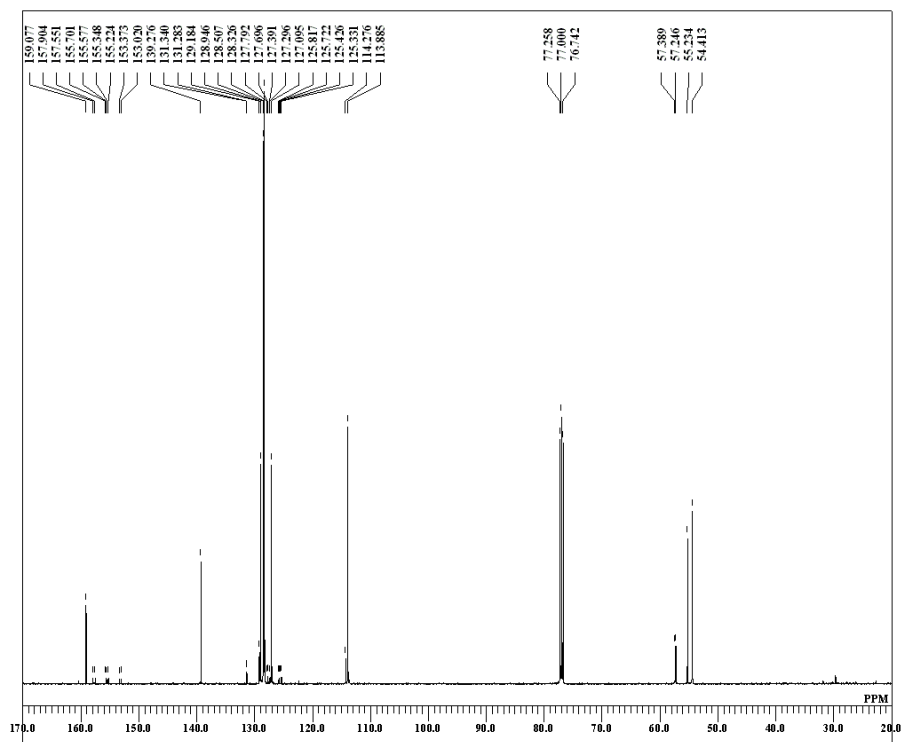
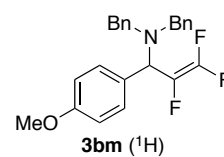


DFILE 1r-2-F-1.jdf
 COMINT 1r-2-F
 DATIM 09-01-2017 17:16:33
 OBNUC 19F
 EXMOD single_pulse_ex2
 OBFREQ 470.62 MHz
 OBSET 0.46 KHz
 OBFIN 0.84 Hz
 POINT 131072
 FREQU 240384.62 Hz
 SCANS 8
 ACQTM 0.5453 sec
 PD 5.0000 sec
 PW1 6.75 usec
 IRNUC 19F
 CTEMP 25.0 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 1.20 Hz
 RGAIN 40

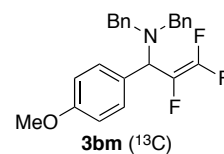


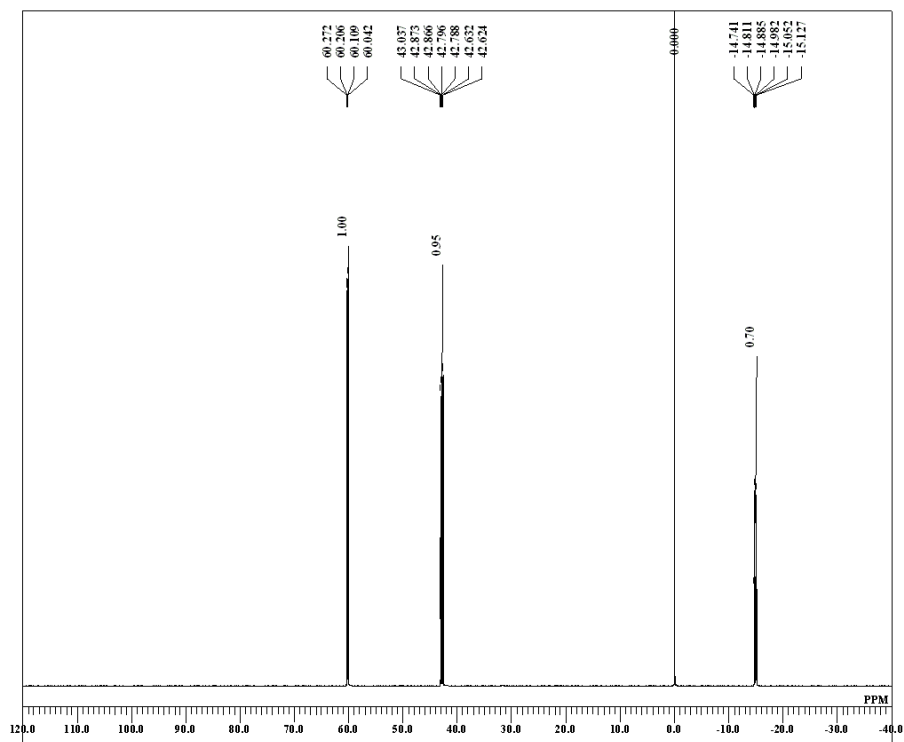


DFILE 2c-H-2.jdf
 COMINT 2c-H
 DATIM 28-01-2017 11:58:45
 OBNUC 1H
 EXMOD single_pulse.ex2
 OBFREQ 500.16 MHz
 OBSET 2.41 KHz
 OBFIN 6.01 Hz
 POINT 16384
 FREQU 9384.38 Hz
 SCANS 8
 ACQTM 1.7459 sec
 PD 5.0000 sec
 PW1 5.70 usec
 IRNUC 1H
 CTEMP 22.9 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.00 Hz
 RGAIN 30

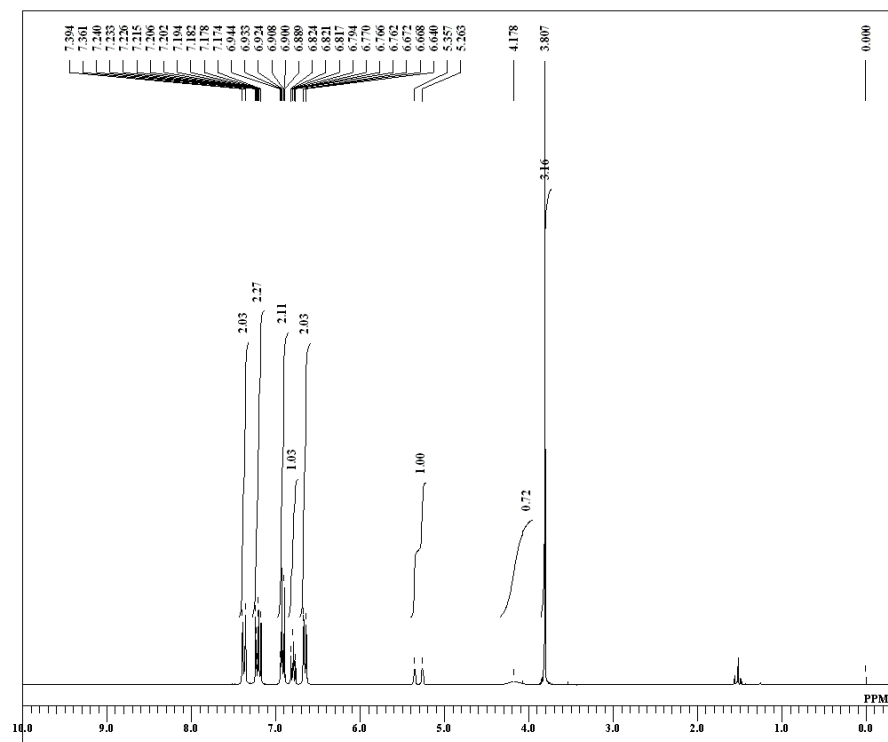
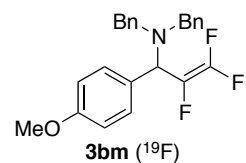


DFILE 2c-C.jdf
 COMINT 3SL-1236-C
 DATIM 08-01-2017 20:03:18
 OBNUC 13C
 EXMOD single_pulse.dec
 OBFREQ 125.77 MHz
 OBSET 7.87 KHz
 OBFIN 4.21 Hz
 POINT 32768
 FREQU 39308.18 Hz
 SCANS 1696
 ACQTM 0.8336 sec
 PD 2.0000 sec
 PW1 3.30 usec
 IRNUC 1H
 CTEMP 20.9 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 1.20 Hz
 RGAIN 56

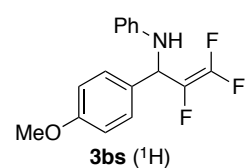


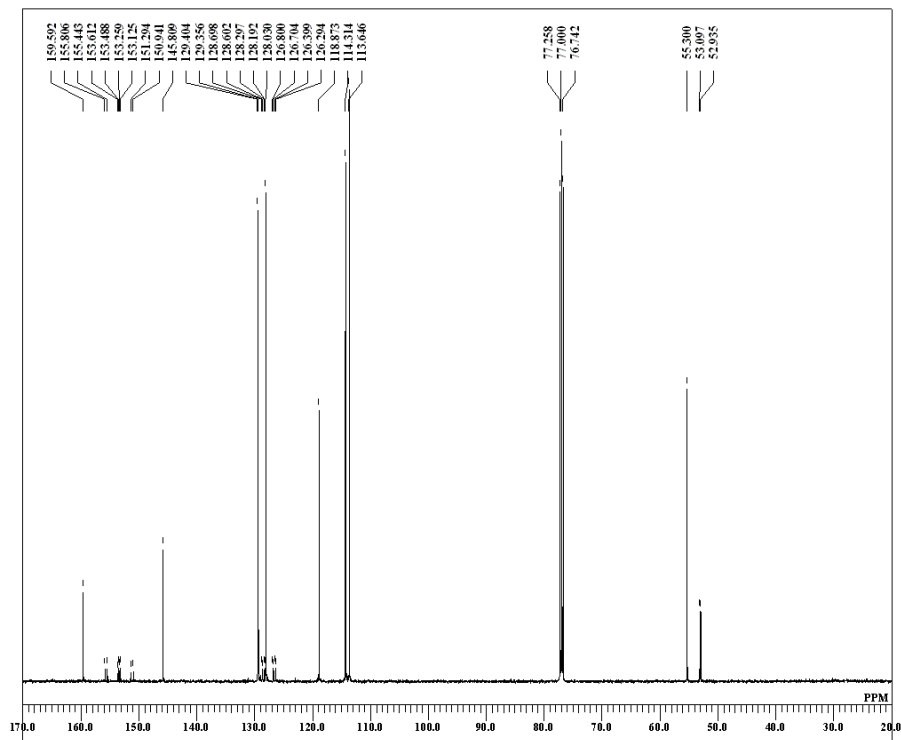


DFILE 2c-F-1j4f
 COMINT 2c-F
 DATIM 09-01-2017 17:20:23
 OBNUC 19F
 EXMOD single_pulse.ex2
 OBFREQ 470.62 MHz
 OBSET 0.46 KHz
 OBFIN 0.84 Hz
 POINT 131072
 FREQU 240384.62 Hz
 SCANS 8
 ACQTM 0.5453 sec
 PD 5.0000 sec
 PW1 6.75 usec
 IRNUC 19F
 CTEMP 25.0 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 1.20 Hz
 RGAIN 44

