

Novel Seleno- and Thio-urea Containing Dihydropyrrol-2-one Analogues as Antibacterial Agents

Shekh Sabir¹, Tsz Tin Yu,¹ Rajesh Kuppasamy,¹ Basmah Almohaywi,² George Iskander,¹ Theerthankar Das,³ Mark Willcox,⁴ David StC. Black,¹ and Naresh Kumar^{1*}

¹ School of Chemistry, The University of New South Wales, NSW 2052 Sydney, Australia; s.sabir@student.unsw.edu.au (S.S.); tsztin.yu@unsw.edu.au (T. T.Y.); r.kuppasamy@ad.unsw.edu.au (R.K.); g.iskanderb@gmail.com (G. I.); d.black@unsw.edu.au (D.S.B.)

² School of Pharmacy, King Khalid University Abha 6142, Saudi Arabia, bal-mohawe@kku.edu.sa (B.A.)

³ Department of Infectious Diseases and Immunology, School of Medical Sciences, The University of Sydney, NSW 2006 Sydney, Australia; das.ashishkumar@sydney.edu.au (T.D.)

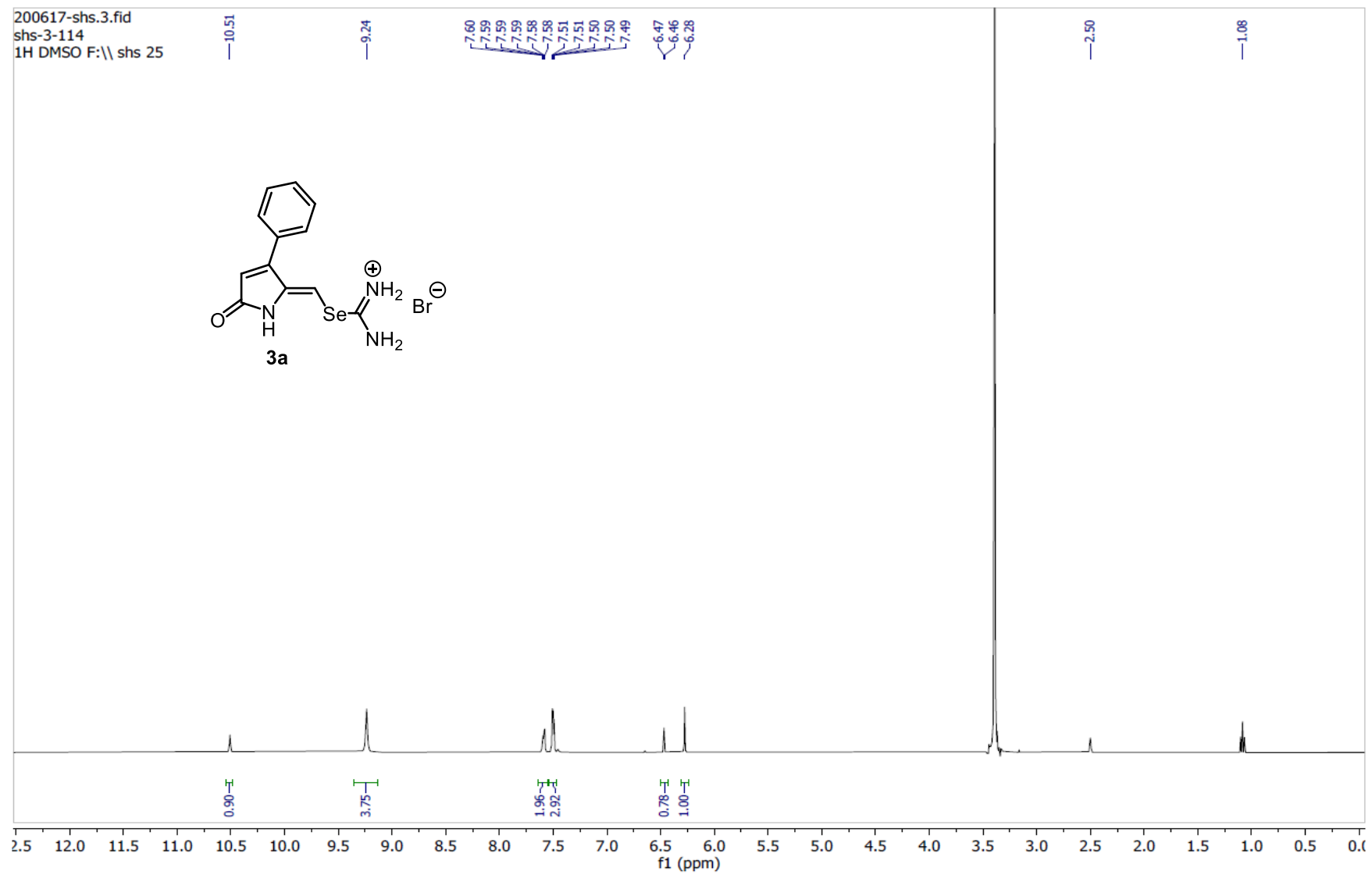
⁴ School of Optometry and Vision Science, The University of New South Wales, NSW 2052 Sydney, m.willcox@unsw.edu.au (M.W.)

* Correspondence: n.kumar@unsw.edu.au; Tel.: +61-29385-4698; Fax: +61-29385-6141

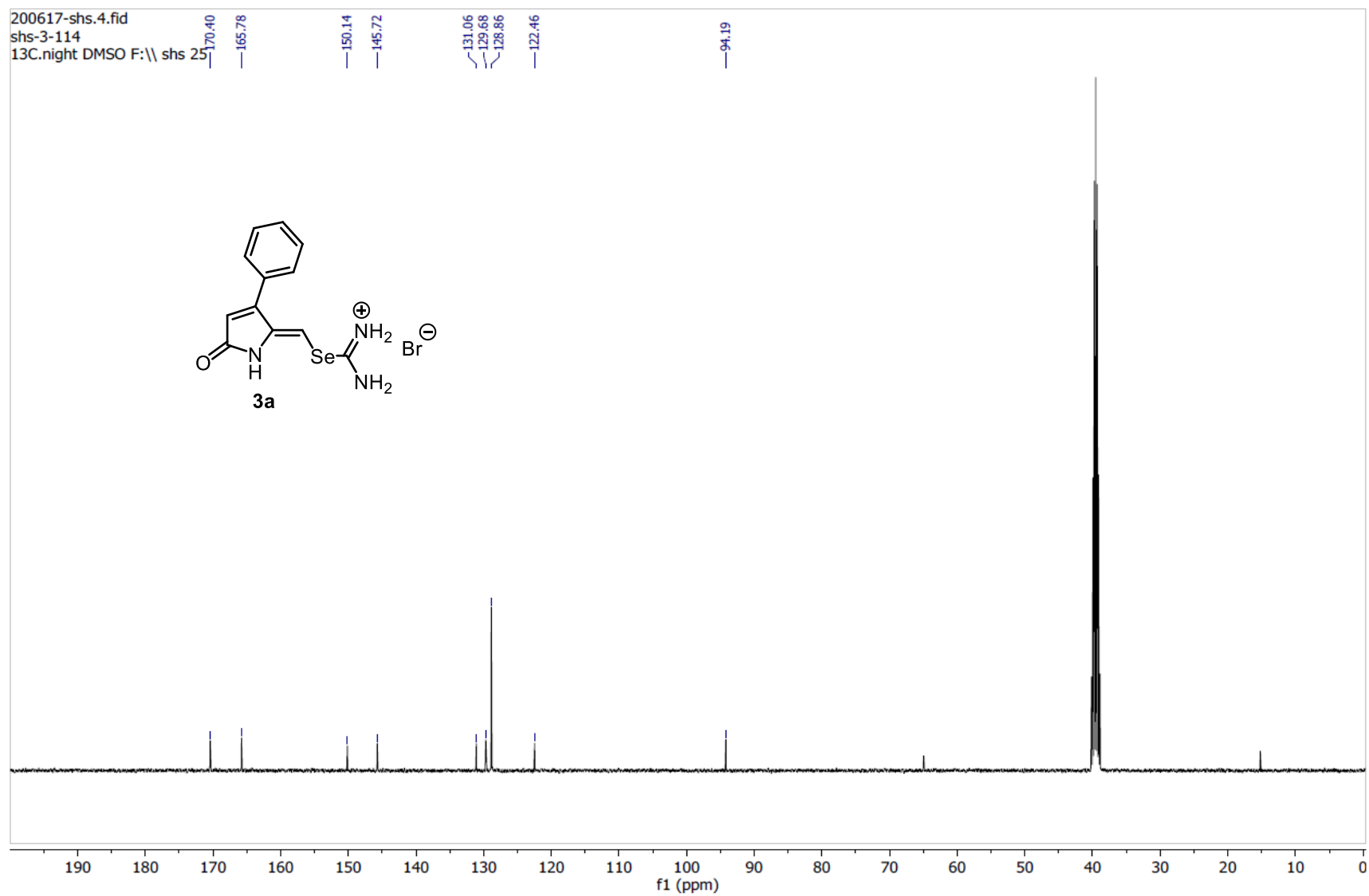
Contents

¹ H and ¹³ C NMR spectra of the compounds	S2-S32
⁷⁷ Se NMR spectrum of compound 3e	S12
HRMS data of the compounds.....	S33-S47
IR Spectra of compounds.....	S48-S52
Growth inhibition data (<i>P.aeruginosa</i> MH602).....	S53

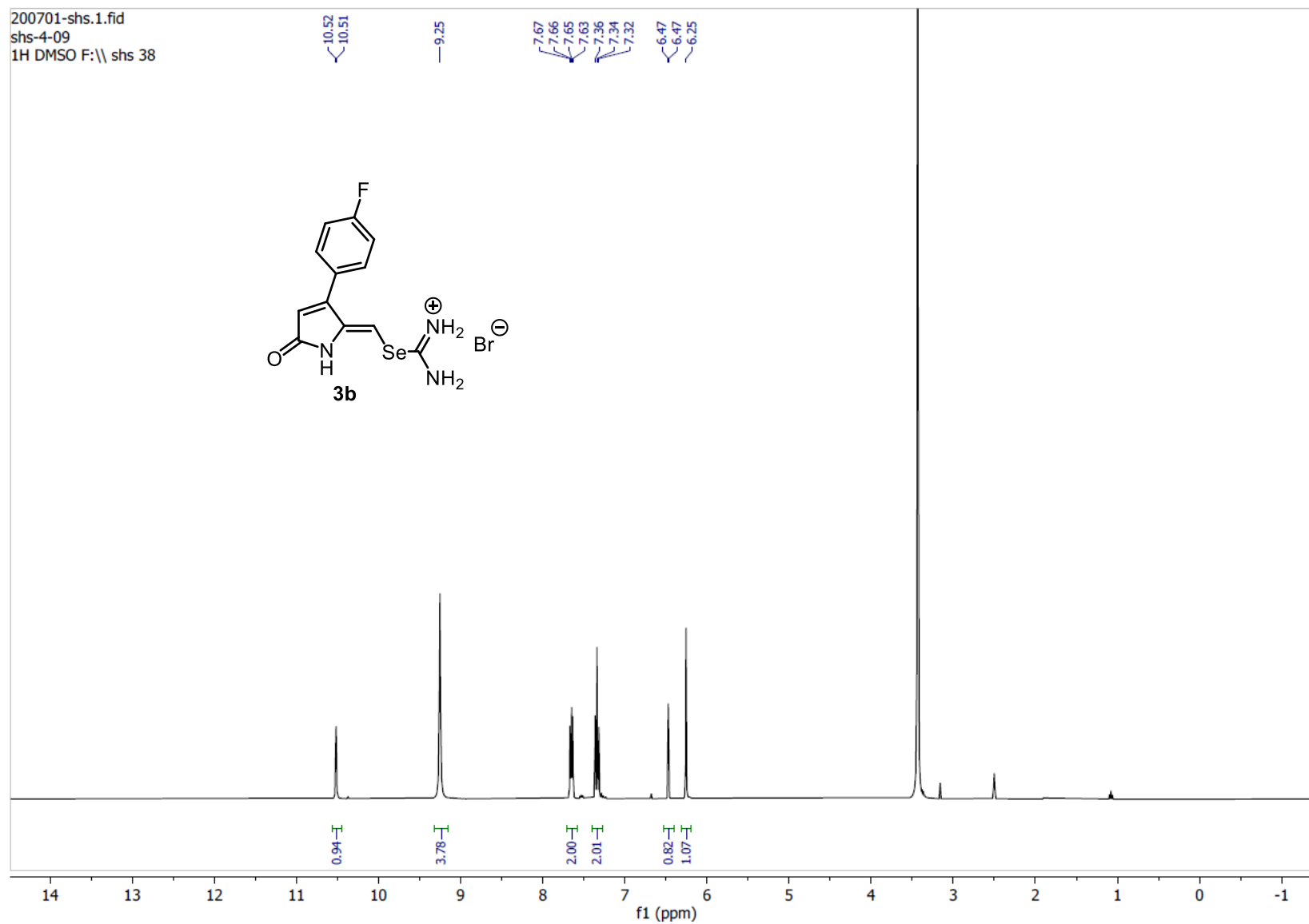
¹H NMR spectrum of compound **3a**



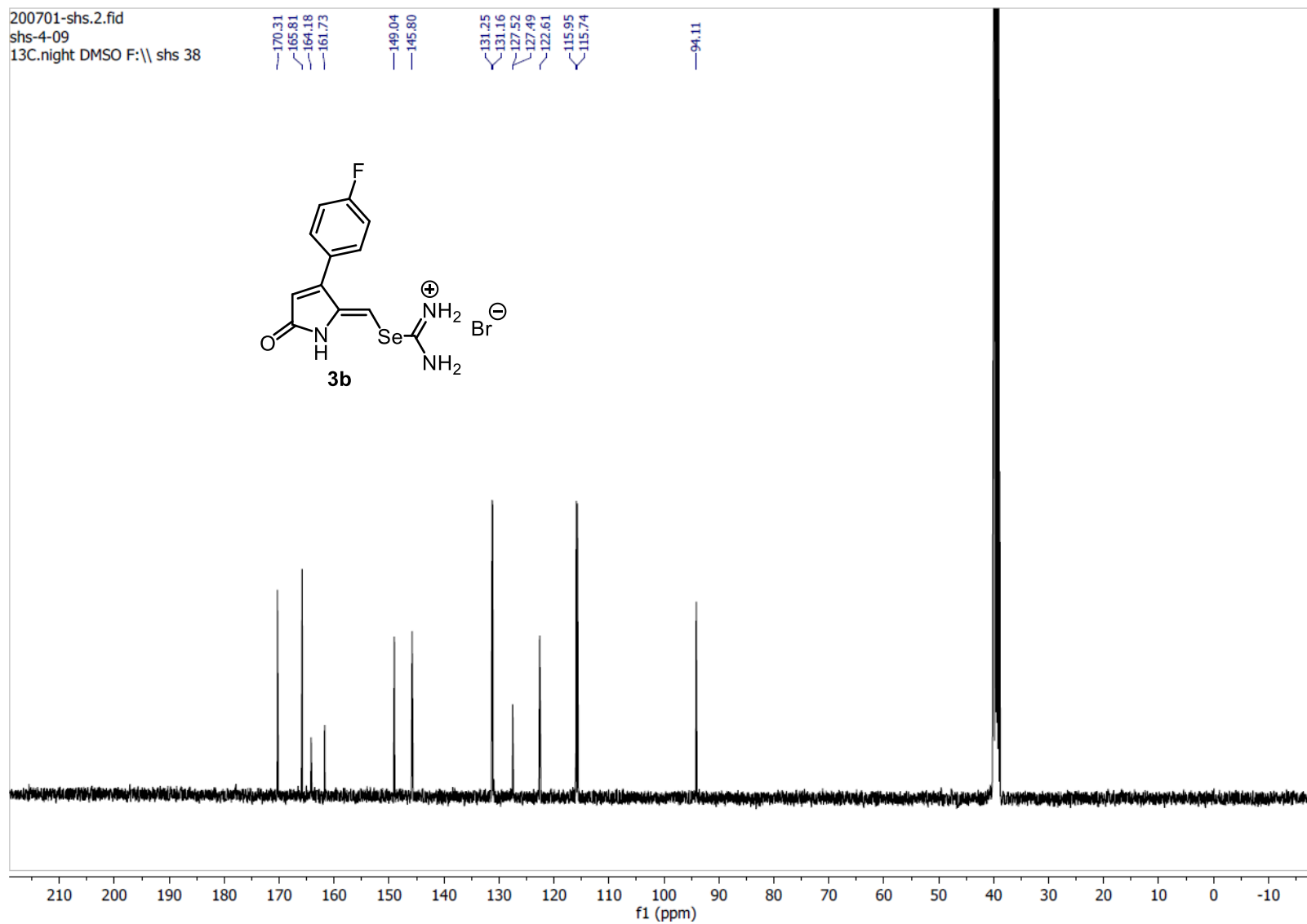
¹³C NMR spectrum of compound **3a**



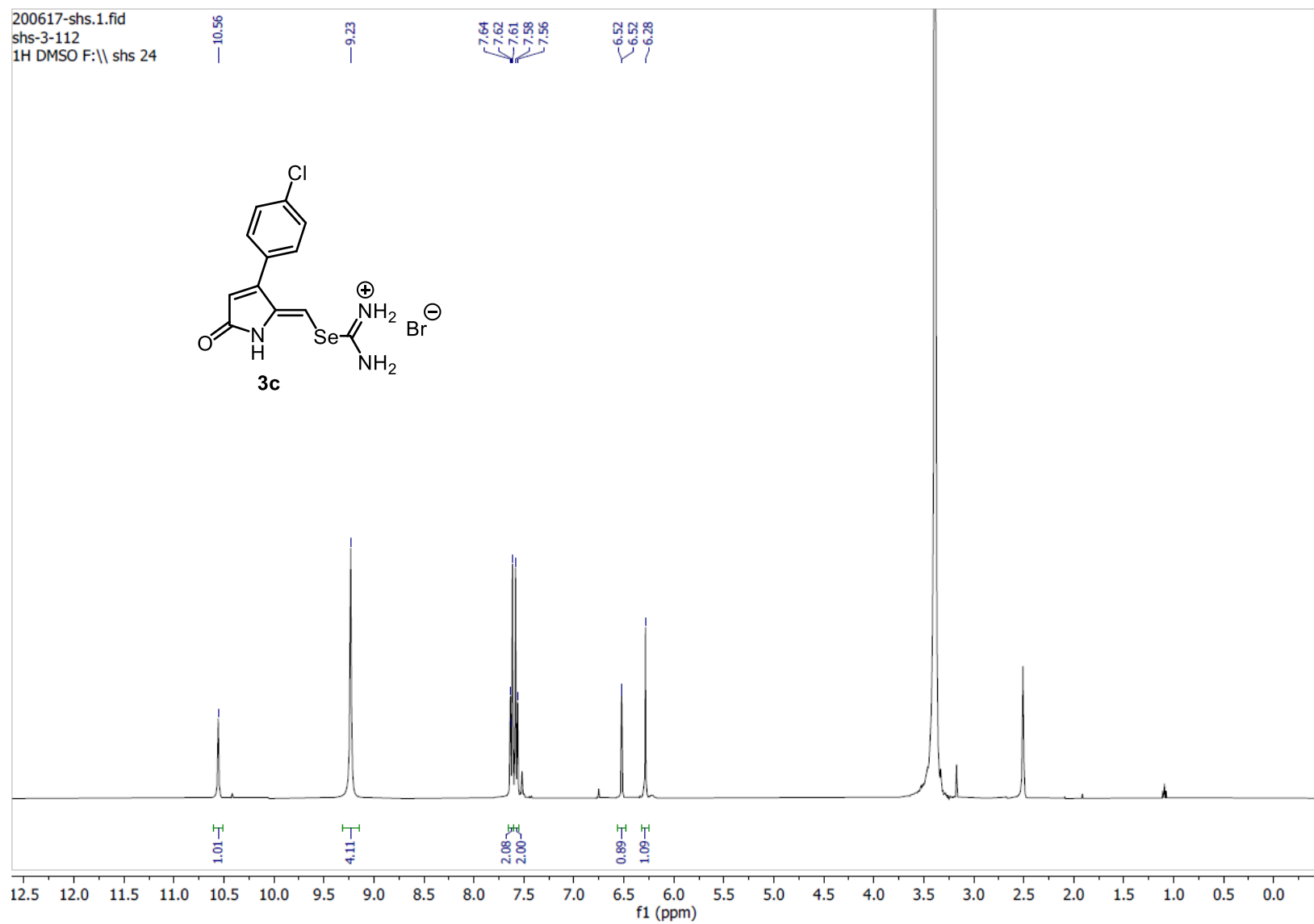
¹H NMR spectrum of compound **3b**



¹³C NMR spectrum of compound **3b**

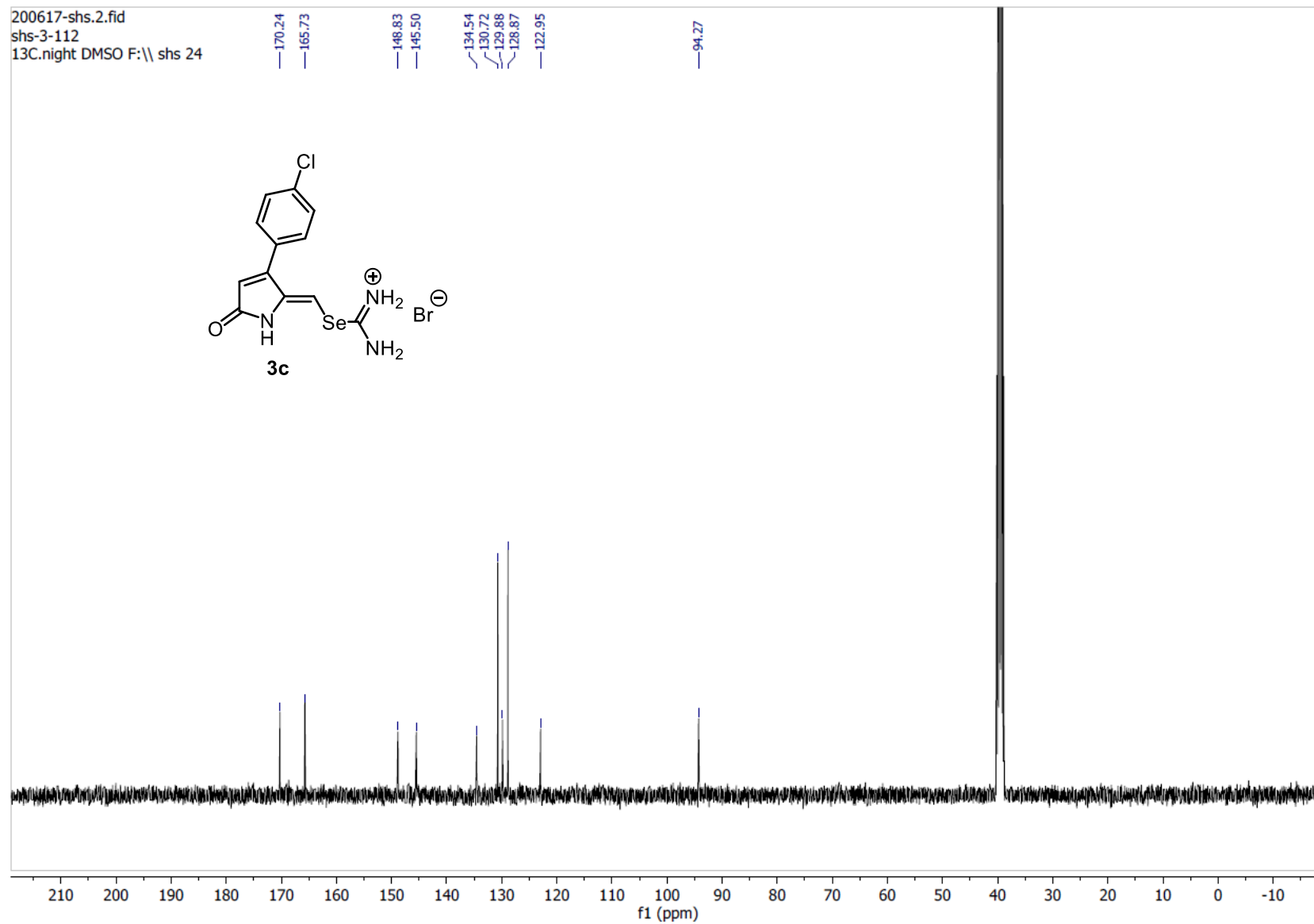
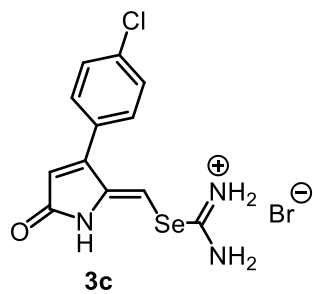


