

Supplementary Materials

Catalytic Enantioselective Synthesis of N-C Axially Chiral Sulfonamides Bearing ortho-disubstituted-Phenyl Groups

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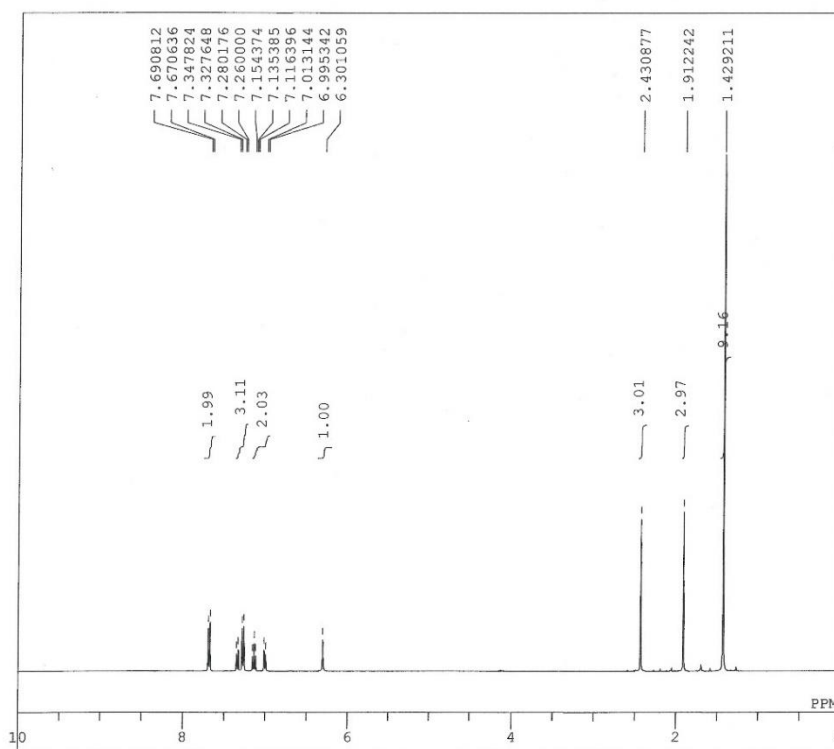
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*Correspondence: kitagawa@shibaura-it.ac.jp; Tel.: +81-3-5859-8161 (O.K.)

(Contents)

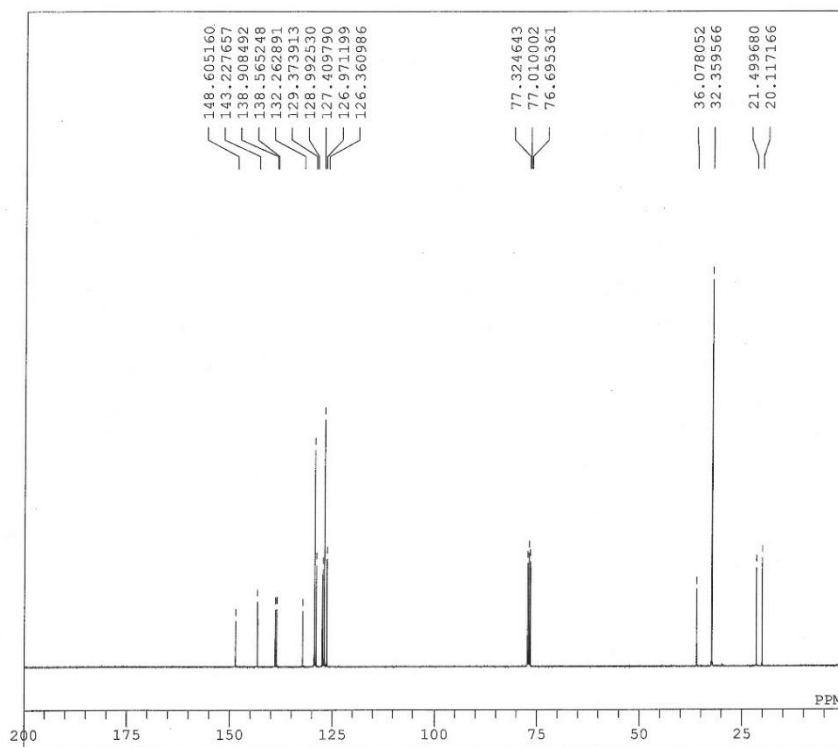
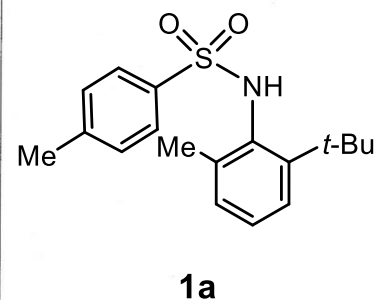
Copies of ¹ H- and ¹³ C-NMR chart of all compounds 1-6	S2-S44
Chiral HPLC chart for the determination of the ee	S45-S64
X-ray crystal data of 2o	S65-S68
Kinetic data for the evaluation of the rotational barriers of 2i and 2r	S69

Copies of ^1H - and ^{13}C -NMR spectra



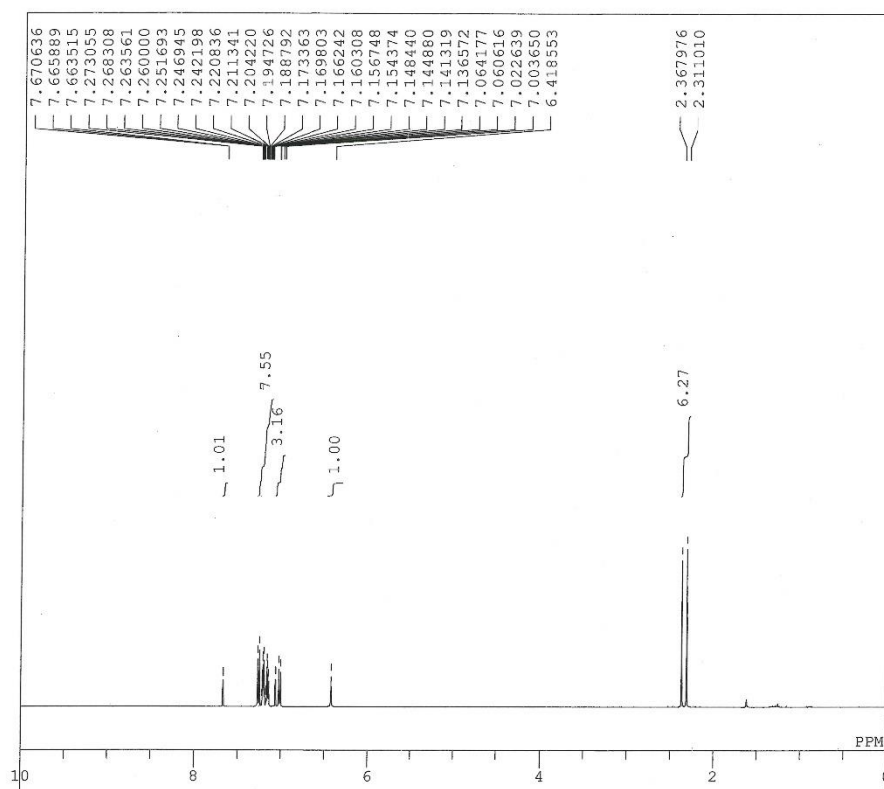
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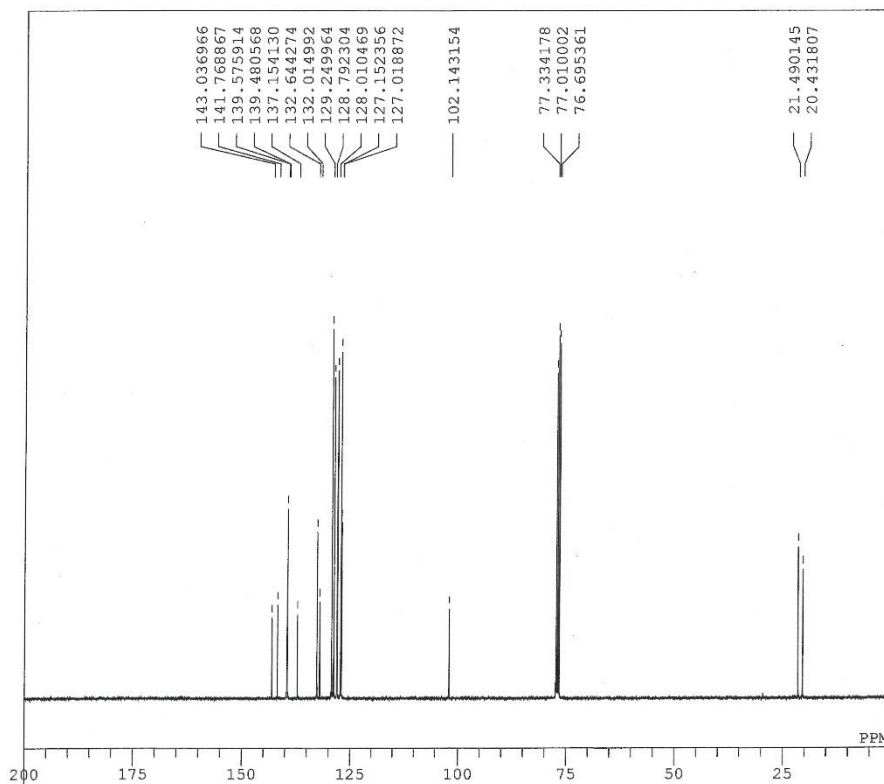
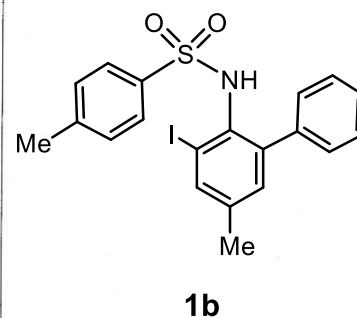


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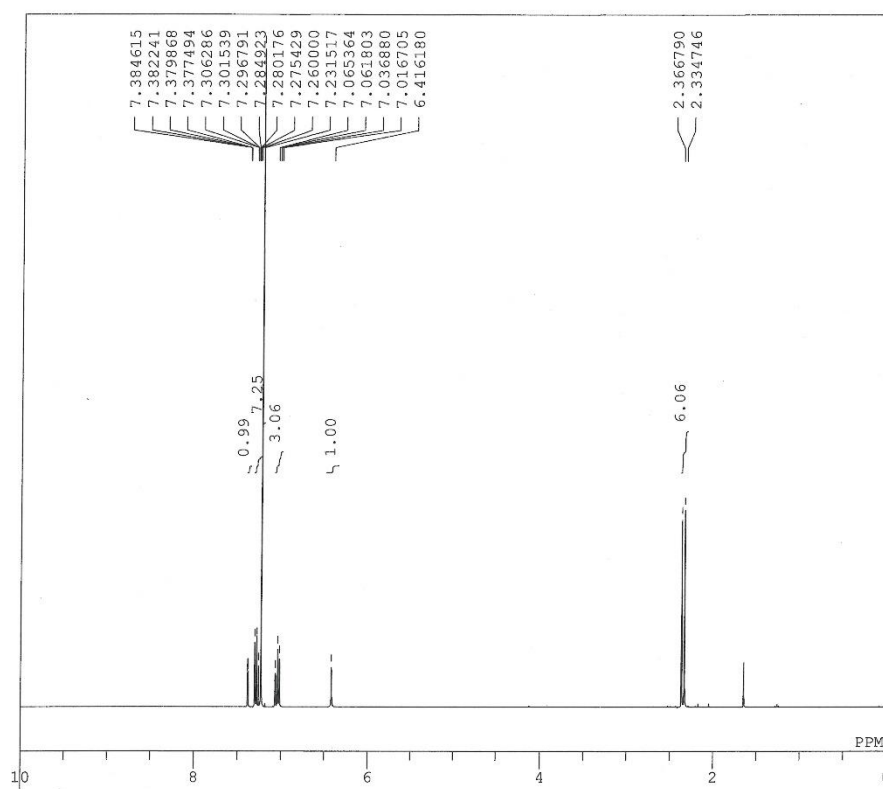
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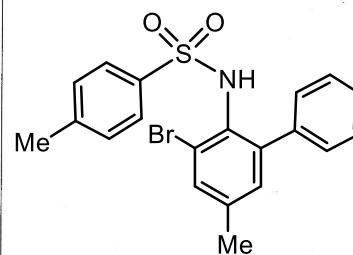
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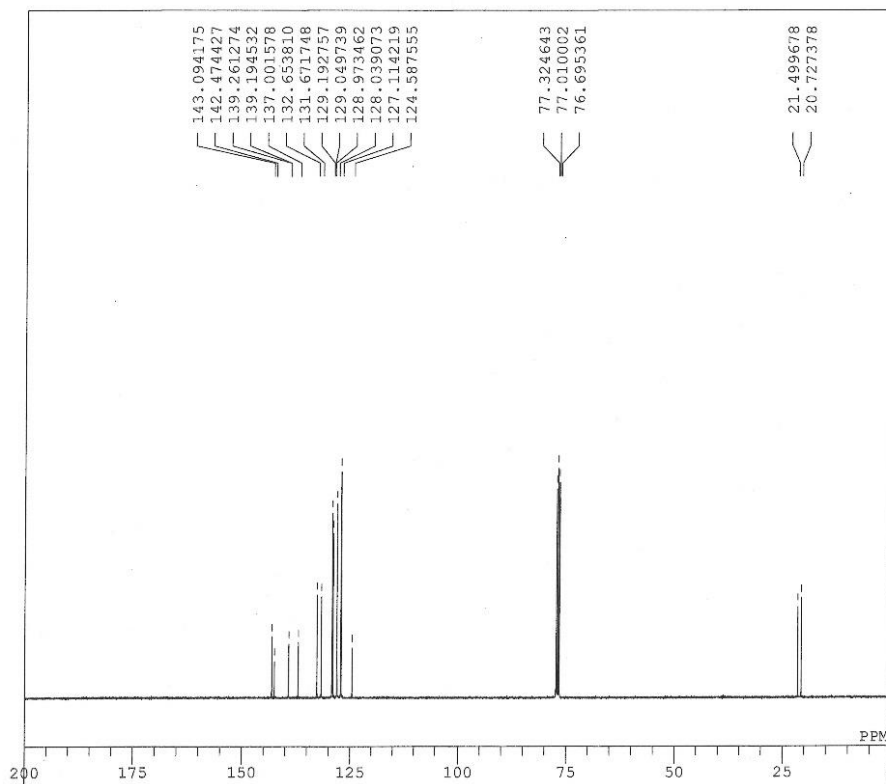
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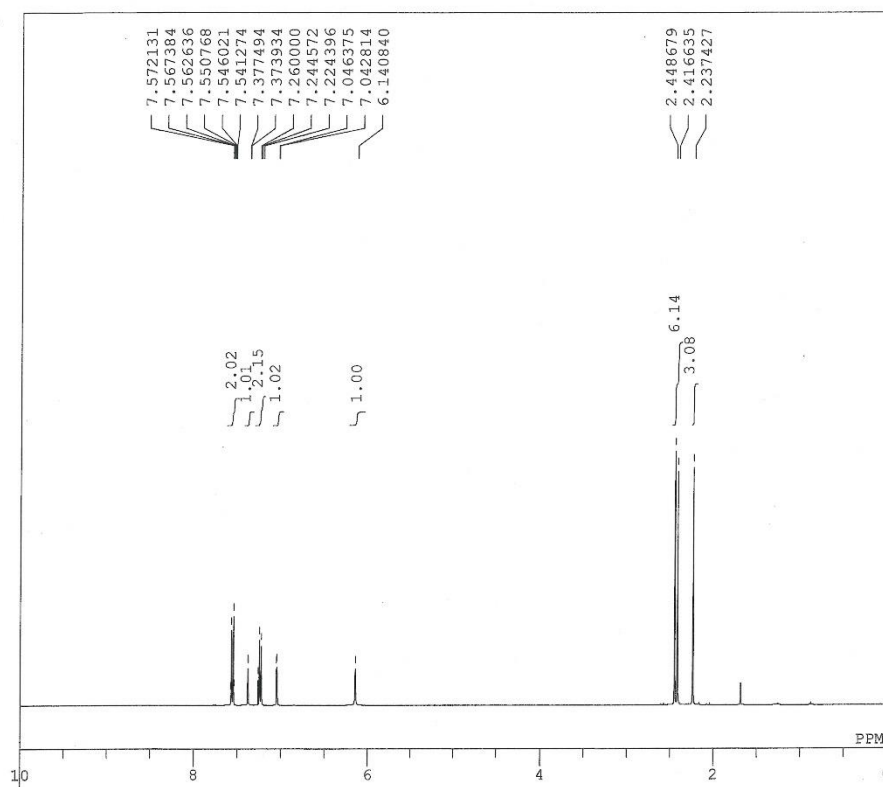
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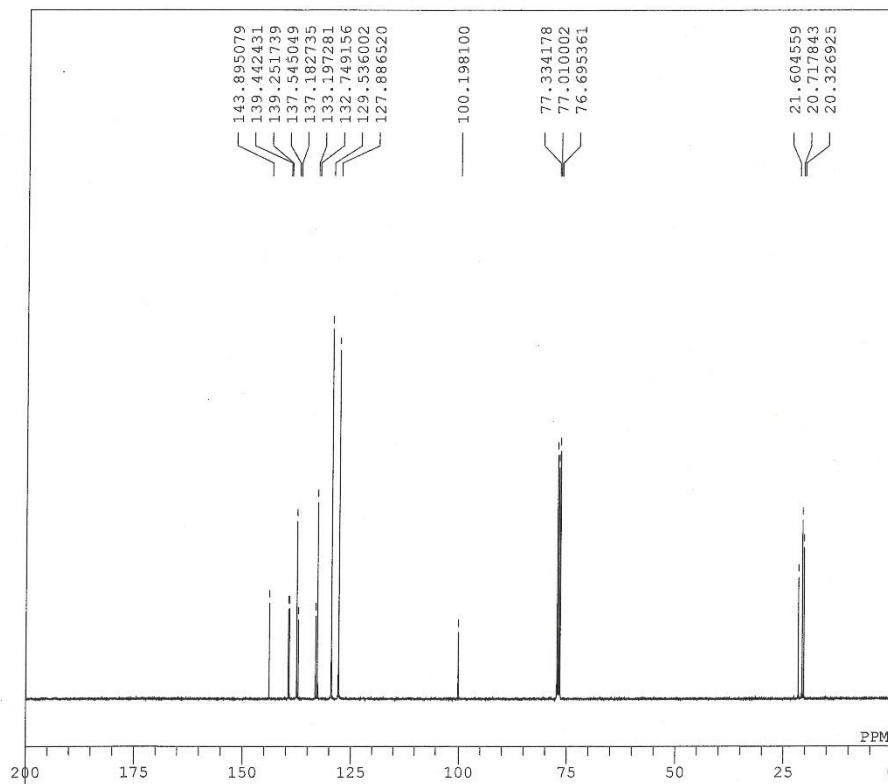
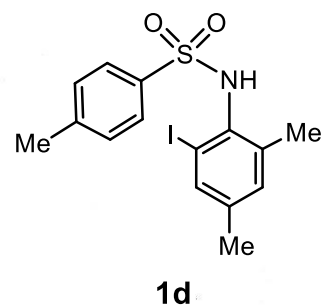
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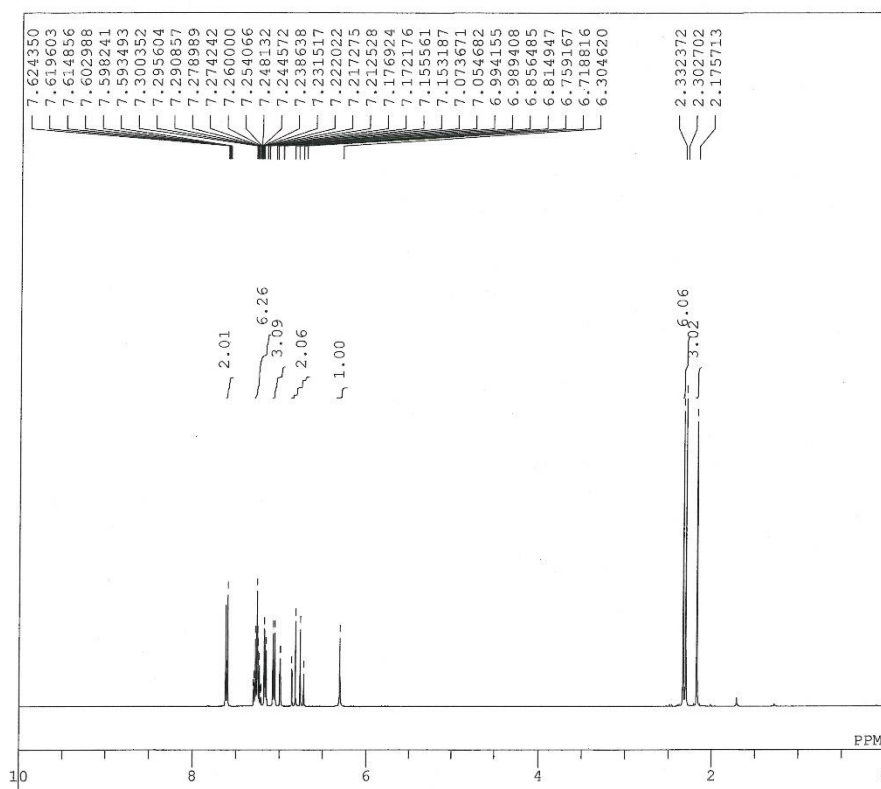
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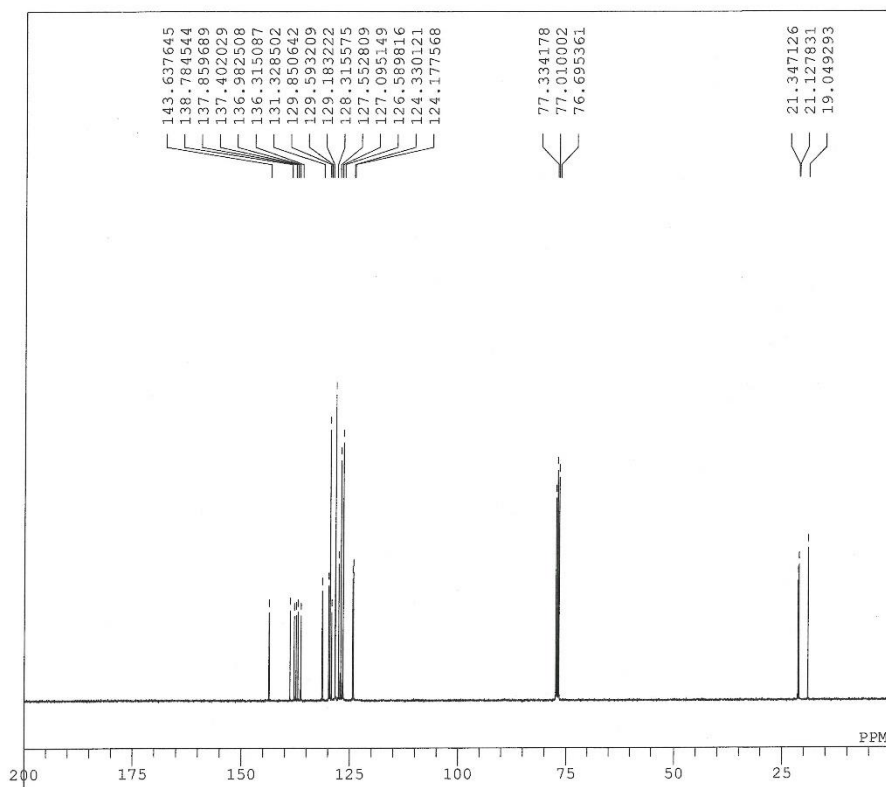


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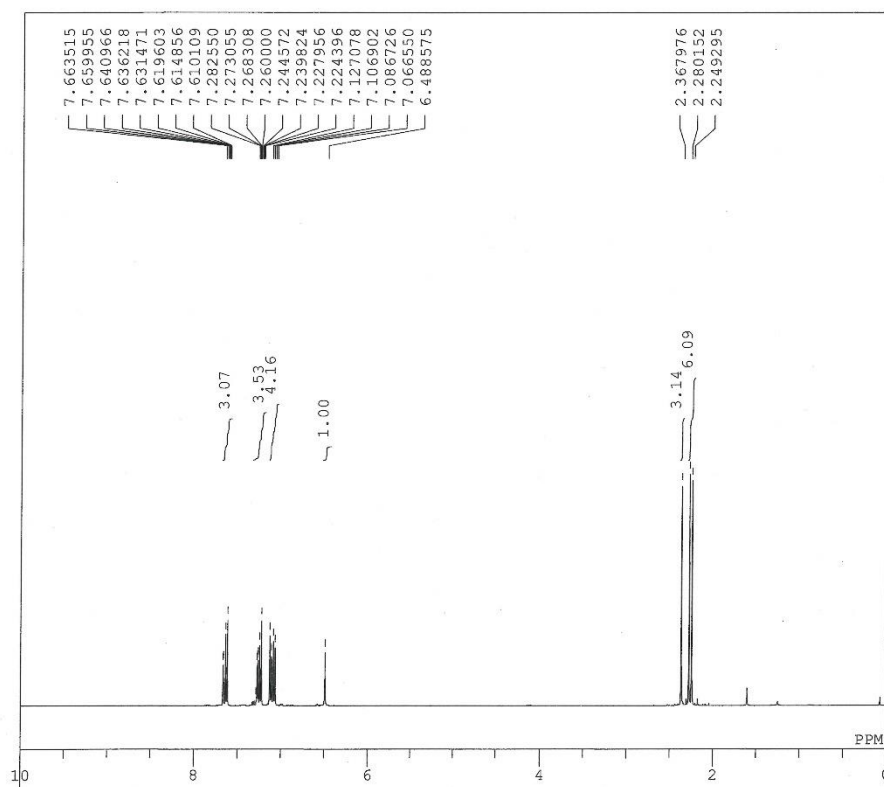
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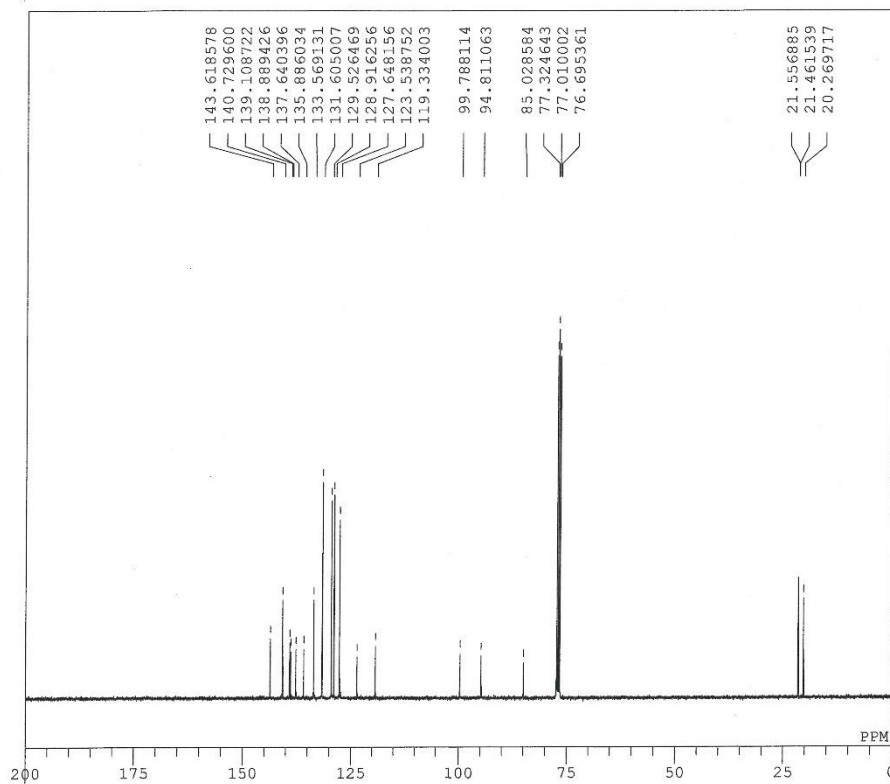
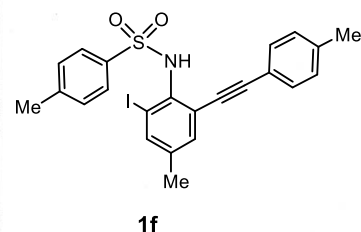