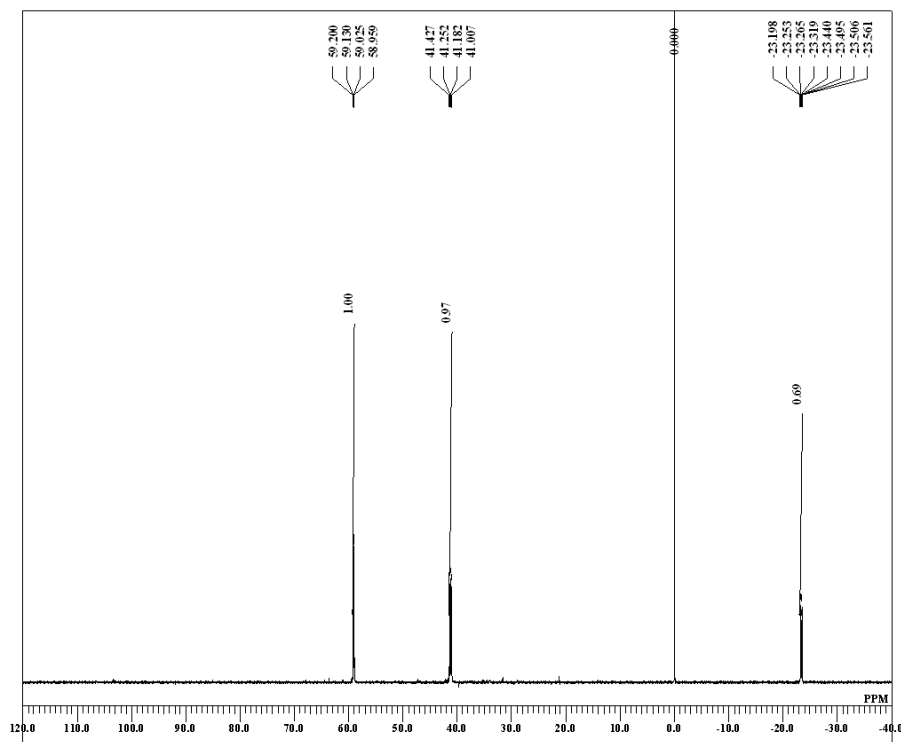
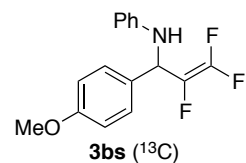


DFILE 3c-2 Jan.,23.2017.als
 COMINT 3c-2 Jan.,23.2017
 DATIM Mon Jan 23 21:44:08 2017
 OBNUC 1H
 EXMOD NON
 OBFREQ 270.05 MHz
 OBSET 112.00 KHz
 OBFIN 5800.00 Hz
 POINT 16384
 FREQU 5401.76 Hz
 SCANS 8
 ACQTM 3.0331 sec
 PD 3.9670 sec
 PW1 5.70 usec
 IRNUC 1H
 CTEMP 24.8 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.10 Hz
 RGAIN 17

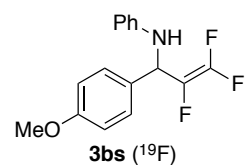


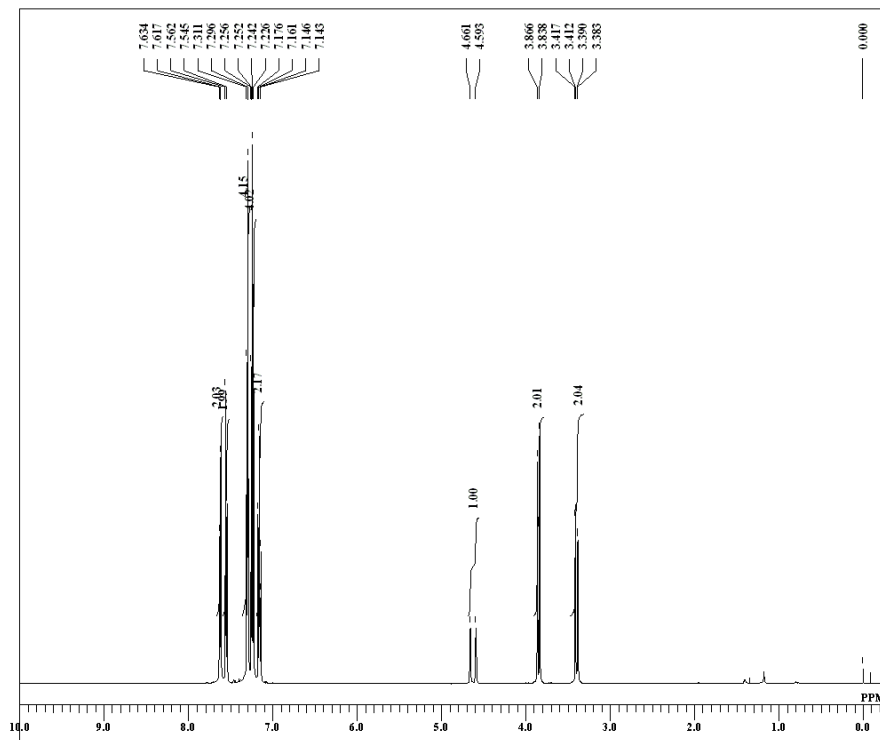


DFILE 3c-C.jdf
 COMINT 3SI-1237-C
 DATIM 08-01-2017 17:32:44
 OBNUC 13C
 EXMOD single_pulse_dec
 OBFREQ 125.77 MHz
 OBSET 7.87 KHz
 OBFIN 4.21 Hz
 POINT 32768
 FREQU 39308.18 Hz
 SCANS 1696
 ACQTM 0.8336 sec
 PD 2.0000 sec
 PW1 3.30 usec
 IRNUC 1H
 CTEMP 21.0 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 1.20 Hz
 RGAIN 56

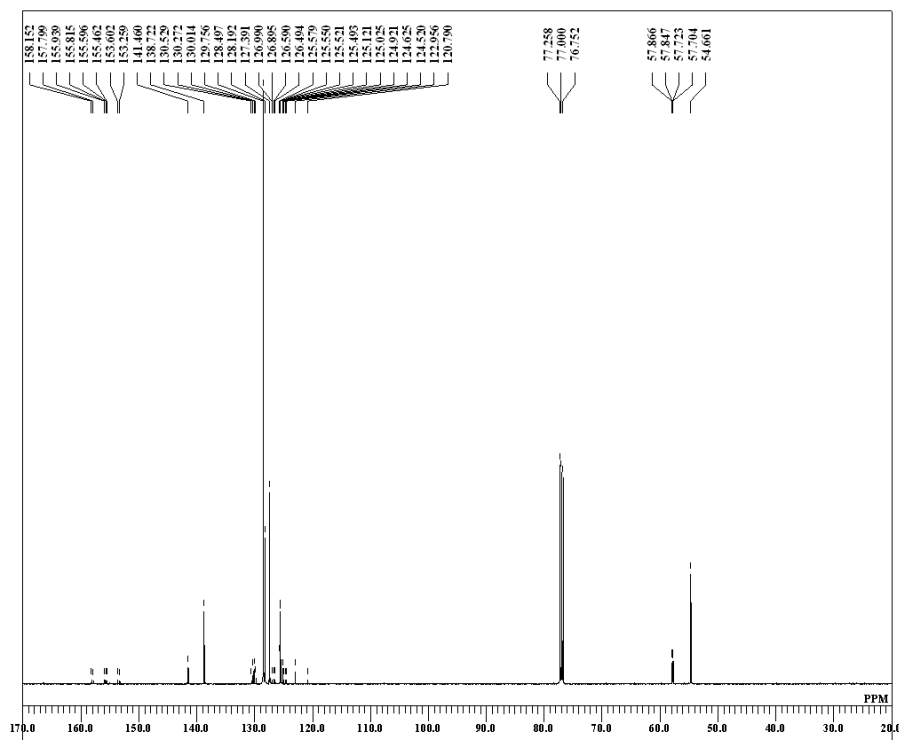
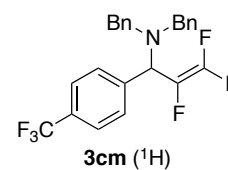


DFILE 3c-F-2.jdf
 COMINT 3c-F
 DATIM 01-02-2017 11:35:44
 OBNUC 19F
 EXMOD single_pulse_ex2
 OBFREQ 470.62 MHz
 OBSET 0.46 KHz
 OBFIN 0.84 Hz
 POINT 131072
 FREQU 240384.62 Hz
 SCANS 8
 ACQTM 0.5453 sec
 PD 5.0000 sec
 PW1 6.75 usec
 IRNUC 19F
 CTEMP 22.5 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 1.20 Hz
 RGAIN 44

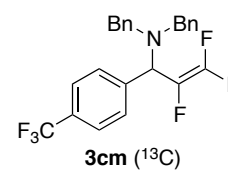


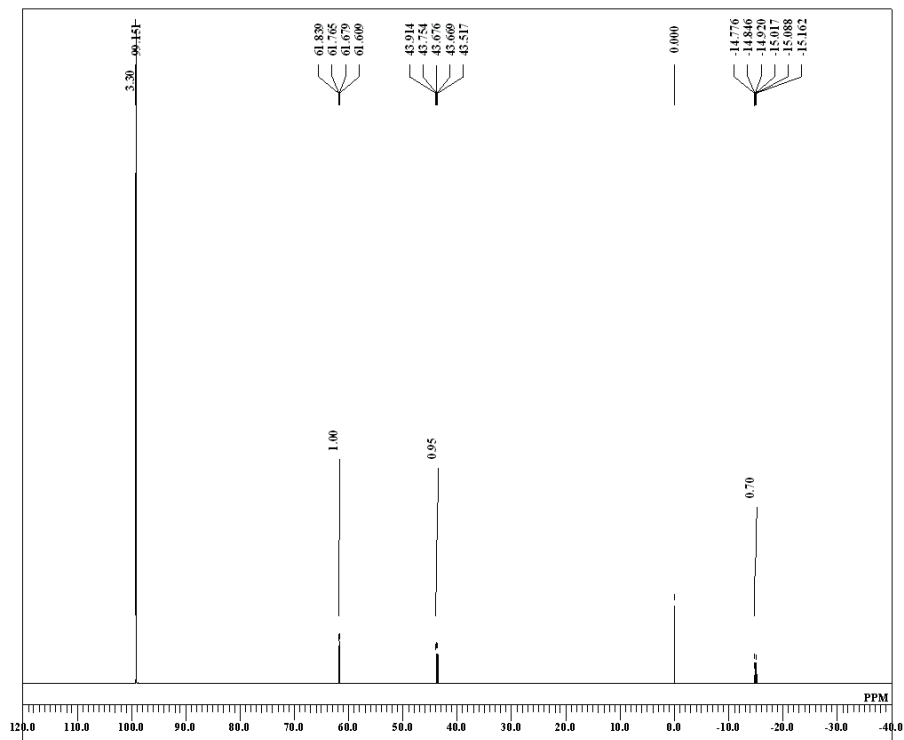


DFILE 3cm.jdf
 COMINT 2b-C-H
 DATIM 21-01-2017 13:37:33
 OBNUC 1H
 EXMOD single_pulse.v2
 OBFRQ 500.16 MHz
 OBSET 2.41 KHz
 OBFIN 6.01 Hz
 POINT 16384
 FREQU 9384.38 Hz
 SCANS 8
 ACQTM 1.7459 sec
 PD 5.0000 sec
 PW1 5.70 usec
 IRNUC 1H
 CTEMP 27.0 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.00 Hz
 RGAIN 34