¹H NMR spectrum of compound **3c**

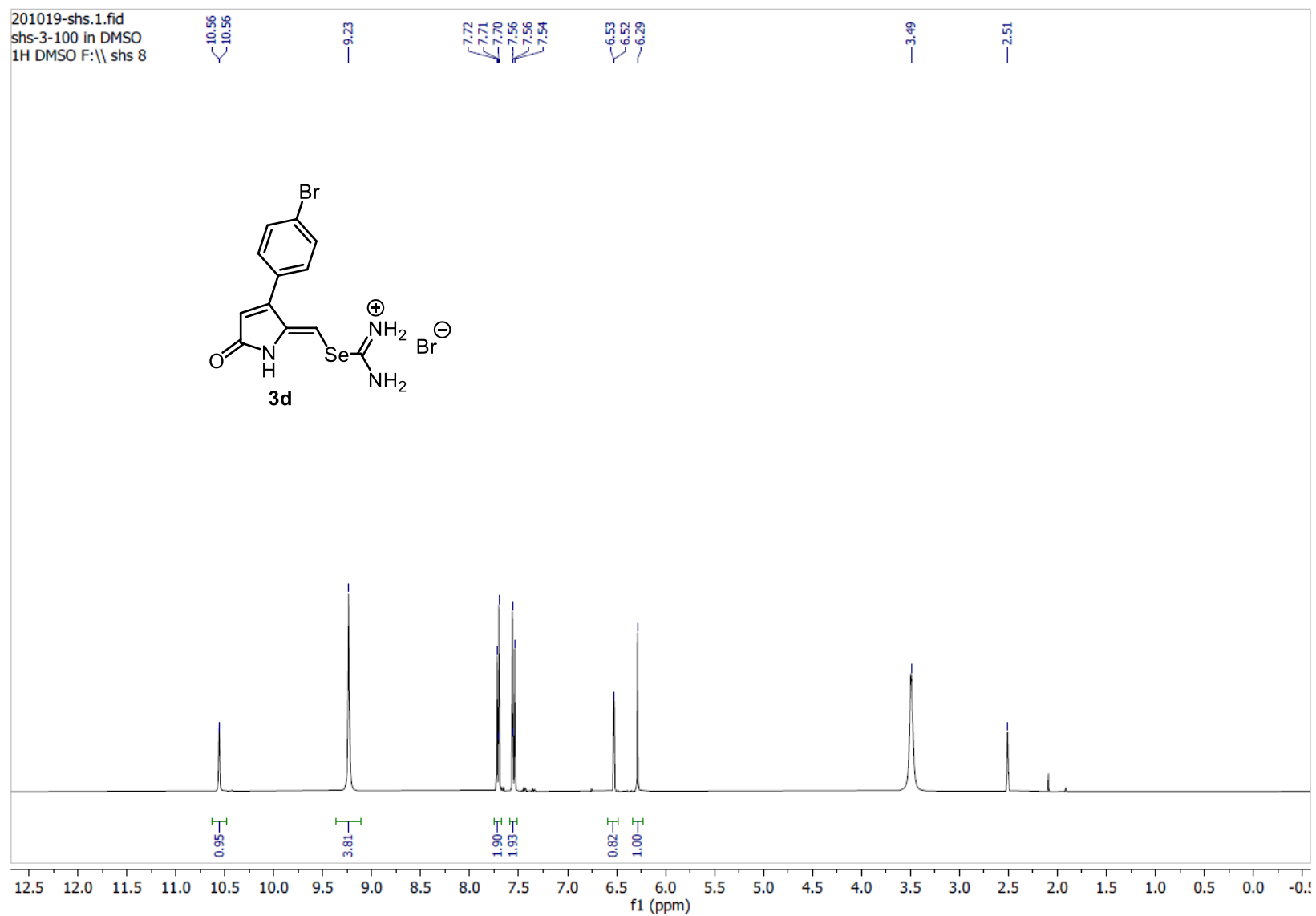


¹³C NMR spectrum of compound **3c**

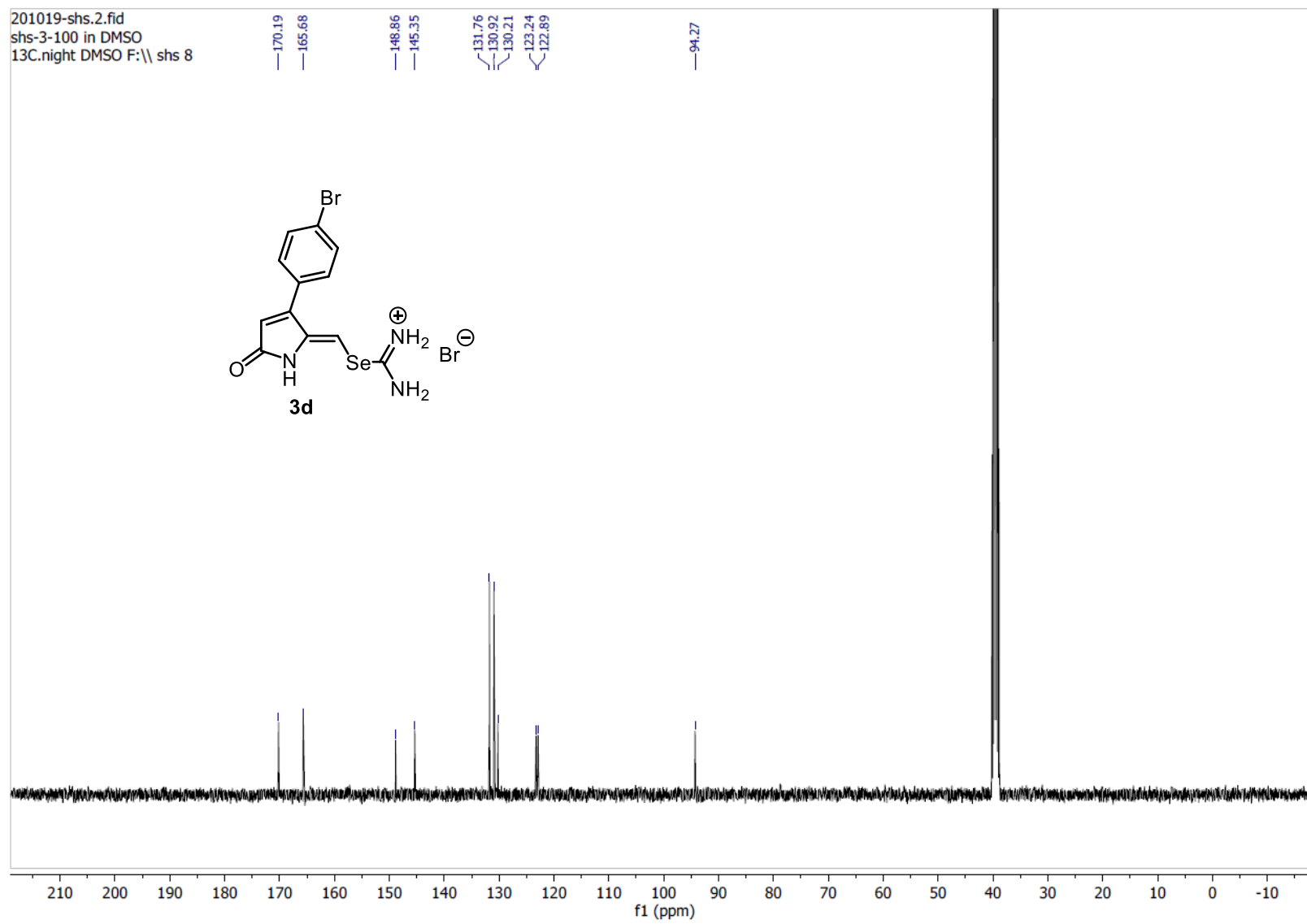
200617-shs.2.fid
shs-3-112
13C.night DMSO F:\ shs 24



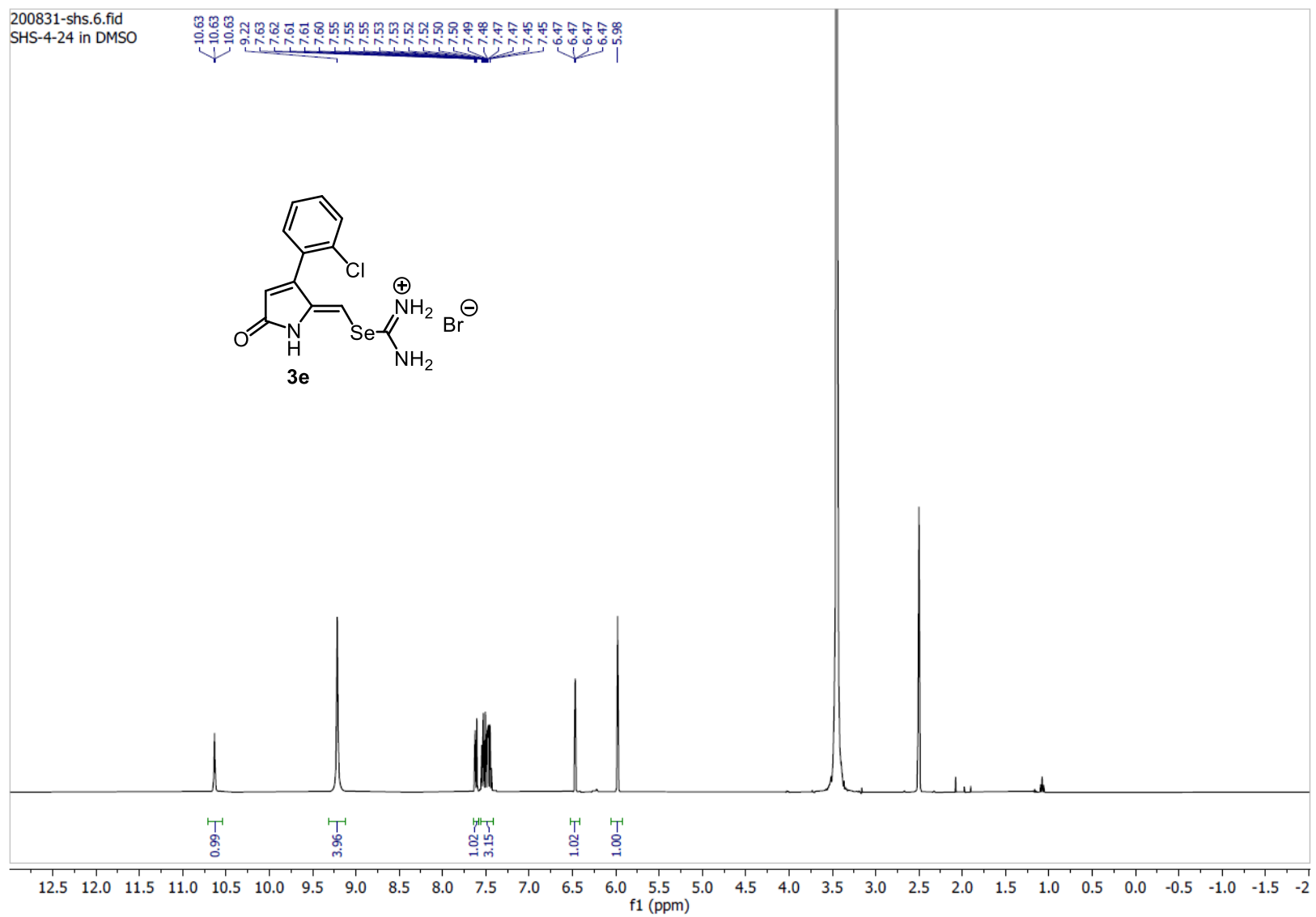
¹H NMR spectrum of compound **3d**



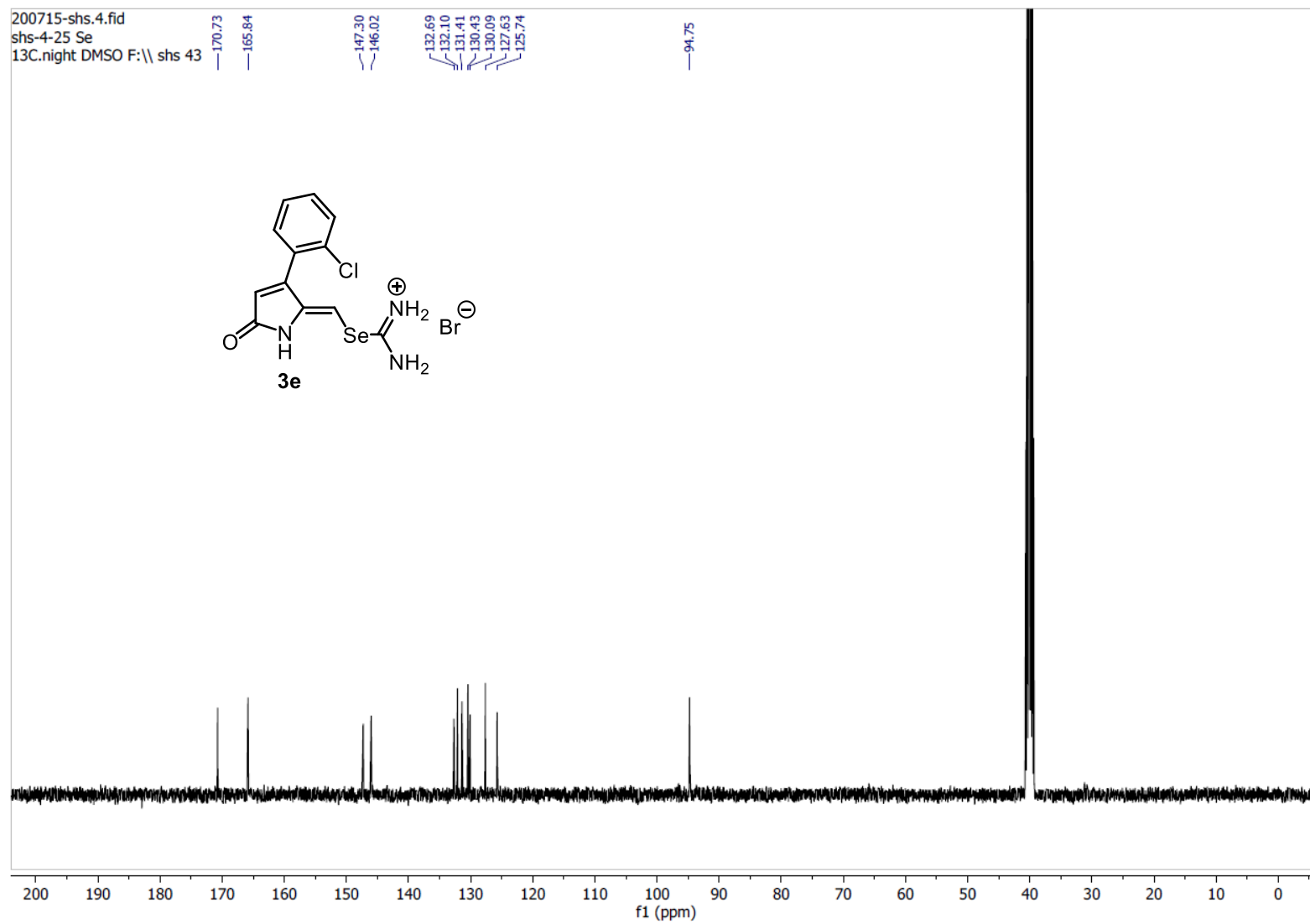
^{13}C NMR spectrum of compound **3d**



¹H NMR spectrum of compound **3e**

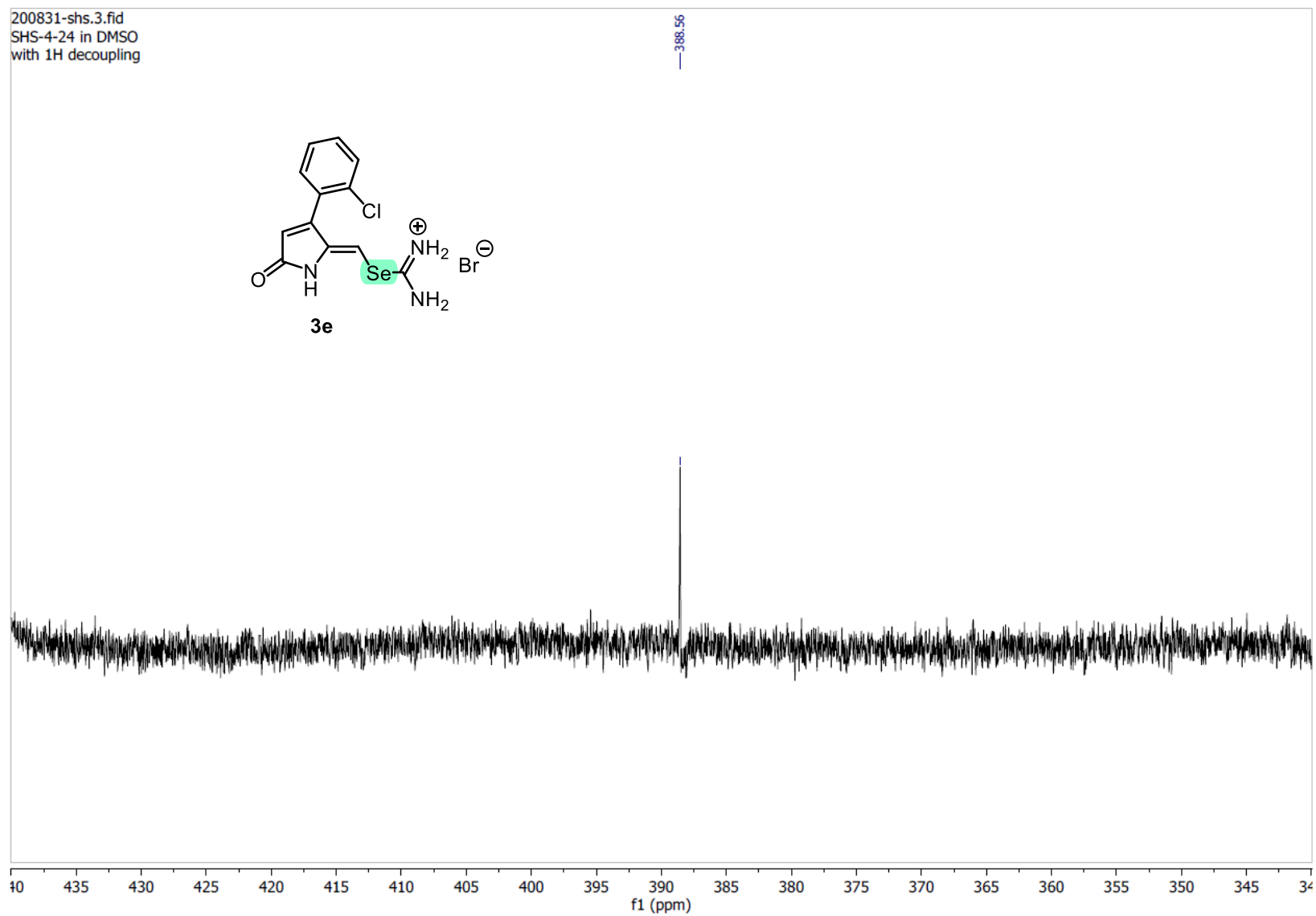
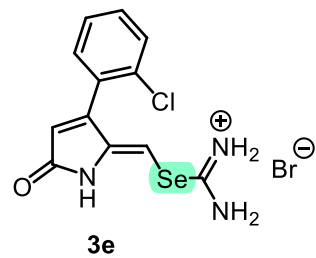


