

Electronic supplementary information (ESI)

A facile synthetic strategy to polysiloxanes containing sulfonyl side groups with high dielectric permittivity

Simon J. Dünki,^{a,b} Eduardo Cuervo-Reyes,^{c,d} Dorina M. Opris^{a*}

^{a.} Swiss Federal Laboratories for Materials Science and Technology Empa, Laboratory for Functional Polymers, Überlandstr. 129, CH-8600, Dübendorf, Switzerland. dorina.opris@empa.ch

^{b.} École Polytechnique Fédérale de Lausanne (EPFL), Institut des Matériaux, Station 12, CH 1015, Lausanne, Switzerland.

^{c.} Swiss Federal Laboratories for Materials Science and Technology Empa, Laboratory of Materials for Energy Conversion, Überlandstr. 129, CH-8600, Dübendorf, Switzerland.

^{d.} Swiss Federal Institute of Technology (ETH), CH-8093 Zürich, Switzerland.

E-mail: dorina.opris@empa.ch

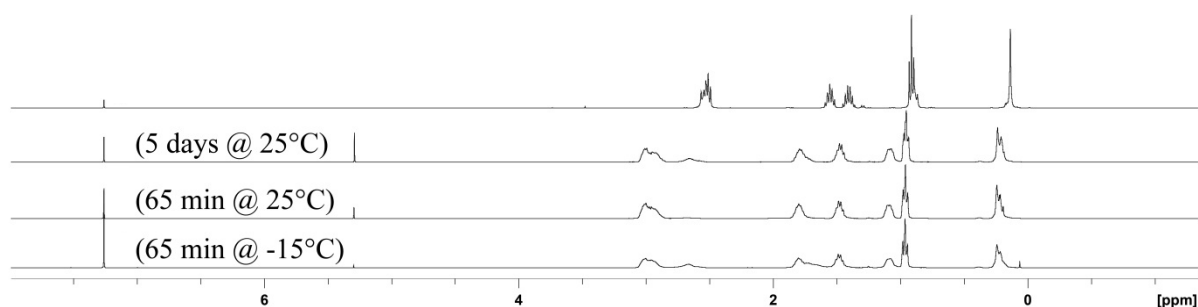


Fig. S1 ¹H NMR spectra of **P1** and of the polymer **P2** obtained at different reaction time and temperature.

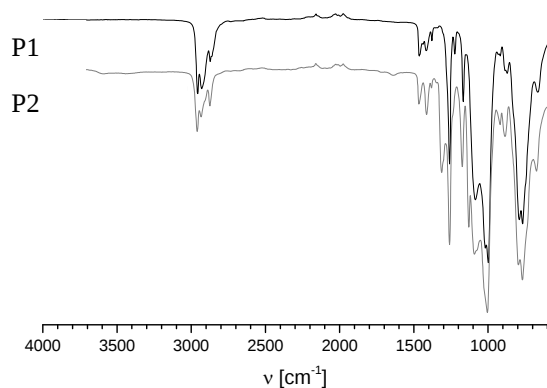


Fig. S2 IR spectra of **P1** and **P2**.

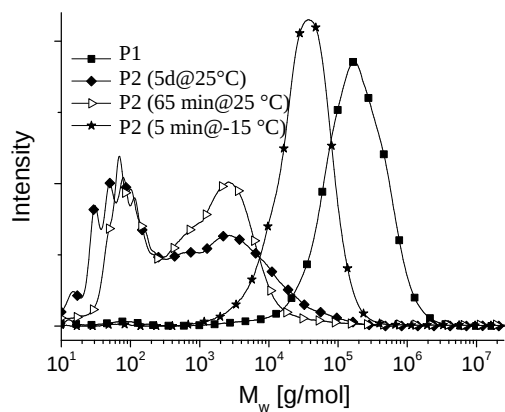


Fig. S3 GPC data of **P1** and the corresponding P2 prepared under different reaction conditions.

TGA Data

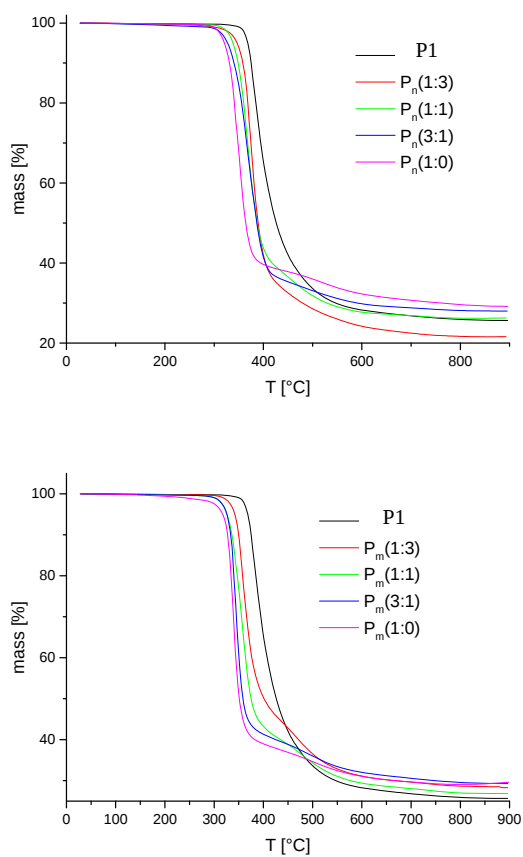
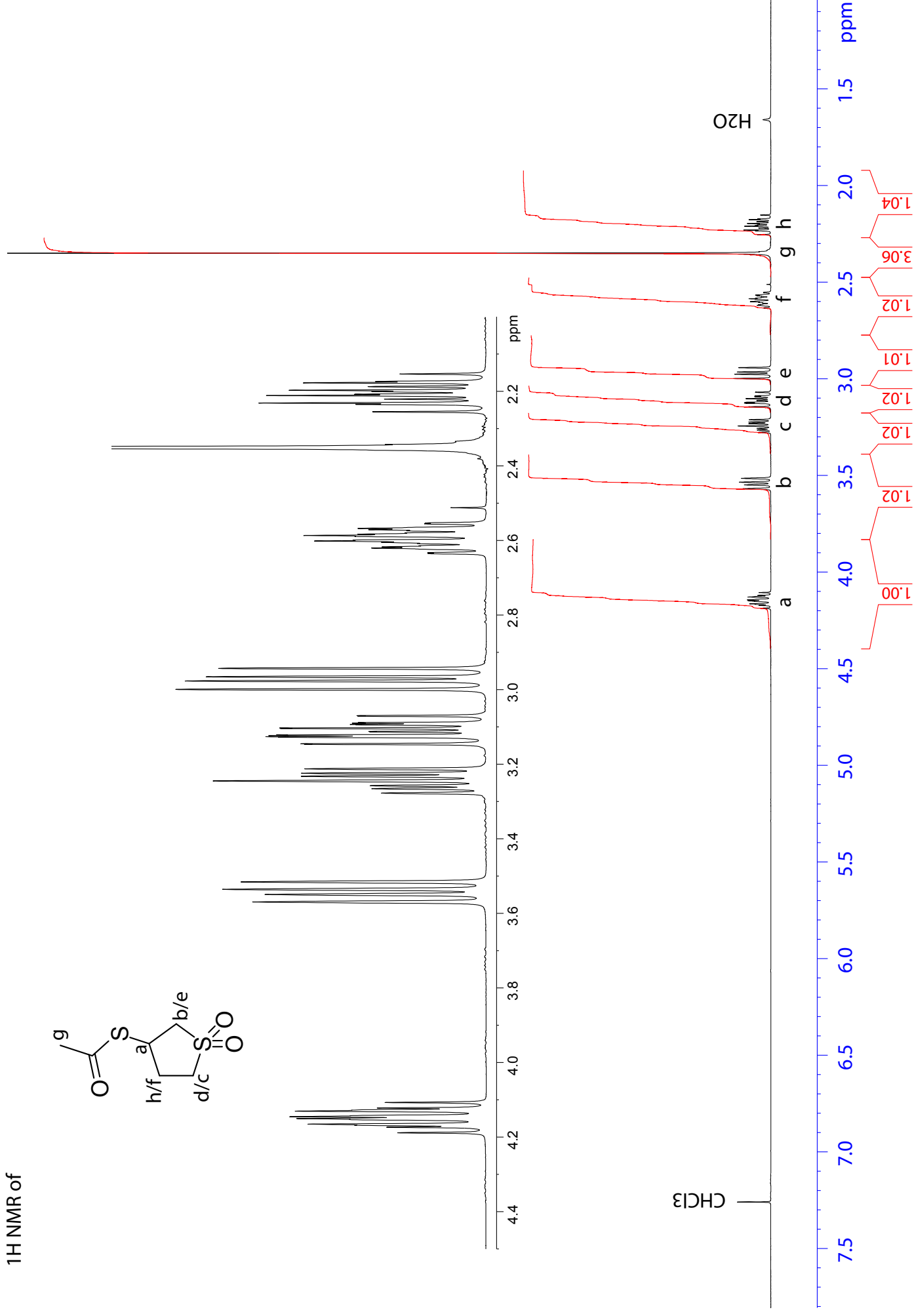
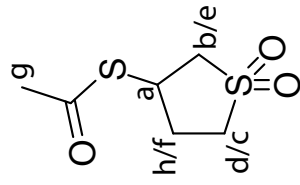
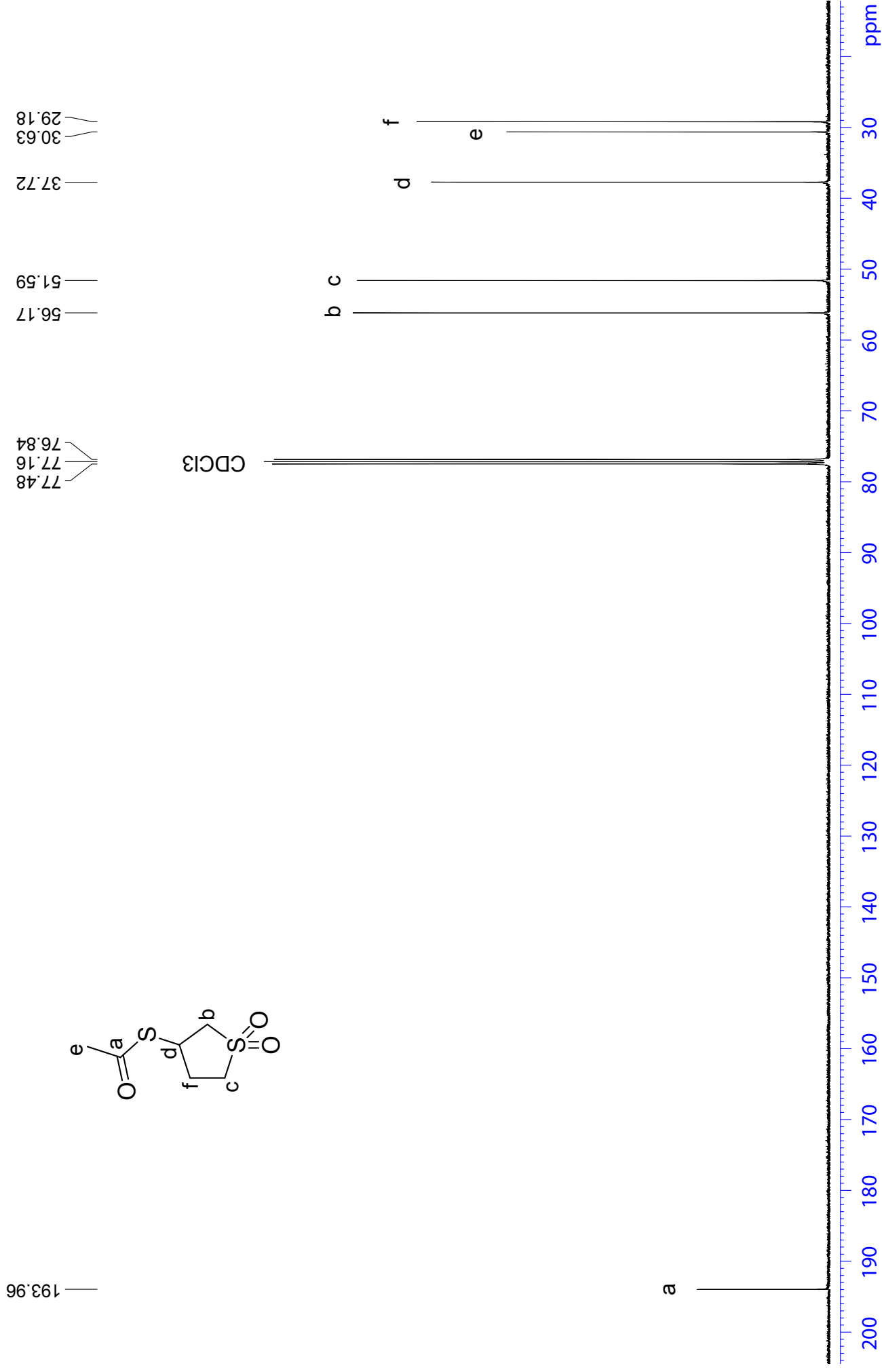


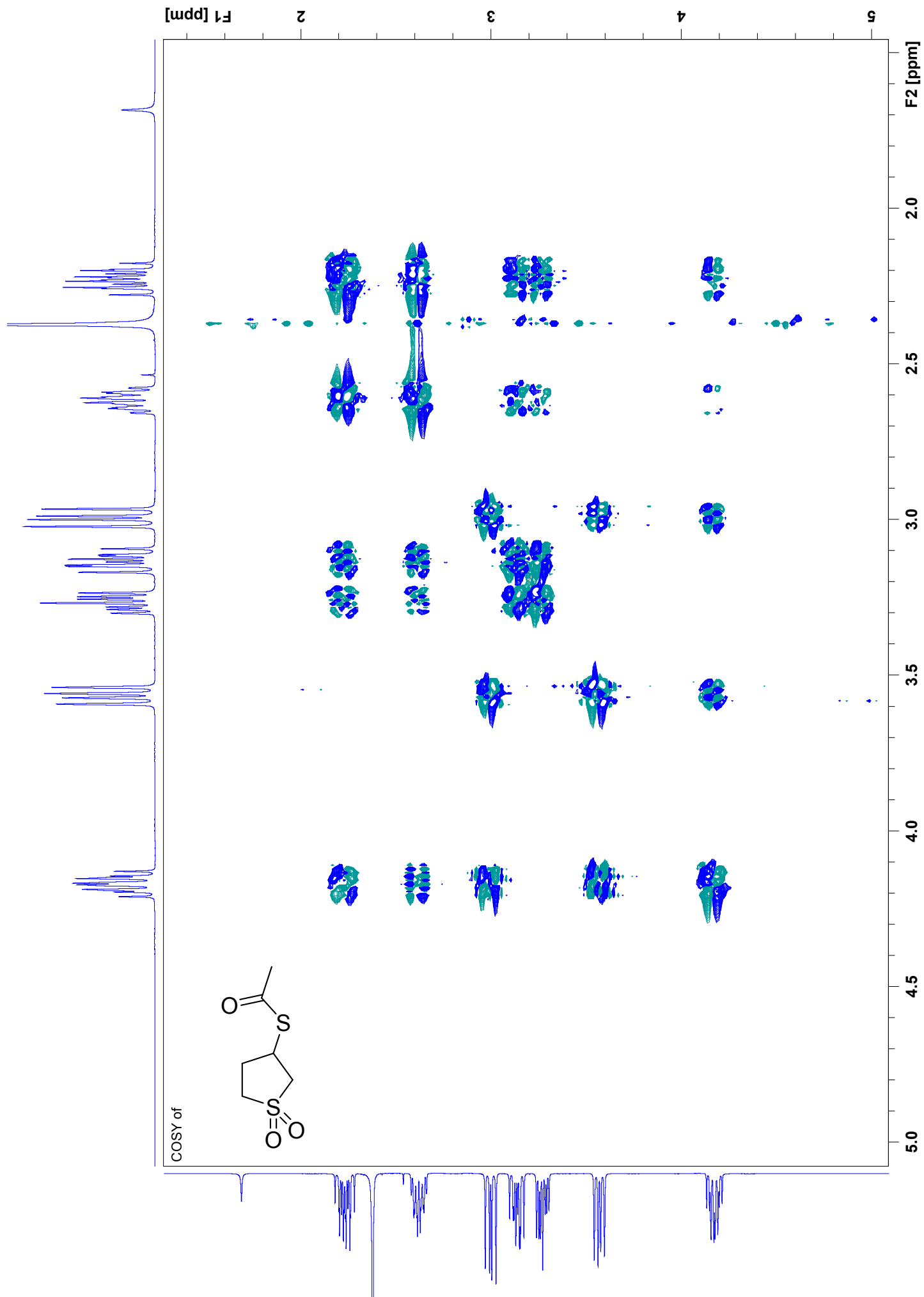
Fig. S4 TGA of **P_m(x:y)** and **P_n(x:y)**.

