

Supporting Information

For

A unique dithiocarbamate chemistry during design & synthesis of novel sperm-immobilizing agents

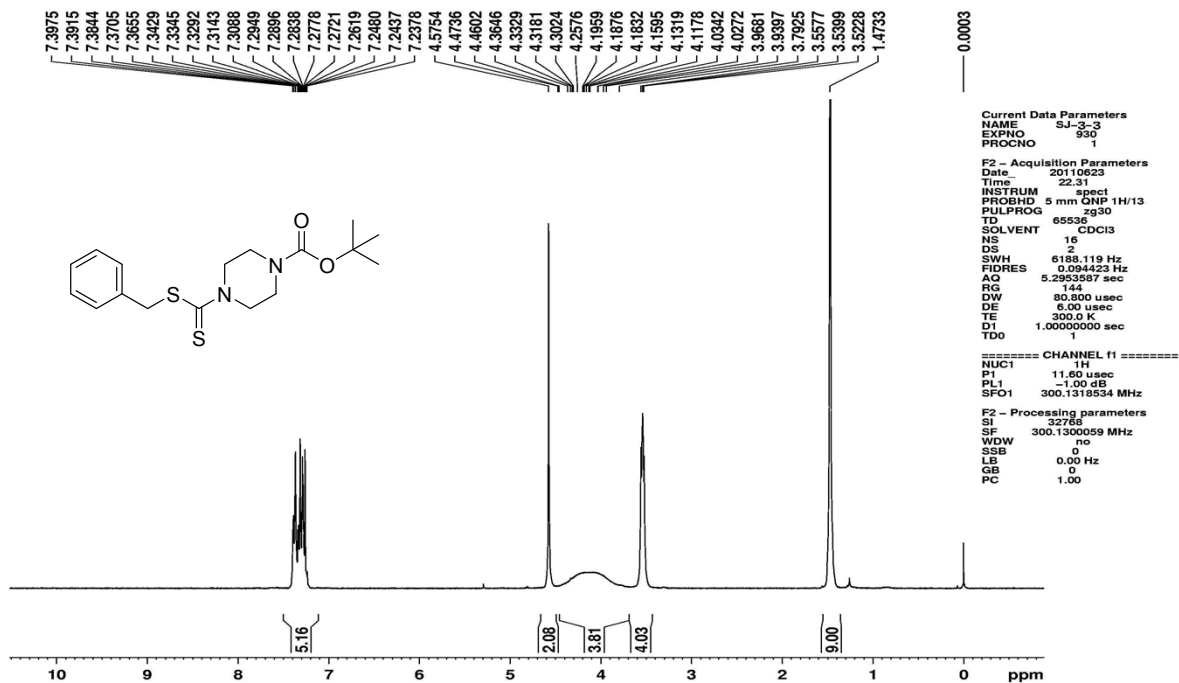
Santosh Jangir,^a Veenu Bala,^{a,d} Nand Lal,^a Lalit Kumar,^a Amit Sarswat,^a Lokesh Kumar,^b Bhavana Kushwaha,^b Pratiksha Singh,^c Praveen Kumar Shukla,^c Jagdamba Prasad Maikhuri,^b Gopal Gupta,^b and Vishnu Lal Sharma^a

^aMedicinal & Process Chemistry Division, ^bEndocrinology Division and ^cMicrobiology Division, CSIR-Central Drug Research Institute, Lucknow-226031 (INDIA);

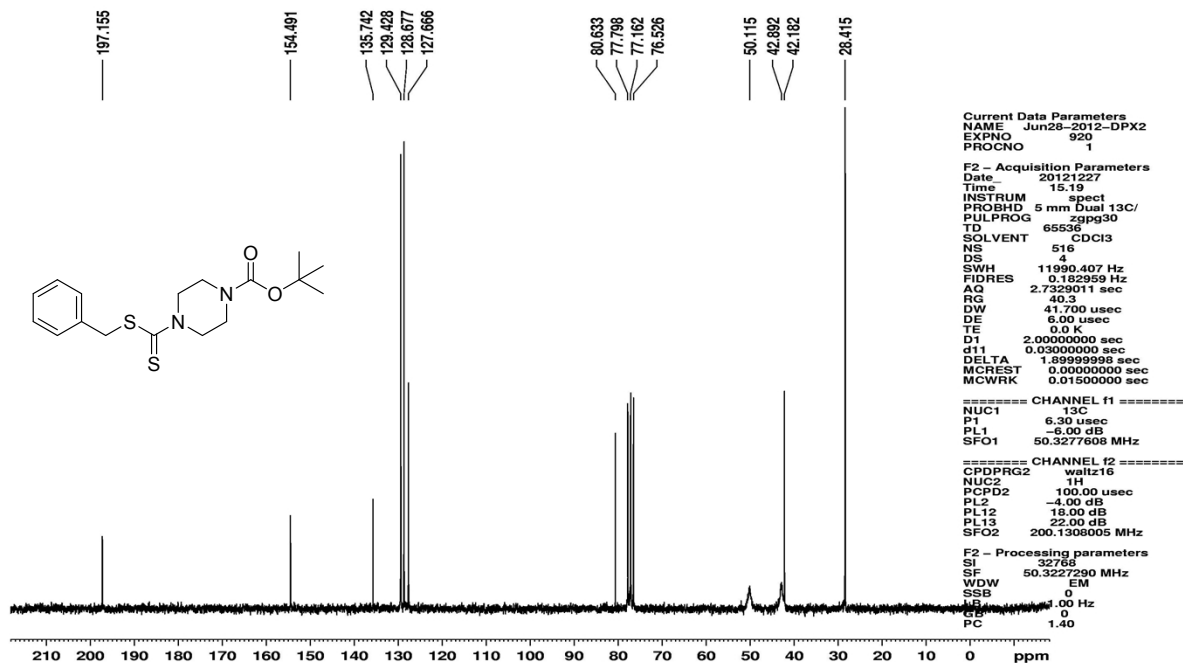
^dAcademy of Scientific & Innovative Research, New Delhi (INDIA)

List of Content

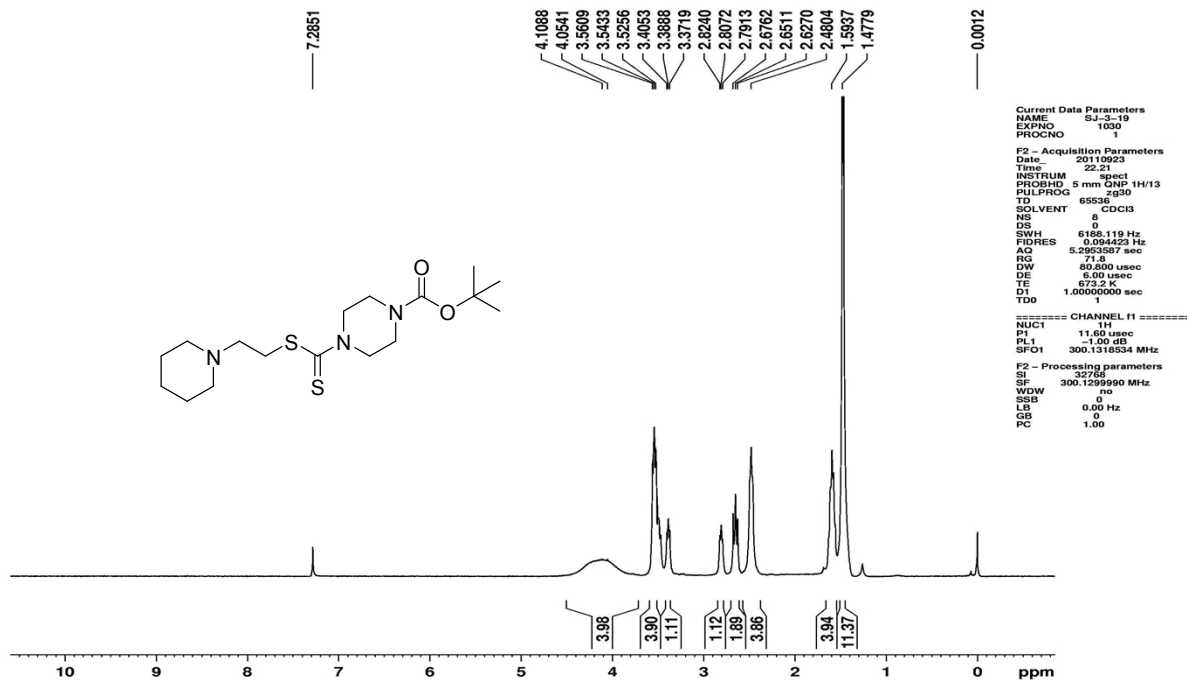
- 1. Scanned copies of ¹H NMR spectra of compounds 4-32**
- 2. Scanned copies of ¹³C NMR spectra of compounds 4 (S1), 5 (S2), 7 (S4), 8 (S5), 9 (S6), 10 (S7), 13 (S9), 14 (S10), 16 (S13), 17 (S15), 18 (S16), 21 (S17), 22 (S19), 23 (S20), 24 (S21), 25 (S23), 26 (S24), 27 (S25), 28 (S27), 29 (S28), 30 (S29), 31 (S31), 32 (S32)**
- 3. Scanned copies of HRMS of compounds 14 (S10), 16 (S14), 18 (S16), 21 (S18), 23 (S20), 24 (S22), 25 (S23), 27 (S26), 29 (S28), 30 (S30), 32 (S32)**
- 4. Scanned copy of mass spectra of reaction mixture (preparation of compound 9) (S11)**



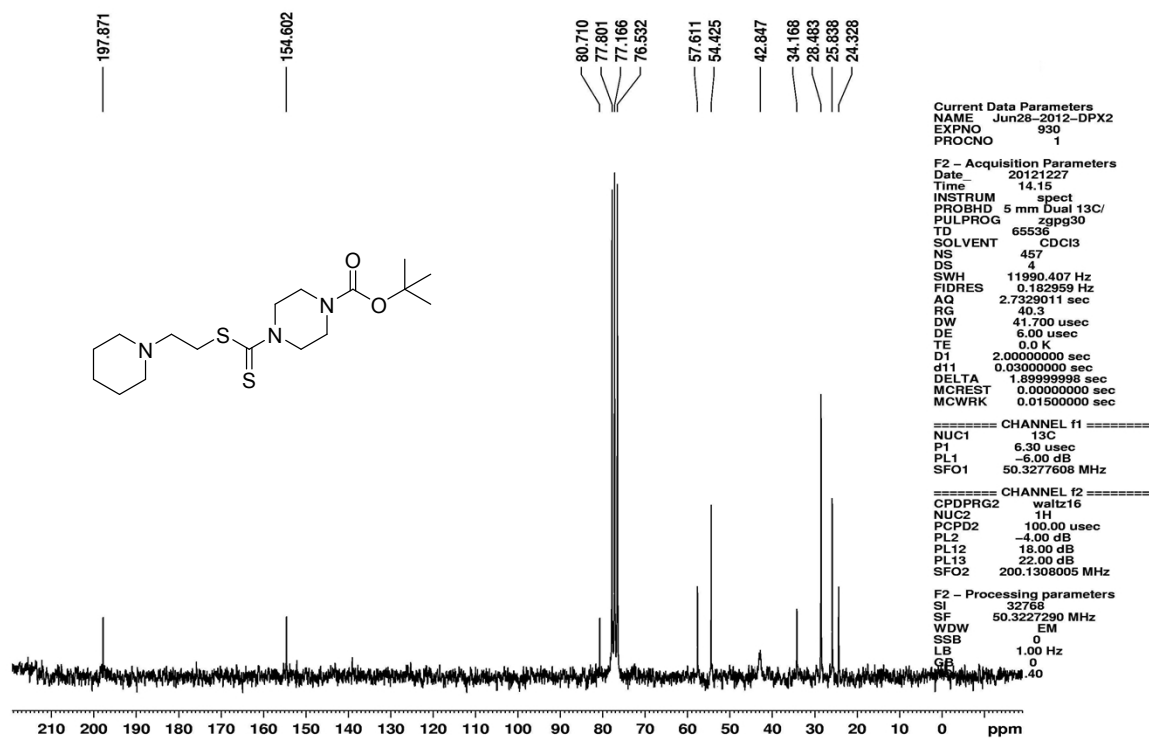
¹H NMR (300MHz, CDCl₃) of compound 4



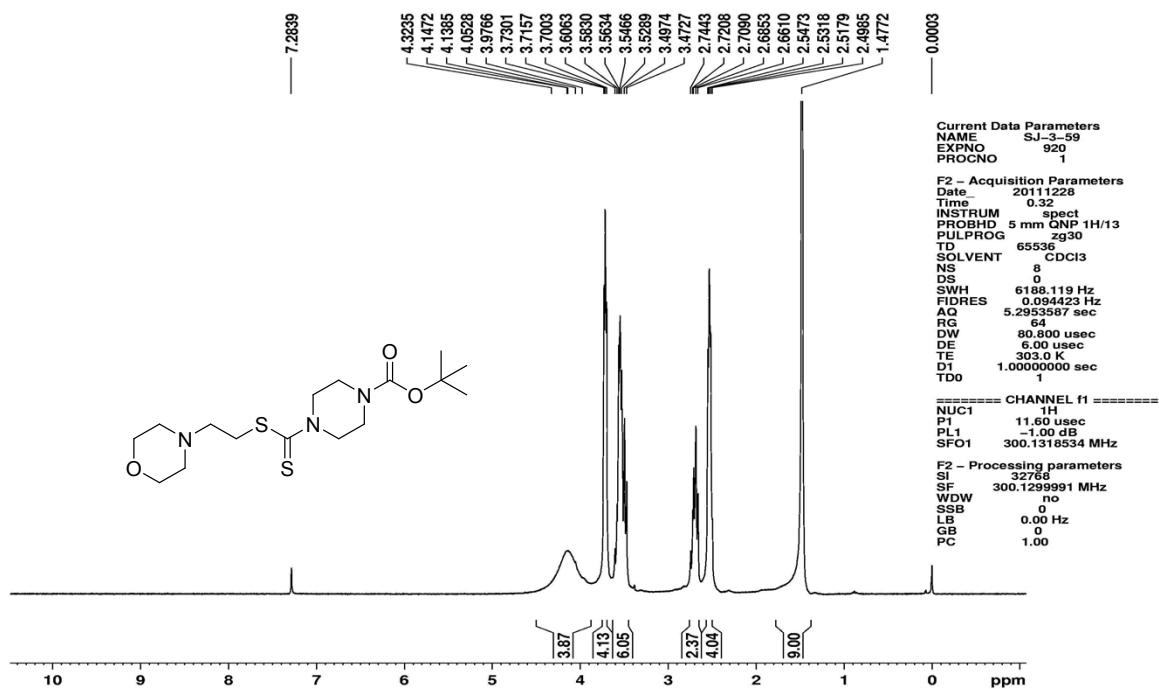
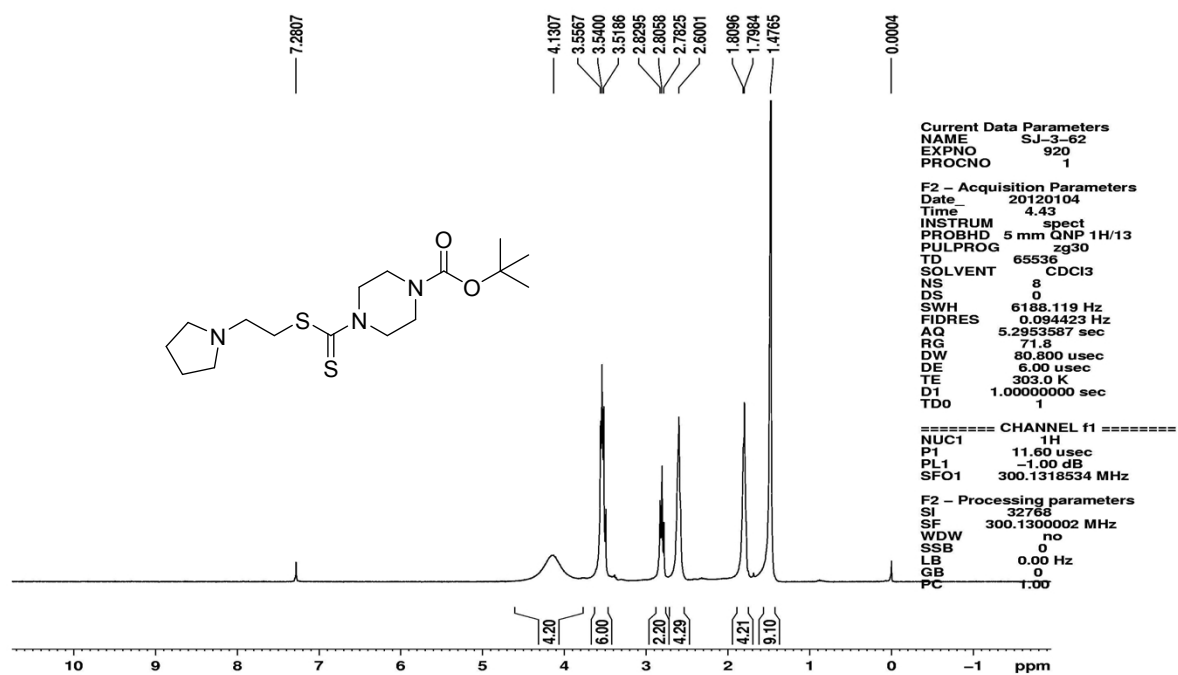
¹³C NMR (50 MHz, CDCl₃) of compound 4

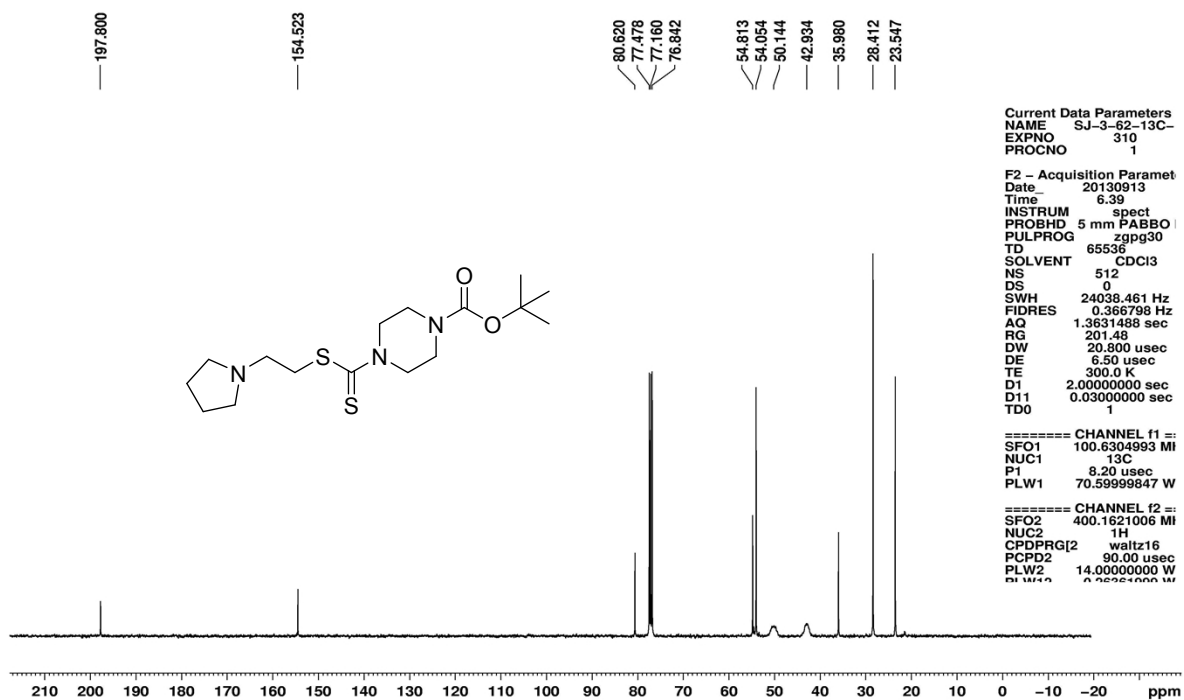
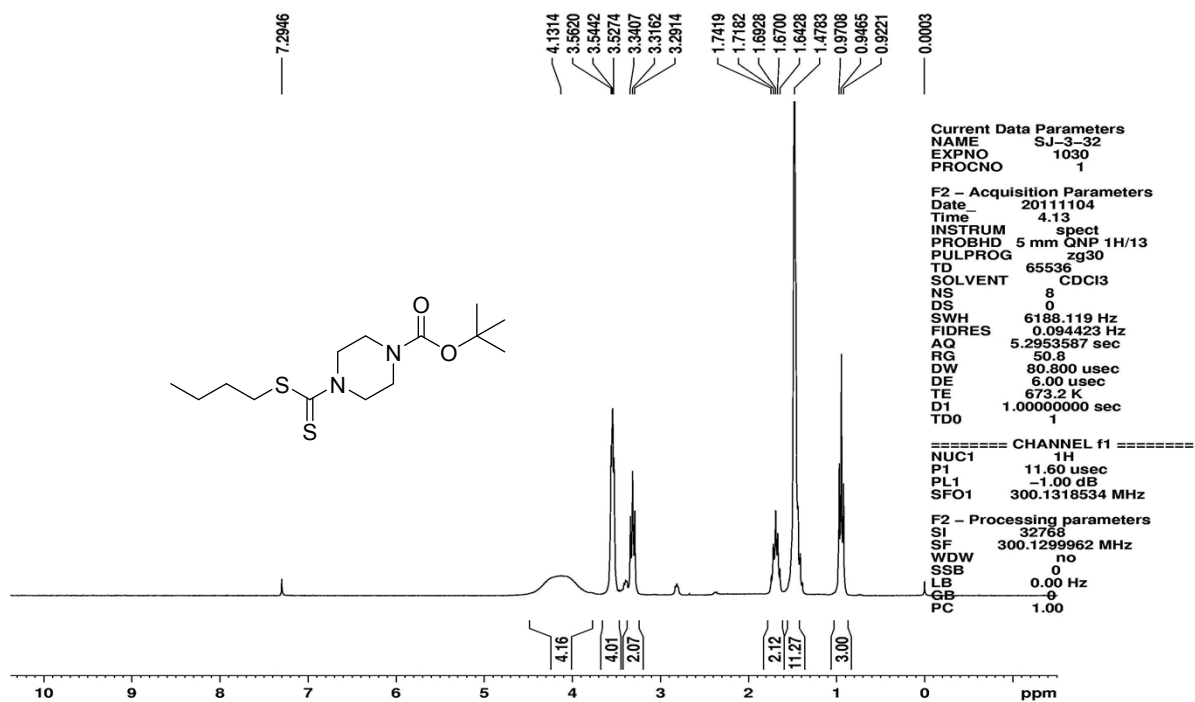