¹³C NMR spectrum of compound **3e**

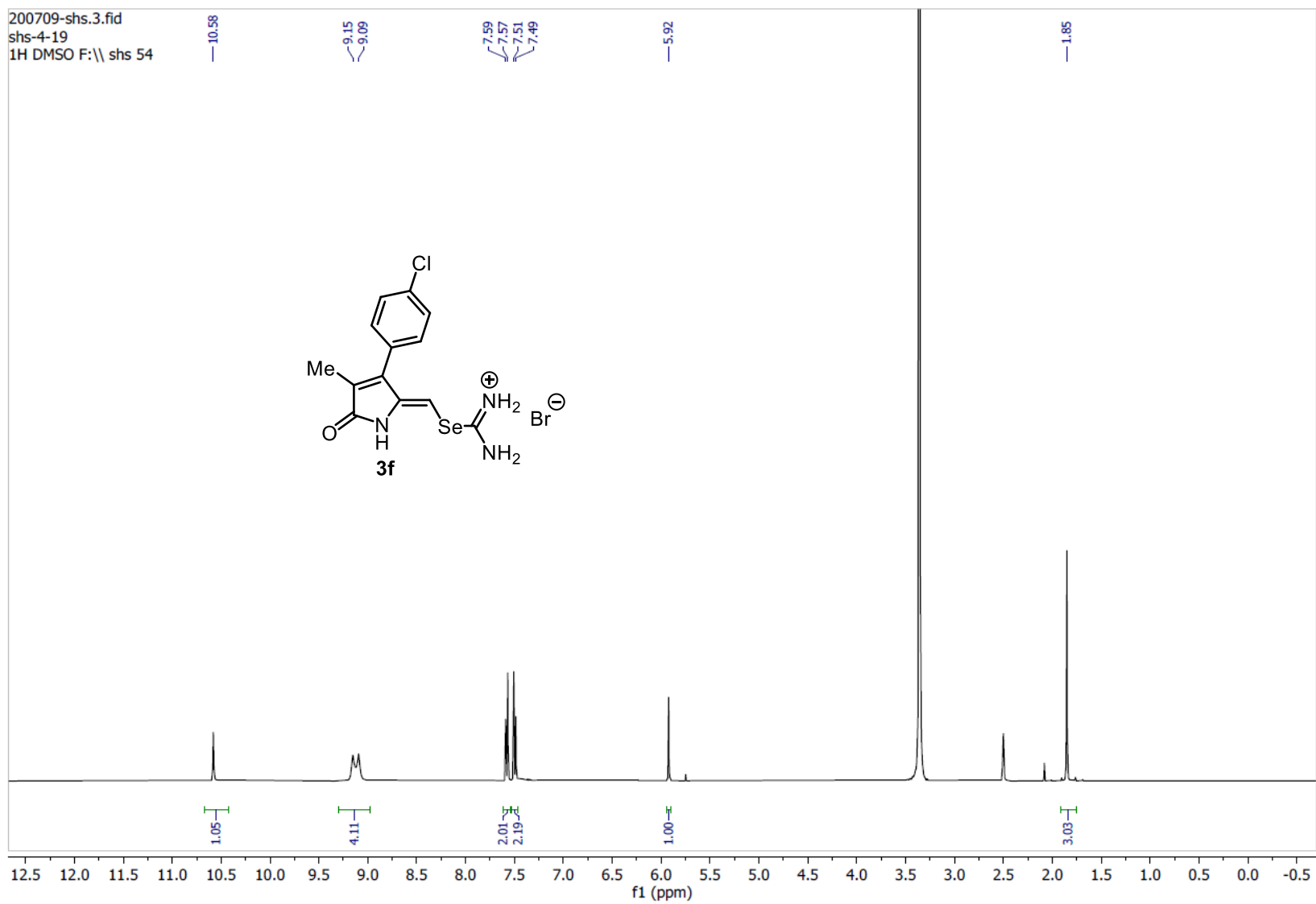


^{77}Se NMR spectrum of compound **3e**

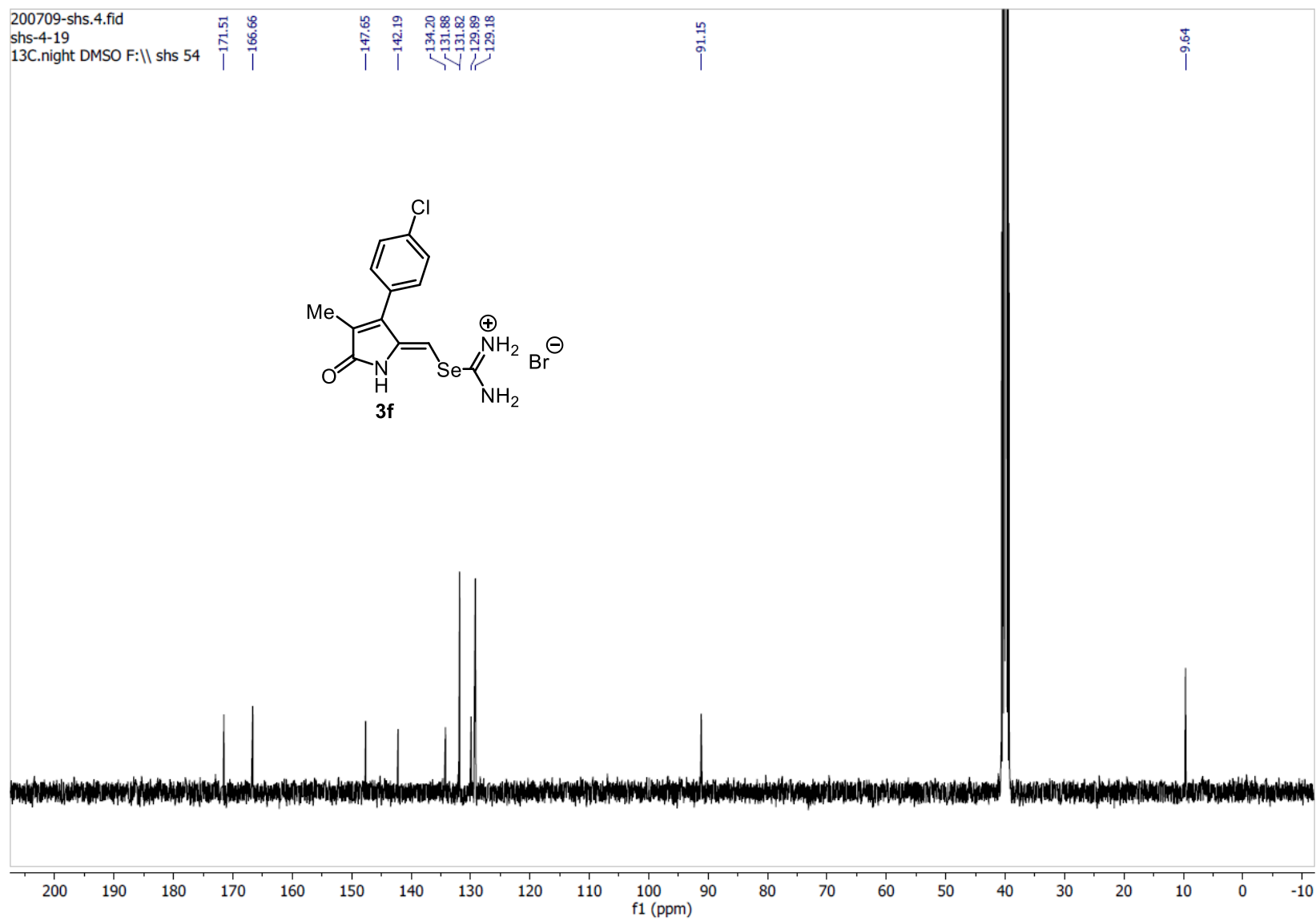
200831-shs.3.fid
SHS-4-24 in DMSO
with ^1H decoupling