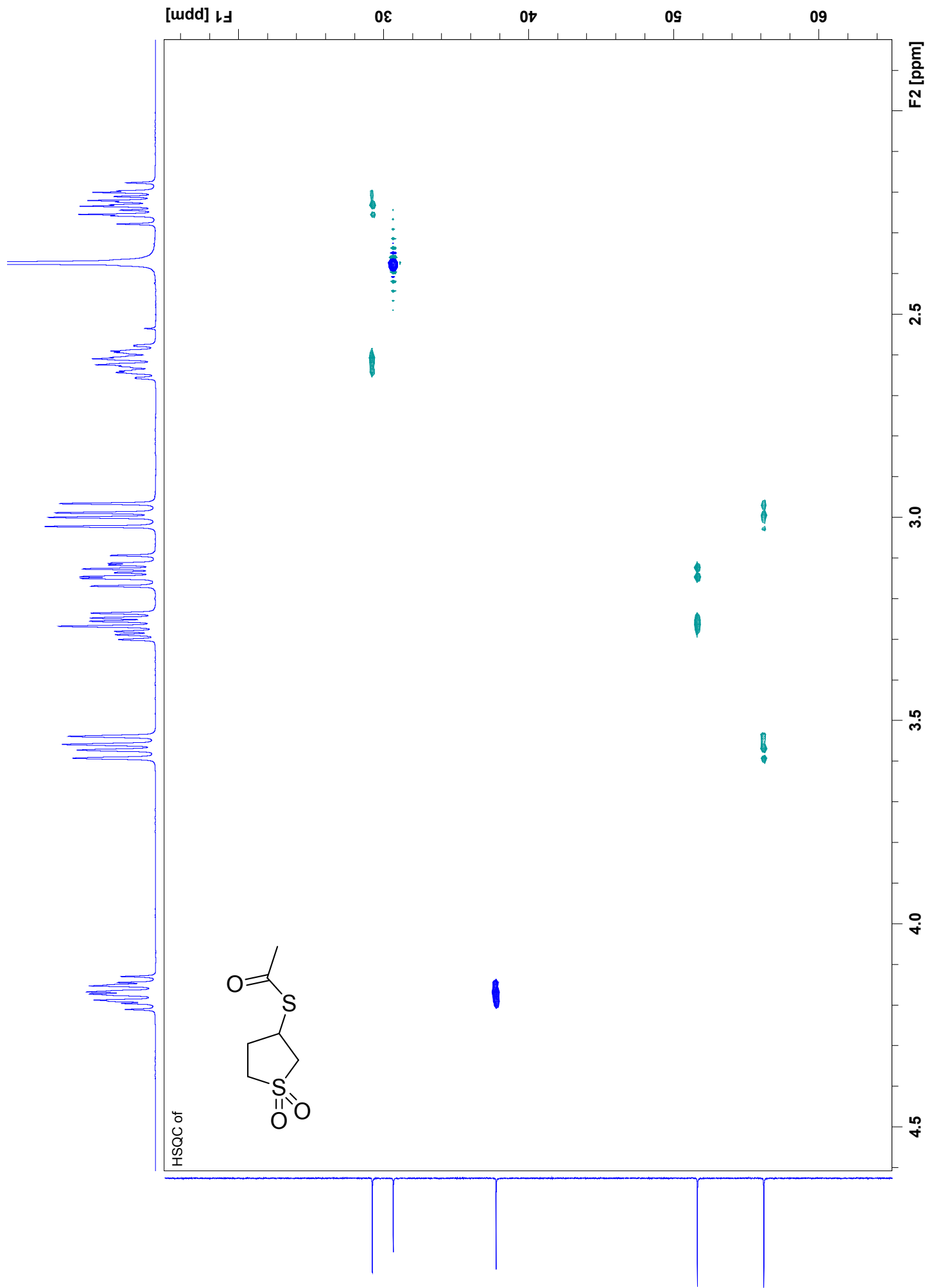
¹H NMR of

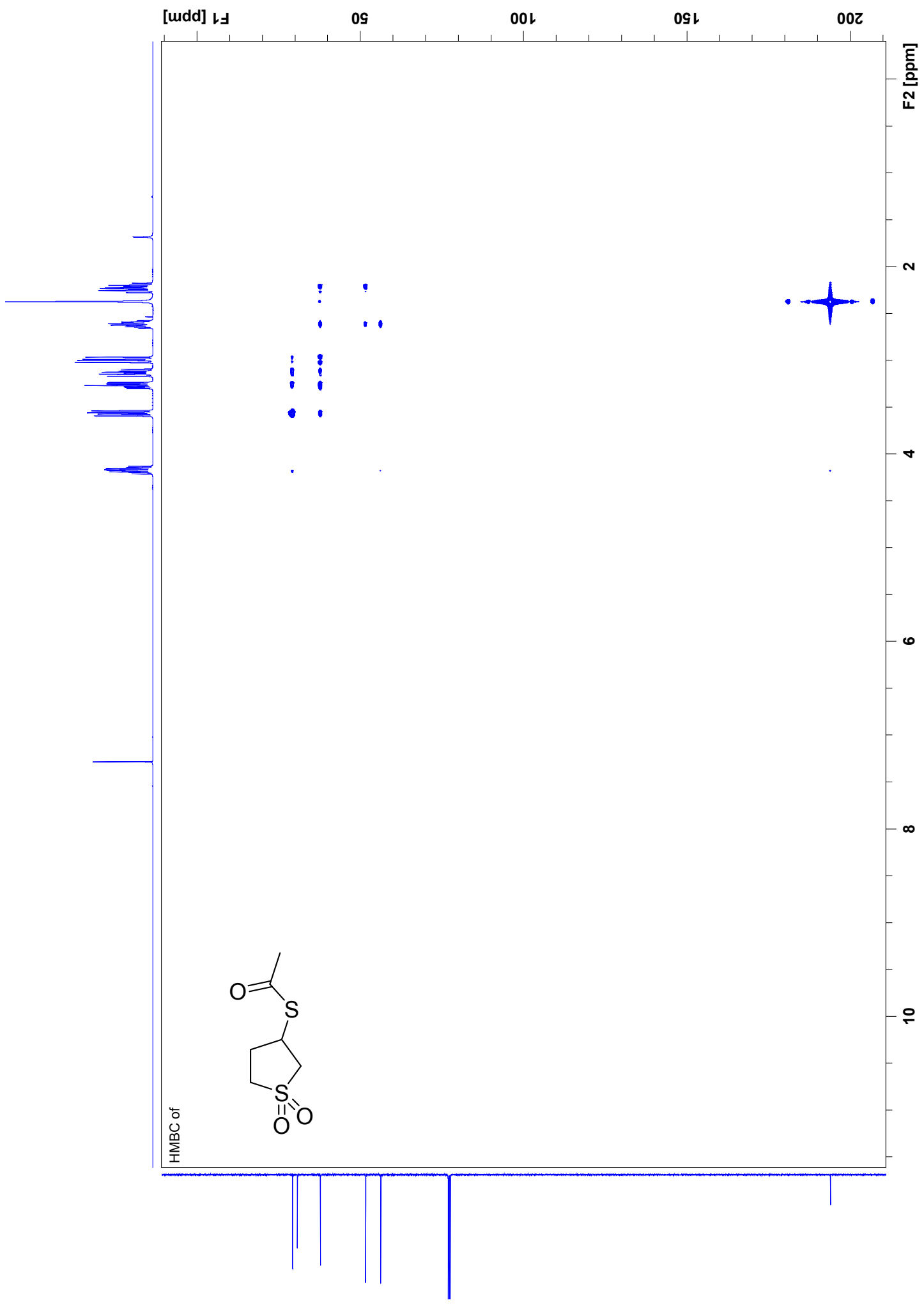


¹³C NMR of



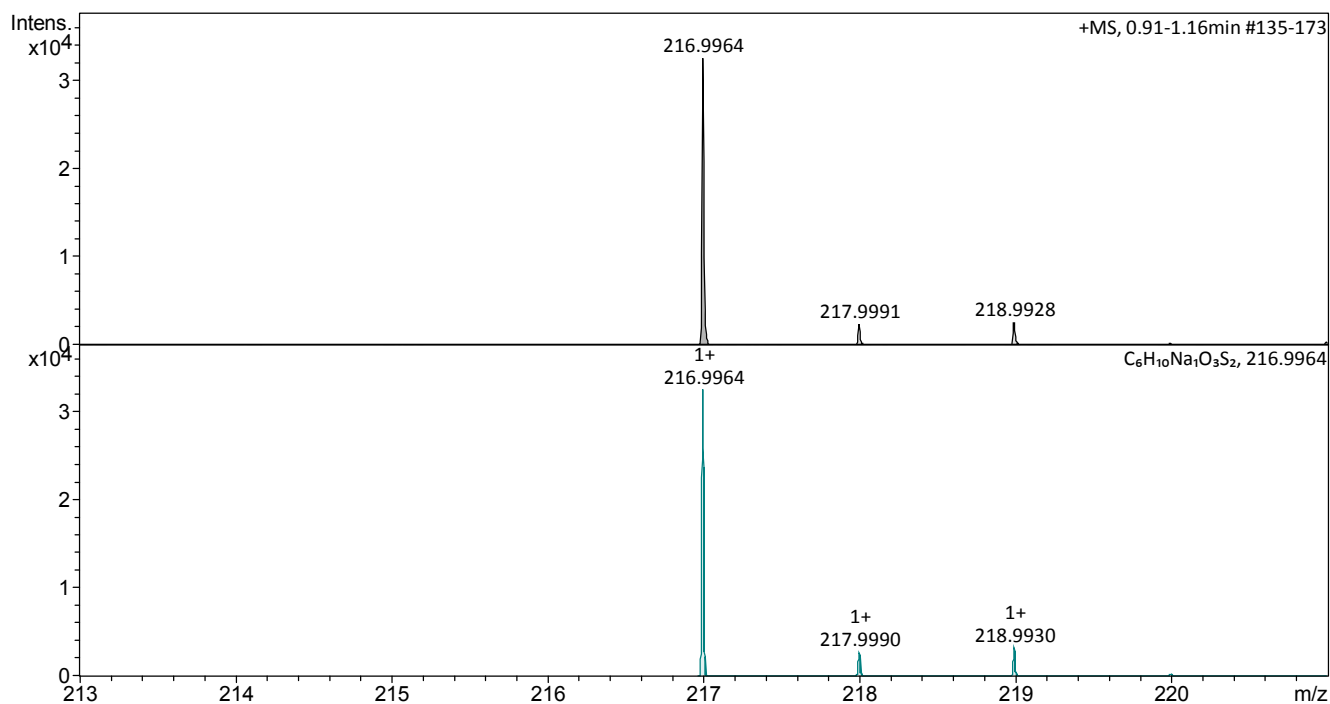
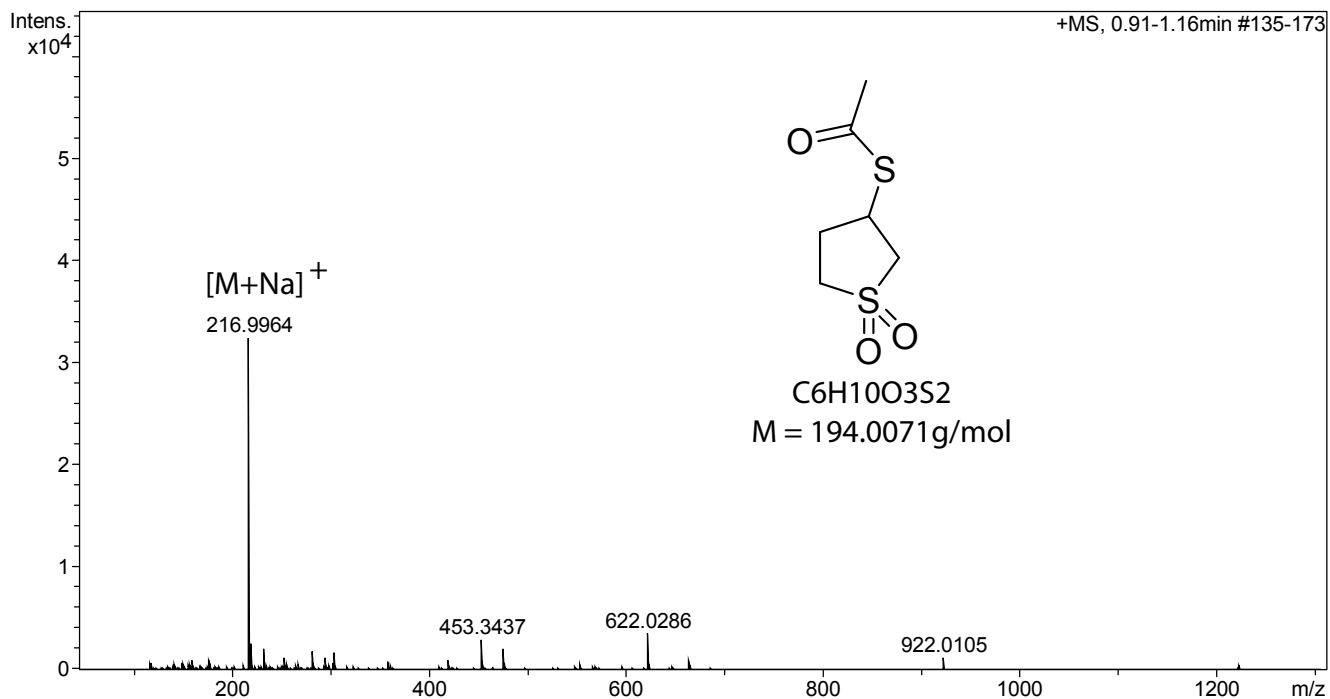