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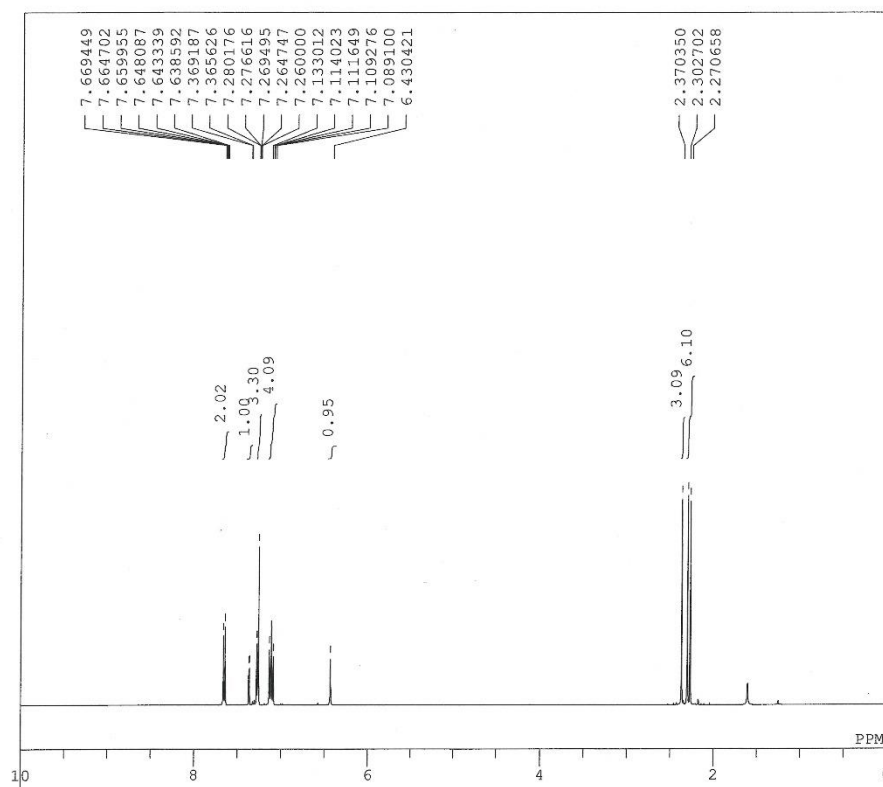
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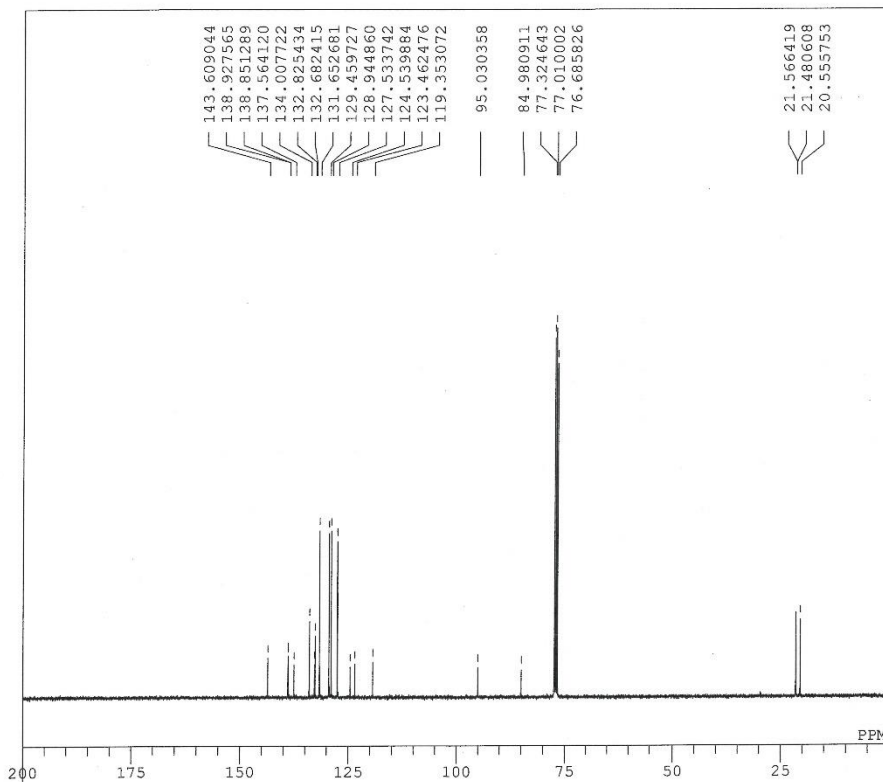
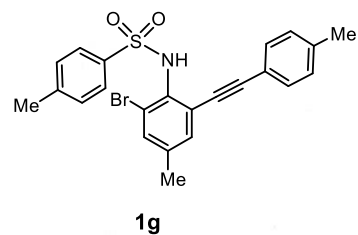
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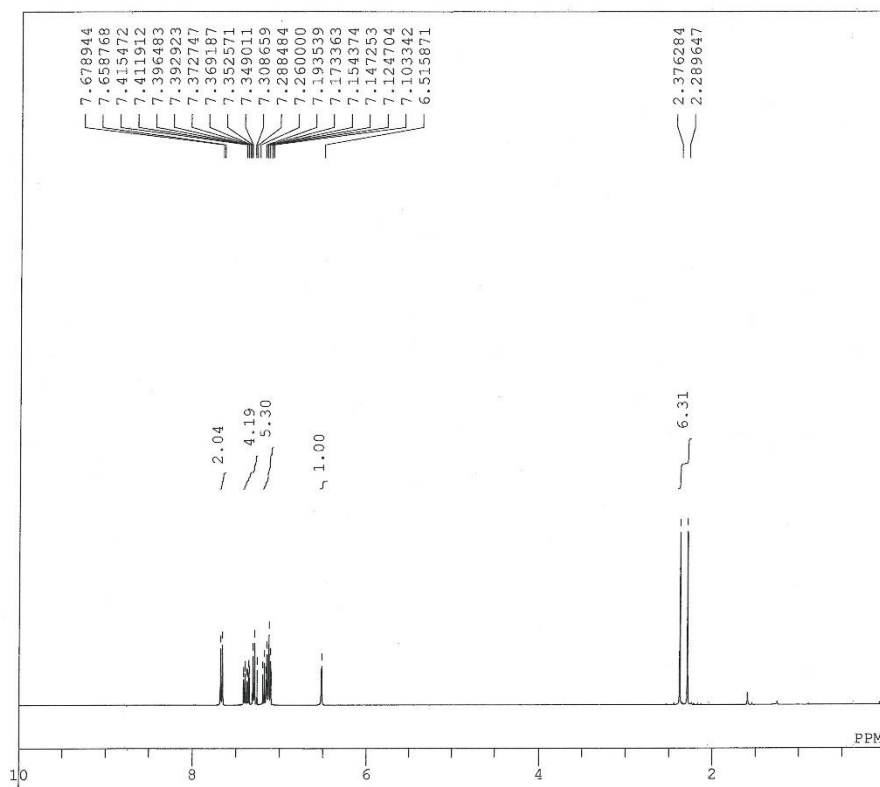
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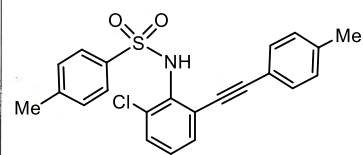
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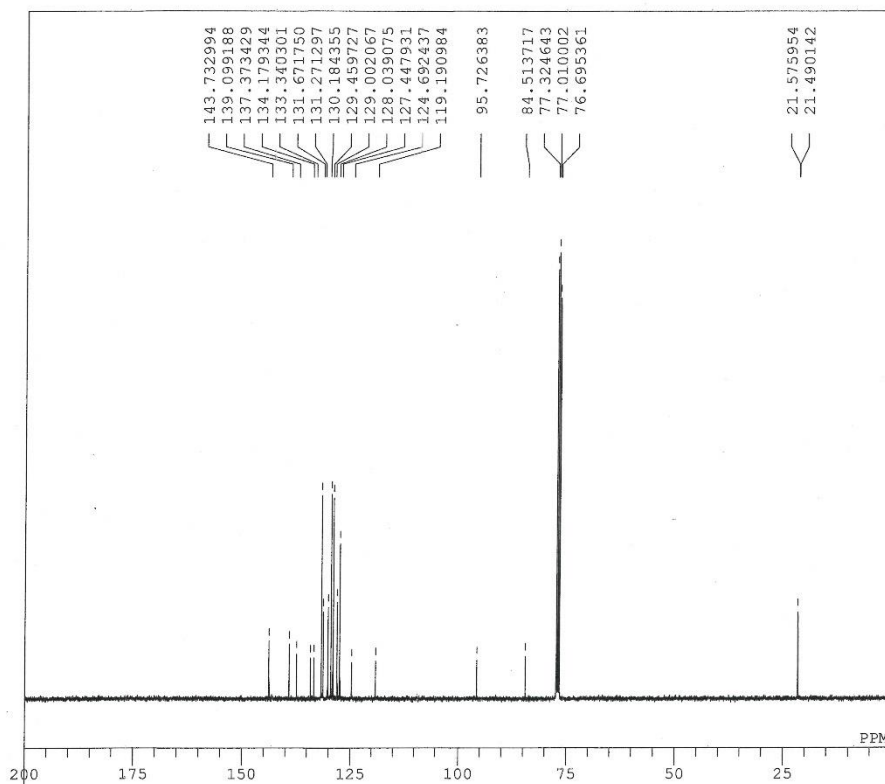
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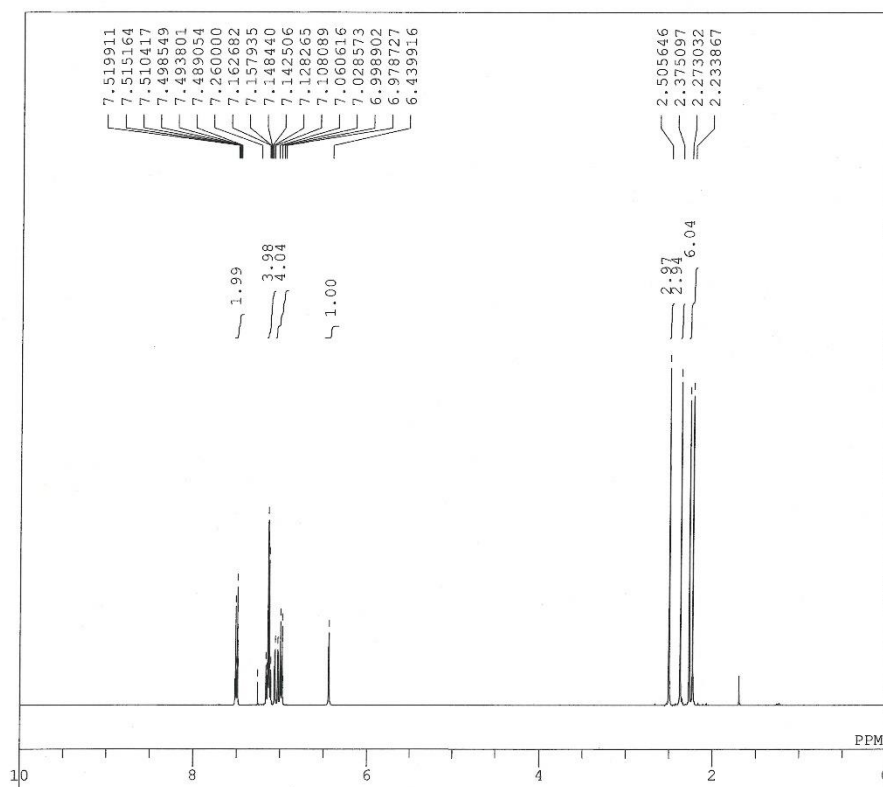
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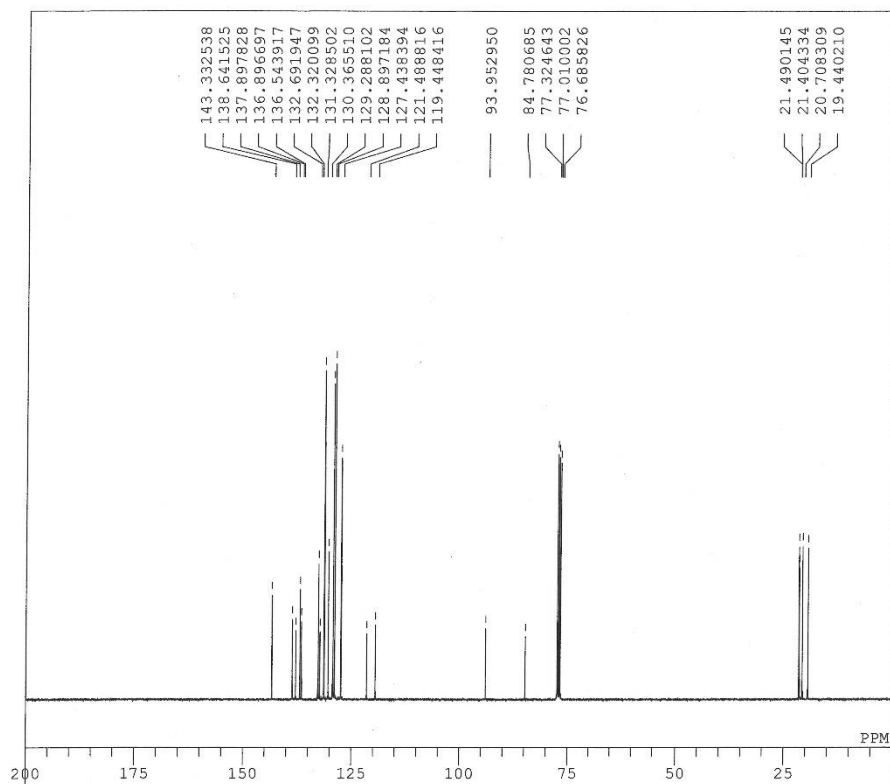
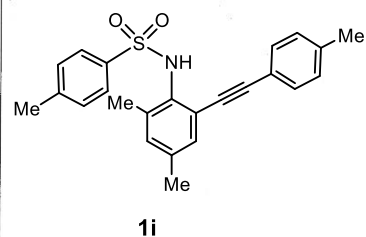
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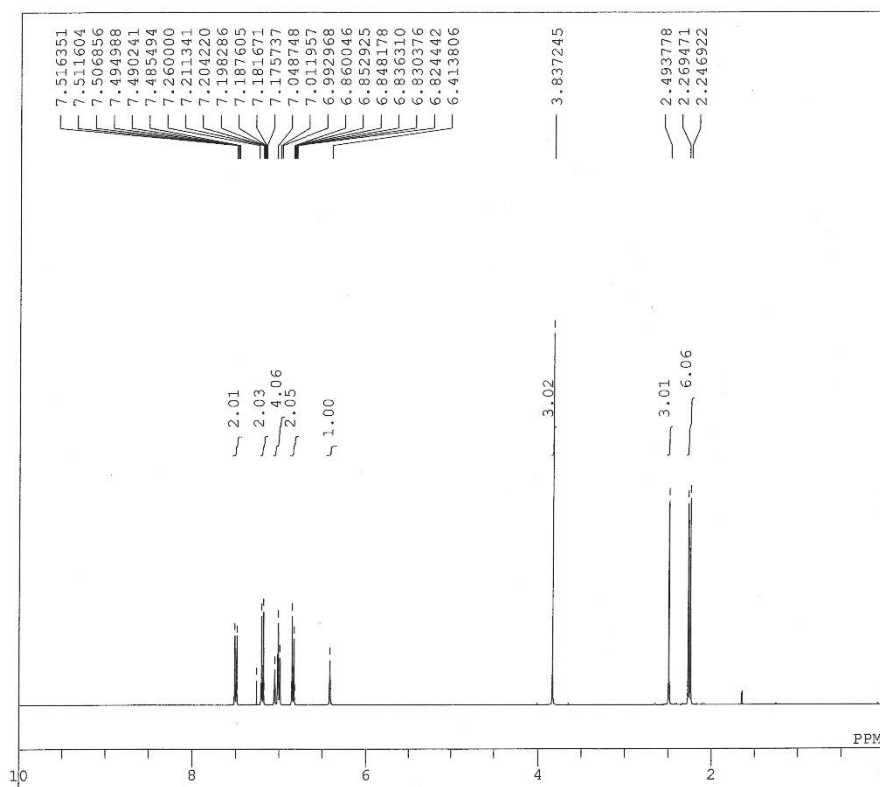
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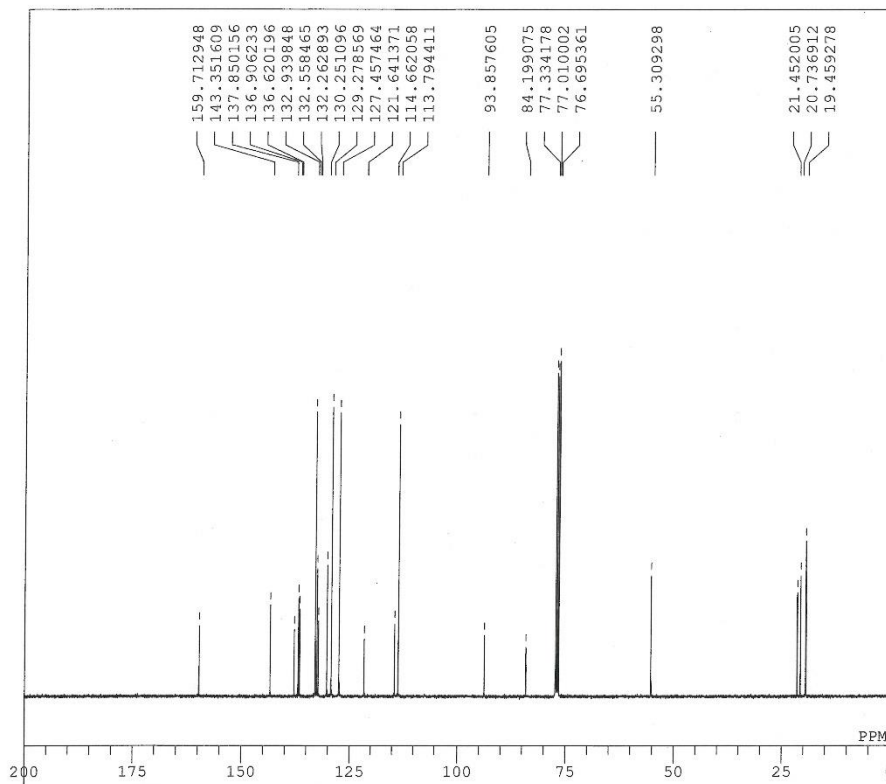
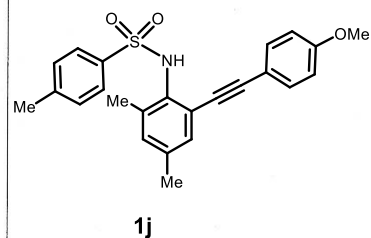
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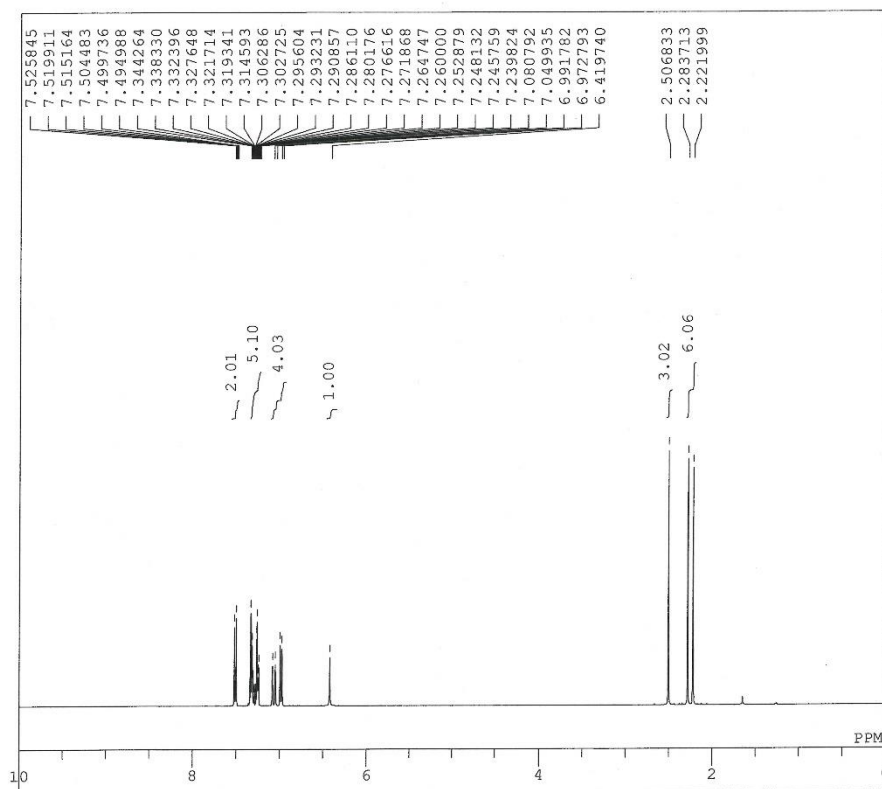
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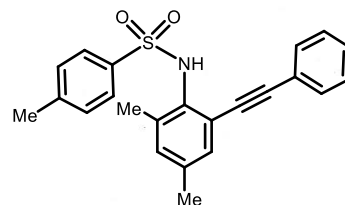
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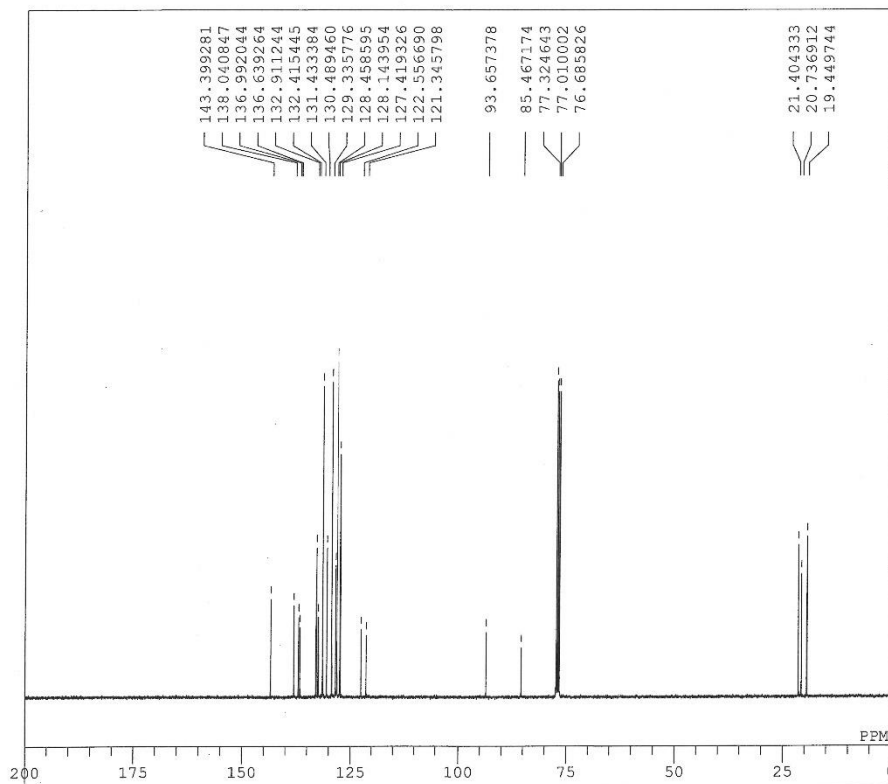
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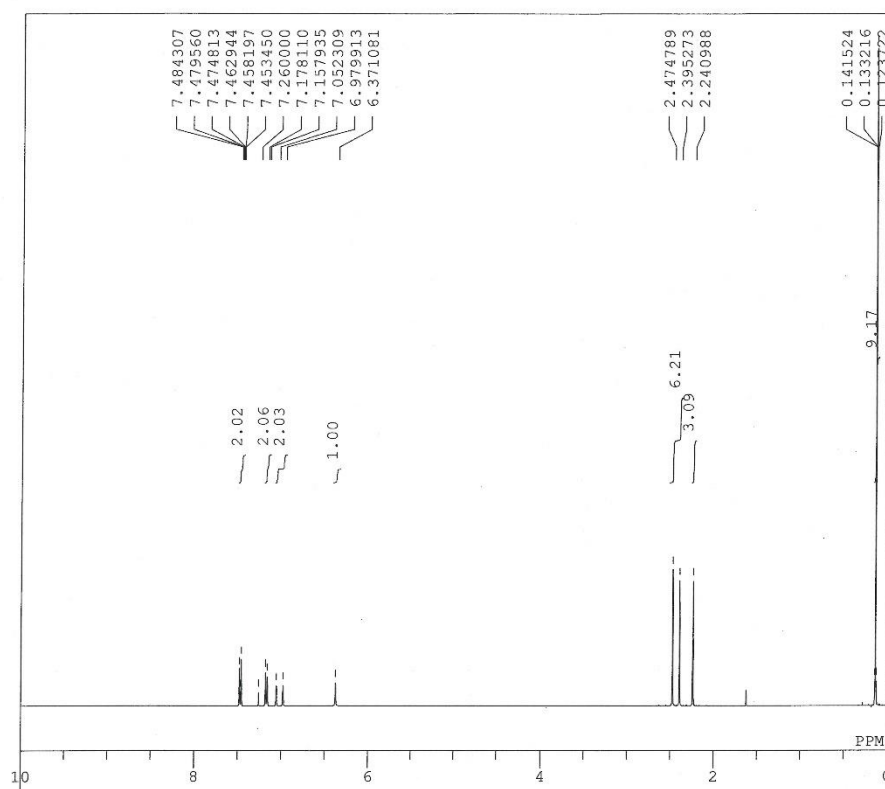
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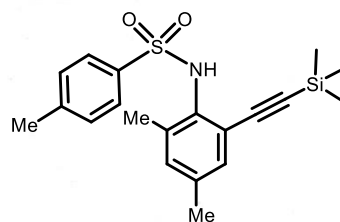
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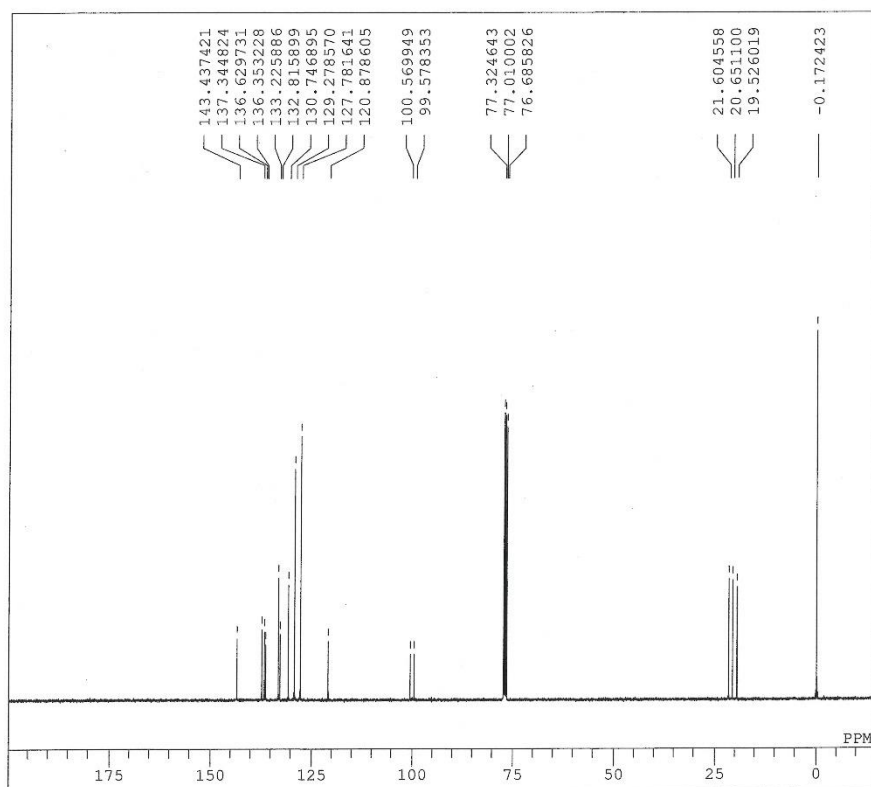
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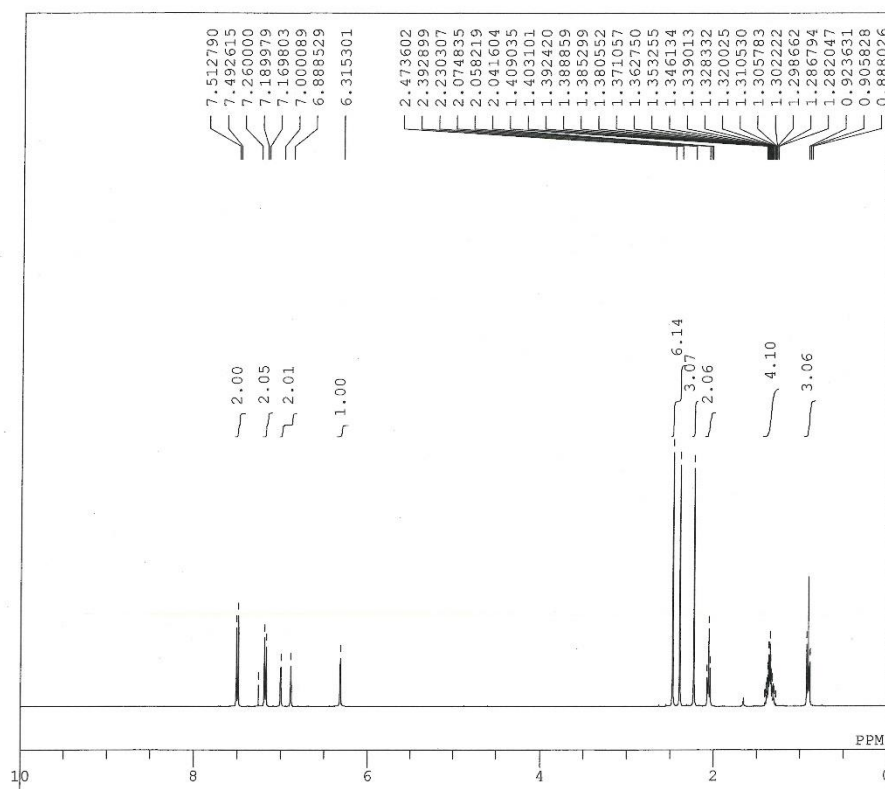
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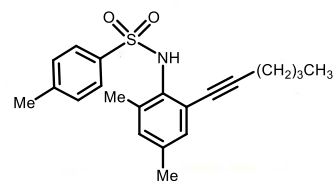
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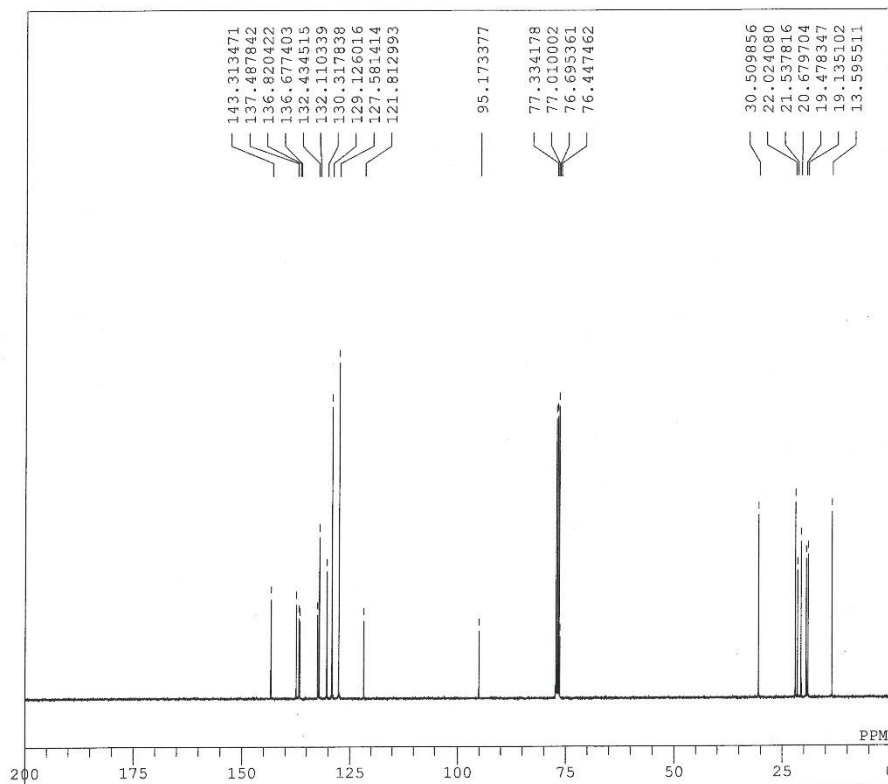
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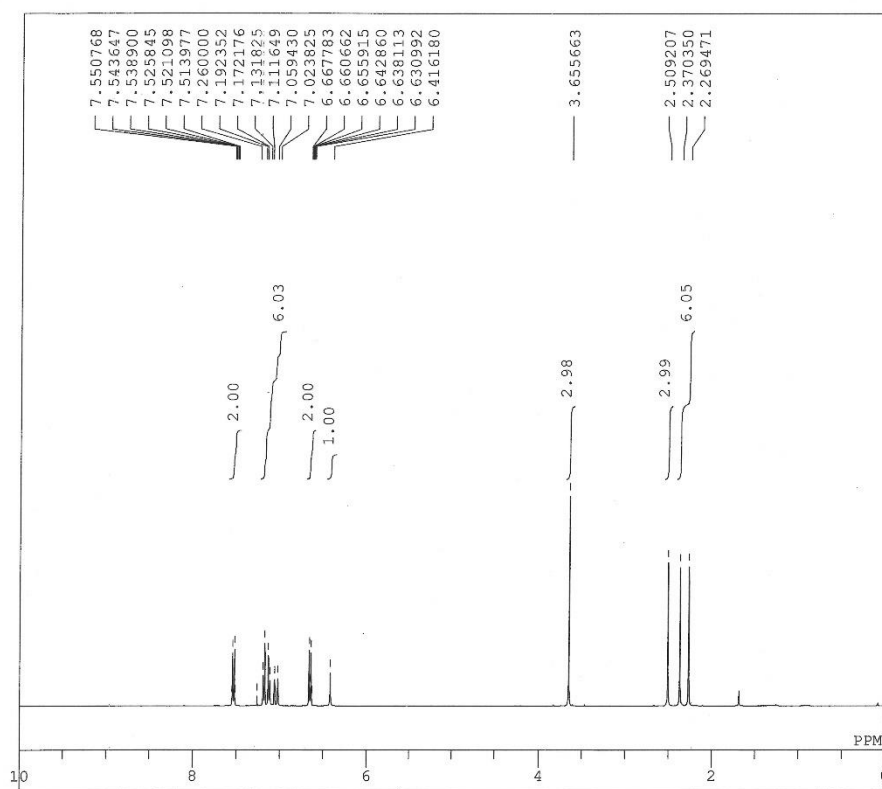
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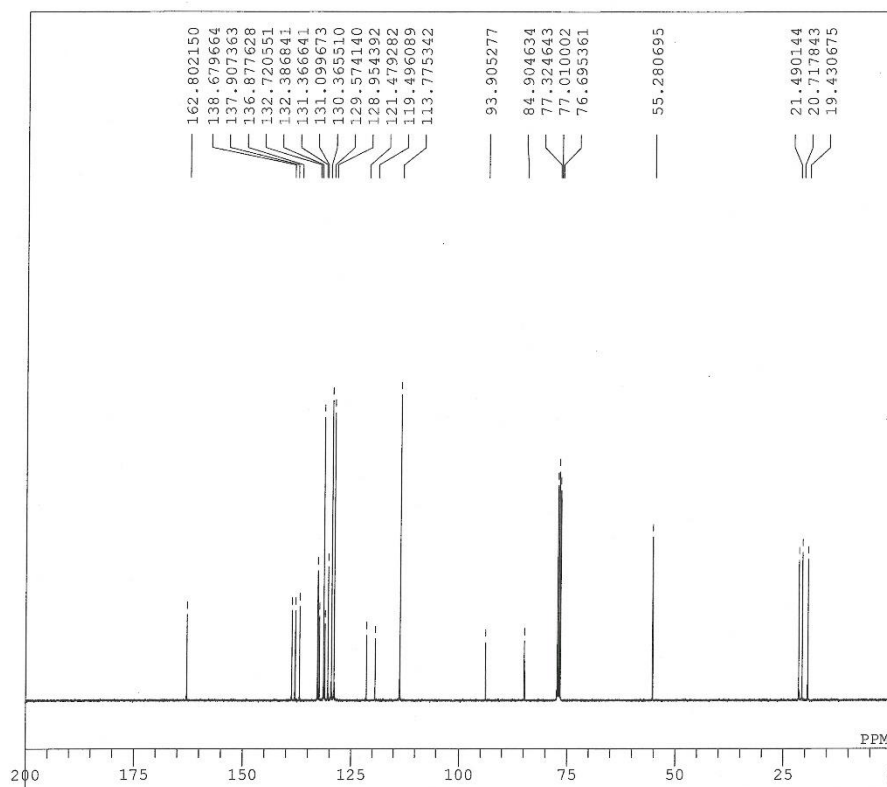
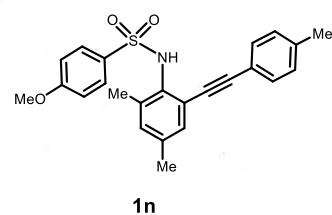
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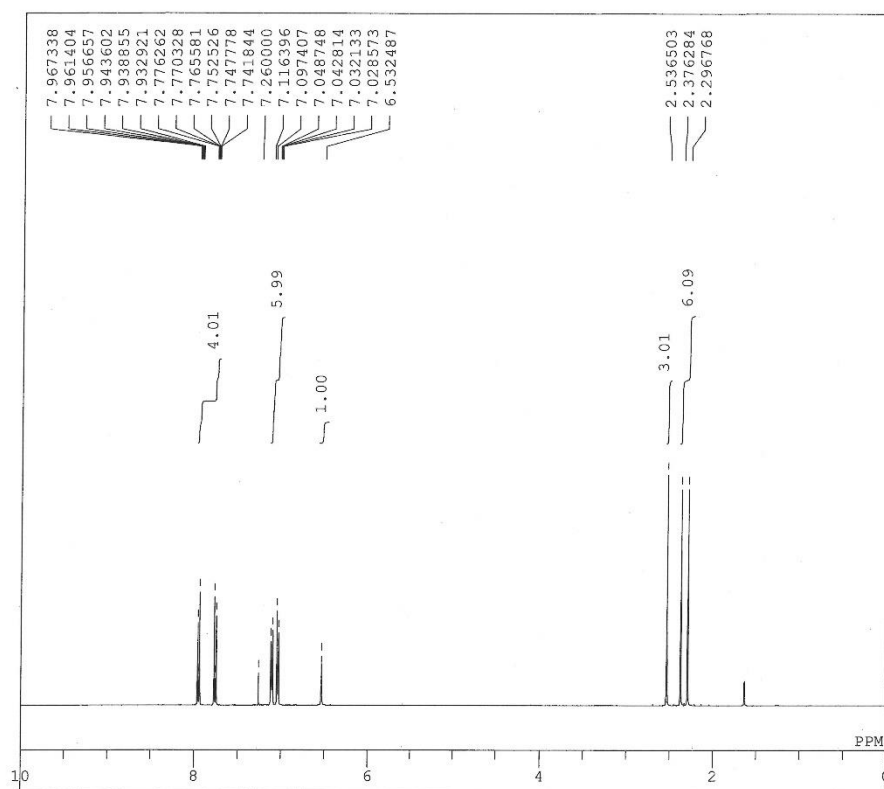
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 OBFRQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 32768
 FREQU 31407.03 Hz
 SCANS 1024
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PW1 3.03 usec
 IRNUC 1H
 CTEMP 19.2 c
 SLVNT CDCL3
 EXREF 77.01 ppm
 BF 1.20 Hz
 RGAIN 60



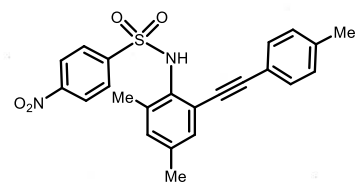
DFILE TF007 20210921-1.als
 COMNT Qn-BOC 1H
 DATIM 2021-09-21 08:42:19
 OBNUC 1H
 EXMOD single pulse.ex2
 OBFRQ 399.78 MHz
 OBSET 4.62 KHz
 OBFIN 5.98 Hz
 POINT 13107
 FREQU 6218.81 Hz
 SCANS 32
 ACQTM 2.1076 sec
 PD 5.0000 sec
 PW1 5.17 usec
 IRNUC 1H
 CTEMP 19.0 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.12 Hz
 RGAIN 30



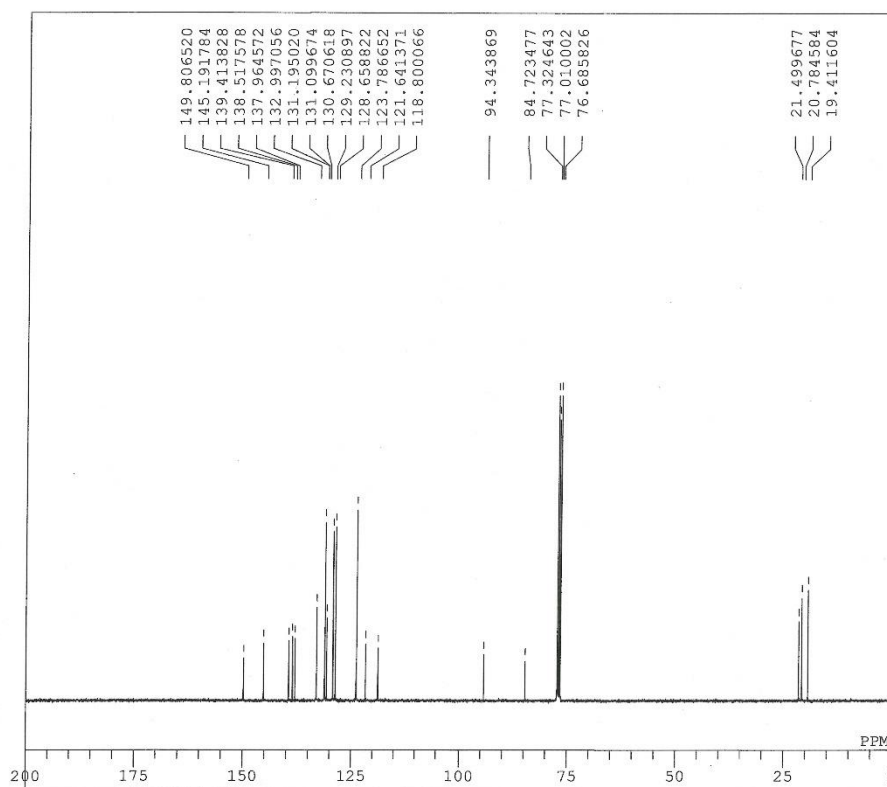
DFILE TF007-13C 20210921-1.als
 COMNT 2021-09-21 09:41:44
 OBNUC 13C
 EXMOD single pulse_dec
 OBFRQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 26214
 FREQU 25125.24 Hz
 SCANS 1024
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PW1 3.03 usec
 IRNUC 1H
 CTEMP 19.3 c
 SLVNT CDCL3
 EXREF 77.01 ppm
 BF 1.20 Hz
 RGAIN 60



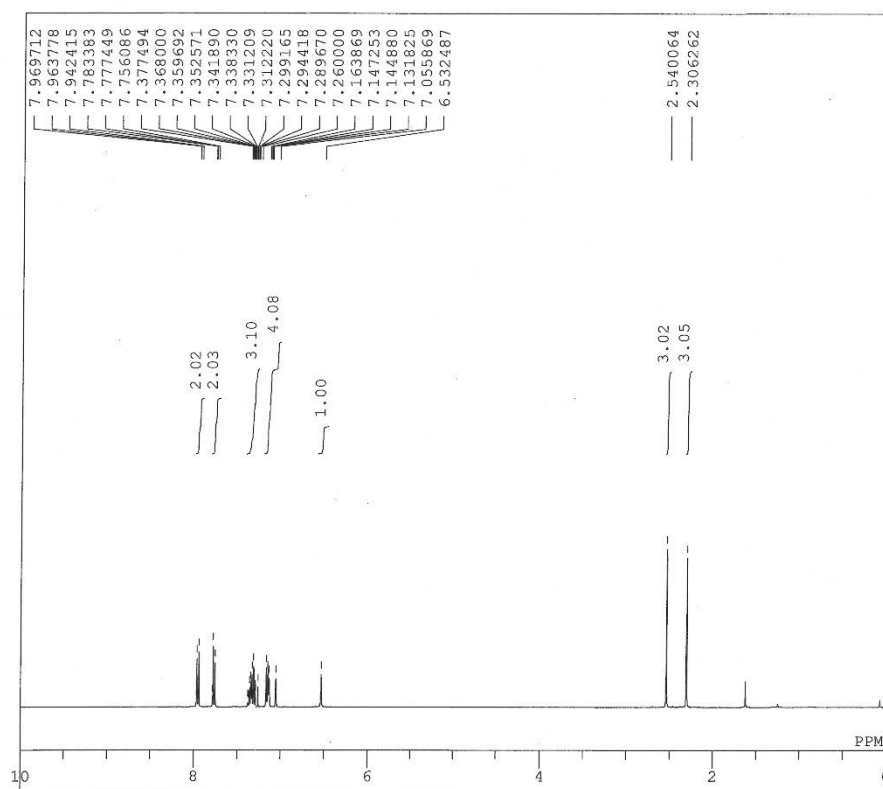
DFILE TT010 20210930-1.als
 COMNT Qn-BOC 1H
 DATIM 2021-09-30 10:19:17
 OBNUC 1H
 EXMOD single pulse.ex2
 OBFRQ 399.78 MHz
 OBSET 4.62 KHz
 OBFIN 5.98 Hz
 POINT 13107
 FREQU 6218.81 Hz
 SCANS 32
 ACQTM 2.1076 sec
 PD 5.0000 sec
 PW1 5.17 usec
 IRNUC 1H
 CTEMP 19.1 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.12 Hz
 RGAIN 34



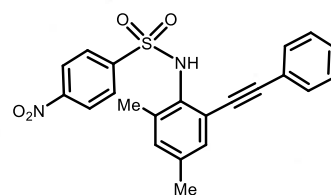
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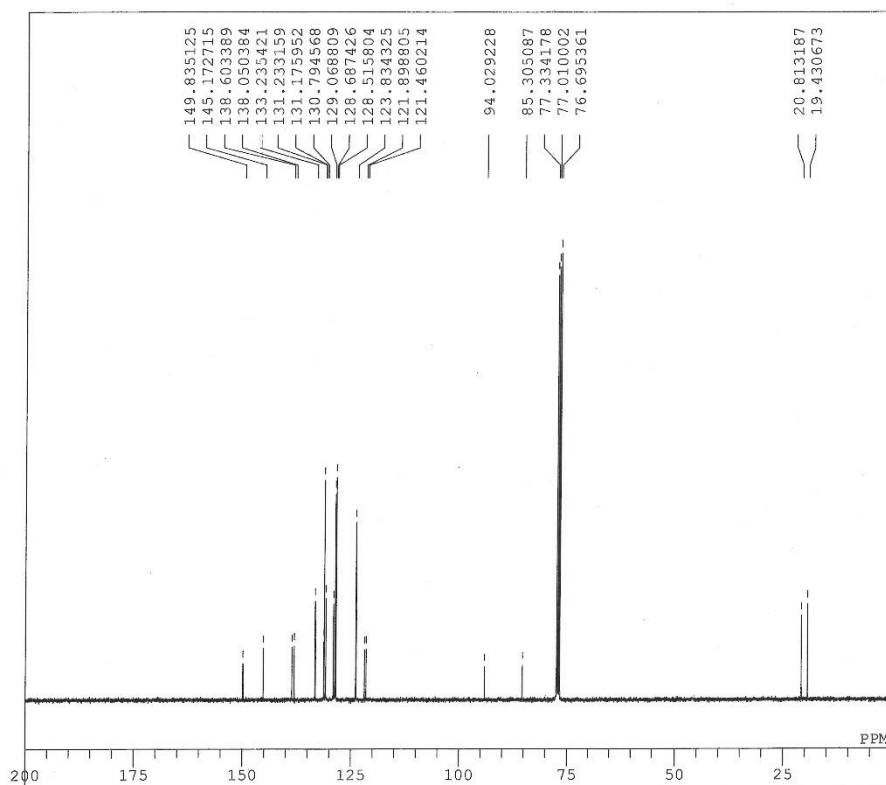
DFILE TT010-13C 20210930-1.als
 COMNT
 DATIM 2021-09-30 18:12:17
 OBNUC 13C
 EXMOD single pulse_dec
 OBFRQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 26214
 FREQU 25125.24 Hz
 SCANS 1024
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PW1 3.03 usec
 IRNUC 1H
 CTEMP 20.3 c
 SLVNT CDCL3
 EXREF 77.01 ppm
 BF 1.20 Hz
 RGAIN 60



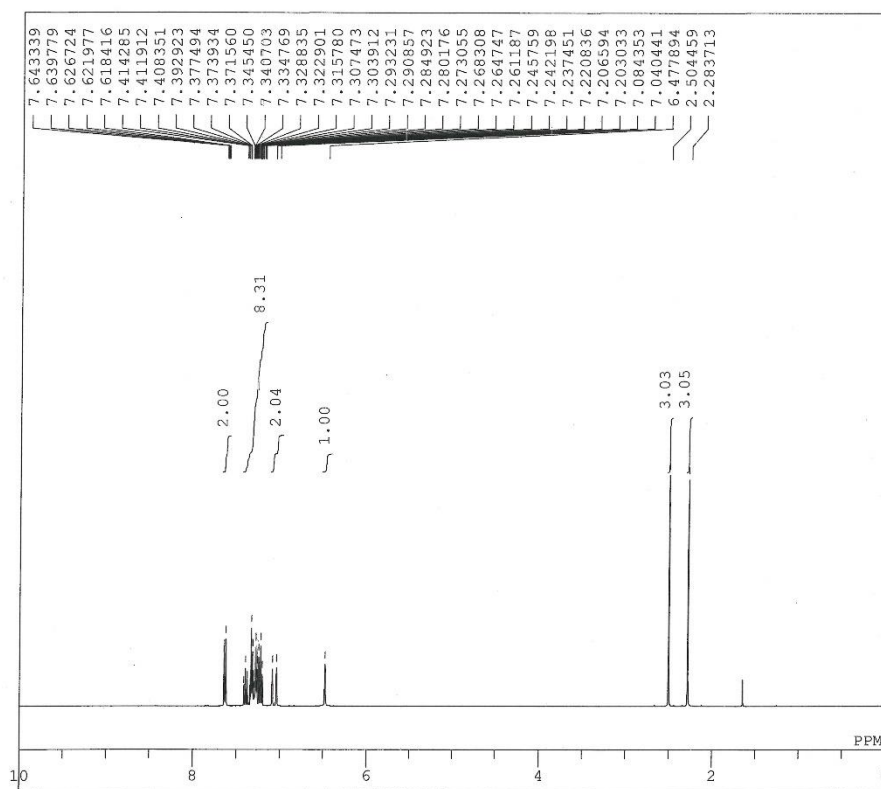
DFILE SF112 20211207-1.als
 COMNT Qn-BOC 1H
 DATIM 2021-12-06 15:50:34
 OBNUC 1H
 EXMOD single pulse.ex2
 OBFRQ 399.78 MHz
 OBSET 4.62 KHz
 OBFIN 5.98 Hz
 POINT 13107
 FREQU 6218.81 Hz
 SCANS 32
 ACQTM 2.1076 sec
 PD 5.0000 sec
 PW1 5.80 usec
 IRNUC 1H
 CTEMP 18.0 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.12 Hz
 RGAIN 34