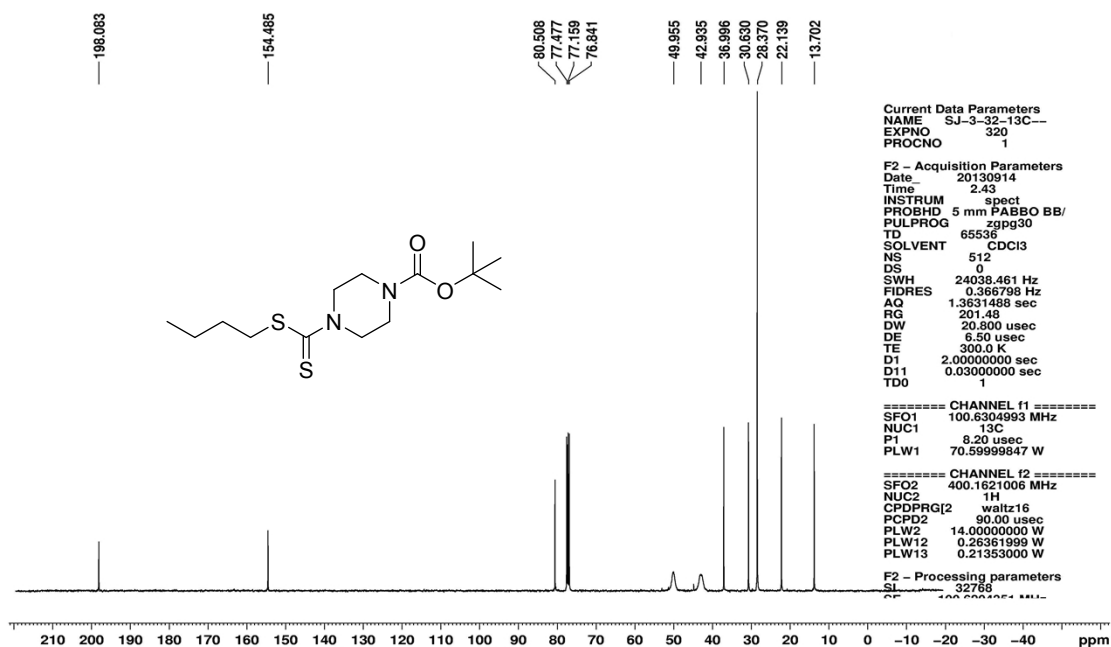
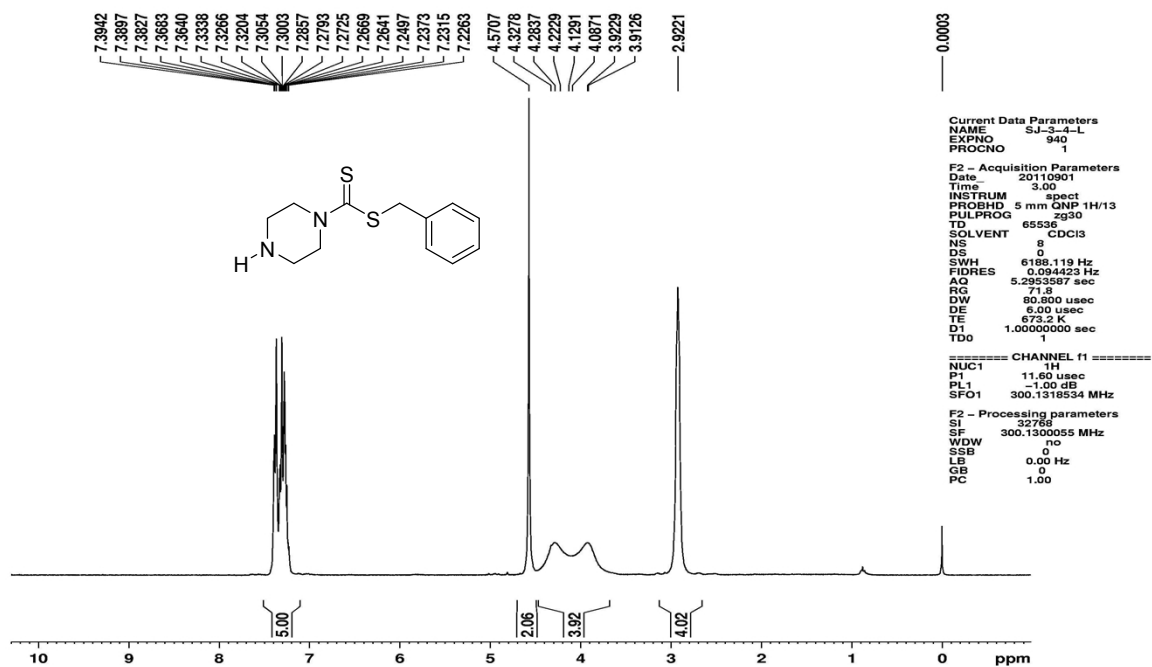
¹H NMR (300MHz, CDCl₃) of compound 5

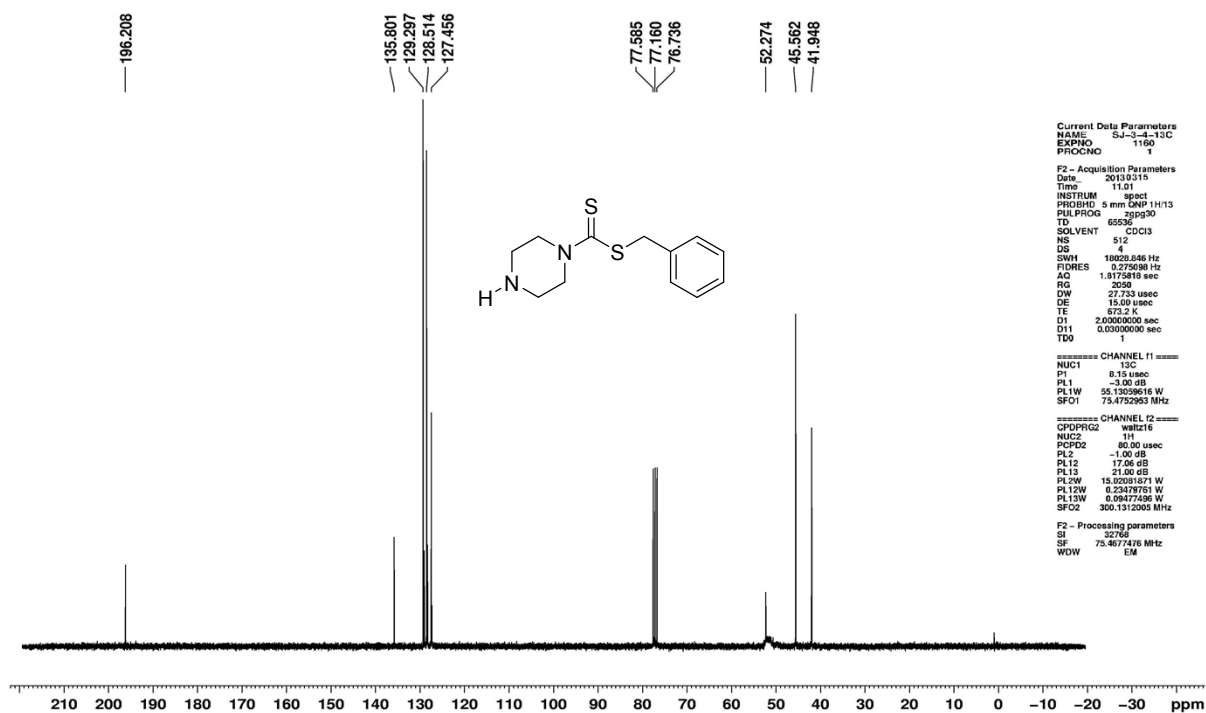


¹³C NMR (50 MHz, CDCl₃) of compound 5

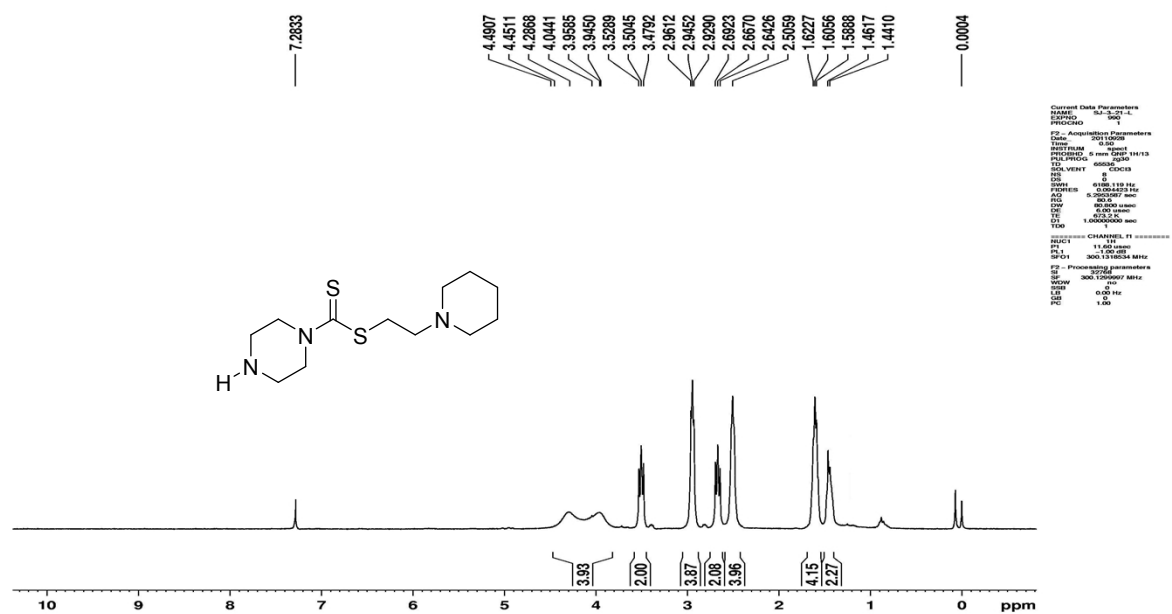
¹H NMR (300MHz, CDCl₃) of compound 6¹H NMR (300 MHz, CDCl₃) of compound 7

 ^{13}C NMR (100 MHz, CDCl_3) of compound 7 ^1H NMR (300 MHz, CDCl_3) of compound 8

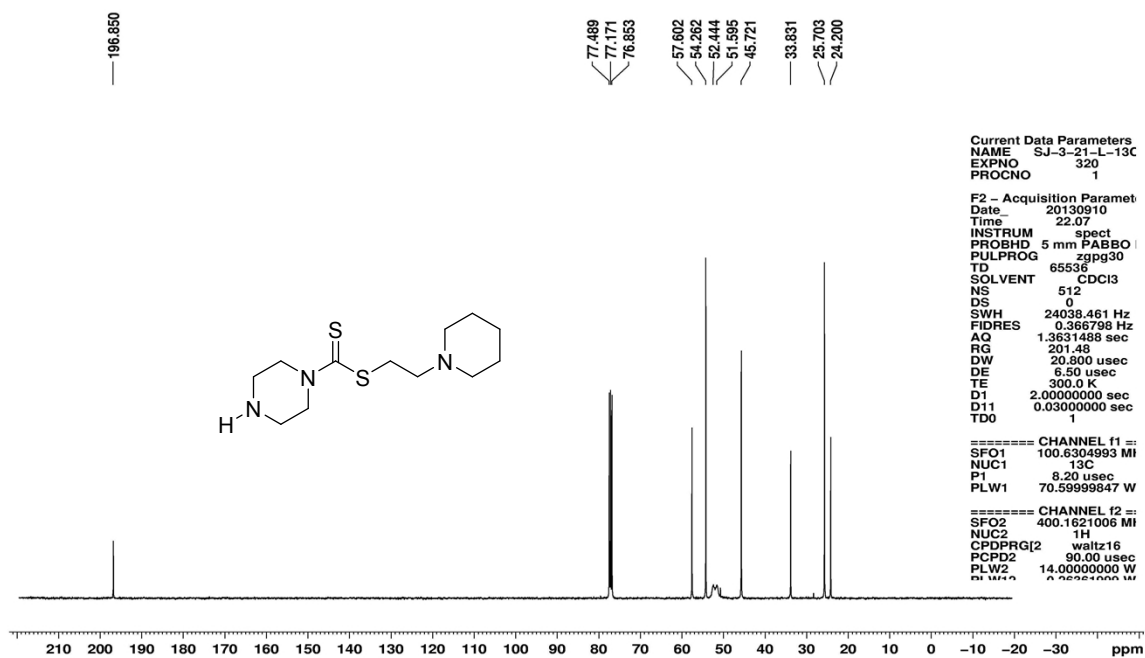
 ^{13}C NMR (100 MHz, CDCl_3) of compound 8 ^1H NMR (300 MHz, CDCl_3) of compound 9



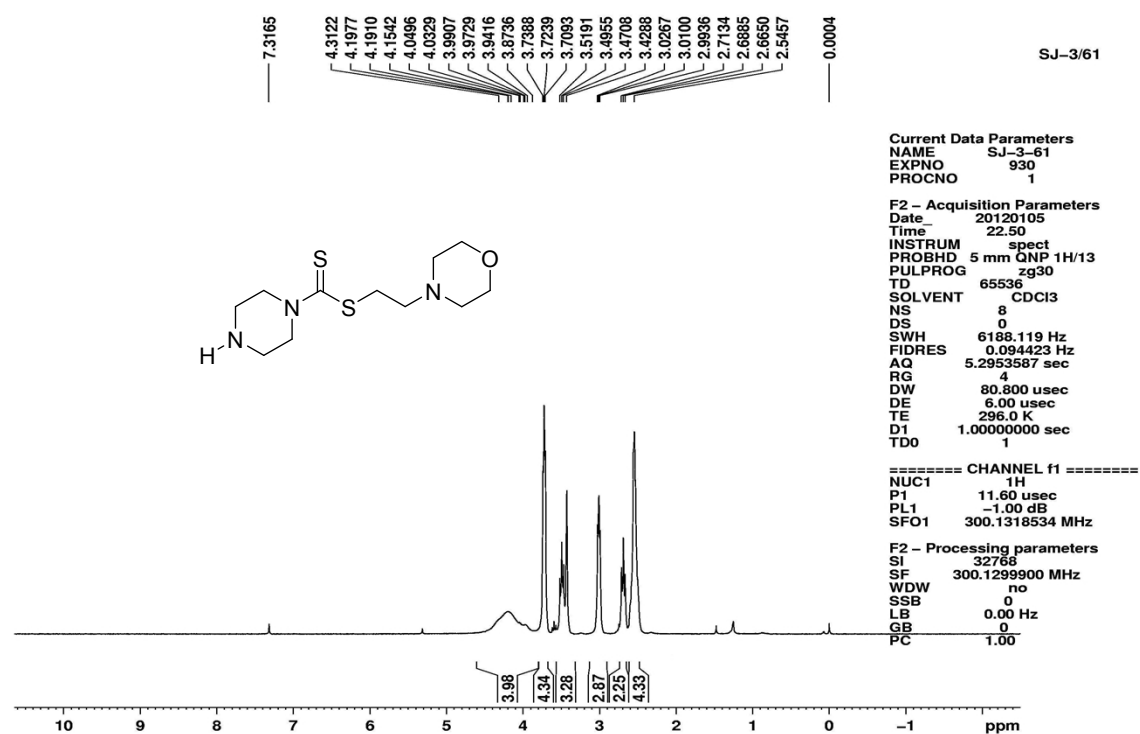
¹³C NMR (75 MHz, CDCl₃) of compound 9



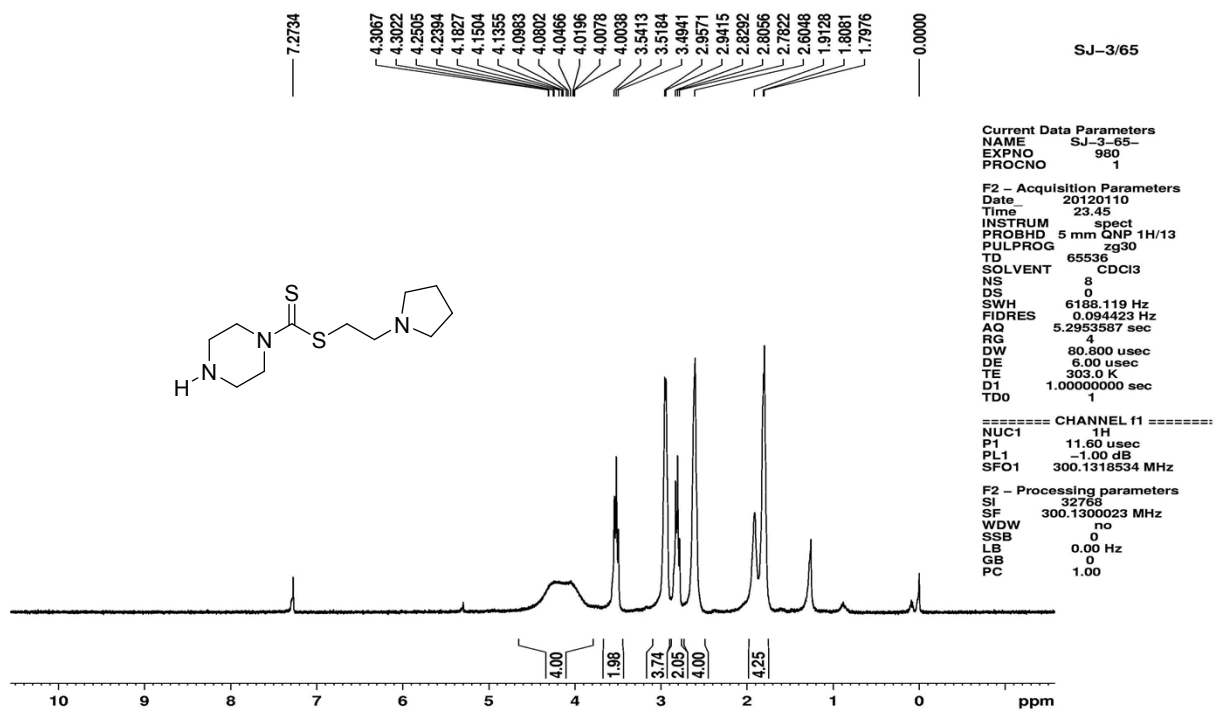
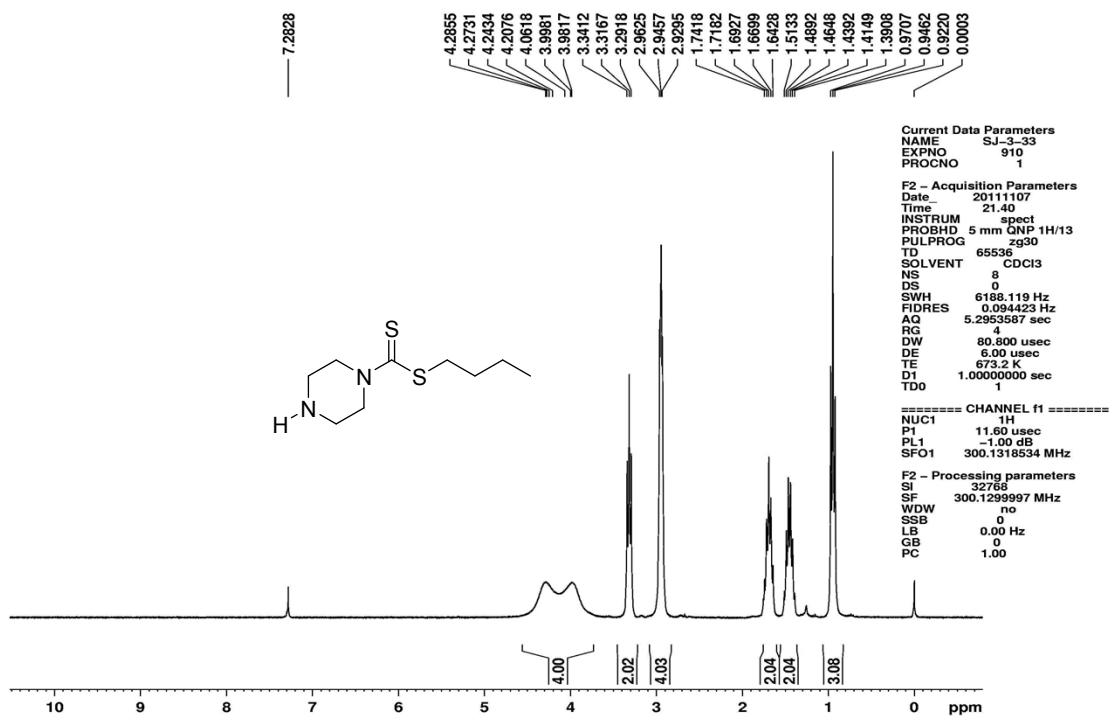
¹H NMR (300 MHz, CDCl₃) of compound 10