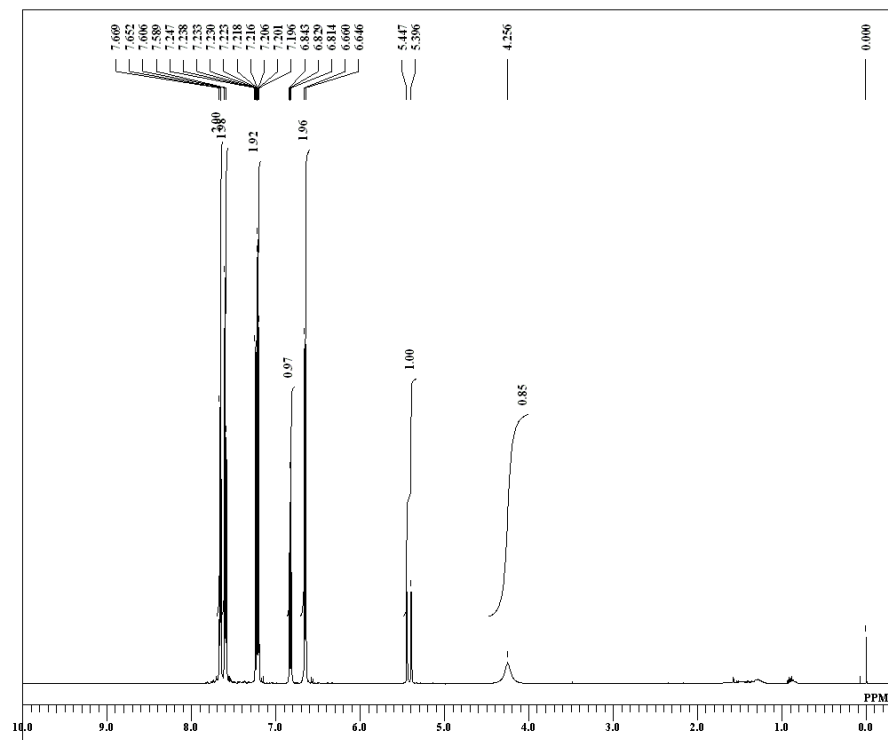
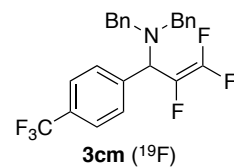


DFILE 2b-C-1.jdf
 COMINT 2b-C
 DATIM 21-01-2017 15:56:00
 OBNUC 13C
 EXMOD single_pulse.dec
 OBFRQ 125.77 MHz
 OBSET 7.87 KHz
 OBFIN 4.21 Hz
 POINT 32768
 FREQU 39308.18 Hz
 SCANS 1696
 ACQTM 0.8336 sec
 PD 2.0000 sec
 PW1 3.30 usec
 IRNUC 1H
 CTEMP 27.7 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 1.20 Hz
 RGAIN 56

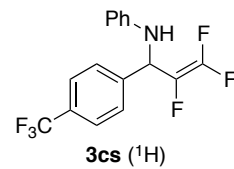


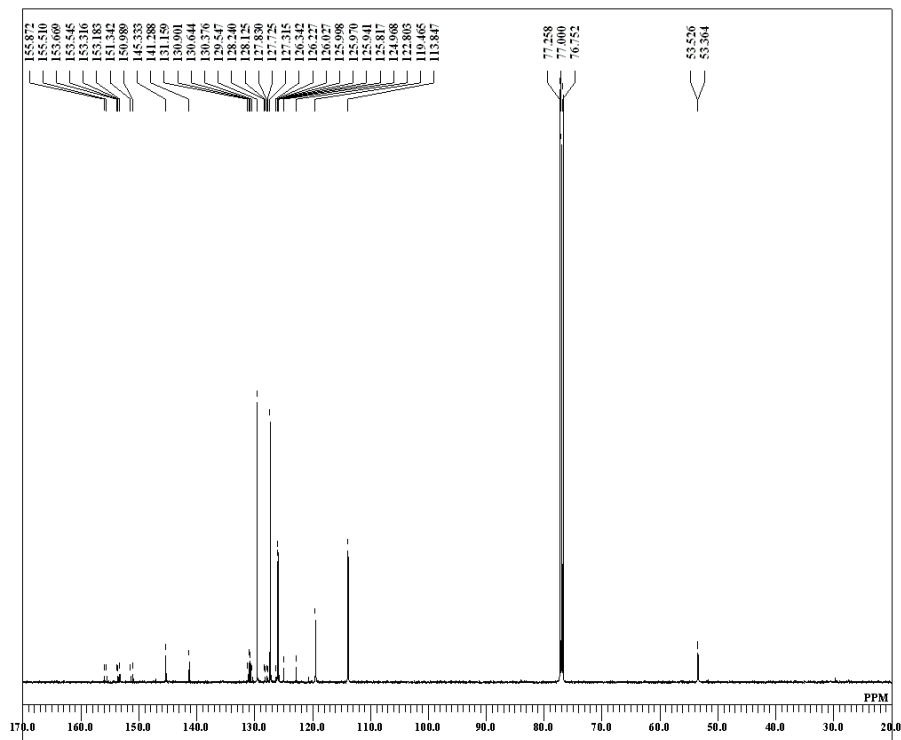


DFILE 2b-F-1.jdf
 COMINT 2b-F
 DATIM 09-01-2017 17:12:33
 OBNUC 19F
 EXMOD single_pulse.ex2
 OBFRQ 470.62 MHz
 OBSET 0.46 KHz
 OBFIN 0.84 Hz
 POINT 131072
 FREQU 240384.62 Hz
 SCANS 8
 ACQTM 0.5453 sec
 PD 5.0000 sec
 PW1 6.75 usec
 IRNUC 19F
 CTEMP 25.0 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 1.20 Hz
 RGAIN 44

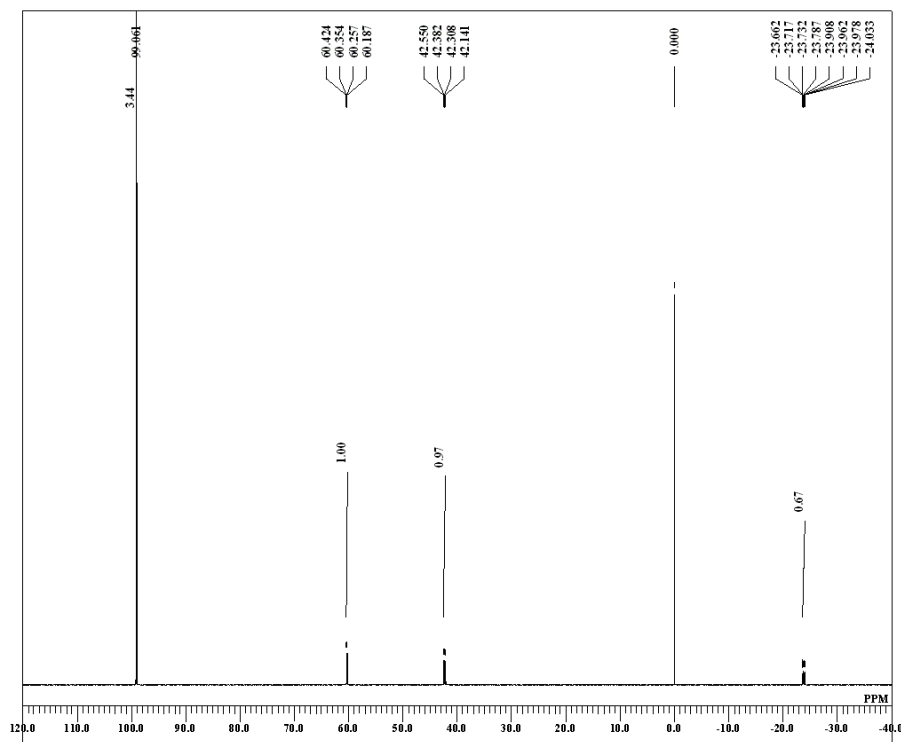
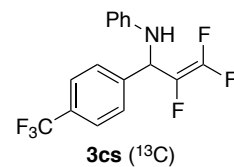


DFILE 3cs.jdf
 COMINT 3b-C-H
 DATIM 24-01-2017 19:30:34
 OBNUC 1H
 EXMOD single_pulse.ex2
 OBFRQ 500.16 MHz
 OBSET 2.41 KHz
 OBFIN 6.01 Hz
 POINT 16384
 FREQU 9384.38 Hz
 SCANS 8
 ACQTM 1.7459 sec
 PD 5.0000 sec
 PW1 5.70 usec
 IRNUC 1H
 CTEMP 23.4 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.10 Hz
 RGAIN 44

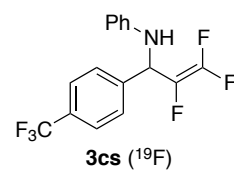


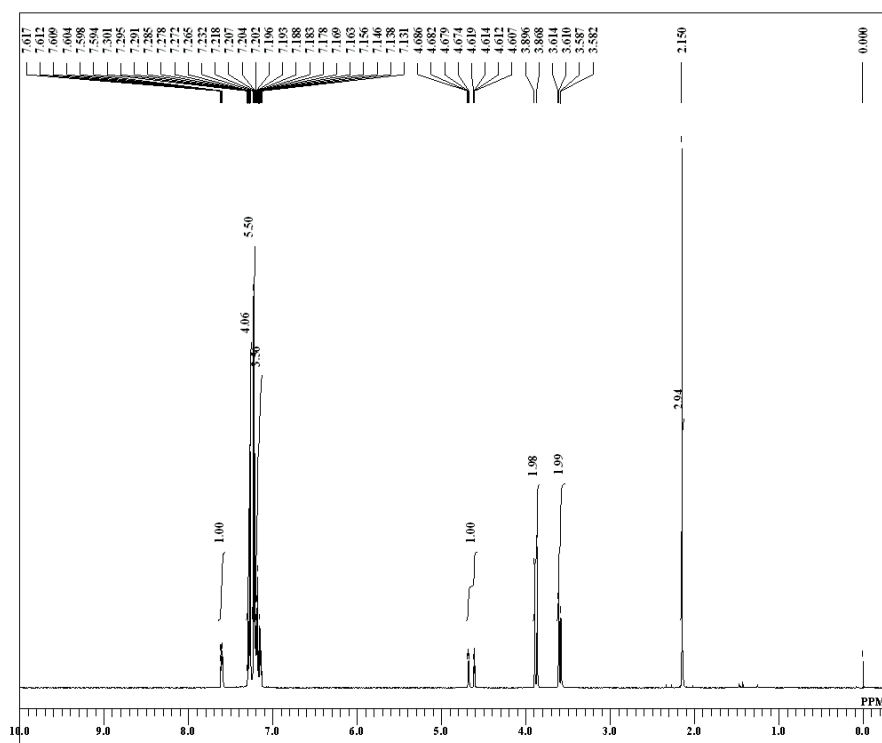


DFILE 3b-C-2.jdf
 COMINT 3b-C
 DATIM 24-01-2017 21:39:55
 OBNUC 13C
 EXMOD single_pulse_dec
 OBFRQ 125.77 MHz
 OBSET 7.87 KHz
 OBFIN 4.21 Hz
 POINT 32768
 FREQU 39308.18 Hz
 SCANS 2715
 ACQTM 0.8336 sec
 PD 2.0000 sec
 PW1 3.30 usec
 IRNUC 1H
 CTEMP 23.5 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 1.20 Hz
 RGAIN 56