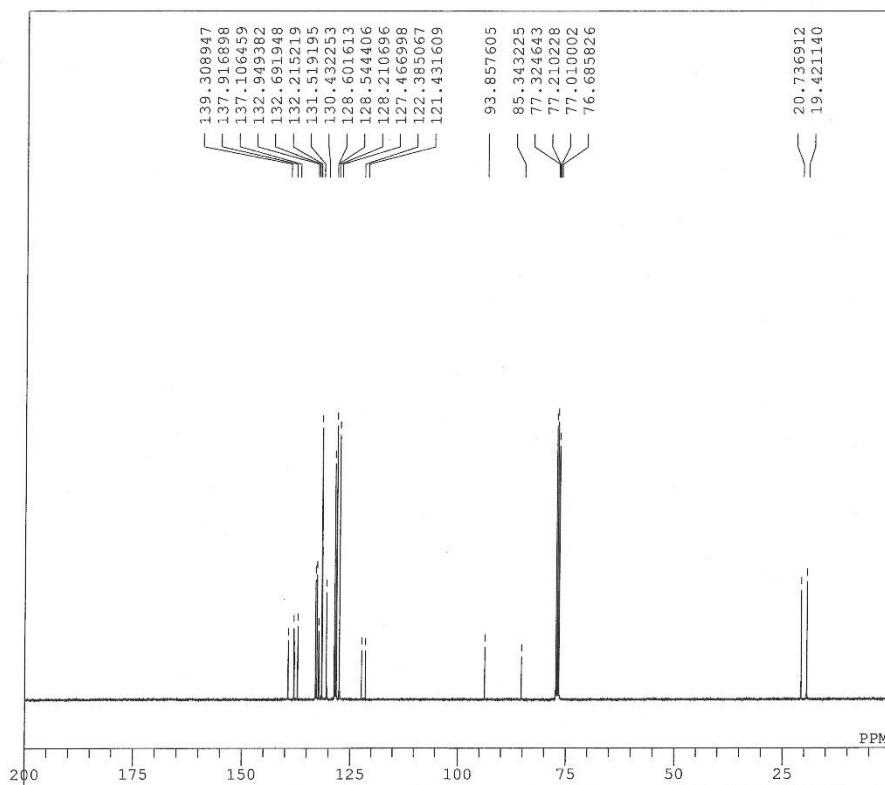
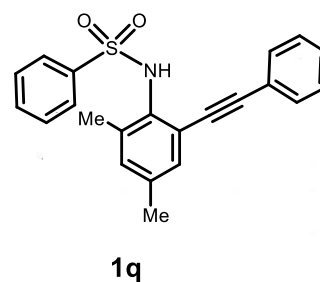
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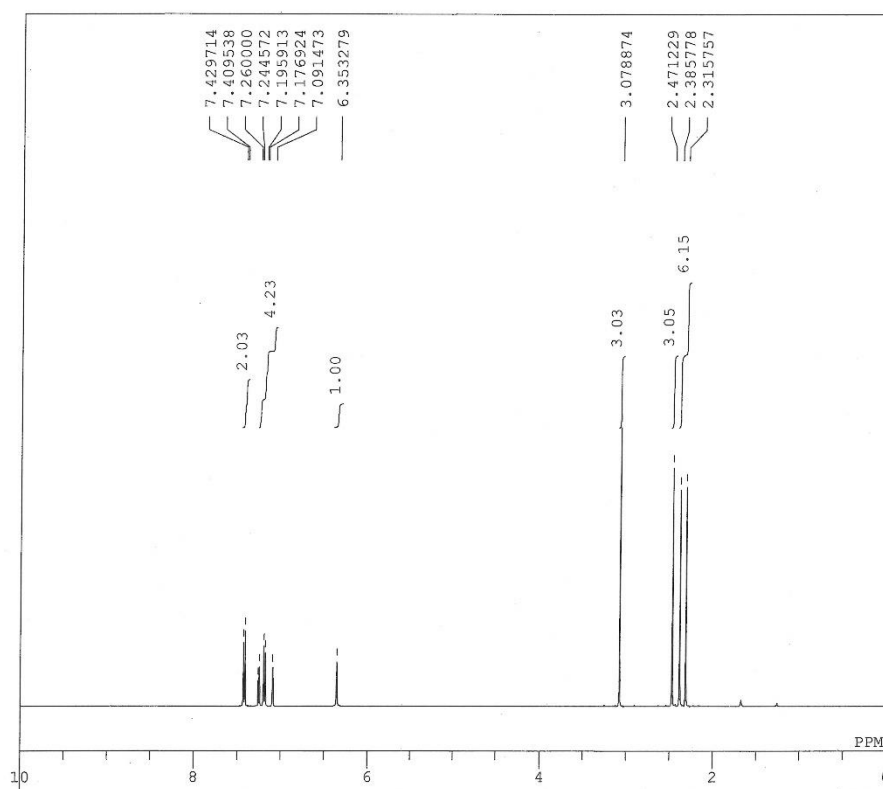
DFILE SF112 13C 20211207-1.als
 COMNT
 DATIM 2021-12-07 10:32:06
 OBNUC 13C
 EXMOD single pulse_dec
 OBFRQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 26214
 FREQU 25125.24 Hz
 SCANS 1024
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PW1 3.23 usec
 IRNUC 1H
 CTEMP 18.1 c
 SLVNT CDCL3
 EXREF 77.01 ppm
 BF 1.20 Hz
 RGAIN 60



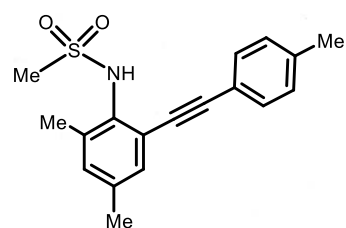
DFILE SF121 20210930-1.als
 COMNT Qn-BOC 1H
 DATIM 2021-09-30 10:30:05
 OBNUC 1H
 EXMOD single pulse.ex2
 OBFRQ 399.78 MHz
 OBSET 4.62 KHz
 OBFIN 5.98 Hz
 POINT 13107
 FREQU 6218.81 Hz
 SCANS 32
 ACQTM 2.1076 sec
 PD 5.0000 sec
 PW1 5.17 usec
 IRNUC 1H
 CTEMP 18.9 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.12 Hz
 RGAIN 30



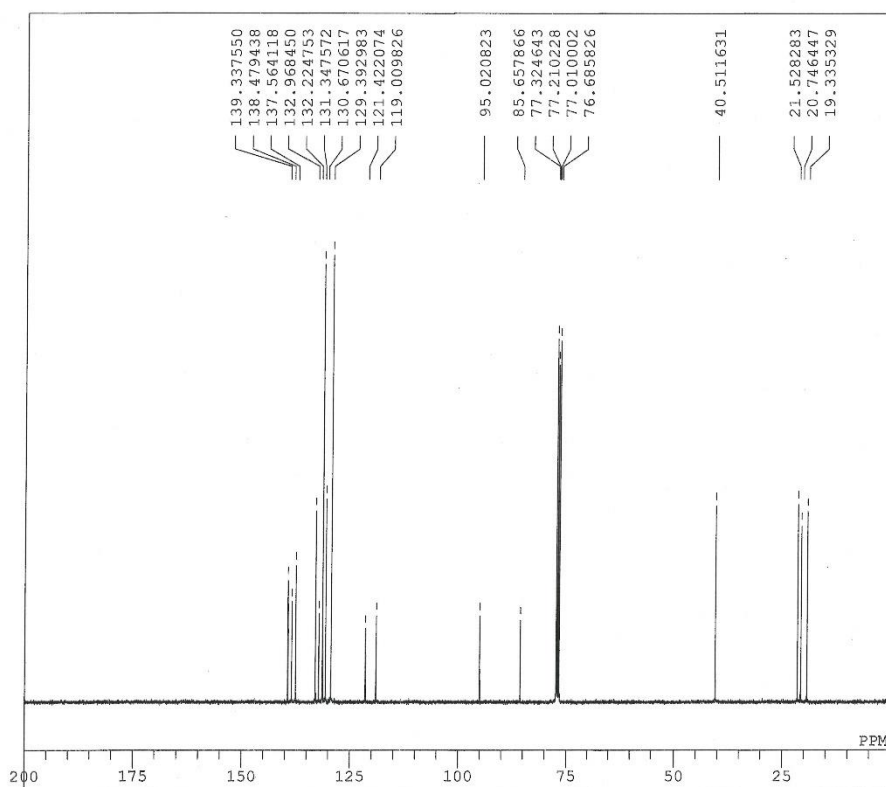
DFILE SF121-13C 20211002-1.als
 COMNT
 DATIM 2021-10-02 09:53:39
 OBNUC 13C
 EXMOD single_pulse_dec
 OBFRQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 26214
 FREQU 25125.24 Hz
 SCANS 1024
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PW1 3.03 usec
 IRNUC 1H
 CTEMP 19.0 c
 SLVNT CDCL3
 EXREF 77.01 ppm
 BF 1.20 Hz
 RGAIN 60



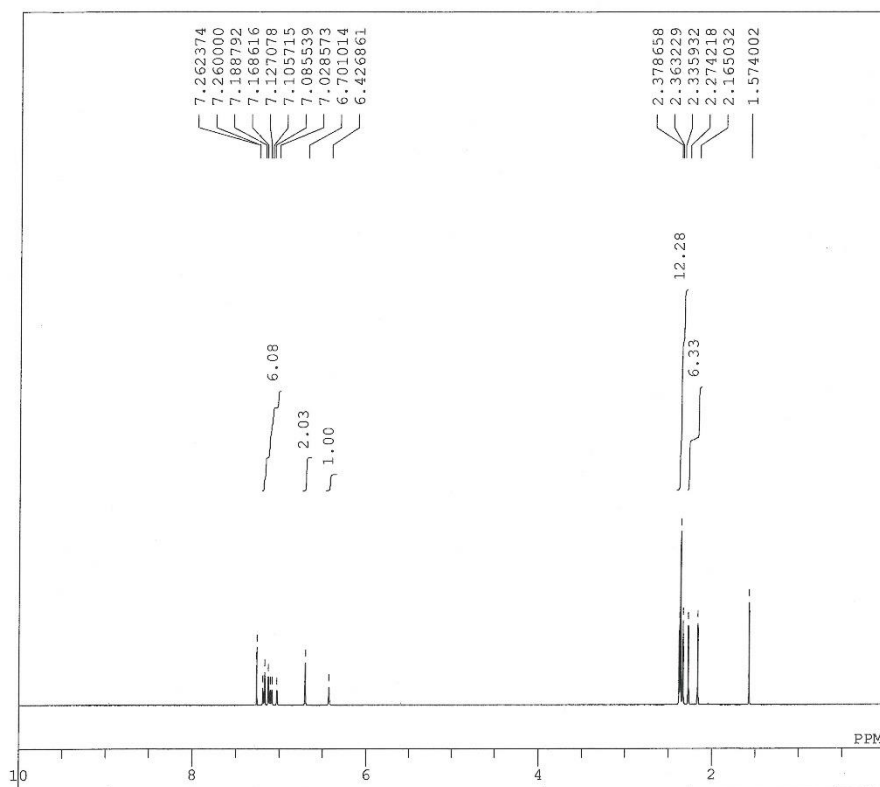
DFILE SF088 20211213-1.als
 COMNT Qn-BOC 1H
 DATIM 2021-12-13 13:28:17
 OBNUC 1H
 EXMOD single_pulse.ex2
 OBFRQ 399.78 MHz
 OBSET 4.62 KHz
 OBFIN 5.98 Hz
 POINT 16384
 FREQU 7773.63 Hz
 SCANS 32
 ACQTM 2.1076 sec
 PD 5.0000 sec
 PW1 5.80 usec
 IRNUC 1H
 CTEMP 18.5 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.12 Hz
 RGAIN 30



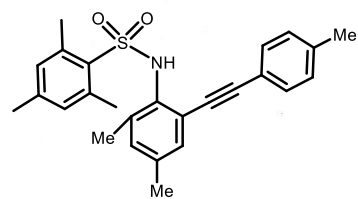
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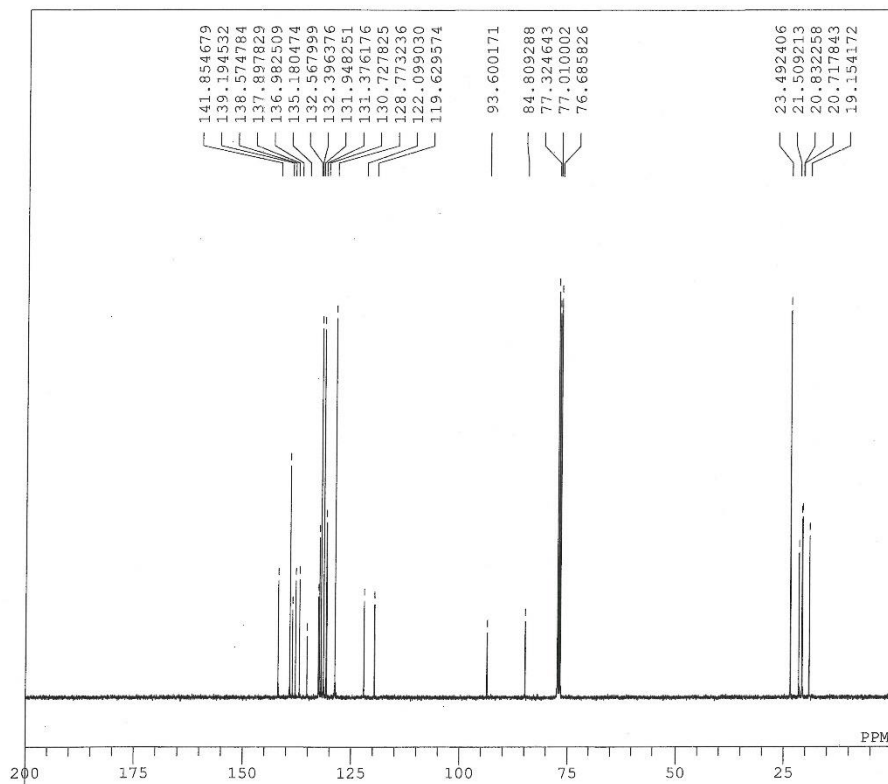
DFILE SF088 13C 20211213-1.als
 COMNT
 DATIM 2021-12-13 09:38:13
 OBNUC 13C
 EXMOD single_pulse_dec
 OBFRQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 32768
 FREQU 31407.03 Hz
 SCANS 1024
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PW1 3.23 usec
 IRNUC 1H
 CTEMP 18.5 c
 SLVNT CDCL3
 EXREF 77.01 ppm
 BF 1.20 Hz
 RGAIN 60



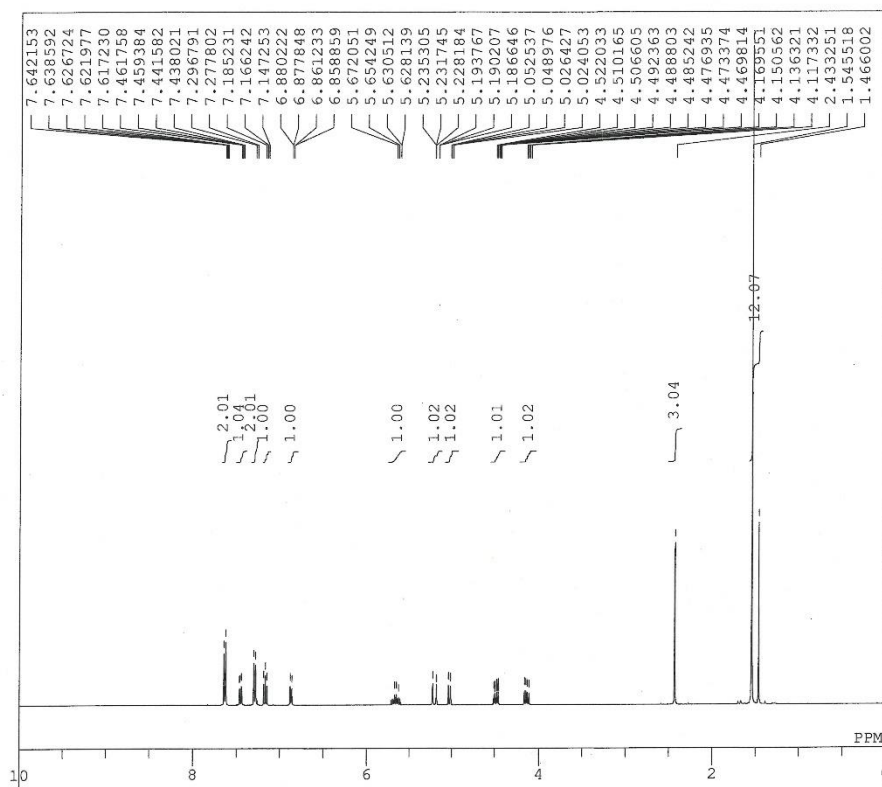
DFILE SF102 20211129-1.als
 COMNT Qn-BOC 1H
 DATIM 2021-11-29 11:57:15
 OBNUC 1H
 EXMOD single pulse.ex2
 OBFRQ 399.78 MHz
 OBSET 4.62 KHz
 OBFIN 5.98 Hz
 POINT 13107
 FREQU 6218.81 Hz
 SCANS 32
 ACQTM 2.1076 sec
 PD 5.0000 sec
 PW1 5.80 usec
 IRNUC 1H
 CTEMP 17.8 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.12 Hz
 RGAIN 36



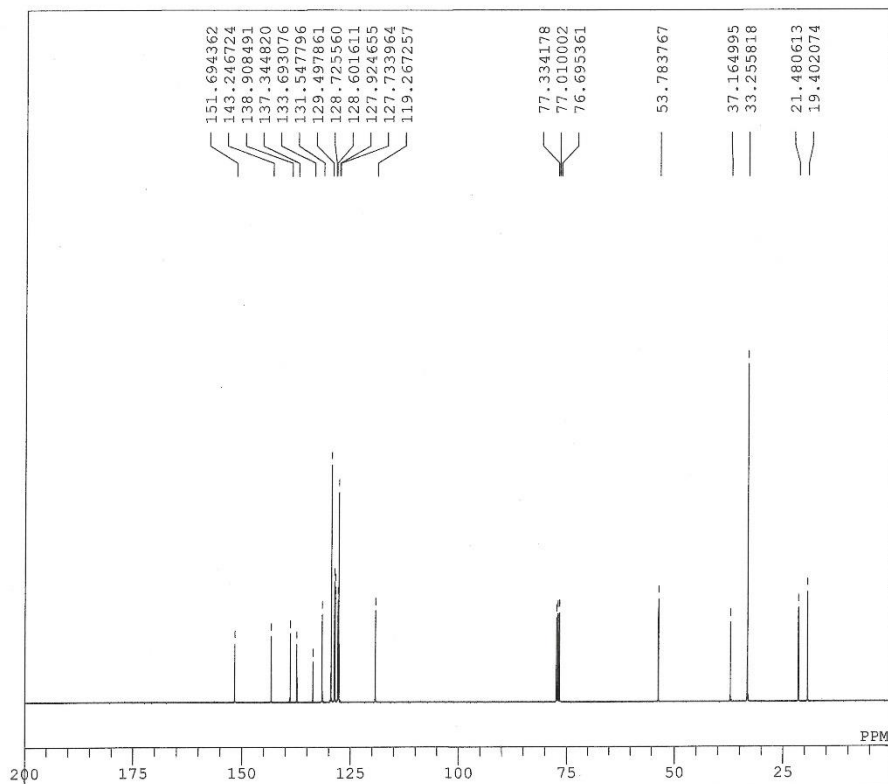
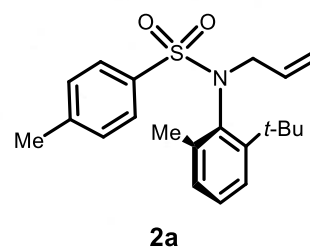
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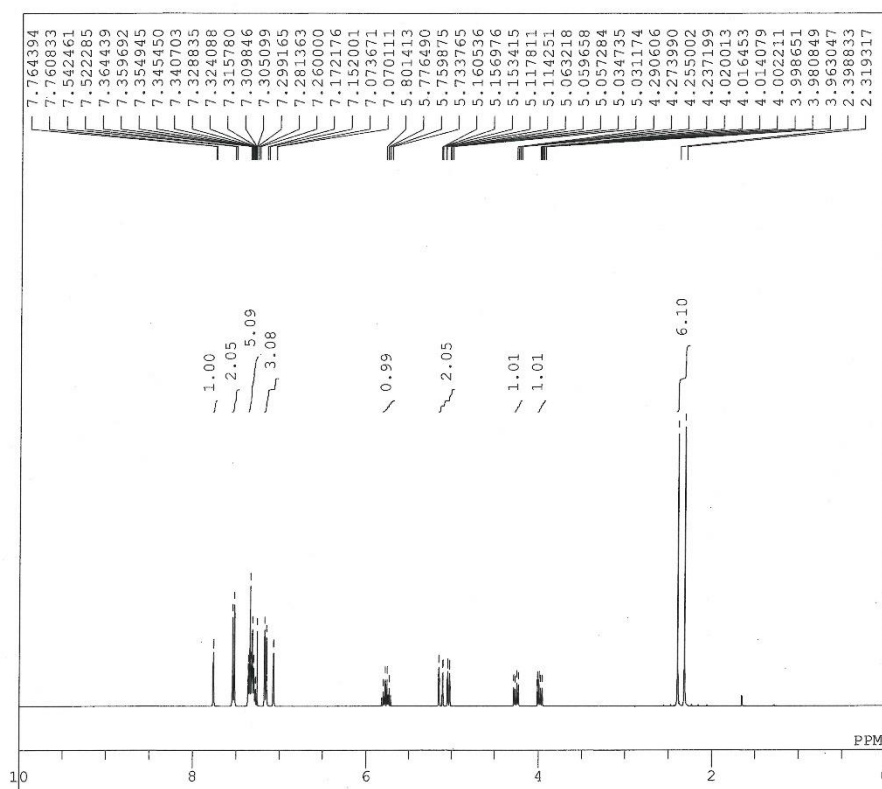
DFILE SF102 13C-2 20211130-1.a
 COMNT
 DATIM 2021-11-30 18:17:36
 OBNUC 13C
 EXMOD single pulse_dec
 OBFRQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 26214
 FREQU 25125.24 Hz
 SCANS 1024
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PW1 3.23 usec
 IRNUC 1H
 CTEMP 19.8 c
 SLVNT CDCL3
 EXREF 77.01 ppm
 BF 1.20 Hz
 RGAIN 60



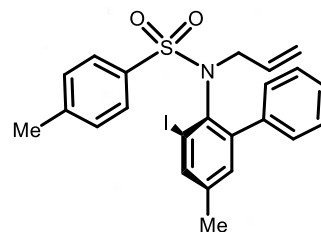
DFILE Y0015 20211008-1.als
 COMNT Qn-BOC 1H
 DATIM 2021-10-08 13:58:12
 OBNUC 1H
 EXMOD single pulse.ex2
 OBFRQ 399.78 MHz
 OBSET 4.62 KHz
 OBFIN 5.98 Hz
 POINT 13107
 FREQU 6218.81 Hz
 SCANS 32
 ACQTM 2.1076 sec
 PD 5.0000 sec
 PW1 5.17 usec
 IRNUC 1H
 CTEMP 18.5 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.12 Hz
 RGAIN 20



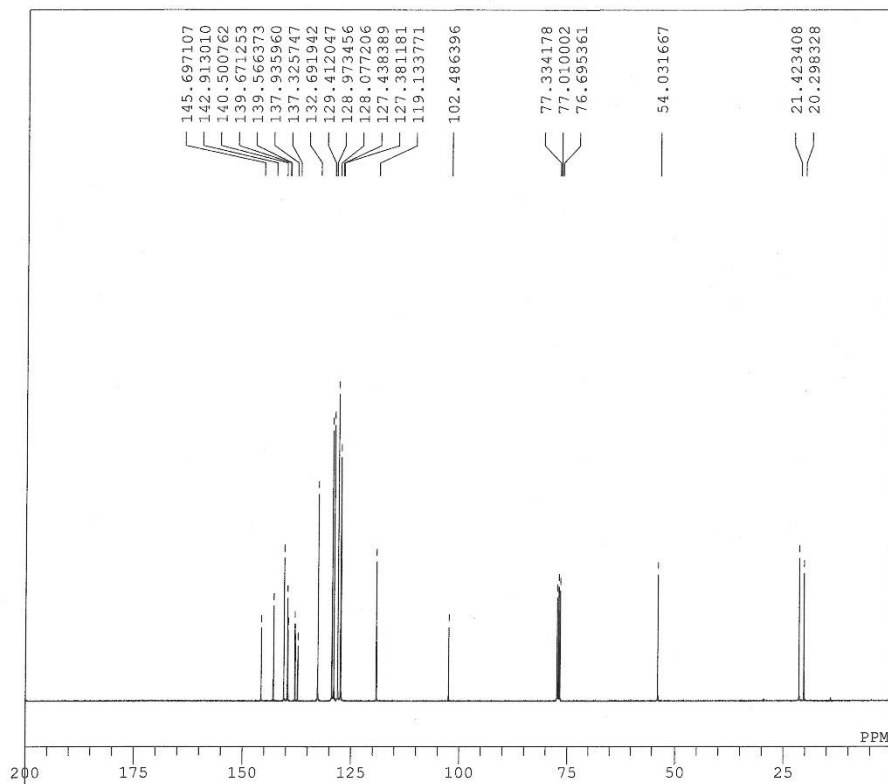
DFILE Y0015-13C 20211008-1.als
 COMNT
 DATIM 2021-10-08 17:31:11
 OBNUC 13C
 EXMOD single pulse_dec
 OBFRQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 32768
 FREQU 31407.03 Hz
 SCANS 1024
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PW1 3.03 usec
 IRNUC 1H
 CTEMP 19.3 c
 SLVNT CDCL3
 EXREF 77.01 ppm
 BF 1.20 Hz
 RGAIN 60



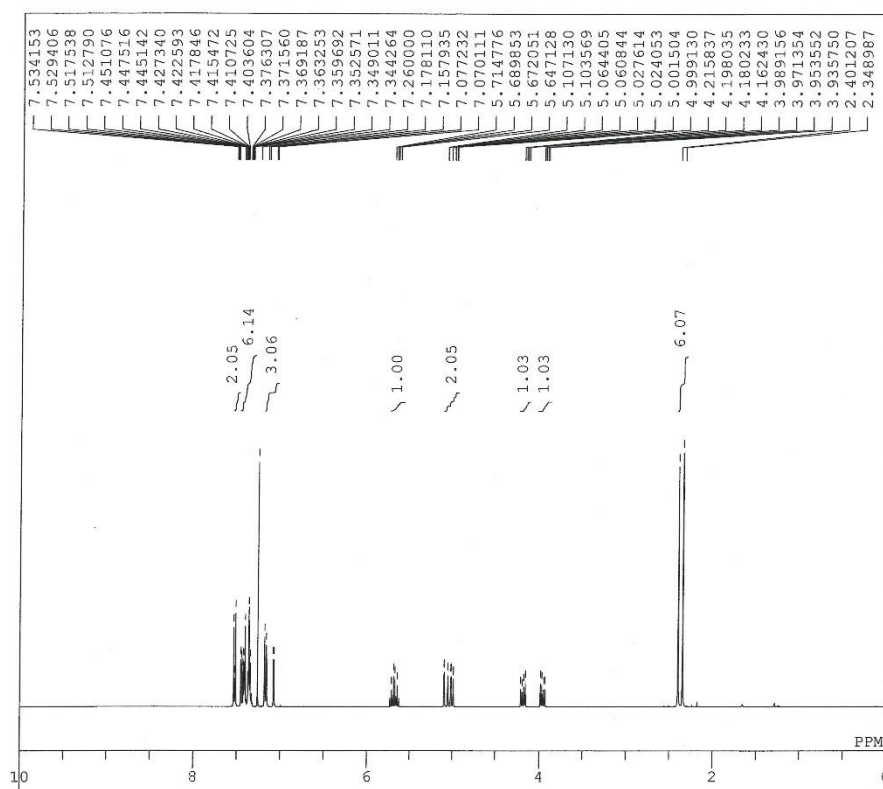
DFILE TT088 20211111-1.als
 COMNT Qn-BOC 1H
 DATIM 2021-11-11 15:20:11
 OBNUC 1H
 EXMOD single pulse.ex2
 OBFRQ 399.78 MHz
 OBSET 4.62 KHz
 OBFIN 5.98 Hz
 POINT 13107
 FREQU 6218.81 Hz
 SCANS 32
 ACQTM 2.1076 sec
 PD 5.0000 sec
 PW1 5.17 usec
 IRNUC 1H
 CTEMP 19.1 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.12 Hz
 RGAIN 24



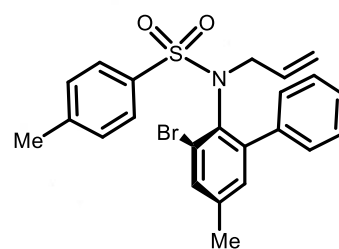
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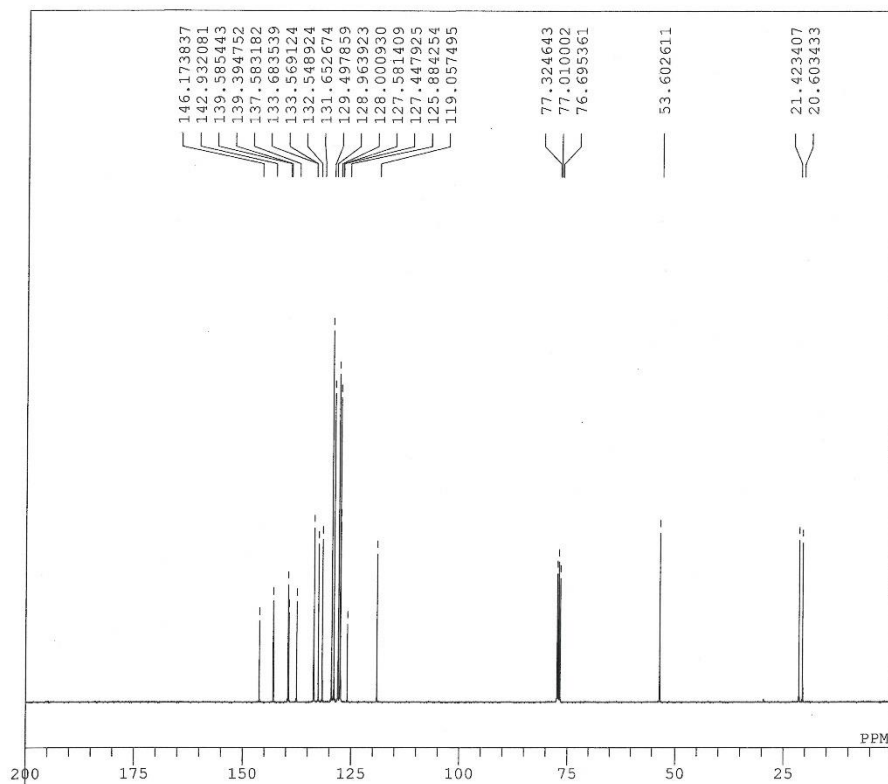
DFILE TT088 carbon 20211027-1.
 COMNT
 DATIM 2021-10-27 20:34:04
 OBNUC 13C
 EXMOD single pulse_dec
 OBFRQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 26214
 FREQU 25125.24 Hz
 SCANS 1024
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PW1 3.03 usec
 IRNUC 1H
 CTEMP 18.5 c
 SLVNT CDCL3
 EXREF 77.01 ppm
 BF 1.20 Hz
 RGAIN 60



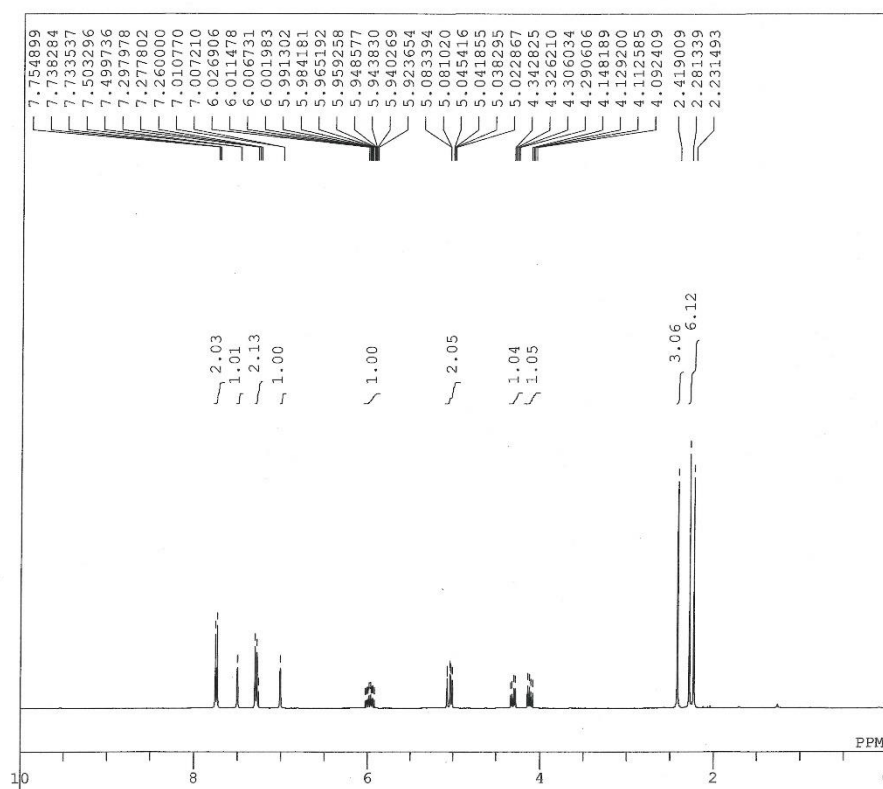
DFILE SF136 20211025-1.als
 COMNT Qn-BOC 1H
 DATIM 2021-10-25 15:16:18
 OBNUC 1H
 EXMOD single_pulse.ex2
 OBFRQ 399.78 MHz
 OBSET 4.62 KHz
 OBFIN 5.98 Hz
 POINT 16384
 FREQU 7773.63 Hz
 SCANS 32
 ACQTM 2.1076 sec
 PD 5.0000 sec
 PW1 5.17 usec
 IRNUC 1H
 CTEMP 17.6 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.12 Hz
 RGAIN 24



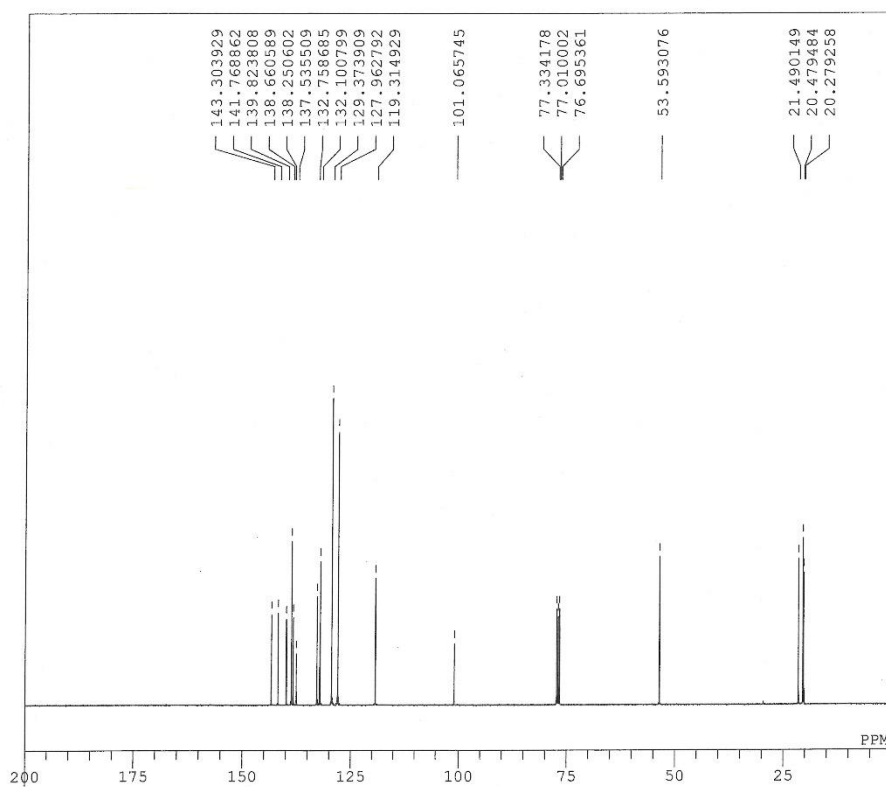
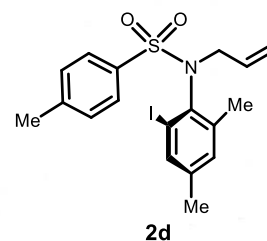
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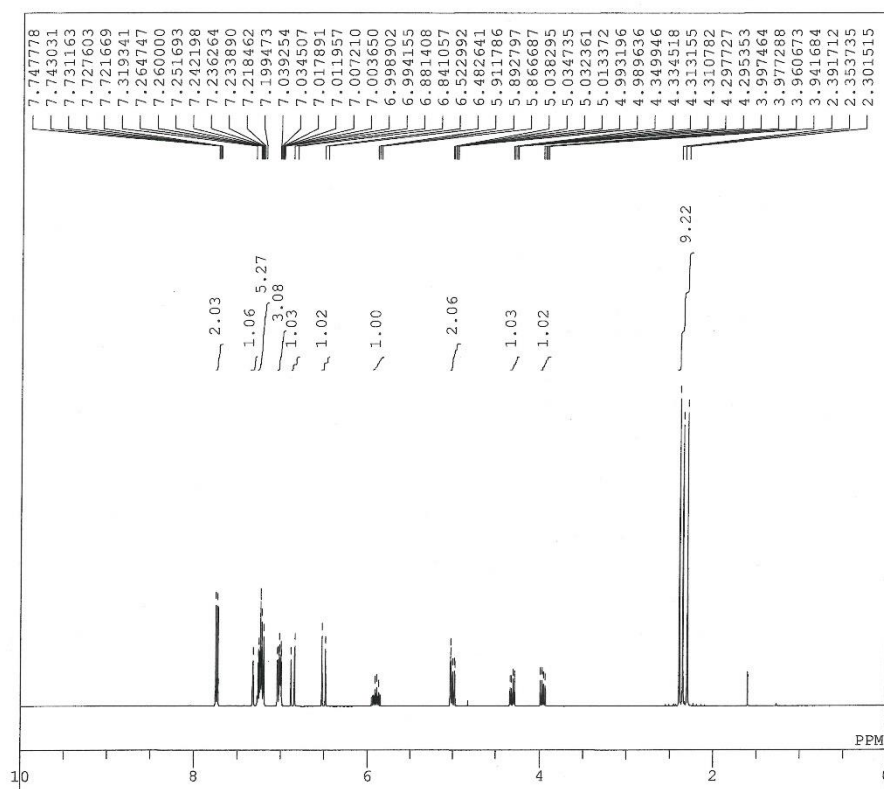
DFILE SF136-13C 20211025-1.als
 COMNT
 DATIM 2021-10-25 18:54:20
 OBNUC 13C
 EXMOD single_pulse_dec
 OBFRQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 32768
 FREQU 31407.03 Hz
 SCANS 1024
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PW1 3.03 usec
 IRNUC 1H
 CTEMP 18.1 c
 SLVNT CDCL3
 EXREF 77.01 ppm
 BF 1.20 Hz
 RGAIN 60



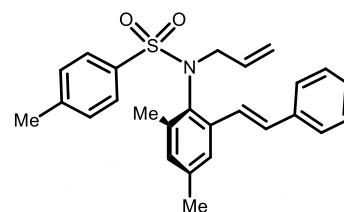
DFILE RK036 20211029-1.als
 COMNT Qn-BOC 1H
 DATIM 2021-10-29 16:08:06
 OBNUC 1H
 EXMOD single pulse.ex2
 OBFRQ 399.78 MHz
 OBSET 4.62 KHz
 OBFIN 5.98 Hz
 POINT 16384
 FREQU 7773.63 Hz
 SCANS 32
 ACQTM 2.1076 sec
 PD 5.0000 sec
 PW1 5.17 usec
 IRNUC 1H
 CTEMP 18.7 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.12 Hz
 RGAIN 22



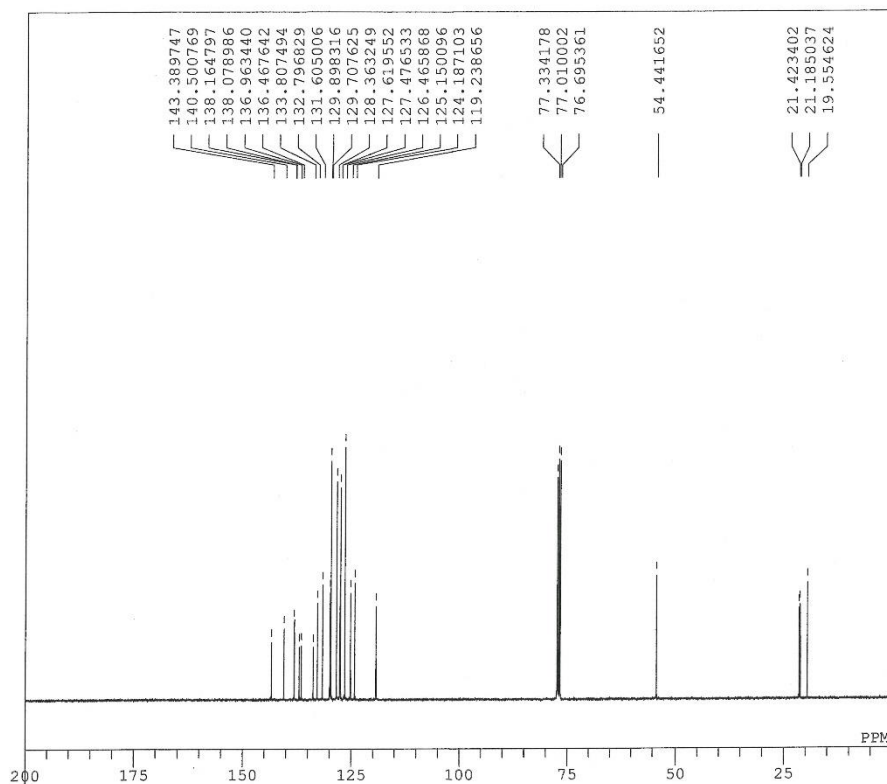
DFILE RK036-13C 20211102-1.als
 COMNT 2021-11-02 09:27:43
 OBNUC 13C
 EXMOD single pulse_dec
 OBFRQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 32768
 FREQU 31407.03 Hz
 SCANS 1024
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PW1 3.03 usec
 IRNUC 1H
 CTEMP 18.5 c
 SLVNT CDCL3
 EXREF 77.01 ppm
 BF 1.20 Hz
 RGAIN 60