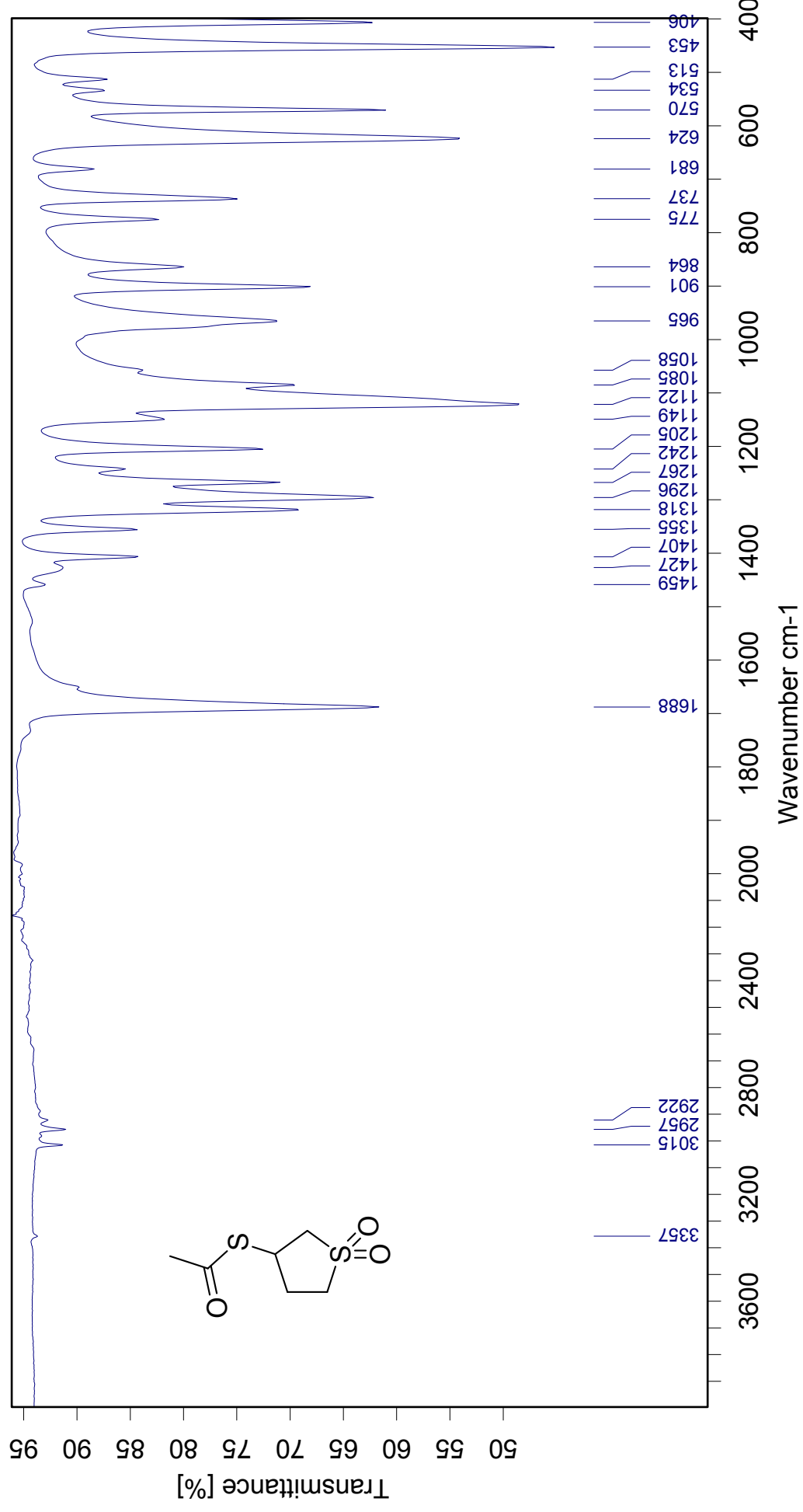


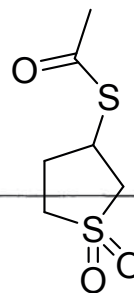
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1300 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source



IR Spectrum of





Molekularformel: C₆ H₁₀ O₃ S₂

Mr = 194.28g/mol

Schmelzpunkt: >100°C

gereinigt: UK aus Toluol

getrocknet: 72h HV / 24h 40°C HV

Bestimmungen: C H O S

Eingang: 11.04.16

Ausgang: 22.04.16

M-161984

Operator: PK

Berechnete Gewichtsanteile:

[C]	37.09%	[H]	5.19%	[O]	24.71%	[S]	33.01%
-----	--------	-----	-------	-----	--------	-----	--------

Gefundene Gewichtsanteile:

Einwaage: 0.922mg

LECO TruSpec Micro

12.04.16

[C] 37.02% [H] 5.02%

Einwaage: 2.306mg

LECO RO-478

22.04.16

[O] 24.64%

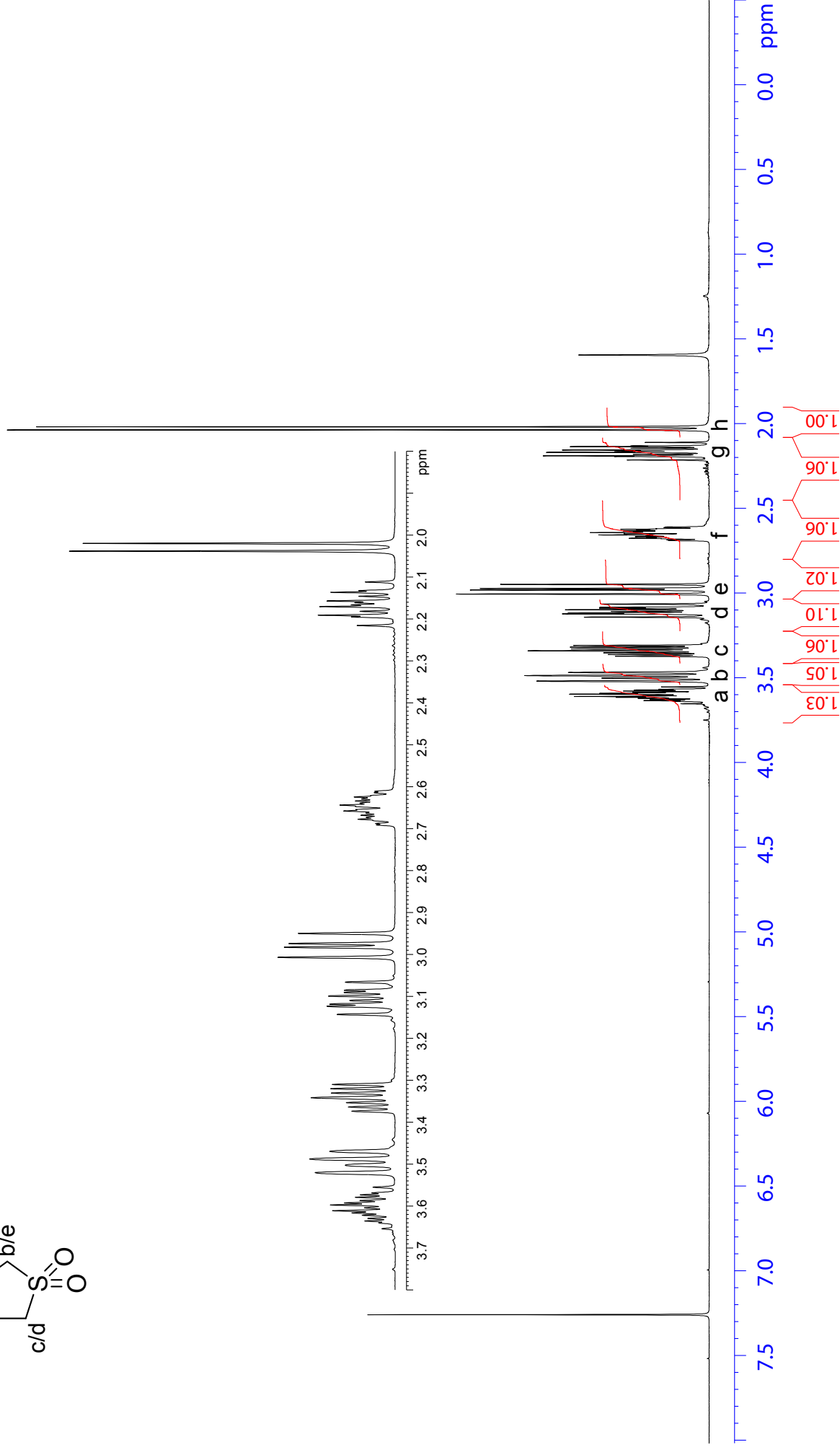
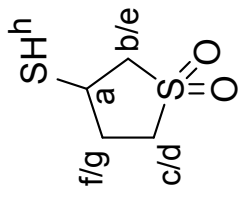
Einwaage: 1.564mg

LECO CHNS-932

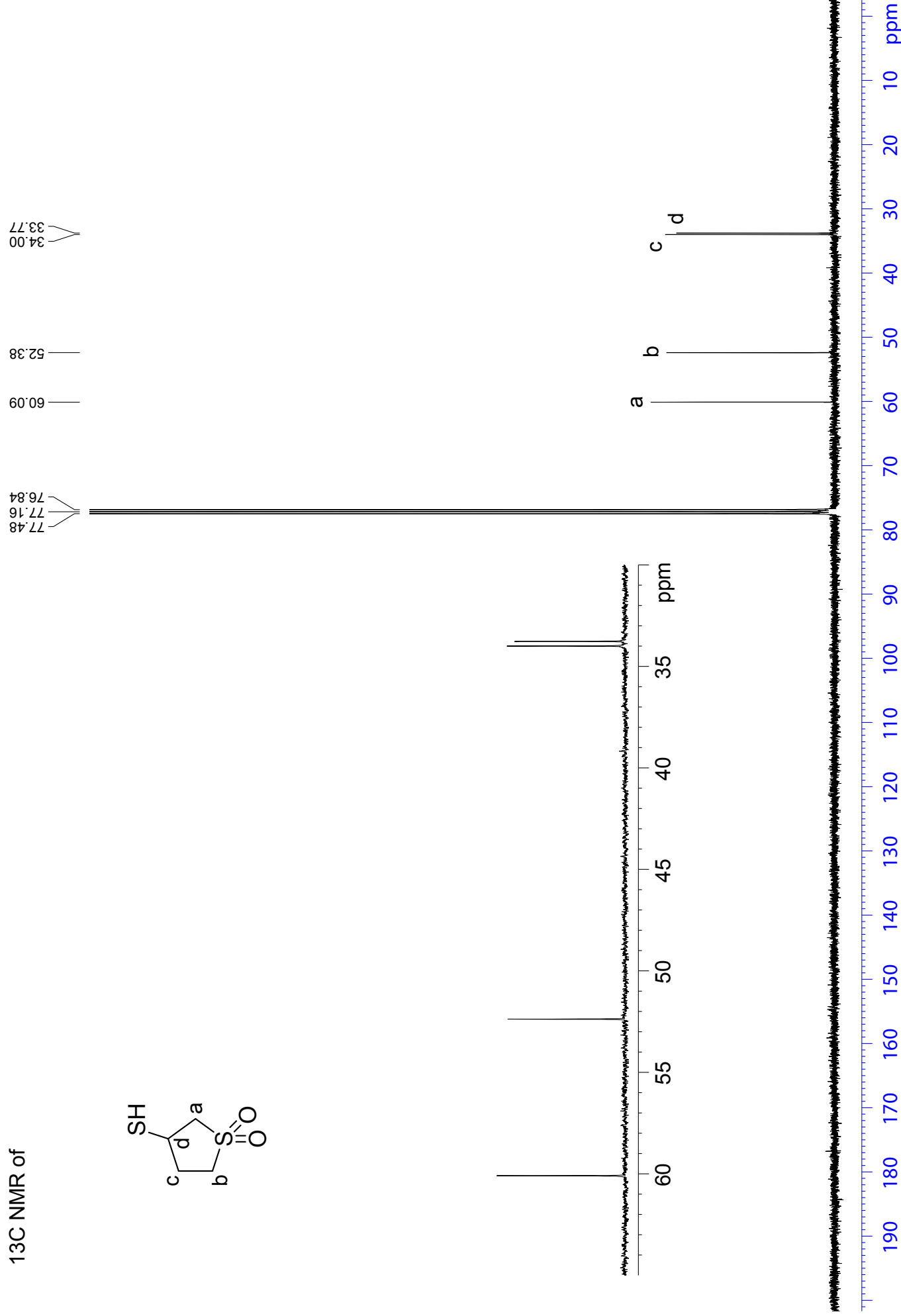
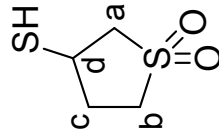
20.04.16