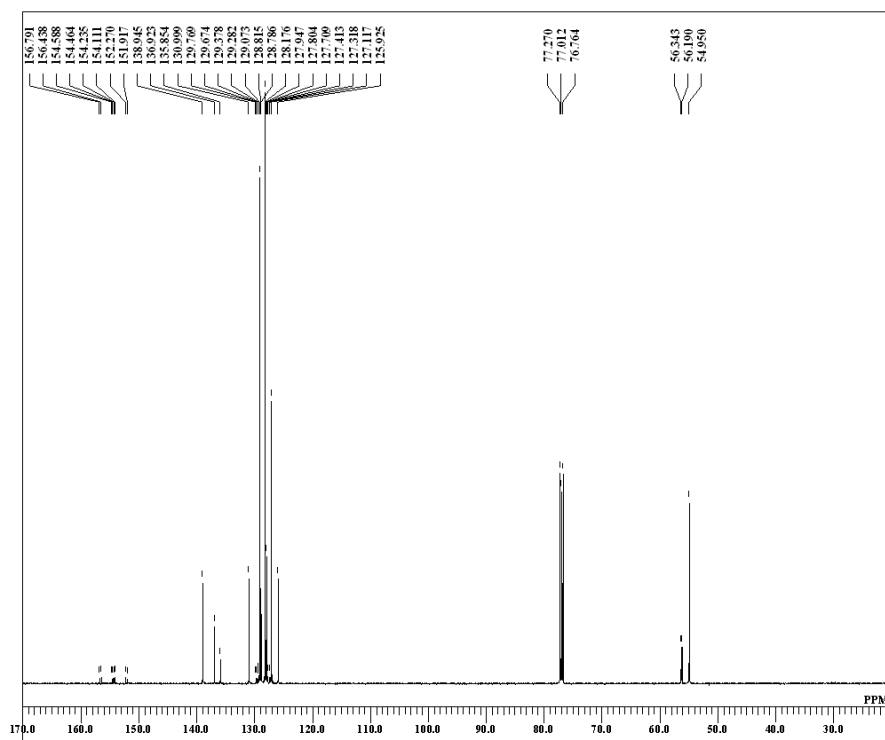
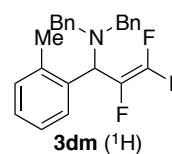


DFILE 3b-3-F-1.jdf
 COMINT 3b-3-F
 DATIM 11-01-2017 17:04:22
 OBNUC 19F
 EXMOD single_pulse.ex2
 OBFRQ 470.62 MHz
 OBSET 0.46 KHz
 OBFIN 0.84 Hz
 POINT 131072
 FREQU 240384.62 Hz
 SCANS 8
 ACQTM 0.5453 sec
 PD 5.0000 sec
 PW1 6.75 usec
 IRNUC 19F
 CTEMP 22.8 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 1.20 Hz
 RGAIN 44

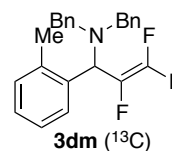


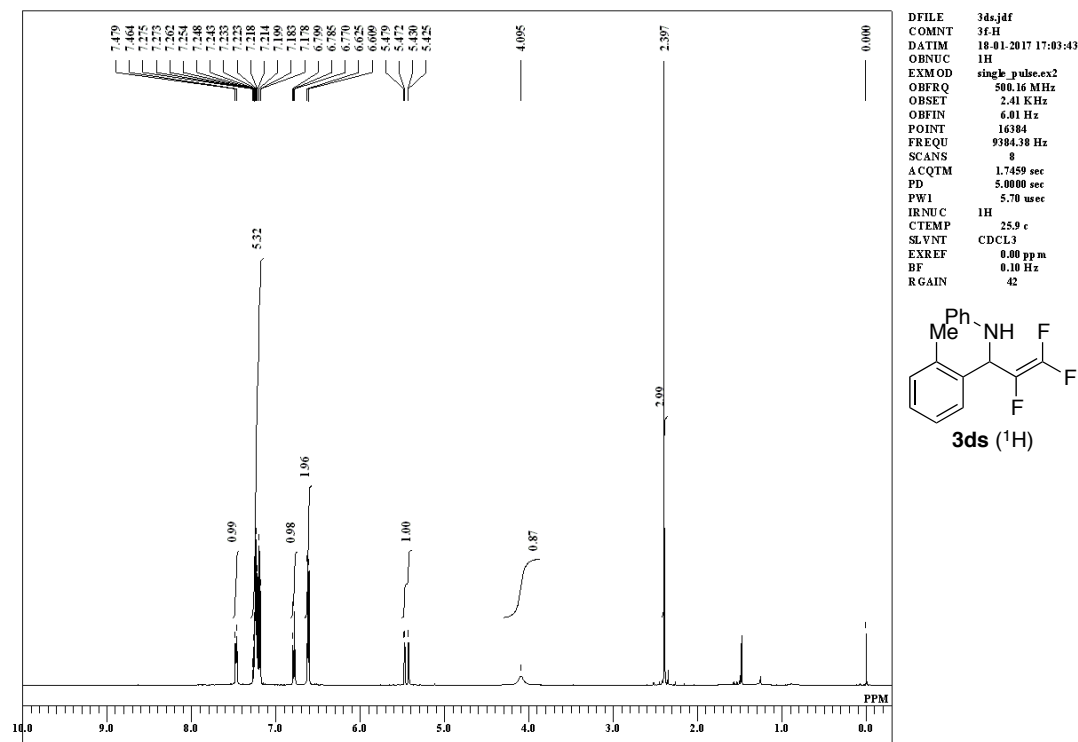
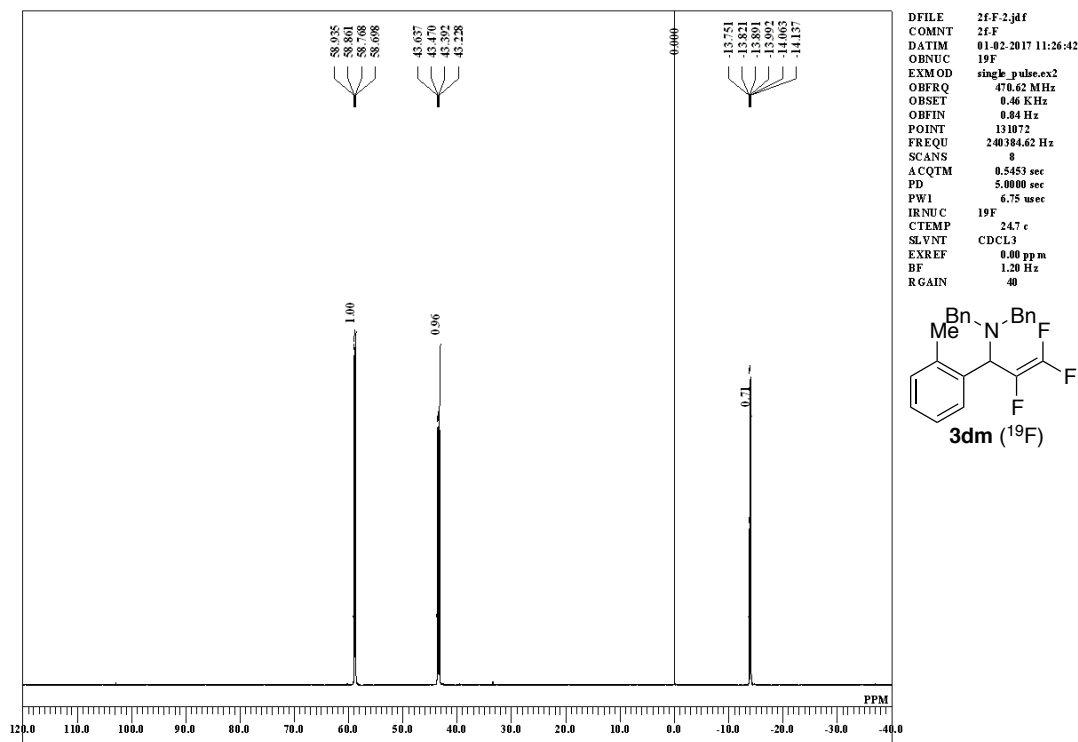


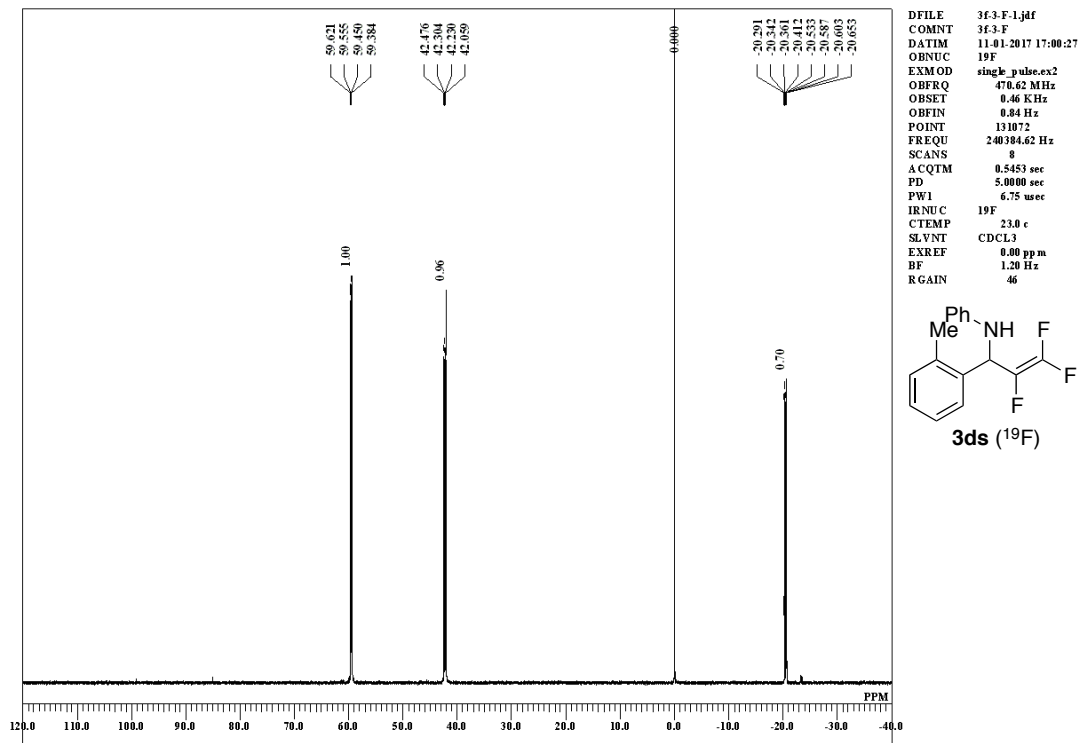
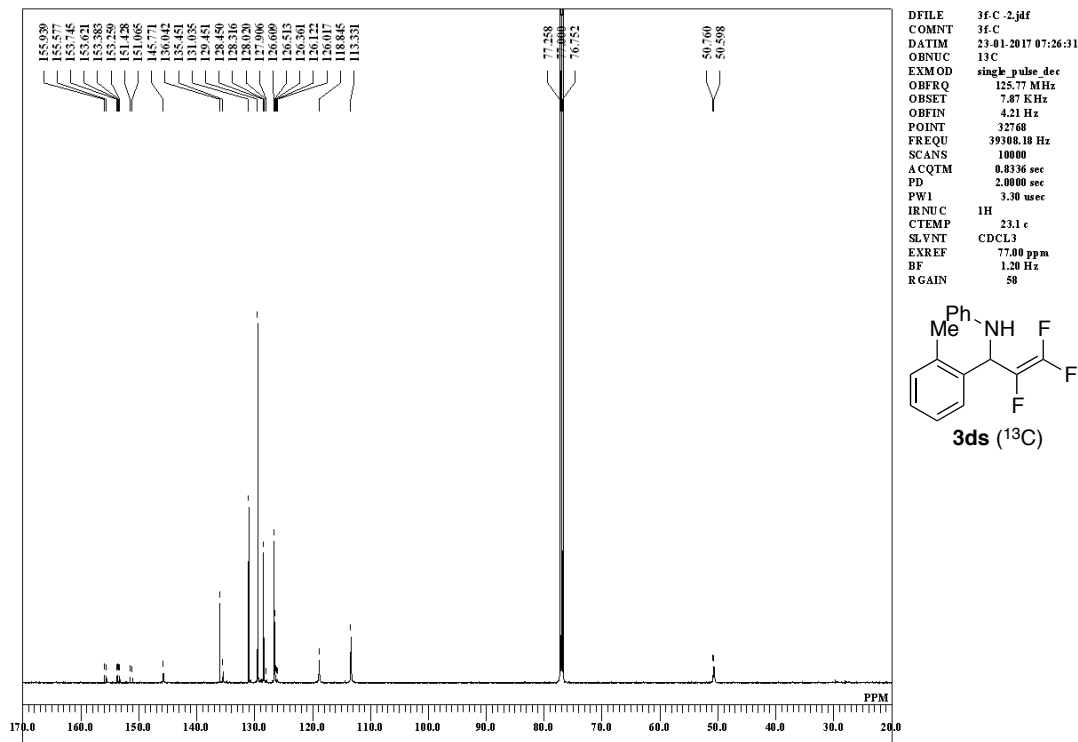
DFILE 3dm.jdf
 COMNT 2f.c H
 DATIM 13-01-2017 11:03:11
 OBNUC 1H
 EXMOD single_pulse.ex2
 OBFRQ 500.16 MHz
 OBSET 2.41 KHz
 OBFIN 6.01 Hz
 POINT 16384
 FREQU 9384.38 Hz
 SCANS 8
 ACQTM 1.7459 sec
 PD 5.0000 sec
 PW1 5.70 usec
 IRNUC 1H
 CTEMP 21.5 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.00 Hz
 RGAIN 30