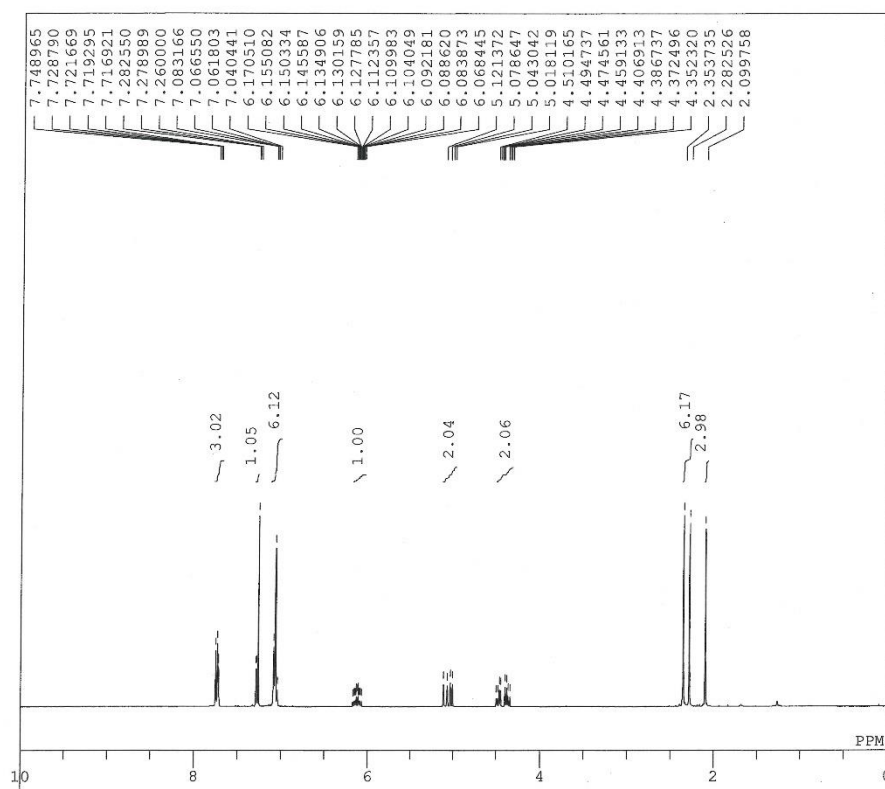
DFILE TT083 20211014-1.als
 COMNT Qn-BOC 1H
 DATIM 2021-10-14 15:49:22
 OBNUC 1H
 EXMOD single_pulse.ex2
 OBFRQ 399.78 MHz
 OBSET 4.62 KHz
 OBFIN 5.98 Hz
 POINT 16384
 FREQU 7773.63 Hz
 SCANS 32
 ACQTM 2.1076 sec
 PD 5.0000 sec
 PW1 5.17 usec
 IRNUC 1H
 CTEMP 18.6 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.12 Hz
 RGAIN 30



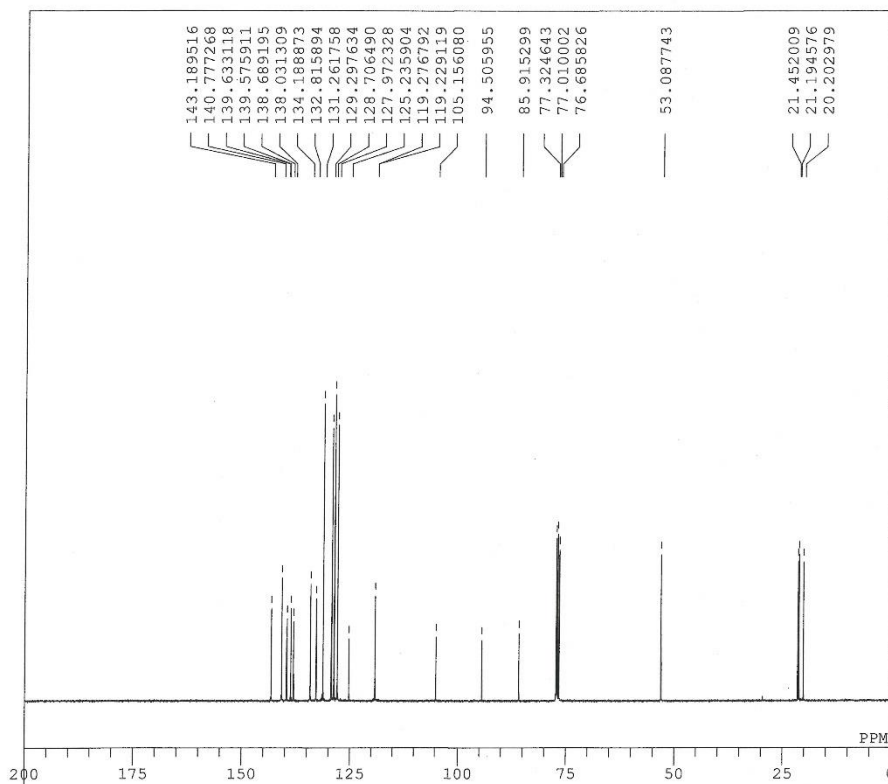
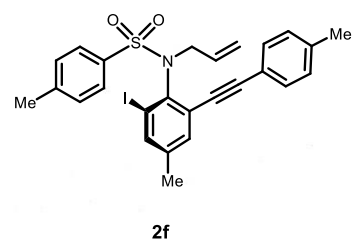
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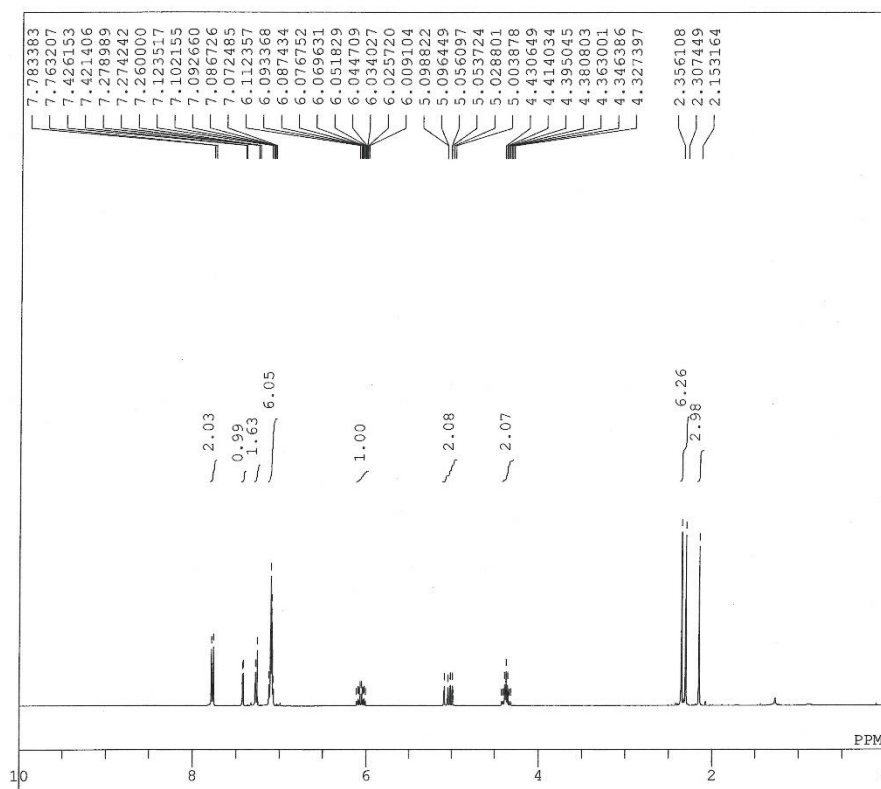
DFILE TT083-13C 20211015-1.als
 COMNT
 DATIM 2021-10-15 09:11:14
 OBNUC 13C
 EXMOD single_pulse_dec
 OBFRQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 32768
 FREQU 31407.03 Hz
 SCANS 1024
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PW1 3.03 usec
 IRNUC 1H
 CTEMP 19.0 c
 SLVNT CDCL3
 EXREF 77.01 ppm
 BF 1.20 Hz
 RGAIN 60



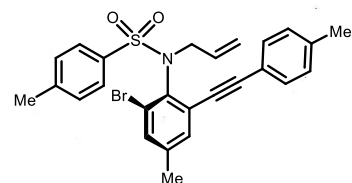
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 COMNT Qn-BOC 1H
 DATIM 2021-11-25 14:03:08
 OBNUC 1H
 EXMOD single pulse.ex2
 OBFRQ 399.78 MHz
 OBSET 4.62 KHz
 OBFIN 5.98 Hz
 POINT 16384
 FREQU 7773.63 Hz
 SCANS 32
 ACQTM 2.1076 sec
 PD 5.0000 sec
 PW1 5.80 usec
 IRNUC 1H
 CTEMP 18.6 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.12 Hz
 RGAIN 26



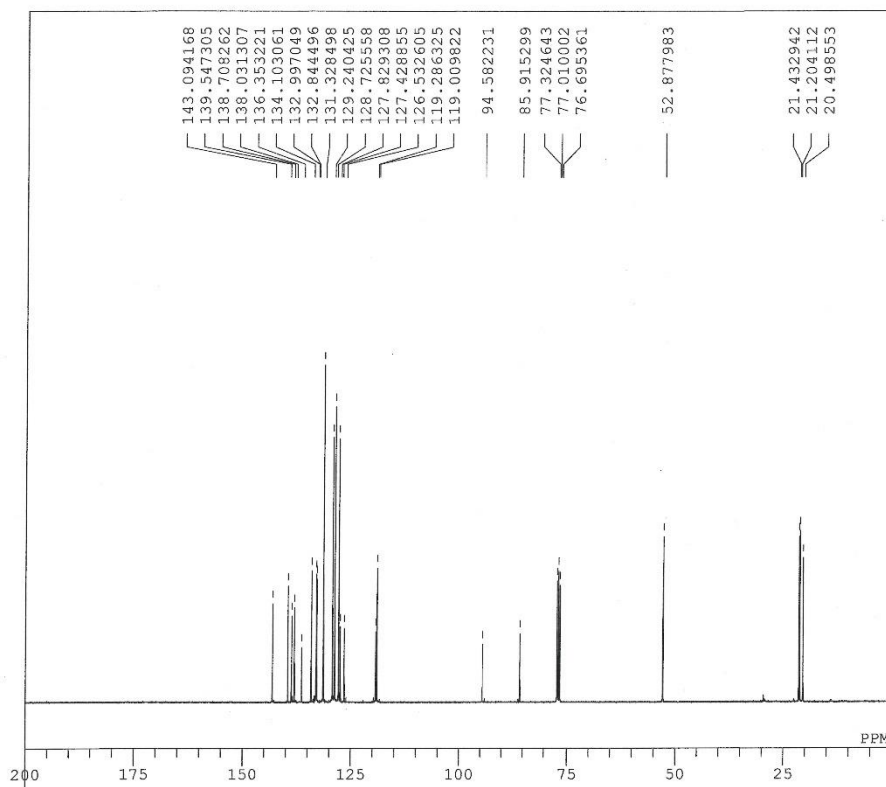
DFILE RK040-13C 20211126-1.jdf
 COMNT 2021-11-26 17:57:28
 OBNUC 13C
 EXMOD single pulse dec
 OBFRQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 32768
 FREQU 31407.03 Hz
 SCANS 1024
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PW1 3.23 usec
 IRNUC 1H
 CTEMP 19.3 c
 SLVNT CDCL3
 EXREF 77.01 ppm
 BF 1.20 Hz
 RGAIN 60



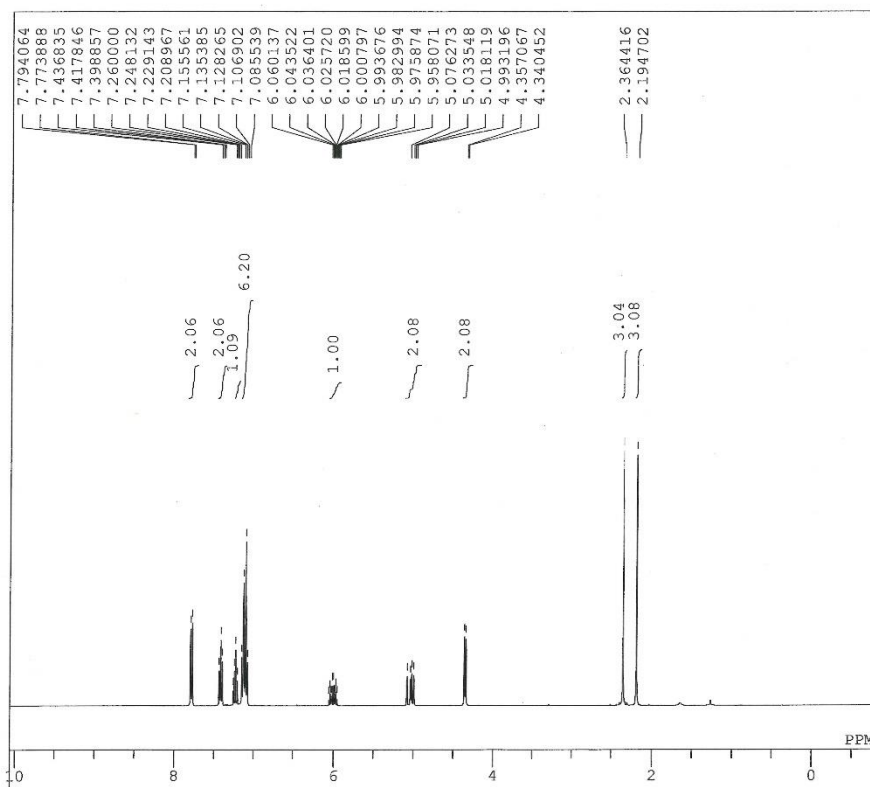
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 DATIM 2021-10-23 12:56:30
 OBNUC 1H
 EXMOD single pulse.ex2
 OBFRQ 399.78 MHz
 OBSET 4.62 KHz
 OBFIN 5.98 Hz
 POINT 13107
 FREQU 6218.81 Hz
 SCANS 32
 ACQTM 2.1076 sec
 PD 5.0000 sec
 PW1 5.17 usec
 IRNUC 1H
 CTEMP 18.1 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.12 Hz
 RGAIN 22



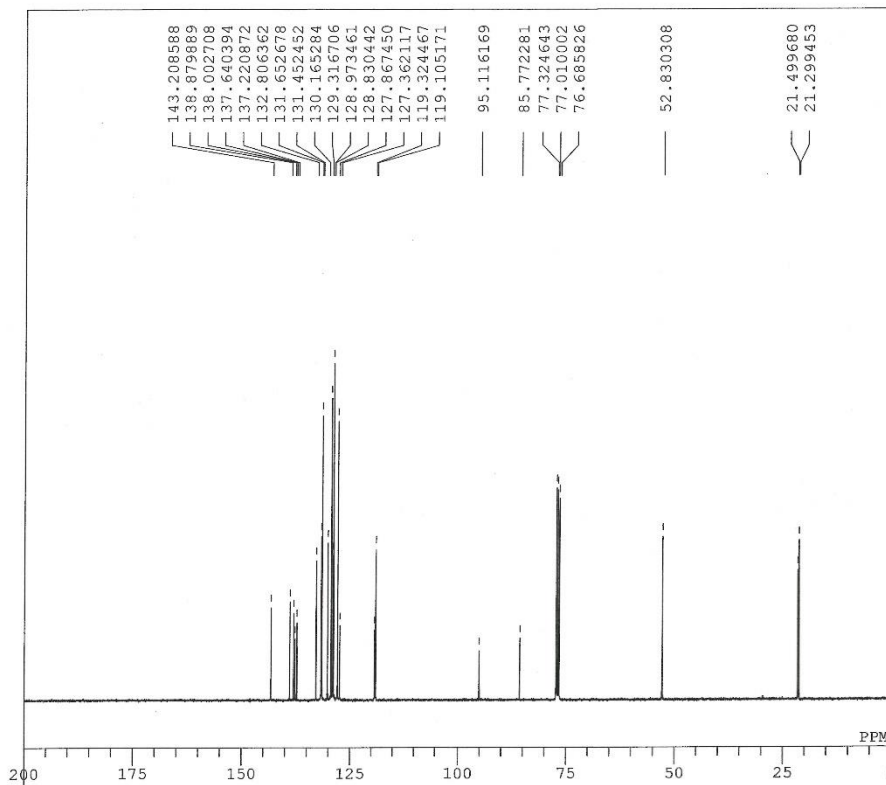
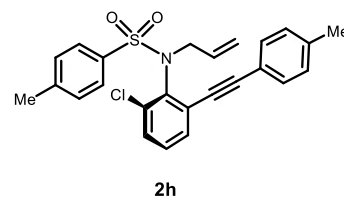
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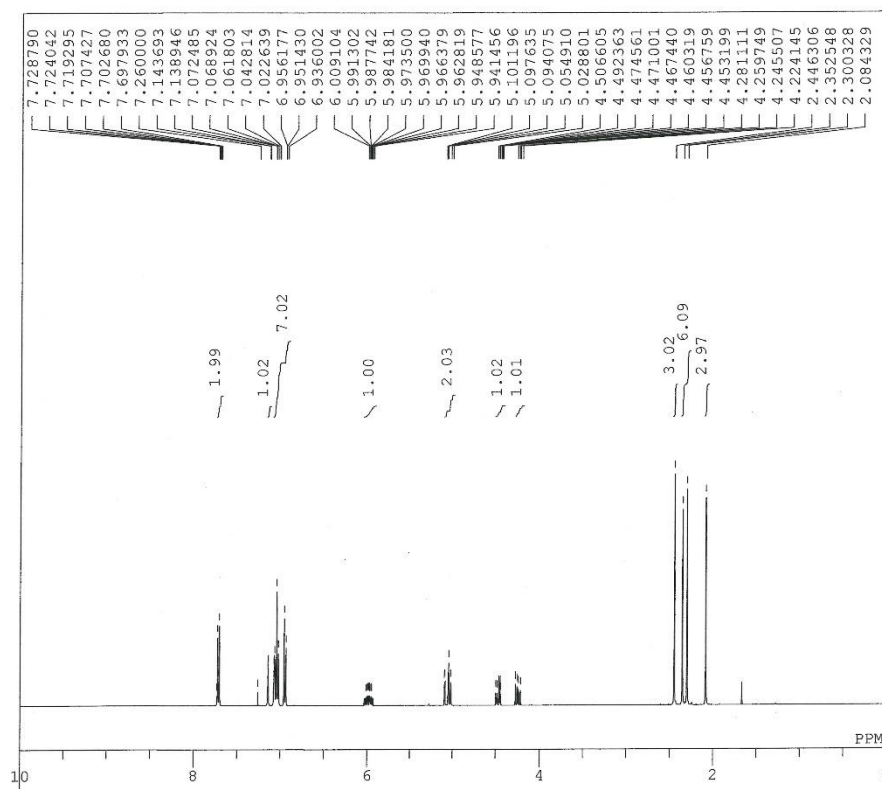
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 COMNT
 DATIM 2021-10-23 10:49:27
 OBNUC 13C
 EXMOD single pulse_dec
 OBFRQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 26214
 FREQU 25125.24 Hz
 SCANS 1024
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PW1 3.03 usec
 IRNUC 1H
 CTEMP 18.0 c
 SLVNT CDCL3
 EXREF 77.01 ppm
 BF 1.20 Hz
 RGAIN 60



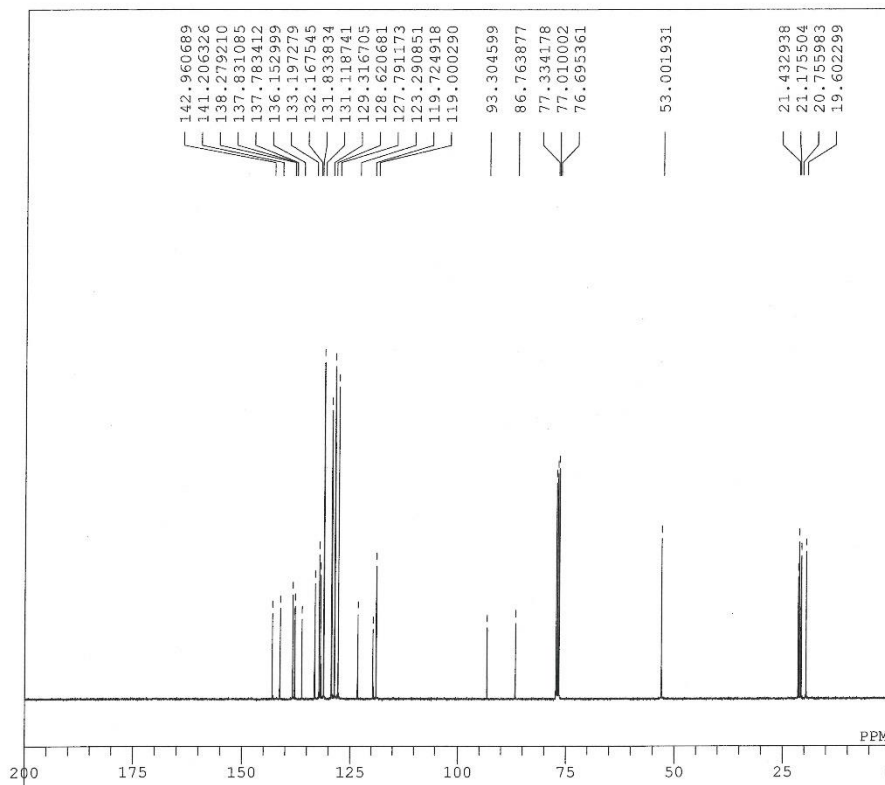
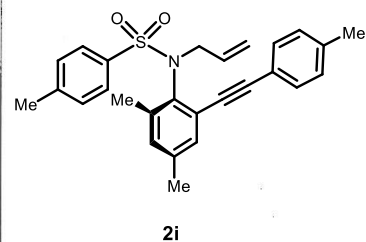
DFILE SF108 20210916-1.als
 COMNT Qn-BOC 1H
 DATIM 2021-09-16 15:42:12
 OBNUC 1H
 EXMOD single pulse.ex2
 OBFRQ 399.78 MHz
 OBSET 4.62 KHz
 OBFIN 5.98 Hz
 POINT 16384
 FREQU 7773.63 Hz
 SCANS 32
 ACQTM 2.1076 sec
 PD 5.0000 sec
 PW1 5.17 usec
 IRNUC 1H
 CTEMP 19.1 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.12 Hz
 RGAIN 30



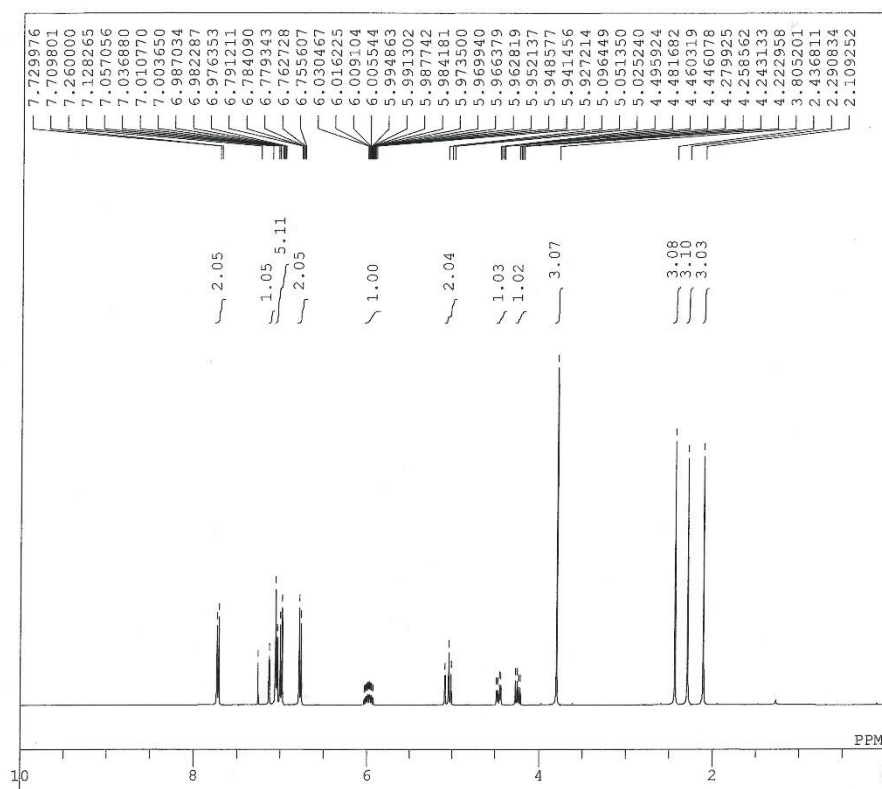
DFILE SF108-13C 20210916-1.als
 COMNT
 DATIM 2021-09-16 18:27:37
 OBNUC 13C
 EXMOD single pulse_dec
 OBFRQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 32768
 FREQU 31407.03 Hz
 SCANS 1024
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PW1 3.03 usec
 IRNUC 1H
 CTEMP 19.3 c
 SLVNT CDCL3
 EXREF 77.01 ppm
 BF 1.20 Hz
 RGAIN 60



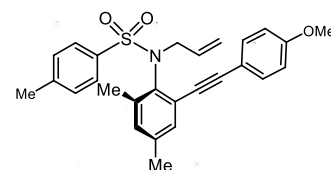
DFILE SF075 20211008-1.als
 COMNT Qn-BOC 1H
 DATIM 2021-10-08 14:09:18
 OBNUC 1H
 EXMOD single_pulse.ex2
 OBFRQ 399.78 MHz
 OBSET 4.62 KHz
 OBFIN 5.98 Hz
 POINT 16384
 FREQU 7773.63 Hz
 SCANS 32
 ACQTM 2.1076 sec
 PD 5.0000 sec
 PW1 5.17 usec
 IRNUC 1H
 CTEMP 18.5 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.12 Hz
 RGAIN 26



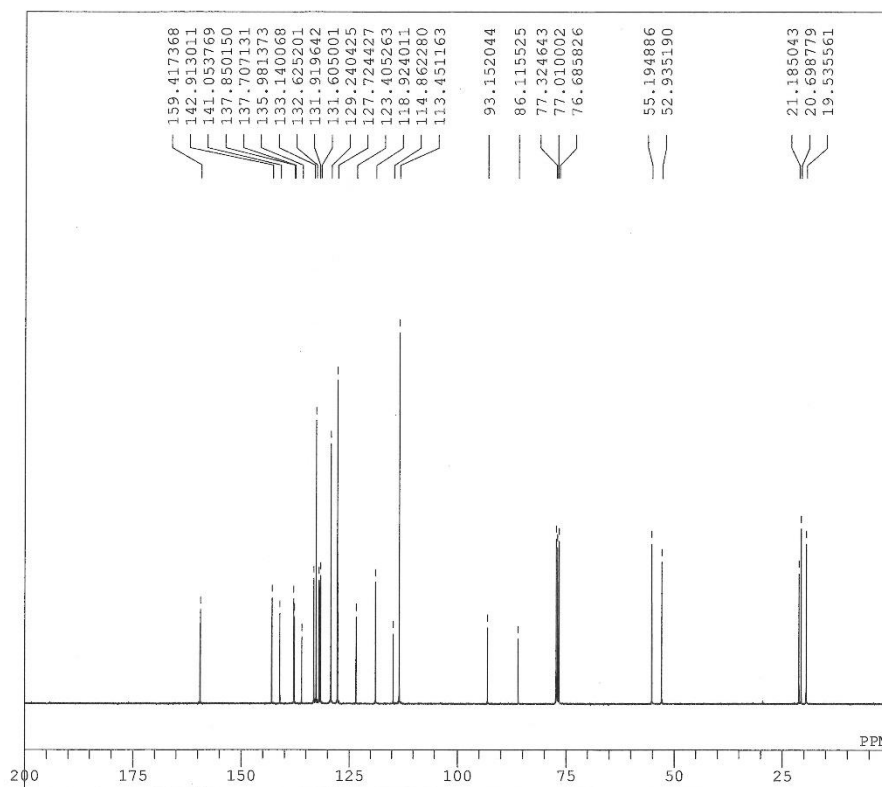
DFILE SF075-13C 20211004-1.als
 COMNT
 DATIM 2021-10-04 18:03:09
 OBNUC 13C
 EXMOD single_pulse_dec
 OBFRQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 32768
 FREQU 31407.03 Hz
 SCANS 1024
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PW1 3.03 usec
 IRNUC 1H
 CTEMP 18.5 c
 SLVNT CDCL3
 EXREF 77.01 ppm
 BF 1.20 Hz
 RGAIN 60



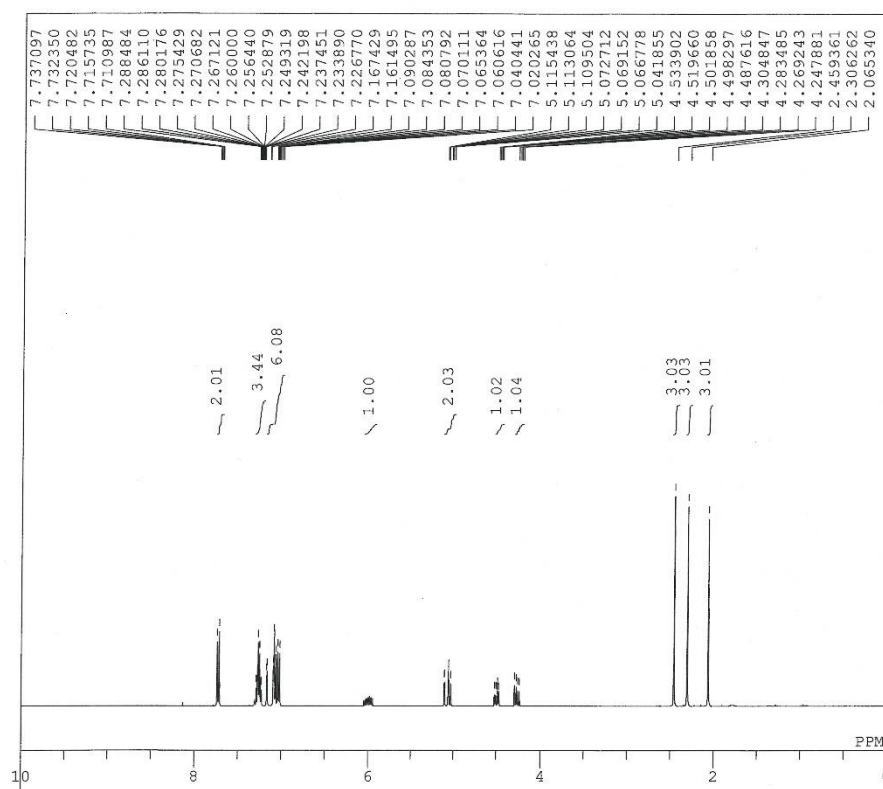
DFILE TF012 20210930-1.als
 COMNT Qn-BOC 1H
 DATIM 2021-09-30 10:08:27
 OBNUC 1H
 EXMOD single_pulse.ex2
 OBFRQ 399.78 MHz
 OBSET 4.62 KHz
 OBFIN 5.98 Hz
 POINT 16384
 FREQU 7773.63 Hz
 SCANS 32
 ACQTM 2.1076 sec
 PD 5.0000 sec
 PW1 5.17 usec
 IRNUC 1H
 CTEMP 19.0 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.12 Hz
 RGAIN 22



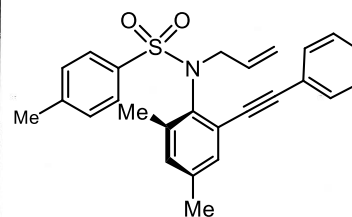
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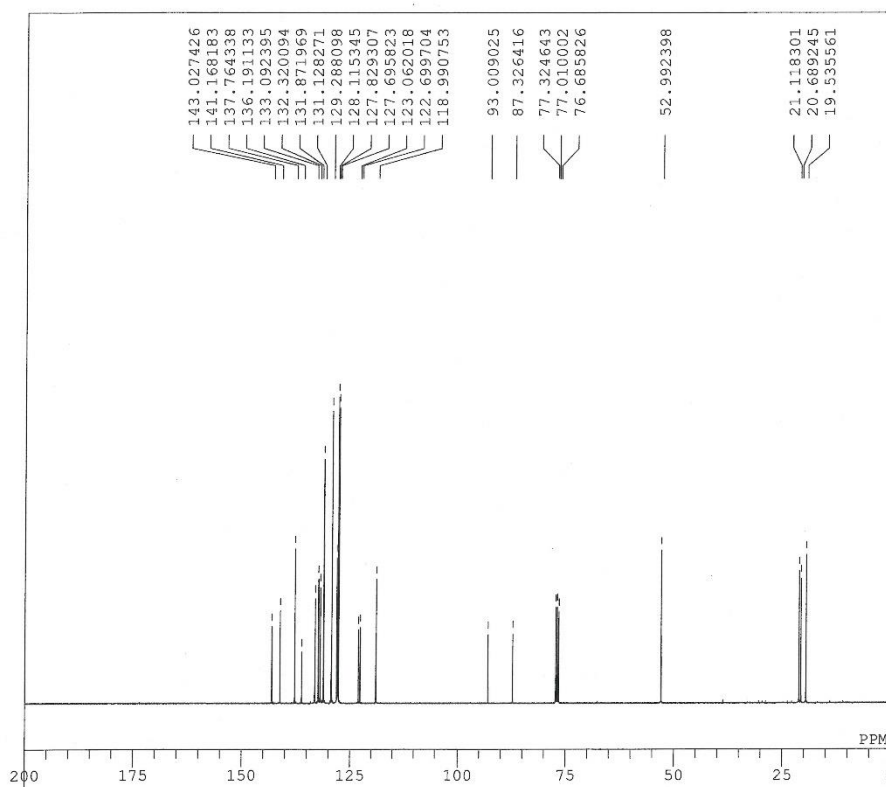
DFILE TF012-13C 20211002-1.als
 COMNT
 DATIM 2021-10-02 10:52:49
 OBNUC 13C
 EXMOD single_pulse_dec
 OBFRQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 26214
 FREQU 25125.24 Hz
 SCANS 1024
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PW1 3.03 usec
 IRNUC 1H
 CTEMP 18.5 c
 SLVNT CDCL3
 EXREF 77.01 ppm
 BF 1.20 Hz
 RGAIN 60



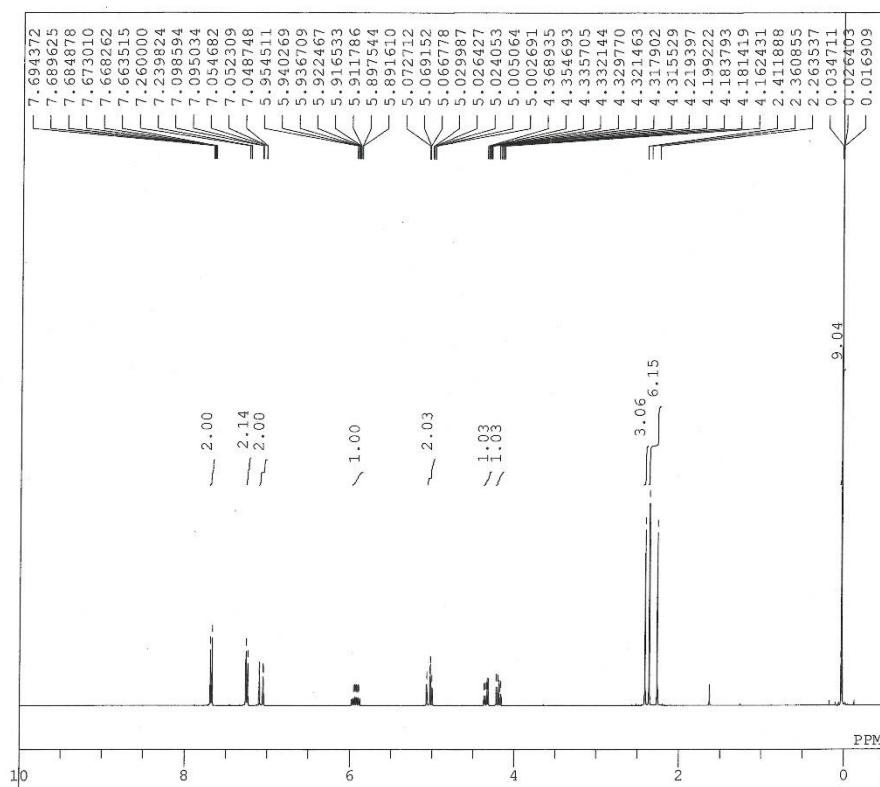
DFILE Y0021 20210927-1.als
 COMNT Qn-BOC 1H
 DATIM 2021-09-27 11:10:30
 OBNUC 1H
 EXMOD single pulse.ex2
 OBFRQ 399.78 MHz
 OBSET 4.62 KHz
 OBFIN 5.98 Hz
 POINT 16384
 FREQU 7773.63 Hz
 SCANS 32
 ACQTM 2.1076 sec
 PD 5.0000 sec
 PW1 5.17 usec
 IRNUC 1H
 CTEMP 18.7 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.12 Hz
 RGAIN 20



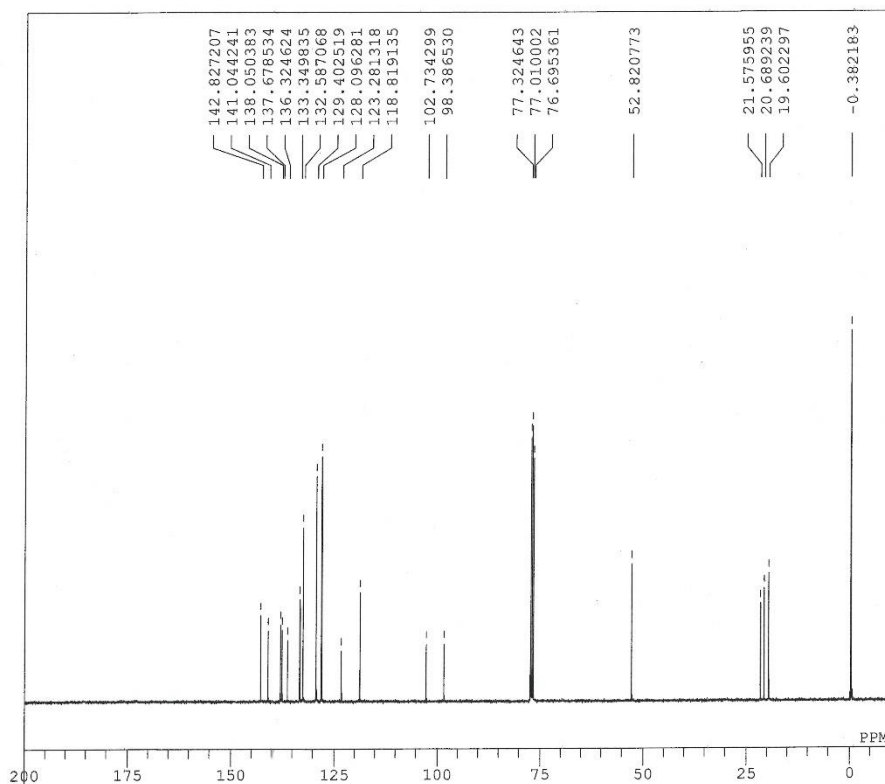
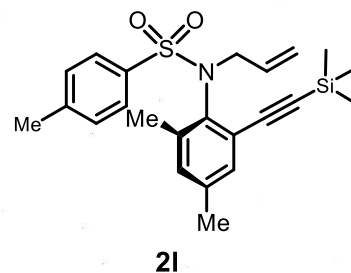
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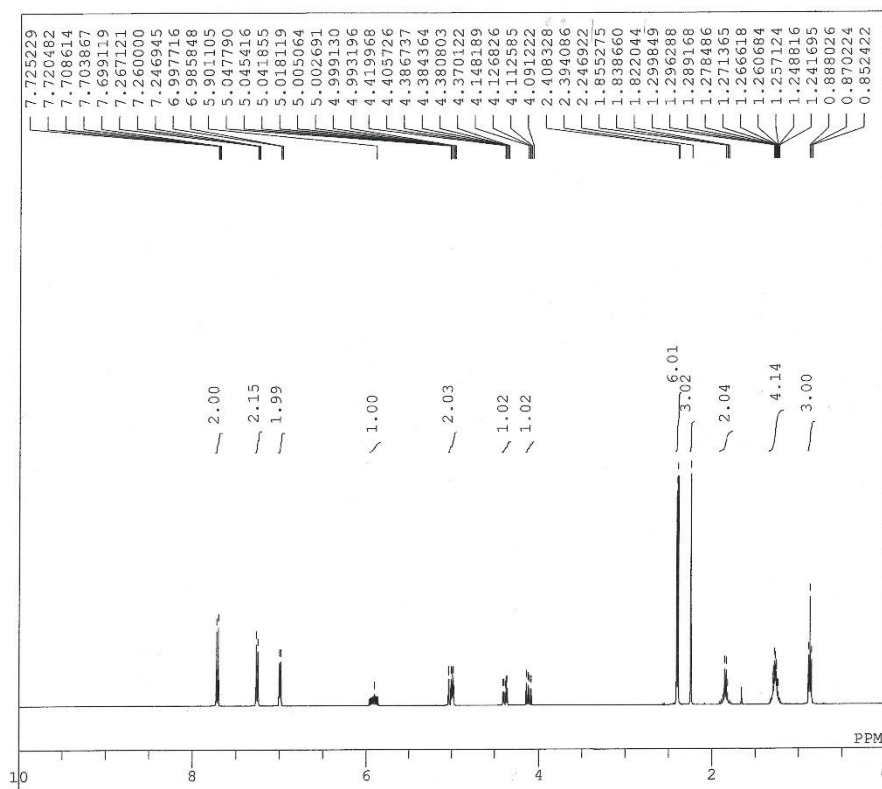
DFILE Y0021-13C 20210924-1.ais
 COMNT
 DATIM 2021-09-24 18:08:11
 OBNUC 13C
 EXMOD single pulse_dec
 OBFRQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 32768
 FREQU 31407.03 Hz
 SCANS 1024
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PW1 3.03 usec
 IRNUC 1H
 CTEMP 19.5 c
 SLVNT CDCL3
 EXREF 77.01 ppm
 BF 1.20 Hz
 RGAIN 60