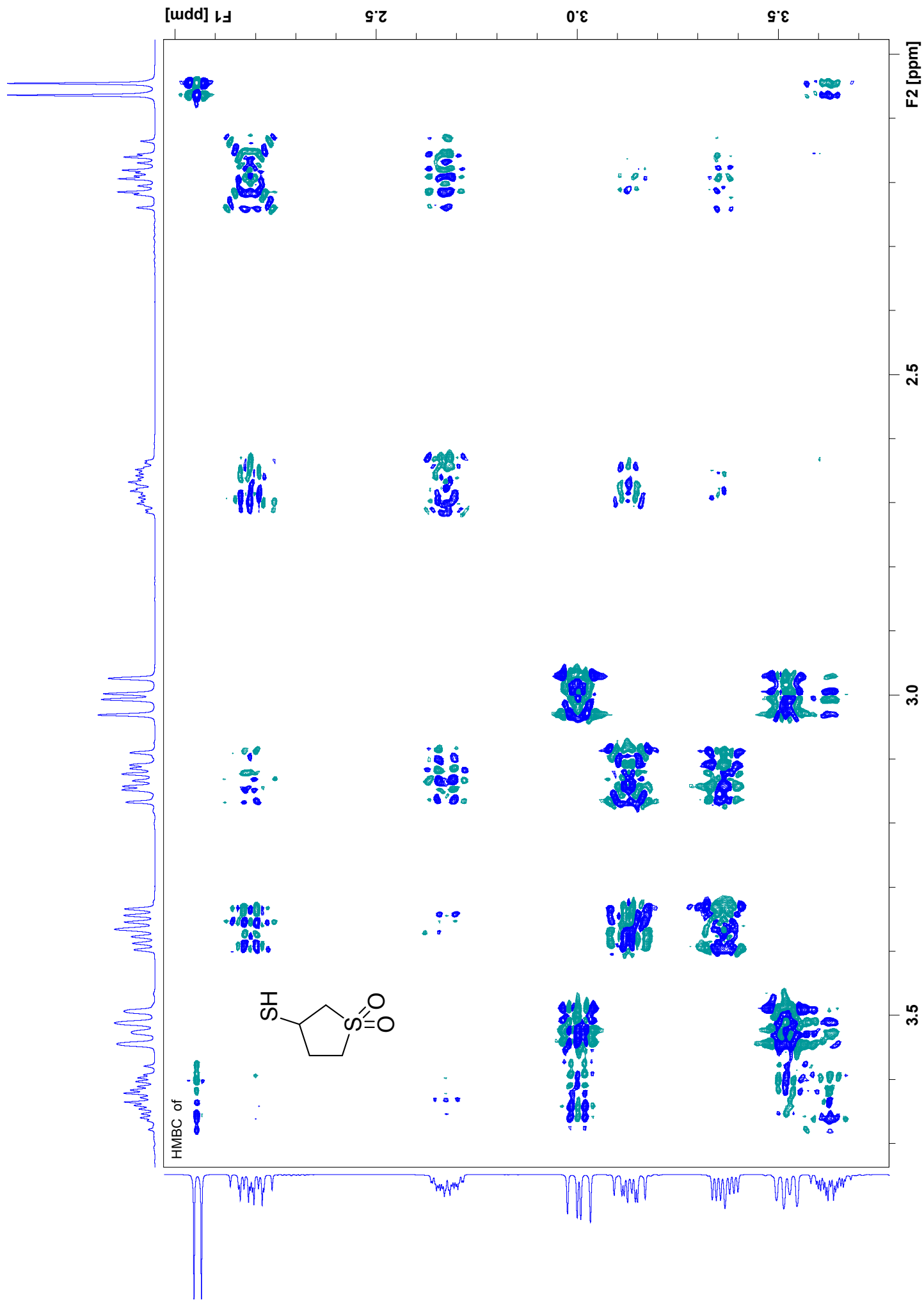
[S] 33.10%

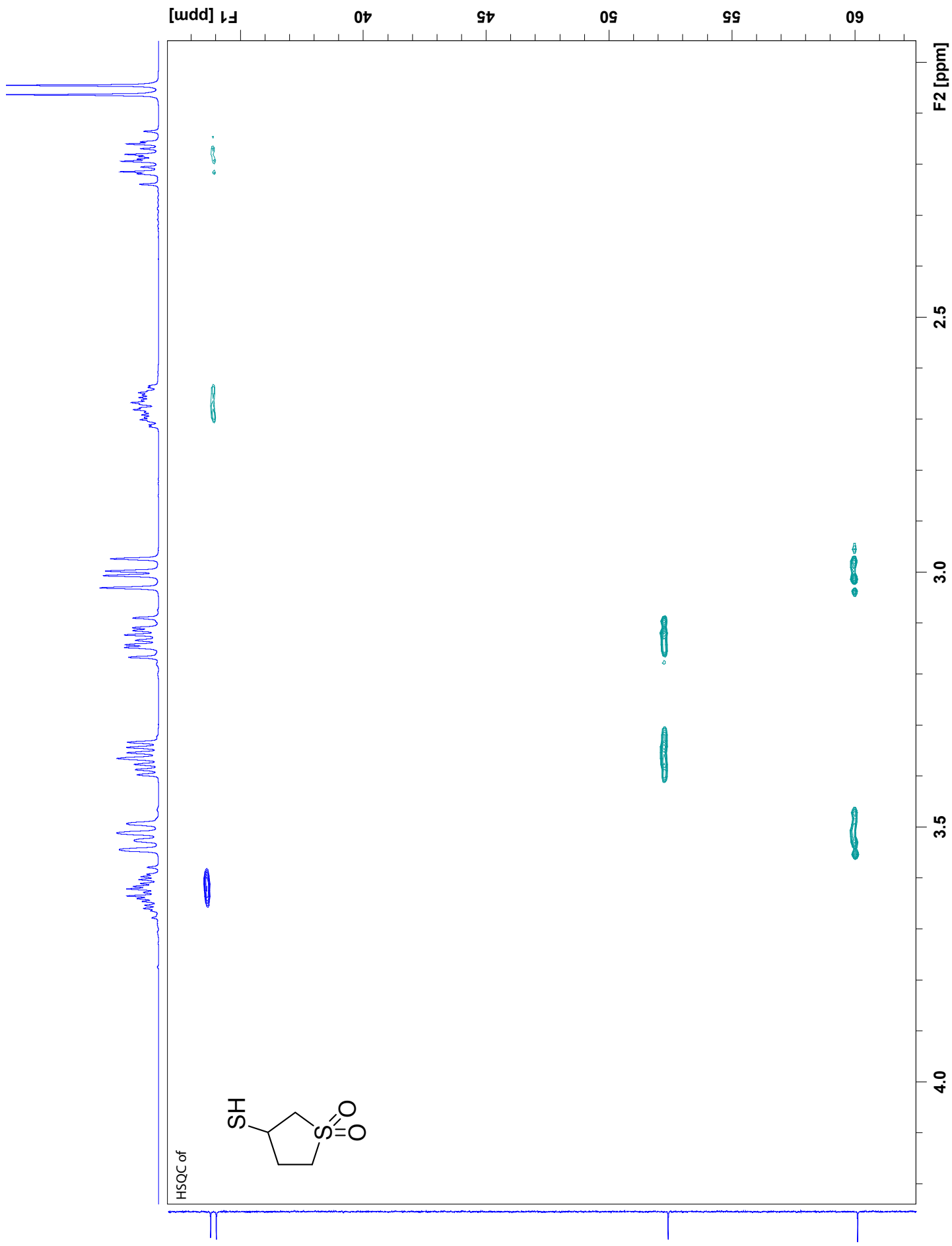
¹H NMR of

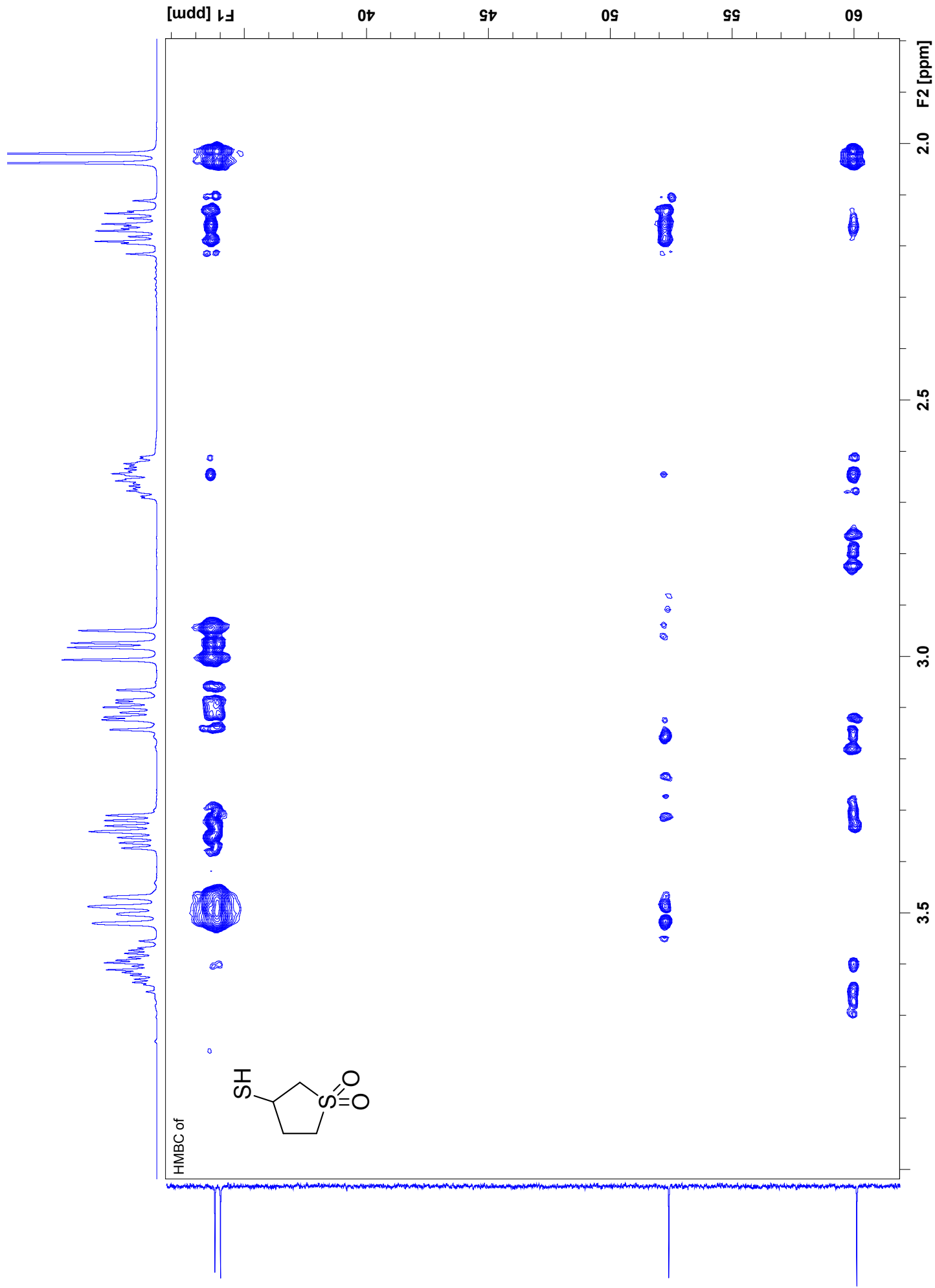


¹³C NMR of



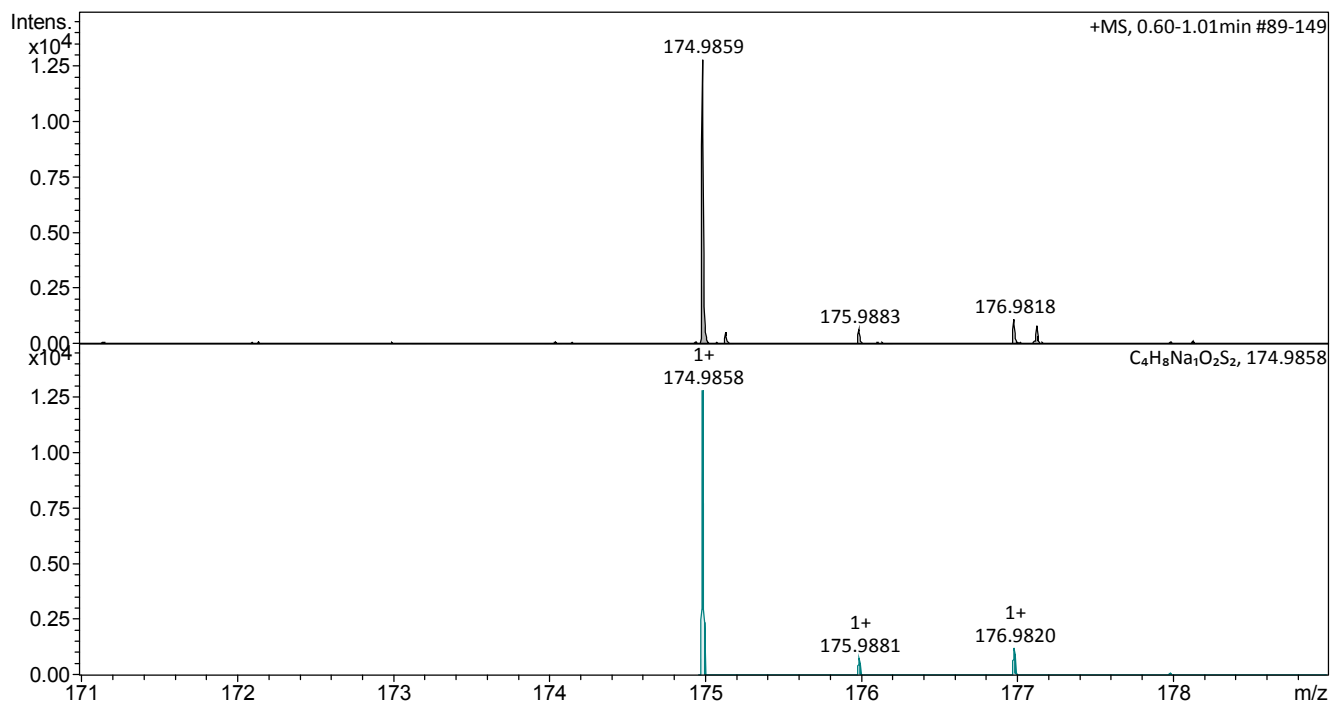
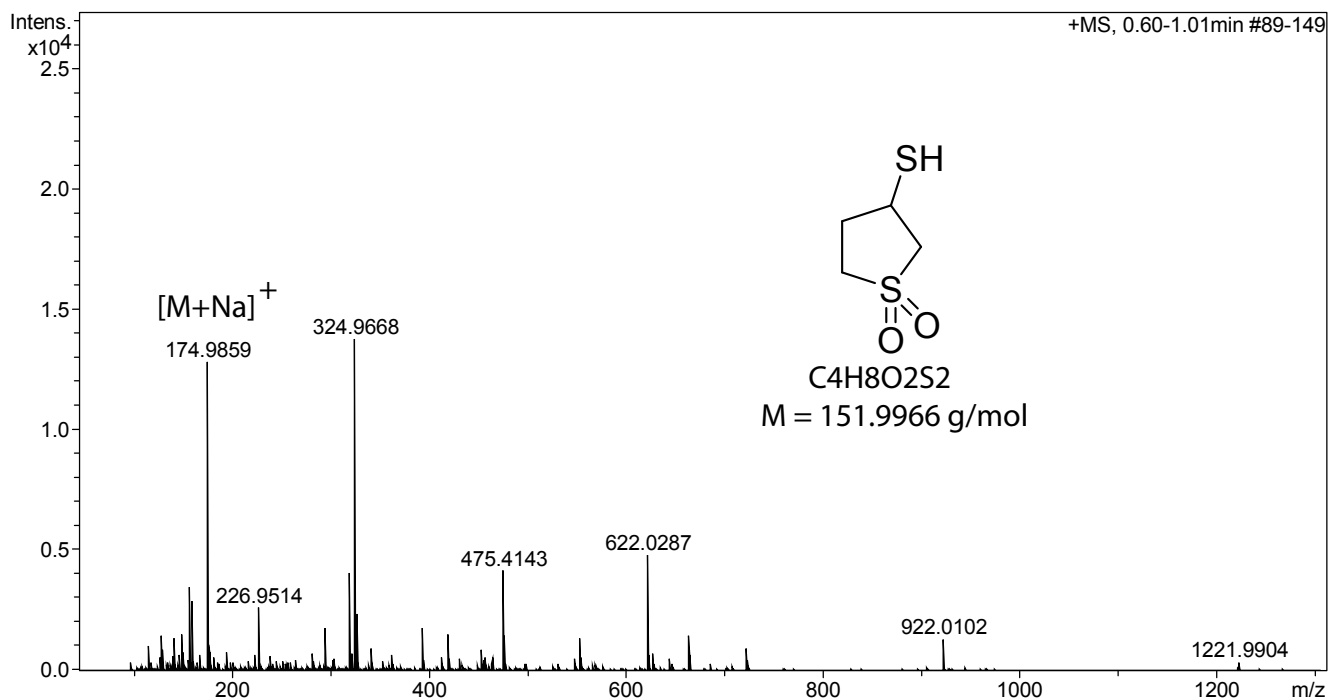