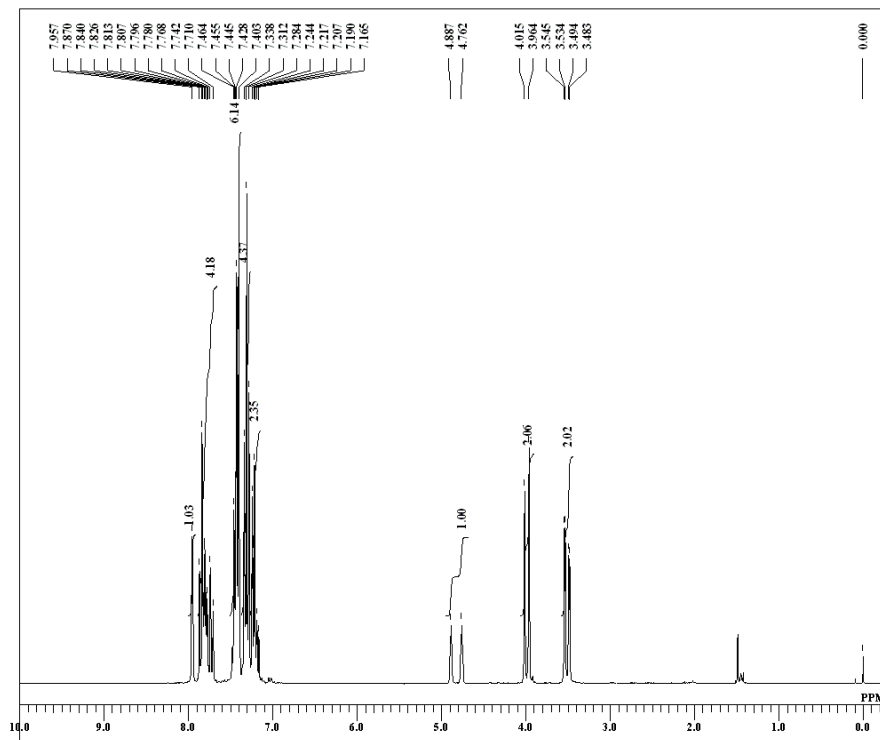


DFILE 2f.c-1.jdf
 COMNT 2f.c
 DATIM 13-01-2017 12:22:06
 OBNUC 13C
 EXMOD single_pulse_dec
 OBFRQ 125.77 MHz
 OBSET 7.87 KHz
 OBFIN 4.21 Hz
 POINT 32760
 FREQU 39308.18 Hz
 SCANS 1650
 ACQTM 0.8336 sec
 PD 2.0000 sec
 PW1 3.30 usec
 IRNUC 13C
 CTEMP 23.2 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 1.20 Hz
 RGAIN 58

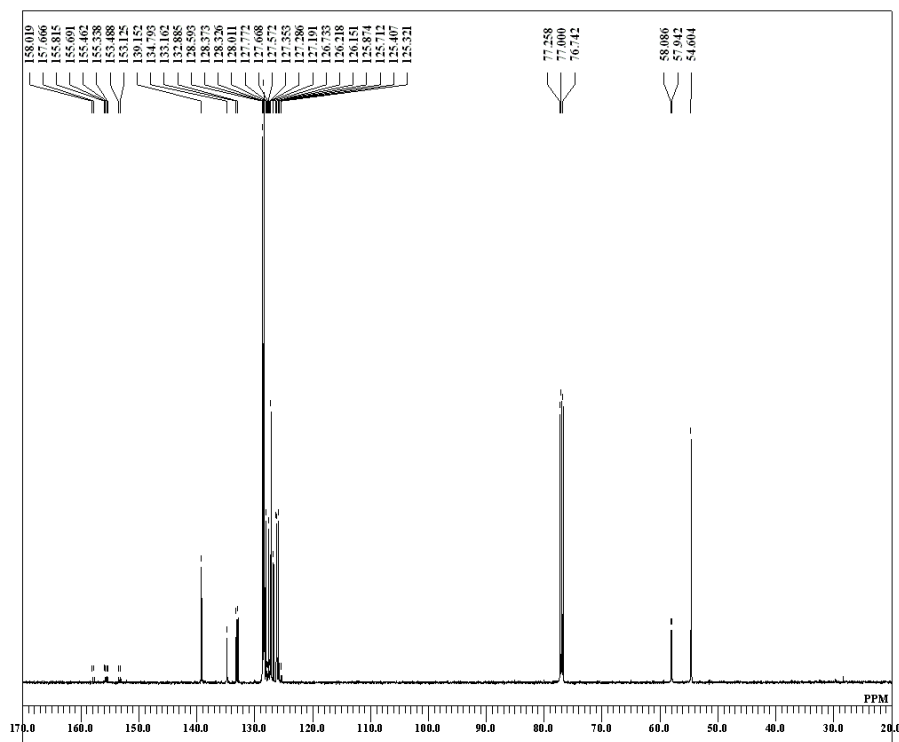
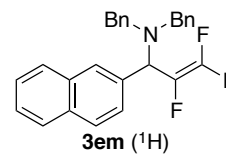




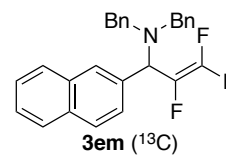


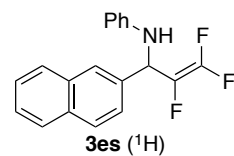
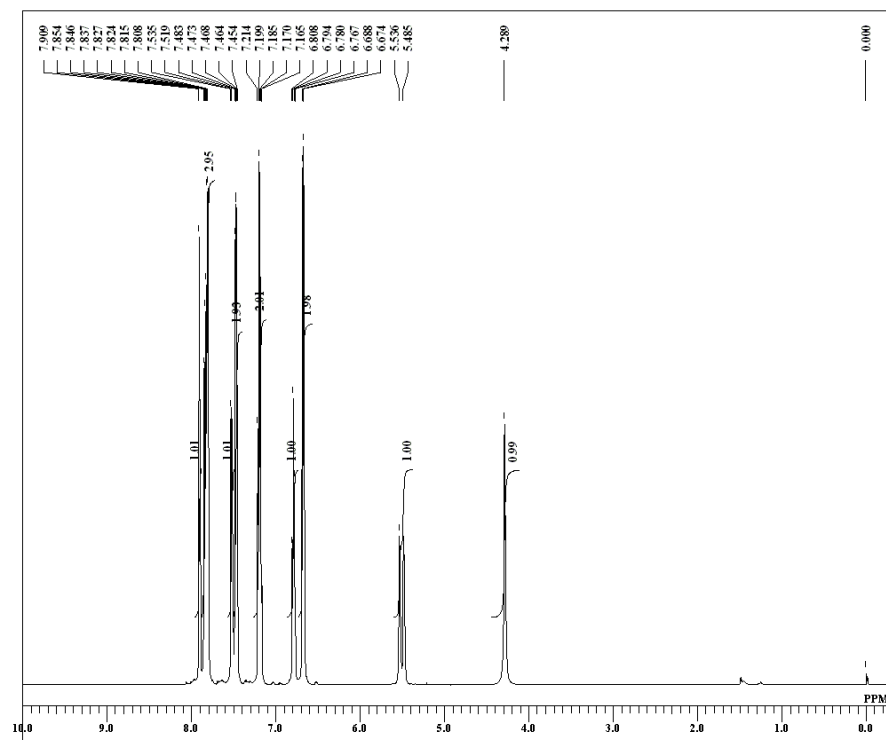
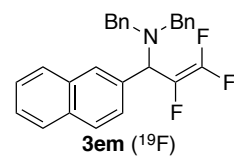
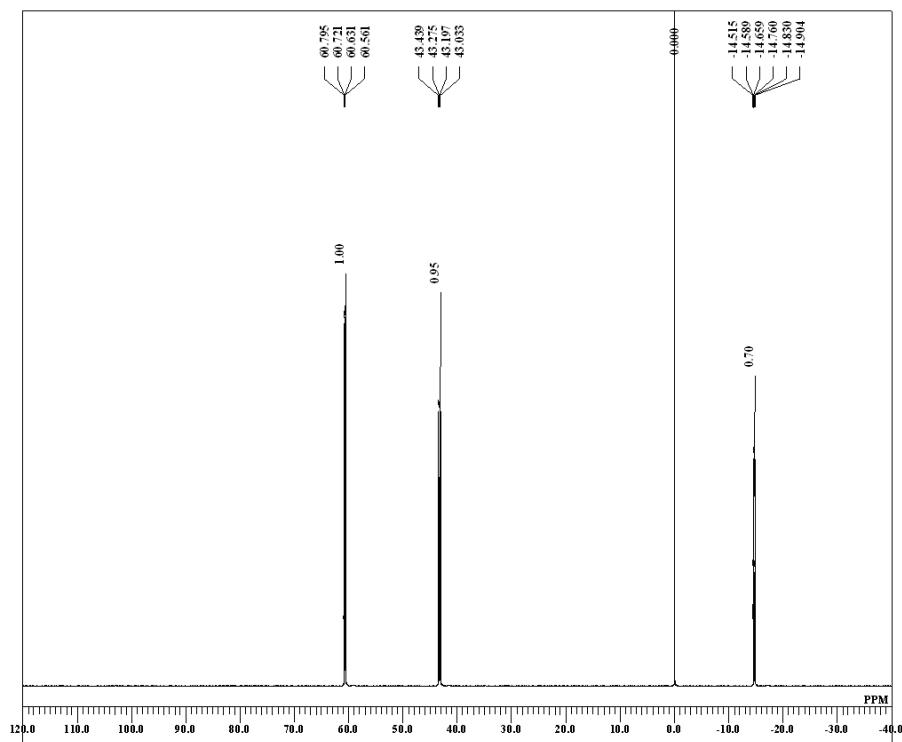