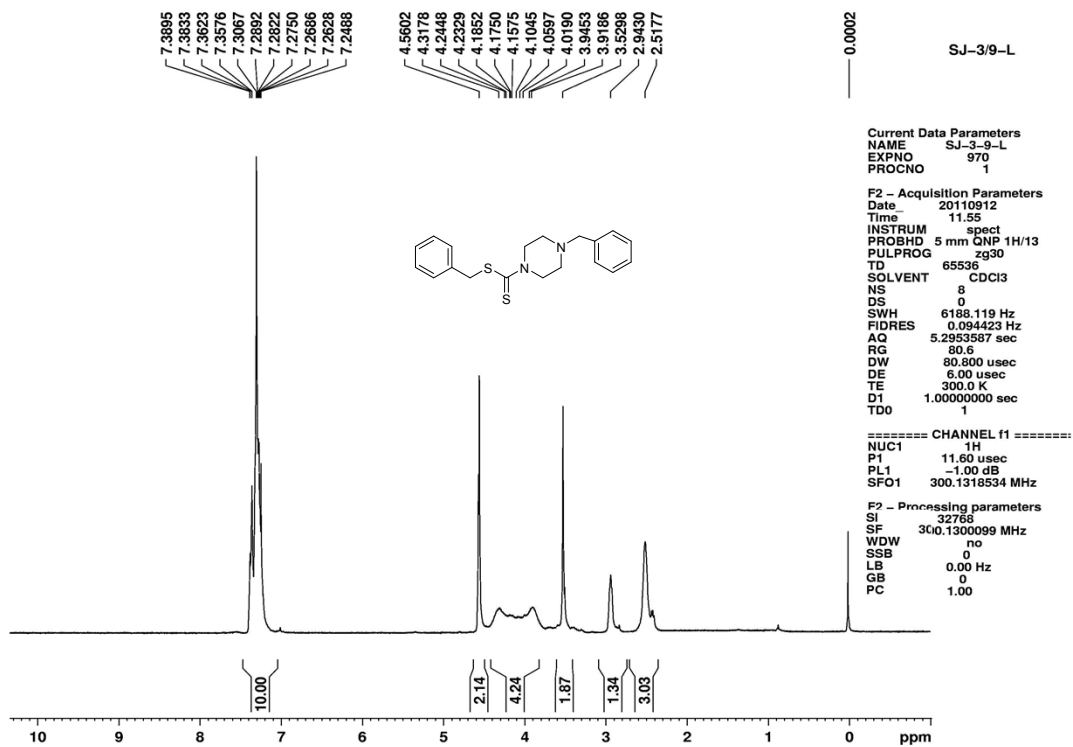


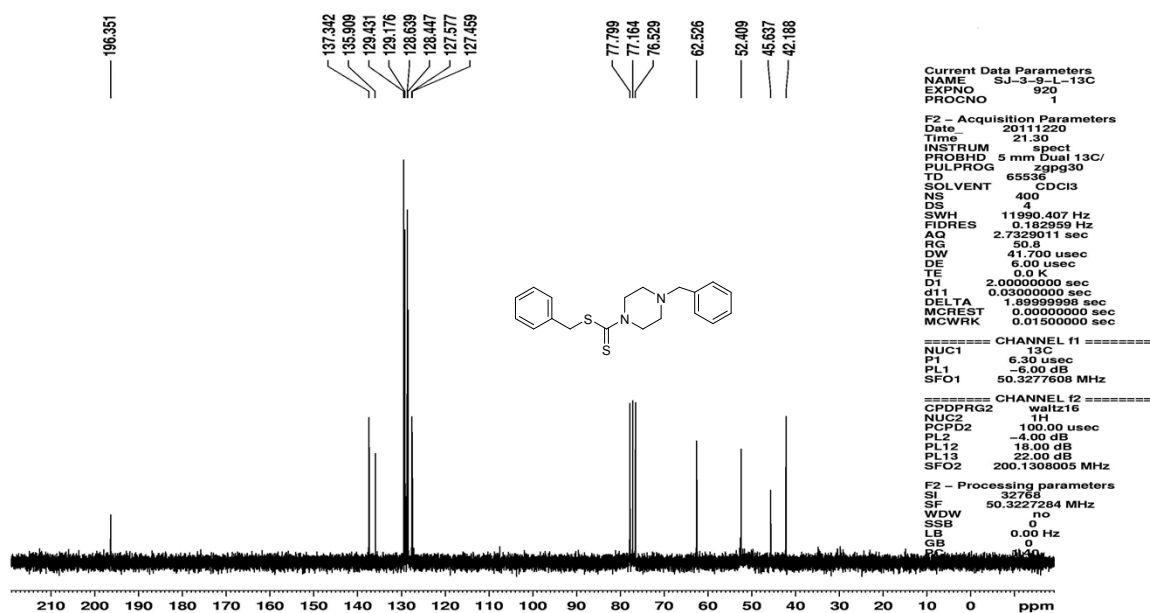
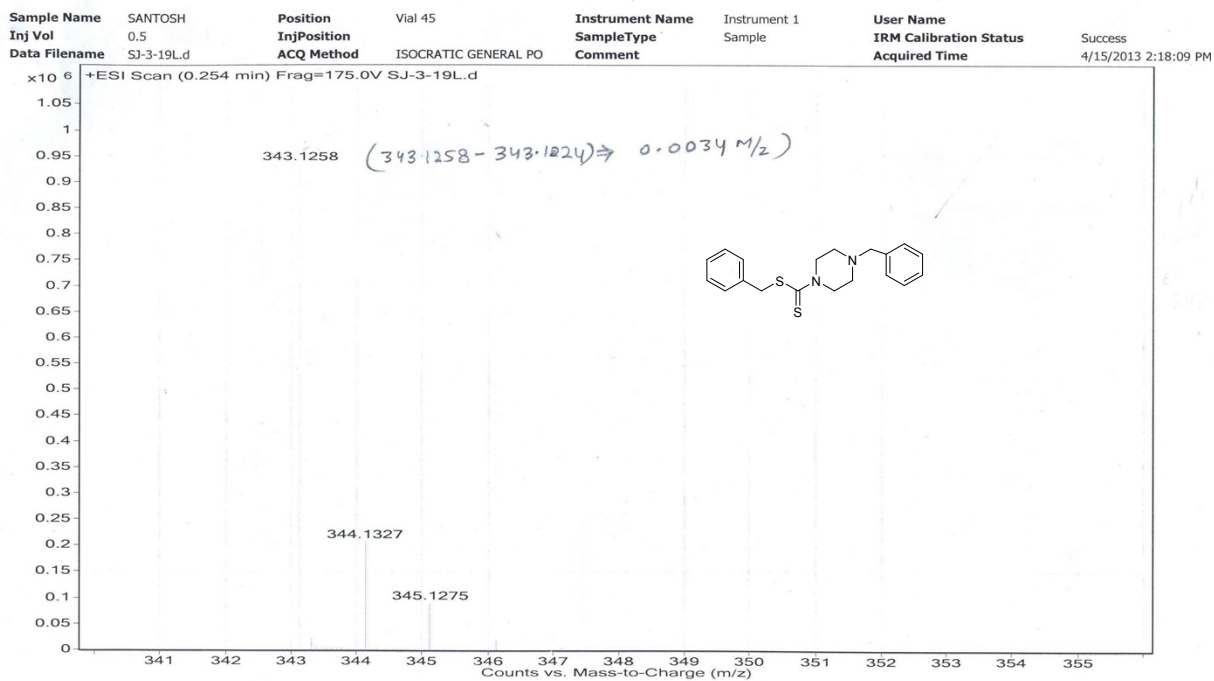
¹³C NMR (100 MHz, CDCl₃) of compound 10



¹H NMR (300 MHz, CDCl₃) of compound 11

¹H NMR (300 MHz, CDCl₃) of compound **12**¹H NMR (300 MHz, CDCl₃) of compound **13**

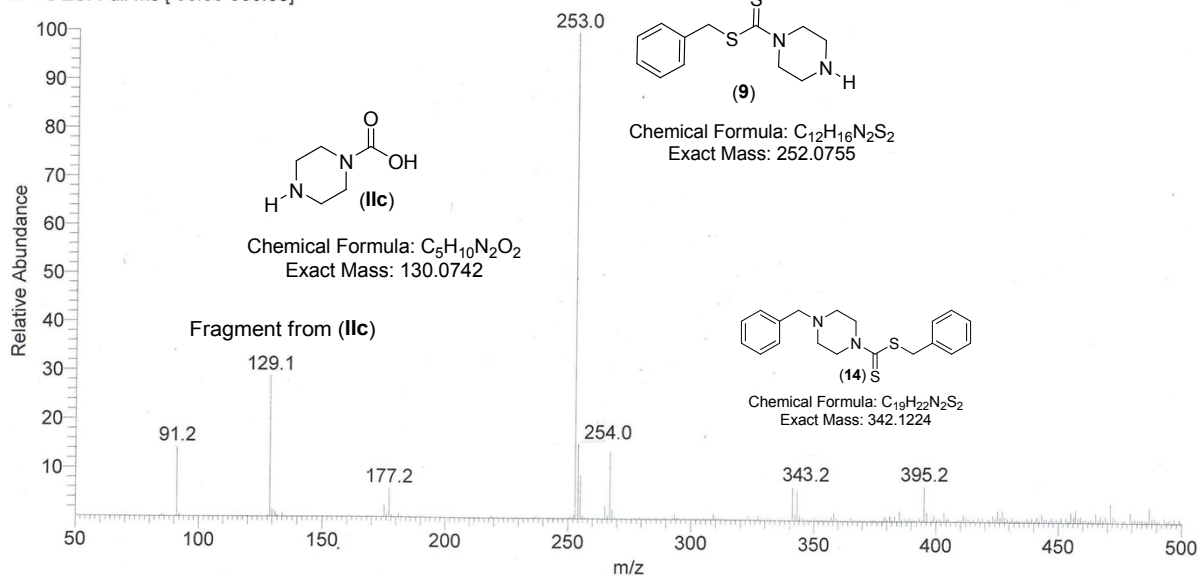
¹³C NMR (100 MHz, CDCl₃) of compound 13¹H NMR (300 MHz, CDCl₃) of compound 14

 ^{13}C NMR (50 MHz, CDCl_3) of compound 14

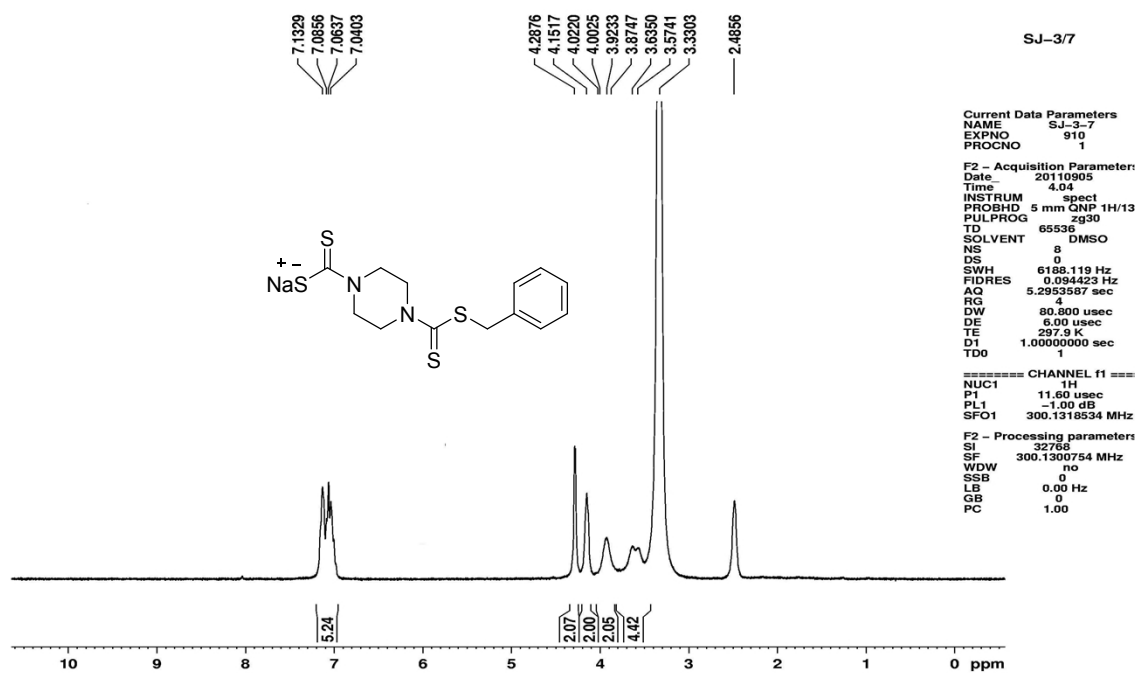
HRMS of compound 14

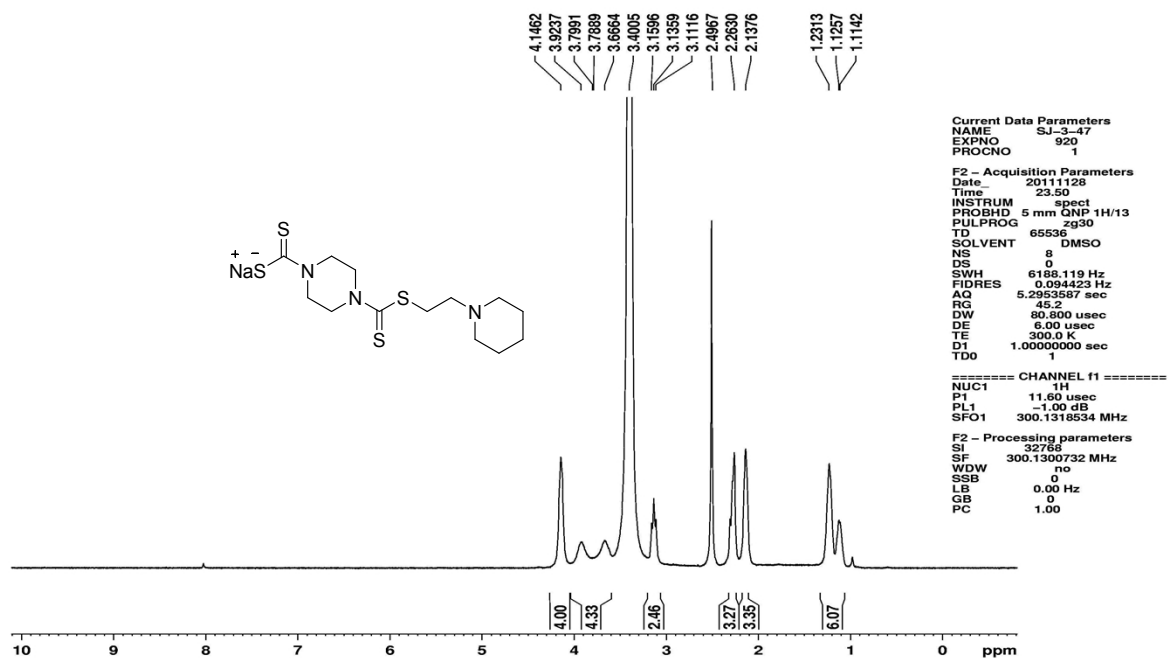
SAIF, CSIR- CDRI, LUCKNOW

Original Data Path: SJ3-4DC-14.RAW
 Current Data Path: C:\DATA2013\15APR13\
 Sample ID: SJ3-4DC
 Acquisition Date: 4/15/2013 5:47:14 PM
 Vial: A:14
 SJ3-4DC-14 #43-97 RT: 0.79-1.81 AV: 55 SB: 2 0.00, 0.00 NL: 3.81E5
 T: + c ESI Full ms [50.00-500.00]

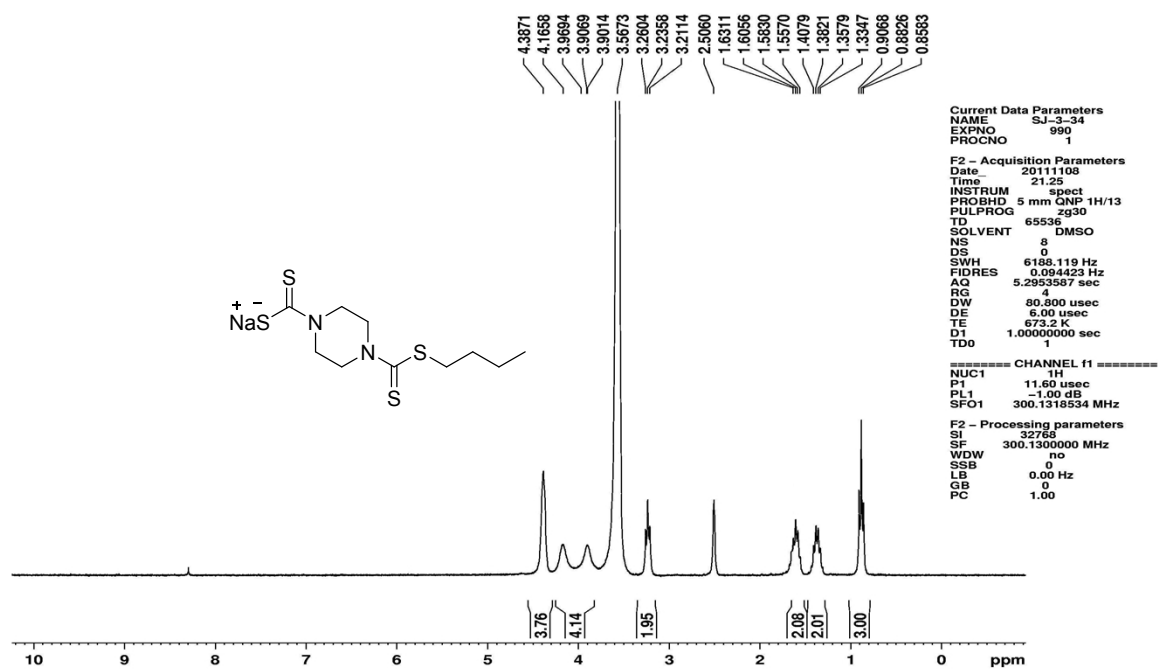


Mass spectra of reaction mixture (preparation of compound 9)