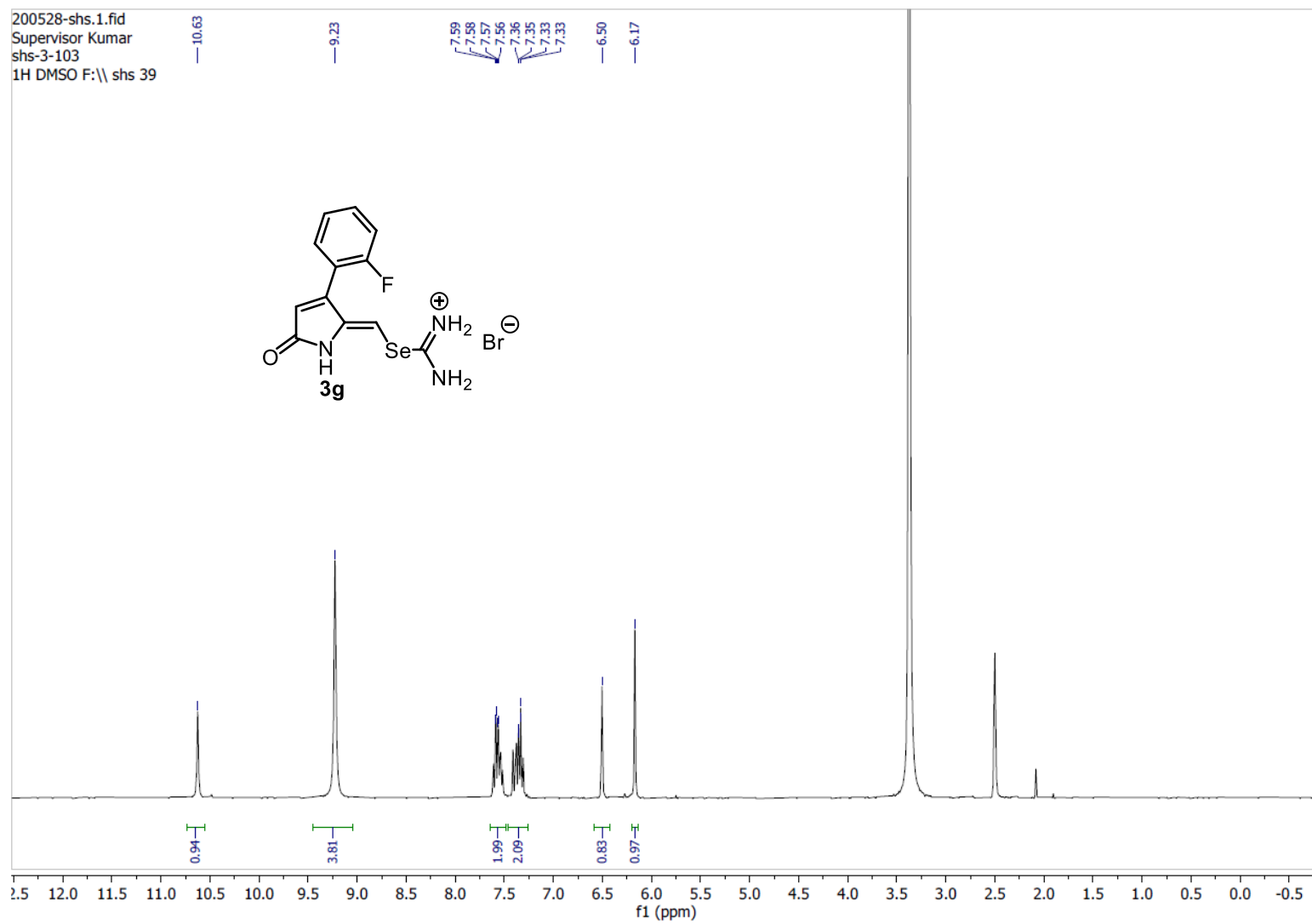
¹H NMR spectrum of compound **3f**



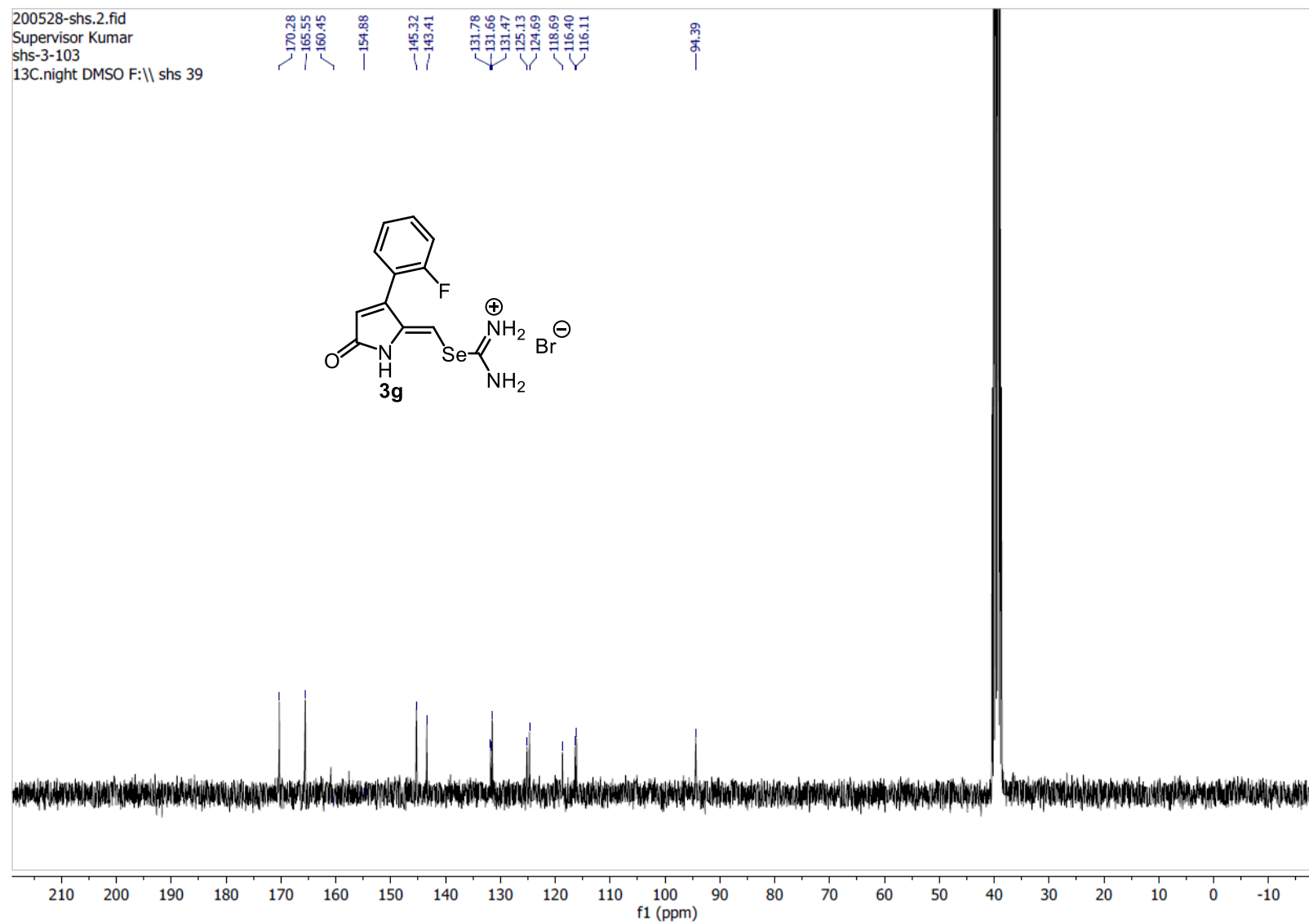
¹³C NMR spectrum of compound **3f**



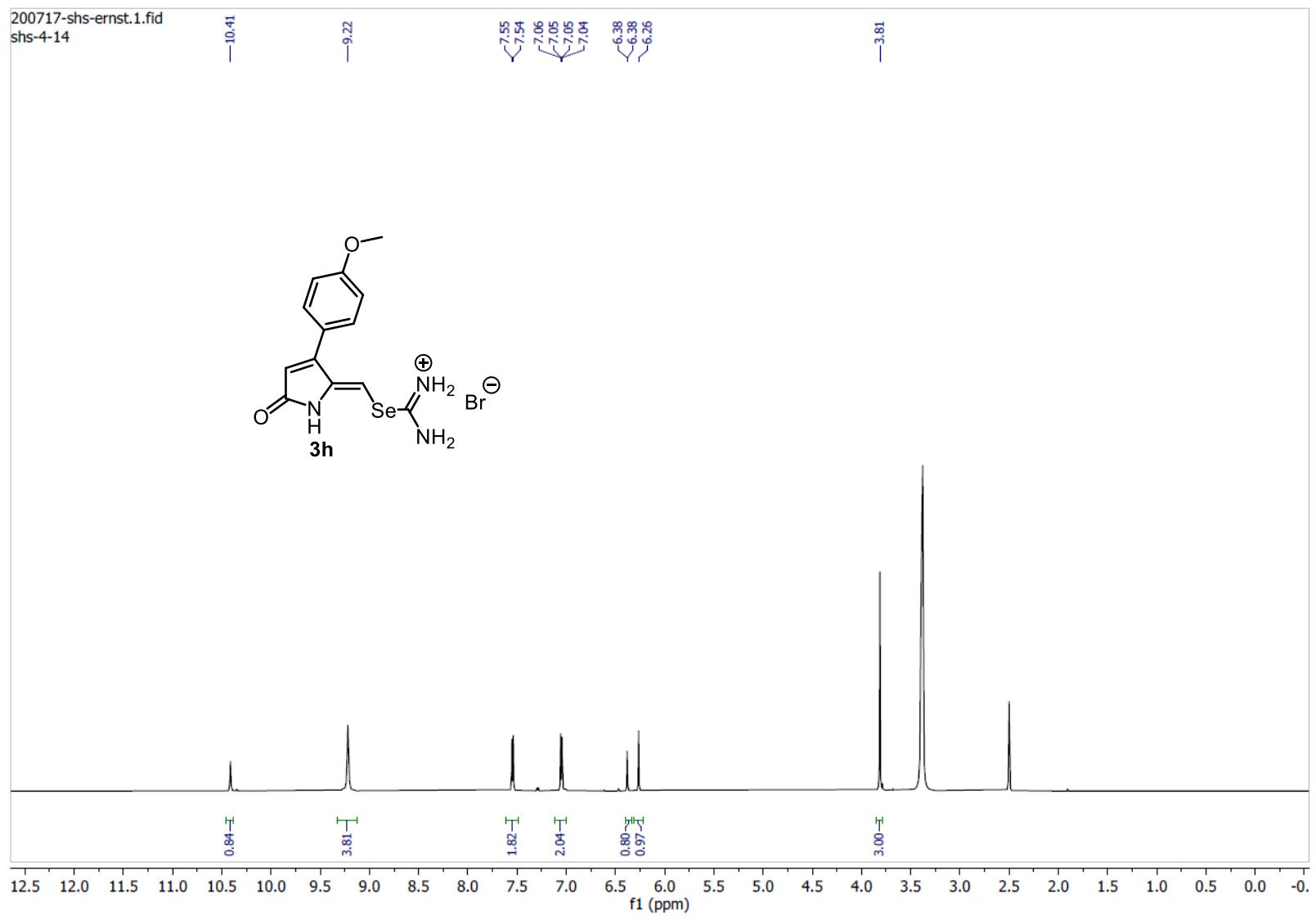
¹H NMR spectrum of compound **3g**



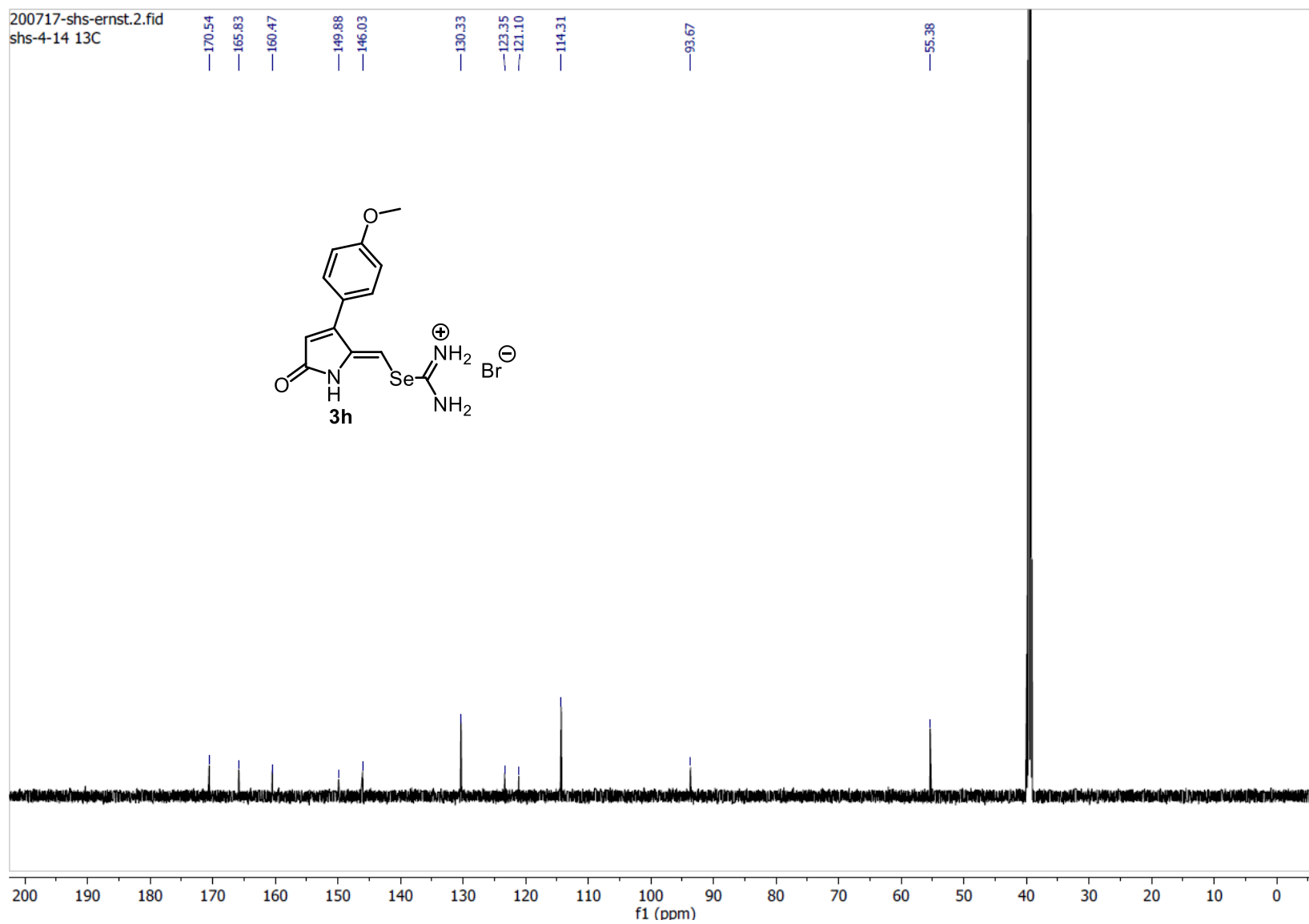
^{13}C NMR spectrum of compound **3g**



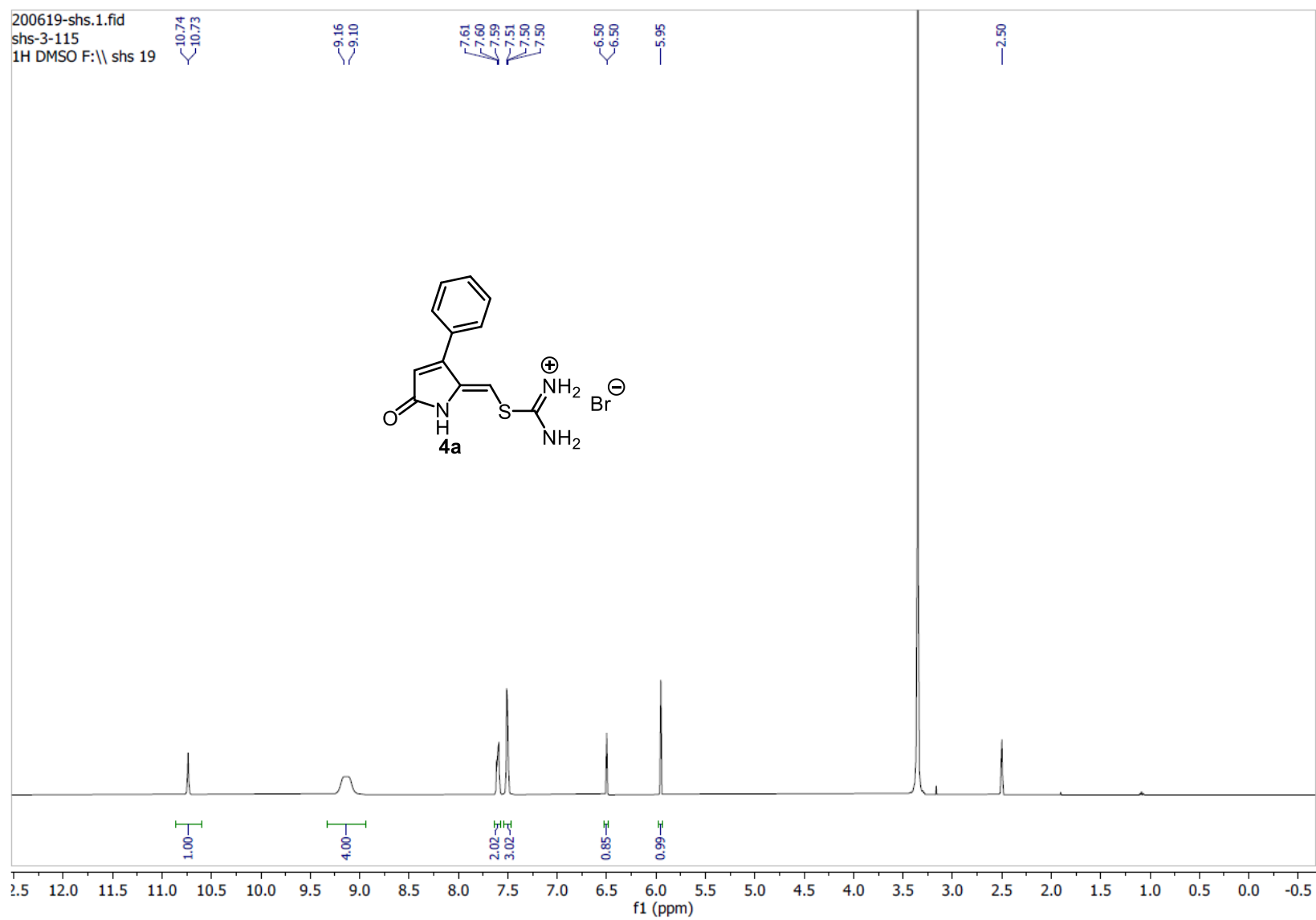
¹H NMR spectrum of compound **3h**



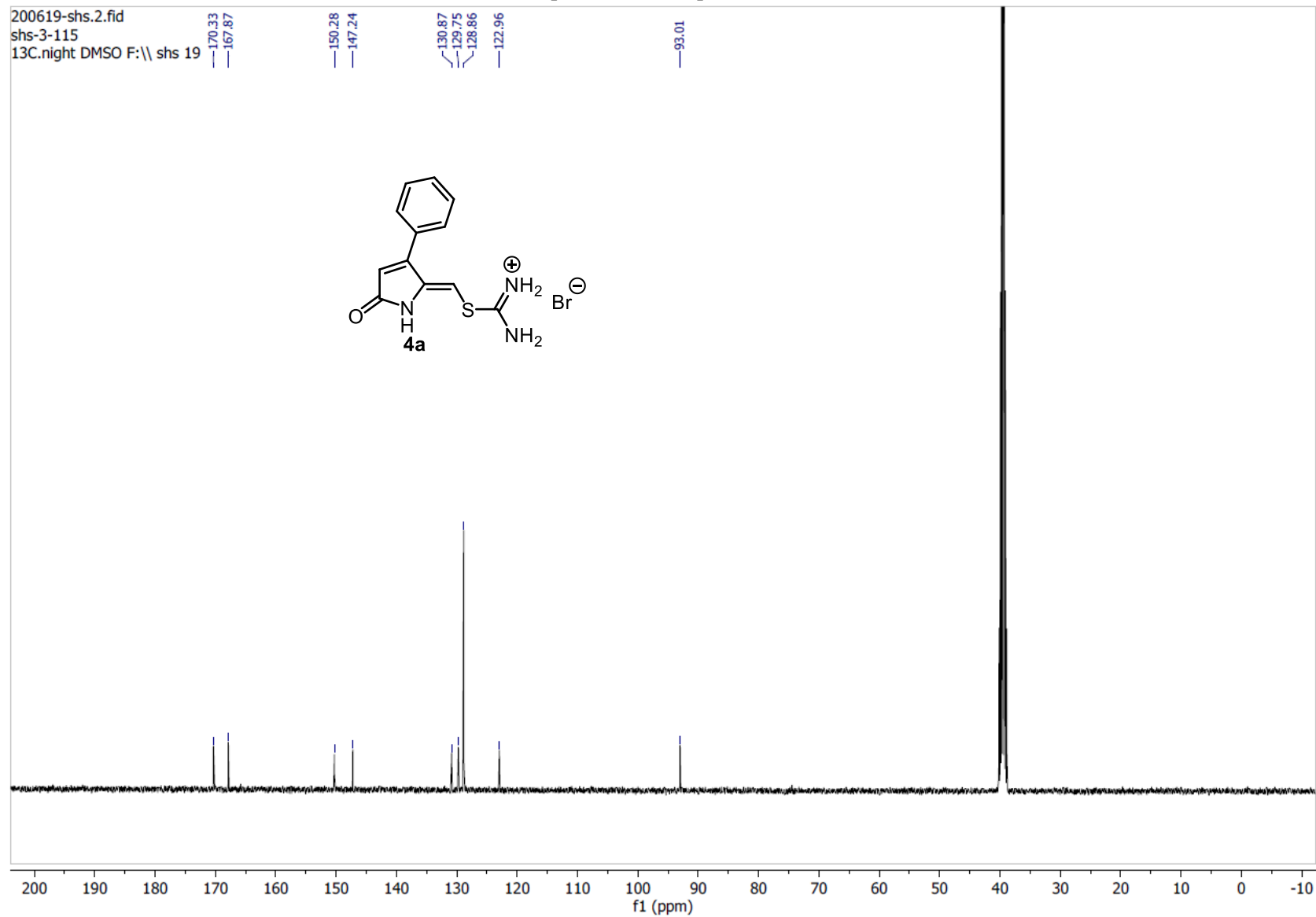
¹³C NMR spectrum of compound **3h**



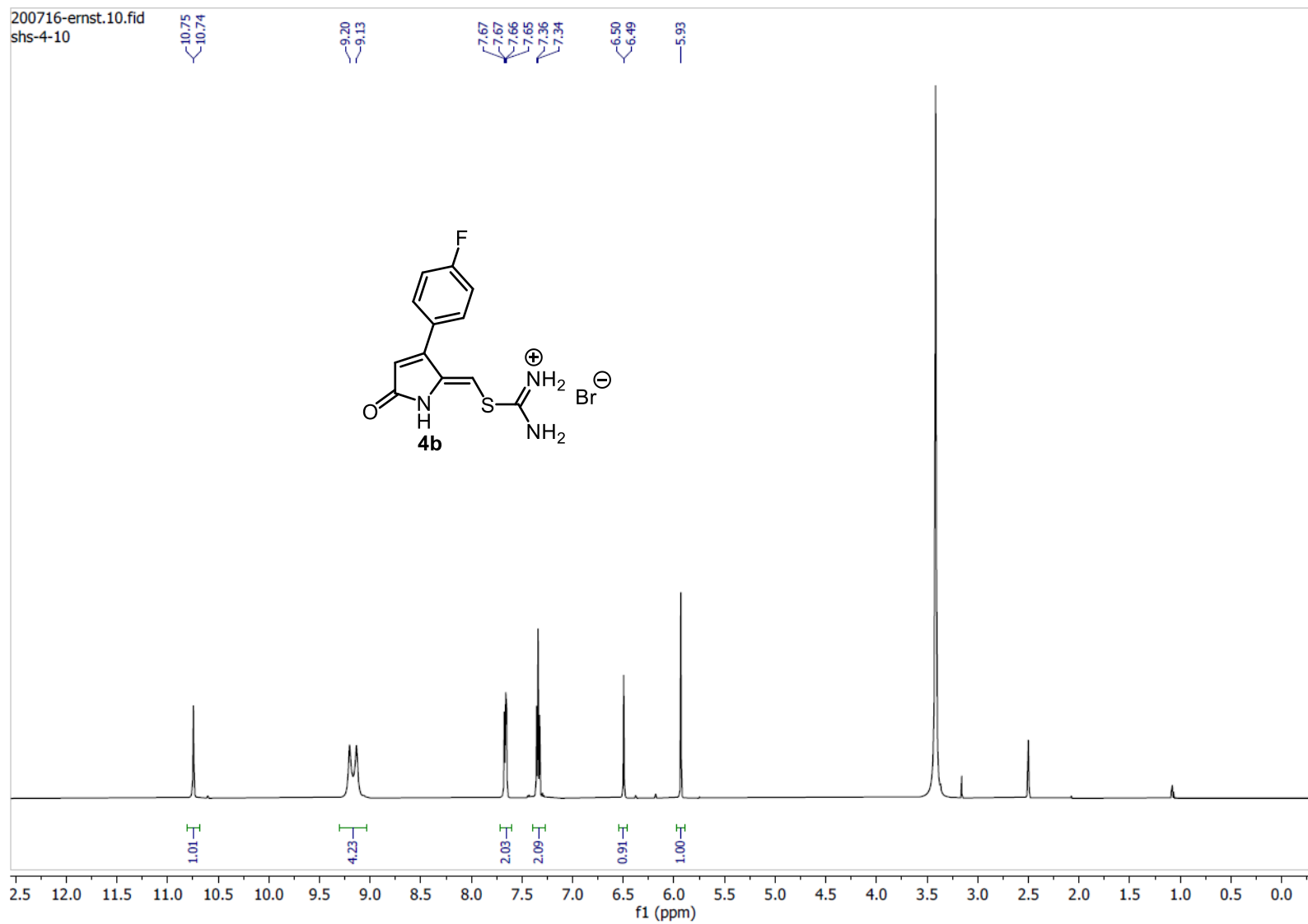
¹H NMR spectrum of compound **4a**