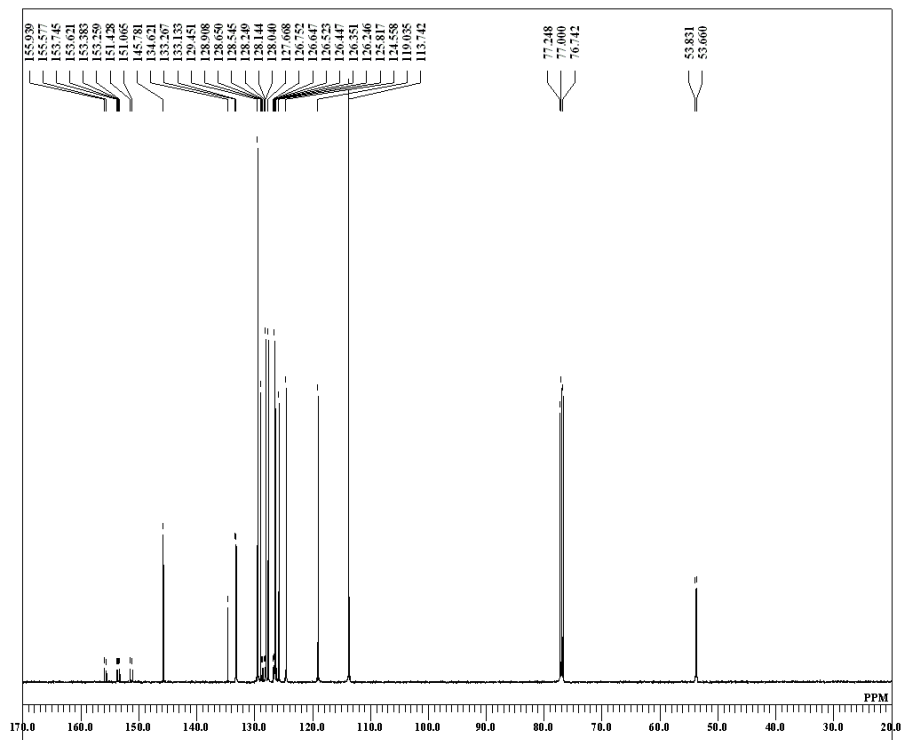
DFILE 3em.ab
 COMINT 2a-5-10
 DATIM Thu Dec 15 16:44:46 2016
 OBNUC ¹H
 EXMOD NON
 OBFRQ 270.05 MHz
 OBSET 112.00 KHz
 OBFIN 5800.00 Hz
 POINT 16384
 FREQU 5401.76 Hz
 SCANS 8
 ACQTM 3.0331 sec
 PD 3.9670 sec
 PW1 5.70 usec
 IRNUC ¹H
 CTEMP 22.4 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.00 Hz
 RGAIN 13



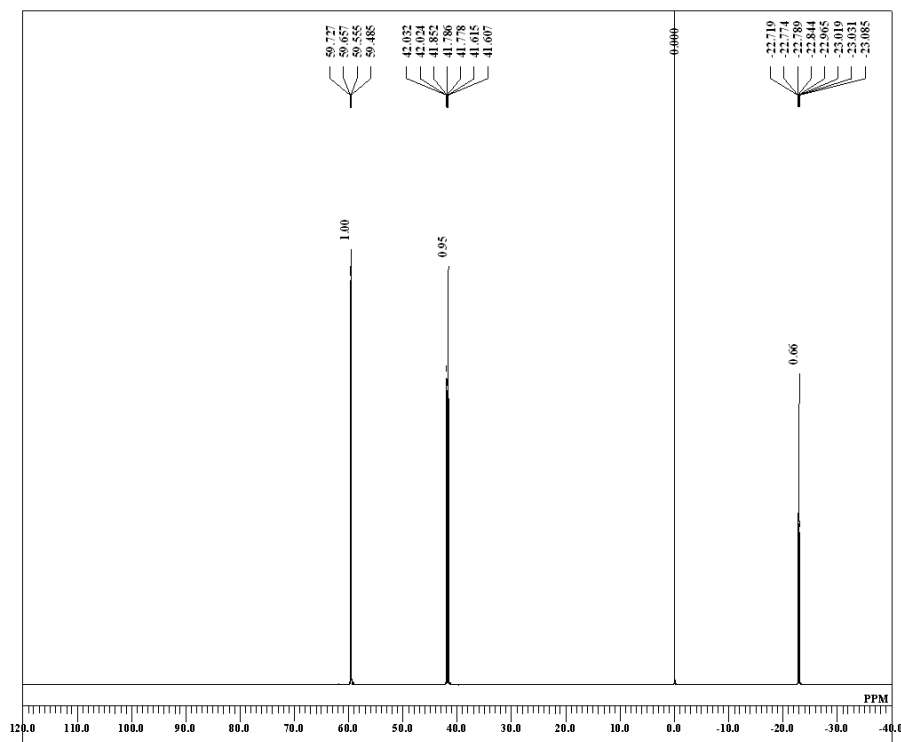
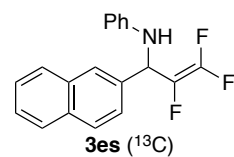
DFILE 2a-C-1.jdf
 COMINT 2a-C-1
 DATIM 16-01-2017 16:00:21
 OBNUC ¹³C
 EXMOD single_pulse_dec
 OBFRQ 125.77 MHz
 OBSET 7.87 KHz
 OBFIN 4.21 Hz
 POINT 32768
 FREQU 39308.18 Hz
 SCANS 1330
 ACQTM 0.8336 sec
 PD 2.0000 sec
 PW1 3.30 usec
 IRNUC ¹H
 CTEMP 23.5 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 1.20 Hz
 RGAIN 58



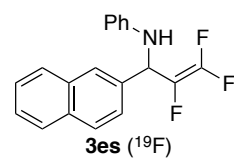


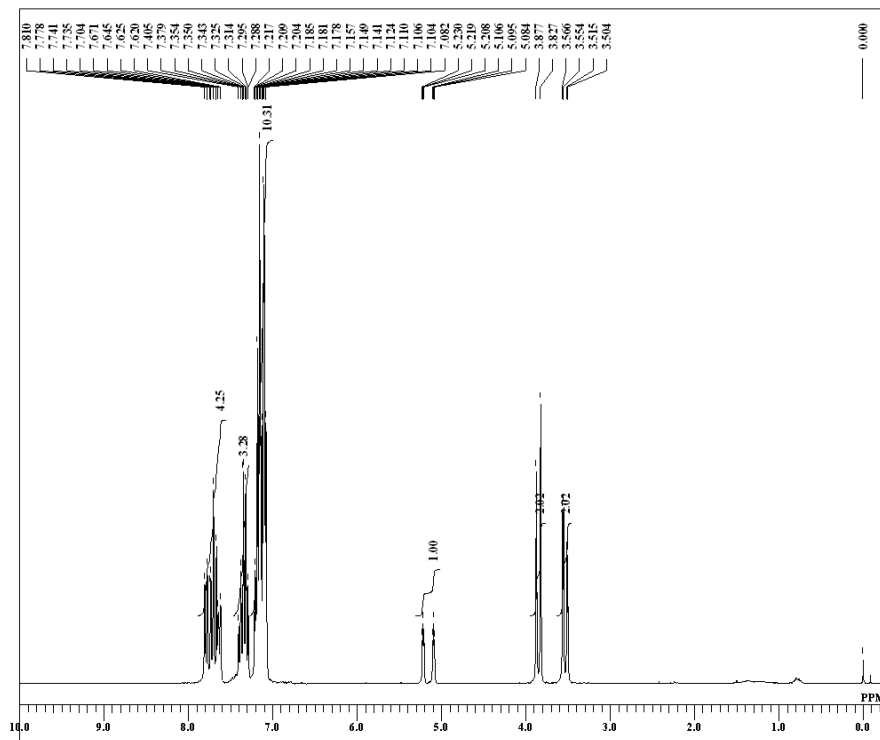


DFILE 3a-C-1.jdf
 COMINT 3a-C
 DATIM 30-12-2016 20:23:48
 OBNUC 13C
 EXMOD single_pulse_dec
 OBFRQ 125.77 MHz
 OBSET 7.87 KHz
 OBFIN 4.21 Hz
 POINT 32768
 FREQU 39308.18 Hz
 SCANS 1639
 ACQTM 0.8336 sec
 PD 2.0000 sec
 PW1 3.30 usec
 IRNUC 1H
 CTEMP 21.0 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 1.20 Hz
 RGAIN 50

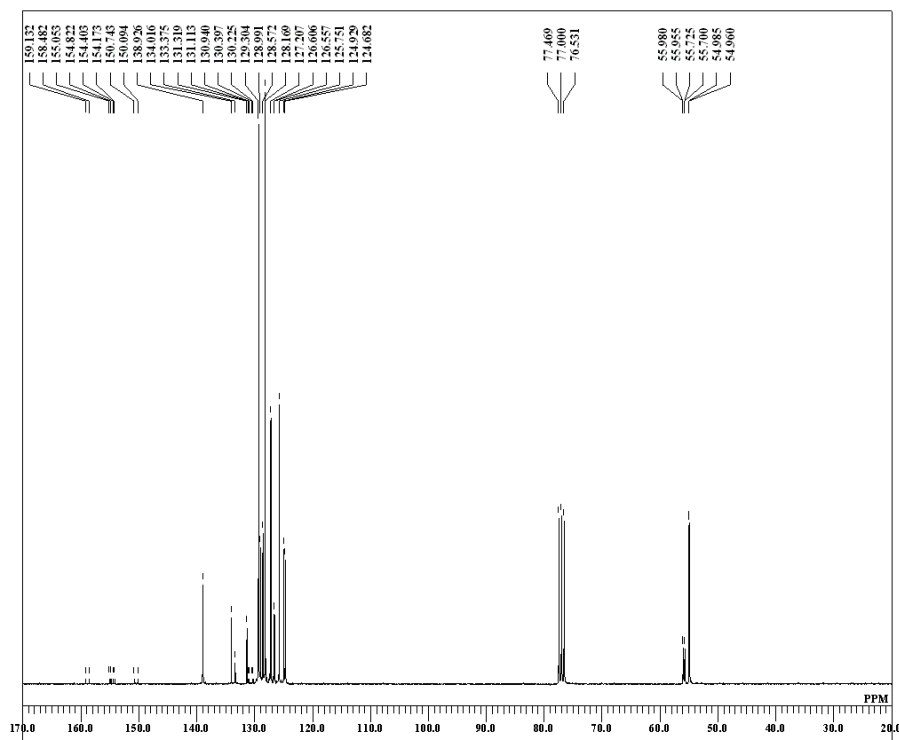
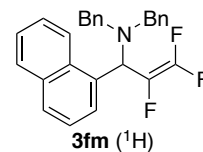


DFILE 3a-F-1.jdf
 COMINT 3a-F
 DATIM 09-01-2017 17:08:35
 OBNUC 19F
 EXMOD single_pulse.ex2
 OBFRQ 470.62 MHz
 OBSET 0.46 KHz
 OBFIN 0.84 Hz
 POINT 131072
 FREQU 240384.62 Hz
 SCANS 8
 ACQTM 0.5453 sec
 PD 5.0000 sec
 PW1 6.75 usec
 IRNUC 19F
 CTEMP 24.9 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 1.20 Hz
 RGAIN 42