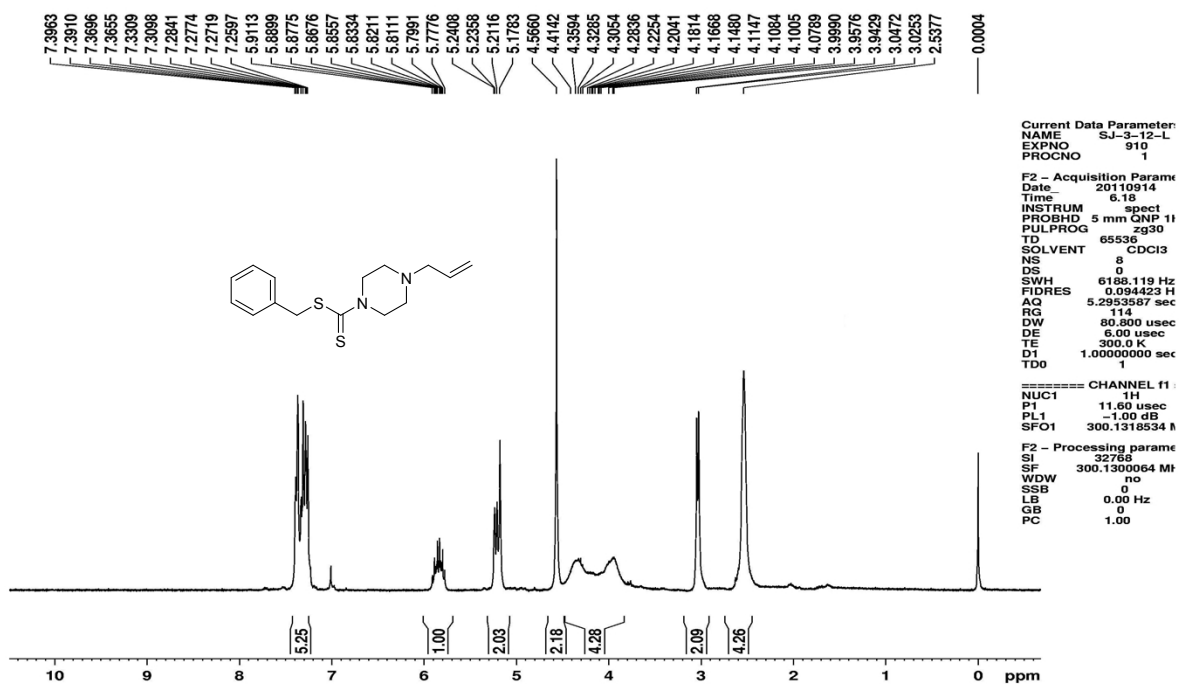
 ^1H NMR (300 MHz, DMSO- d_6) of compound 15



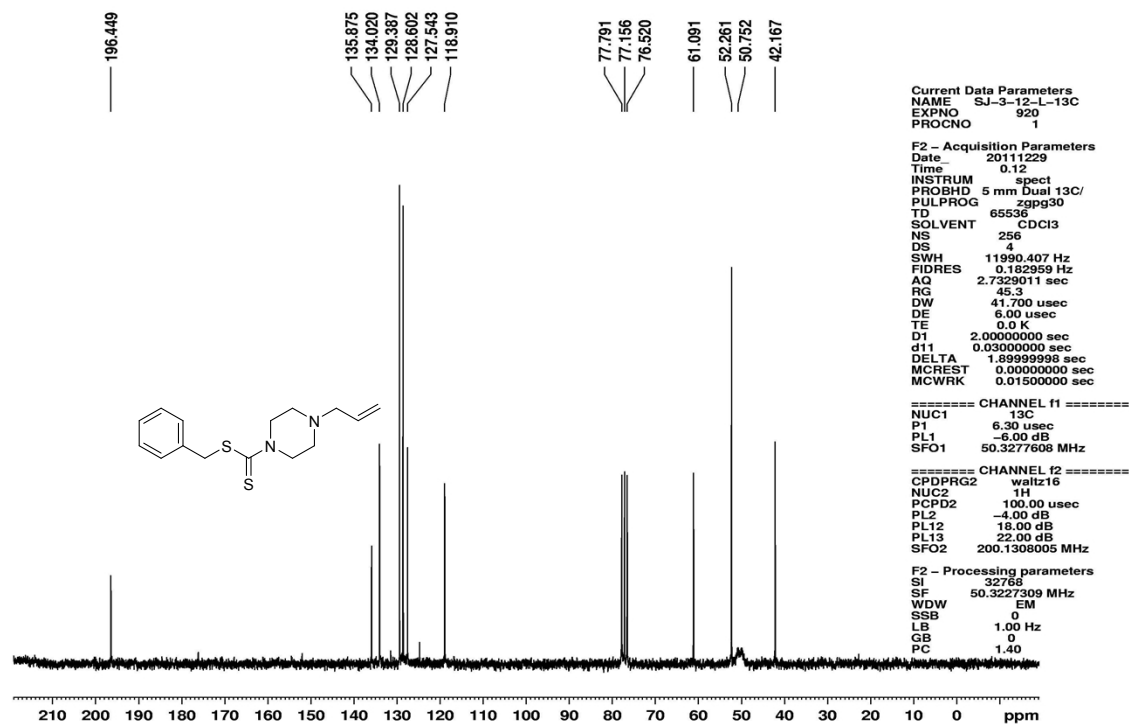
^1H NMR (300 MHz, DMSO- d_6) of compound **19**



^1H NMR (300 MHz, DMSO- d_6) of compound **20**

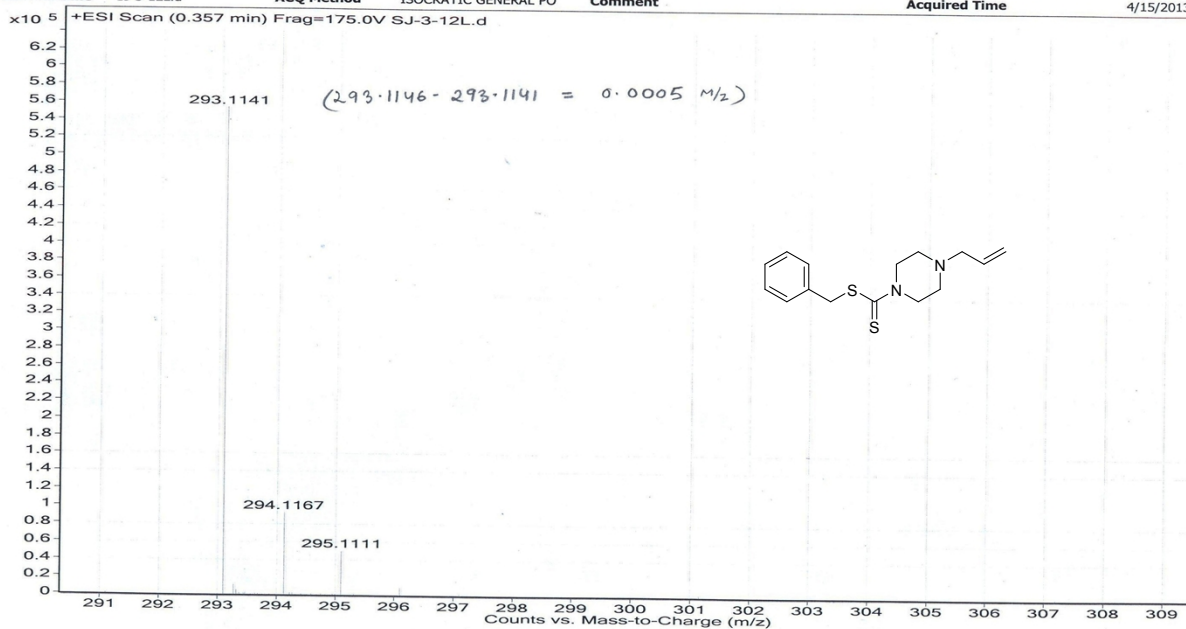


¹H NMR (300 MHz, CDCl₃) of compound 16

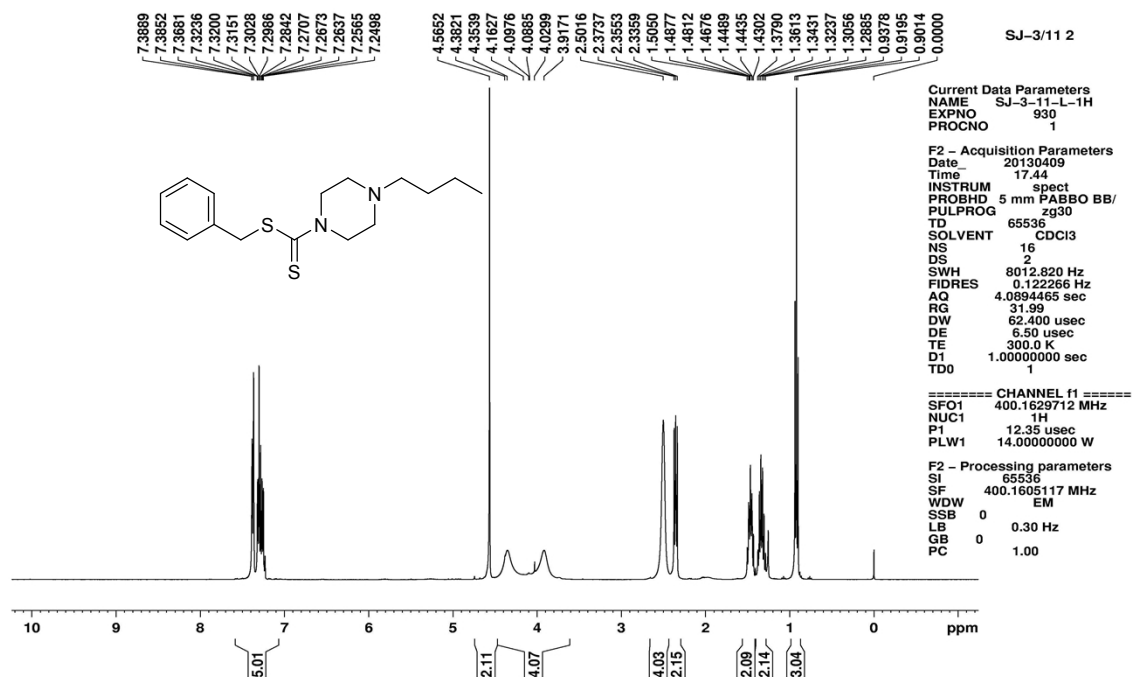


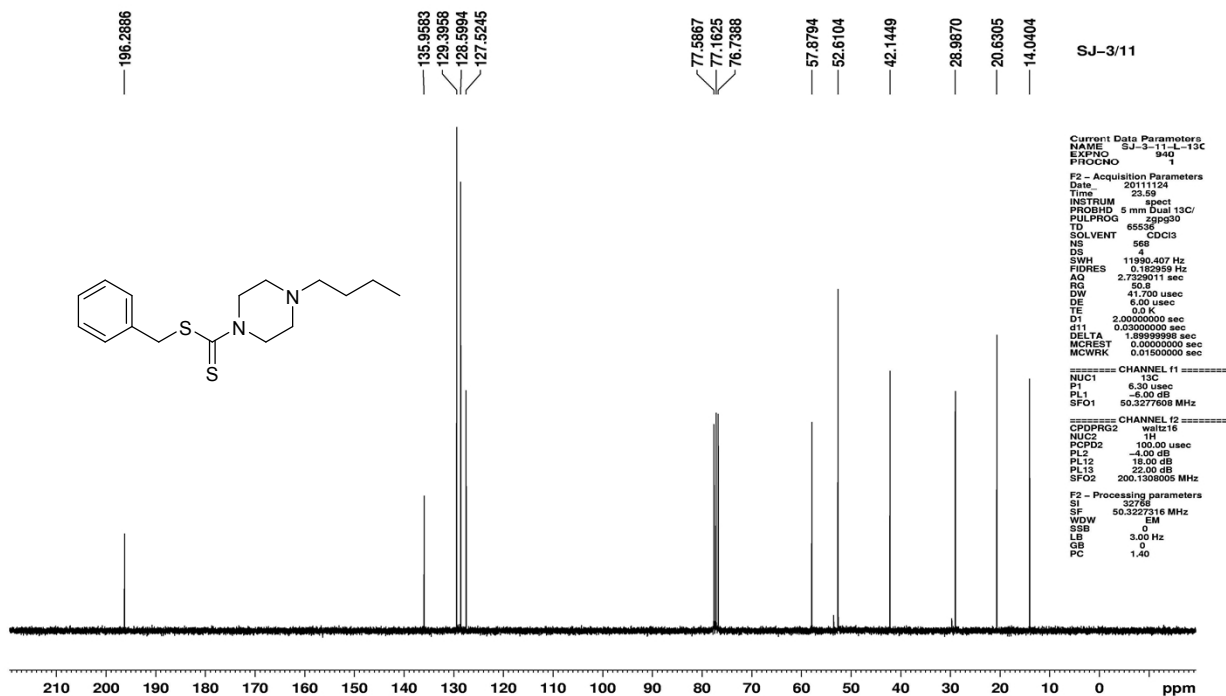
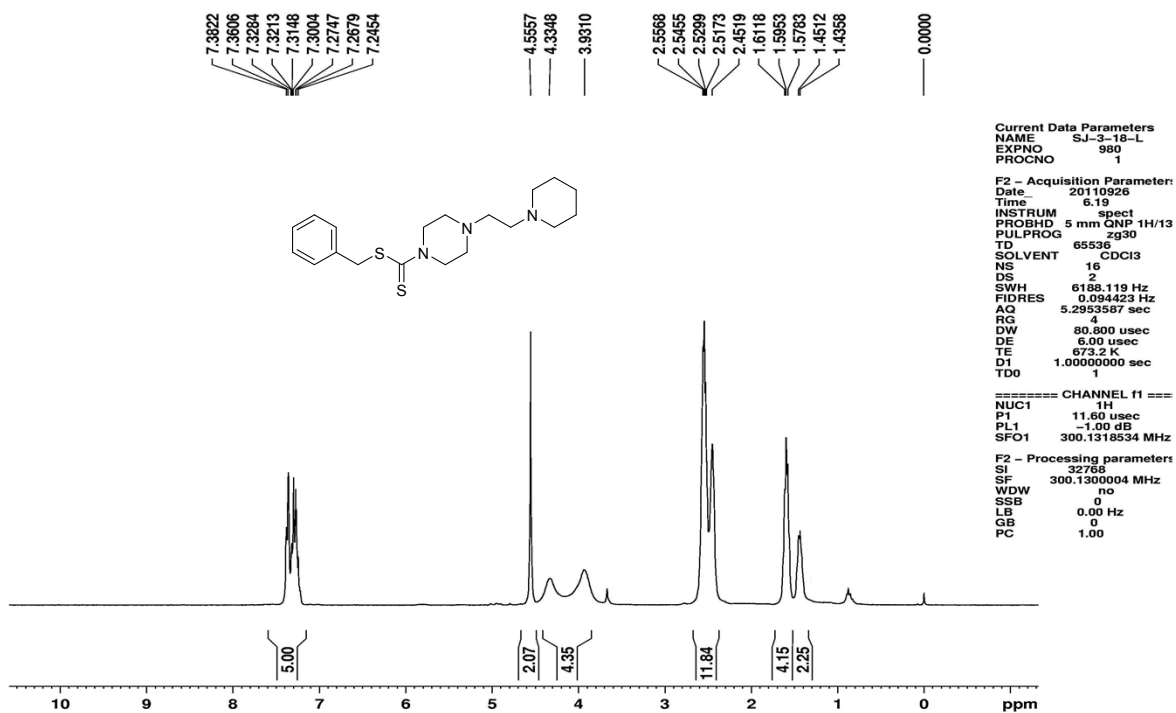
¹³C NMR (50.3 MHz, CDCl₃) of compound 16

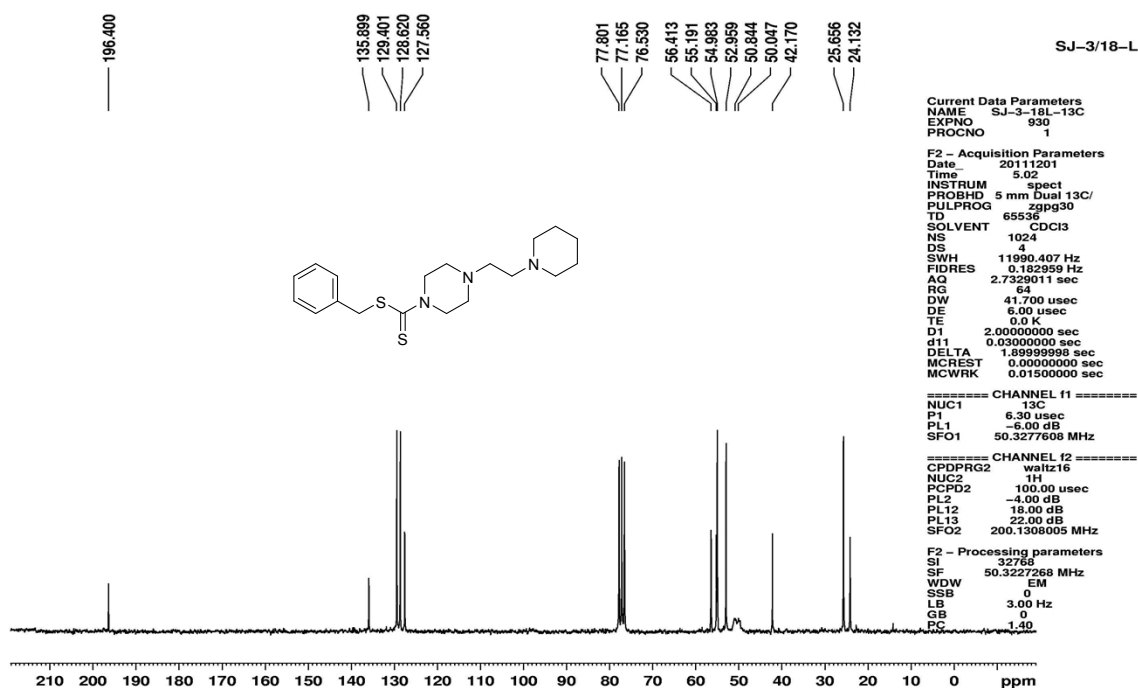
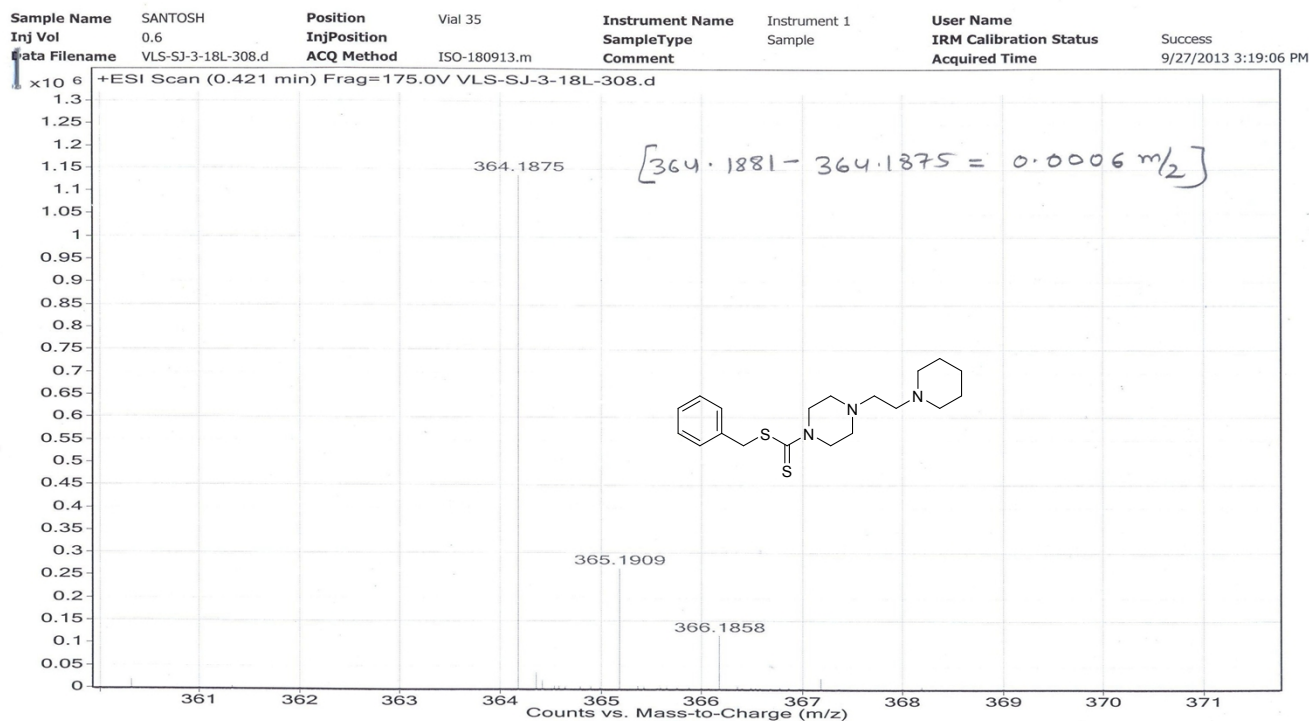
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 Data Filename SJ-3-12L.d ACQ Method ISOCRATIC GENERAL PO SampleType Comment Acquired Time 4/15/2013 2:14:30 PM