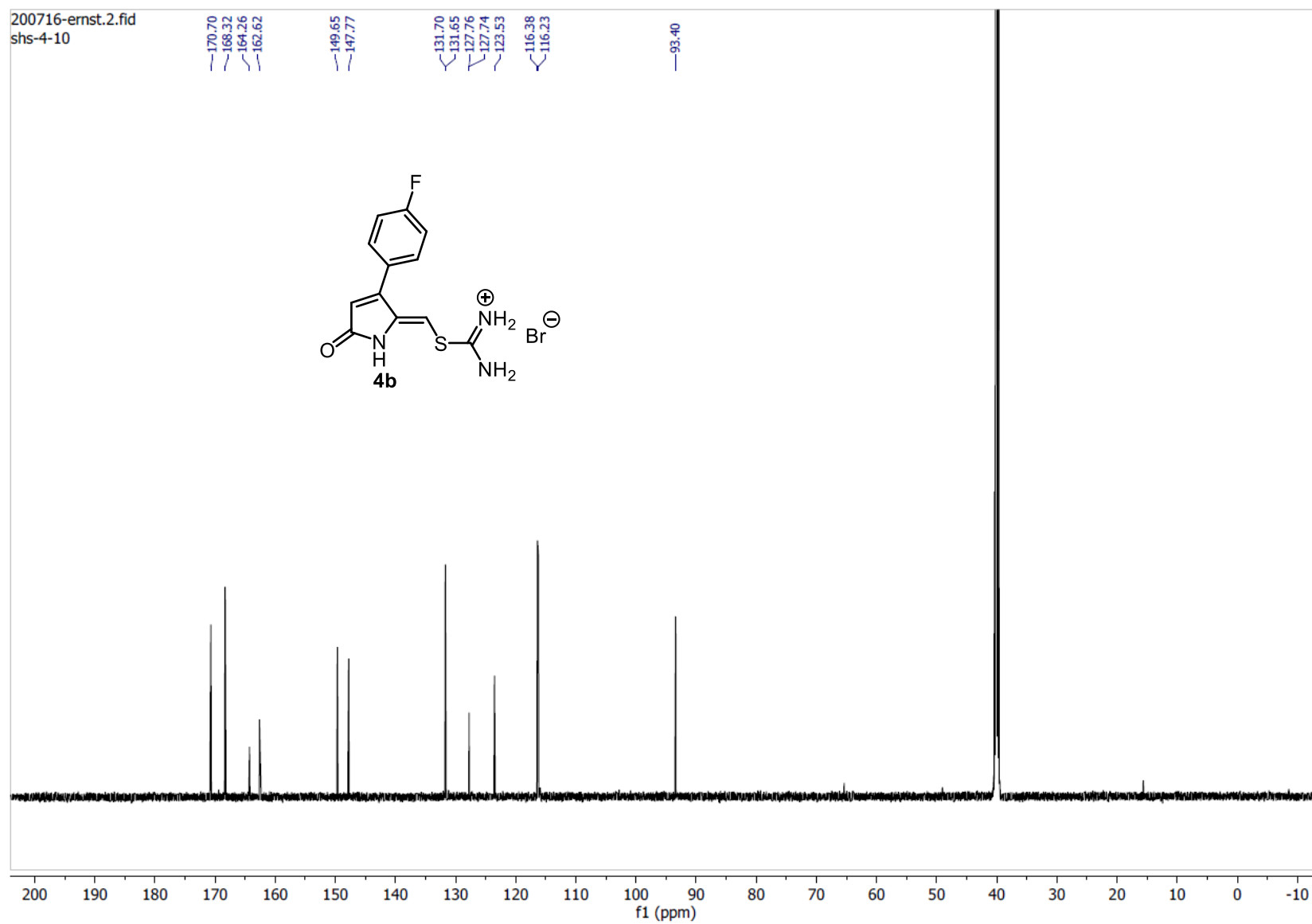
¹³C NMR spectrum of compound **4a**



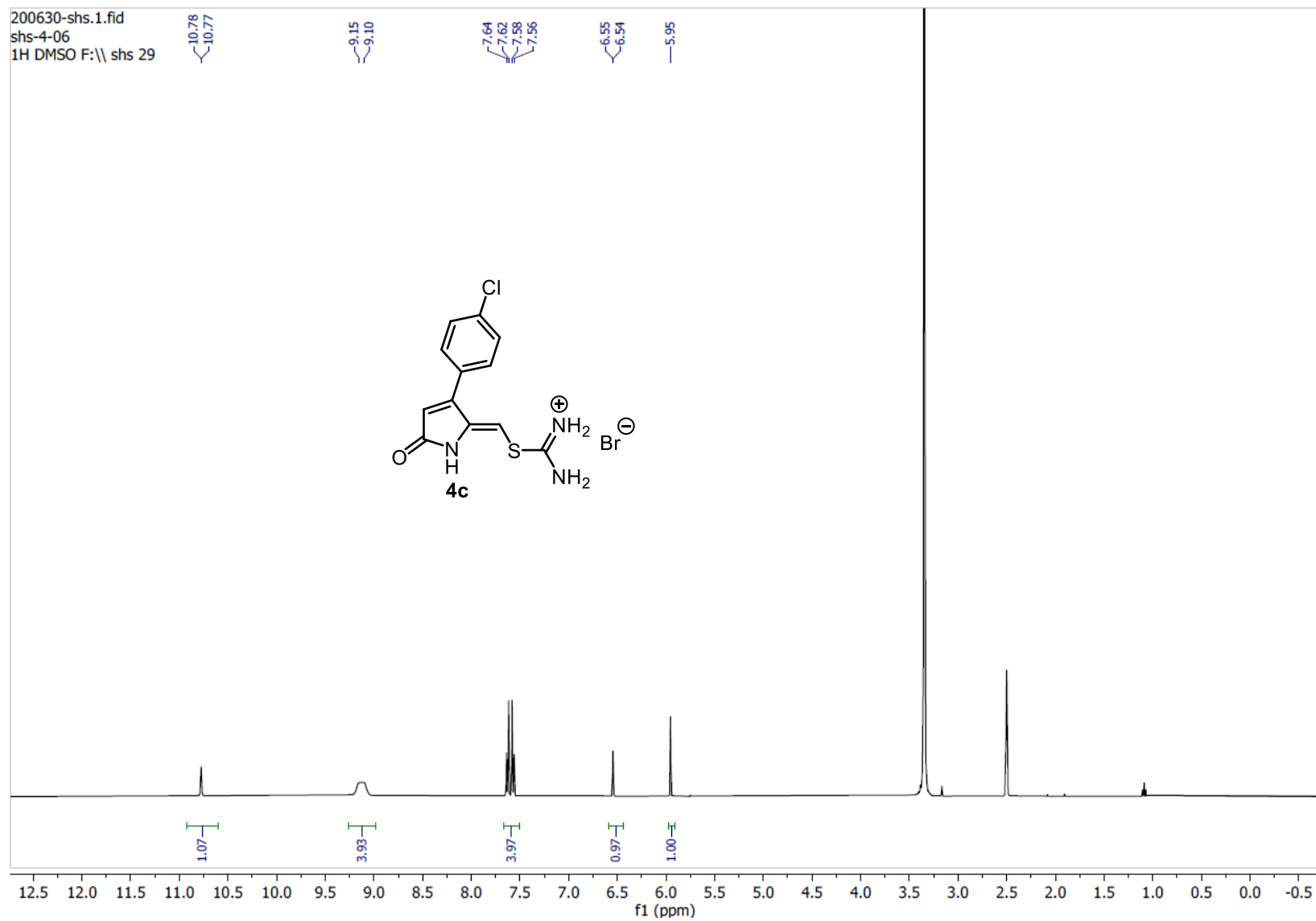
¹H NMR spectrum of compound **4b**



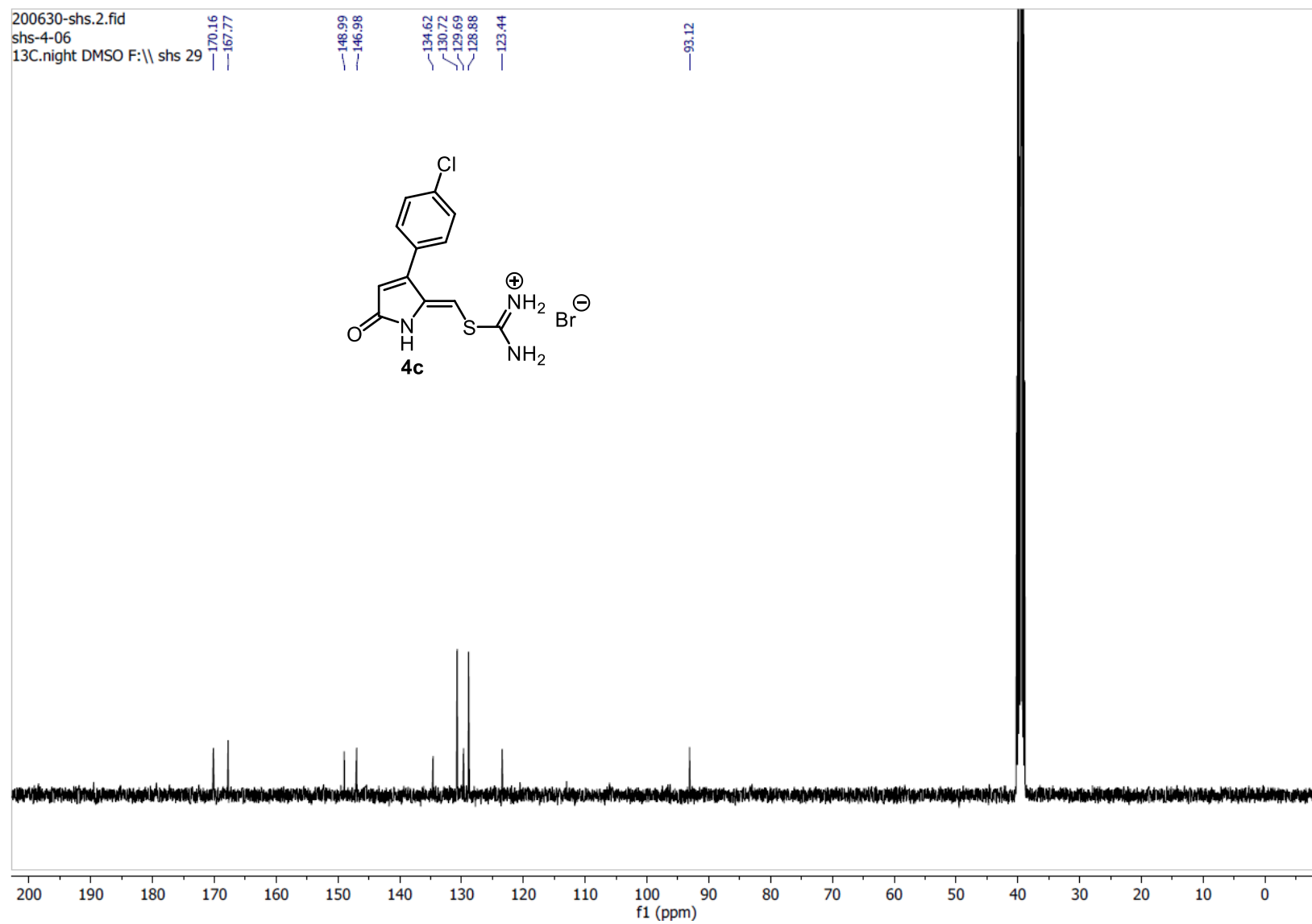
¹³C NMR spectrum of compound **4b**



¹H NMR spectrum of compound **4c**

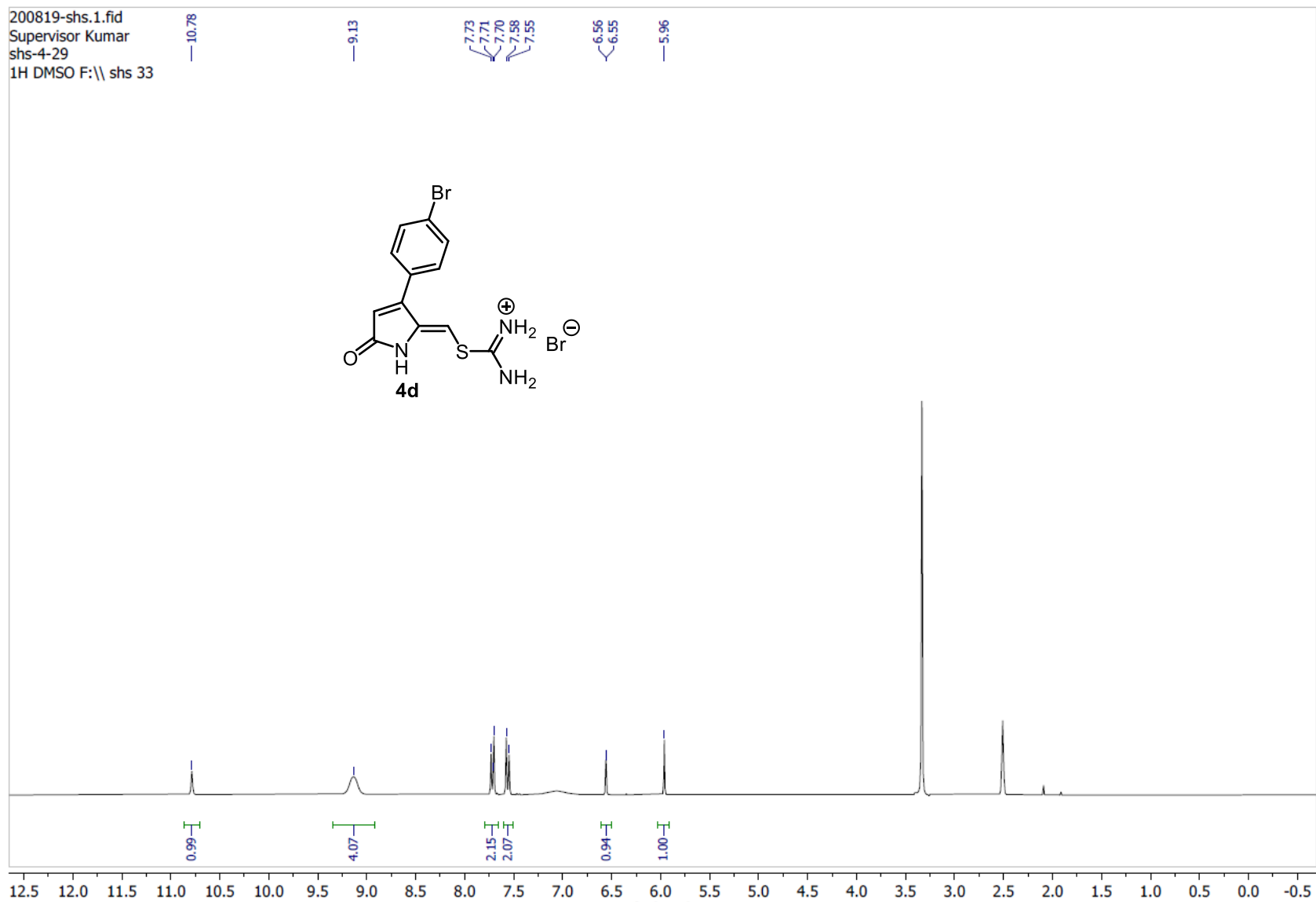


¹³C NMR spectrum of compound **4c**

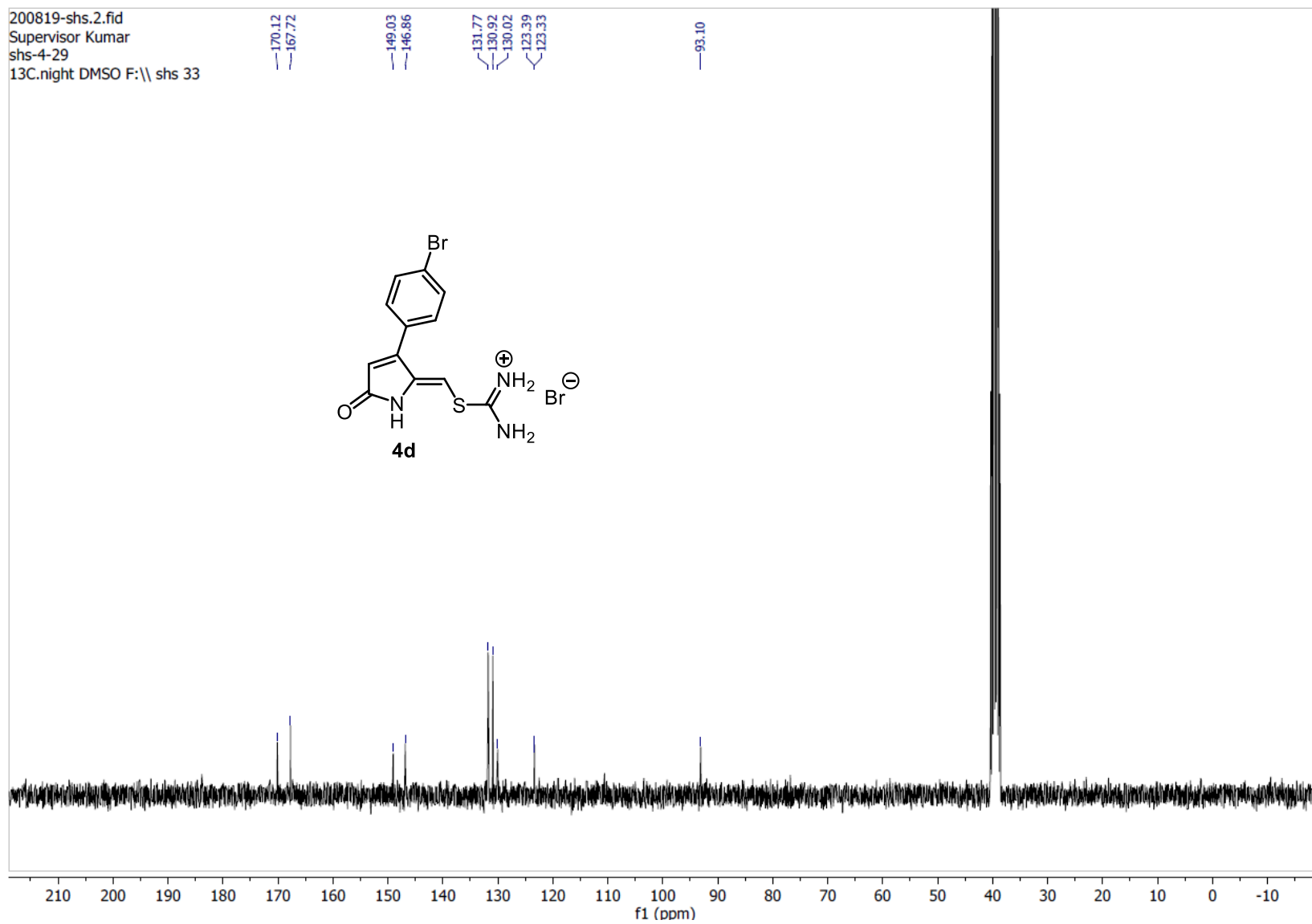


¹H NMR spectrum of compound **4d**

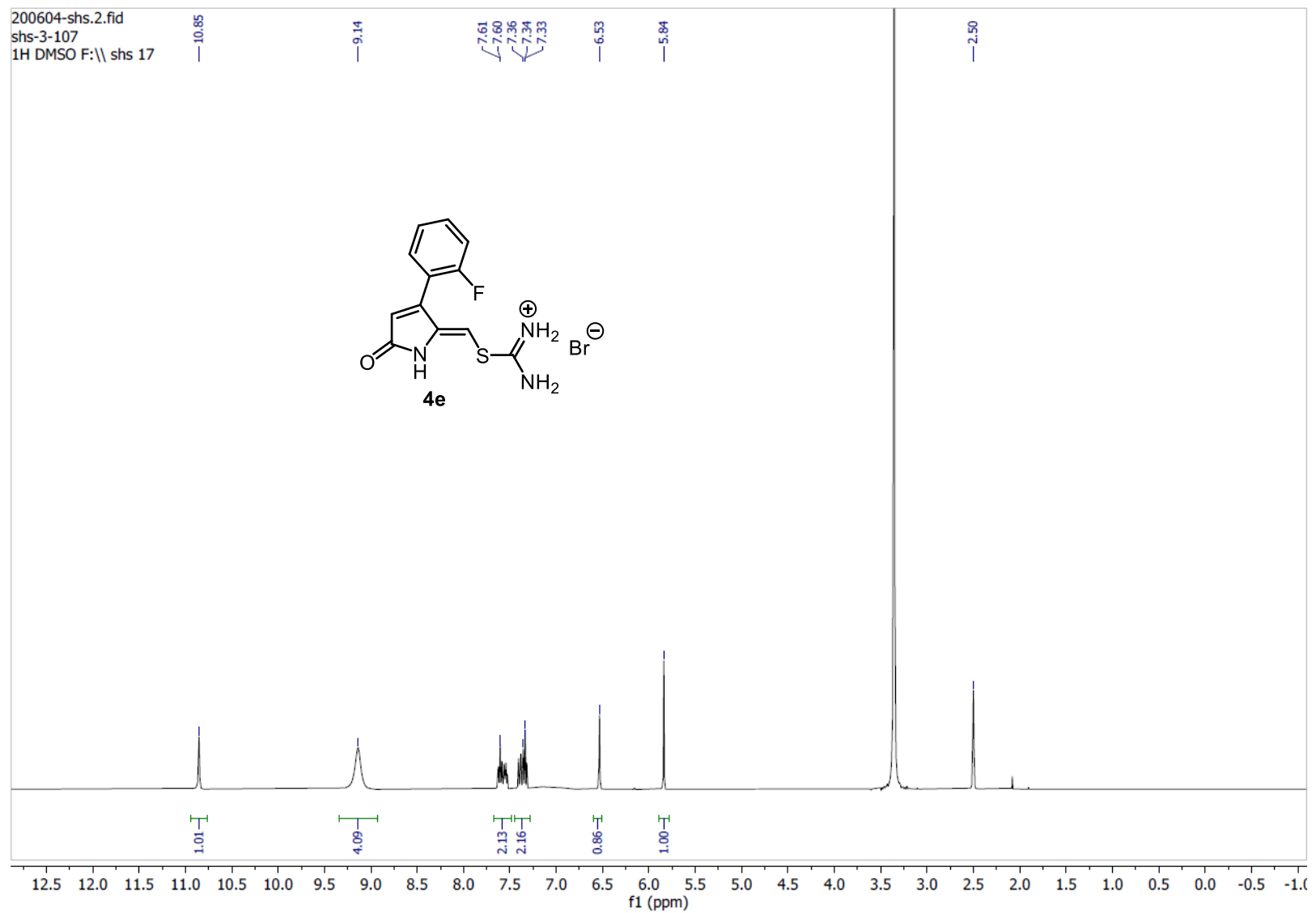
200819-shs.1.fid
Supervisor Kumar
shs-4-29
1H DMSO F:\ shs 33