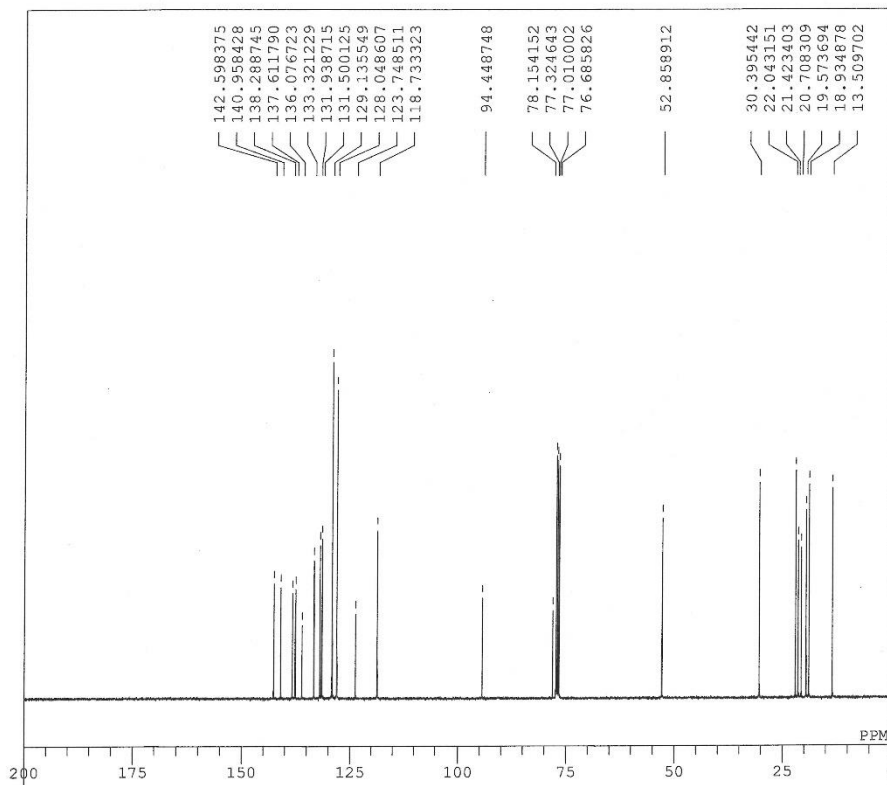
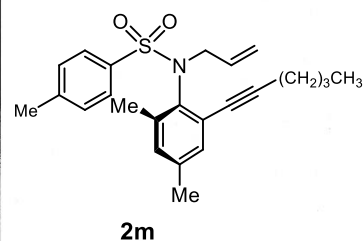
DFILE TT064 20211123-1.als
 COMNT Qn-BOC 1H
 DATIM 2021-11-23 14:49:48
 OBNUC 1H
 EXMOD single_pulse.ex2
 OBFREQ 399.78 MHz
 OBSET 4.62 KHz
 OBFIN 5.98 Hz
 POINT 13107
 FREQU 6218.81 Hz
 SCANS 32
 ACQTM 2.1076 sec
 PD 5.0000 sec
 PW1 5.80 usec
 IRNUC 1H
 CTEMP 18.8 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.12 Hz
 RGAIN 30



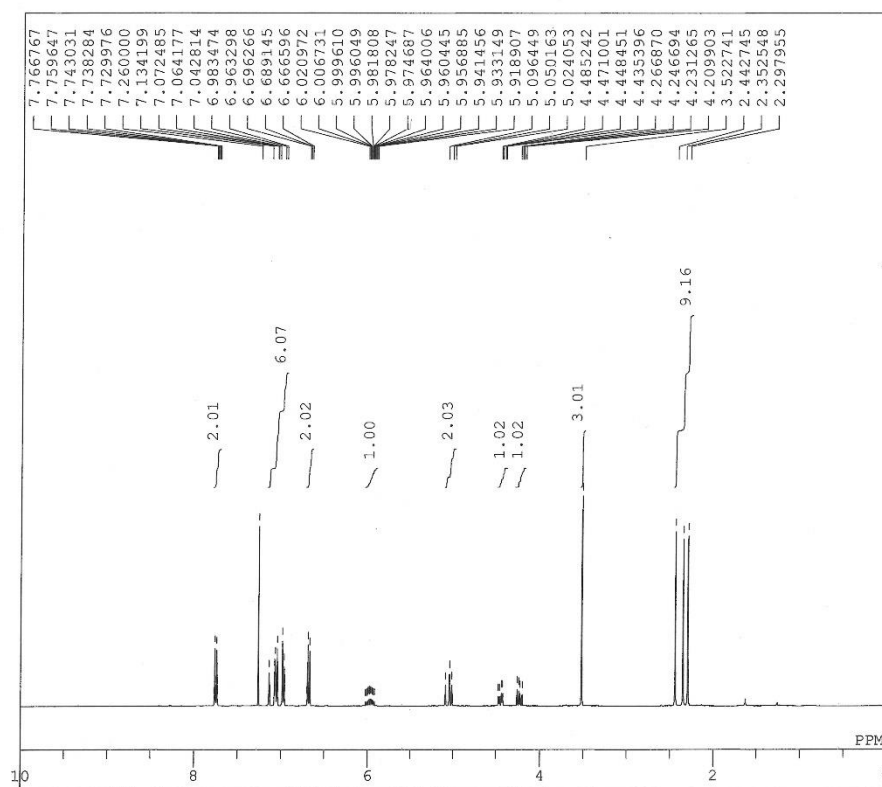
DFILE TT064-13C 20211123-1.als
 COMNT
 DATIM 2021-11-23 18:01:60
 OBNUC 13C
 EXMOD single_pulse_dec
 OBFREQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 32768
 FREQU 31407.03 Hz
 SCANS 1024
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PW1 3.23 usec
 IRNUC 1H
 CTEMP 19.1 c
 SLVNT CDCL3
 EXREF 77.01 ppm
 BF 1.20 Hz
 RGAIN 60



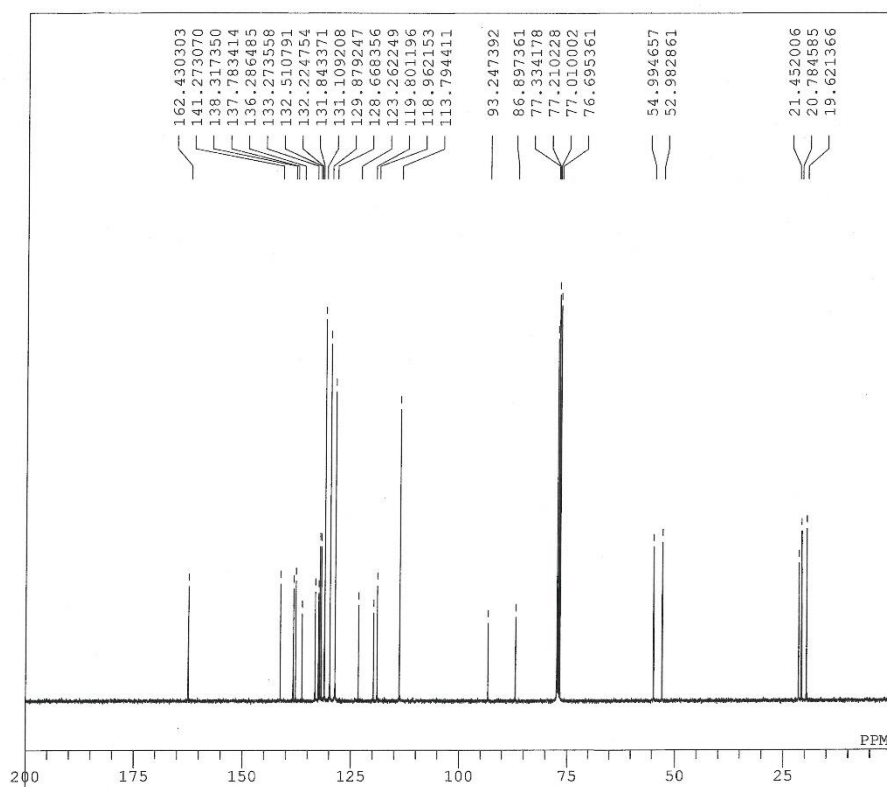
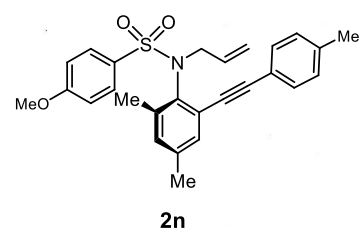
DFILE SF138 20211121-1.jdf
 COMNT Qn-BOC 1H
 DATIM 2021-11-21 17:14:58
 OBNUC 1H
 EXMOD single pulse.ex2
 OBFRQ 399.78 MHz
 OBSET 4.62 KHz
 OBFIN 5.98 Hz
 POINT 16384
 FREQU 7773.63 Hz
 SCANS 32
 ACQTM 2.1076 sec
 PD 5.0000 sec
 PW1 5.80 usec
 IRNUC 1H
 CTEMP 18.5 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.12 Hz
 RGAIN 26



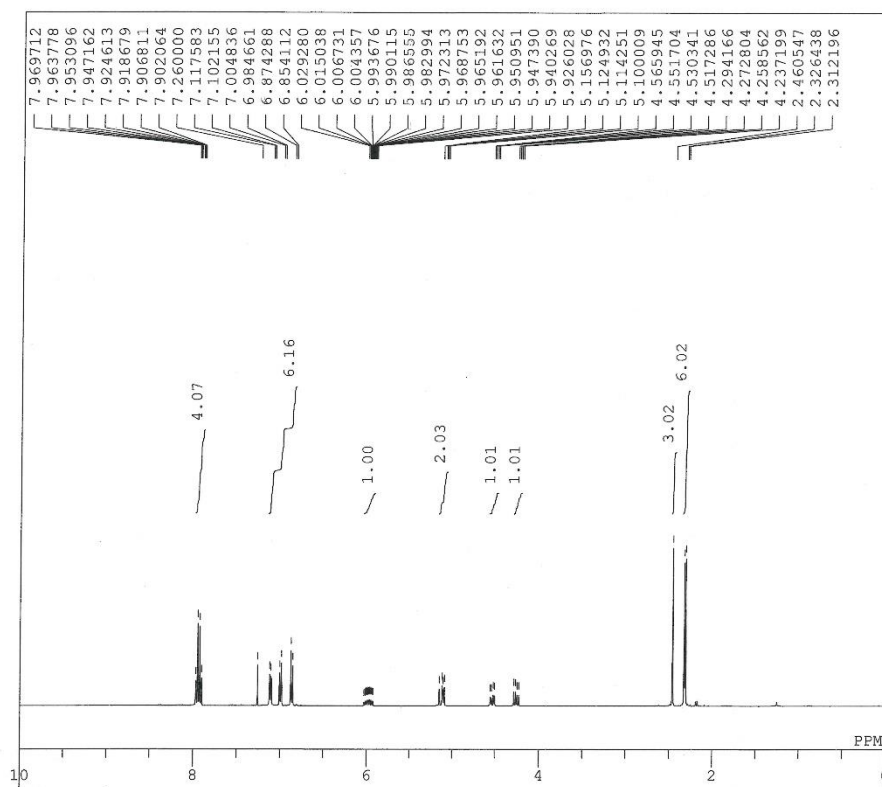
DFILE SF138-13C 20211121-1.jdf
 COMNT
 DATIM 2021-11-21 17:01:13
 OBNUC 13C
 EXMOD single pulse_dec
 OBFRQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 32768
 FREQU 31407.03 Hz
 SCANS 1024
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PW1 3.23 usec
 IRNUC 1H
 CTEMP 19.0 c
 SLVNT CDCL3
 EXREF 77.01 ppm
 BF 1.20 Hz
 RGAIN 60



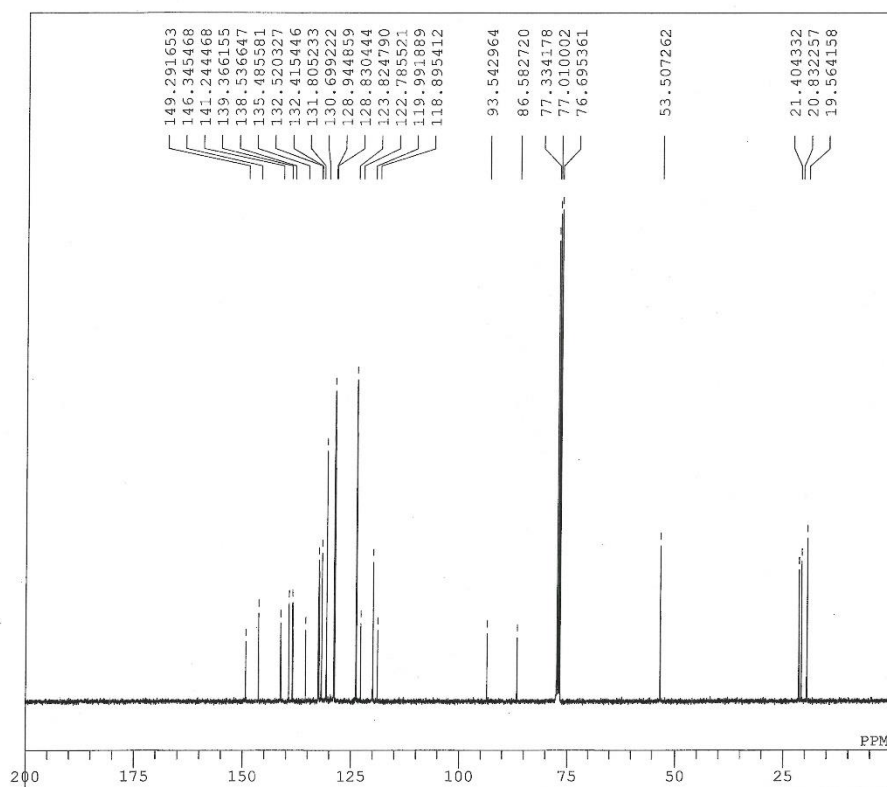
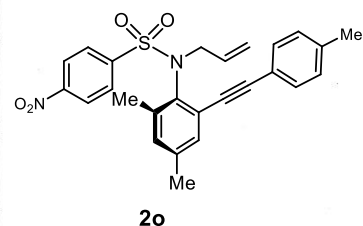
DFILE TF008 20211203 sin-1.als
 COMNT Qn-BOC 1H
 DATIM 2021-12-03 15:28:44
 OBNUC 1H
 EXMOD single_pulse.ex2
 OBFRQ 399.78 MHz
 OBSET 4.62 KHz
 OBFIN 5.98 Hz
 POINT 13107
 FREQU 6218.81 Hz
 SCANS 32
 ACQTM 2.1076 sec
 PD 5.0000 sec
 PW1 5.80 usec
 IRNUC 1H
 CTEMP 18.6 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.12 Hz
 RGAIN 30



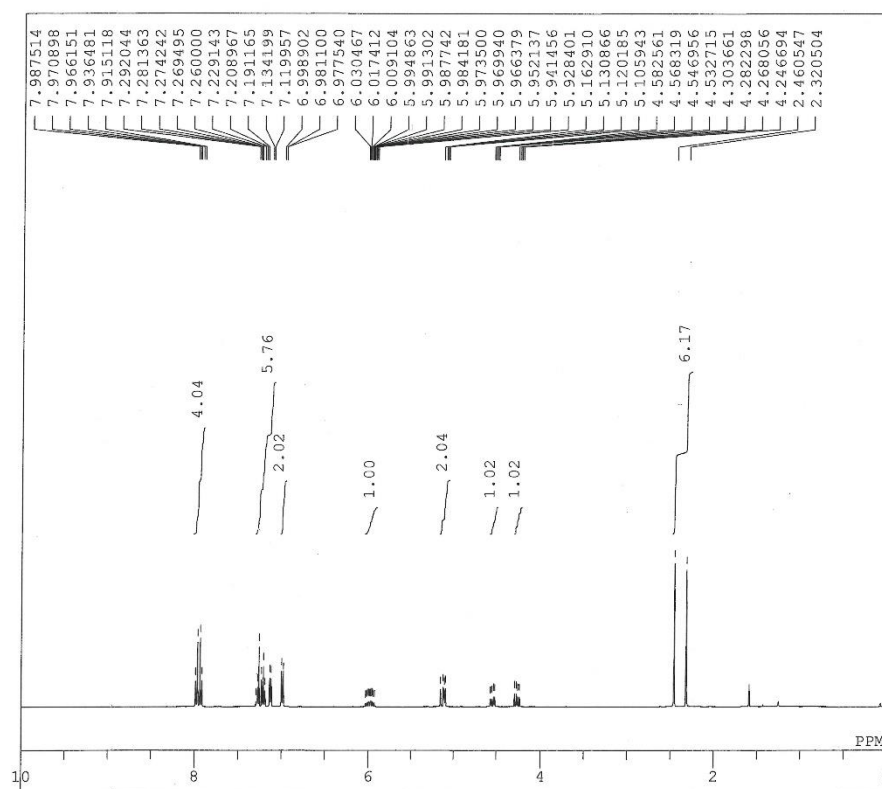
DFILE TF008 13C 20211204-1.als
 COMNT 2021-12-04 10:39:27
 OBNUC 13C
 EXMOD single_pulse_dec
 OBFRQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 32768
 FREQU 31407.03 Hz
 SCANS 1024
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PW1 3.23 usec
 IRNUC 1H
 CTEMP 18.4 c
 SLVNT CDCL3
 EXREF 77.01 ppm
 BF 1.20 Hz
 RGAIN 60



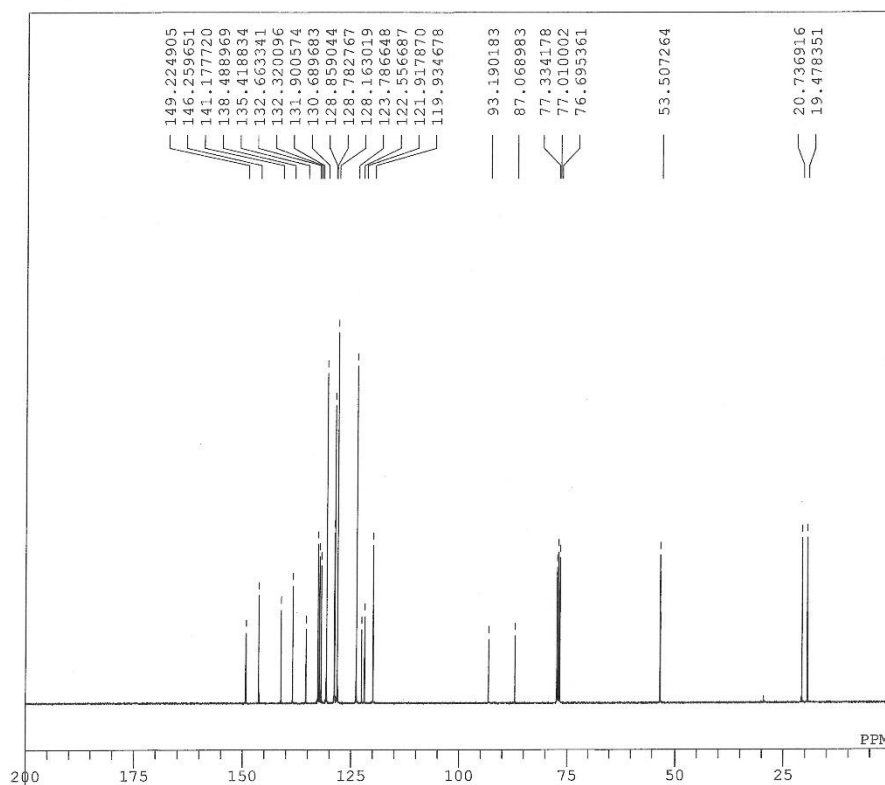
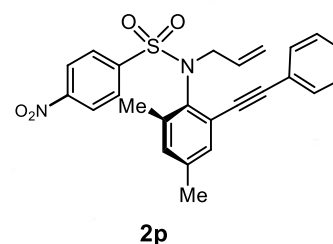
DFILE TT011 20211204-1.als
 COMNT Qn-BOC 1H
 DATIM 2021-12-04 10:51:14
 OBNUC 1H
 EXMOD single pulse.ex2
 OBFRQ 399.78 MHz
 OBSET 4.62 KHz
 OBFIN 5.98 Hz
 POINT 13107
 FREQU 6218.81 Hz
 SCANS 32
 ACQTM 2.1076 sec
 PD 5.0000 sec
 PW1 5.80 usec
 IRNUC 1H
 CTEMP 18.0 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.12 Hz
 RGAIN 30



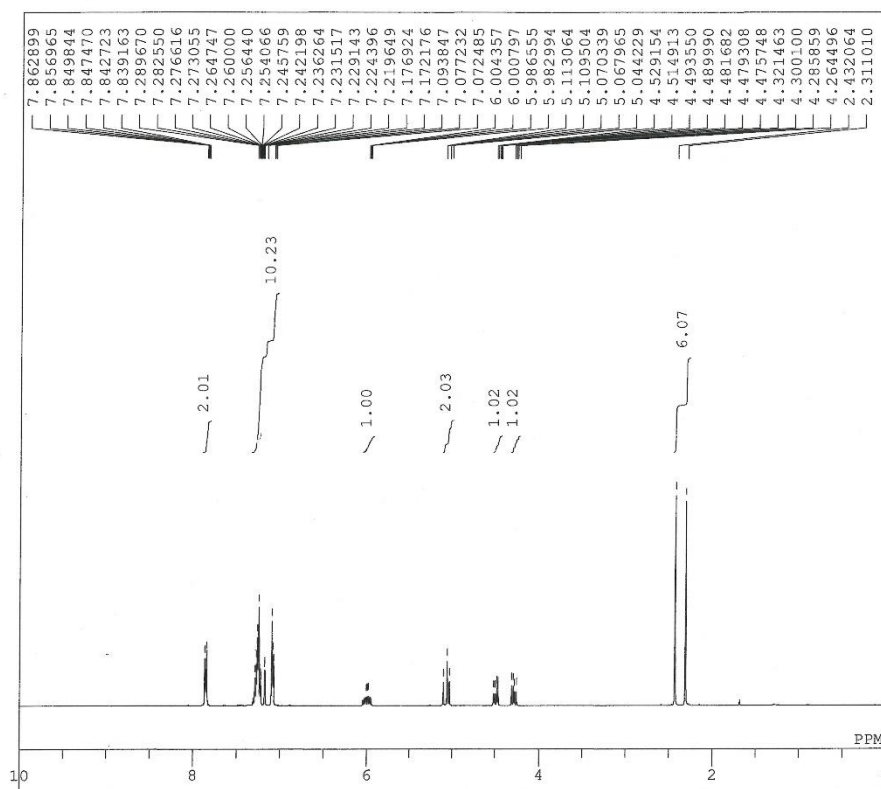
DFILE TT011 13C 20211203-1.als
 COMNT
 DATIM 2021-12-03 09:32:53
 OBNUC 13C
 EXMOD single pulse_dec
 OBFRQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 26214
 FREQU 25125.24 Hz
 SCANS 1024
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PW1 3.23 usec
 IRNUC 1H
 CTEMP 17.6 c
 SLVNT CDCL3
 EXREF 77.01 ppm
 BF 1.20 Hz
 RGAIN 60



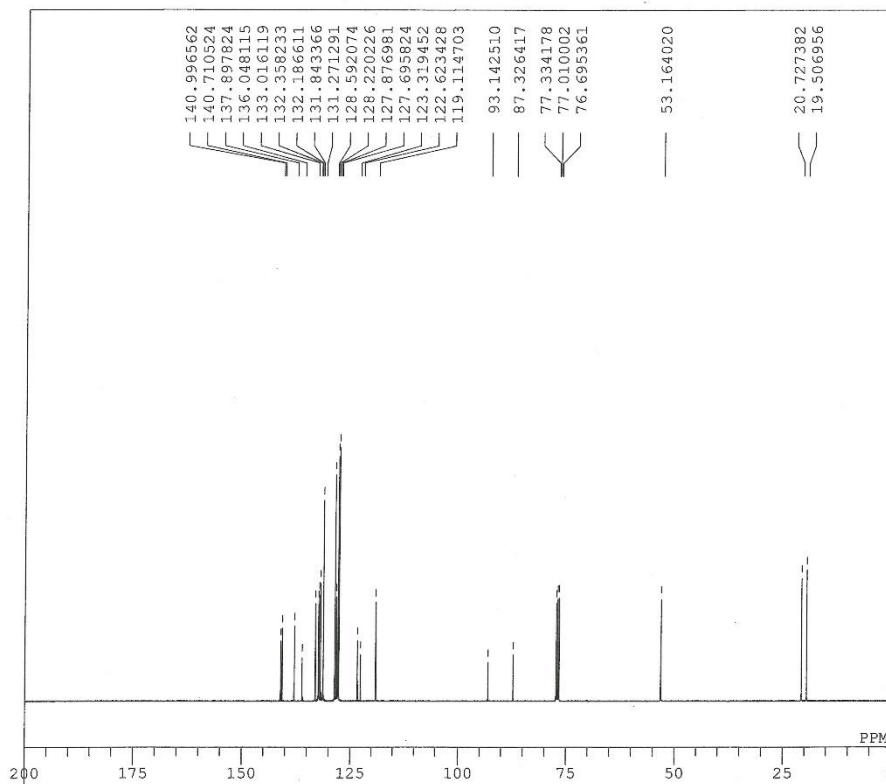
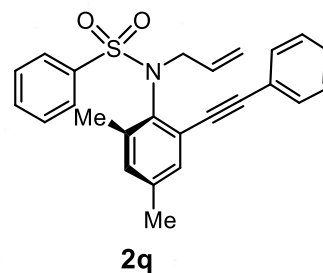
DFILE RK020 20211129-1.als
 COMNT Qn-BOC 1H
 DATIM 2021-11-29 12:21:25
 OBNUC 1H
 EXMOD single_pulse.ex2
 OBFRQ 399.78 MHz
 OBSET 4.62 KHz
 OBFIN 5.98 Hz
 POINT 13107
 FREQU 6218.81 Hz
 SCANS 32
 ACQTM 2.1076 sec
 PD 5.0000 sec
 PW1 5.80 usec
 IRNUC 1H
 CTEMP 17.9 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.12 Hz
 RGAIN 30



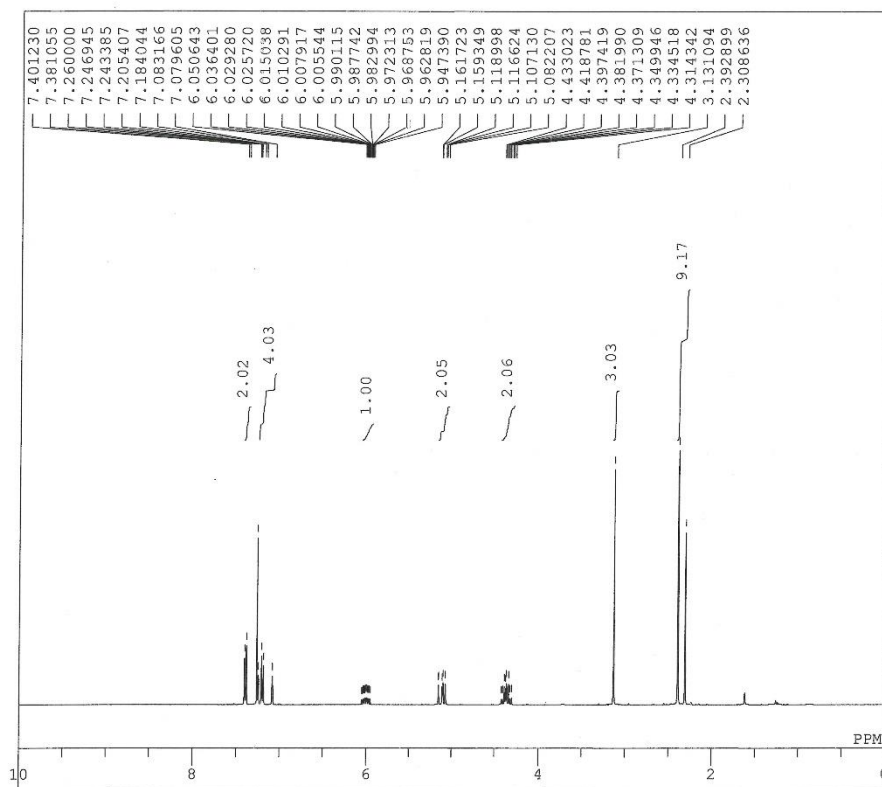
DFILE SF094 13C 20211202-1.als
 COMNT
 DATIM 2021-12-02 09:37:24
 OBNUC 13C
 EXMOD single_pulse_dec
 OBFRQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 26214
 FREQU 25125.24 Hz
 SCANS 1024
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PW1 3.23 usec
 IRNUC 1H
 CTEMP 17.9 c
 SLVNT CDCL3
 EXREF 77.01 ppm
 BF 1.20 Hz
 RGAIN 60



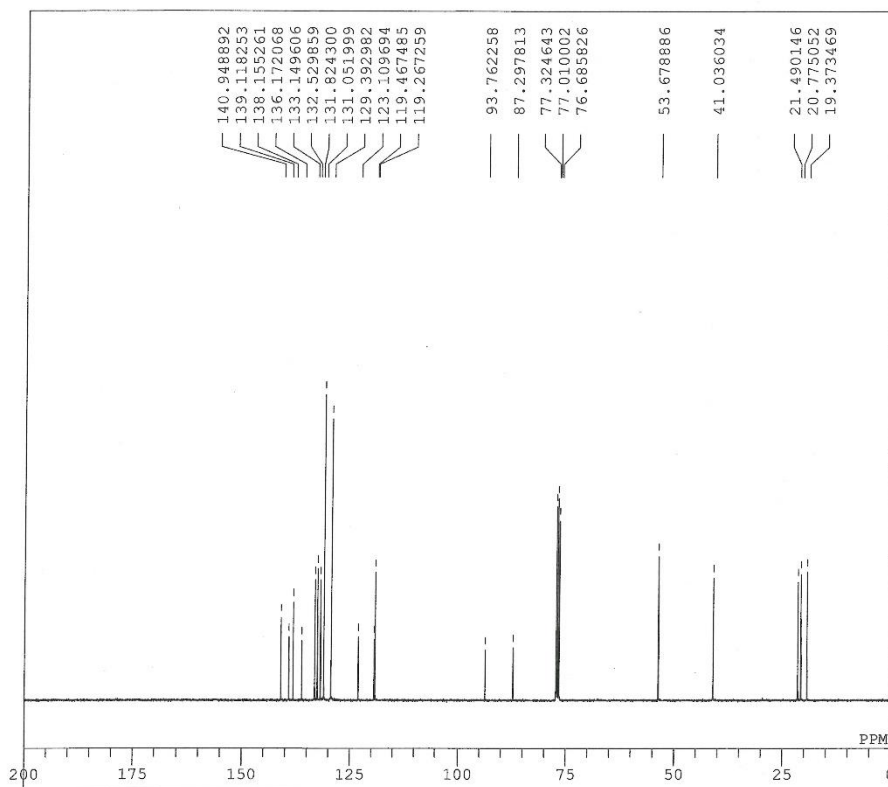
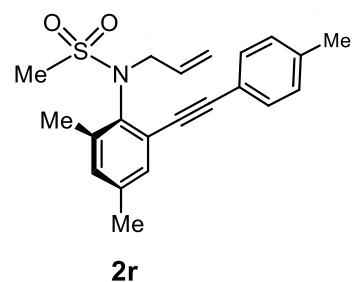
DFILE SF122 20210927-1.als
 COMNT Qn-BOC 1H
 DATIM 2021-09-27 11:33:23
 OBNUC 1H
 EXMOD single pulse.ex2
 OBFRQ 399.78 MHz
 OBSET 4.62 KHz
 OBFIN 5.98 Hz
 POINT 13107
 FREQU 6218.81 Hz
 SCANS 32
 ACQTM 2.1076 sec
 PD 5.0000 sec
 PW1 5.17 usec
 IRNUC 1H
 CTEMP 18.9 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.12 Hz
 RGAIN 22



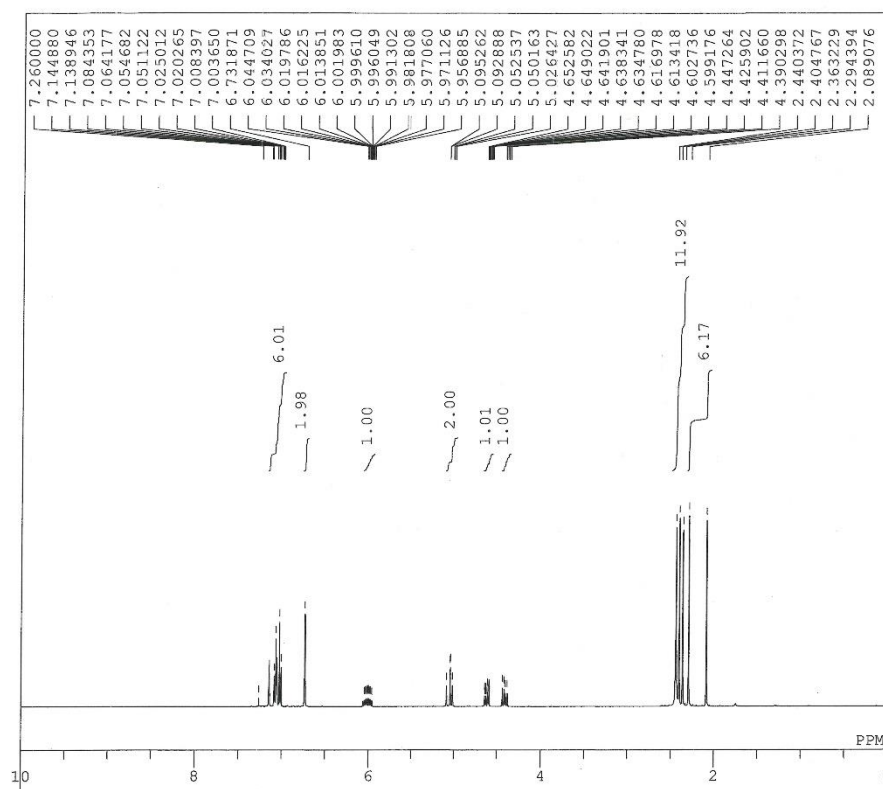
DFILE SF122-13C 20210928-1.als
 COMNT 2021-09-28 09:45:01
 OBNUC 13C
 EXMOD single pulse_dec
 OBFRQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 26214
 FREQU 25125.24 Hz
 SCANS 1024
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PW1 3.03 usec
 IRNUC 1H
 CTEMP 19.2 c
 SLVNT CDCL3
 EXREF 77.01 ppm
 BF 1.20 Hz
 RGAIN 60



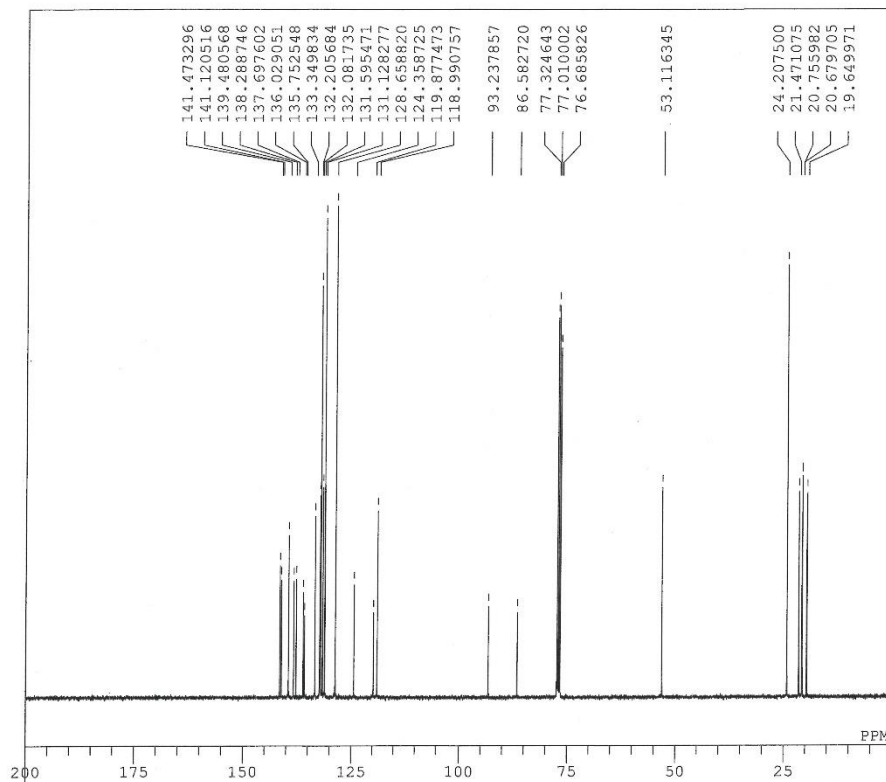
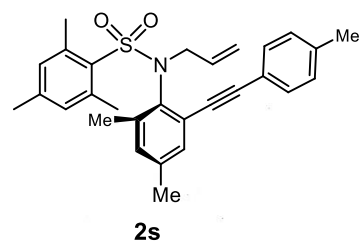
DFILE SF094 20211129-1.als
 COMNT Qn-BOC 1H
 DATIM 2021-11-29 12:09:12
 OBNUC 1H
 EXMOD single pulse.ex2
 OBFRQ 399.78 MHz
 OBSET 4.62 KHz
 OBFIN 5.98 Hz
 POINT 13107
 FREQU 6218.81 Hz
 SCANS 32
 ACQTM 2.1076 sec
 PD 5.0000 sec
 PW1 5.80 usec
 IRNUC 1H
 CTEMP 17.6 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.12 Hz
 RGAIN 30



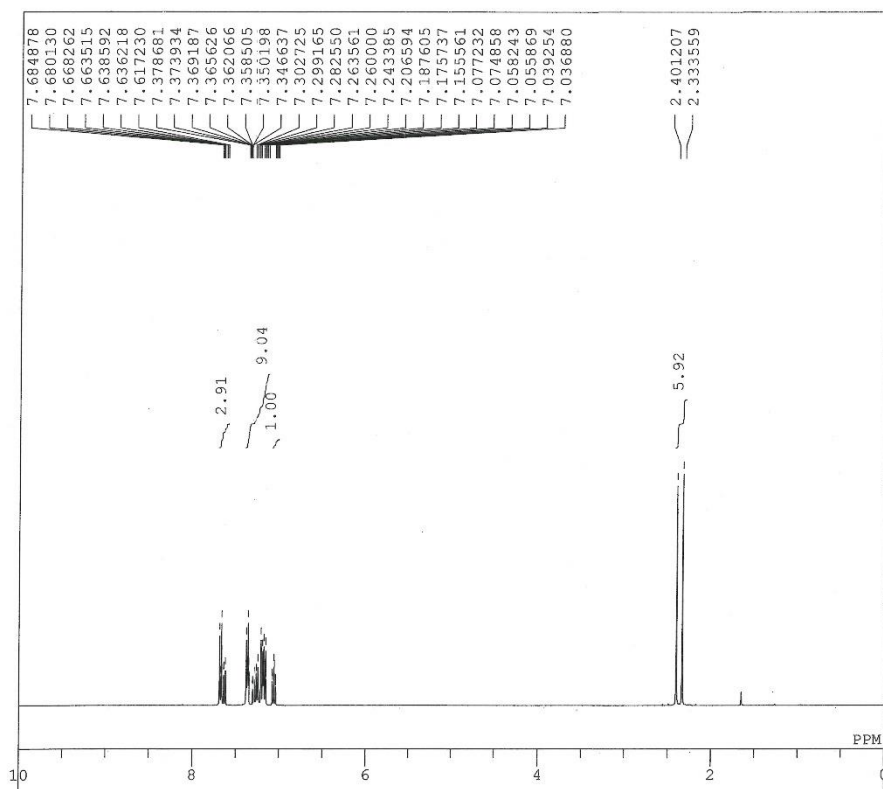
DFILE RK020 13C 20211201-1.als
 COMNT 2021-12-01 19:42:38
 OBNUC 13C
 EXMOD single pulse_dec
 OBFRQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 26214
 FREQU 25125.24 Hz
 SCANS 1024
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PW1 3.23 usec
 IRNUC 1H
 CTEMP 18.8 c
 SLVNT CDCL3
 EXREF 77.01 ppm
 BF 1.20 Hz
 RGAIN 60