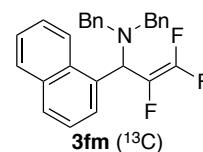


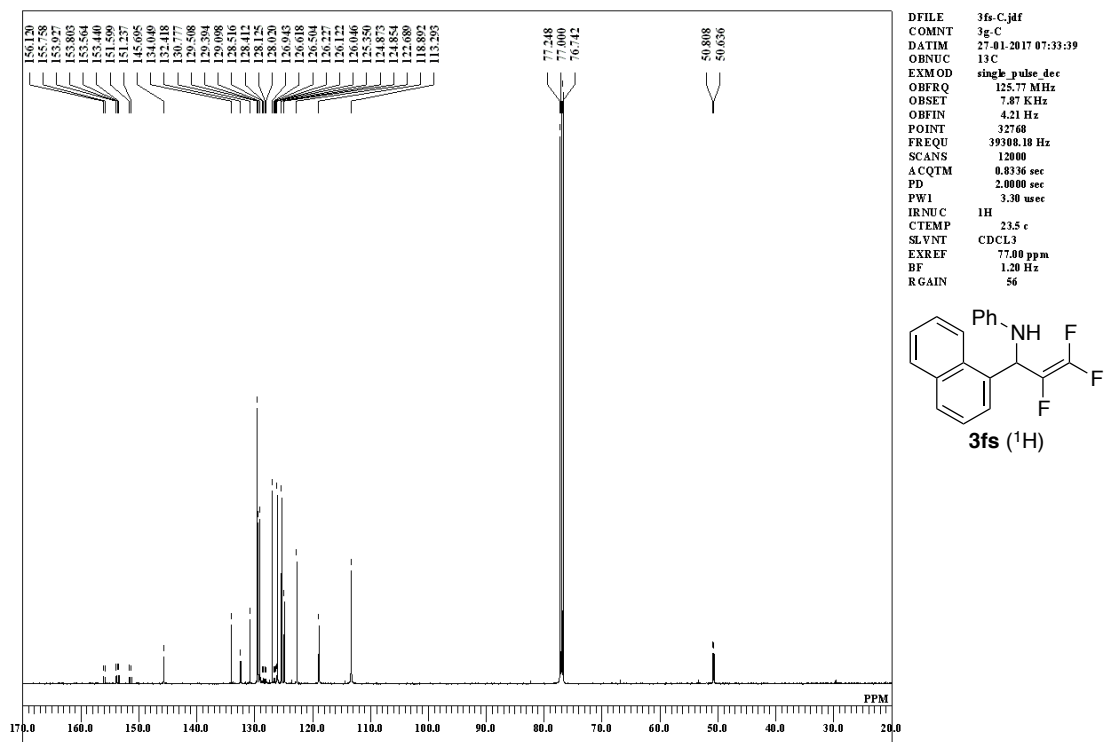
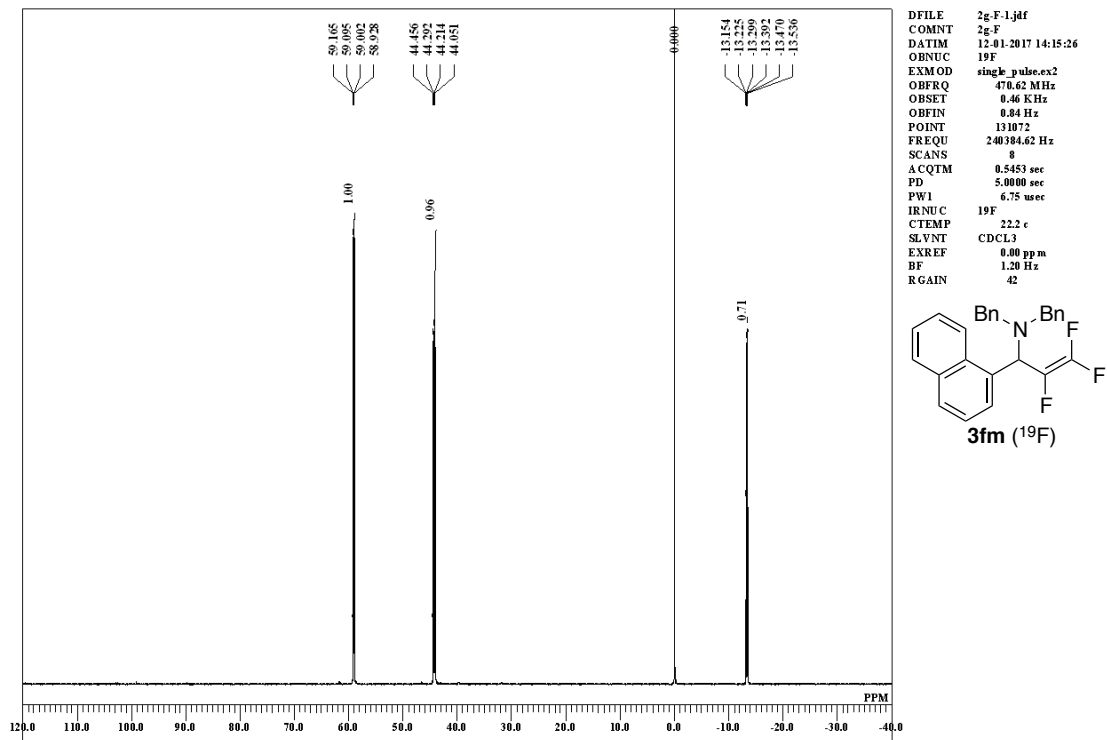


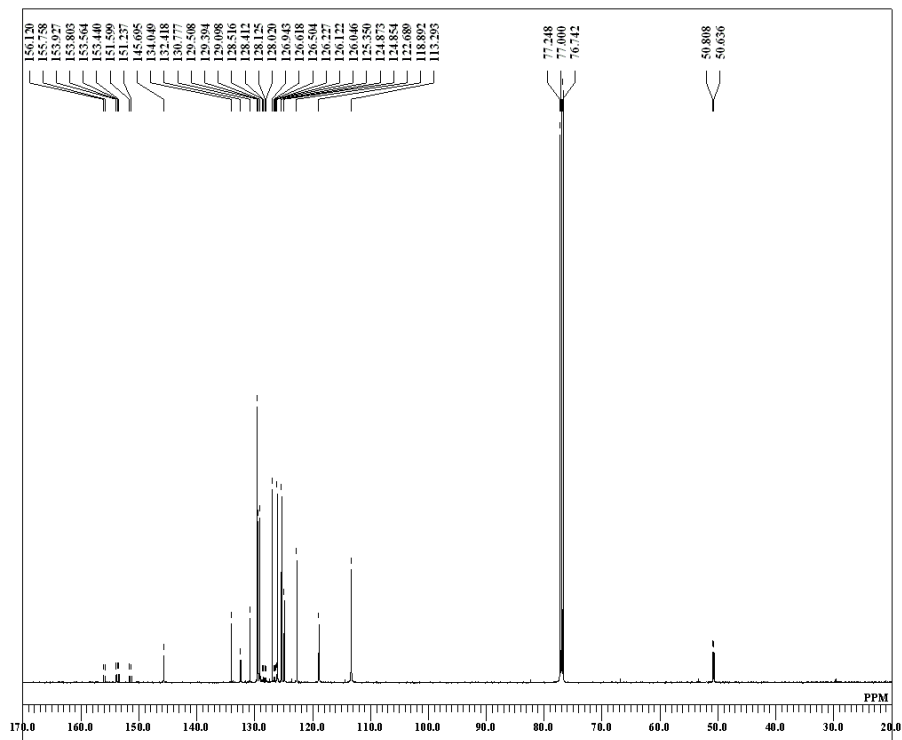
DFILE 3fm.als
 COMINT 2g. C H
 DATIM Tue Jan 24 00:32:27 2017
 OBNUC 1H
 EXMOD NON
 OBFREQ 270.05 MHz
 OBSET 112.00 KHz
 OBFIN 5800.00 Hz
 POINT 16384
 FREQU 5401.76 Hz
 SCANS 8
 ACQTM 3.0331 sec
 PD 3.9670 sec
 PW1 5.70 usec
 IRNUC 1H
 CTEMP 24.4 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.00 Hz
 RGAIN 14



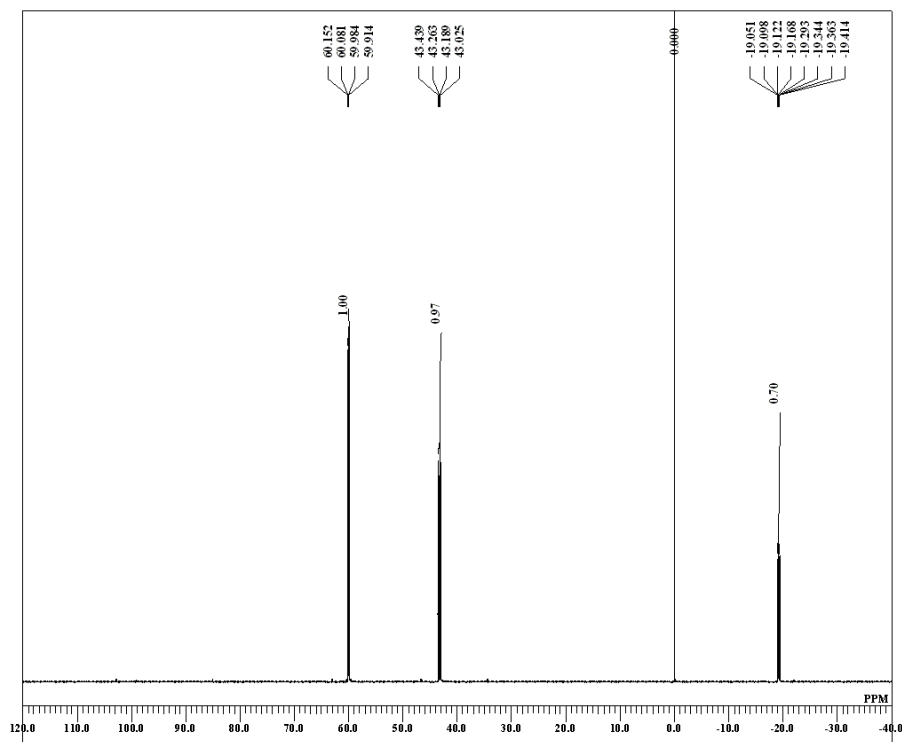
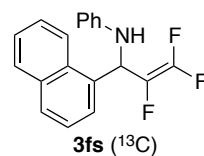
DFILE 2g. C.als
 COMINT 2g. C
 DATIM Tue Jan 24 08:54:52 2017
 OBNUC 13C
 EXMOD BCM
 OBFREQ 67.80 MHz
 OBSET 135.00 KHz
 OBFIN 5200.00 Hz
 POINT 32768
 FREQU 18306.64 Hz
 SCANS 10000
 ACQTM 1.7900 sec
 PD 1.2100 sec
 PW1 4.70 usec
 IRNUC 1H
 CTEMP 24.0 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 1.20 Hz
 RGAIN 28