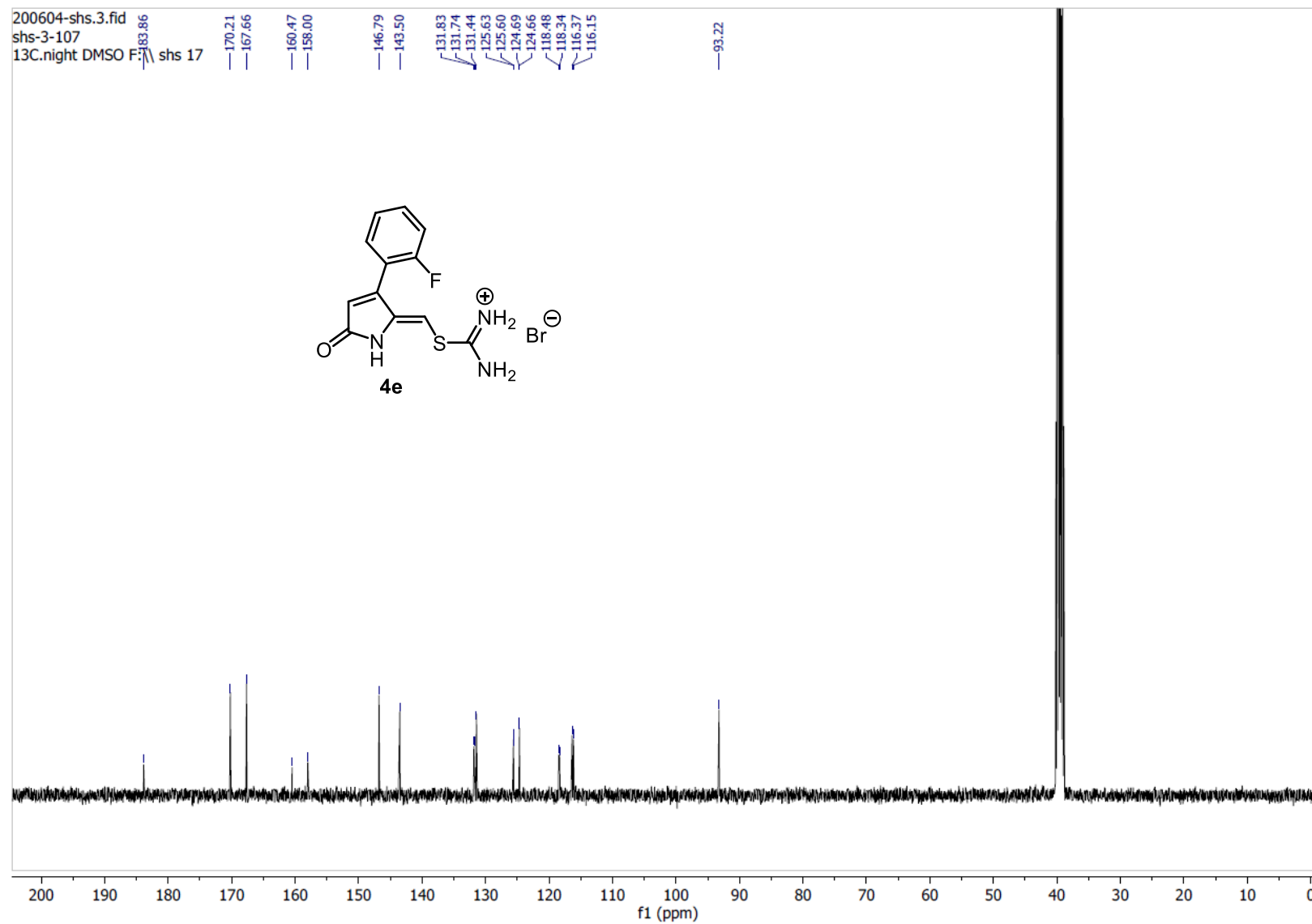
¹³C NMR spectrum of compound **4d**



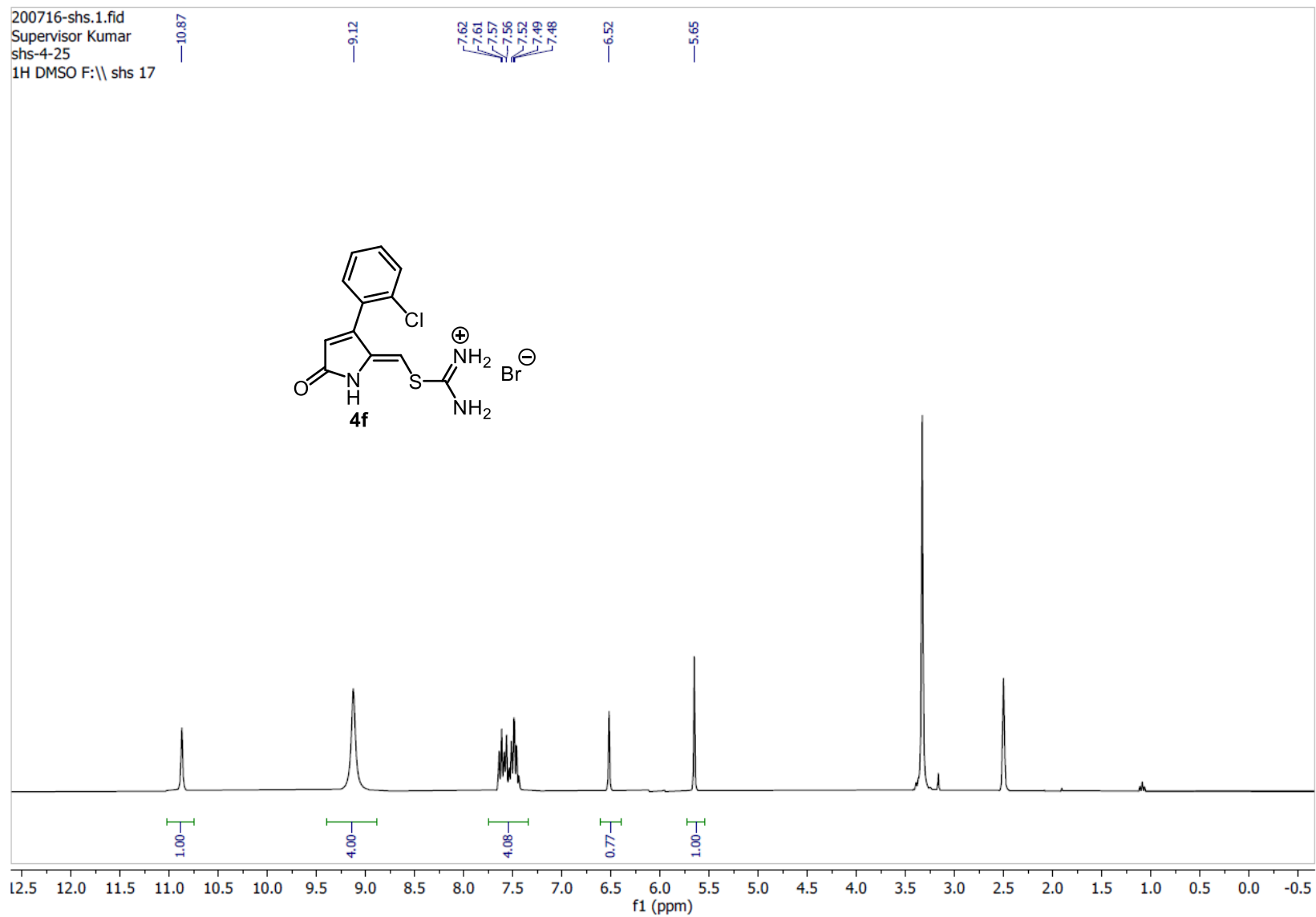
¹H NMR spectrum of compound **4e**



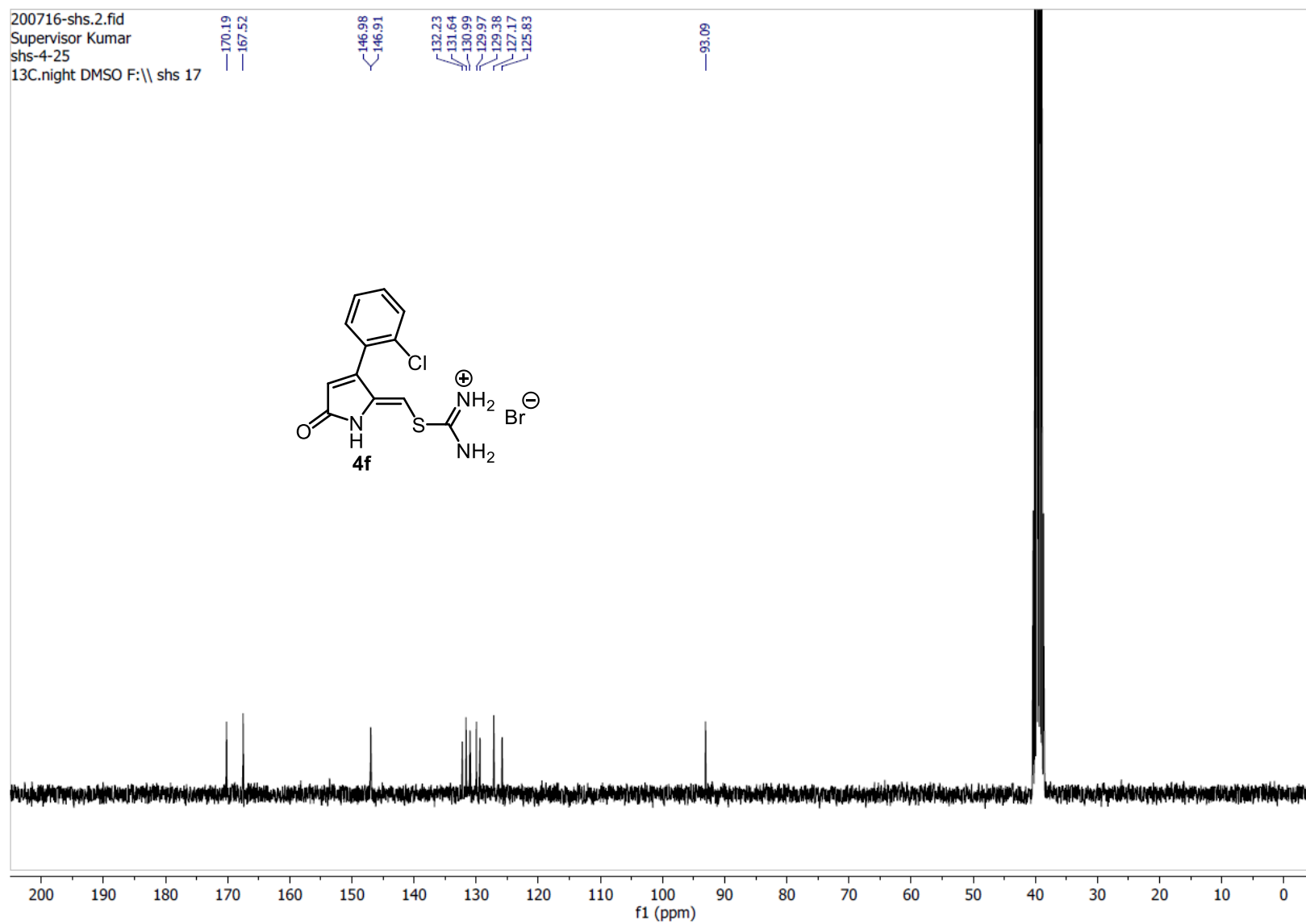
¹³C NMR spectrum of compound **4e**



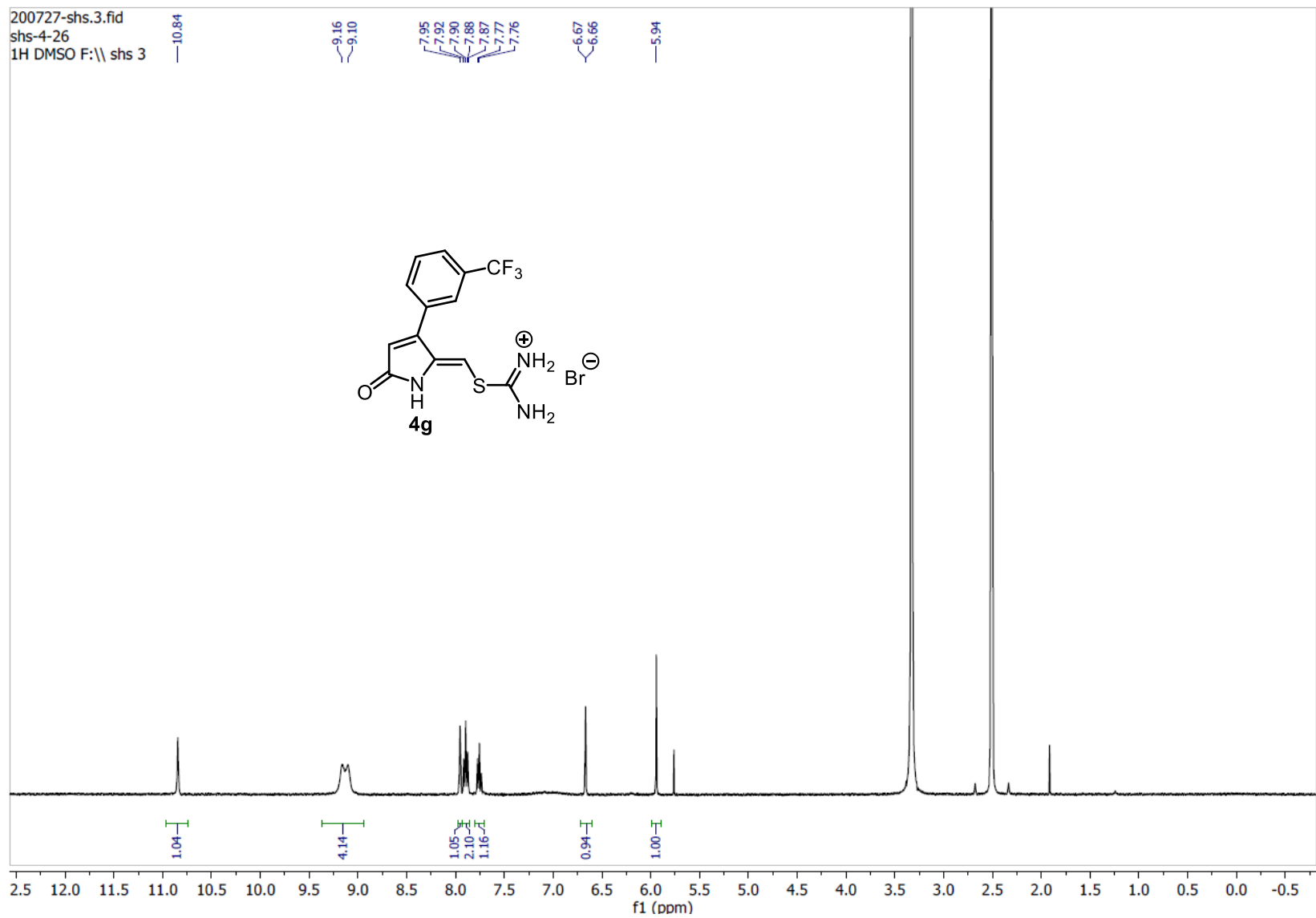
¹H NMR spectrum of compound **4f**



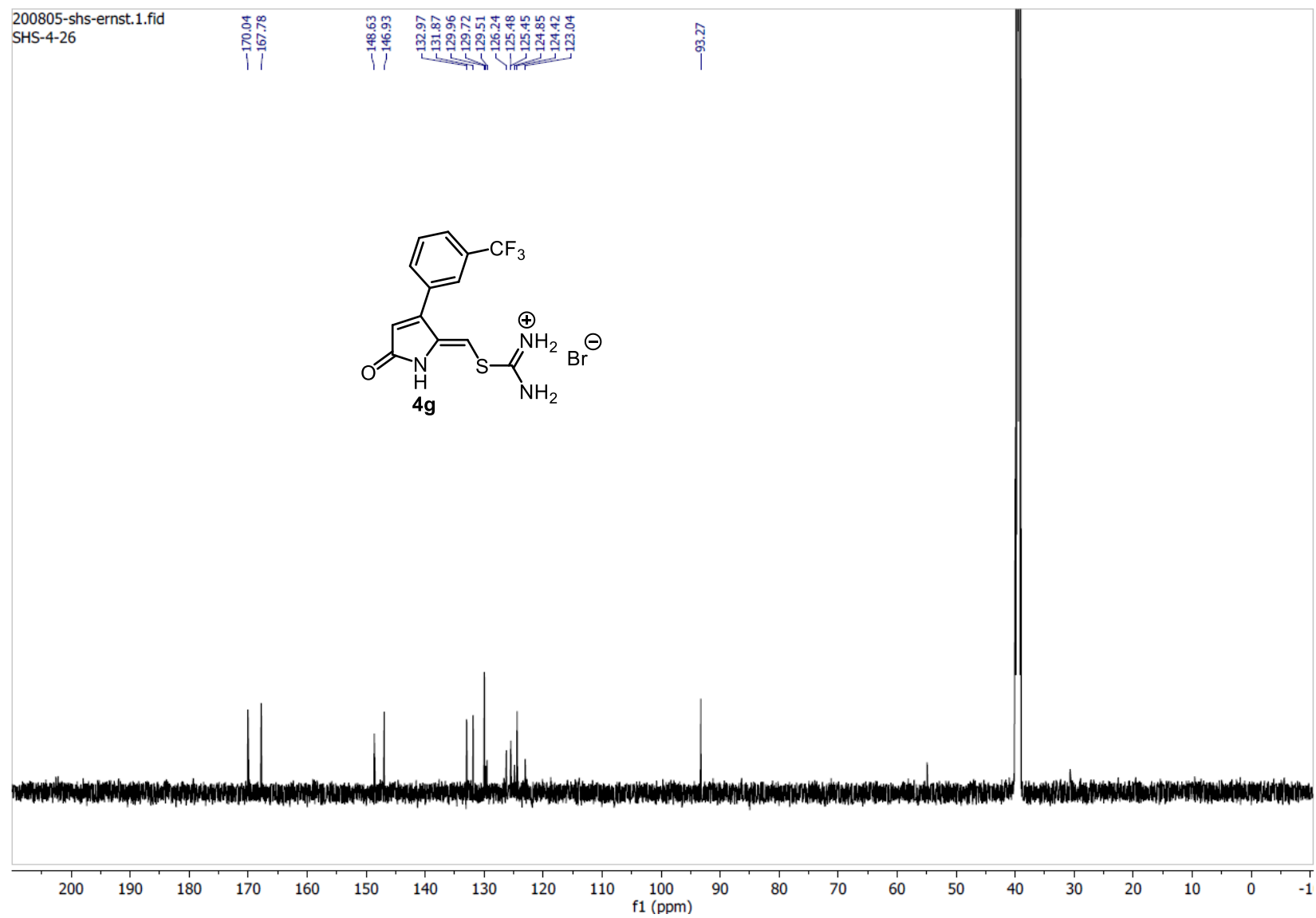
¹³C NMR spectrum of compound **4f**



¹H NMR spectrum of compound **4g**



¹³C NMR spectrum of compound **4g**



Sample submission report

Sample Analysis Request # **3073456**
Samples submitted by **Shekh Sabir**
Date run **2020-11-17**
Operator **Chowdhury Sarowar**
Report prepared by **Chowdhury Sarowar**

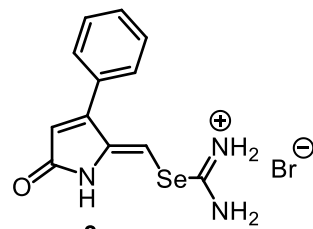
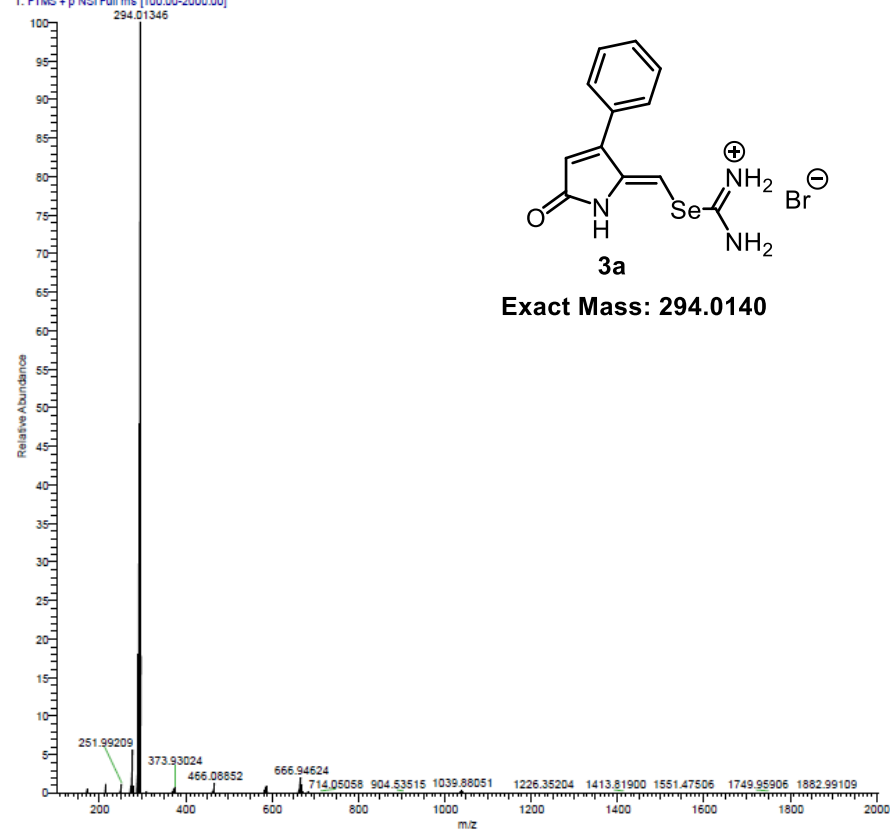


Notes:

Sample: shs-3-114

Full spectrum

shs-3-114_Pos_Full #6-8 RT: 0.30-0.41 Av: 3 NL: 9.32E8
T: FTMS + p NSI Full ms [100.00-2000.00]



Exact Mass: 294.0140

Sample submission report

Sample Analysis Request # **3073456**
Samples submitted by **Shekh Sabir**
Date run **2020-11-17**
Operator **Chowdhury Sarowar**
Report prepared by **Chowdhury Sarowar**

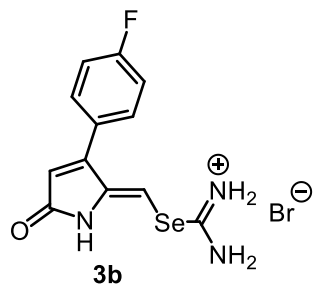
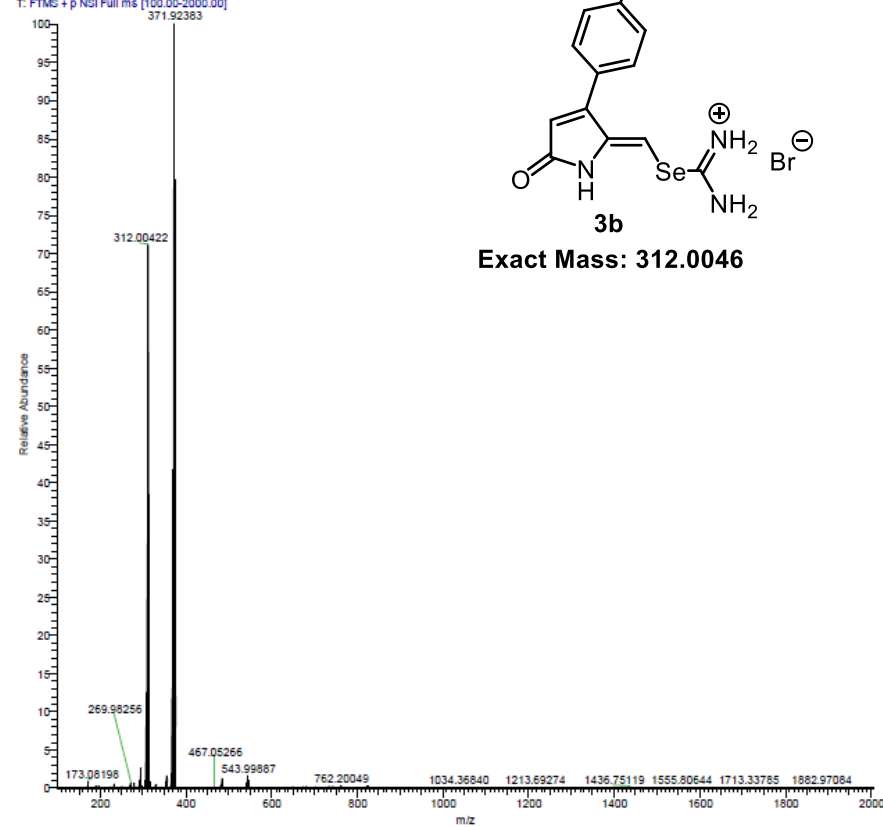


Notes:

Sample: shs-4-09

Full spectrum

shs-4-09_Pos_Full.ms#1-17 RT: 0.02-0.91 AV: 17 NL: 3.24E8
T: FTMS + p NSI Full ms [100.00-2000.00]



Exact Mass: 312.0046

Sample submission report

Sample Analysis Request # **3073456**
Samples submitted by **Shekh Sabir**
Date run **2020-11-17**
Operator **Chowdhury Sarowar**
Report prepared by **Chowdhury Sarowar**

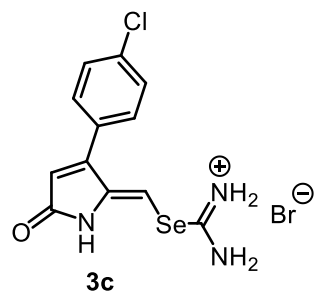
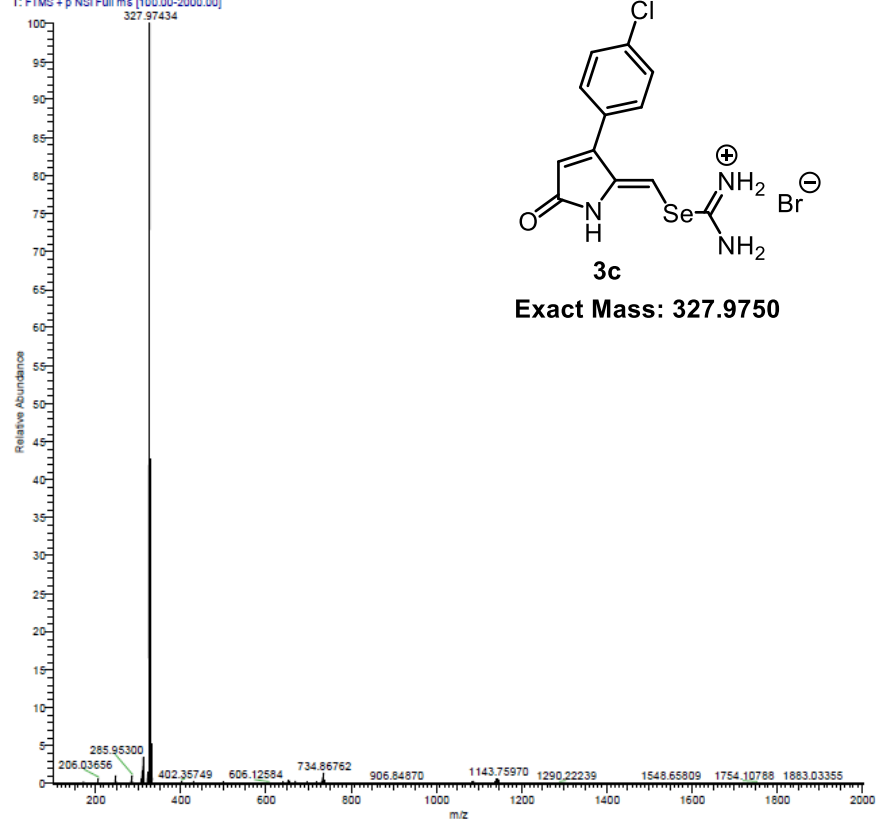


Notes:

Sample: shs-3-112

Full spectrum

shs-3-112_Pos_Full #2-9 RT: 0.08-0.47 AV: 8 NL: 5.87E8
T: FTMS + p NSI Full ms [100.00-2000.00]



Exact Mass: 327.9750

Sample submission report

Sample Analysis Request # **3073456**
Samples submitted by **Shekh Sabir**
Date run 2020-11-17
Operator Chowdhury Sarowar
Report prepared by Chowdhury Sarowar

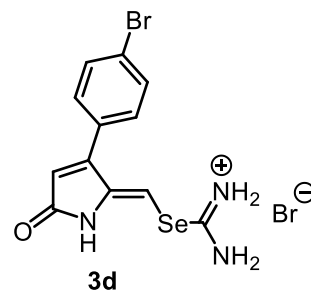
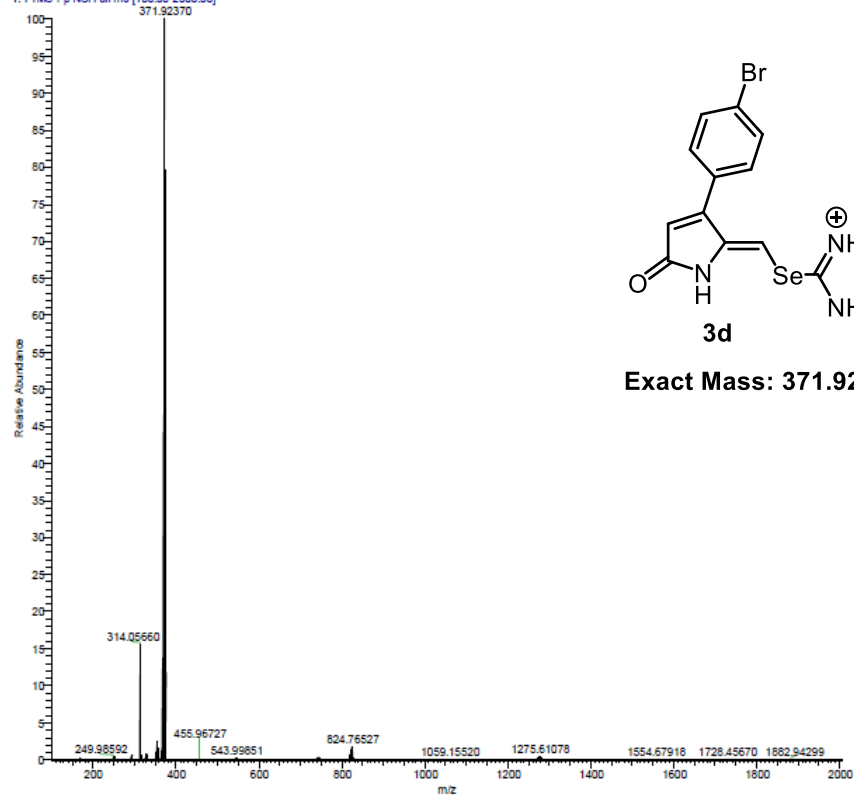


Notes:

Sample: shs-3-100

Full spectrum

shs-3-100_Pos_Full#1-7 RT: 0.02-0.35 Av: 7 NL: 2.71E8
T: FTMS + p NSI Full ms [100.00-2000.00]



Exact Mass: 371.9245

Sample submission report

Sample Analysis Request # **2997593**
Samples submitted by **Sabir, Shekh**
Date run **2020-08-11**
Operator **Chowdhury Sarowar**
Report prepared by **Chowdhury Sarowar**

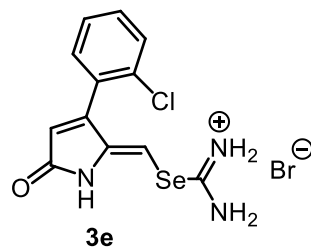
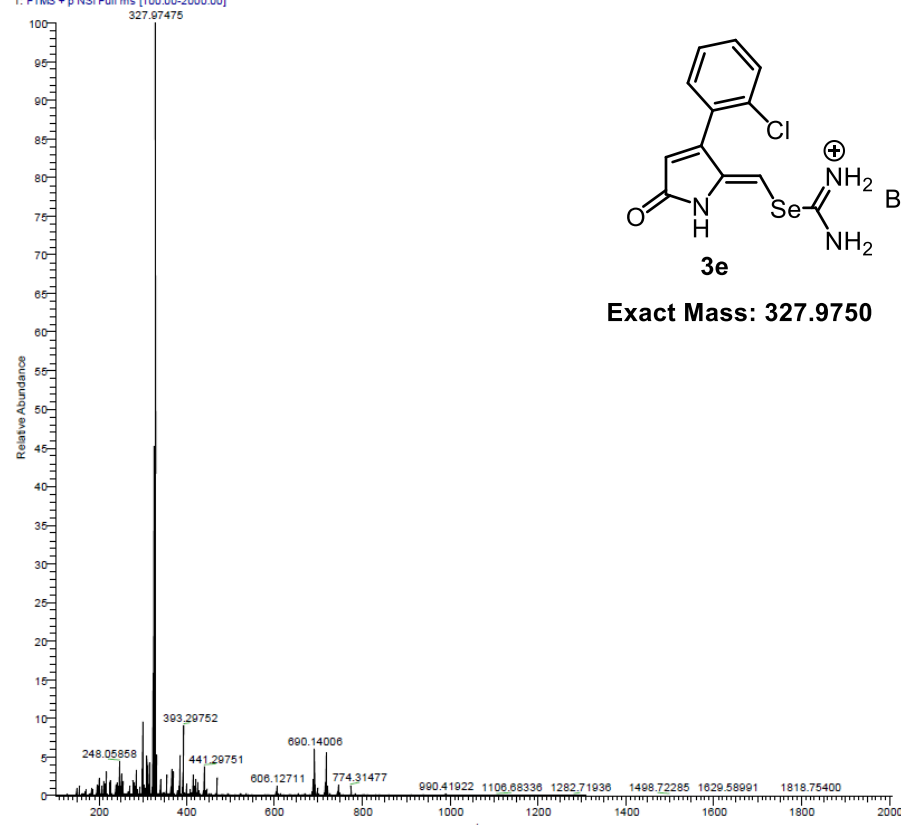


Notes:

Sample: shs-3-24

Full spectrum

shs-3-24_Pos_Full #13-23 RT: 0.73-1.31 AV: 11 NL: 5.61E7
T: FTMS + p NSI Full ms [100.00-2000.00]



Exact Mass: 327.9750

Sample submission report

Sample Analysis Request # **3073456**
Samples submitted by **Shekh Sabir**
Date run 2020-11-17
Operator Chowdhury Sarowar
Report prepared by Chowdhury Sarowar

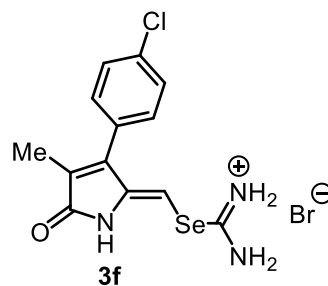
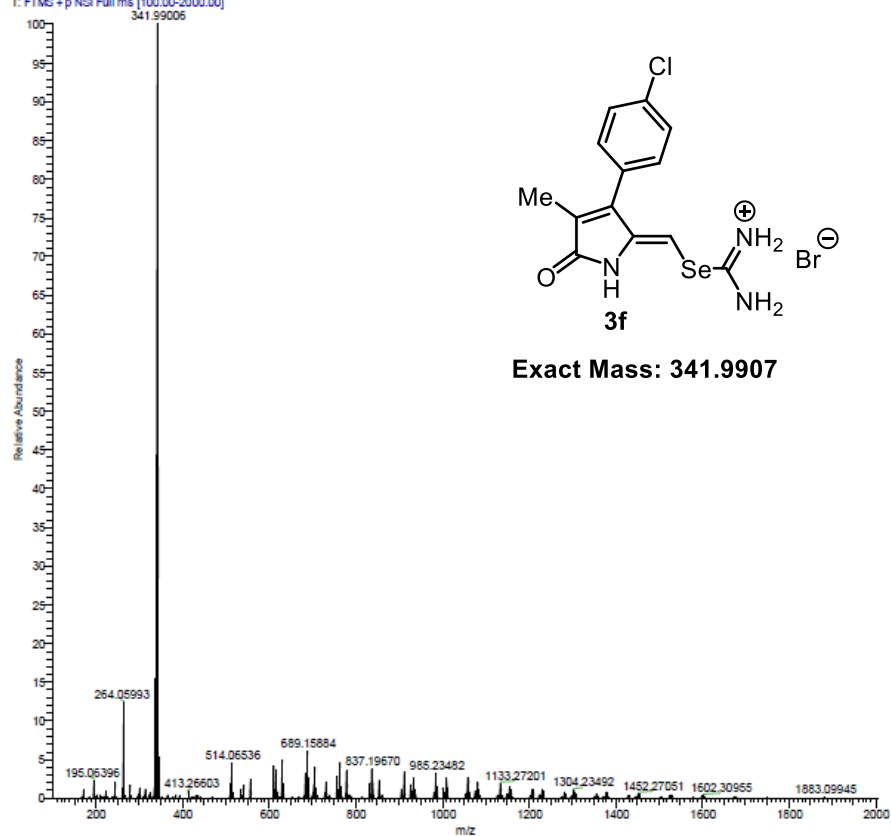


Notes:

Sample: shs-4-19

Full spectrum

shs-4-19_Pos_Full #1-7 RT: 0.02-0.36 Av: 7 NL: 1.62E8
T: FTMS +p NSI Full ms [100.00-2000.00]