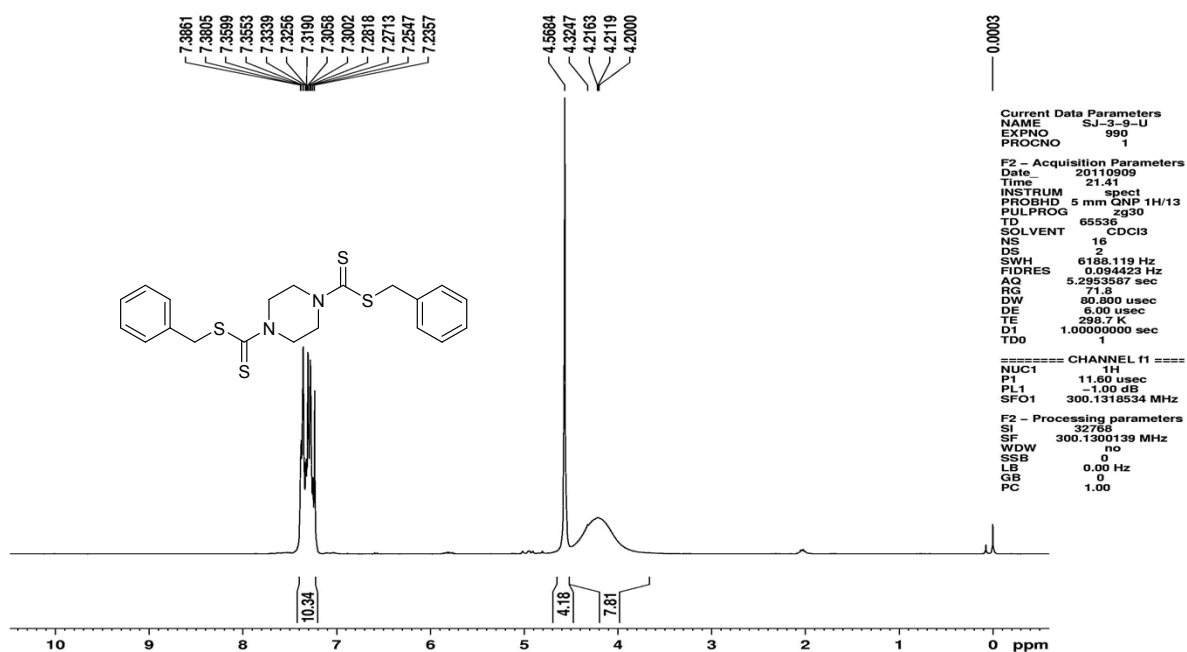
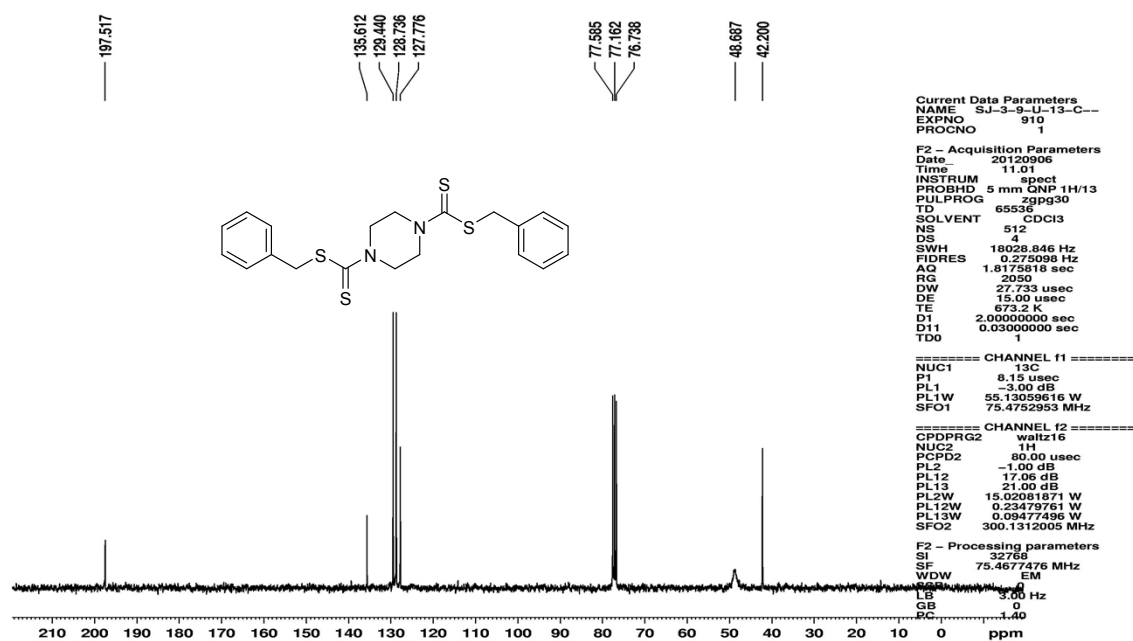
HRMS of compound 16

¹H NMR (300 MHz, CDCl₃) of compound 17

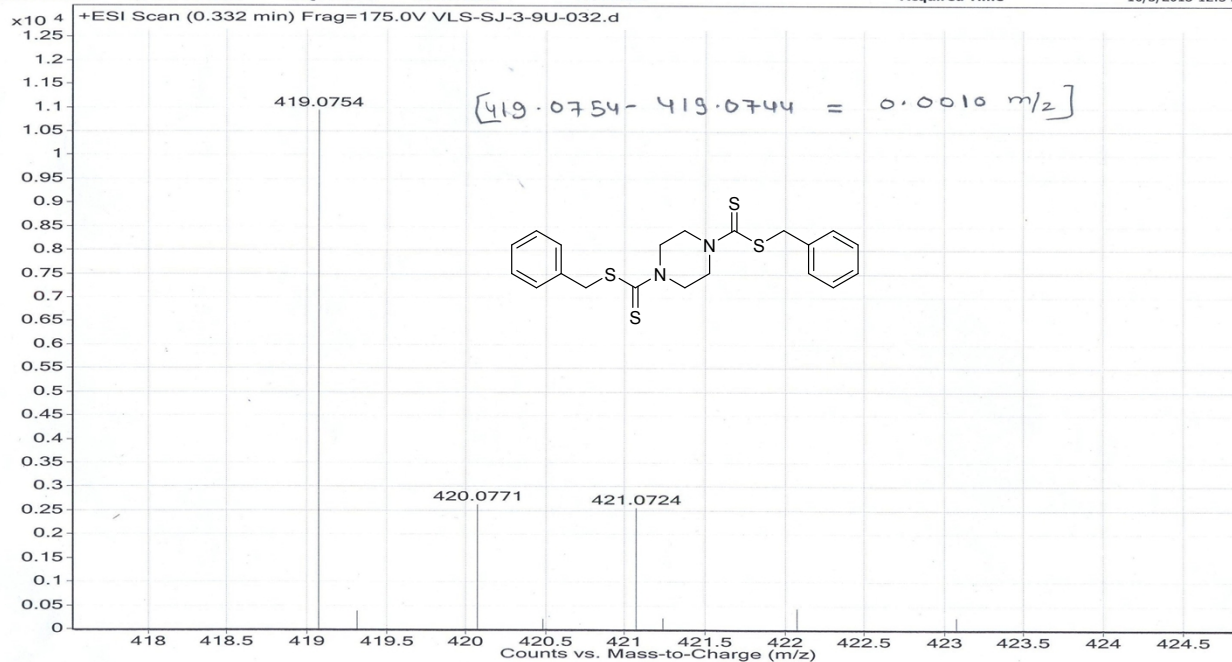
 ^{13}C NMR (50 MHz, CDCl_3) of compound 17 ^1H NMR (300 MHz, CDCl_3) of compound 18

¹³C NMR (50 MHz, CDCl₃) of compound 18

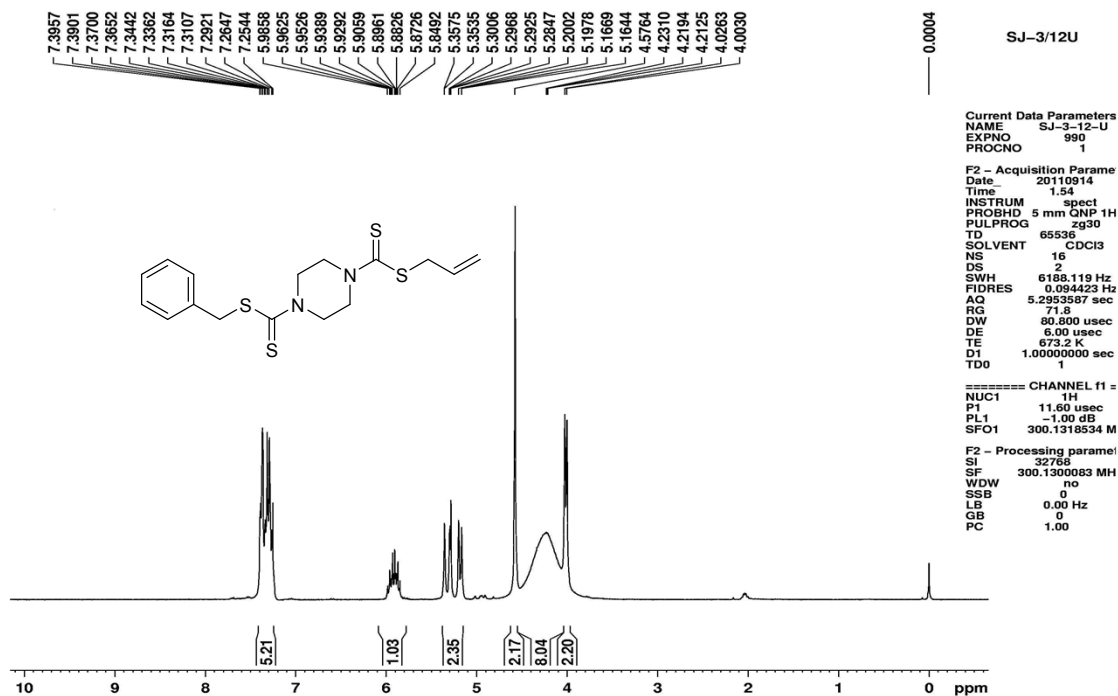
HRMS of compound 18

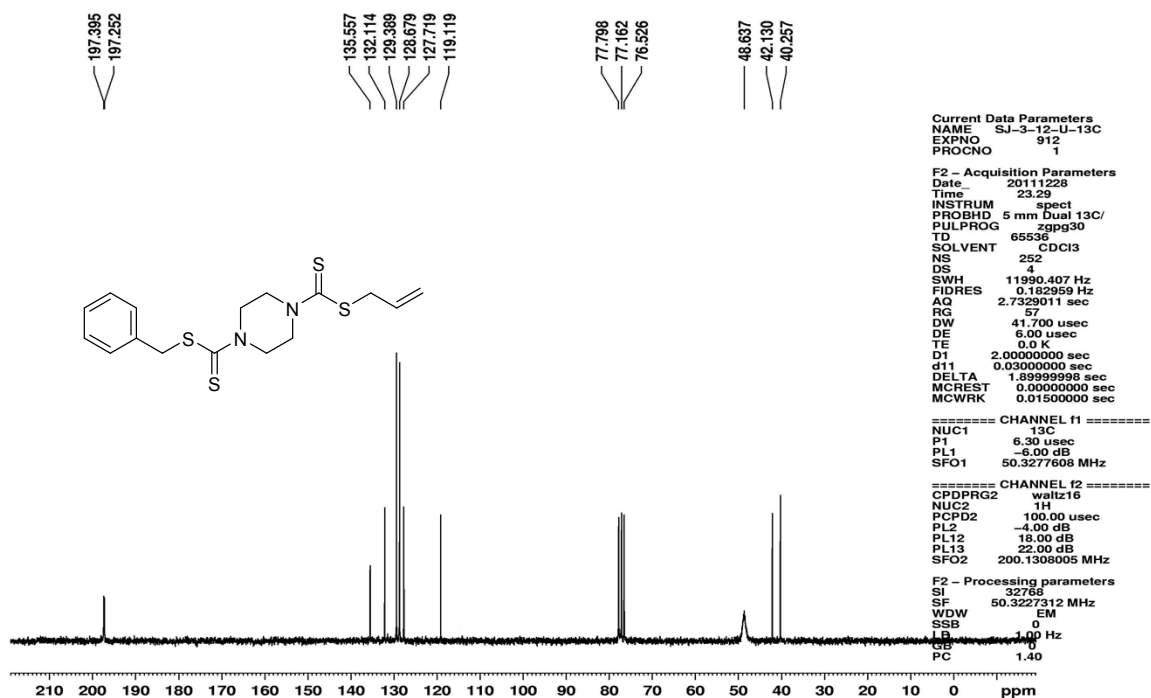
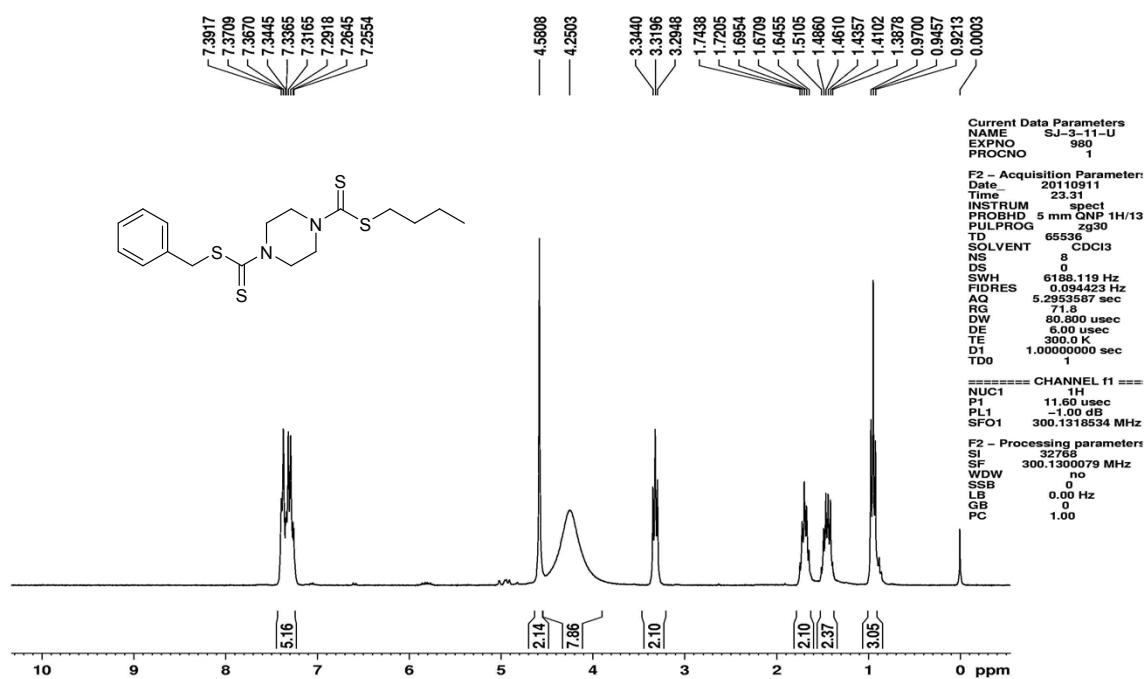
¹H NMR (300 MHz, CDCl₃) of compound 21¹³C NMR (75 MHz, CDCl₃) of compound 21

Sample Name SANTOSH Position Vial 41 Instrument Name Instrument 1 User Name
 Inj Vol 1 InjPosition SampleType Sample IRM Calibration Status Success
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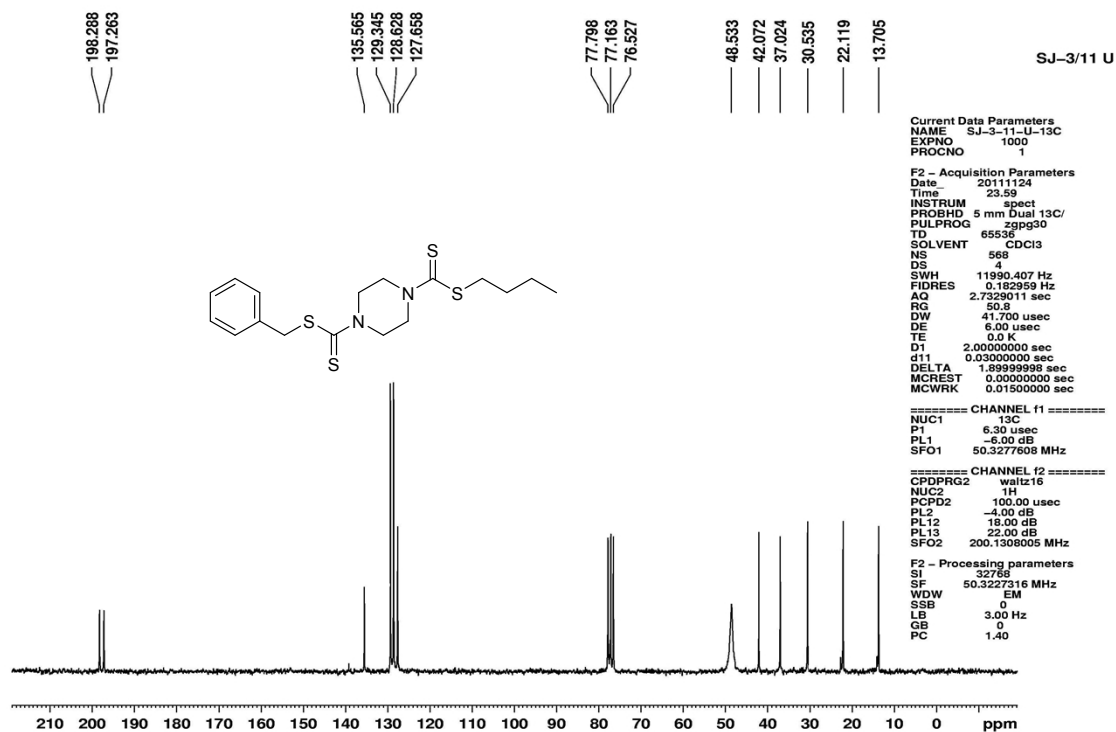
HRMS of compound 21

¹H NMR (300 MHz, CDCl₃) of compound 22

¹³C NMR (50 MHz, CDCl₃) of compound 22

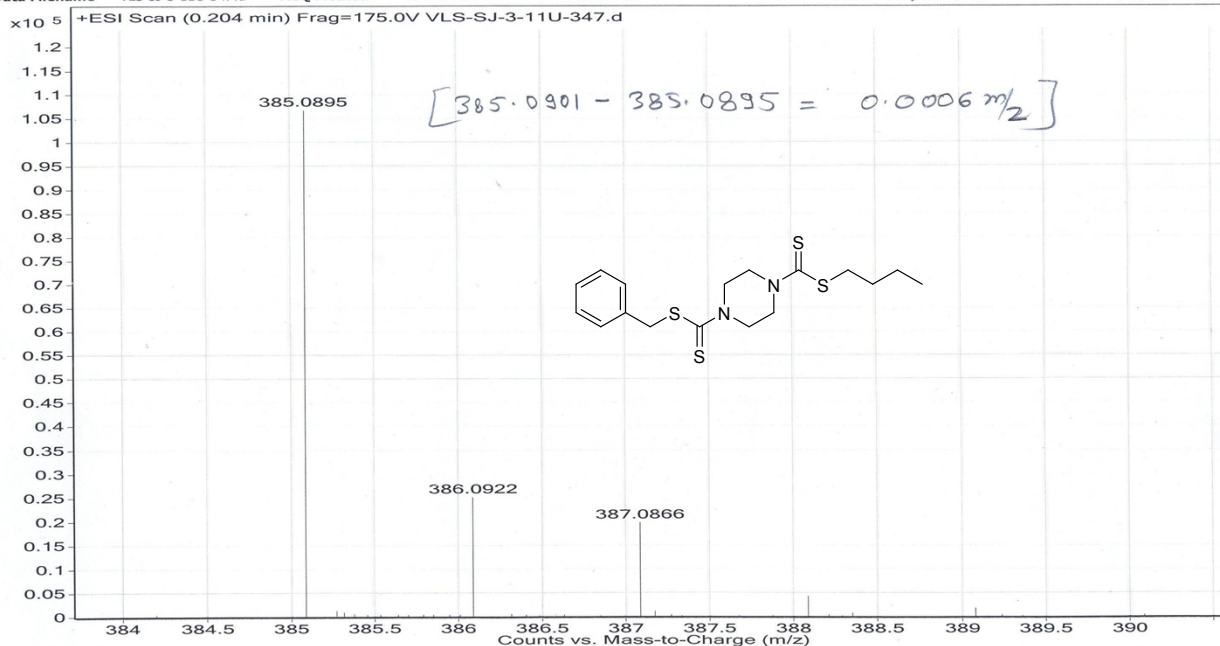
¹H NMR (300 MHz, CDCl₃) of compound **23**