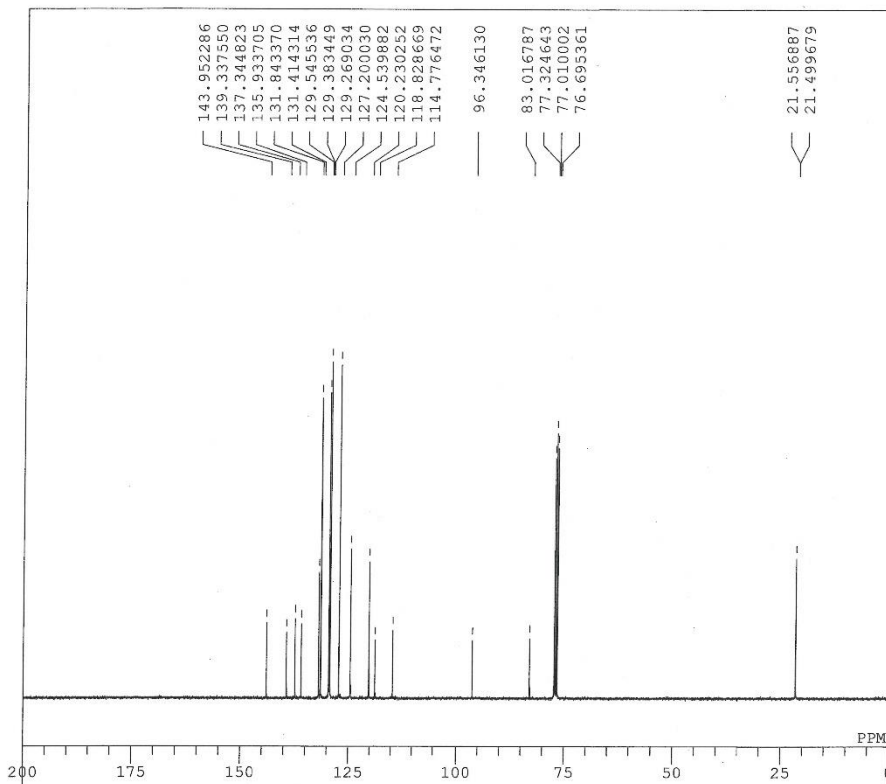
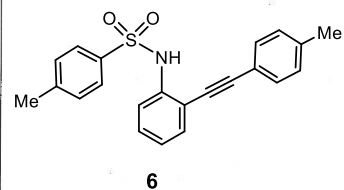
DFILE TT020 20210922-1.als
 COMNT Qn-BOC 1H
 DATIM 2021-09-22 17:22:21
 OBNUC 1H
 EXMOD single pulse.ex2
 OBFRQ 399.78 MHz
 OBSET 4.62 KHz
 OBFIN 5.98 Hz
 POINT 13107
 FREQU 6218.81 Hz
 SCANS 32
 ACQTM 2.1076 sec
 PD 5.0000 sec
 PW1 5.17 usec
 IRNUC 1H
 CTEMP 20.4 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.12 Hz
 RGAIN 30



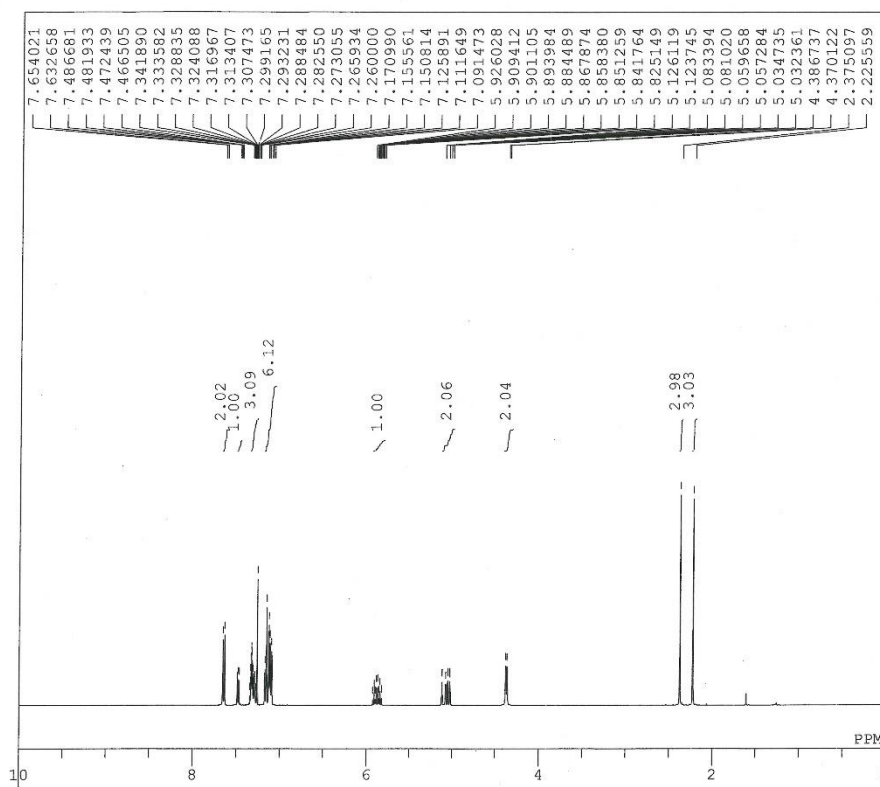
DFILE TT020 13C 20211217-1.als
 COMNT 2021-12-17 09:43:06
 OBNUC 13C
 EXMOD single pulse_dec
 OBFRQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 32768
 FREQU 31407.03 Hz
 SCANS 1024
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PW1 3.23 usec
 IRNUC 1H
 CTEMP 18.0 c
 SLVNT CDCL3
 EXREF 77.01 ppm
 BF 1.20 Hz
 RGAIN 60



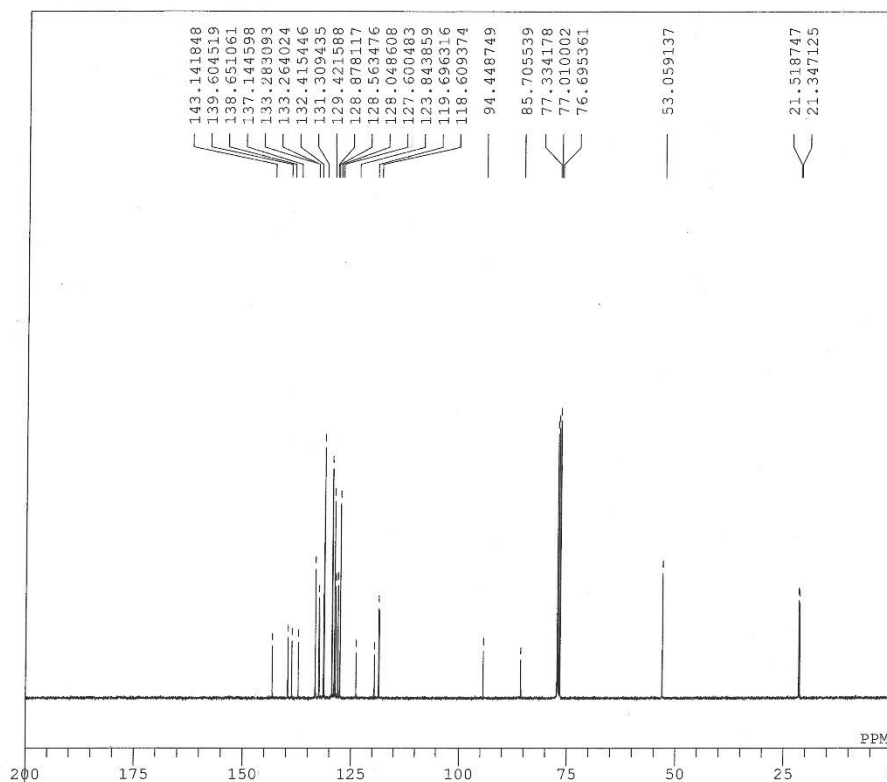
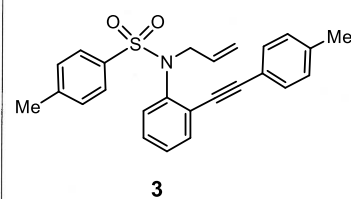
DFILE Y0024-2 20211209-1.als
COMNT Qn-BOC 1H
DATIM 2021-12-09 15:50:05
OBNUC 1H
EXMOD single_pulse.ex2
OBFRQ 399.78 MHz
OBSET 4.62 KHz
OBFIN 5.98 Hz
POINT 16384
FREQU 7773.63 Hz
SCANS 32
ACQTM 2.1076 sec
PD 5.0000 sec
PW1 5.80 usec
IRNUC 1H
CTEMP 18.8 c
SLVNT CDCL3
EXREF 7.26 ppm
BF 0.12 Hz
RGAIN 30



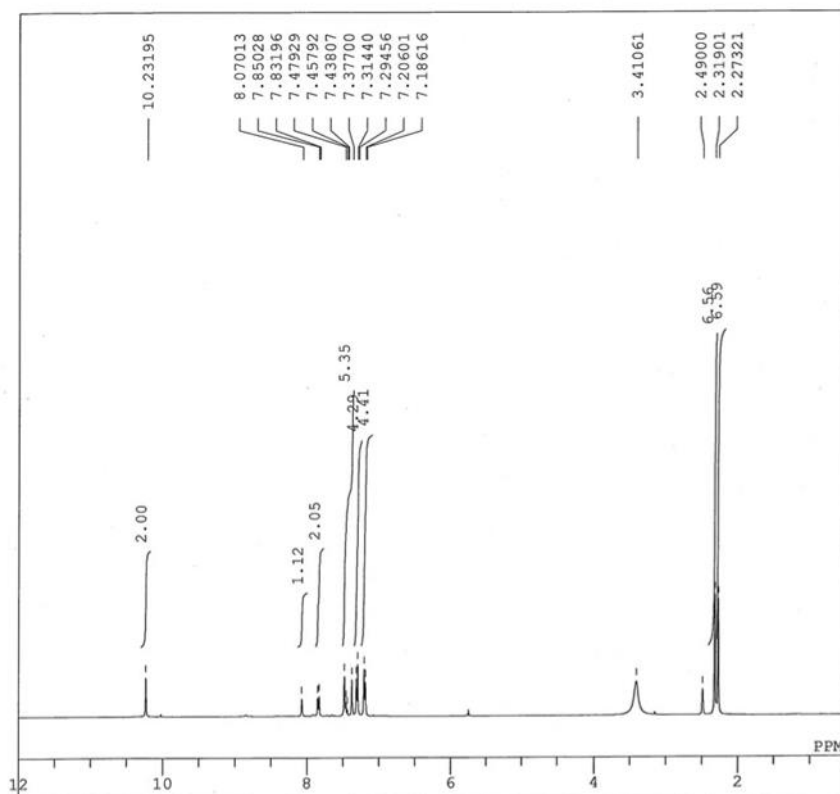
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COMNT
DATIM 2021-12-09 18:15:52
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 32768
FREQU 31407.03 Hz
SCANS 1024
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.23 usec
IRNUC 1H
CTEMP 18.7 c
SLVNT CDCL3
EXREF 77.01 ppm
BF 1.20 Hz
RGAIN 60



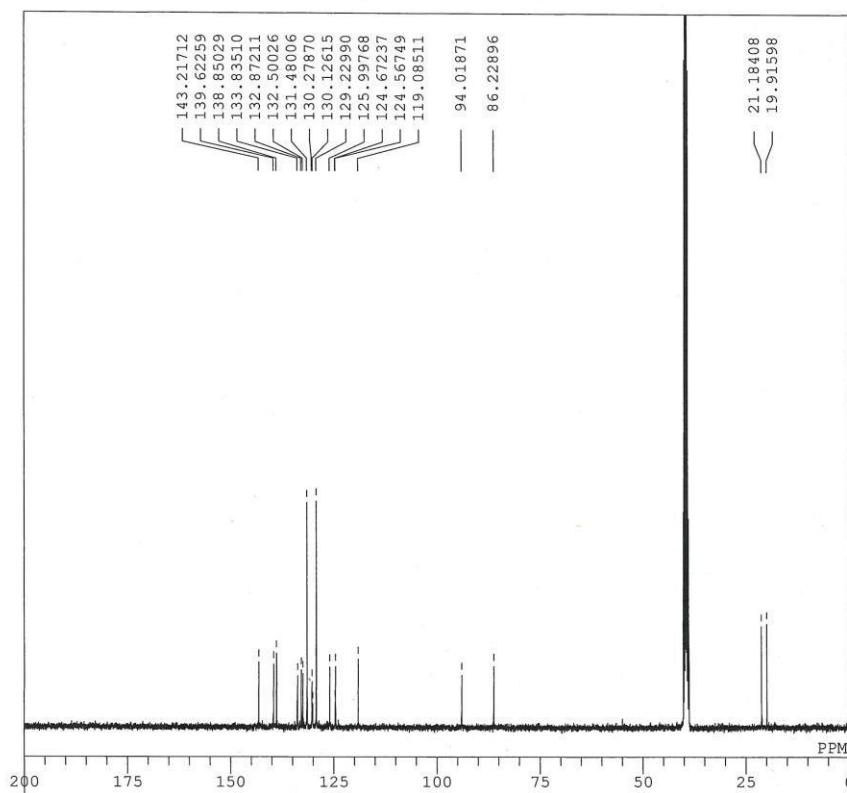
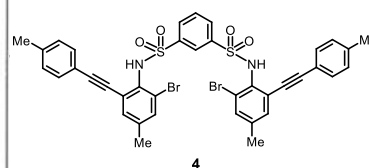
DFILE Y0027 acetone removal 20
 COMNT Qn-BOC 1H
 DATIM 2021-12-15 14:44:50
 OBNUC 1H
 EXMOD single pulse.ex2
 OBFRQ 399.78 MHz
 OBSET 4.62 KHz
 OBFIN 5.98 Hz
 POINT 16384
 FREQU 7773.63 Hz
 SCANS 32
 ACQTM 2.1076 sec
 PD 5.0000 sec
 PW1 5.80 usec
 IRNUC 1H
 CTEMP 17.6 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.12 Hz
 RGAIN 30



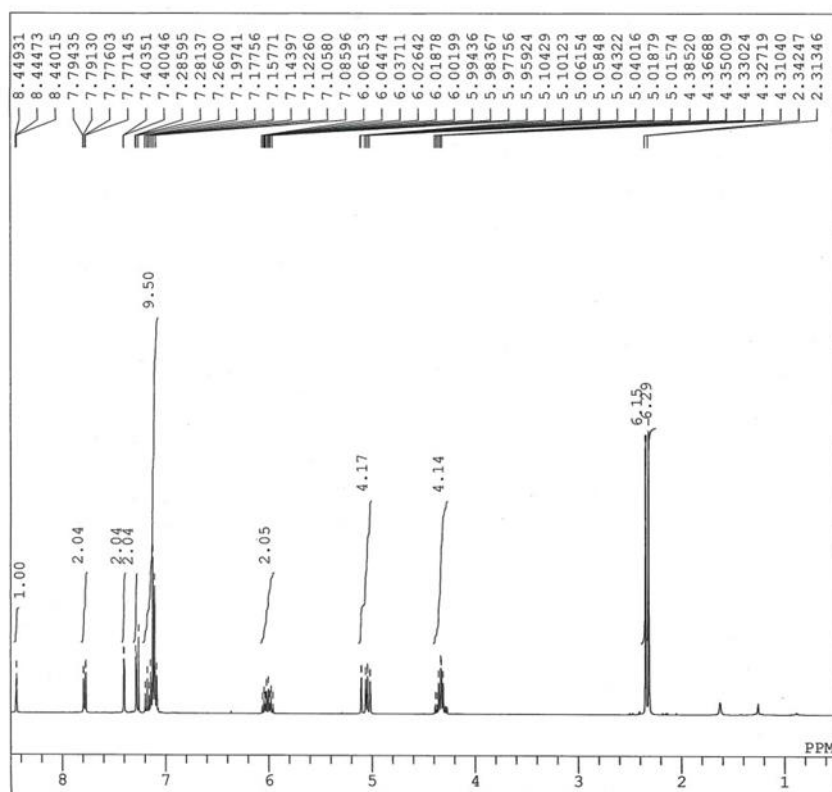
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 COMNT 2021-12-15 17:57:60
 OBNUC 13C
 EXMOD single pulse_dec
 OBFRQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 32768
 FREQU 31407.03 Hz
 SCANS 1024
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PW1 3.23 usec
 IRNUC 1H
 CTEMP 18.9 c
 SLVNT CDCL3
 EXREF 77.01 ppm
 BF 1.20 Hz
 RGAIN 60



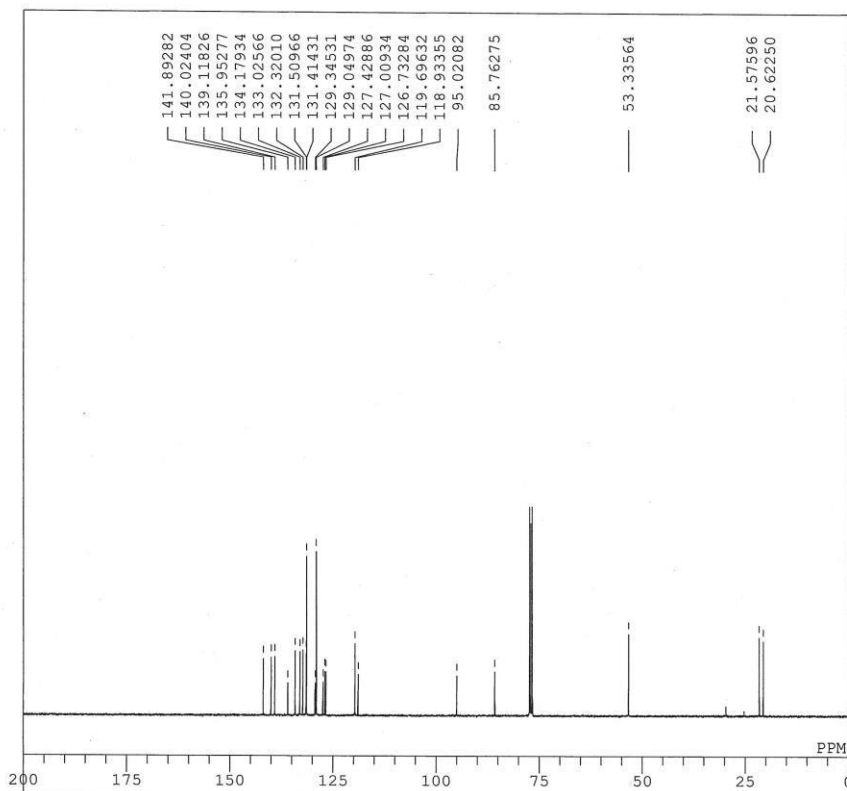
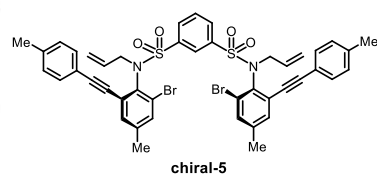
DFILE Y0013 20201215 DMSO 2-1.a)
 COMNT Qn-BOC 1H
 DATIM 2020-12-15 10:49:15
 OBNUC 1H
 EXMOD single pulse.ex2
 OBFRQ 399.78 MHz
 OBSET 5.19 KHz
 OBFIN 6.74 Hz
 POINT 13107
 FREQU 7999.88 Hz
 SCANS 32
 ACQTM 1.6384 sec
 PD 5.0000 sec
 PW1 5.17 usec
 IRNUC 1H
 CTEMP 17.1 c
 SLVNT DMSO
 EXREF 2.49 ppm
 BF 0.12 Hz
 RGAIN 36



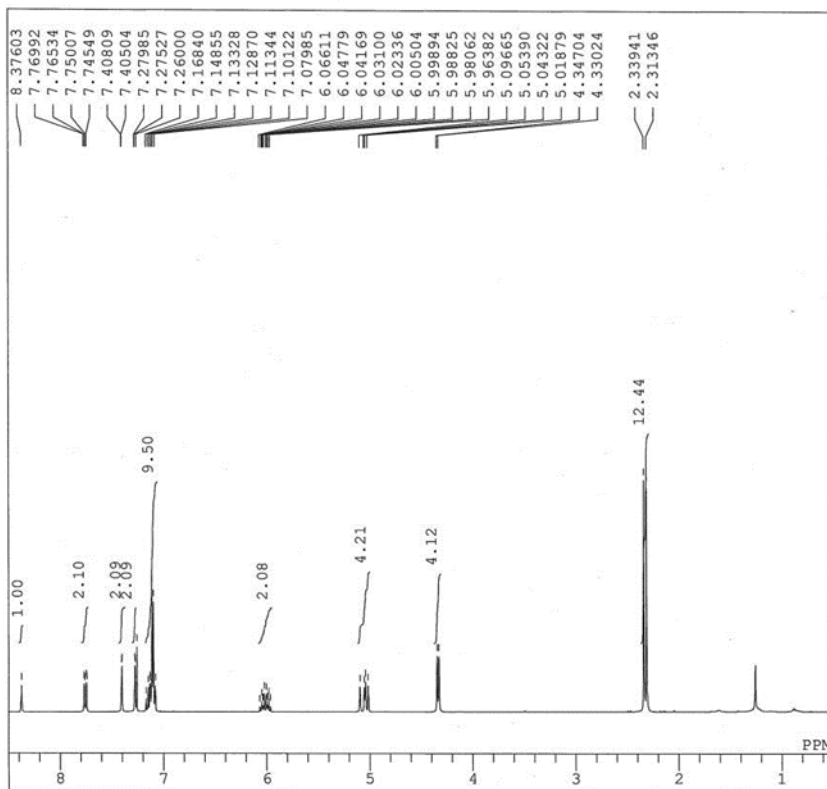
DFILE Y0013 20201216 DMSO 13C-1.
 COMNT
 DATIM 2020-12-16 12:58:59
 OBNUC 13C
 EXMOD single pulse_dec
 OBFRQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 26214
 FREQU 25125.24 Hz
 SCANS 1024
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PW1 2.87 usec
 IRNUC 1H
 CTEMP 16.4 c
 SLVNT DMSO
 EXREF 39.50 ppm
 BF 1.20 Hz
 RGAIN 60



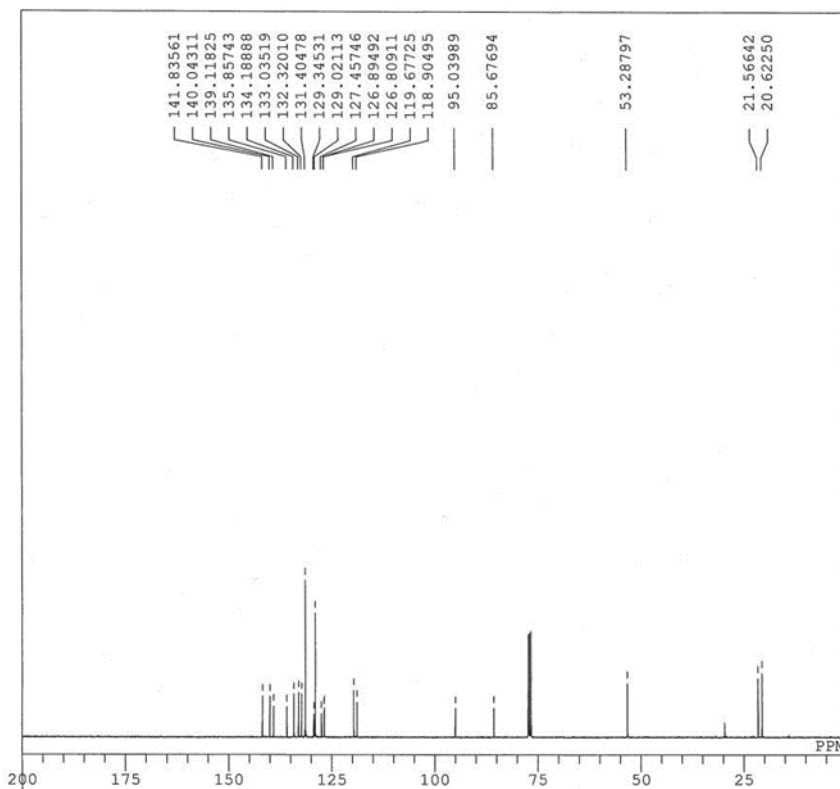
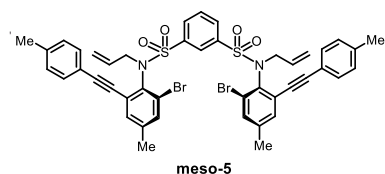
DFILE CN125 jyunnchiral 20201124
 COMNT Qn-BOC 1H
 DATIM 2020-11-24 13:26:23
 OBNUC 1H
 EXMOD single_pulse.ex2
 OBFRQ 399.78 MHz
 OBSET 5.19 KHz
 OBFIN 6.74 Hz
 POINT 13107
 FREQU 7999.88 Hz
 SCANS 32
 ACQTM 1.6384 sec
 PD 5.0000 sec
 PW1 5.17 usec
 IRNUC 1H
 CTEMP 16.1 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.12 Hz
 RGAIN 30



DFILE CN122 mplc 1st rac 13c 20
 COMNT
 DATIM 2020-09-29 13:42:03
 OBNUC 13C
 EXMOD single_pulse_dec
 OBFRQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 26214
 FREQU 25125.24 Hz
 SCANS 1024
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PW1 2.87 usec
 IRNUC 1H
 CTEMP 15.9 c
 SLVNT CDCL3
 EXREF 77.01 ppm
 BF 1.20 Hz
 RGAIN 60

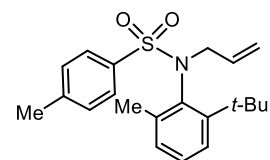
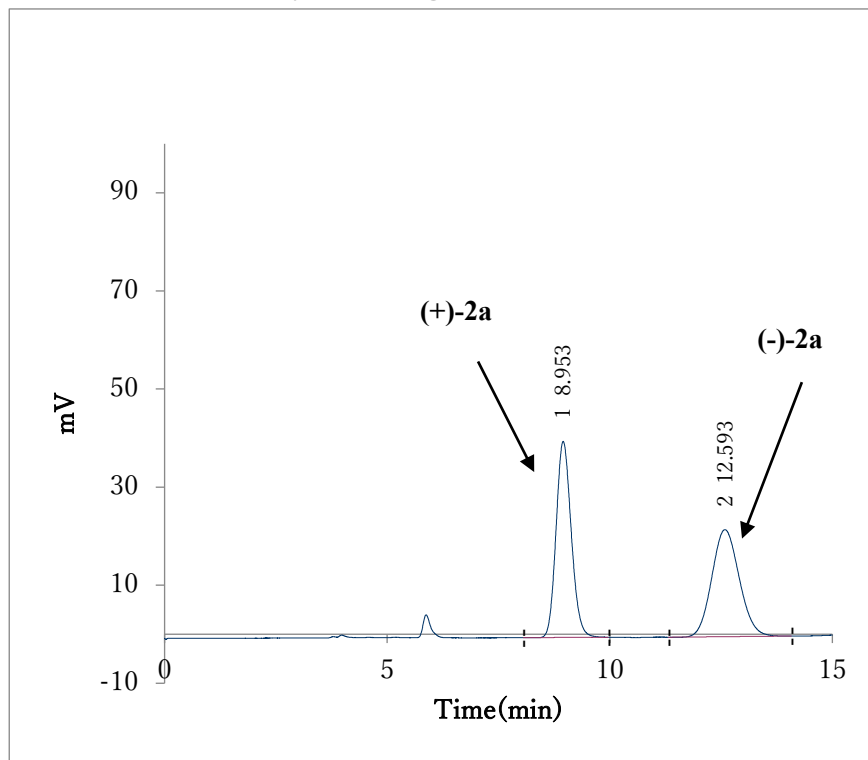


DFILE CN122 2nd 20201222-1.jdf
 COMNT Qn-BOC 1H
 DATIM 2020-12-22 13:48:33
 OBNUC 1H
 EXMOD single_pulse.ex2
 OBFRQ 399.78 MHz
 OBSET 5.19 KHz
 OBFIN 6.74 Hz
 POINT 16384
 FREQU 10000.00 Hz
 SCANS 32
 ACQTM 1.6384 sec
 PD 5.0000 sec
 PW1 5.17 usec
 IRNUC 1H
 CTEMP 15.8 c
 SLVNT CDCL3
 EXREF 7.26 ppm
 BF 0.12 Hz
 RGAIN 30



DFILE CN122 2nd 13c 20201222-1.a
 COMNT
 DATIM 2020-12-22 14:48:04
 OBNUC 13C
 EXMOD single_pulse_dec
 OBFRQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 26214
 FREQU 25125.24 Hz
 SCANS 1024
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PW1 2.87 usec
 IRNUC 1H
 CTEMP 16.8 c
 SLVNT CDCL3
 EXREF 77.01 ppm
 BF 1.20 Hz
 RGAIN 60

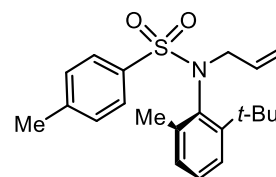
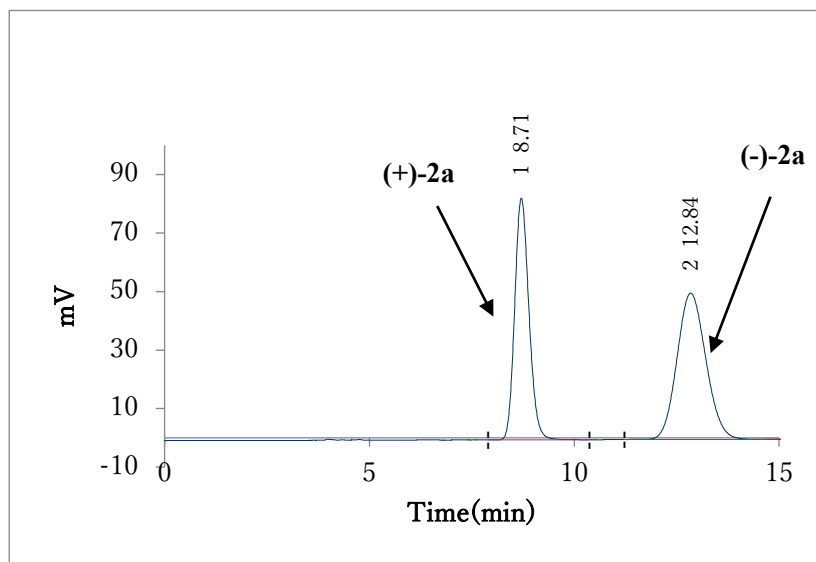
HPLC analysis using a chiral column for the determination of the ee



rac-2a

AS-H
eluent : 15% IPA in hexane
flow rate : 0.800 ml/min

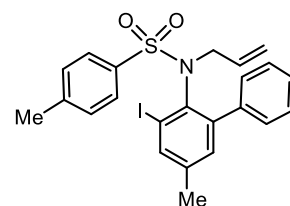
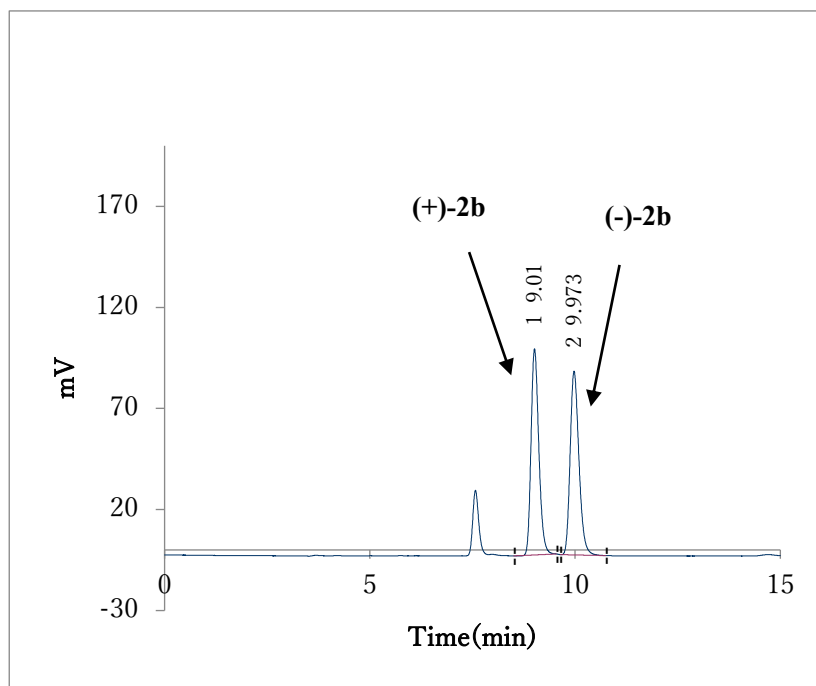
No.	Rt	Area	Area(%)	Height
1	8.953	946346.6	50.3	39991
2	12.593	934059.8	49.7	21825
		1880406	100	61816



2a

AS-H
eluent : 15% IPA in hexane
flow rate : 0.800 ml/min

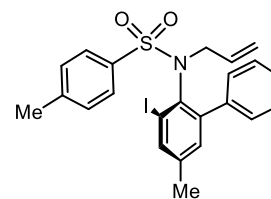
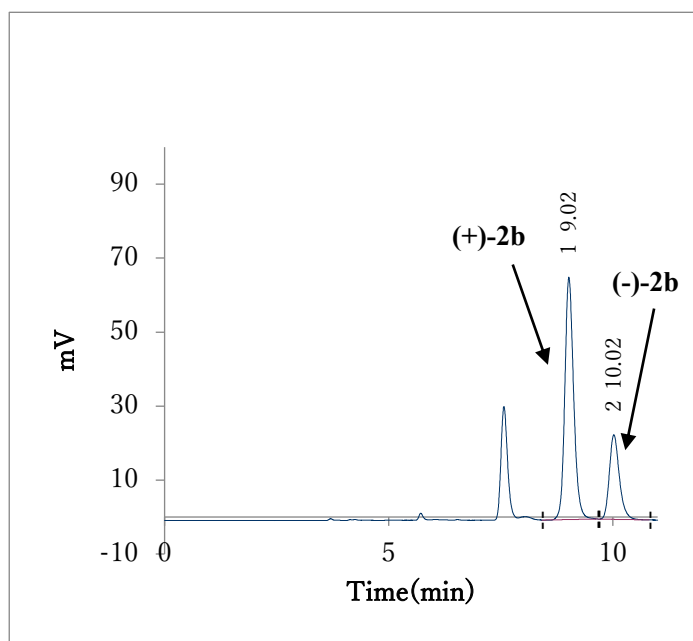
No.	Rt	Area	Area(%)	Height
1	8.71	1998473	45	82653
2	12.84	2447382	55	50024
		4445855	100	132677



rac-2b

OD-3
eluent : 15% IPA in hexane
flow rate : 0.800 ml/min

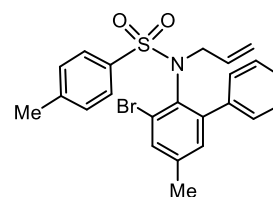
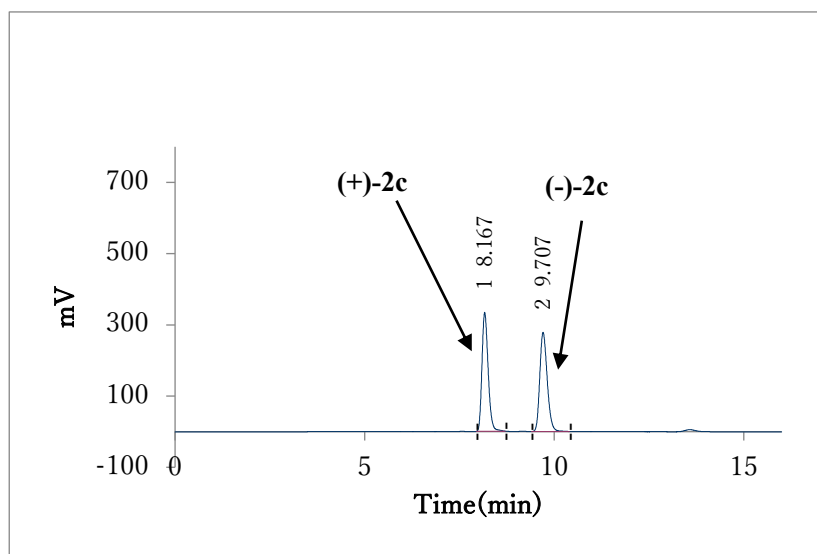
No.	Rt	Area	Area(%)	Height
1	9.01	1335462	49.8	102013
2	9.973	1348567	50.2	90983
		2684030	100	192996



2b

OD-3
eluent : 15% IPA in hexane
flow rate : 0.800 ml/min

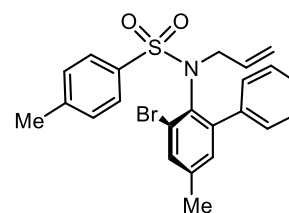
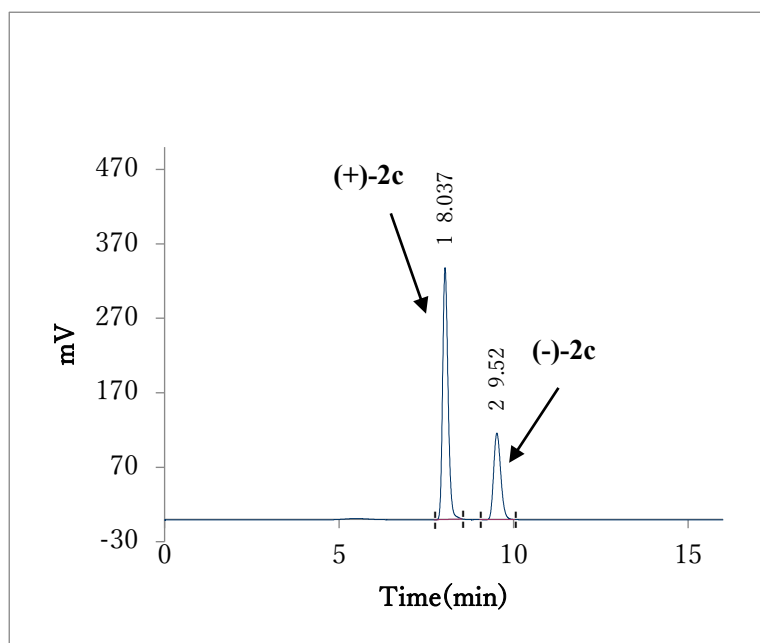
No.	Rt	Area	Area(%)	Height
1	9.02	897741.6	71.7	65538
2	10.02	353680.6	28.3	22887
		1251422	100	88425



rac-2c

OD-3
eluent : 15% IPA in hexane
flow rate : 0.800 ml/min

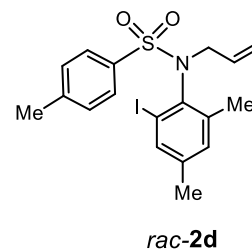
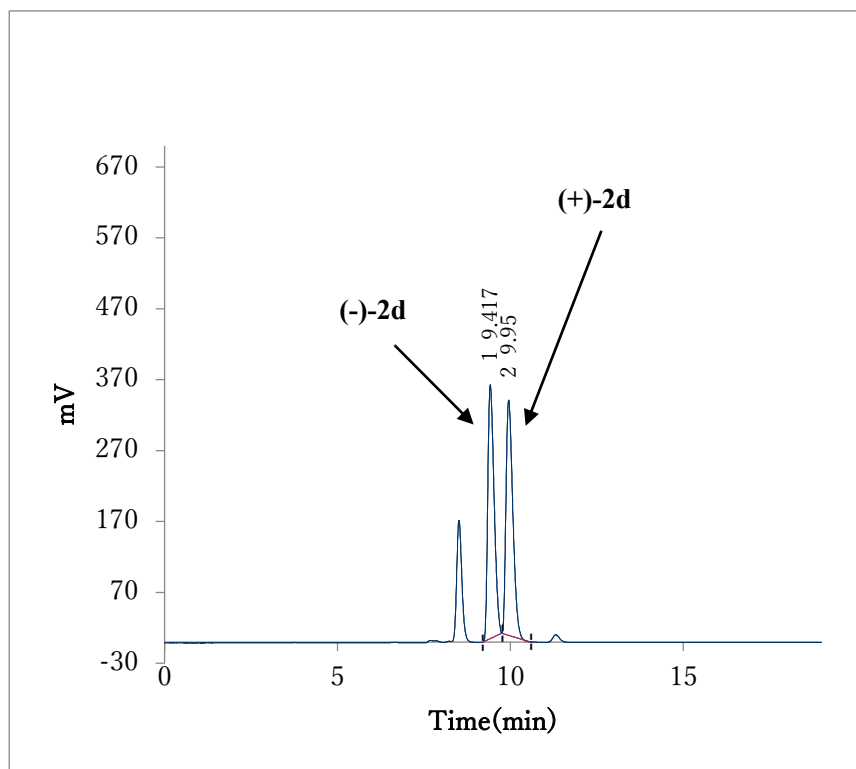
No.	Rt	Area	Area(%)	Height
1	8.167	3774489	49.9	334226
2	9.707	3784213	50.1	278629
		7558702	100	