Exact Mass: 341.9907

Sample submission report

Sample Analysis Request # **3073456**
Samples submitted by **Shekh Sabir**
Date run **2020-11-17**
Operator **Chowdhury Sarowar**
Report prepared by **Chowdhury Sarowar**

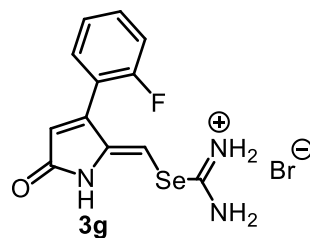
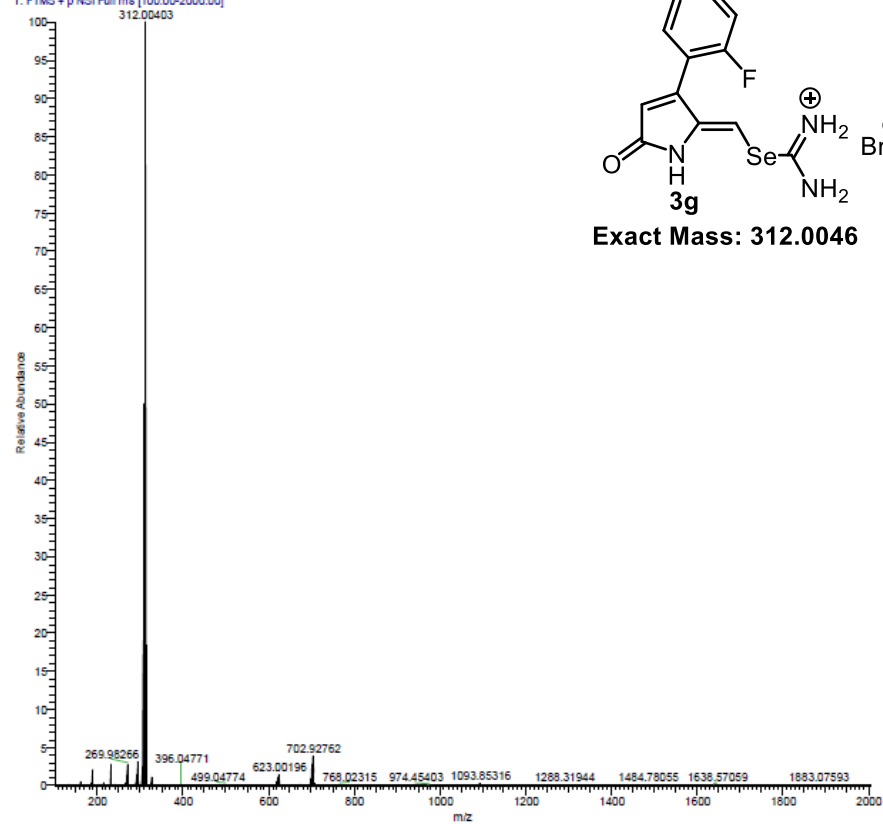


Notes:

Sample: shs-3-103

Full spectrum

shs-3-103_Pos_Full #1-7 RT: 0.02-0.36 Av: 7 NL: 5.58E8
T: FTMS + p NSI Full ms [100.00-2000.00]



Exact Mass: 312.0046

Sample submission report

Sample Analysis Request # **3073456**
Samples submitted by **Shekh Sabir**
Date run **2020-11-17**
Operator **Chowdhury Sarowar**
Report prepared by **Chowdhury Sarowar**

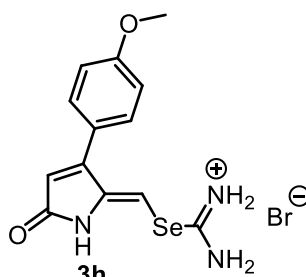
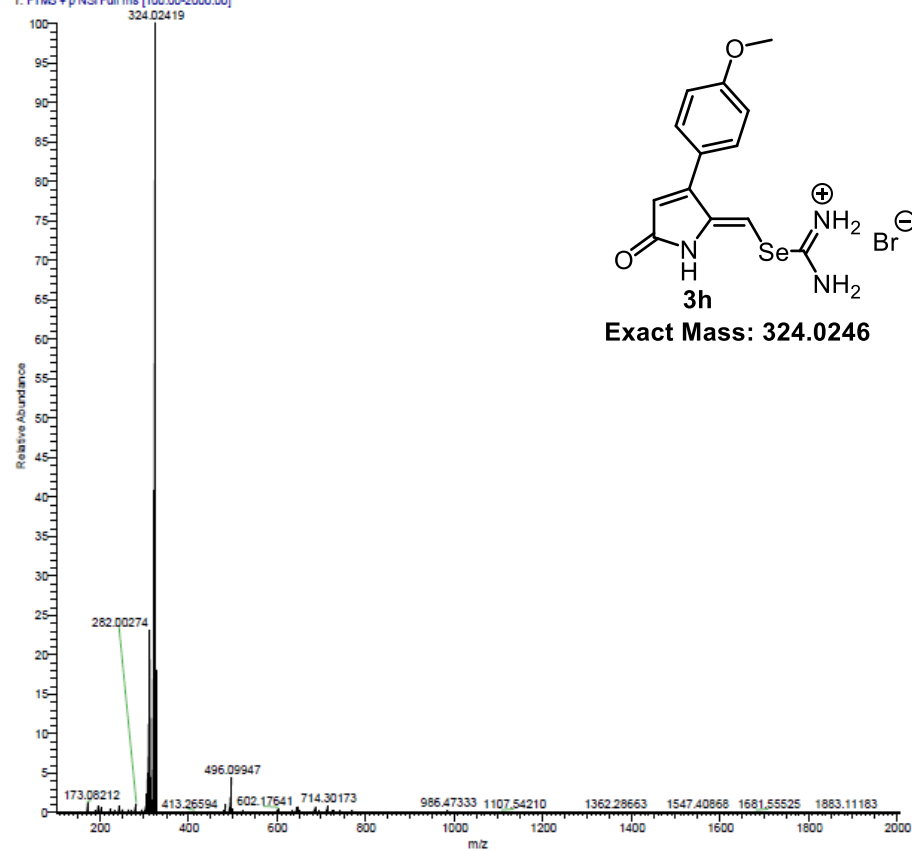


Notes:

Sample: shs-4-14

Full spectrum

shs-4-14_Pos_Full #1-18 RT: 0.02-0.97 AV: 18 NL: 1.54E8
T: FTMS + p NSI Full ms [100.00-2000.00]



Exact Mass: 324.0246

Sample submission report

Sample Analysis Request # **3073456**
Samples submitted by **Shekh Sabir**
Date run **2020-11-17**
Operator **Chowdhury Sarowar**
Report prepared by **Chowdhury Sarowar**

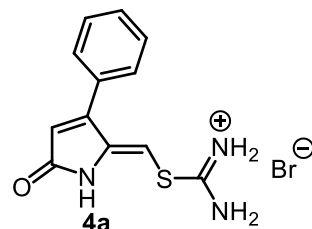
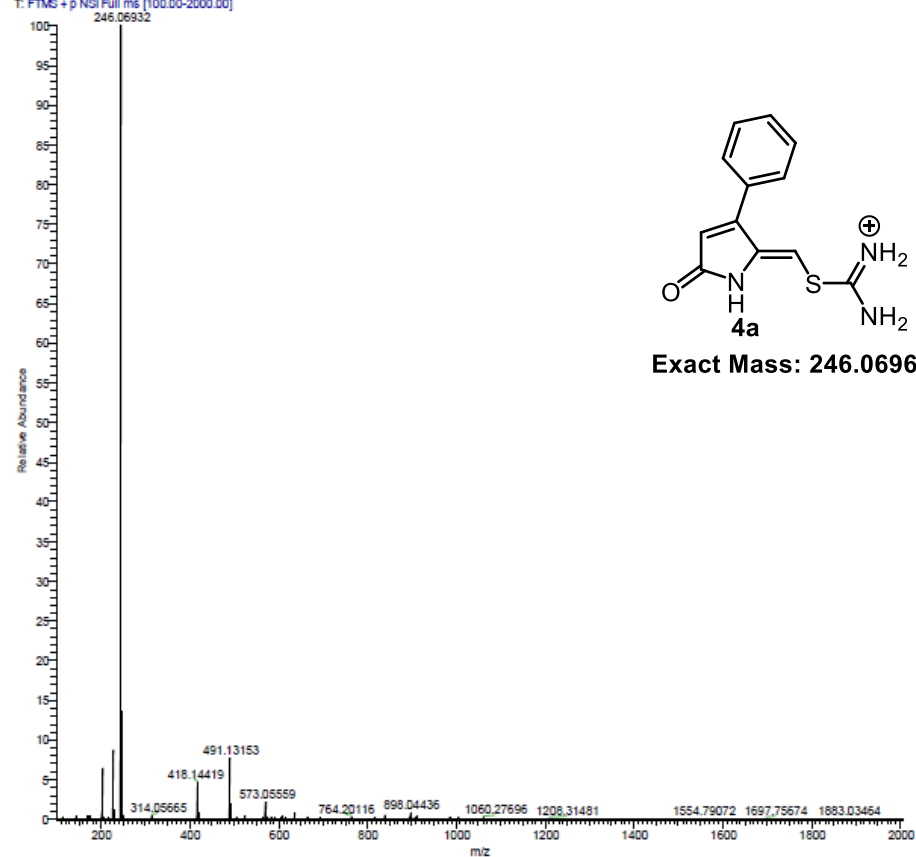


Notes:

Sample: shs-3-115

Full spectrum

shs-3-115_Pos_Full#15-20 RT: 0.80-1.08 AV: 6 NL: 3.42E8
T: FTMS + p NSI Full ms [100.00-2000.00]



Exact Mass: 246.0696

Sample submission report

Sample Analysis Request # **3073456**
Samples submitted by **Shekh Sabir**
Date run **2020-11-17**
Operator **Chowdhury Sarowar**
Report prepared by **Chowdhury Sarowar**

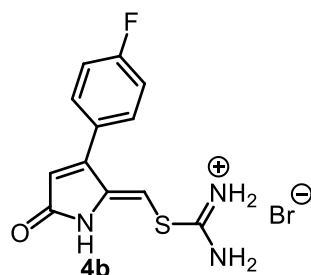
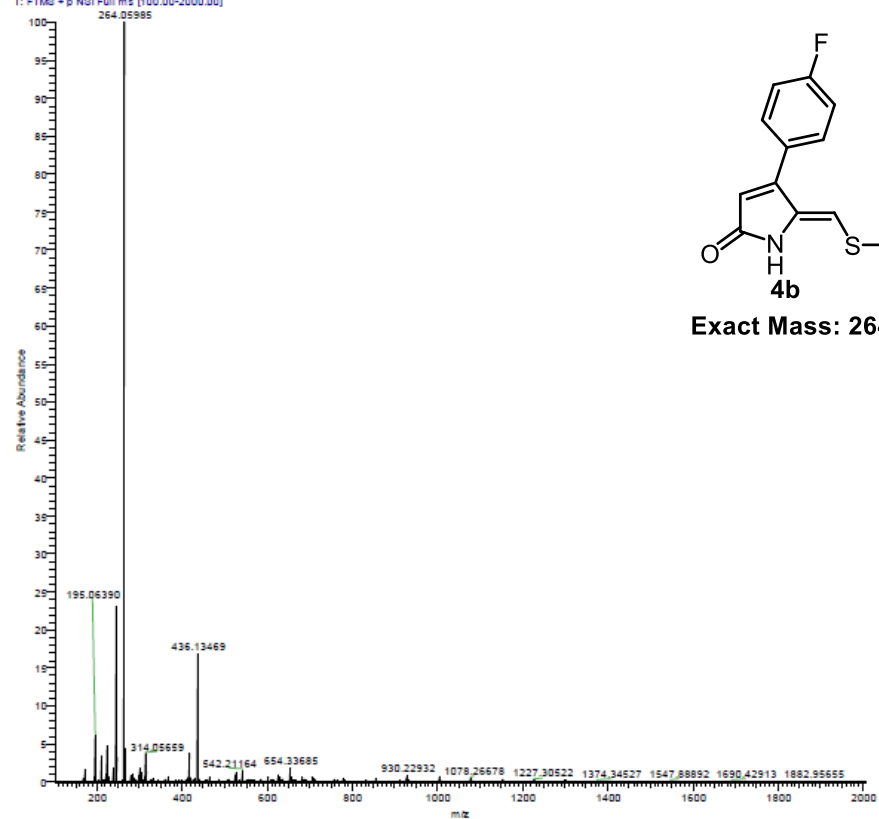


Notes:

Sample: shs-4-10

Full spectrum

shs-4-10_Pos_Full #2-12 RT: 0.08-0.63 AV: 11 NL: 2.49E8
T: FTMS - p NSI Full ms (100.00-2000.00)



Exact Mass: 264.0601

Sample submission report

Sample Analysis Request # **3073456**
Samples submitted by **Shekh Sabir**
Date run **2020-11-17**
Operator **Chowdhury Sarwar**
Report prepared by **Chowdhury Sarwar**

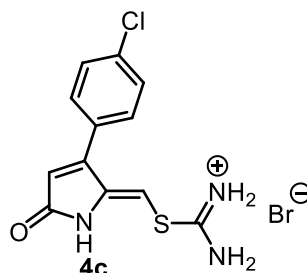
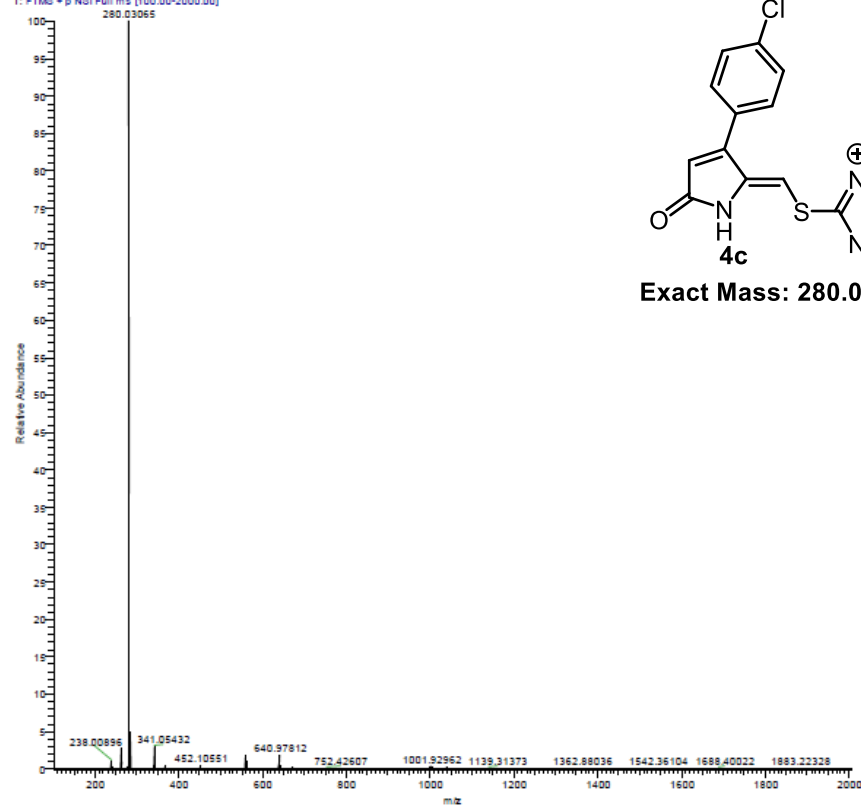


Notes:

Sample: shs-4-06

Full spectrum

shs-4-06_Pos_Full #8-18 RT: 0.41-0.97 AV: 11 NL: 6.24E8
T: FTMS - p NCI Full ms (100.00-2000.00)



Exact Mass: 280.0306

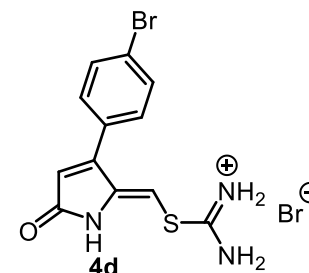
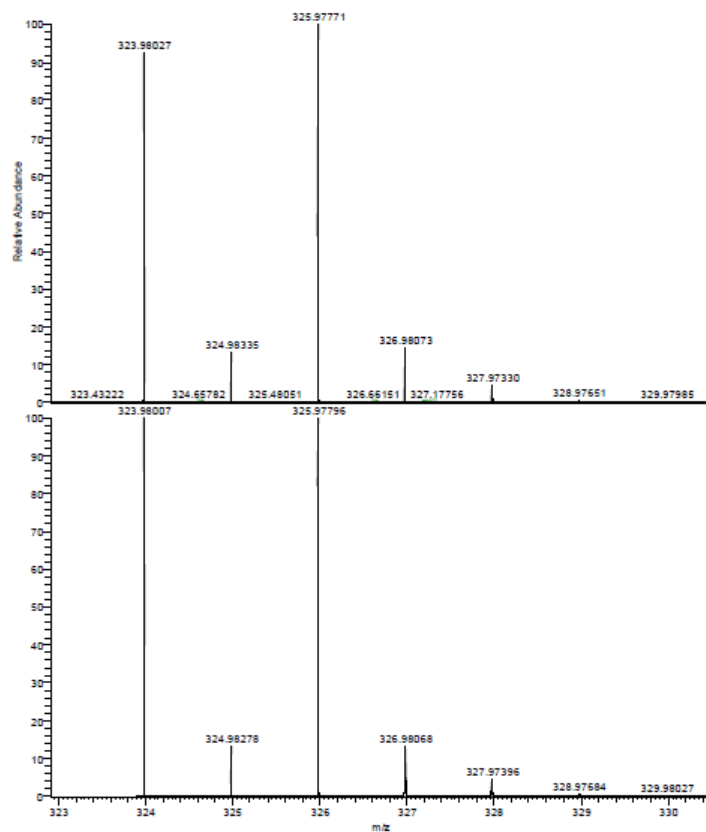
Sample submission report

Sample Analysis Request # **3073456**
Samples submitted by **Shekh Sabir**
Date run **2020-11-17**
Operator **Chowdhury Sarowar**
Report prepared by **Chowdhury Sarowar**



Notes:

Zoomed spectrum



Exact Mass: 323.9801

Sample submission report

Sample Analysis Request # **3073456**
Samples submitted by **Shekh Sabir**
Date run **2020-11-17**
Operator **Chowdhury Sarowar**
Report prepared by **Chowdhury Sarowar**

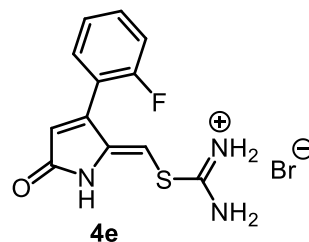
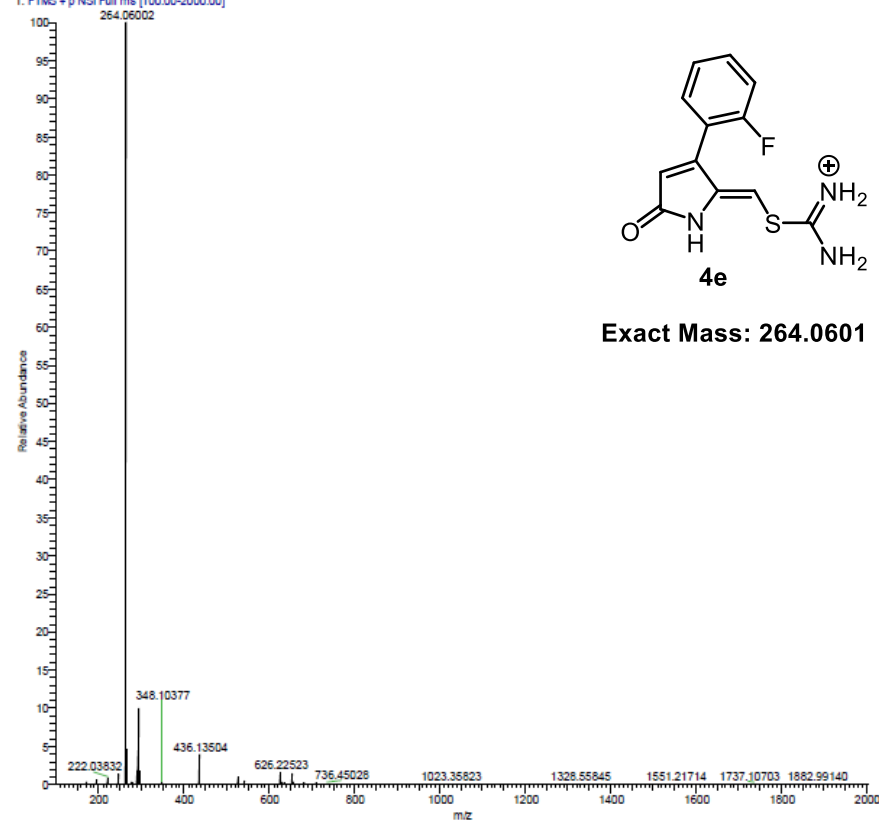


Notes:

Sample: shs-3-107

Full spectrum

shs-3-107_Pos_Full #1-7 RT: 0.02-0.36 AV: 7 NL: 2.00E8
T: FTMS + p NSI Full ms [100.00-2000.00]

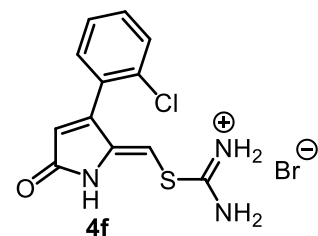
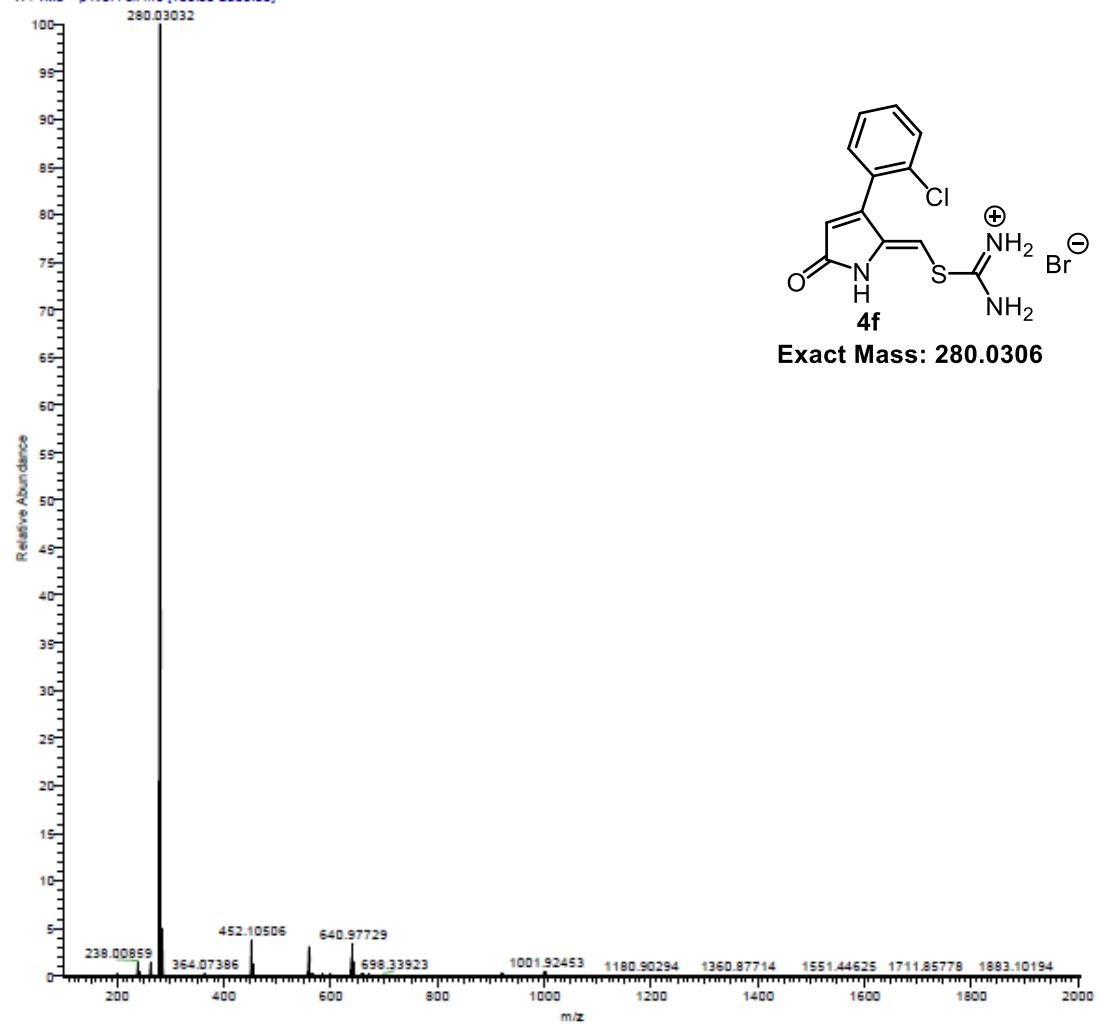