S20

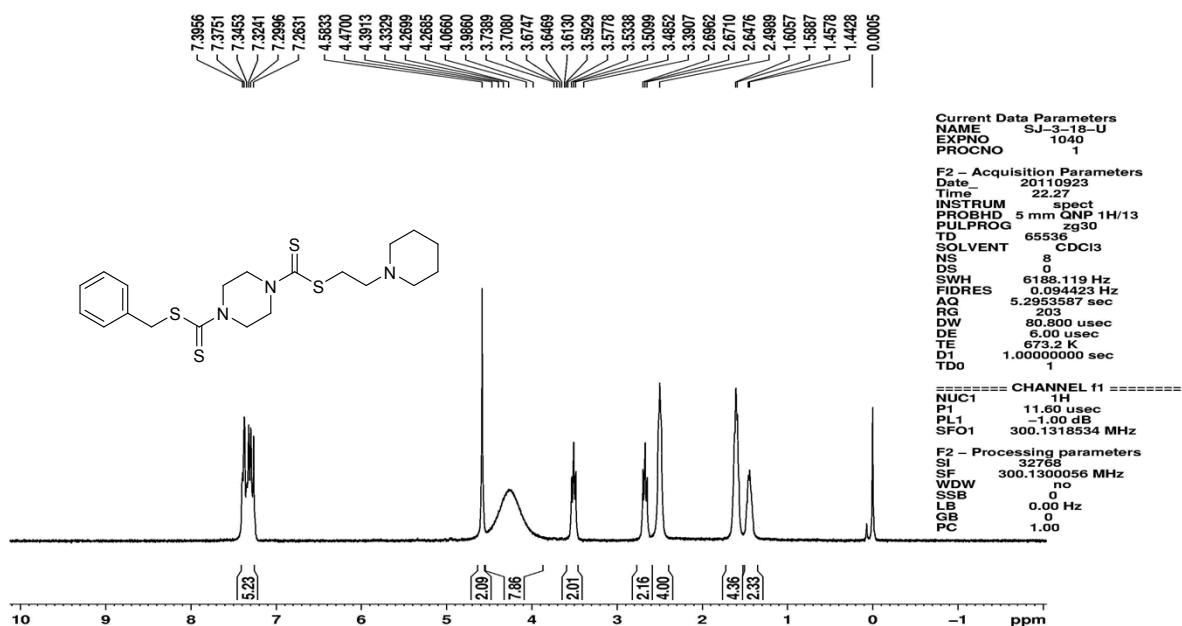
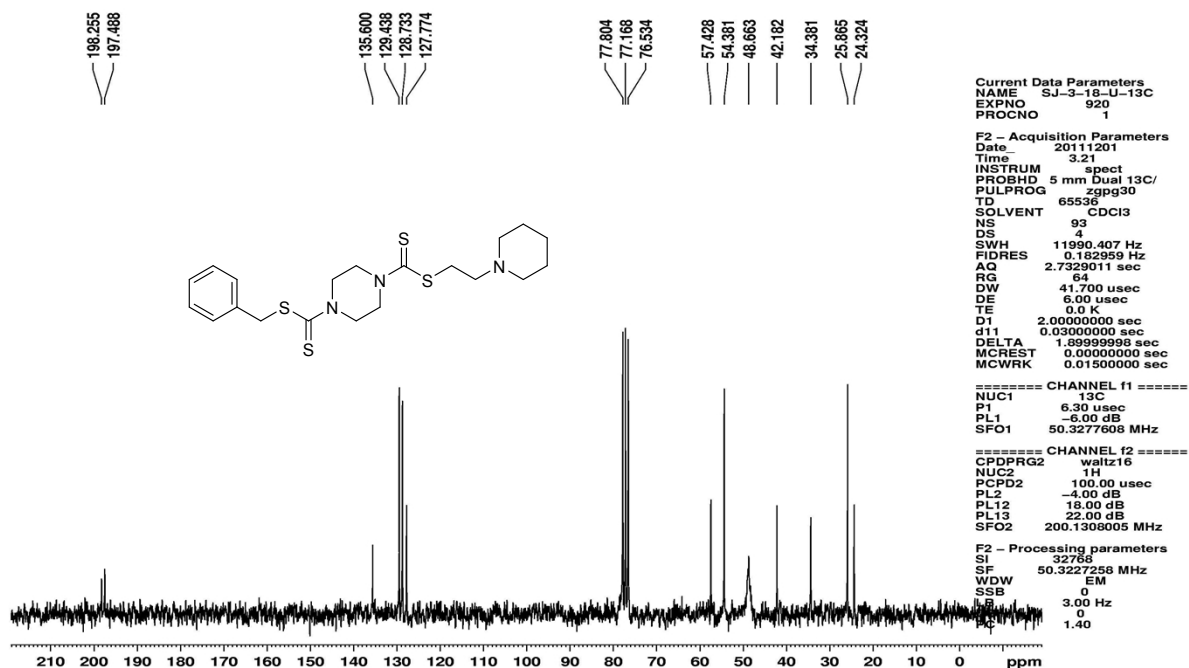


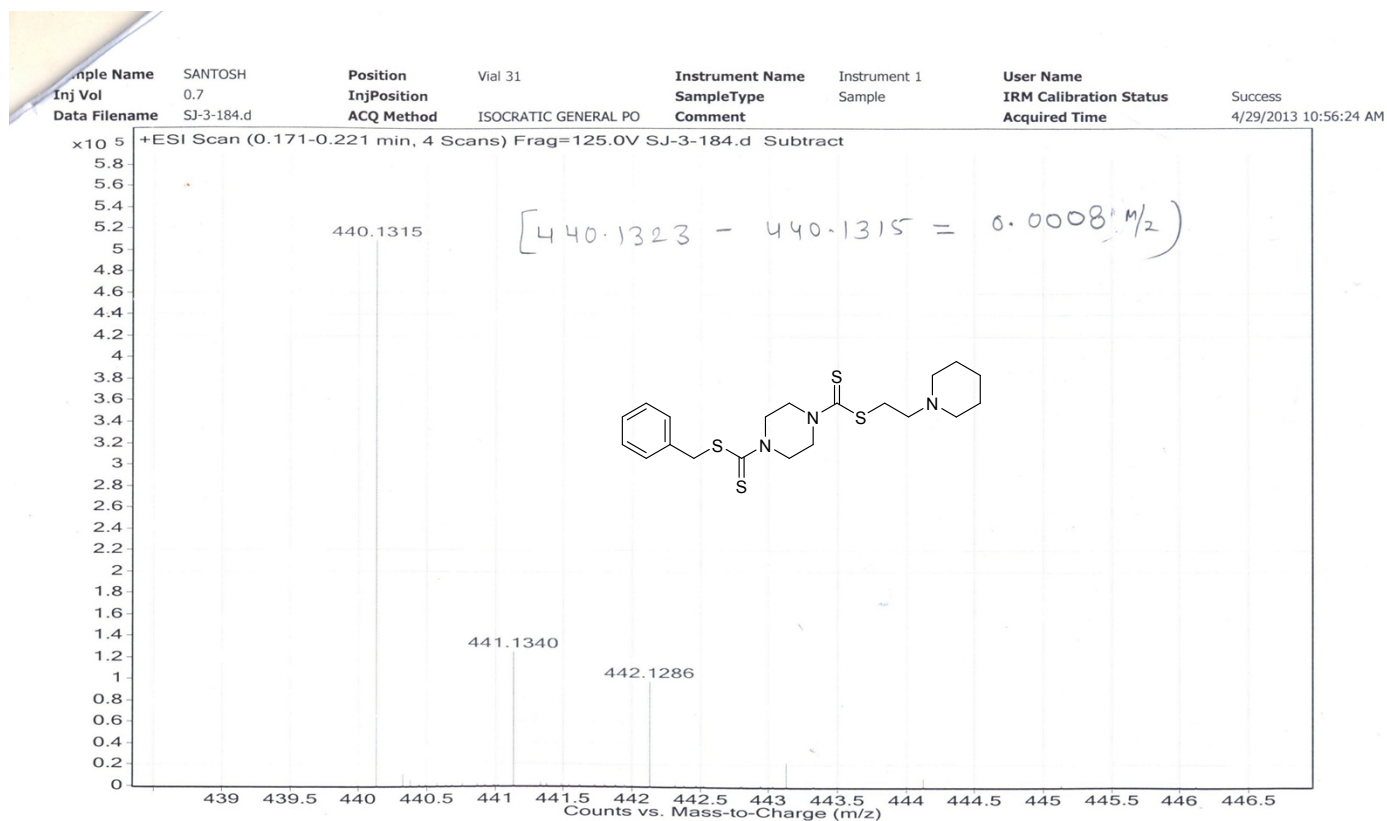
¹³C NMR (50 MHz, CDCl₃) of compound **23**

Sample Name	Dr. SHARMA	Position	Vial 42	Instrument Name	Instrument 1	User Name	
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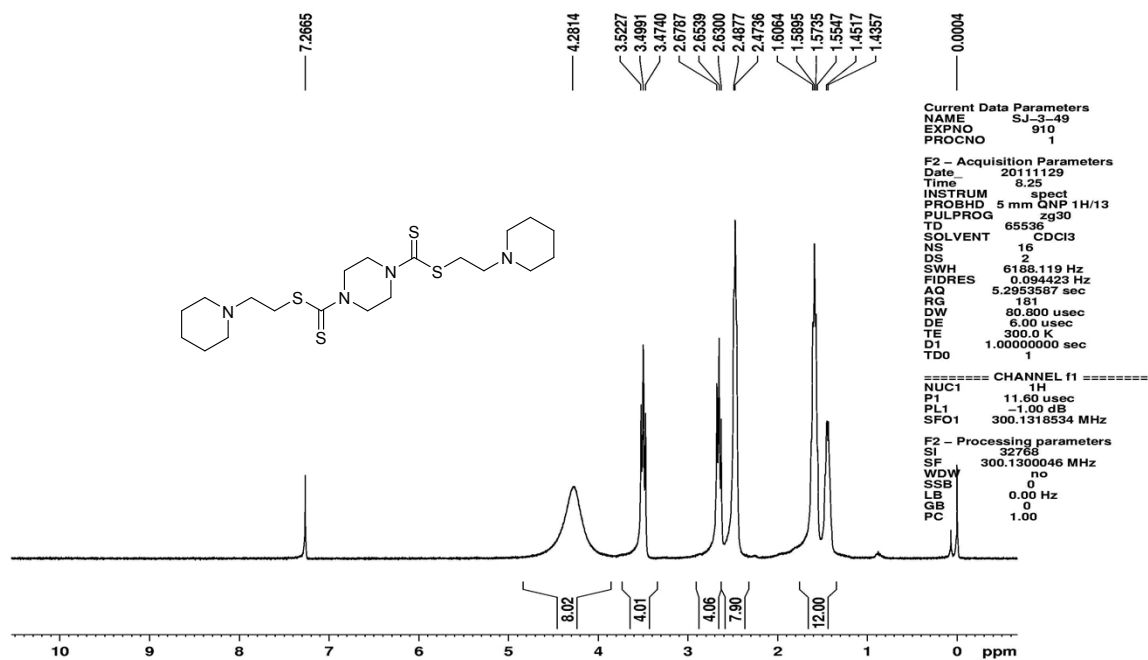


HRMS of compound **23**

¹H NMR (300 MHz, CDCl₃) of compound 24¹³C NMR (50 MHz, CDCl₃) of compound 24



HRMS of compound 24



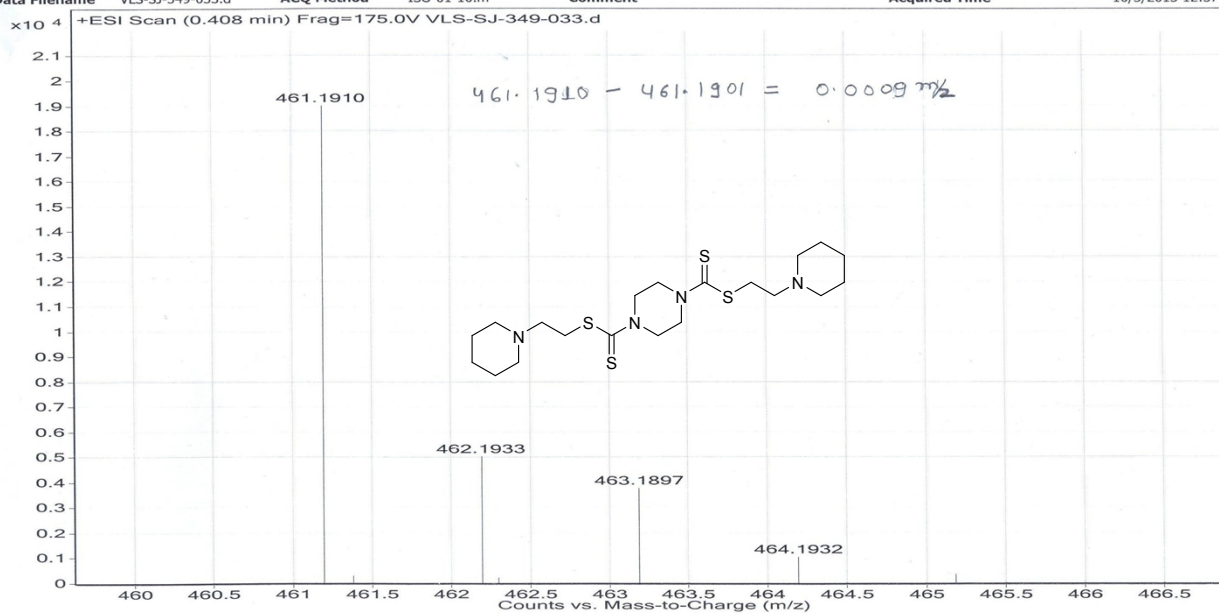
¹H NMR (300 MHz, CDCl₃) of compound 25

S23

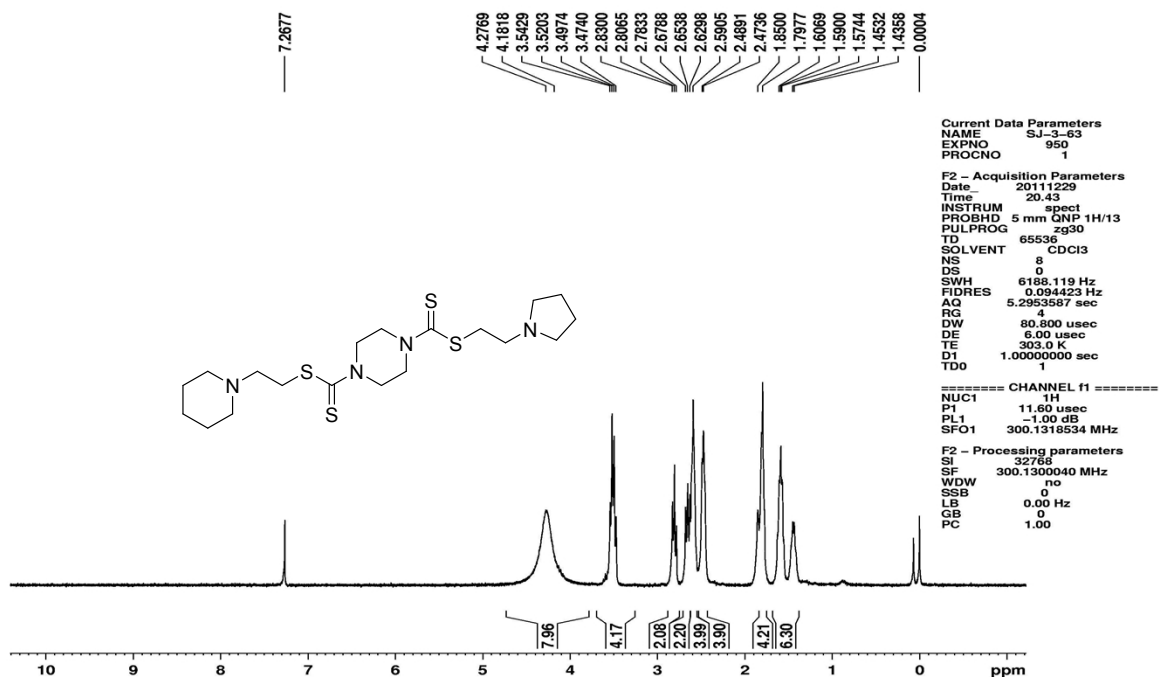


¹³C NMR (50 MHz, CDCl₃) of compound 25

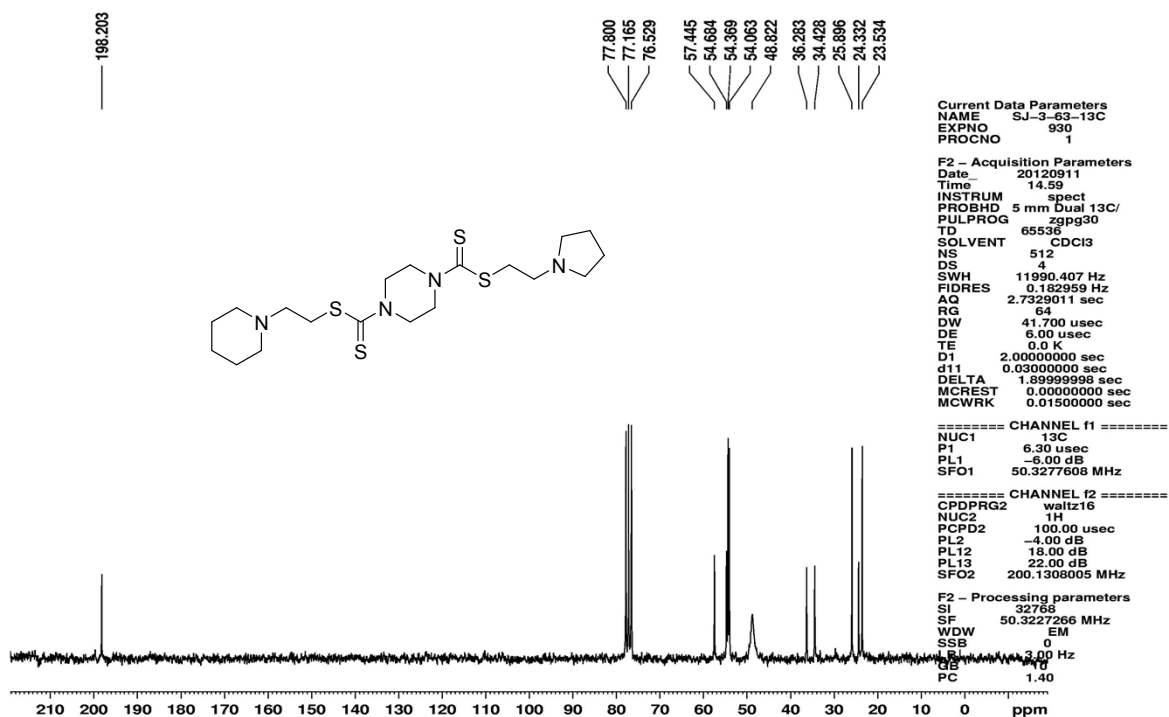
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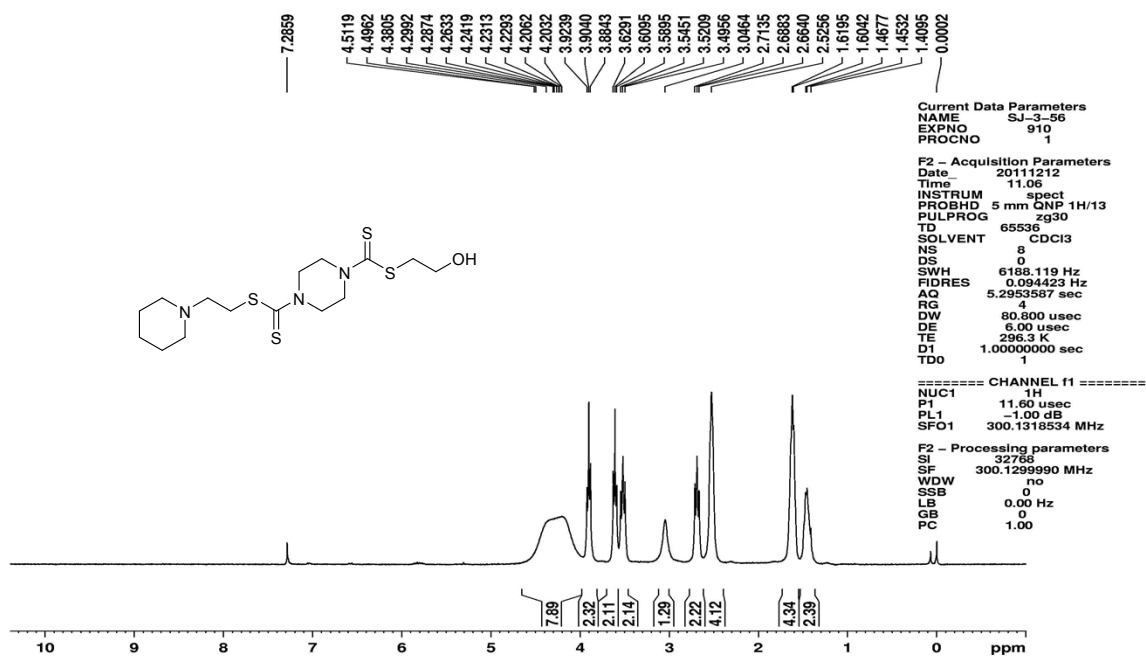
HRMS of compound 25