2c

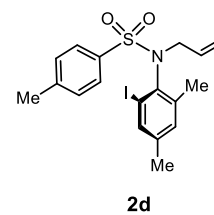
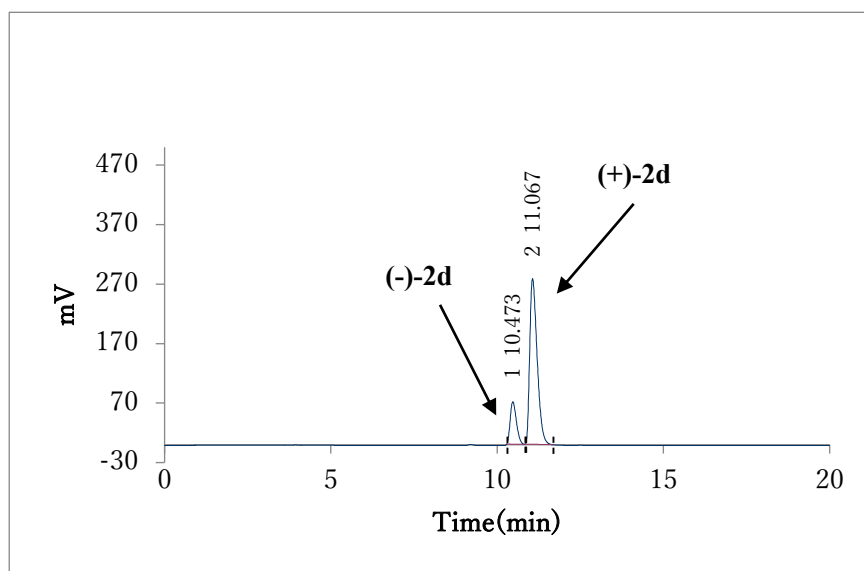
OD-3
eluent : 15% IPA in hexane
flow rate : 0.800 ml/min

No.	Rt	Area	Area(%)	Height
1	8.037	3637341	69	337996
2	9.52	1631538	31	116315
		5268879	100	454311



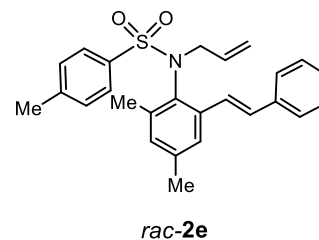
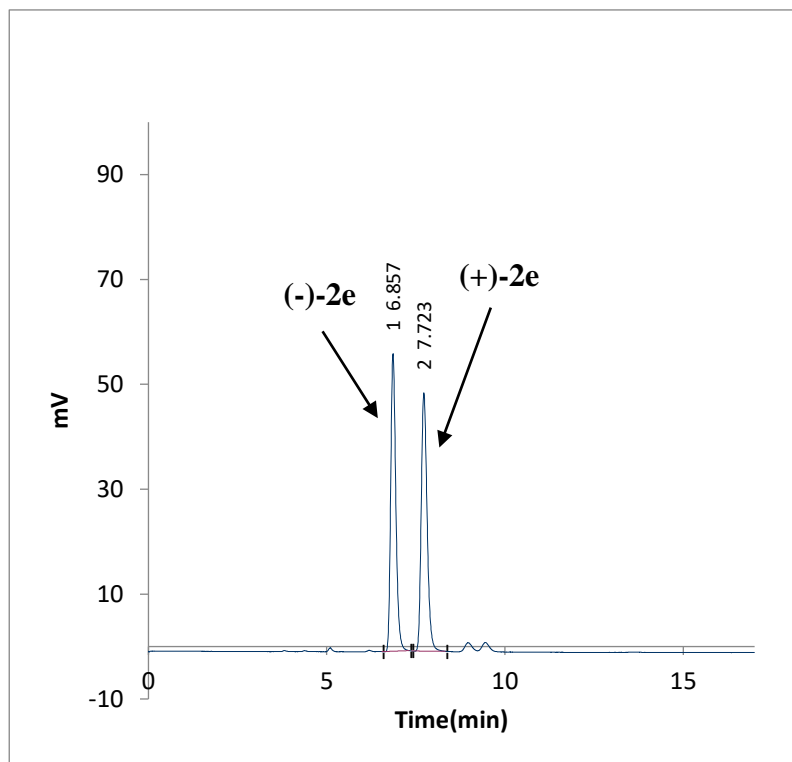
OD-3
eluent : 3% IPA in hexane
flow rate : 0.800 ml/min

No.	Rt	Area	Area(%)	Height
1	9.417	4555926	50.1	358224
2	9.95	4543942	49.9	332272
		9099868	100	690496



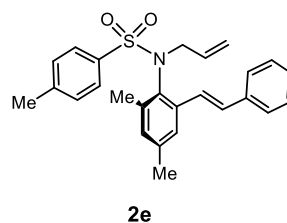
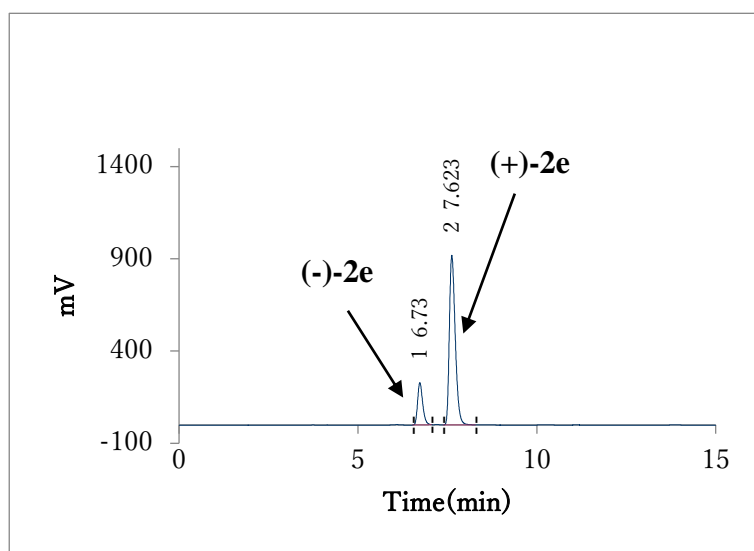
OD-3
eluent : 3% IPA in hexane
flow rate : 0.800 ml/min

No.	Rt	Area	Area(%)	Height
1	10.473	917391.8	17.6	71148
2	11.067	4289202	82.4	278279
		5206593	100	349427



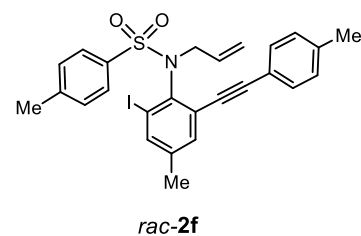
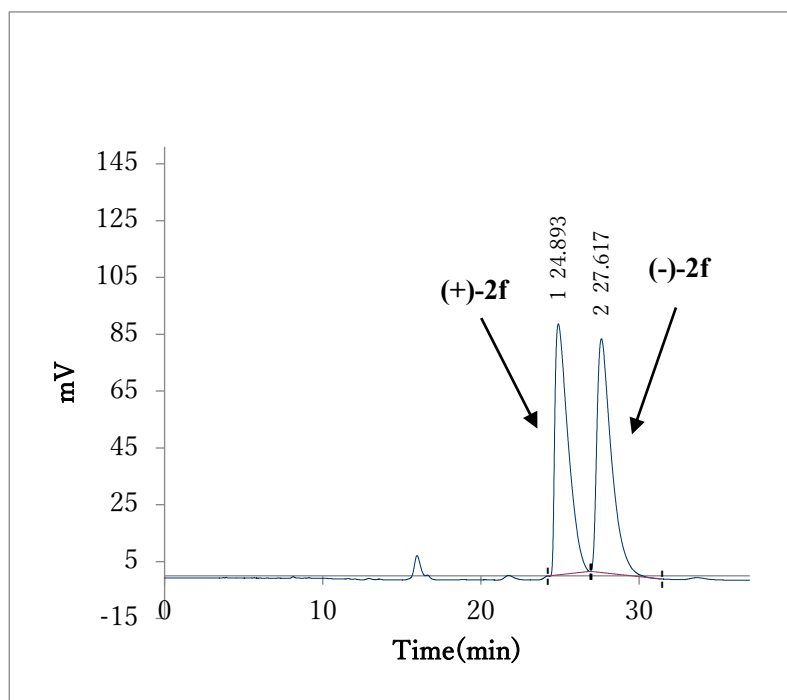
OD-3
eluent : 15% IPA in hexane
flow rate : 0.800 ml/min

No.	Rt	Area	Area(%)	Height
1	6.857	566012	50.2	56774
2	7.723	562544.7	49.8	49290
		1128557	100	106064

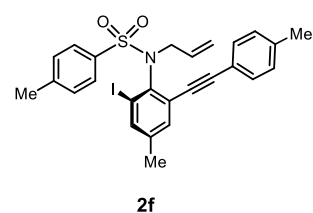
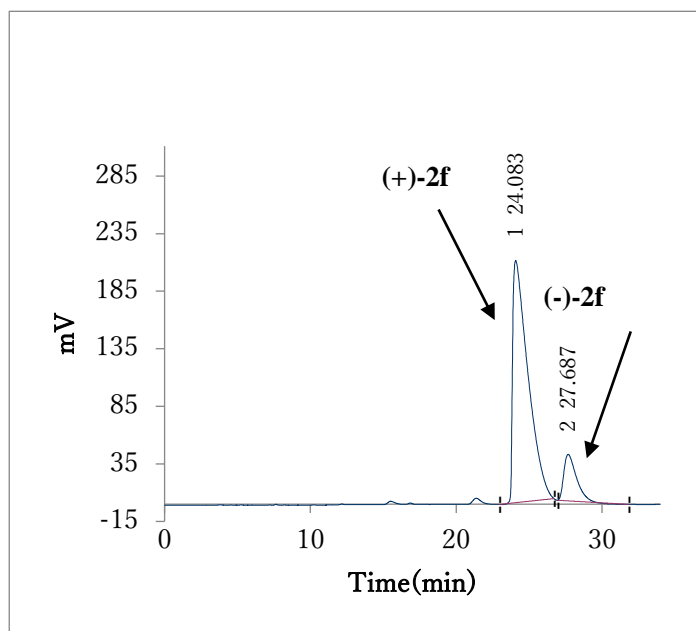


OD-3
eluent : 15% IPA in hexane
flow rate : 0.800 ml/min

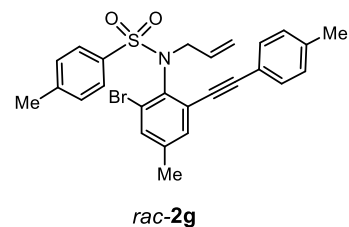
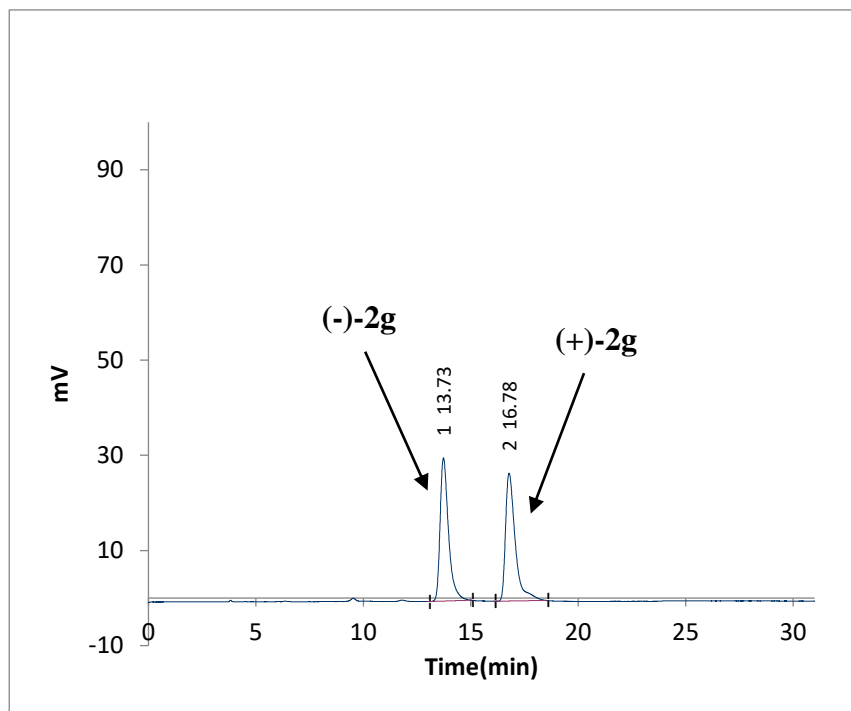
No.	Rt	Area	Area(%)	Height
1	6.73	2245655	17.6	229431
2	7.623	10527822	82.4	919828
		12773477	100	1149259



OD-3
eluent : 3% IPA in hexane
flow rate : 0.800 ml/min

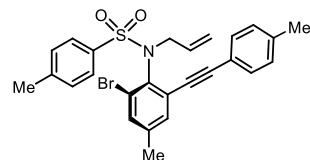
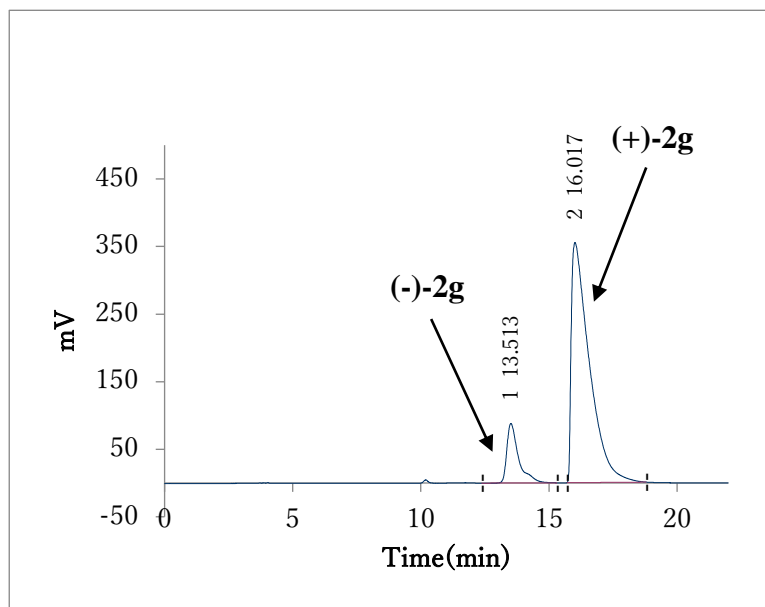


OD-3
eluent : 3% IPA in hexane
flow rate : 0.800 ml/min



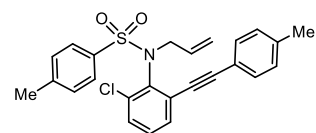
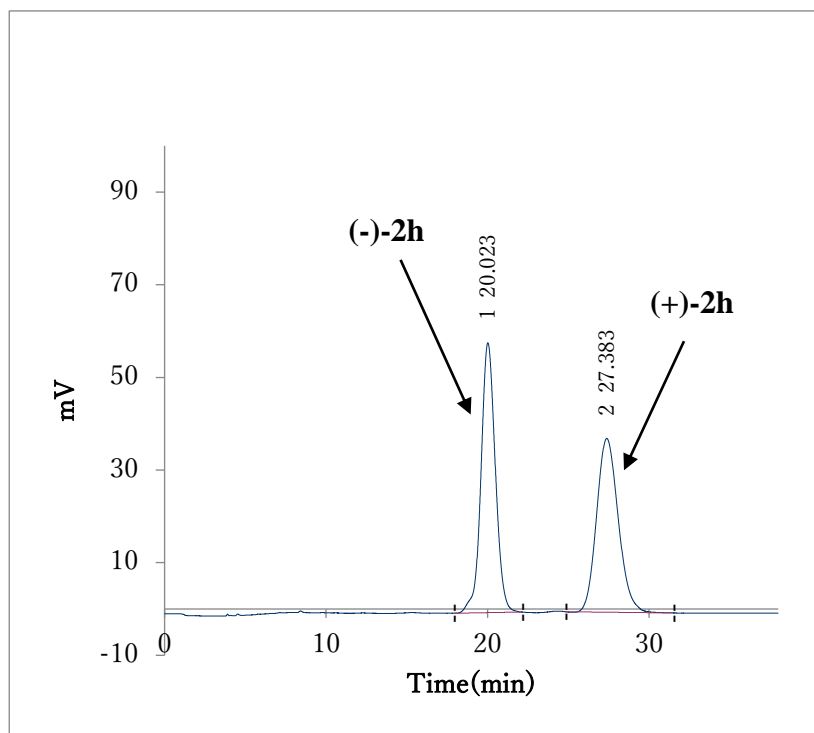
rac-2g
 OD-3
 eluent : 5% IPA in hexane
 flow rate : 0.800 ml/min

No.	Rt	Area	Area(%)	Height
1	13.73	818781.6	49.2	30108
2	16.78	846494.6	50.8	26893
		1665276	100	57001



2g
 OD-3
 eluent : 5% IPA in hexane
 flow rate : 0.800 ml/min

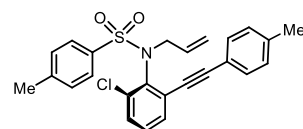
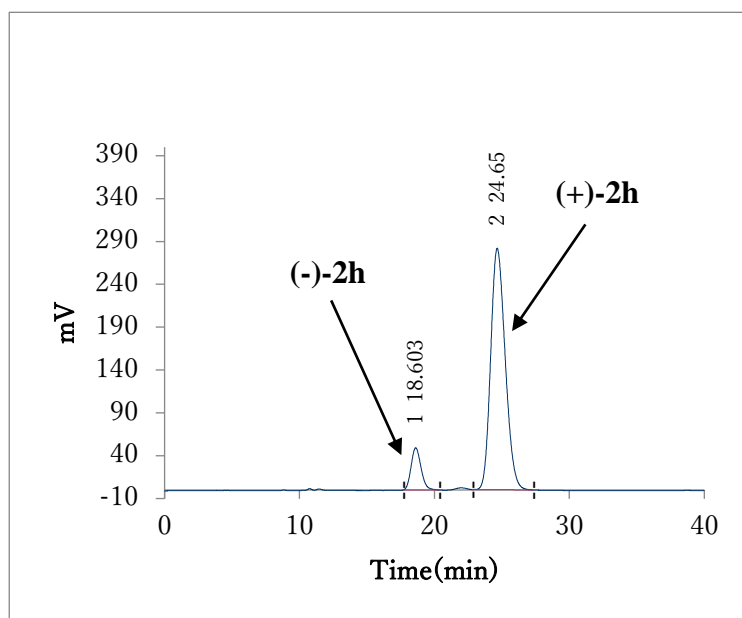
No.	Rt	Area	Area(%)	Height
1	13.513	2792384	13.8	88046
2	16.017	17404710	86.2	355501
		20197094	100	443547



rac-2h

AS-H
eluent : 15% IPA in hexane
flow rate : 0.800 ml/min

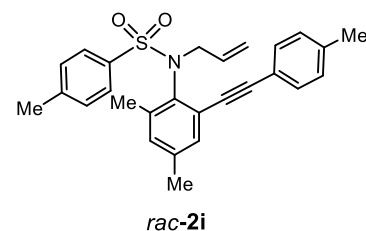
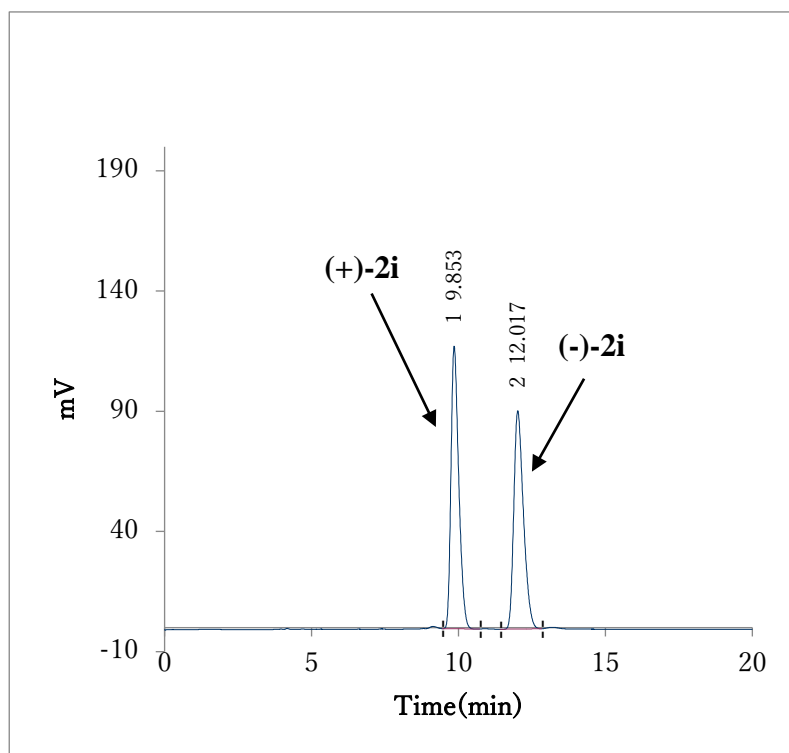
No.	Rt	Area	Area(%)	Height
1	20.023	3607239	50.8	58265
2	27.383	3498382	49.2	37534
		7105622	100	95799



2h

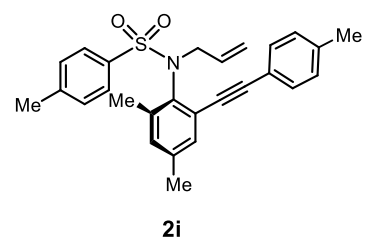
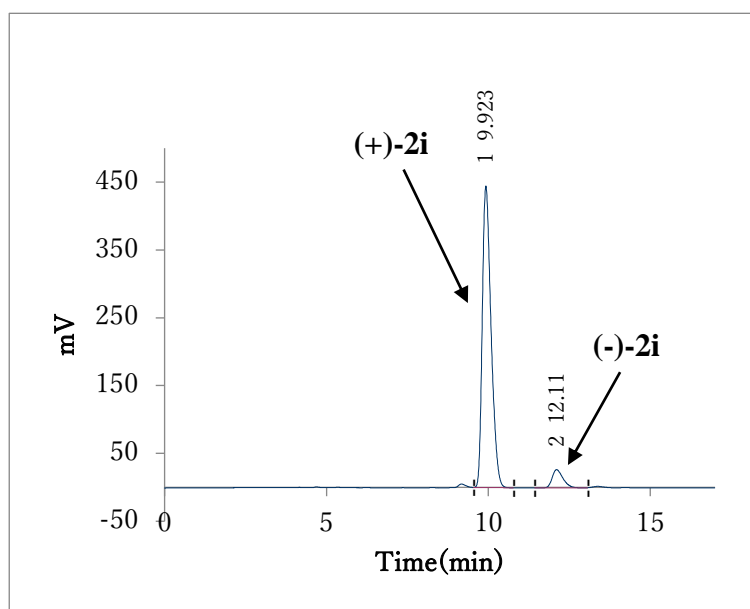
AS-H
eluent : 15% IPA in hexane
flow rate : 0.800 ml/min

No.	Rt	Area	Area(%)	Height
1	18.603	2516148	10.7	49327
2	24.65	21061843	89.3	281780
		23577991	100	331107



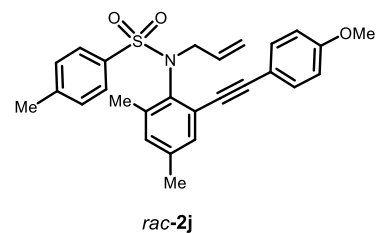
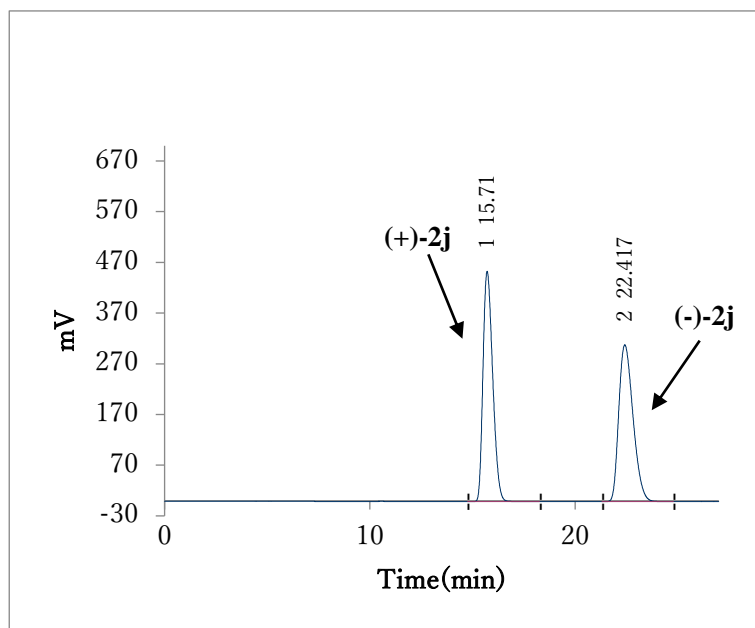
AD-H
eluent : 15% IPA in hexane
flow rate : 0.800 ml/min

No.	Rt	Area	Area(%)	Height
1	9.853	2160478	51.1	117545
2	12.017	2070706	48.9	90830
		4231184	100	208375



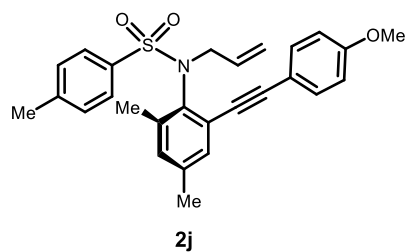
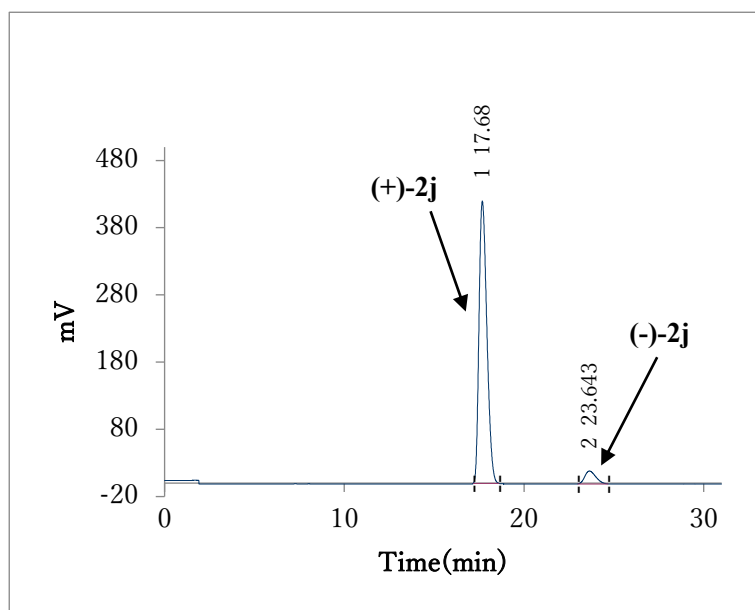
AD-H
eluent : 15% IPA in hexane
flow rate : 0.800 ml/min

No.	Rt	Area	Area(%)	Height
1	9.923	8352218	93.1	444591
2	12.11	616146.6	6.9	26956
		8968364	100	471547



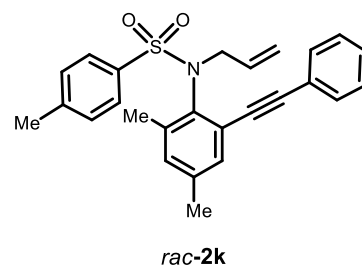
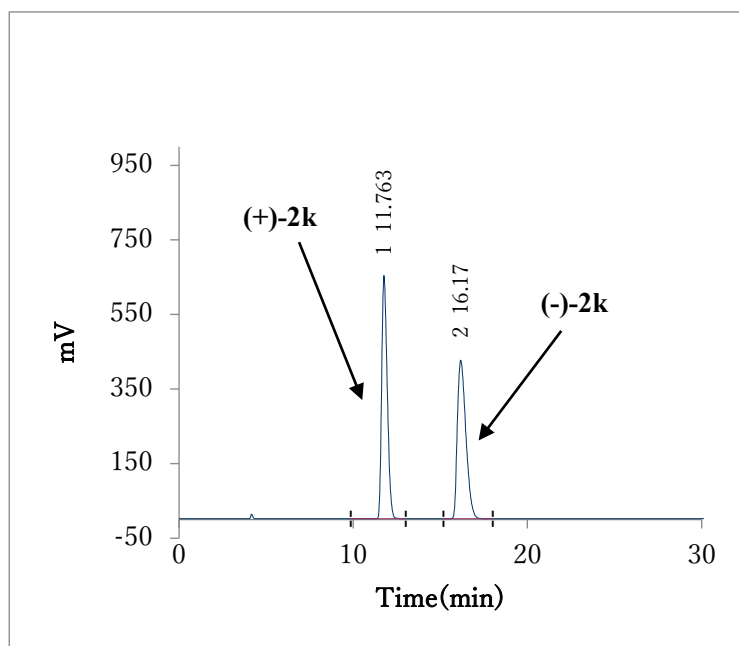
rac-2j
AD-H
eluent : 15% IPA in hexane
flow rate : 0.800 ml/min

No.	Rt	Area	Area(%)	Height
1	15.71	14871225	50	454163
2	22.417	14882932	50	309231
		29754157	100	763394

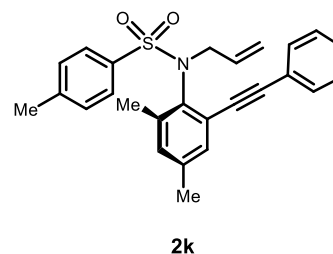
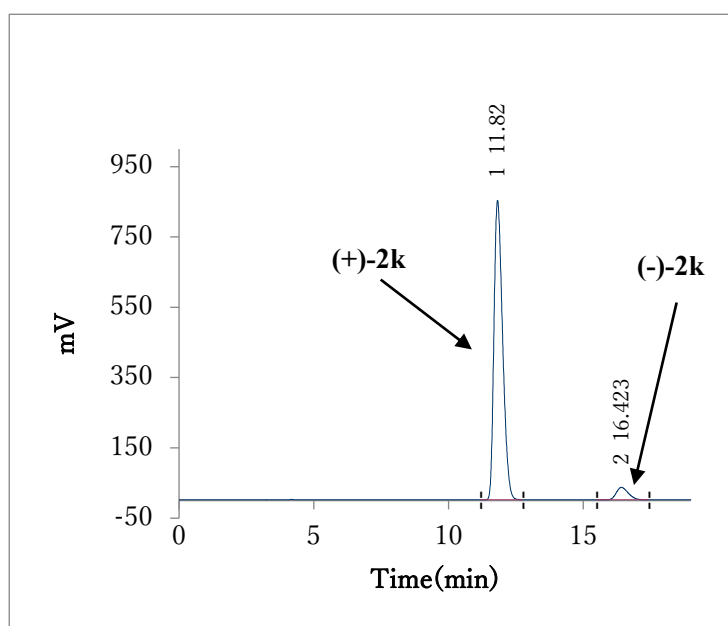


2j
AD-H
eluent : 15% IPA in hexane
flow rate : 0.800 ml/min

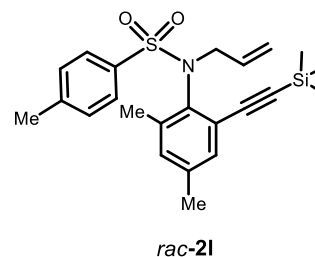
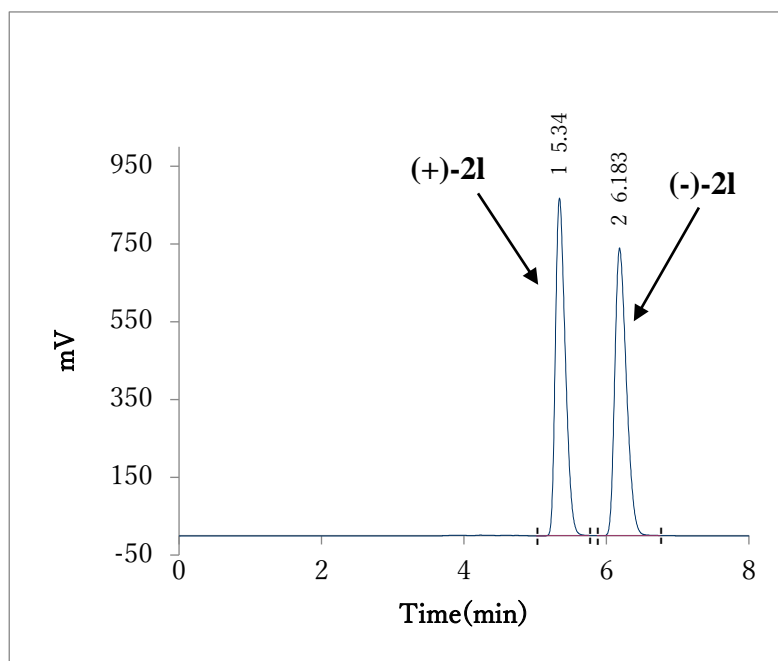
No.	Rt	Area	Area(%)	Height
1	17.68	12792973	94	420224
2	23.643	812021.8	6	19140
		13604994	100	439364



AD-H
eluent : 15% IPA in hexane
flow rate : 0.800 ml/min

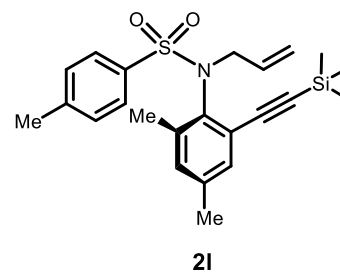
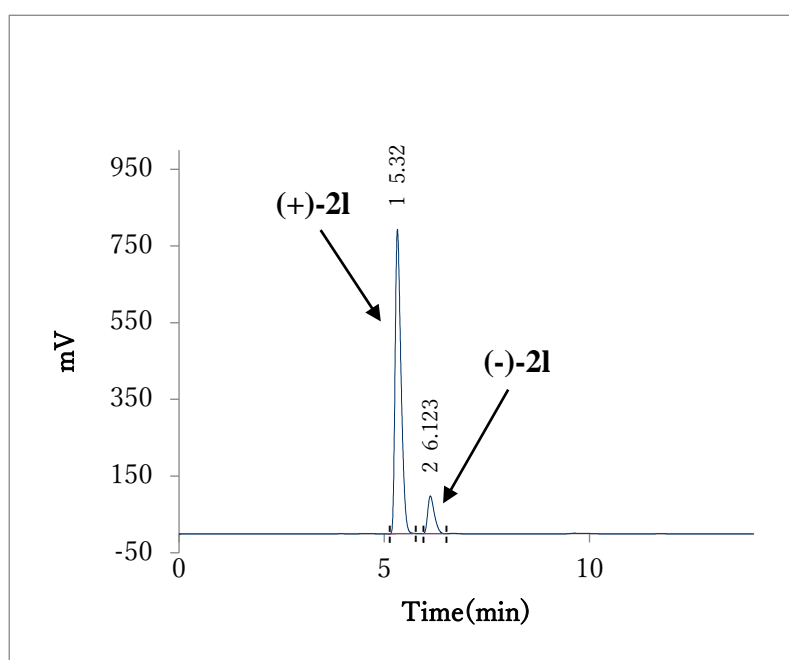


AD-H
eluent : 15% IPA in hexane
flow rate : 0.800 ml/min



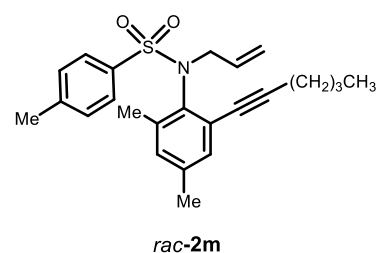
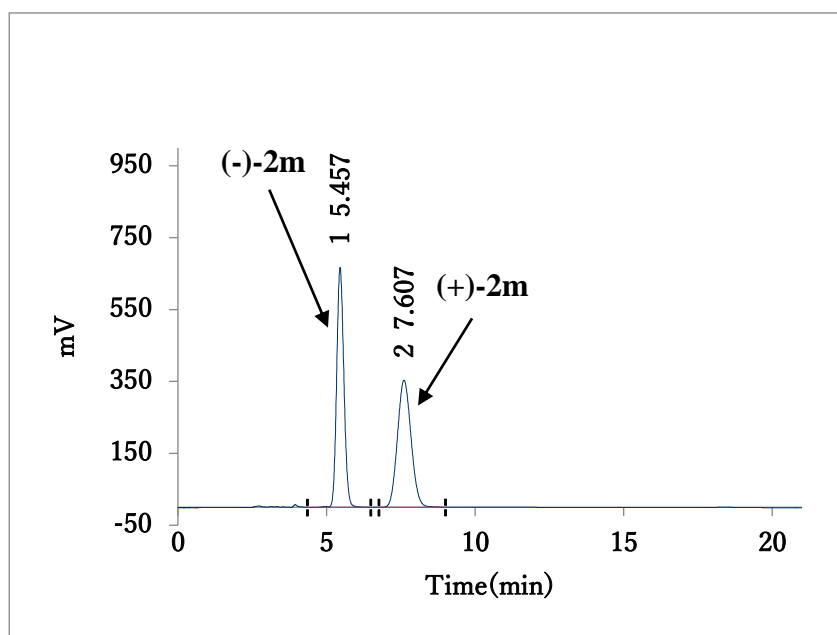
AD-H
eluent : 15% IPA in hexane
flow rate : 0.800 ml/min

No.	Rt	Area	Area(%)	Height
1	5.34	8351457	50	868501
2	6.183	8354624	50	739717
		16706081	100	1608218



AD-H
eluent : 15% IPA in hexane
flow rate : 0.800 ml/min

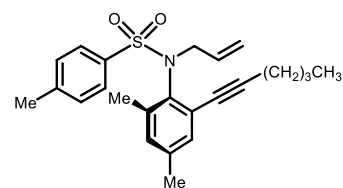
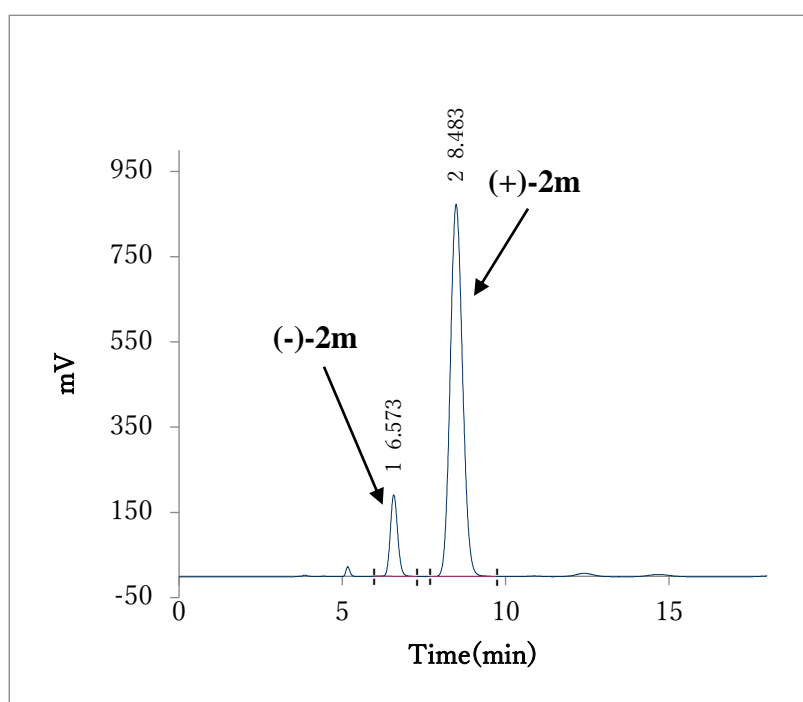
No.	Rt	Area	Area(%)	Height
1	5.32	7899865	87.6	793544
2	6.123	1116536	12.4	98740
		9016401	100	892284



rac-2m

AS-H
eluent : 15% IPA in hexane
flow rate : 0.800 ml/min

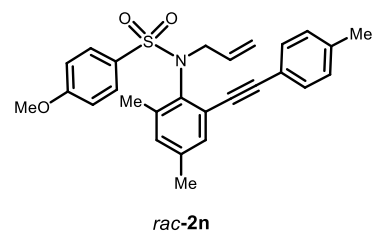
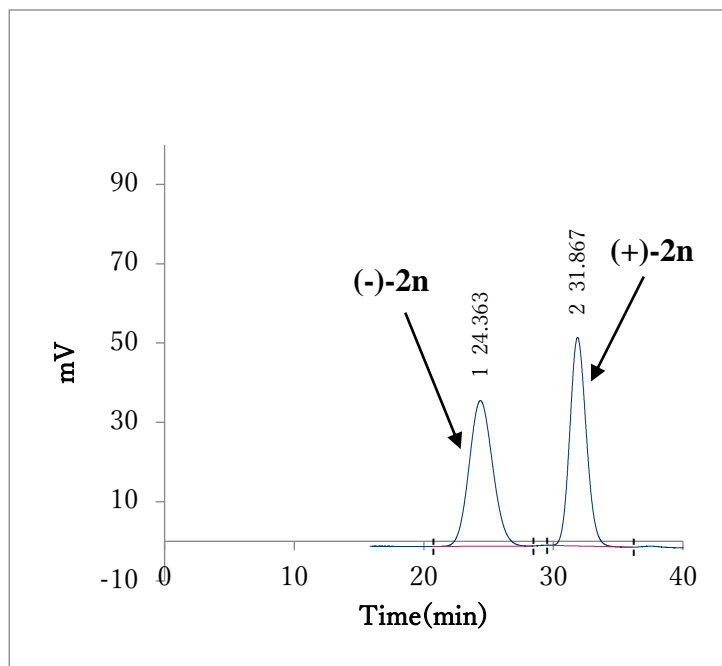
No.	Rt	Area	Area(%)	Height
1	5.457	11207659	50	667207
2	7.607	11217198	50	353275
		22424857	100	1020482