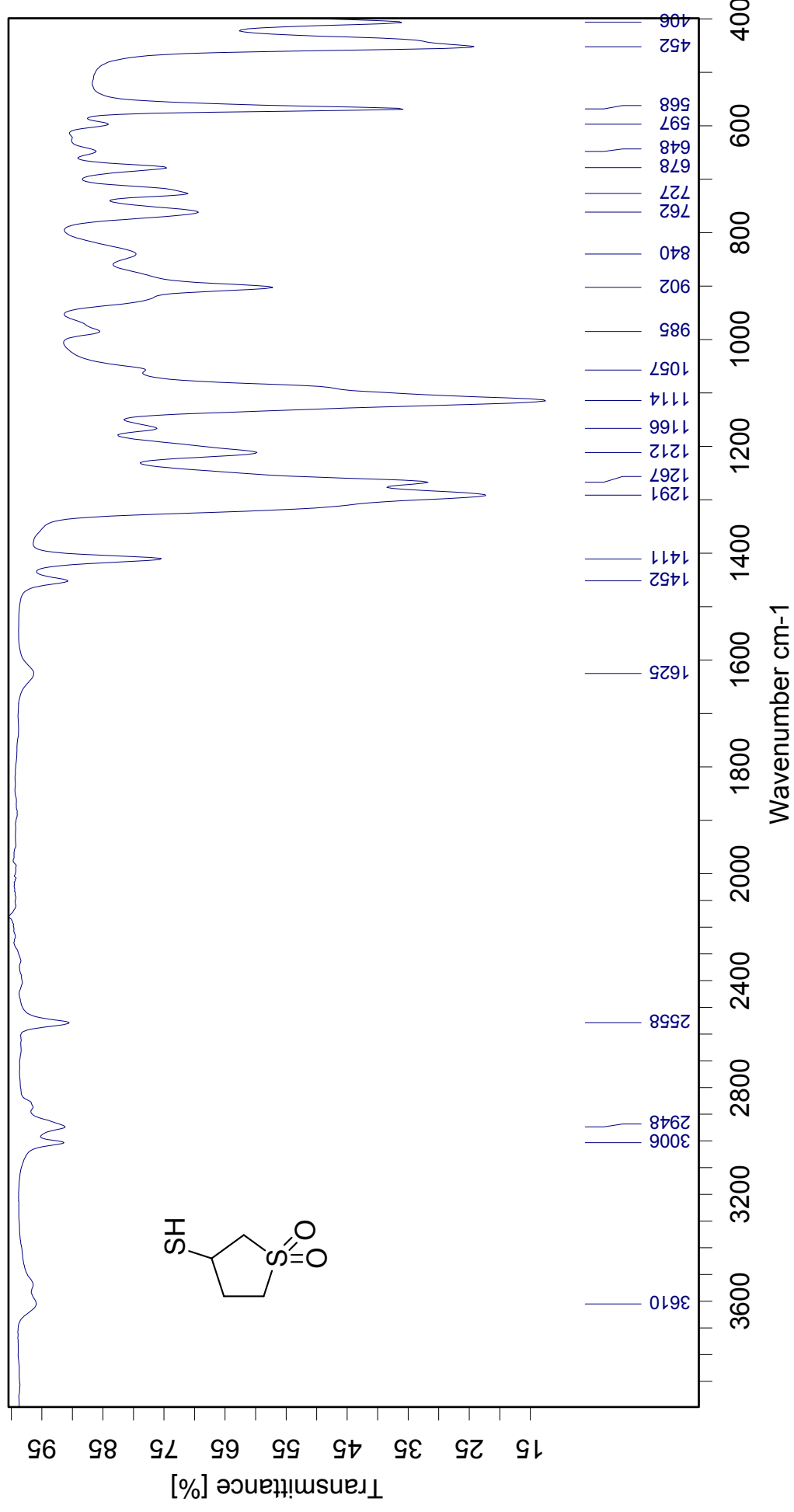


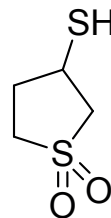
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1300 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source



IR Spectrum of





Molekularformel: C₄ H₈ O₂ S₂

Mr = 152.24g/mol

Siedepunkt: 182°C/1.2mbar

gereinigt: Dest.

getrocknet: ????

Bestimmungen: C H O S

Eingang: 11.04.16

Ausgang: 22.04.16

M-161985

Operator: SM

Berechnete Gewichtsanteile:

[C]	31.56%	[H]	5.30%	[O]	21.02%	[S]	42.13%
-----	--------	-----	-------	-----	--------	-----	--------

Gefundene Gewichtsanteile:

Einwaage: 2.415mg

LECO CHNS-932

[C] 31.42% [H] 5.32%

12.04.16

Einwaage: 2.004mg

LECO RO-478

[O] 21.25%

22.04.16

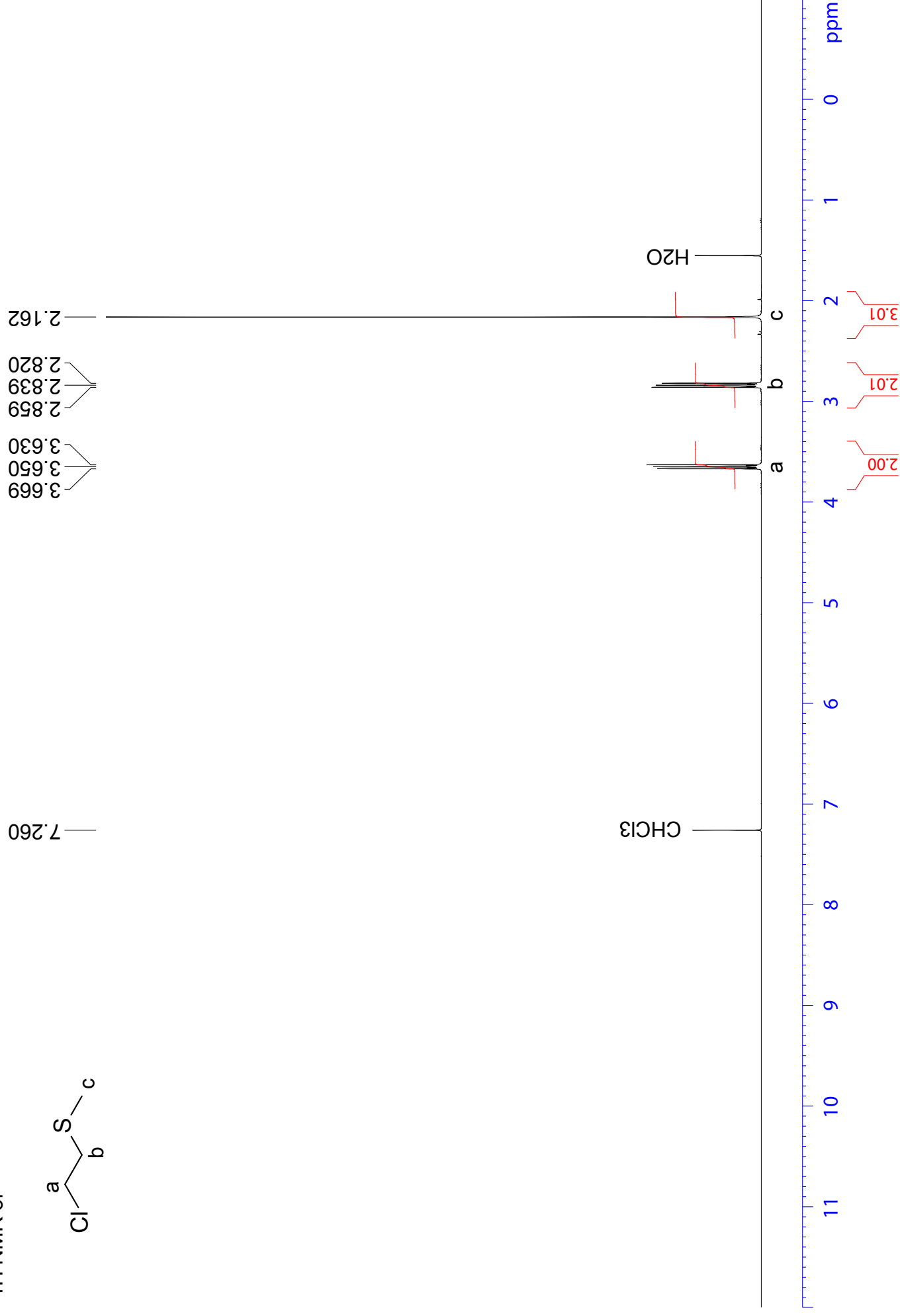
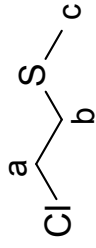
Einwaage: 1.890mg

LECO CHNS-932

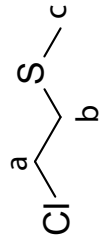
[S] 42.29%

20.04.16

¹H NMR of



¹³C NMR of



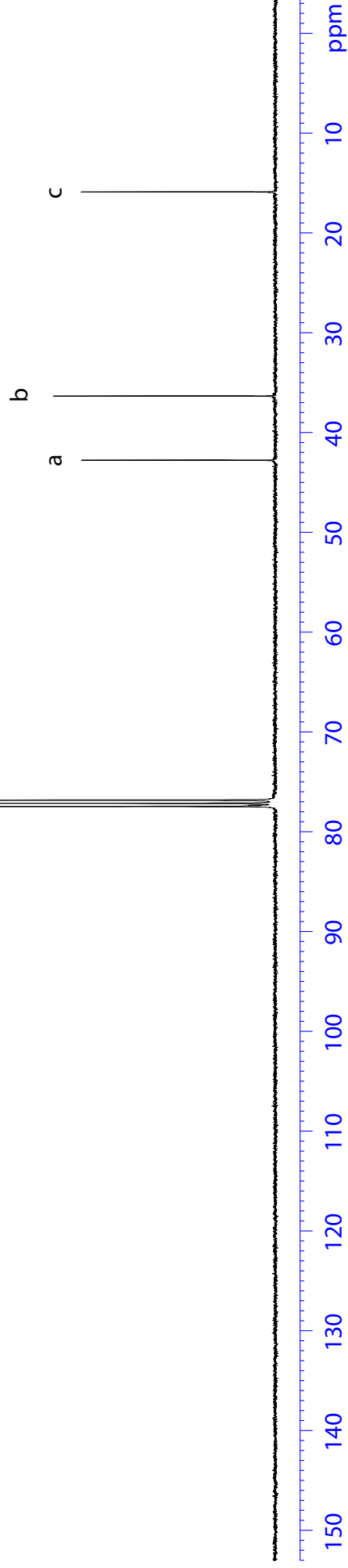
77.48
77.16
76.84

42.78

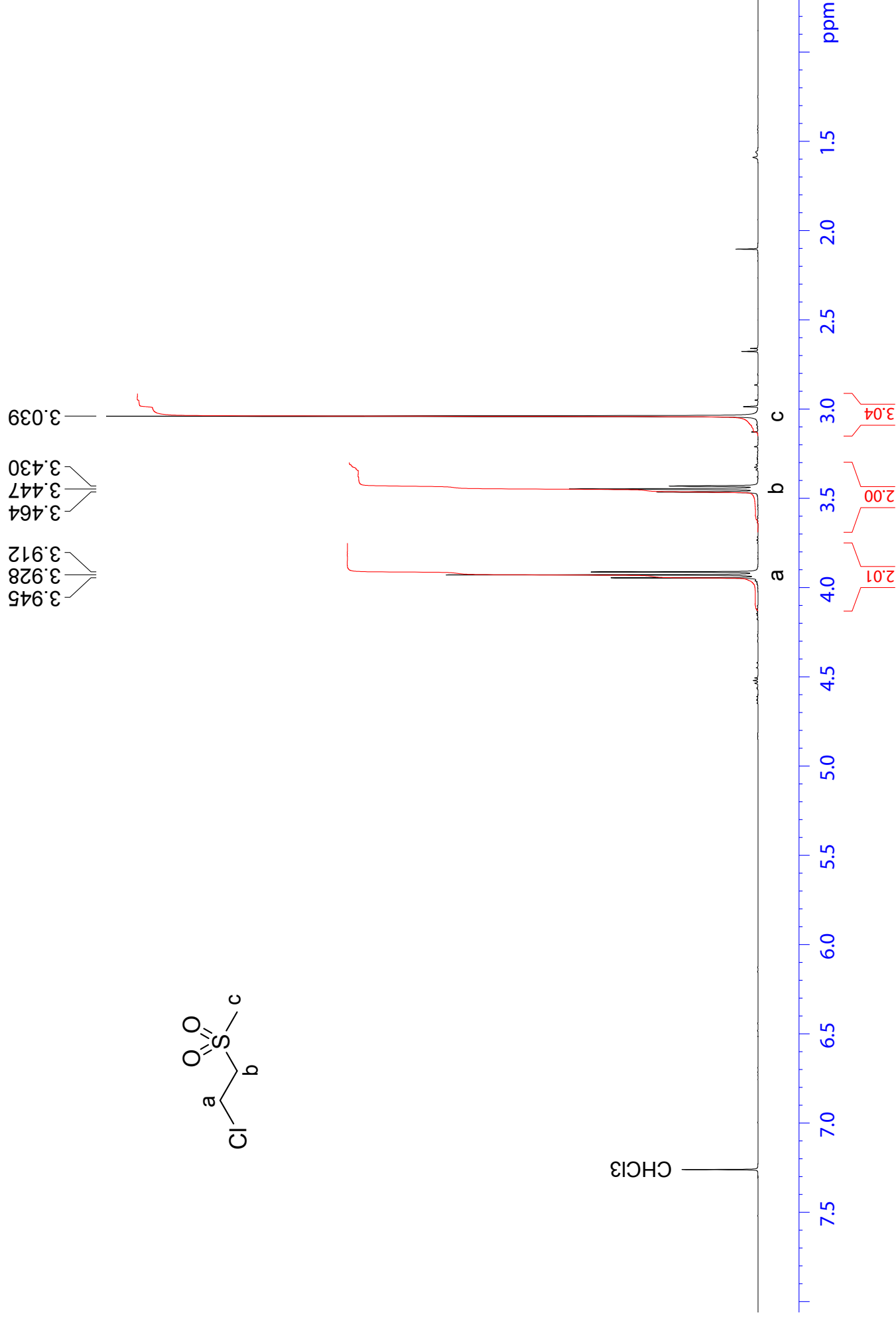
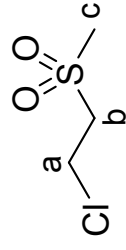
36.34

15.89

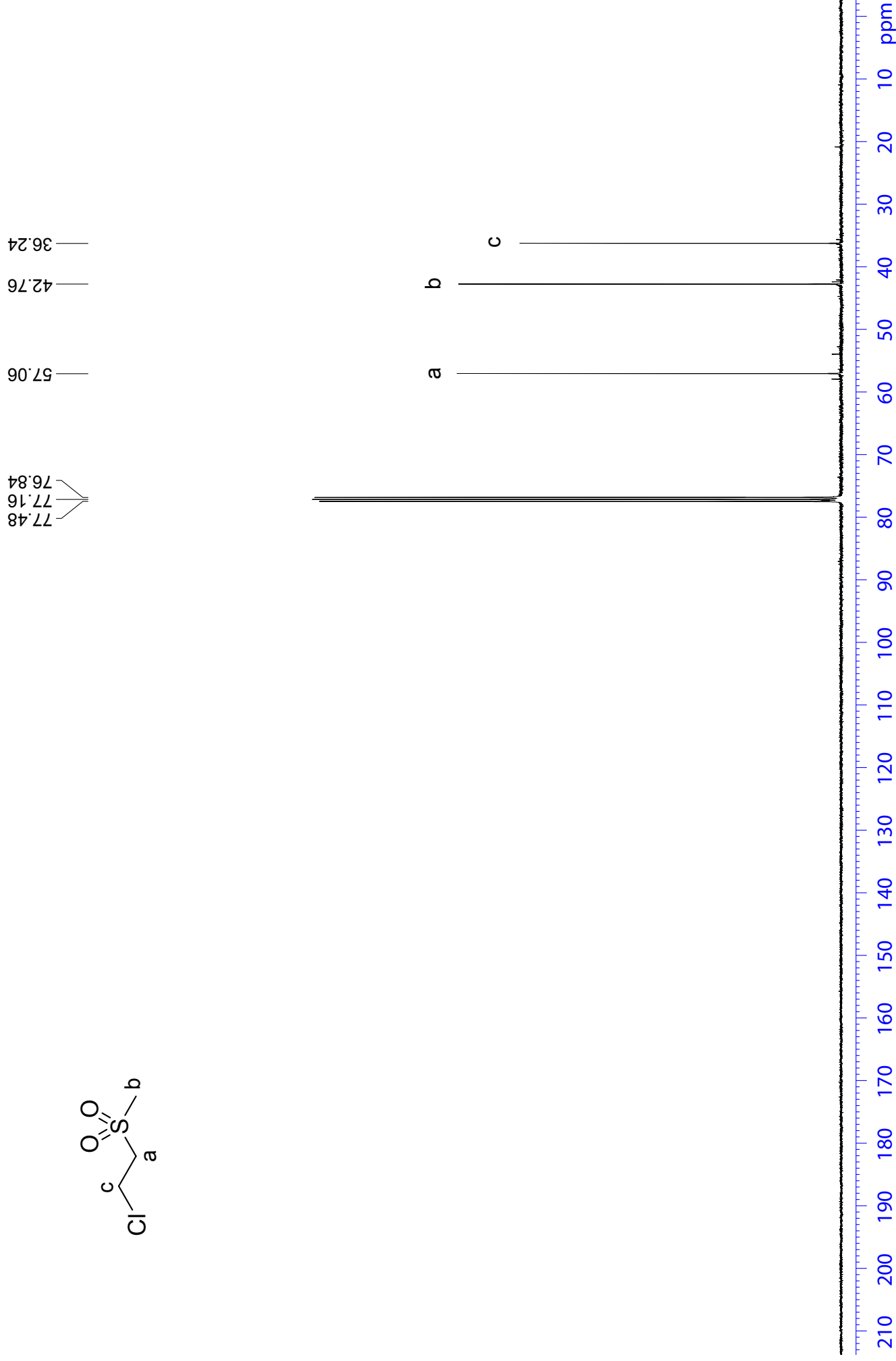
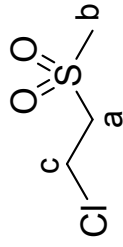
CDCl₃