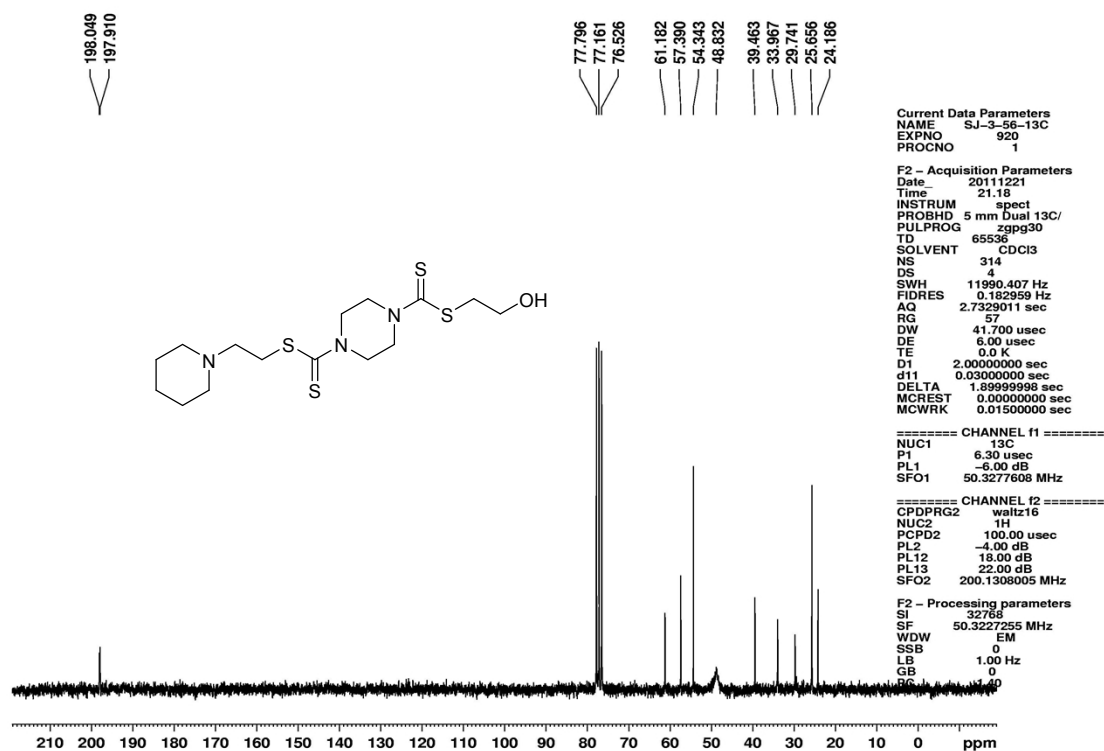
¹H NMR (300 MHz, CDCl₃) of compound 26



¹³C NMR (50 MHz, CDCl₃) of compound 26

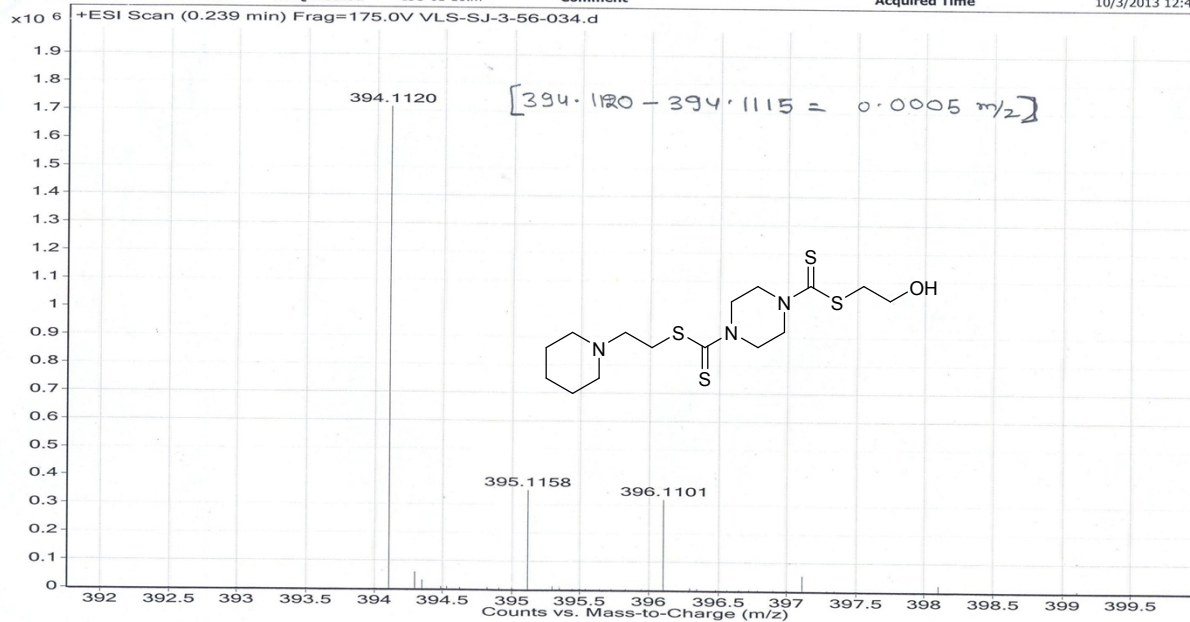


¹H NMR (300 MHz, CDCl₃) of compound **27**

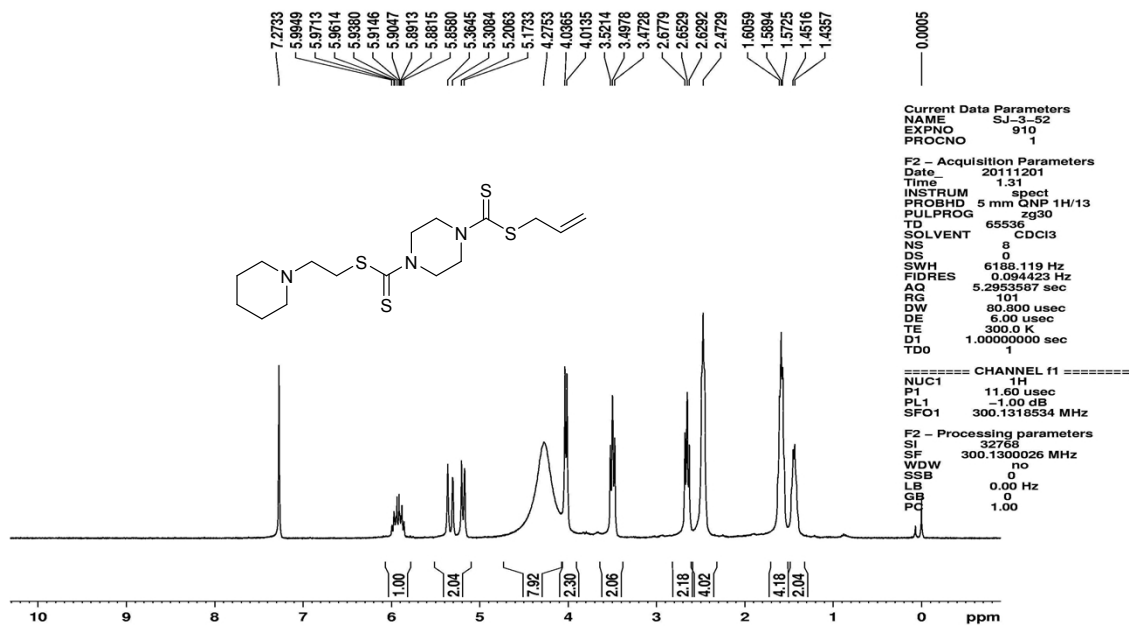


¹³C NMR (50 MHz, CDCl₃) of compound **27**

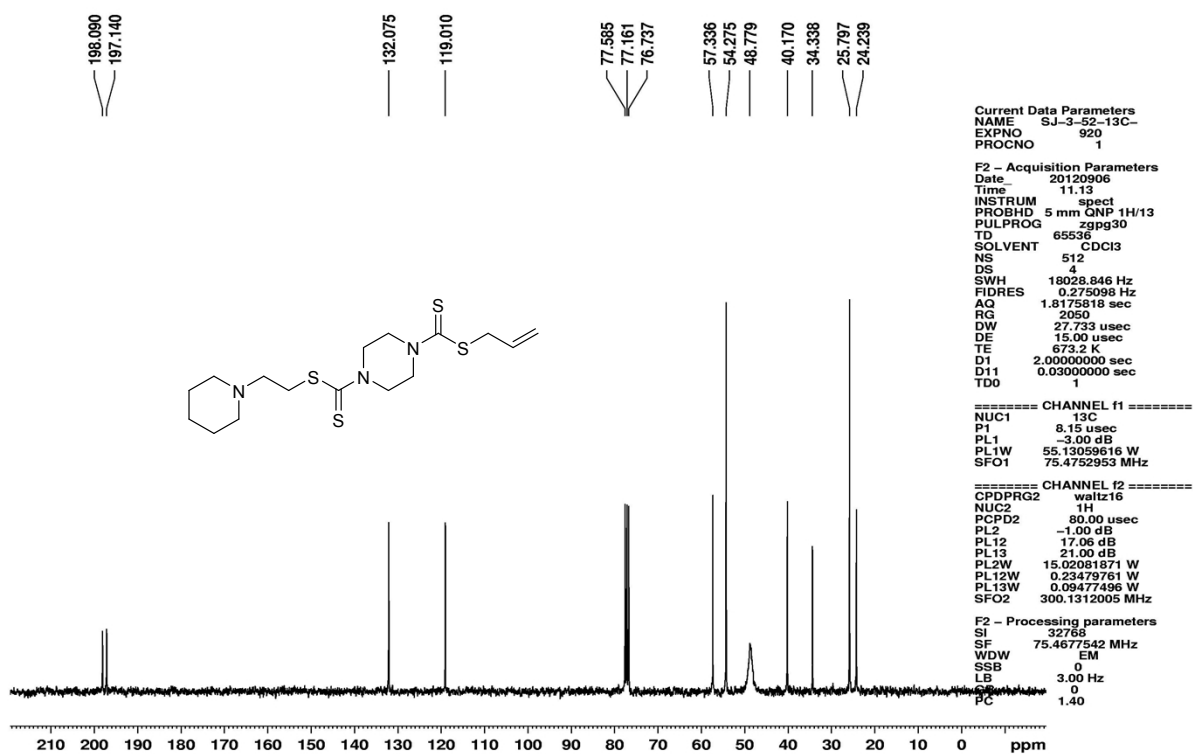
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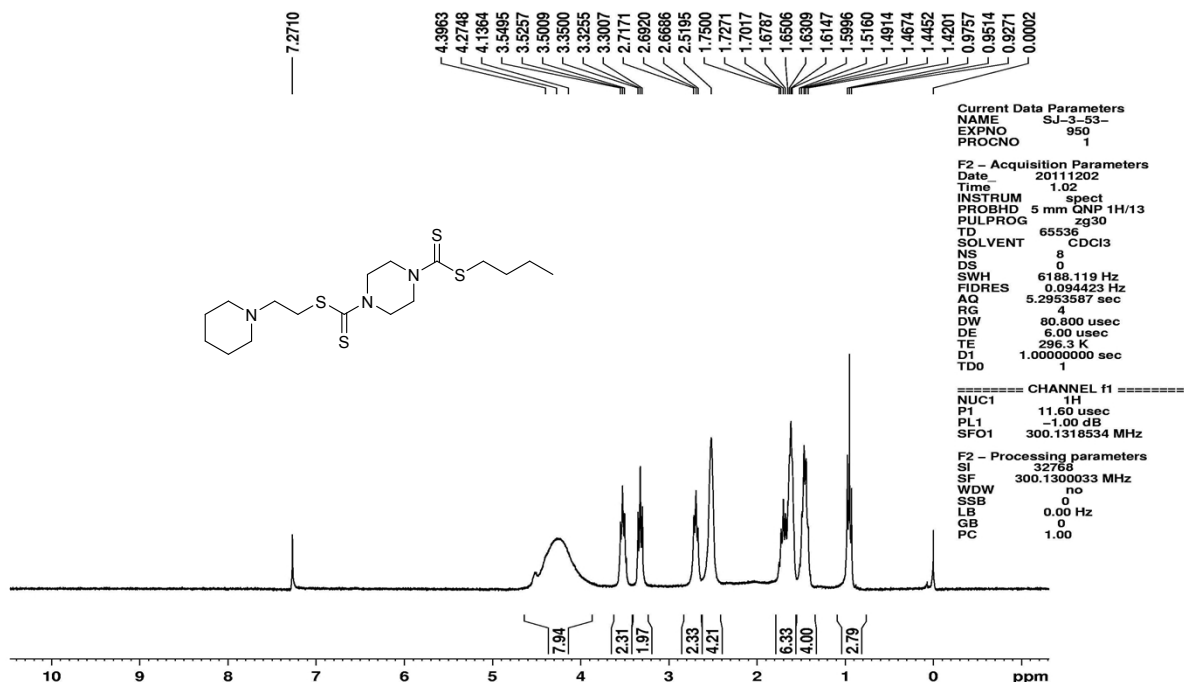
HRMS of compound 27



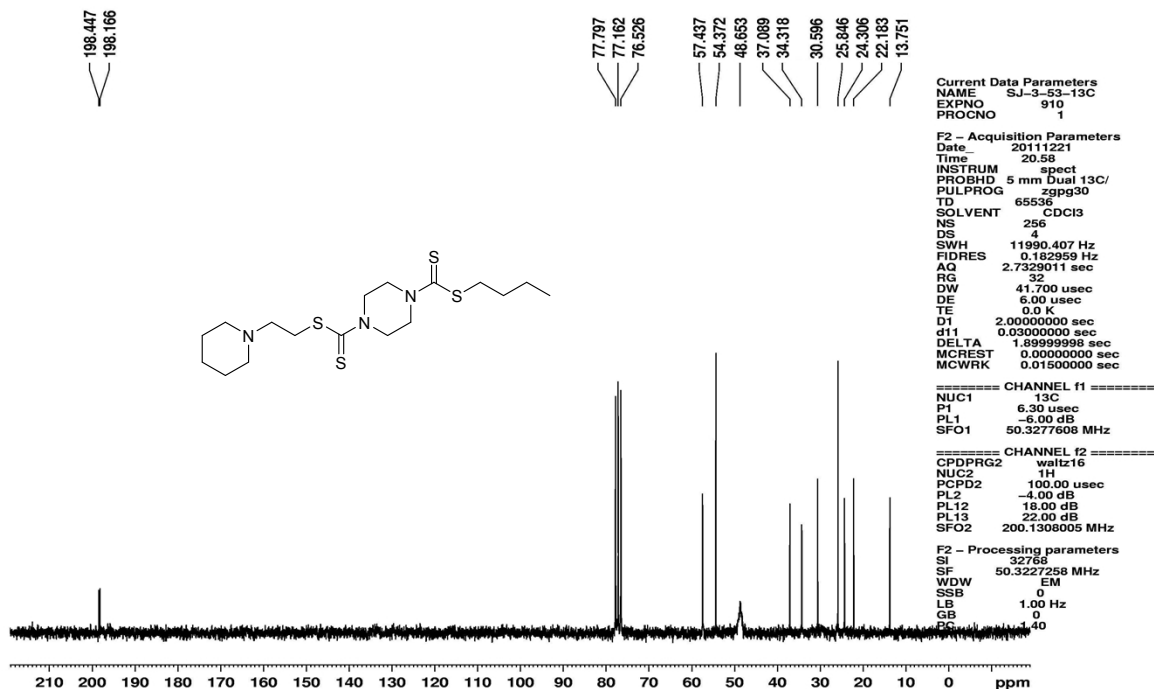
¹H NMR (300 MHz, CDCl₃) of compound 28



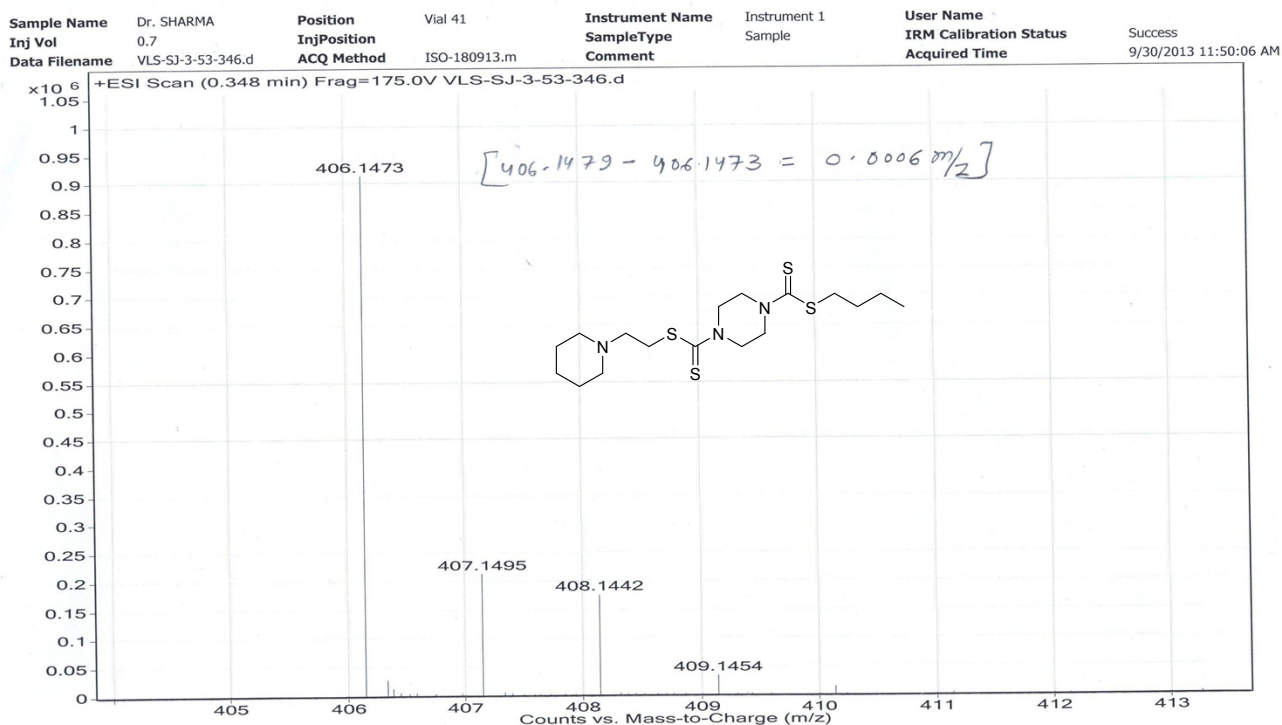
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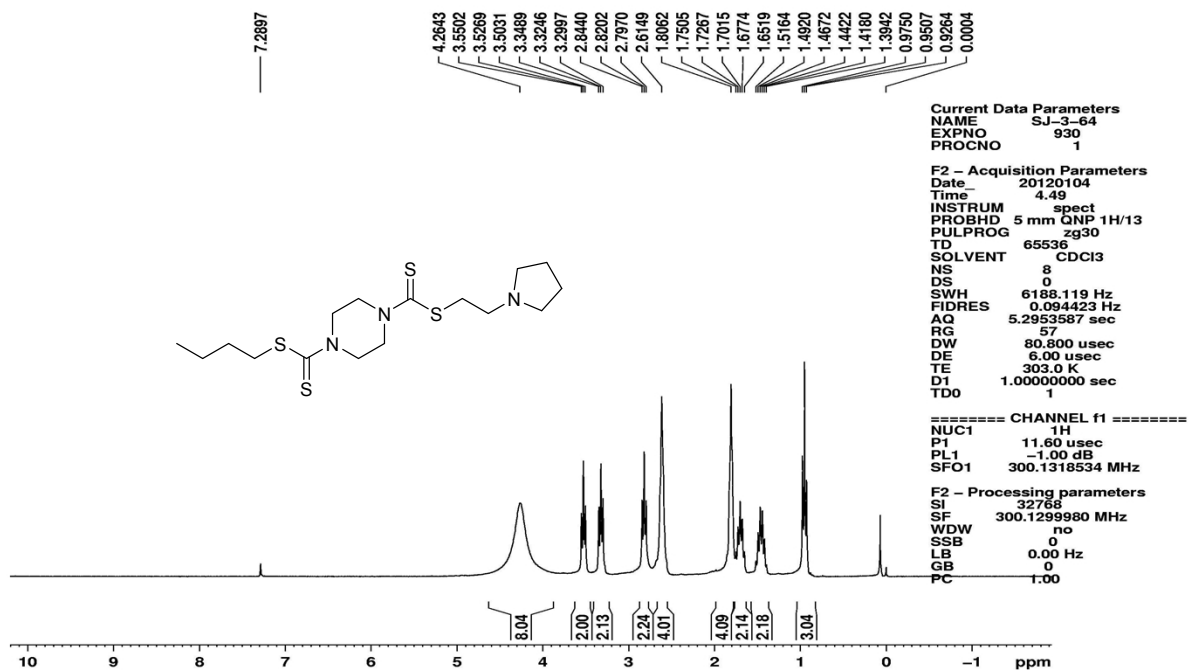
¹H NMR (300 MHz, CDCl₃) of compound 29