2m

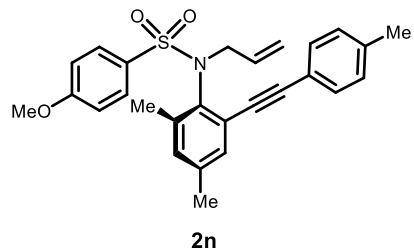
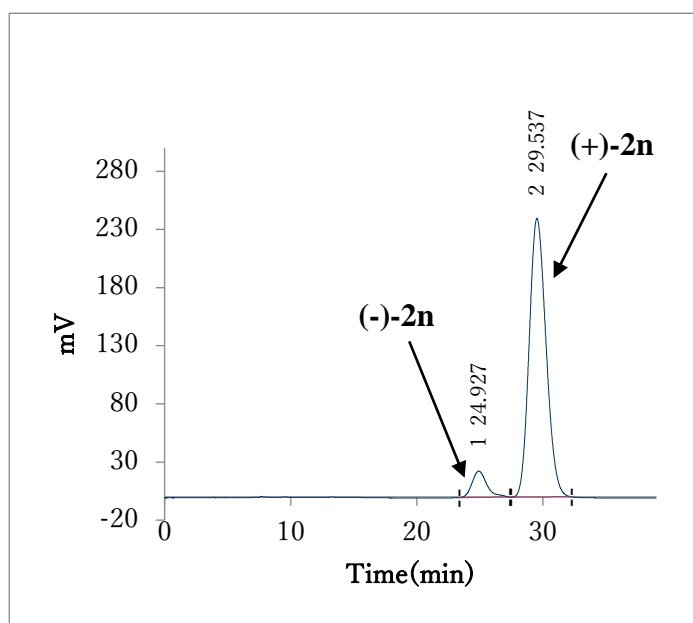
AS-H
eluent : 15% IPA in hexane
flow rate : 0.800 ml/min

No.	Rt	Area	Area(%)	Height
1	6.573	2984160	11.5	191397
2	8.483	22926038	88.5	873678
		25910198	100	1065075



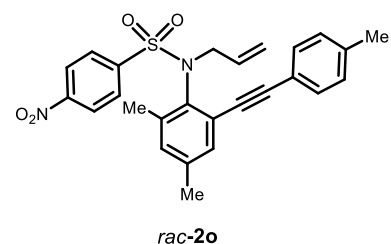
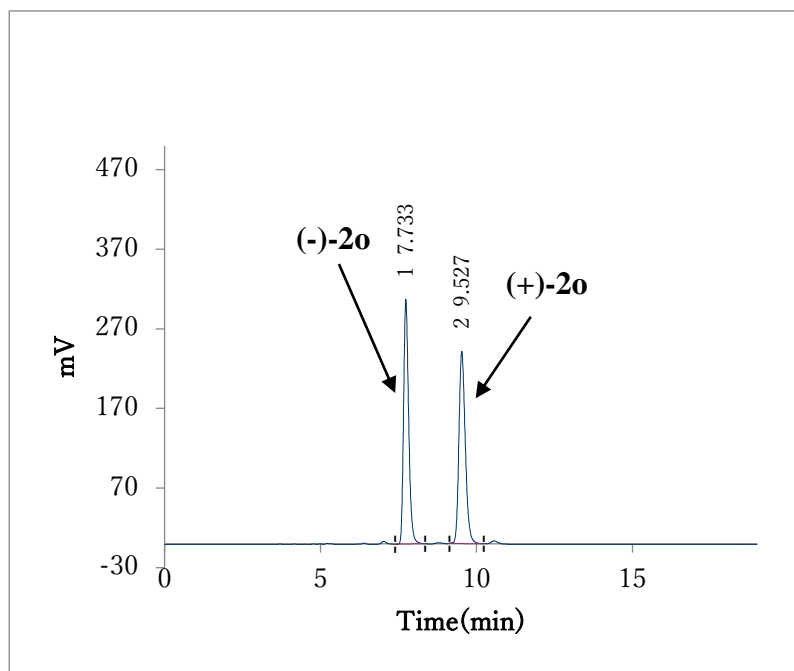
rac-2n
AS-H
eluent : 5% IPA in hexane
flow rate : 0.800 ml/min

No.	Rt	Area	Area(%)	Height
1	24.363	4648267	50.1	36764
2	31.867	4630188	49.9	52617
		9278454	100	89381



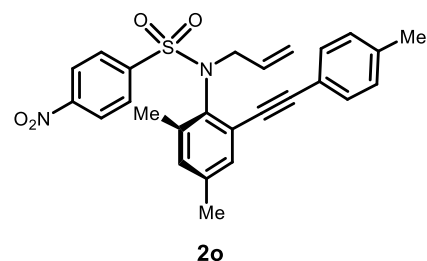
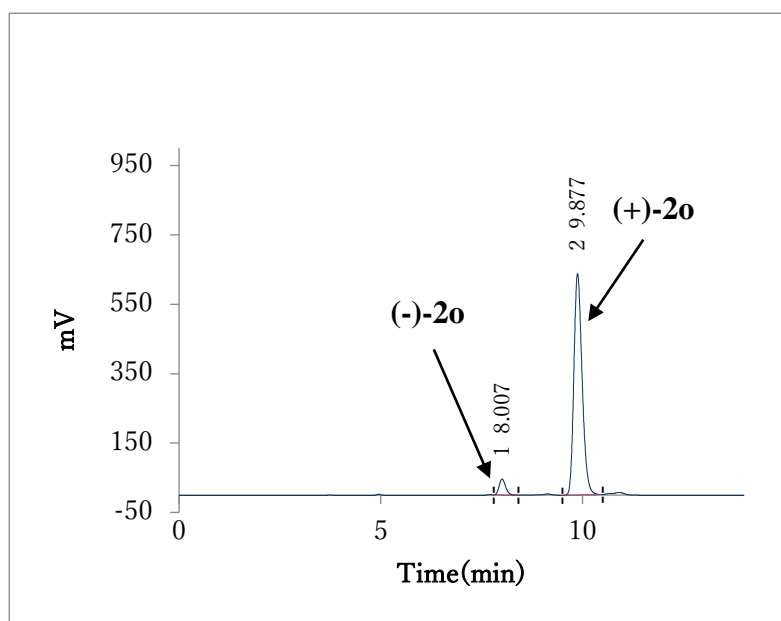
2n
AS-H
eluent : 5% IPA in hexane
flow rate : 0.800 ml/min

No.	Rt	Area	Area(%)	Height
1	24.927	1836889	7.6	22609
2	29.537	22208298	92.4	239673
		24045187	100	262282



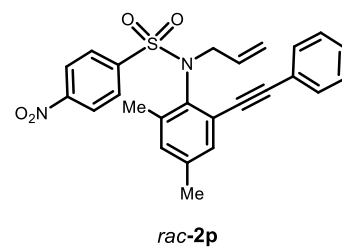
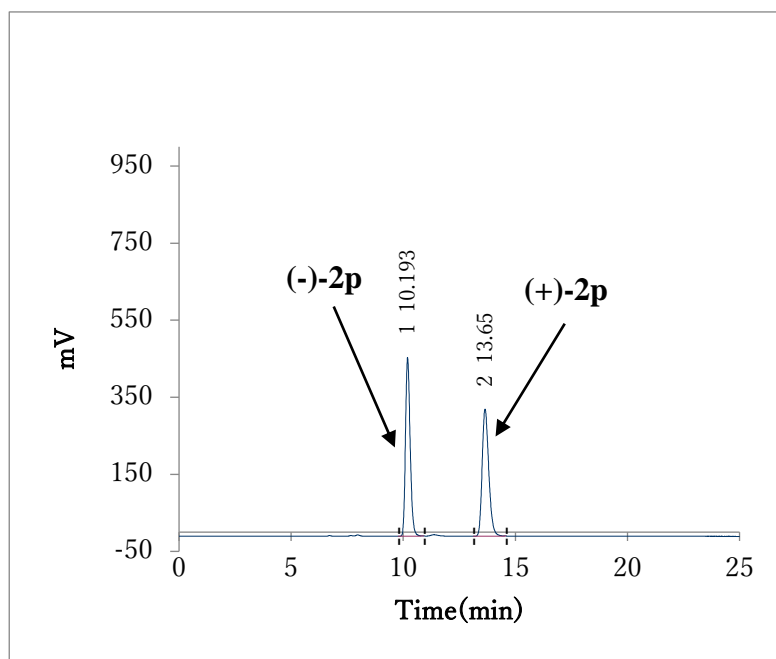
rac-2o
 OD-3
 eluent : 15% IPA in hexane
 flow rate : 0.800 ml/min

No.	Rt	Area	Area(%)	Height
1	7.733	3467087	50.3	307779
2	9.527	3420459	49.7	241565
		6887546	100	549344



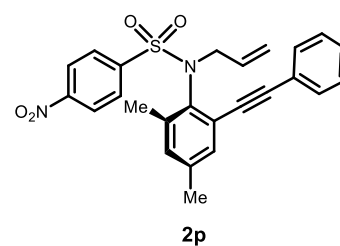
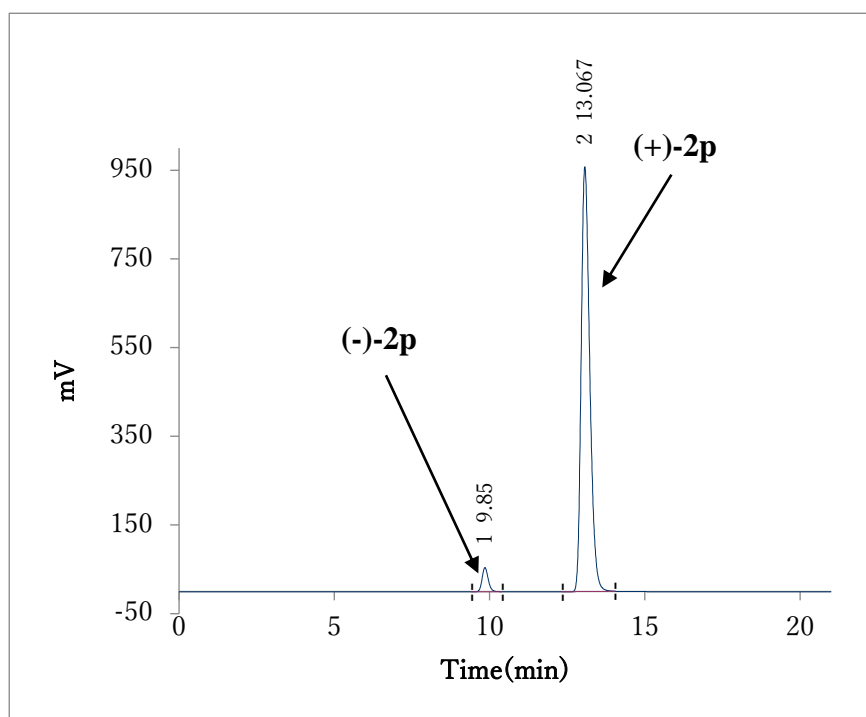
2o
 OD-3
 eluent : 15% IPA in hexane
 flow rate : 0.800 ml/min

No.	Rt	Area	Area(%)	Height
1	8.007	511222.6	5.3	45935
2	9.877	9046738	94.7	638258
		9557961	100	684193



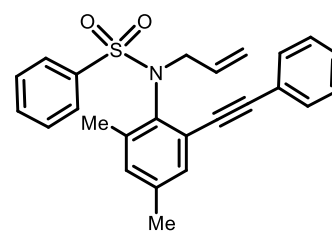
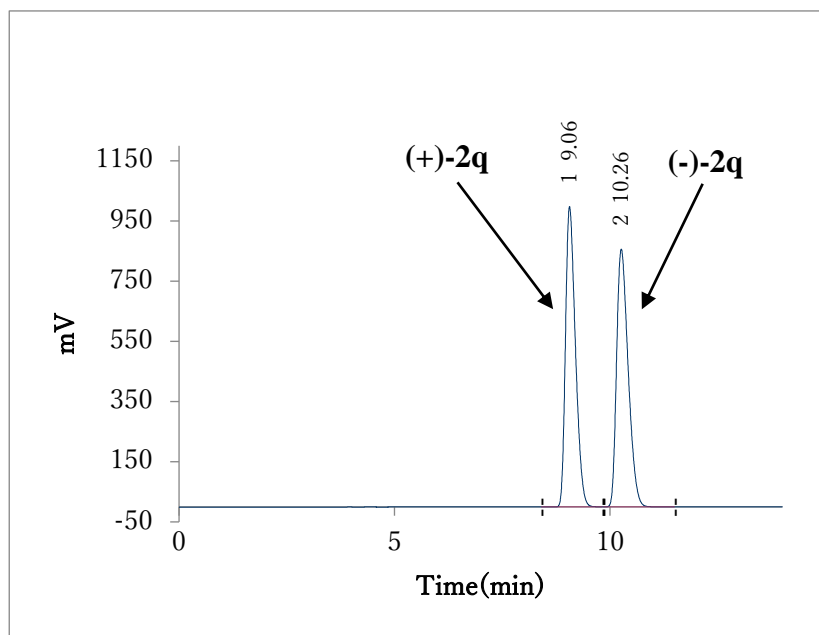
rac-2p
 OD-3
 eluent : 15% IPA in hexane
 flow rate : 0.800 ml/min

No.	Rt	Area	Area(%)	Height
1	10.193	6732828	50	463875
2	13.65	6736503	50	329762
		13469331	100	793637



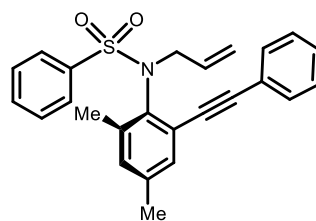
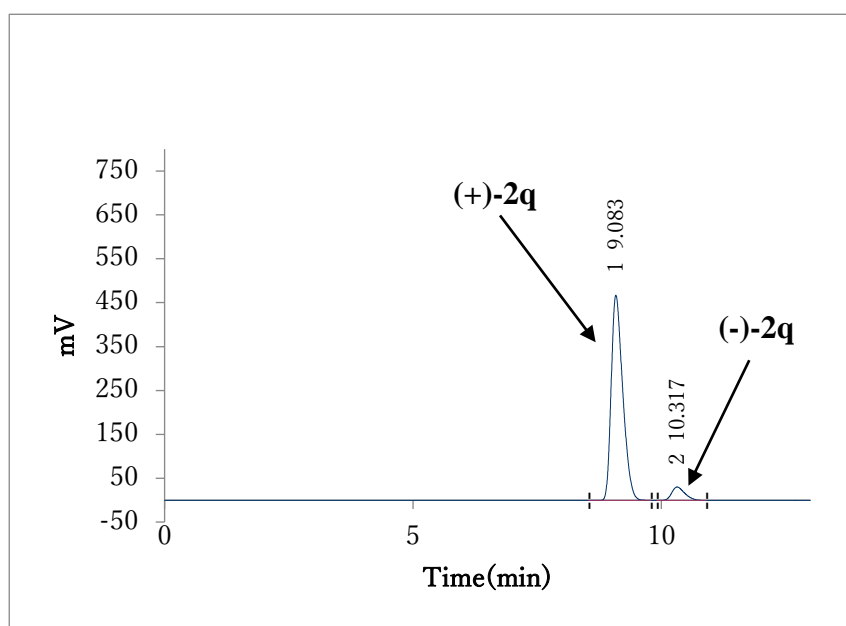
2p
 OD-3
 eluent : 15% IPA in hexane
 flow rate : 0.800 ml/min

No.	Rt	Area	Area(%)	Height
1	9.85	742086.5	3.9	54500
2	13.067	18326906	96.1	958185
		19068993	100	1012685



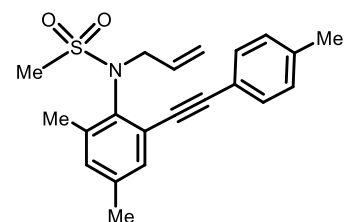
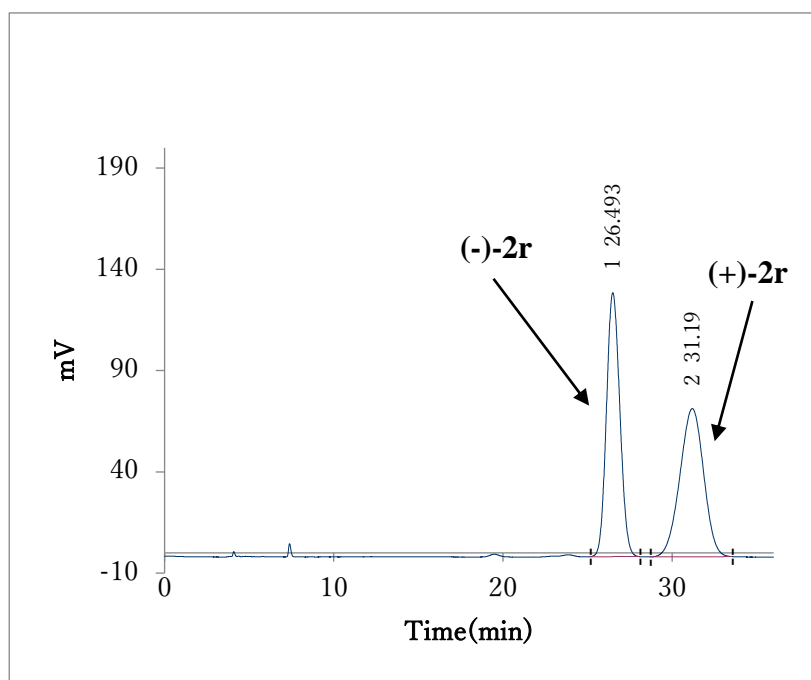
rac-2q

AD-H
eluent : 15% IPA in hexane
flow rate : 0.800 ml/min



2q

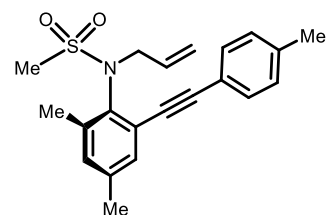
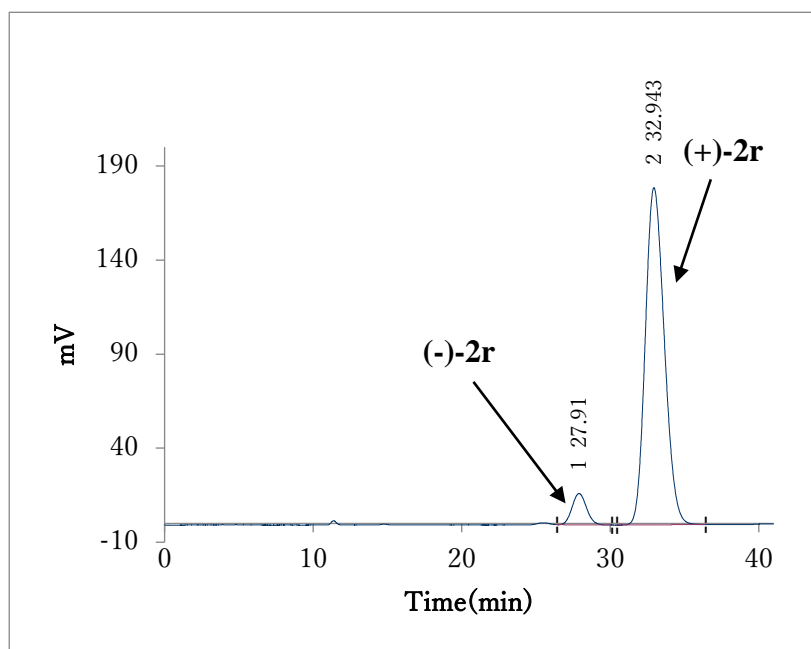
AD-H
eluent : 15% IPA in hexane
flow rate : 0.800 ml/min



rac-2r

AS-H
eluent : 5% IPA in hexane
flow rate : 0.800 ml/min

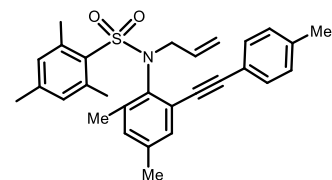
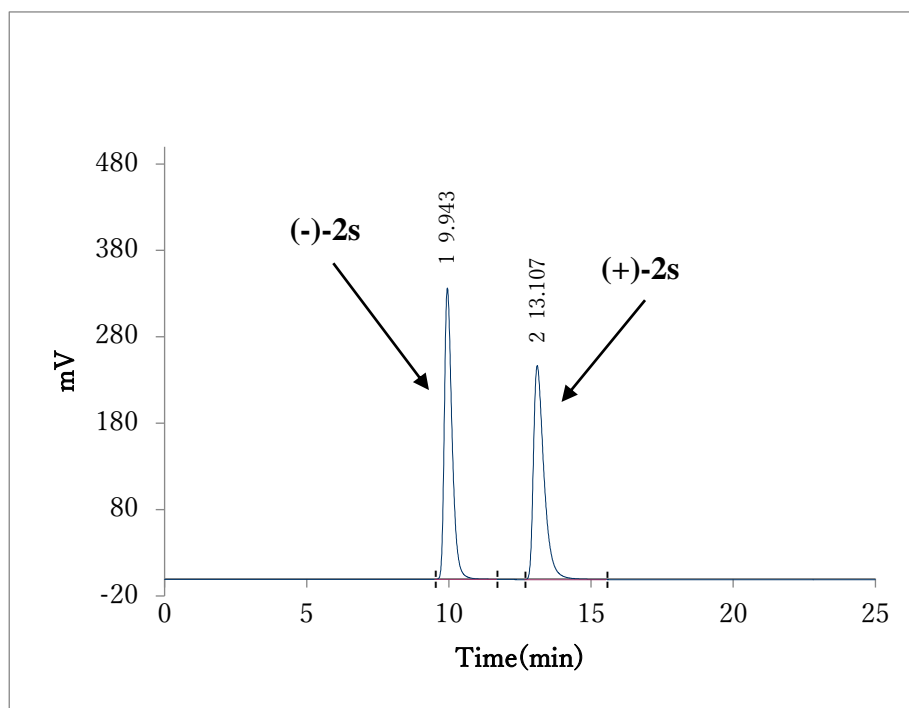
No.	Rt	Area	Area(%)	Height
1	26.493	7173448	50.1	130271
2	31.19	7146590	49.9	73200
		14320038	100	203471



2r

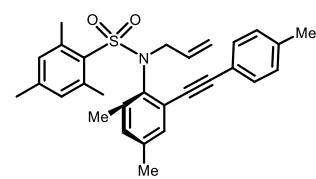
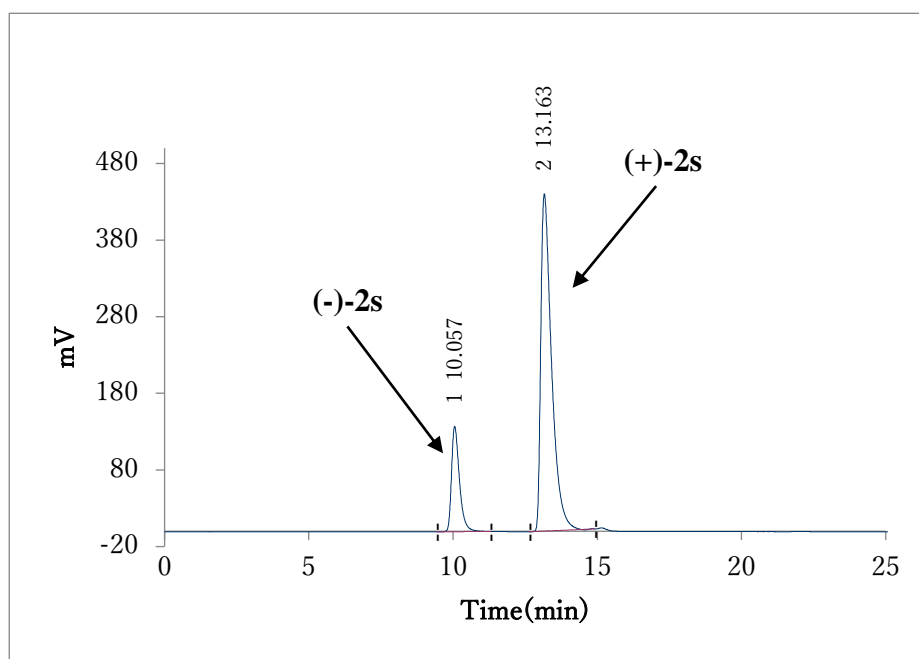
AS-H
eluent : 5% IPA in hexane
flow rate : 0.800 ml/min

No.	Rt	Area	Area(%)	Height
1	27.91	1123997	6.6	16653
2	32.943	15902586	93.4	179203
		17026584	100	195856



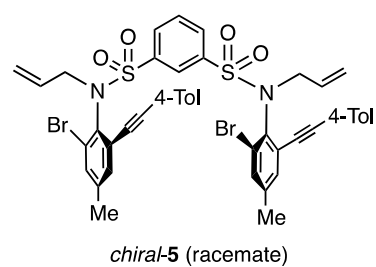
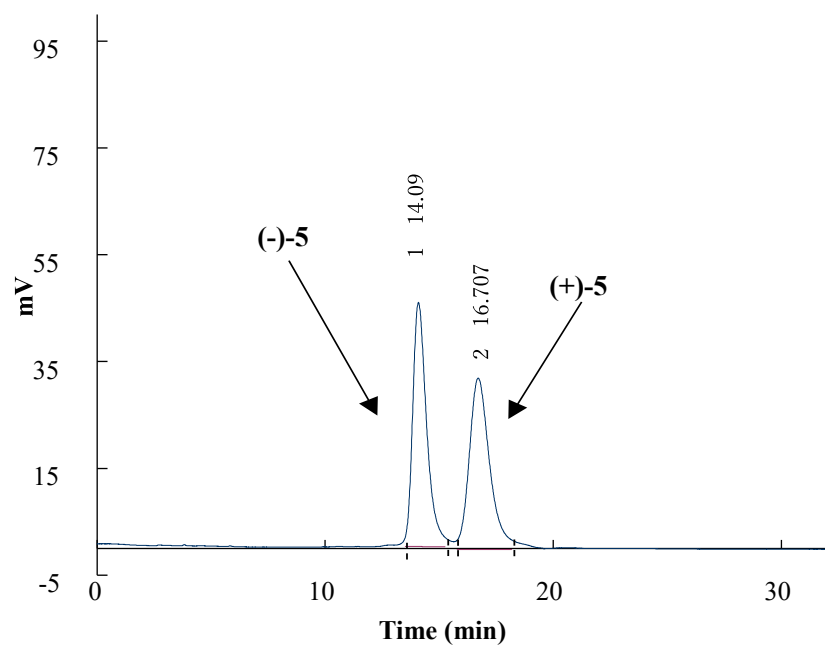
rac-2s
 OD-3
 eluent : 1% IPA in hexane
 flow rate : 0.800 ml/min

No.	Rt	Area	Area(%)	Height
1	9.943	6343040	49.8	337423
2	13.107	6385348	50.2	247913
		12728388	100	585336



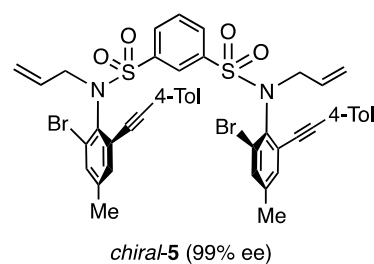
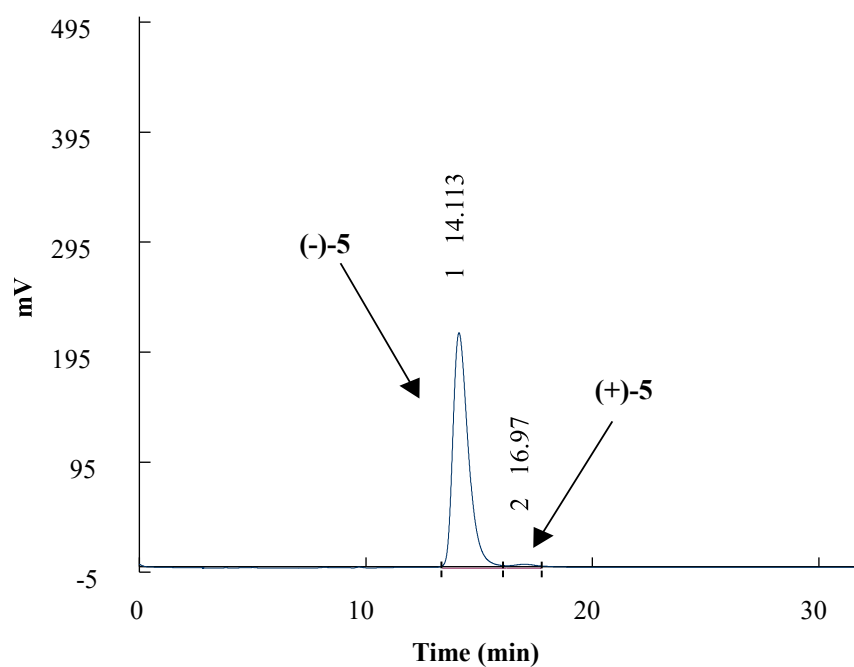
2s
 OD-3
 eluent : 1% IPA in hexane
 flow rate : 0.800 ml/min

No.	Rt	Area	Area(%)	Height
1	10.057	2618016	18.7	137592
2	13.163	11401047	81.3	440314
		14019063	100	577906



AD-H
eluent: 10% IPA in hexane
flow rate: 0.80 min

No.	Rt	Area	Area(%)	Height
1	14.09	1749424	50.4	43960
2	16.707	1724361	49.6	30351
		3473784	100	74311



AD-H
eluent: 10% IPA in hexane
flow rate: 0.80 min

No.	Rt	Area	Area(%)	Height
1	14.113	9878409	99.3	211717
2	16.97	67729.6	0.7	1424
		9946139	100	213141

X-Ray crystal data of **2o** (CheckCIF/PLATON report)

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) hk210406a_a

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: hk210406a_a

Bond precision:	C-C = 0.0070 Å	Wavelength=0.71073
Cell:	a=10.3010 (16)	b=9.0527 (14) c=25.570 (4)
	alpha=90	beta=99.171 (5) gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	2354.0 (6)	2354.0 (6)
Space group	P 21	P 21
Hall group	P 2yb	P 2yb
Moiety formula	C26 H24 N2 O4 S	C26 H24 N2 O4 S
Sum formula	C26 H24 N2 O4 S	C26 H24 N2 O4 S
Mr	460.53	460.53
Dx, g cm ⁻³	1.299	1.299
Z	4	4
Mu (mm ⁻¹)	0.173	0.173
F000	968.0	968.0
F000'	968.92	
h, k, lmax	12, 10, 30	12, 10, 30
Nref	8327 [4452]	8236
Tmin, Tmax	0.946, 0.986	0.830, 0.990
Tmin'	0.936	

Correction method= # Reported T Limits: Tmin=0.830 Tmax=0.990

AbsCorr = MULTI-SCAN

$$\text{Theta (max)} = 25.027$$

R(reflections)= 0.0511 (6426)

```
wR2 (reflections) =
```

0.1191 (8236)

$$S = 1.040$$

Npar= 601

The following ALERTS were generated. Each ALERT has the format

```
test-name ALERT alert-type alert-level.
```

Click on the hyperlinks for more details of the test.



Alert level C

PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax < 18)	7.38	Note
PLAT220_ALERT_2_C NonSolvent Resd 2 C Ueq(max)/Ueq(min) Range	3.4	Ratio
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds	0.00698	Ang.
PLAT911 ALERT 3 C Missing FCF Refl Between Thmin & STh/L=	0.595	13 Report



Alert level G

PLAT371_ALERT_2_G	Long	C(sp2)-C(sp1) Bond	C6	-	C7	.	1.44 Ang.
PLAT371_ALERT_2_G	Long	C(sp2)-C(sp1) Bond	C8	-	C9	.	1.43 Ang.
PLAT371_ALERT_2_G	Long	C(sp2)-C(sp1) Bond	C32	-	C33	.	1.44 Ang.
PLAT371_ALERT_2_G	Long	C(sp2)-C(sp1) Bond	C34	-	C35	.	1.45 Ang.
PLAT883_ALERT_1_G	No Info/Value for	_atom_sites_solution_primary	.				Please Do !
PLAT909_ALERT_3_G	Percentage of I>2sig(I)	Data at Theta(Max)	Still				47% Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s)	Below Theta(Min).					2 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in	Embedded .res File					1 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive	Residual Density.					0 Info
PLAT992_ALERT_5_G	Repd & Actual reflns number	gt Values Differ by					3 Check

0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully

4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

10 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

7 ALERT type 2 Indicator that the structure model may be wrong or deficient

5 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

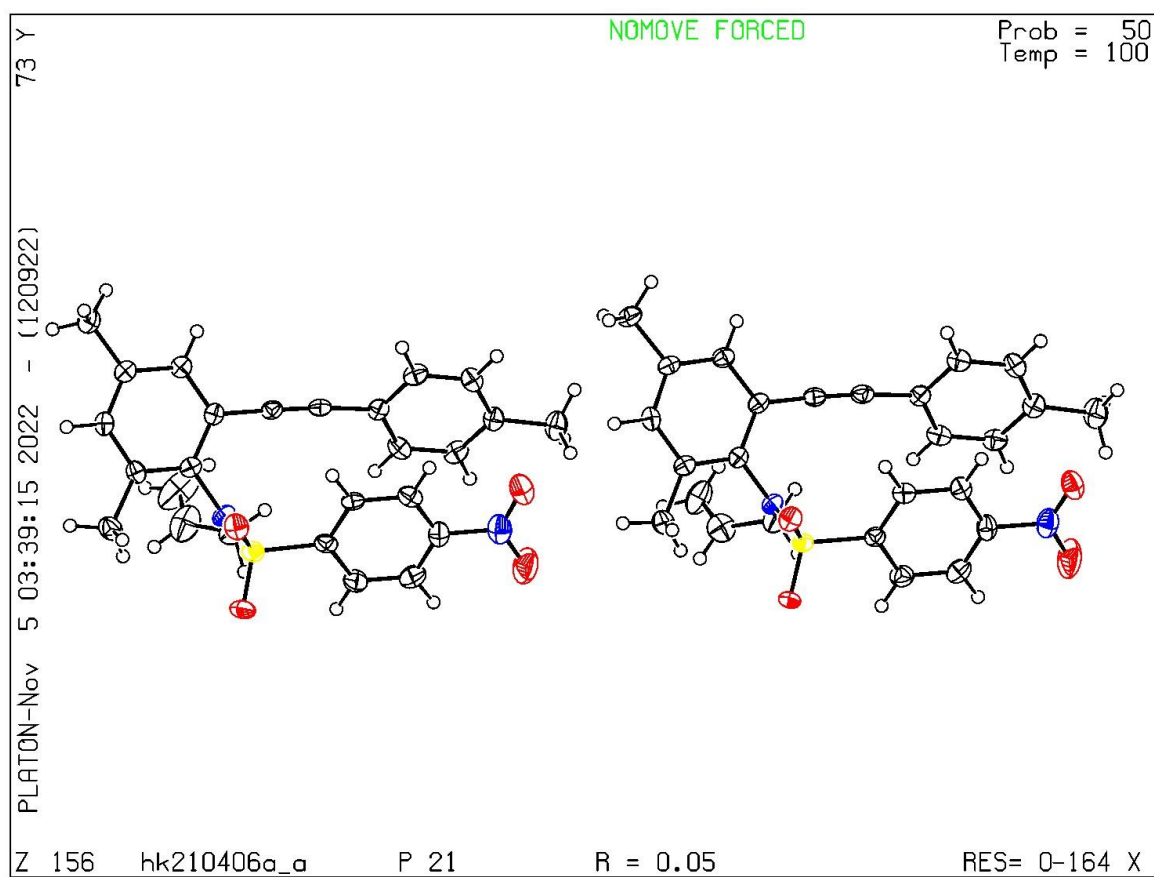
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

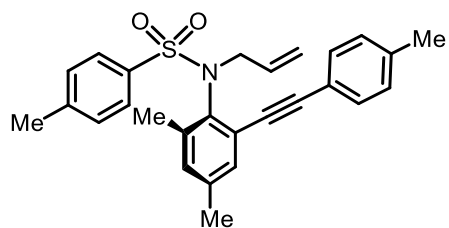
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 12/09/2022; check.def file version of 09/08/2022

Datablock hk210406a_a - ellipsoid plot



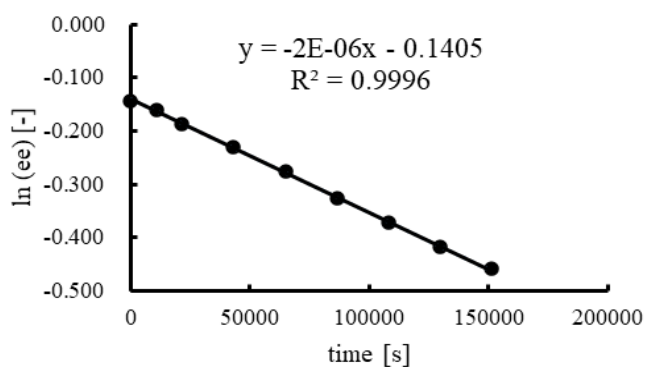
Evaluation of rotational barrier of **2i**, **2r**



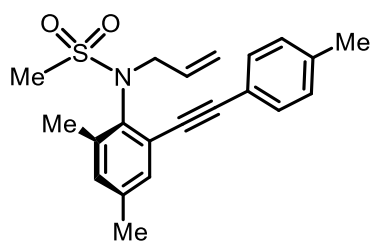
2i

$\Delta G^\ddagger = 28.7$ kcal/mol

60 °C	
time (h)	ee (%)
0	87
3	85
6	83
12	79
30	69
42	63



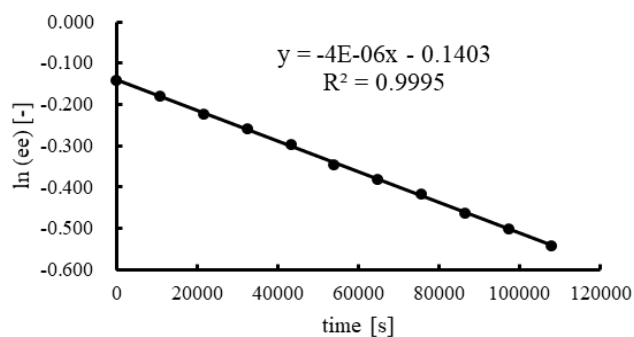
temp (°C)	k (s ⁻¹)	ΔG^\ddagger (kcal/mol)	t _{1/2} (days)
60	1.06×10 ⁻⁶	28.7	7.6



2r

$\Delta G^\ddagger = 28.3$ kcal/mol

60 °C	
time (h)	ee (%)
0	87
3	84
6	80
12	74
30	58
33	57



temp (°C)	k (s ⁻¹)	ΔG^\ddagger (kcal/mol)	t _{1/2} (days)
60	1.89×10 ⁻⁶	28.3	4.3