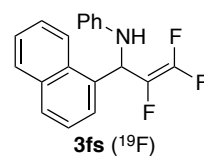


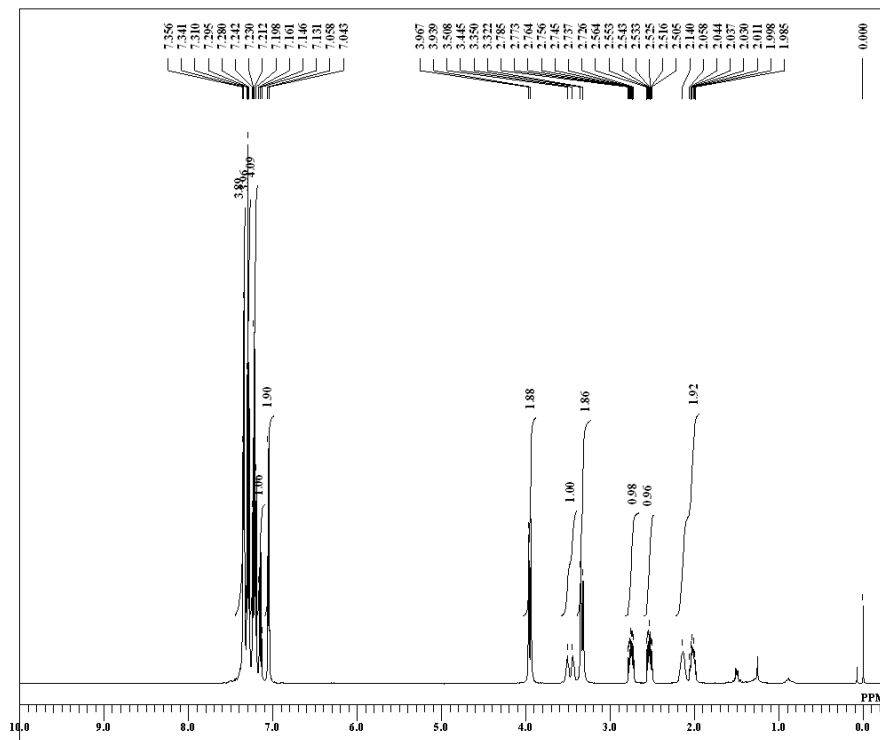


DFILE 3fs-C.jdf
 COMINT 3g-C
 DATIM 27-01-2017 07:33:39
 OBNUC 13C
 EXMOD single_pulse_dec
 OBFREQ 125.77 MHz
 OBSET 7.87 KHz
 OBFIN 4.21 Hz
 POINT 32768
 FREQU 39308.18 Hz
 SCANS 12000
 ACQTM 0.8336 sec
 PD 2.0000 sec
 PW1 3.30 usec
 IRNUC 1H
 CTEMP 23.5 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 1.20 Hz
 RGAIN 56

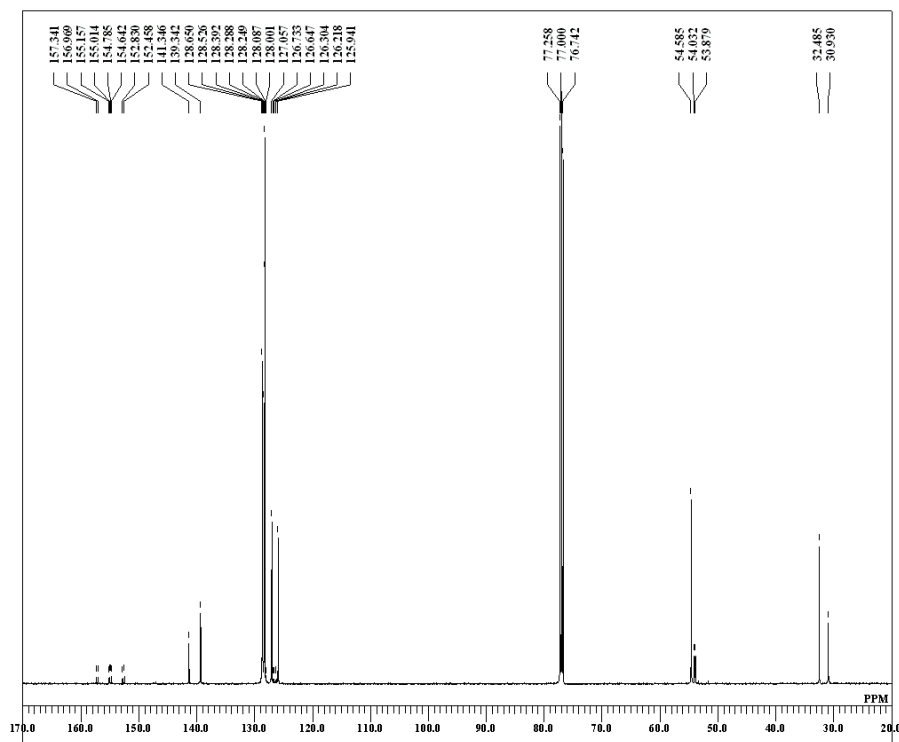
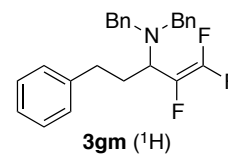


DFILE 3g-F-1.jdf
 COMINT 3g-F
 DATIM 01-02-2017 11:30:56
 OBNUC 19F
 EXMOD single_pulse.ex2
 OBFREQ 470.62 MHz
 OBSET 0.46 KHz
 OBFIN 0.84 Hz
 POINT 131072
 FREQU 240384.62 Hz
 SCANS 8
 ACQTM 0.5453 sec
 PD 5.0000 sec
 PW1 6.75 usec
 IRNUC 19F
 CTEMP 23.1 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 1.20 Hz
 RGAIN 42

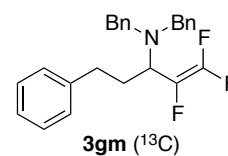


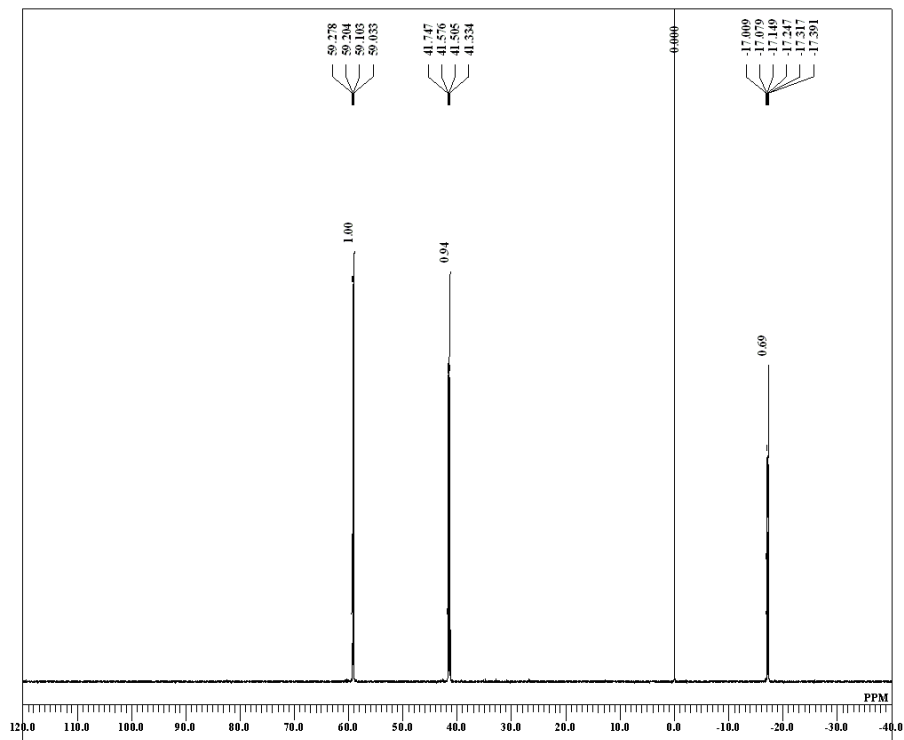


DFILE 3gm.jdf
 COMINT 2d.C-H
 DATIM 15-01-2017 19:55:33
 OBNUC 1H
 EXMOD single_pulse.v2
 OBFREQ 500.16 MHz
 OBSET 2.41 KHz
 OBFIN 6.01 Hz
 POINT 16384
 FREQU 9384.38 Hz
 SCANS 8
 ACQTM 1.7459 sec
 PD 5.0000 sec
 PW1 5.70 usec
 IRNUC 1H
 CTEMP 23.0 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.00 Hz
 RGAIN 36

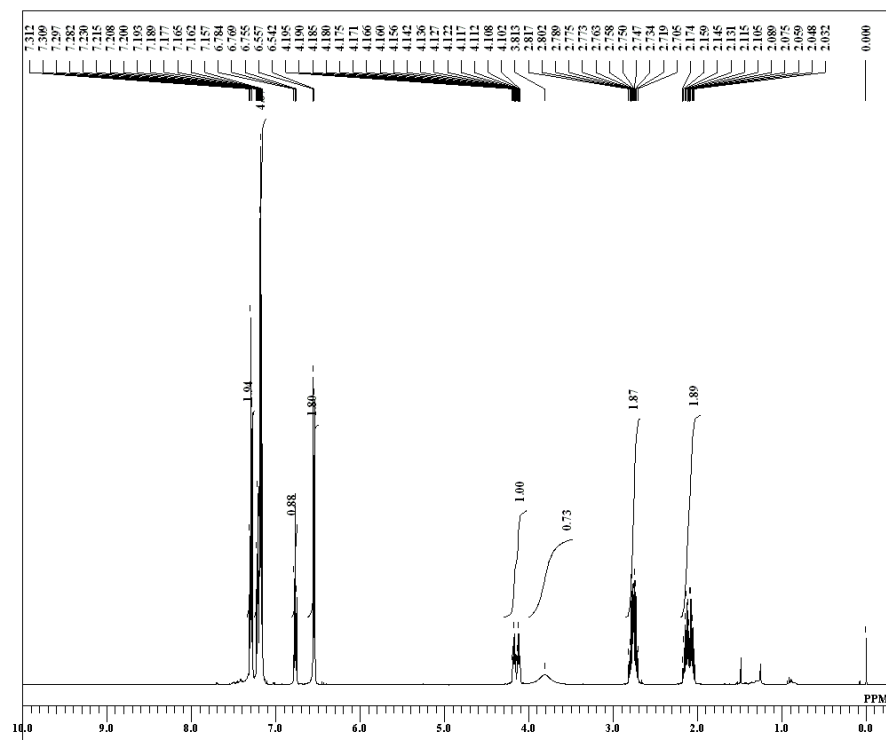
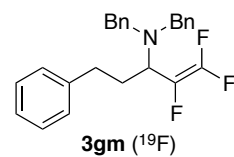


DFILE 2d.C-2.jdf
 COMINT 2d.C
 DATIM 25-01-2017 05:39:21
 OBNUC 13C
 EXMOD single_pulse.dec
 OBFREQ 125.77 MHz
 OBSET 7.87 KHz
 OBFIN 4.21 Hz
 POINT 32768
 FREQU 39308.18 Hz
 SCANS 8400
 ACQTM 0.8336 sec
 PD 2.0000 sec
 PW1 3.30 usec
 IRNUC 1H
 CTEMP 23.4 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 1.20 Hz
 RGAIN 58





DFILE 2d-FR1 F-2-jdf
 COMINT 2d-FR1 F
 DATIM 13-01-2017 10:56:00
 OBNUC 19F
 EXMOD single_pulse.ex2
 OBFRQ 470.62 MHz
 OBSET 0.46 KHz
 OBFIN 0.84 Hz
 POINT 131072
 FREQU 240384.62 Hz
 SCANS 8
 ACQTM 0.5453 sec
 PD 5.0000 sec
 PW1 6.75 usec
 IRNUC 19F
 CTEMP 21.2 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 1.20 Hz
 RGAIN 44



DFILE 3gs.jdf
 COMINT 3d.C.H
 DATIM 19-01-2017 15:59:31
 OBNUC 1H
 EXMOD single_pulse.ex2
 OBFRQ 500.16 MHz
 OBSET 2.41 KHz
 OBFIN 6.01 Hz
 POINT 16384
 FREQU 9384.38 Hz
 SCANS 8
 ACQTM 1.7459 sec
 PD 5.0000 sec
 PW1 5.70 usec
 IRNUC 1H
 CTEMP 22.1 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.10 Hz
 RGAIN 30