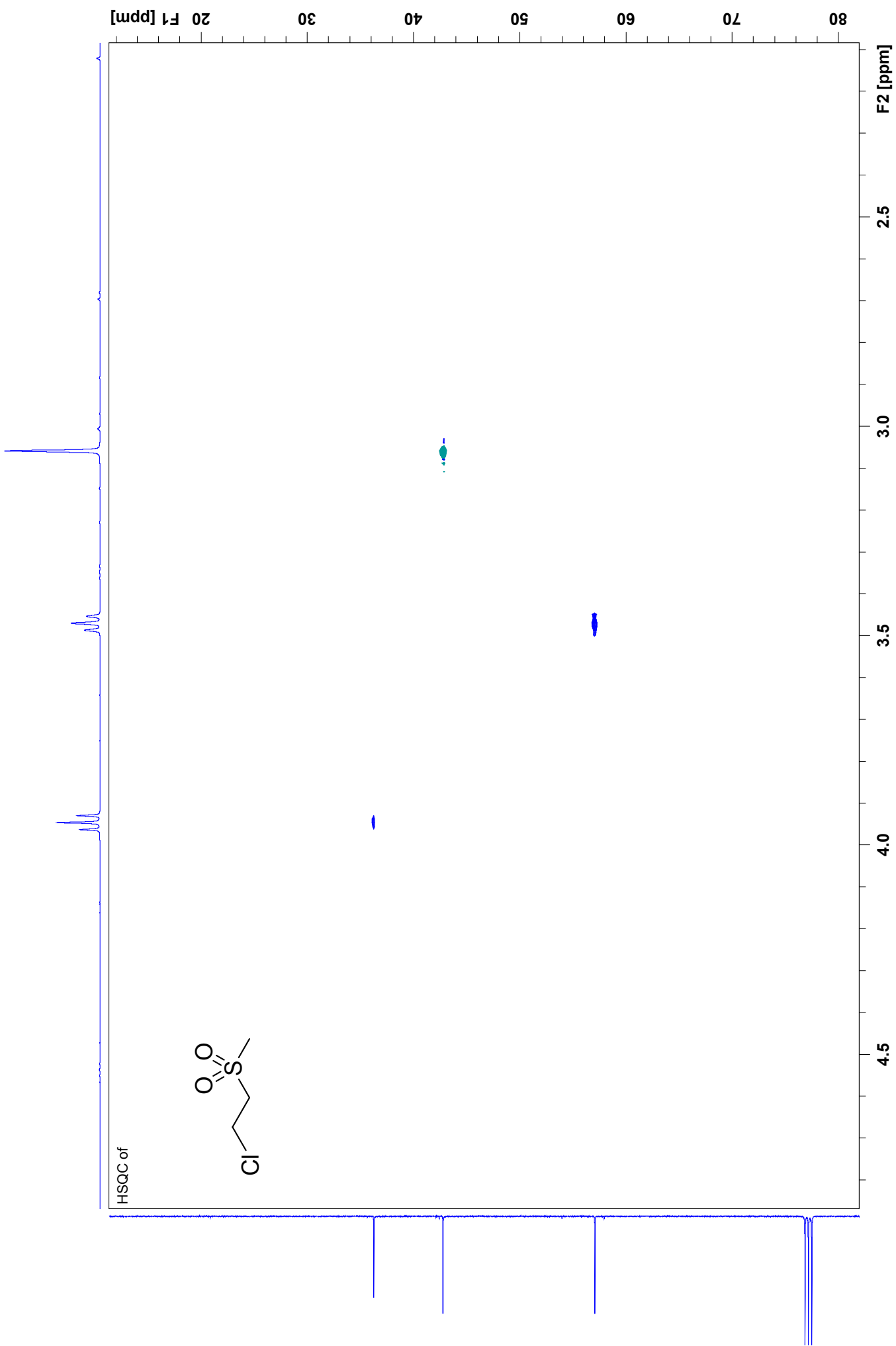


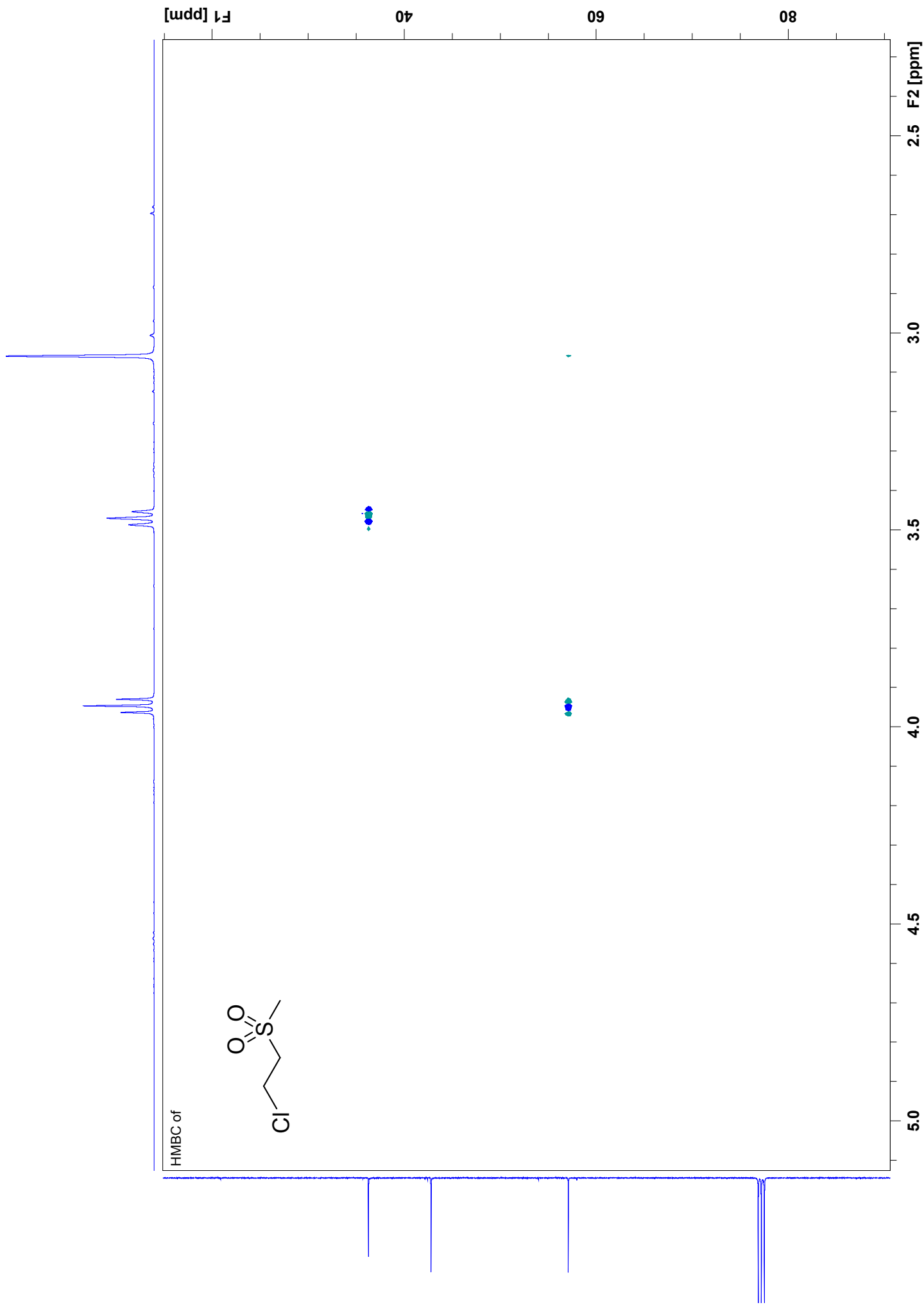
¹H NMR of



¹³C NMR of

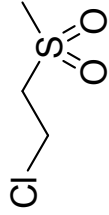






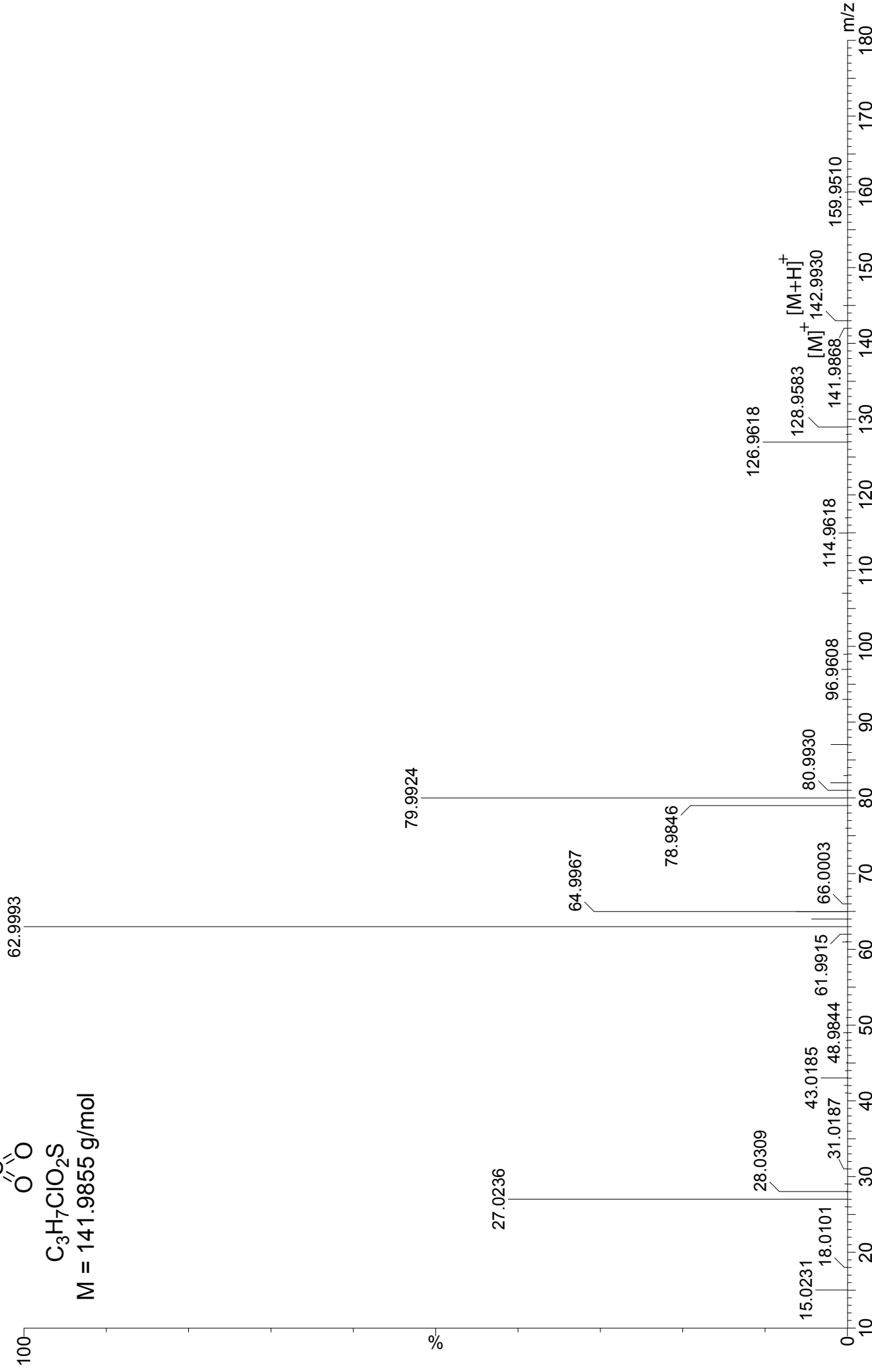
MS of

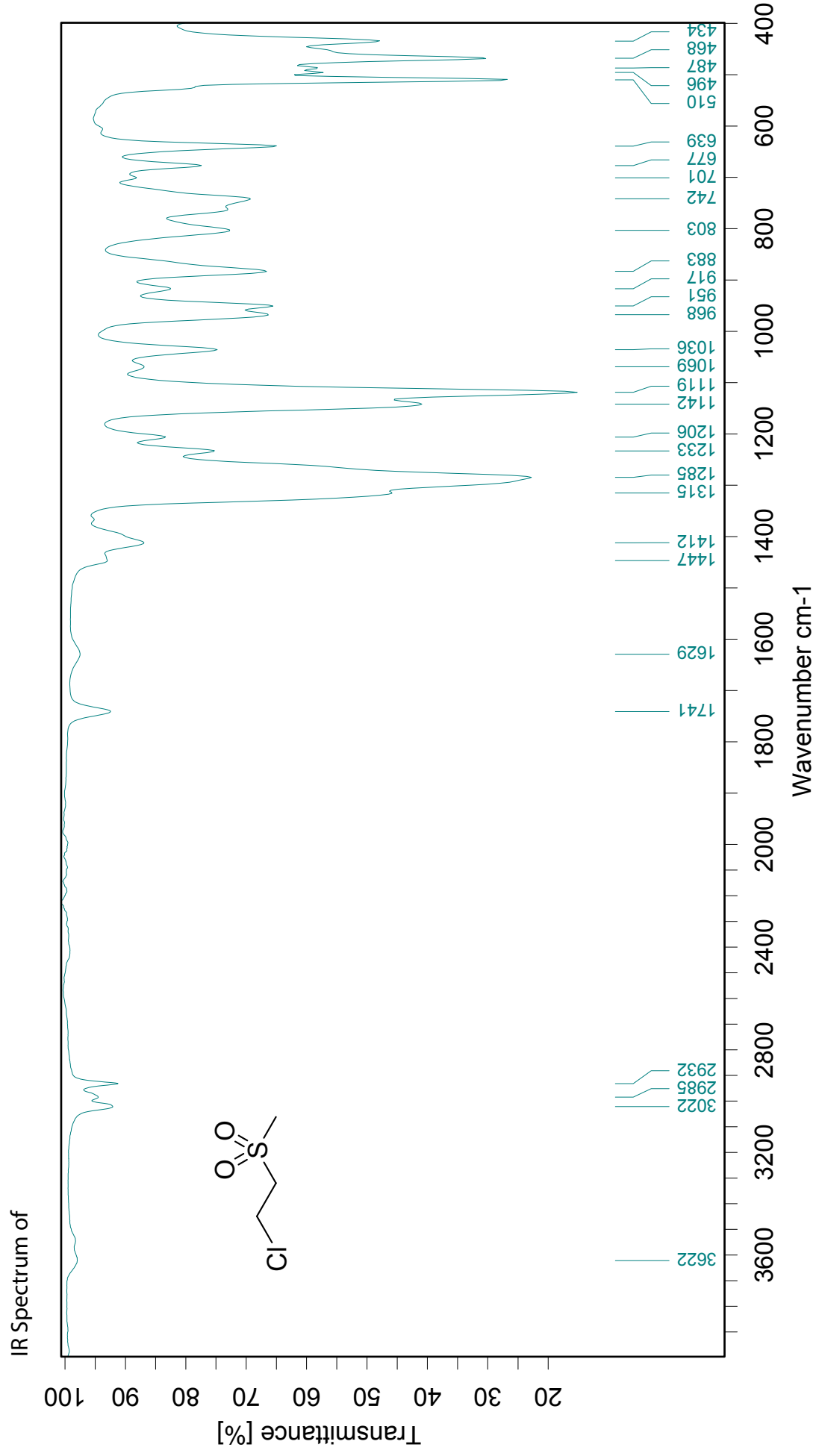
Magnet EI+
6.32e3

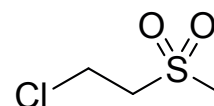


$\text{C}_3\text{H}_7\text{ClO}_2\text{S}$

M = 141.9855 g/mol







Molekularformel: C₃ H₇ O₂ S Cl

Mr = 142.61g/mol

Siedepunkt: 110°C, 0.15mbar

gereinigt: Dest.