Exact Mass: 264.0601

Sample: shs-4-25

Full spectrum

shs-4-25_Pos_Full #8-13 RT: 0.41-0.69 AV: 6 NL: 6.51E8
T: FTMS + p NSI Full ms [100.00-2000.00]



Exact Mass: 280.0306

Sample submission report

Sample Analysis Request # **3073456**
Samples submitted by **Shekh Sabir**
Date run **2020-11-17**
Operator **Chowdhury Sarwar**
Report prepared by **Chowdhury Sarwar**

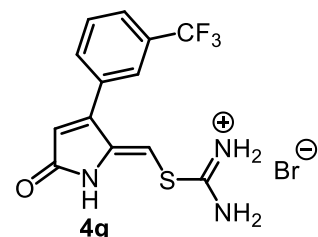
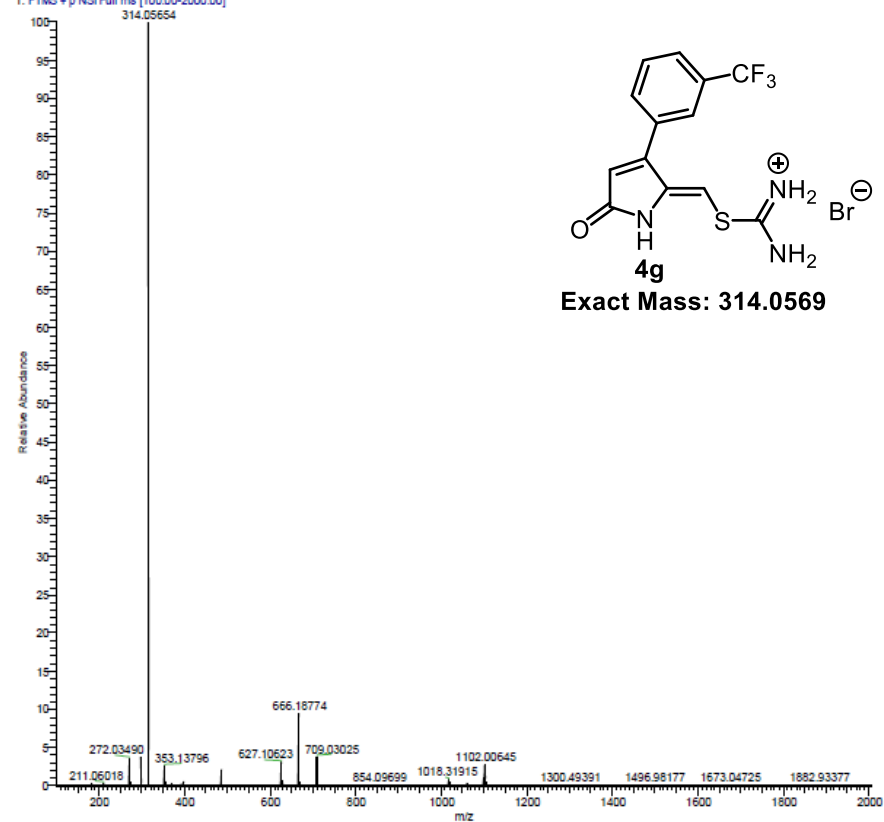


Notes:

Sample: shs-3-26

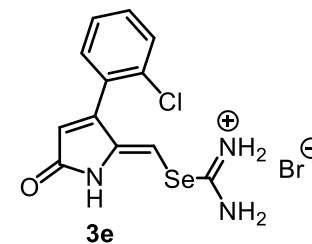
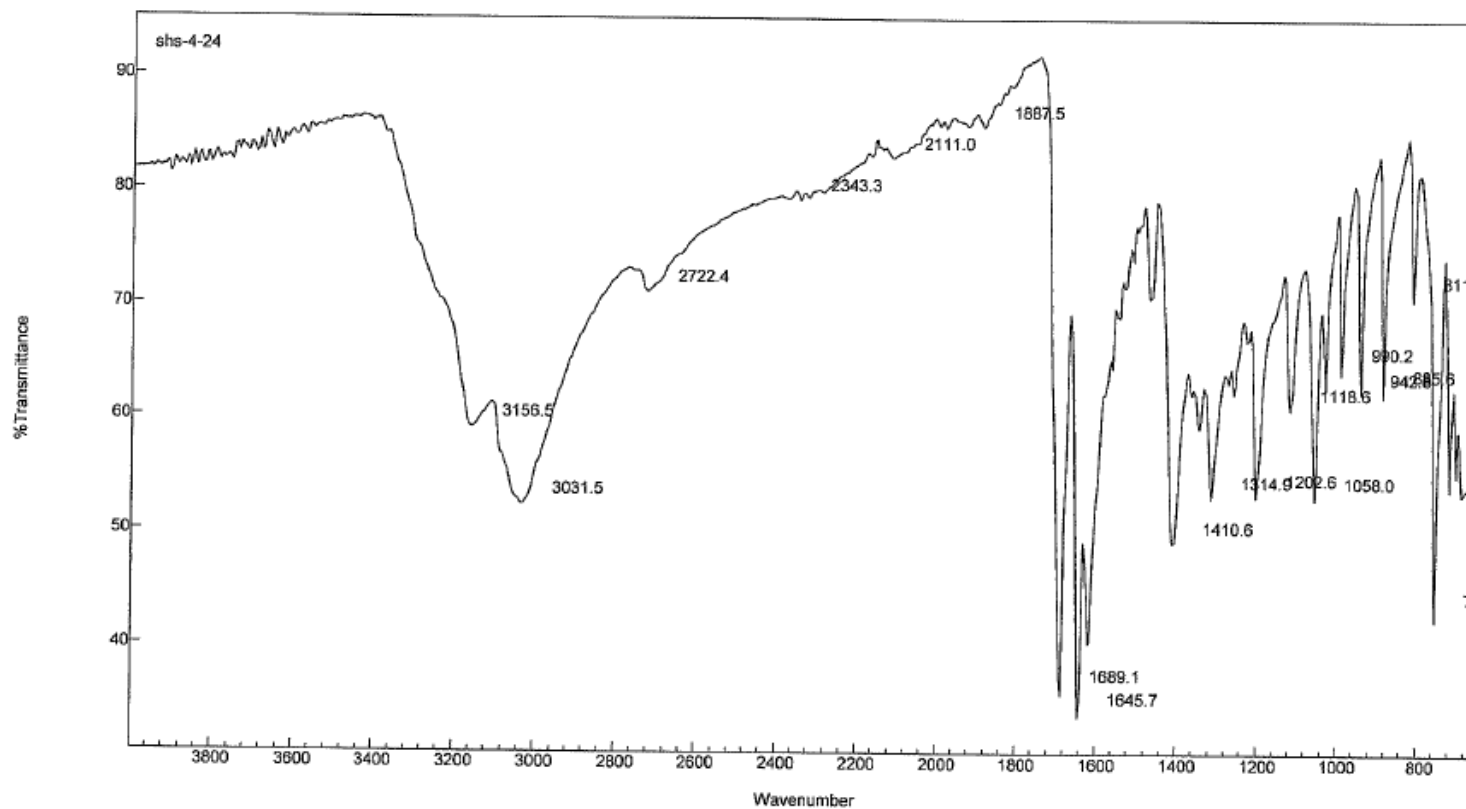
Full spectrum

shs-3-26_Pos_Full #5-12 RT: 0.25-0.64 AV: 8 NL: 4.93E8
T: FTMS + p NSI Full ms [100.00-2000.00]



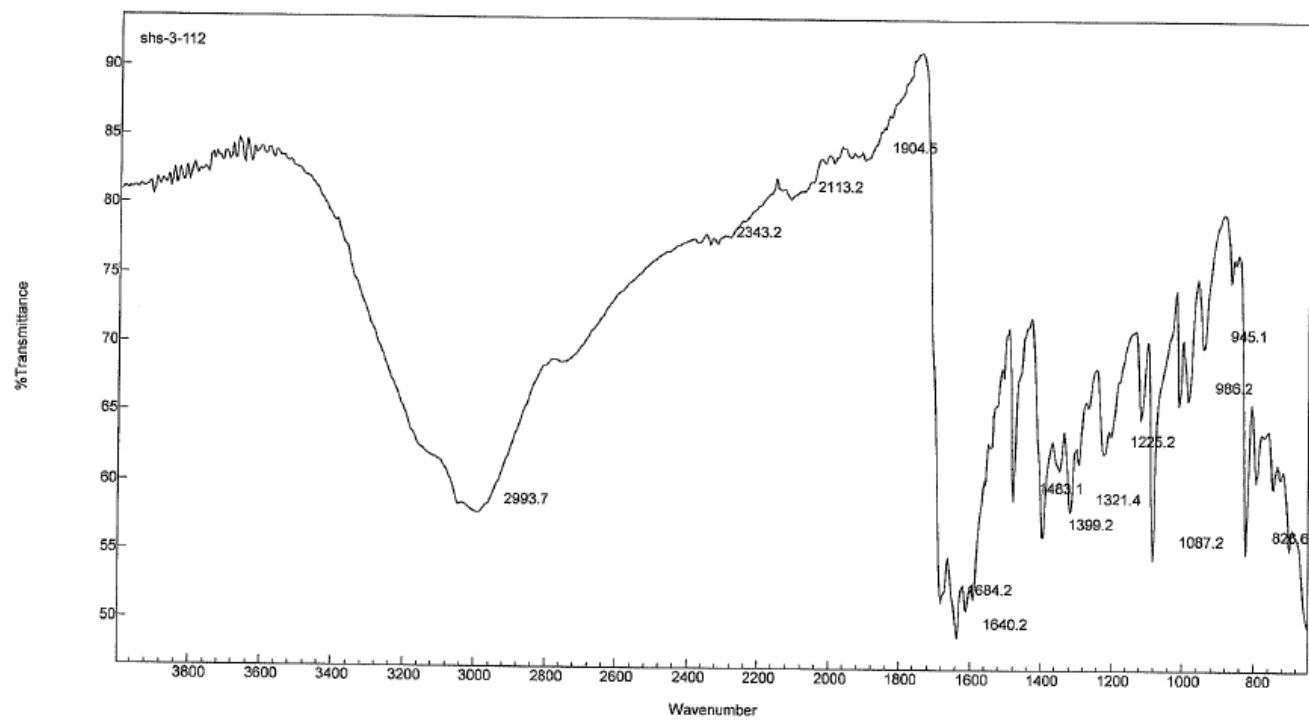
Exact Mass: 314.0569

Agilent Resolutions Pro

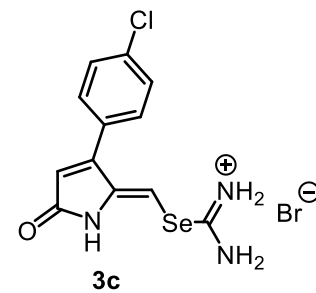


Name
shs-4-24

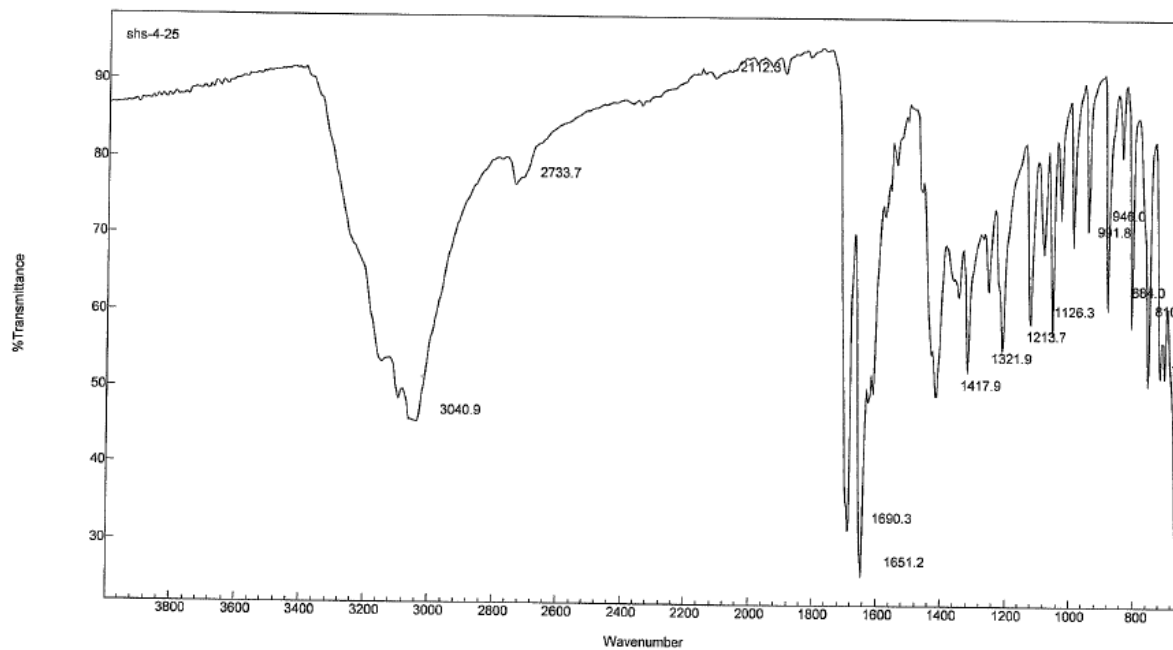
Agilent Resolutions Pro



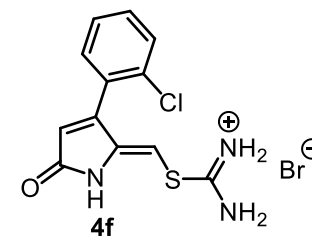
Name
shs-3-112



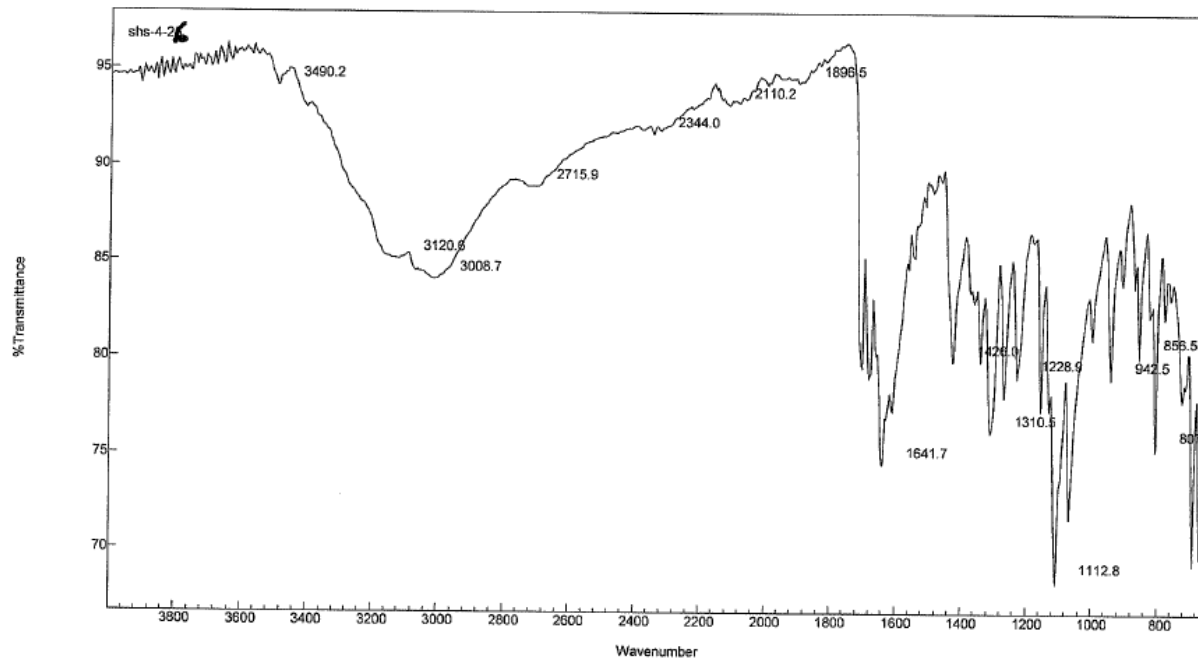
Agilent Resolutions Pro



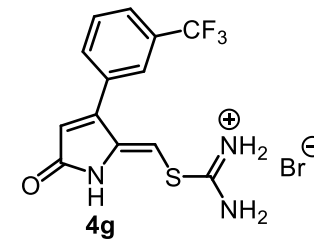
Name
shs-4-25



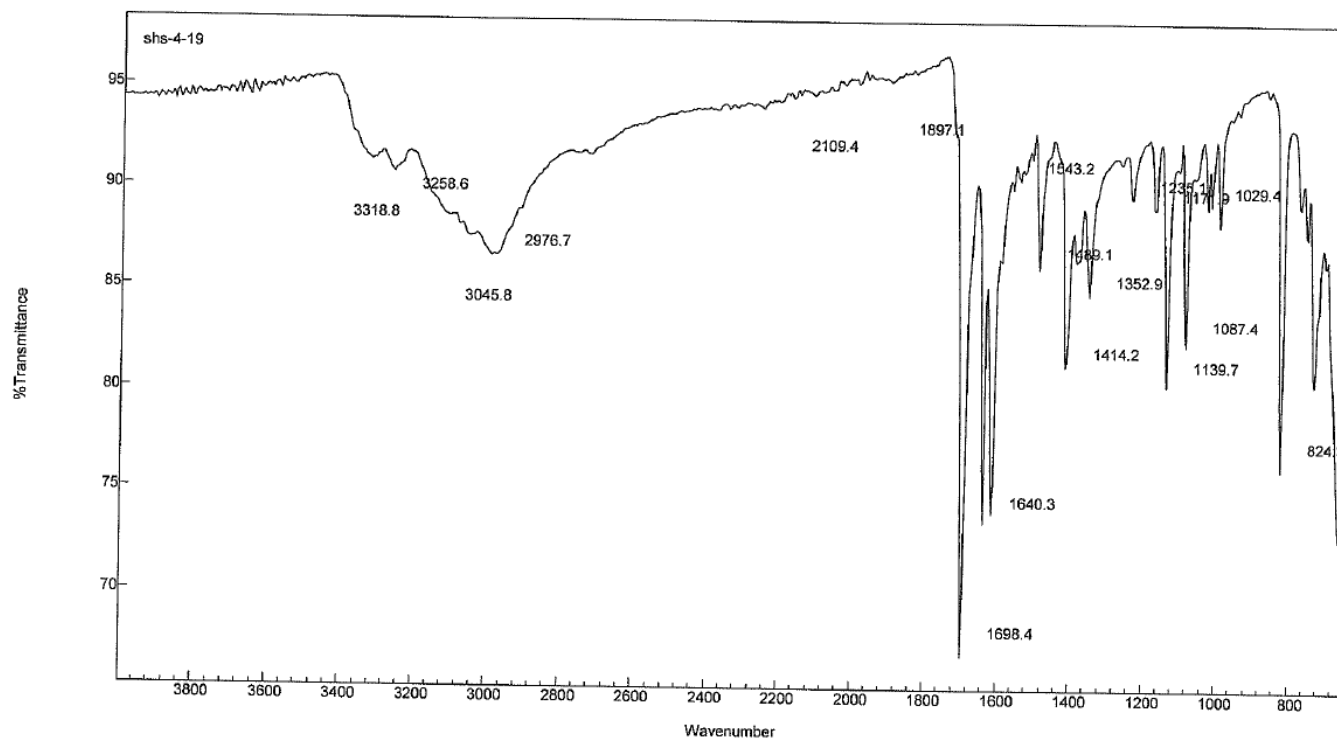
Agilent Resolutions Pro 4-26



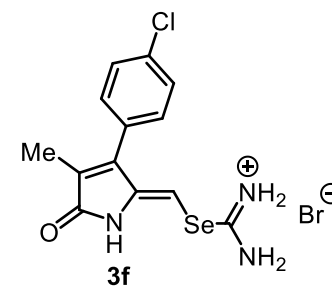
Name
shs-4-25



Agilent Resolutions Pro



Name
shs-4-19



Effect on bacterial growth

Compound	% Growth inhibition data (<i>P. aeruginosa</i> MH602)		
	125 μ M	61.5 μ M	31 μ M
3a	49.8 \pm 7.6	33.7 \pm 7.6	19.2 \pm 3.6
3b	26.9 \pm 3.4	12.4 \pm 1.8	7.9 \pm 7.2
3c	41.1 \pm 6.8	32.2 \pm 2.7	22.8 \pm 3.3
3d	39.5 \pm 2.7	31.8 \pm 3.3	16.7 \pm 3.0
3e	36.2 \pm 7.5	25.8 \pm 4.6	10.5 \pm 4.5
3f	23.7 \pm 3.4	12.4 \pm 1.8	7.9 \pm 7.2
3g	32.1 \pm 6.8	21.3 \pm 2.8	9.2 \pm 8.1
3h	26.9 \pm 14.4	21.8 \pm 3.2	1.3 \pm 1.13
4a	18.9 \pm 11.3	7.7 \pm 4.1	3.3 \pm 2.3
4b	10.4 \pm 9.1	4.4 \pm 4.4	0.0 \pm 0.0
4c	30.0 \pm 3.9	19.5 \pm 2.3	10.6 \pm 7.3
4d	34.9 \pm 2.2	25.3 \pm 7.9	15.2 \pm 4.0
4e	55.6 \pm 3.4	43.4 \pm 6.9	30.0 \pm 2.2
4f	33.3 \pm 7.2	33.9 \pm 5.7	33.1 \pm 5.8
4g	58.9 \pm 5.5	46.8 \pm 4.3	36.0 \pm 8.9
Fu 30	50.2 \pm 3.4	40.5 \pm 21.9	22.8 \pm 8.1