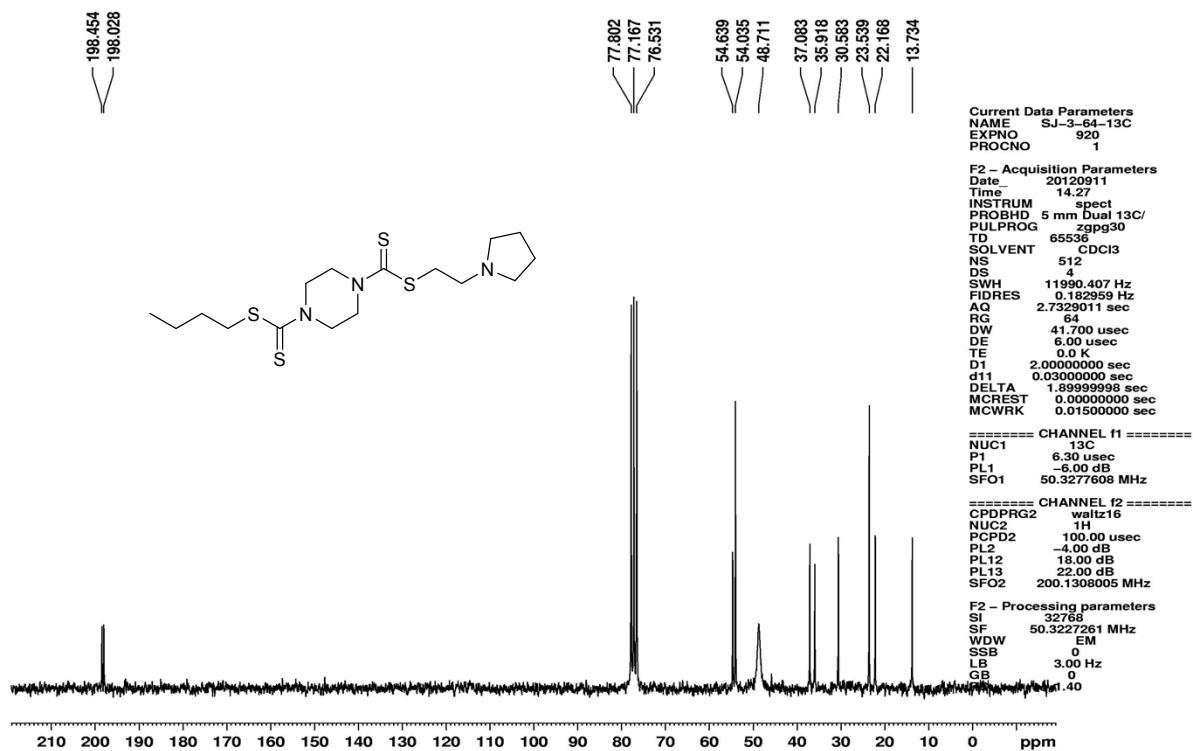
¹³C NMR (50 MHz, CDCl₃) of compound 29



HRMS of compound 29

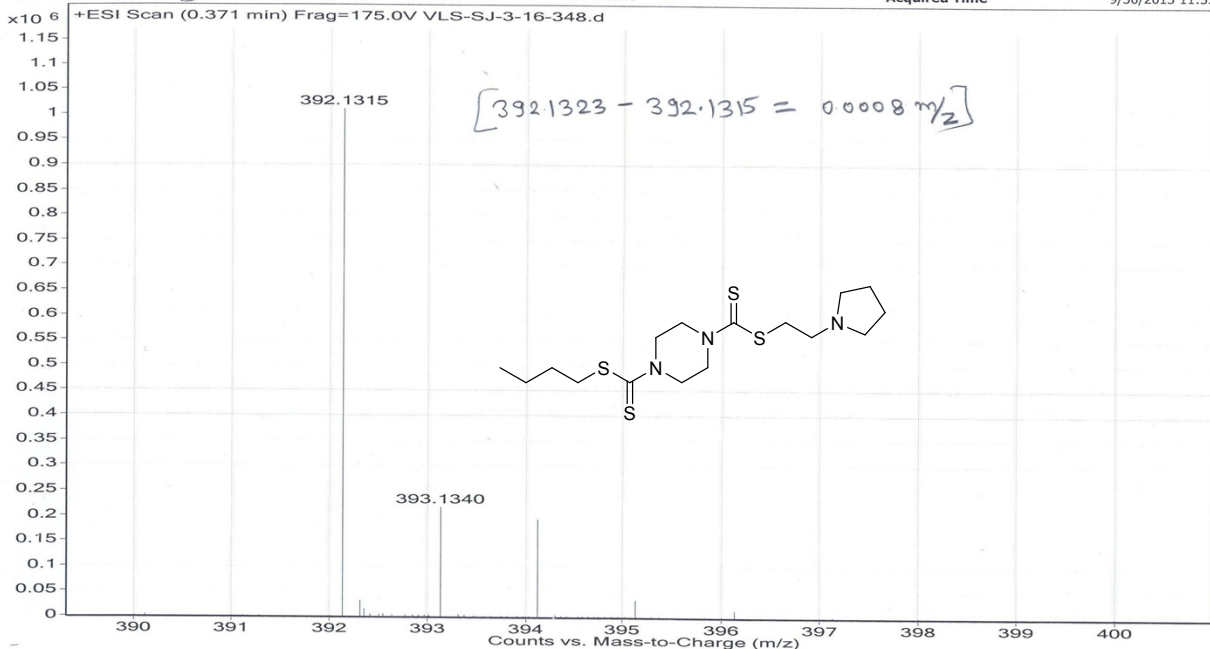


¹H NMR (300 MHz, CDCl₃) of compound 30

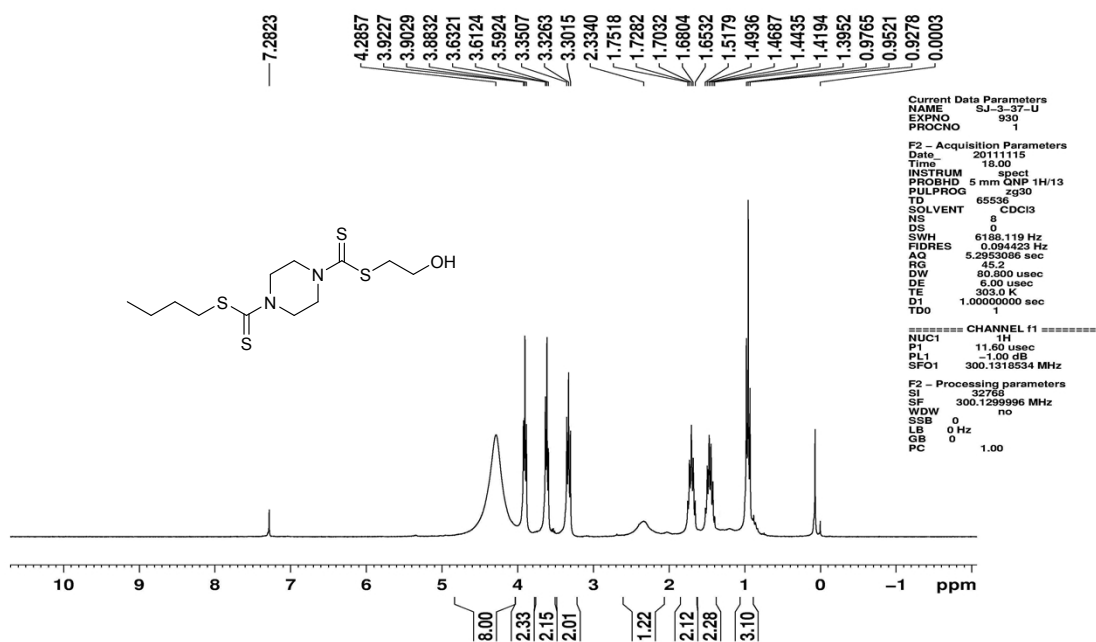


¹³C NMR (50 MHz, CDCl₃) of compound 30

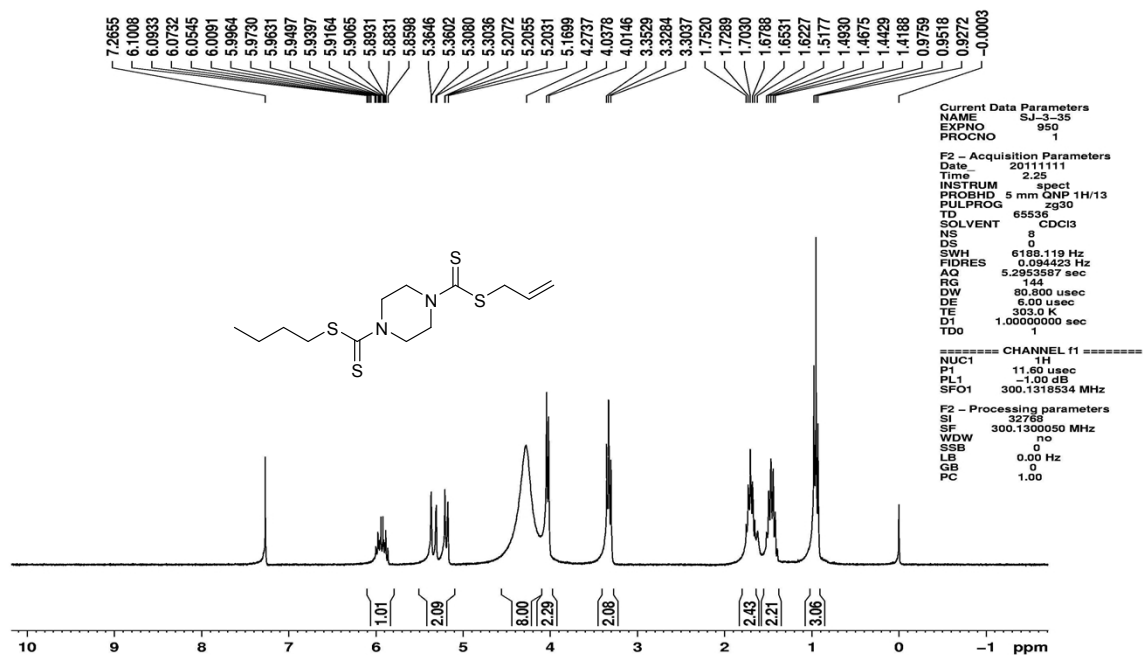
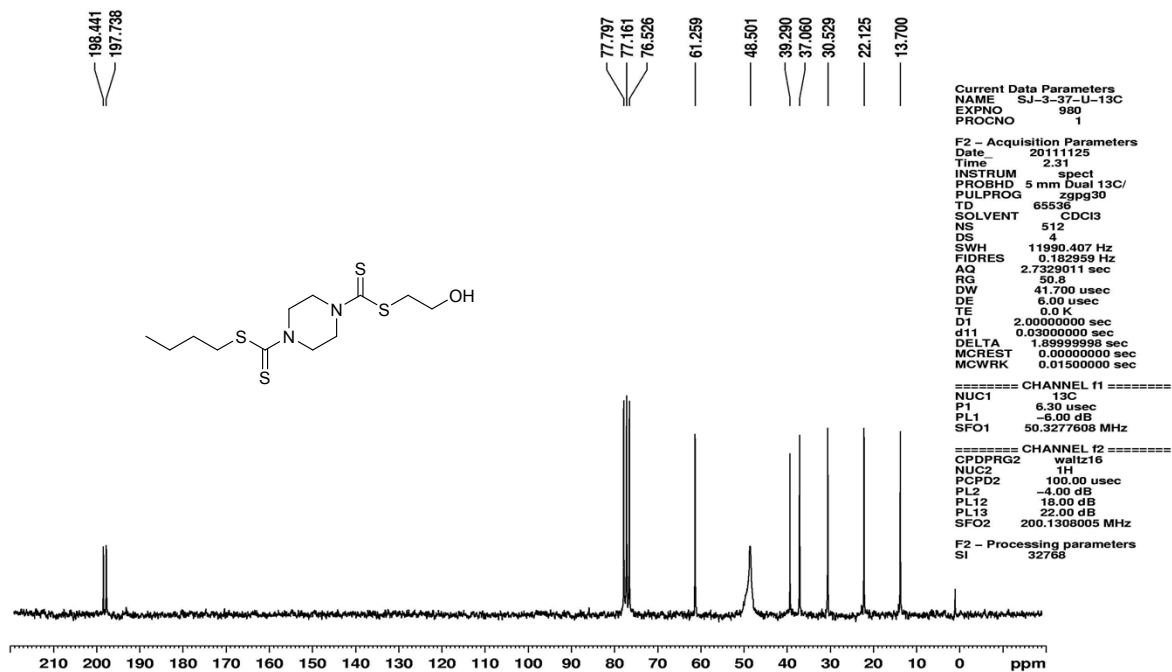
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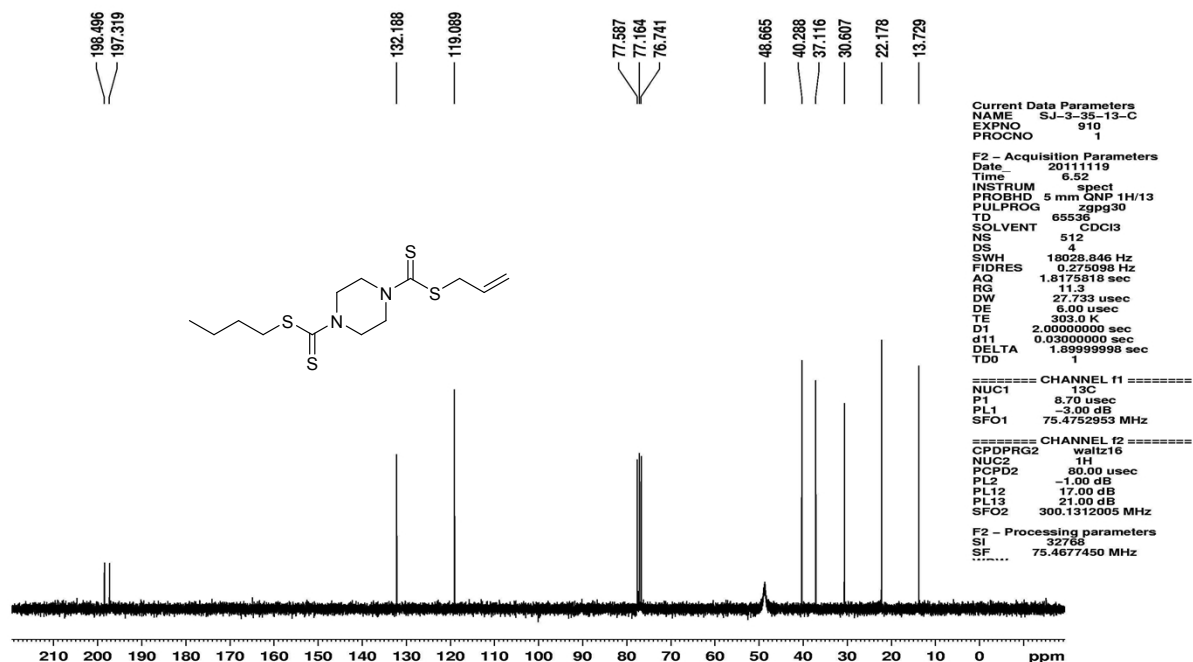


HRMS of compound 30

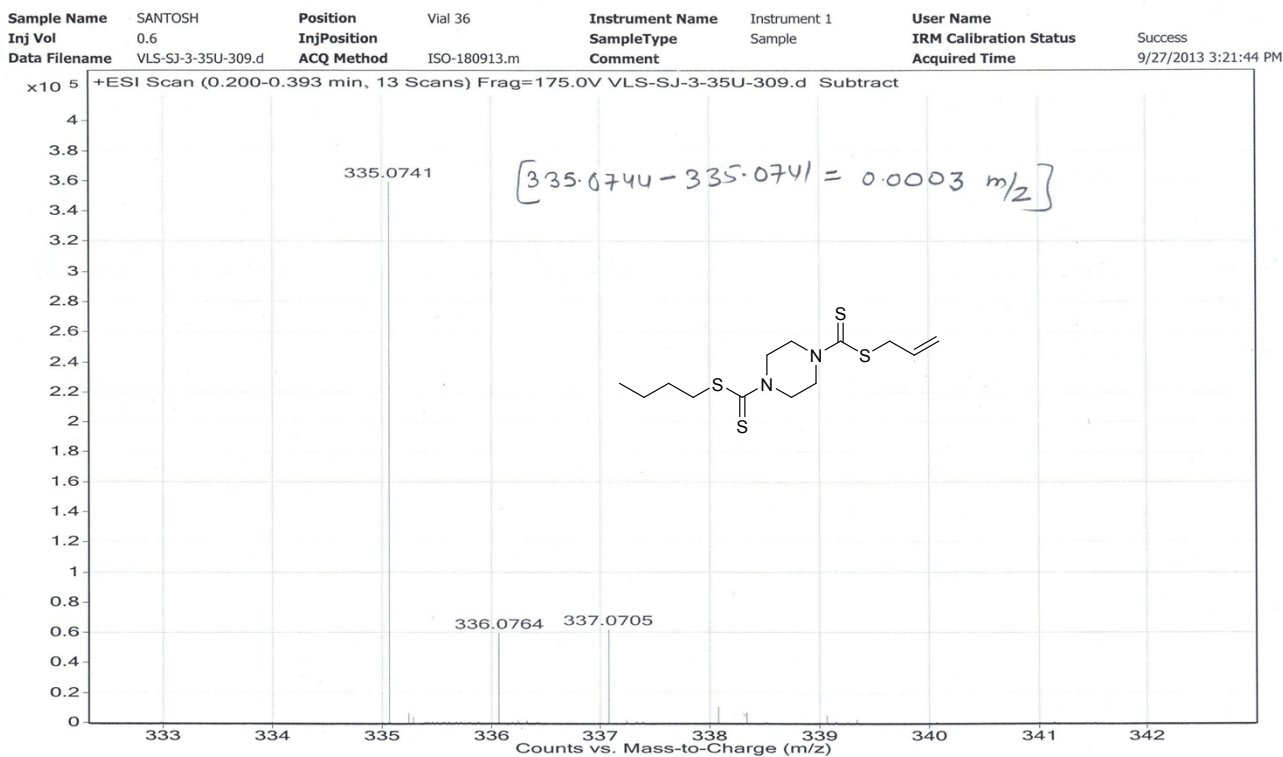


¹H NMR (300 MHz, CDCl₃) of compound 31





^{13}C NMR (75 MHz, CDCl_3) of compound 32



HRMS of compound 32