getrocknet:

Bestimmungen: C H O S

Eingang: 14.06.16

Ausgang: 22.06.16

M-162423

Operator: PK

Berechnete Gewichtsanteile:

[C]	25.27%	[H]	4.95%	[O]	22.44%	[S]	22.49%	[Cl]	24.86%
-----	--------	-----	-------	-----	--------	-----	--------	------	--------

Gefundene Gewichtsanteile:

Einwaage: 1.022mg

LECO TruSpec Micro

[C] 25.15% [H] 4.97%

14.06.16

Einwaage: 1.732mg

LECO RO-478

[O] 22.73%

22.06.16

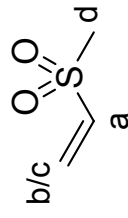
Einwaage: 1.945mg

LECO CHNS-932

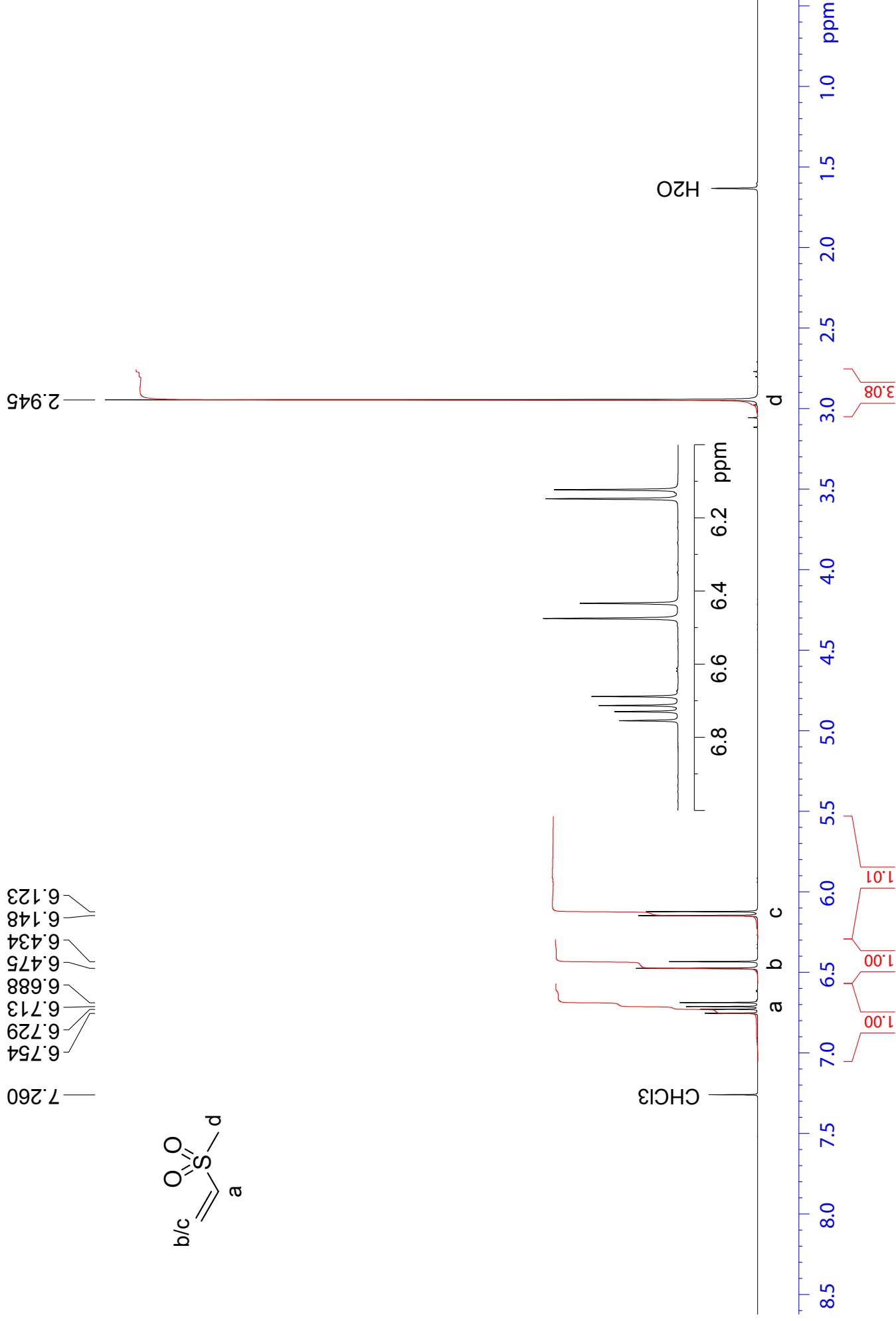
[S] 22.20%

16.06.16

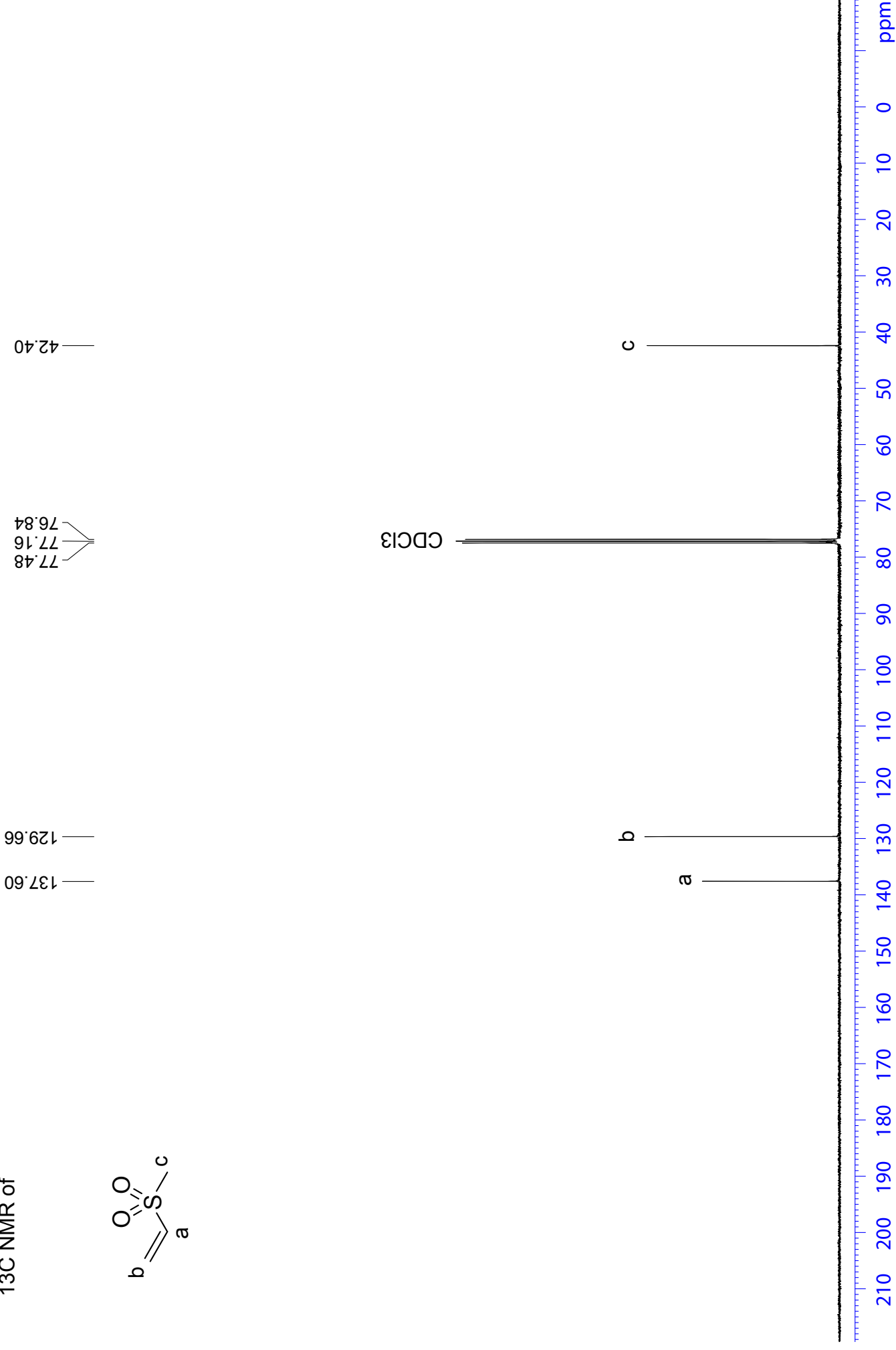
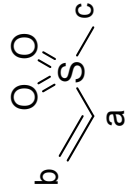
¹H NMR of

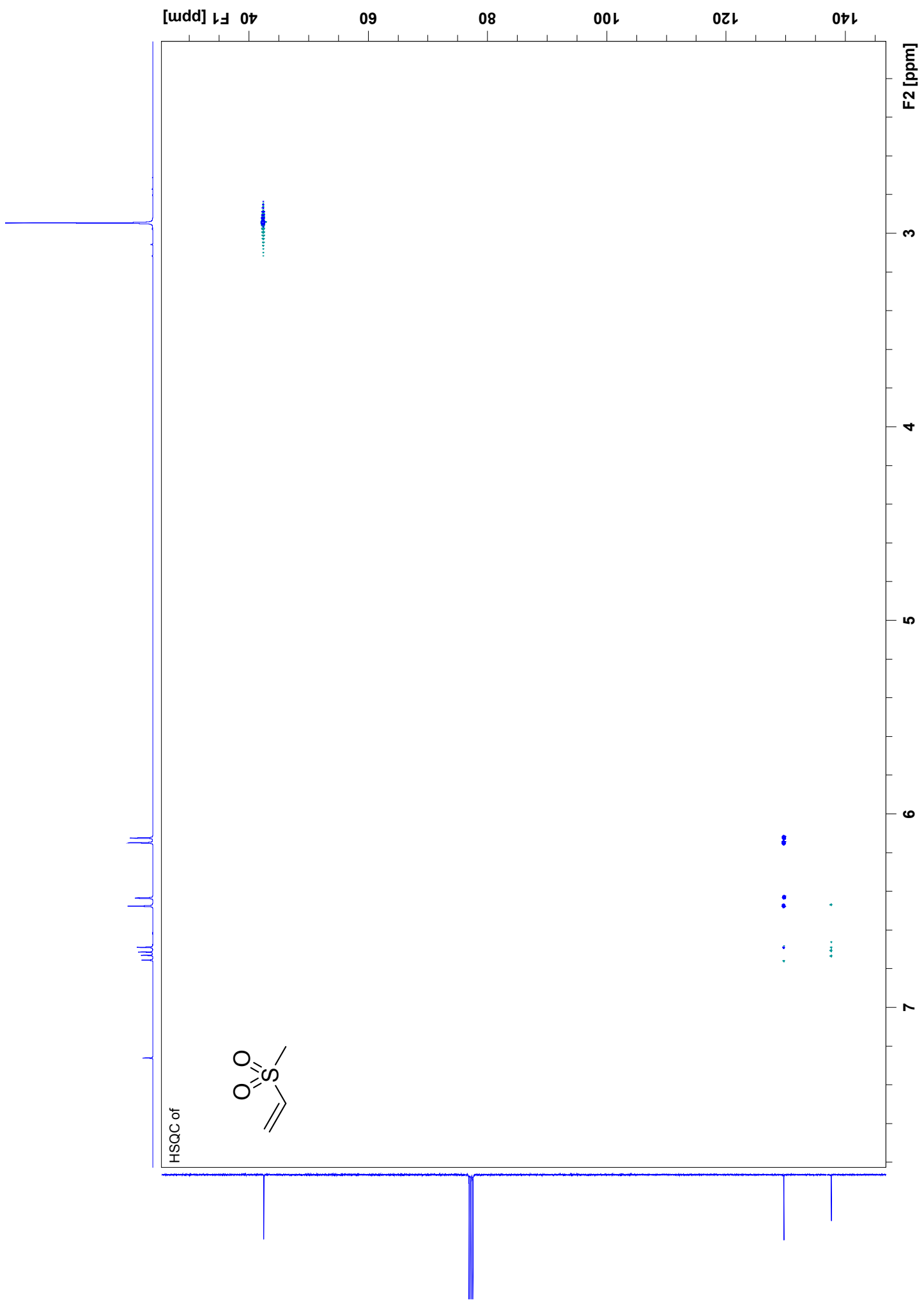


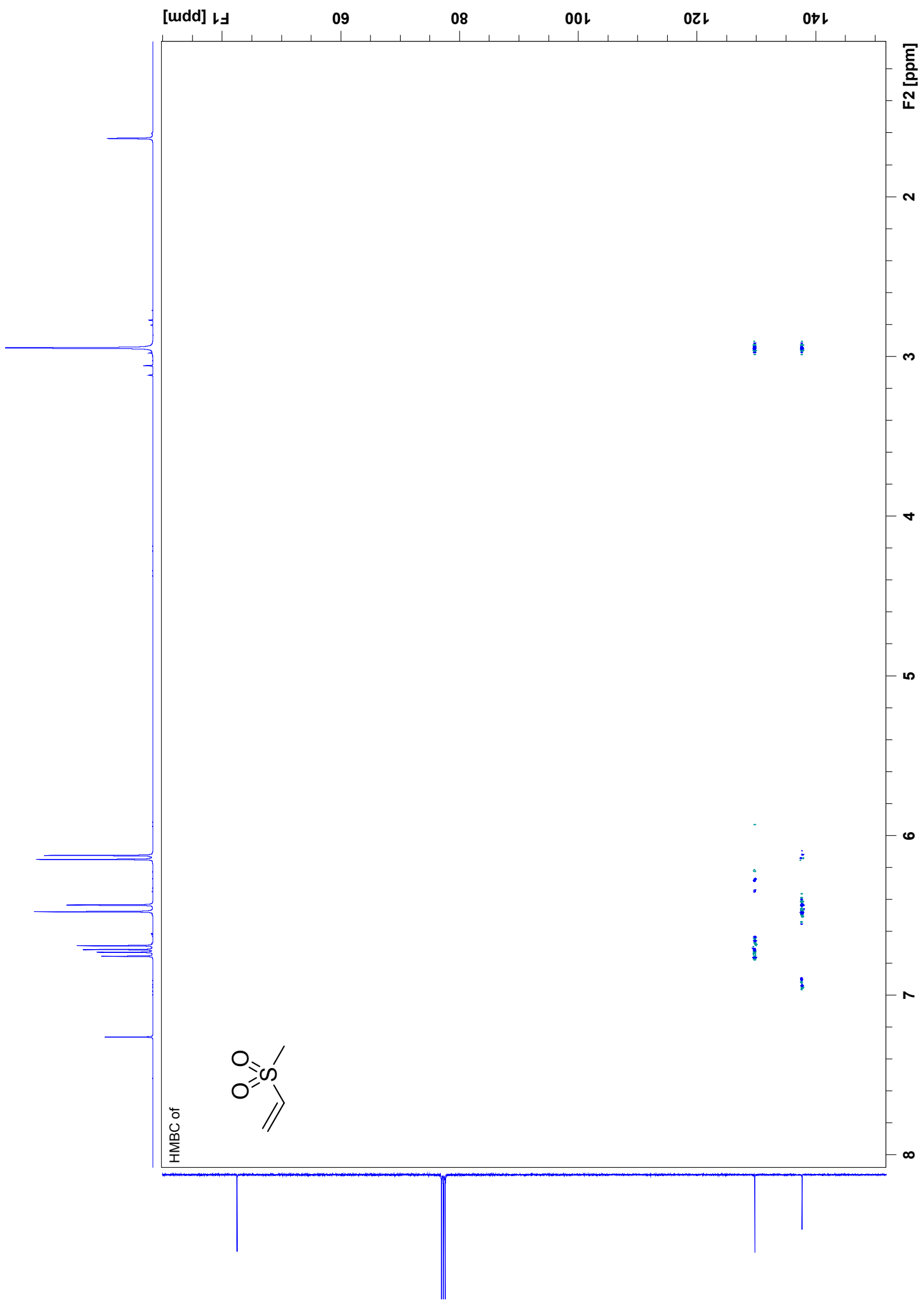
7.260
6.754
6.729
6.713
6.688
6.475
6.434
6.148
6.123

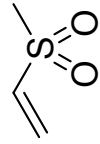


¹³C NMR of

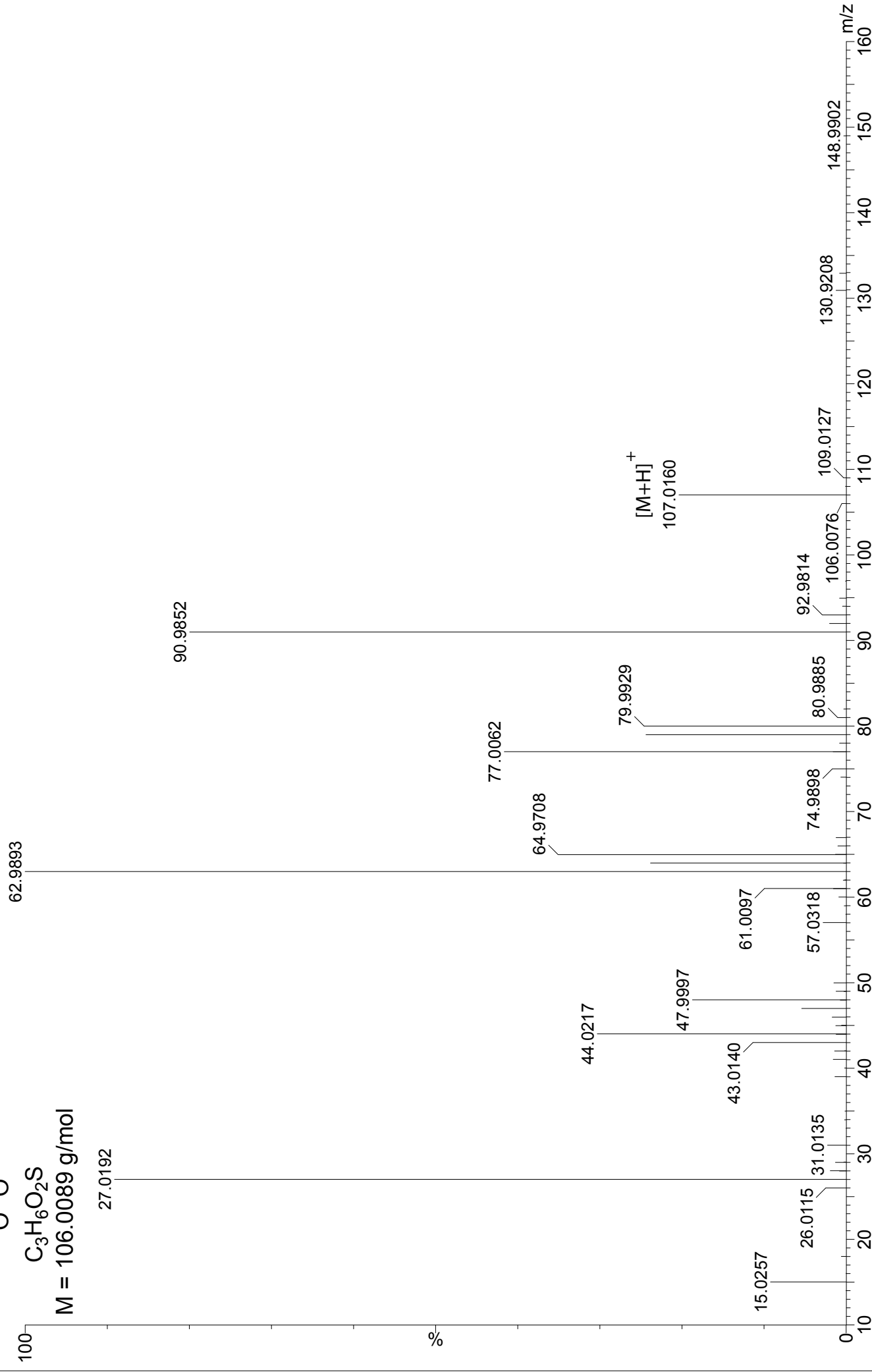




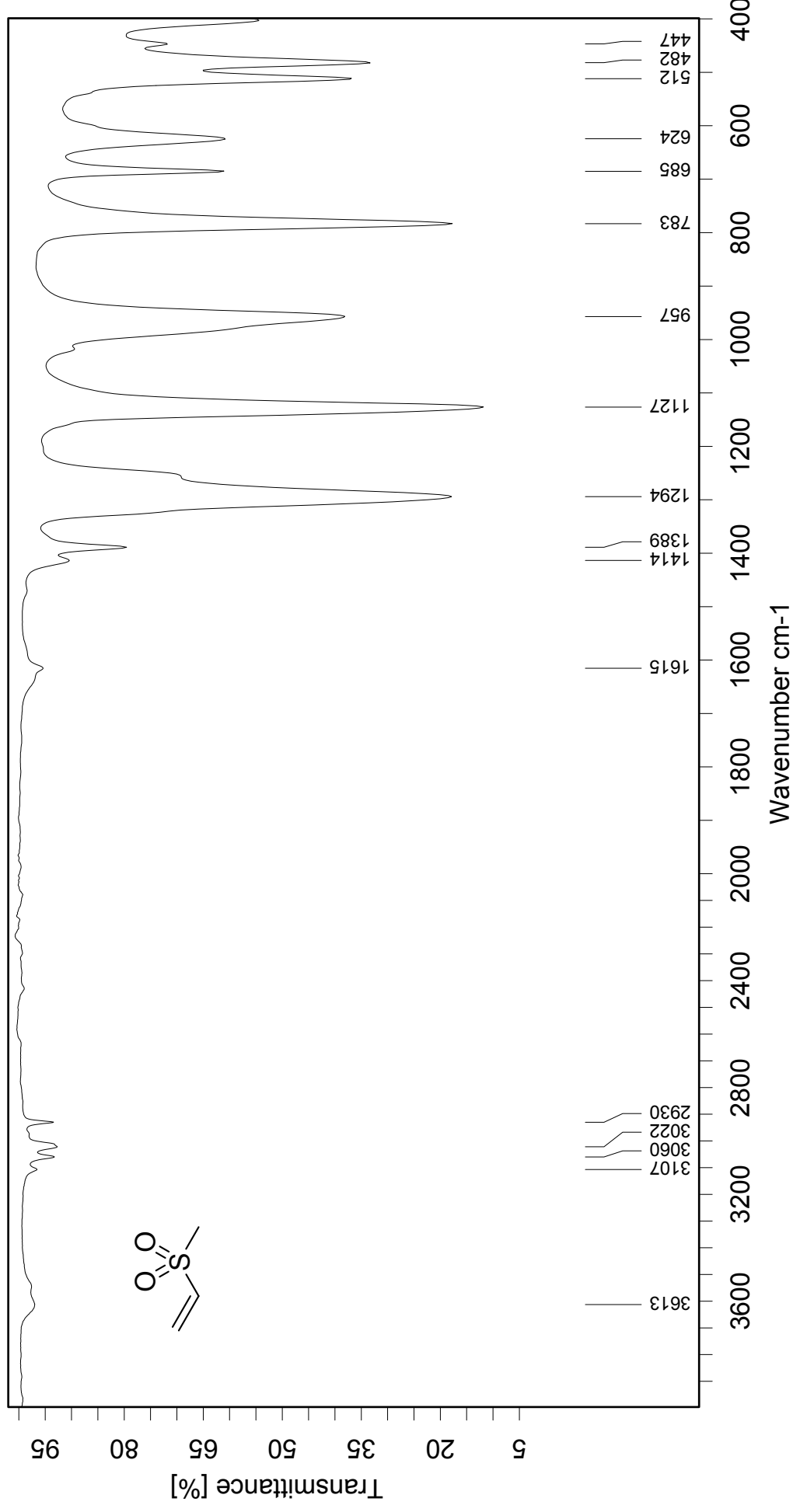


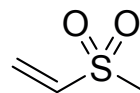
 $\text{C}_3\text{H}_6\text{O}_2\text{S}$

M = 106.0089 g/mol



IR Spectrum of





Molekularformel: C₃ H₆ O₂ S

Mr = 106.15g/mol

Siedepunkt: ?

gereinigt: Dest.

getrocknet: 75°C, 0.15mbar

Bestimmungen: C H O S

Eingang: 14.06.16

Ausgang: 22.06.16

M-162424

Operator: SM

Berechnete Gewichtsanteile:

[C]	33.95%	[H]	5.70%	[O]	30.15%	[S]	30.21%
-----	--------	-----	-------	-----	--------	-----	--------

Gefundene Gewichtsanteile:

Einwaage: 1.897mg

LECO CHNS-932

14.06.16

[C] 32.98% [H] 6.16%

Einwaage: 2.180mg

LECO CHNS-932

14.06.16

[C] 33.17% [H] 6.24%

Einwaage: 2.103mg

LECO RO-478

22.06.16

[O] 30.74%

Einwaage: 1.967mg

LECO RO-478

22.06.16

[O] 30.82%

Einwaage: 1.341mg

LECO CHNS-932

16.06.16

[S] 29.79%

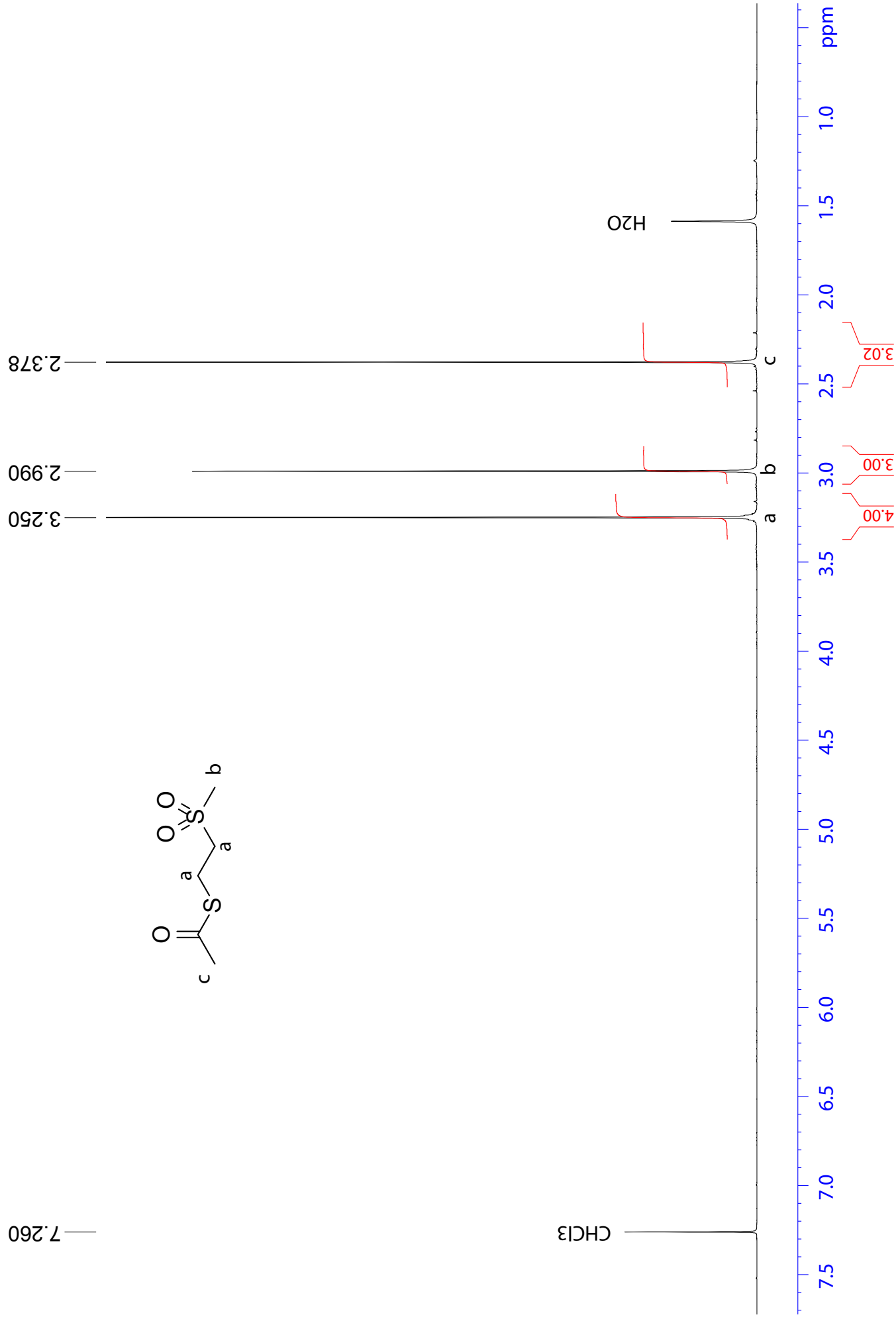
Einwaage: 1.567mg

LECO CHNS-932

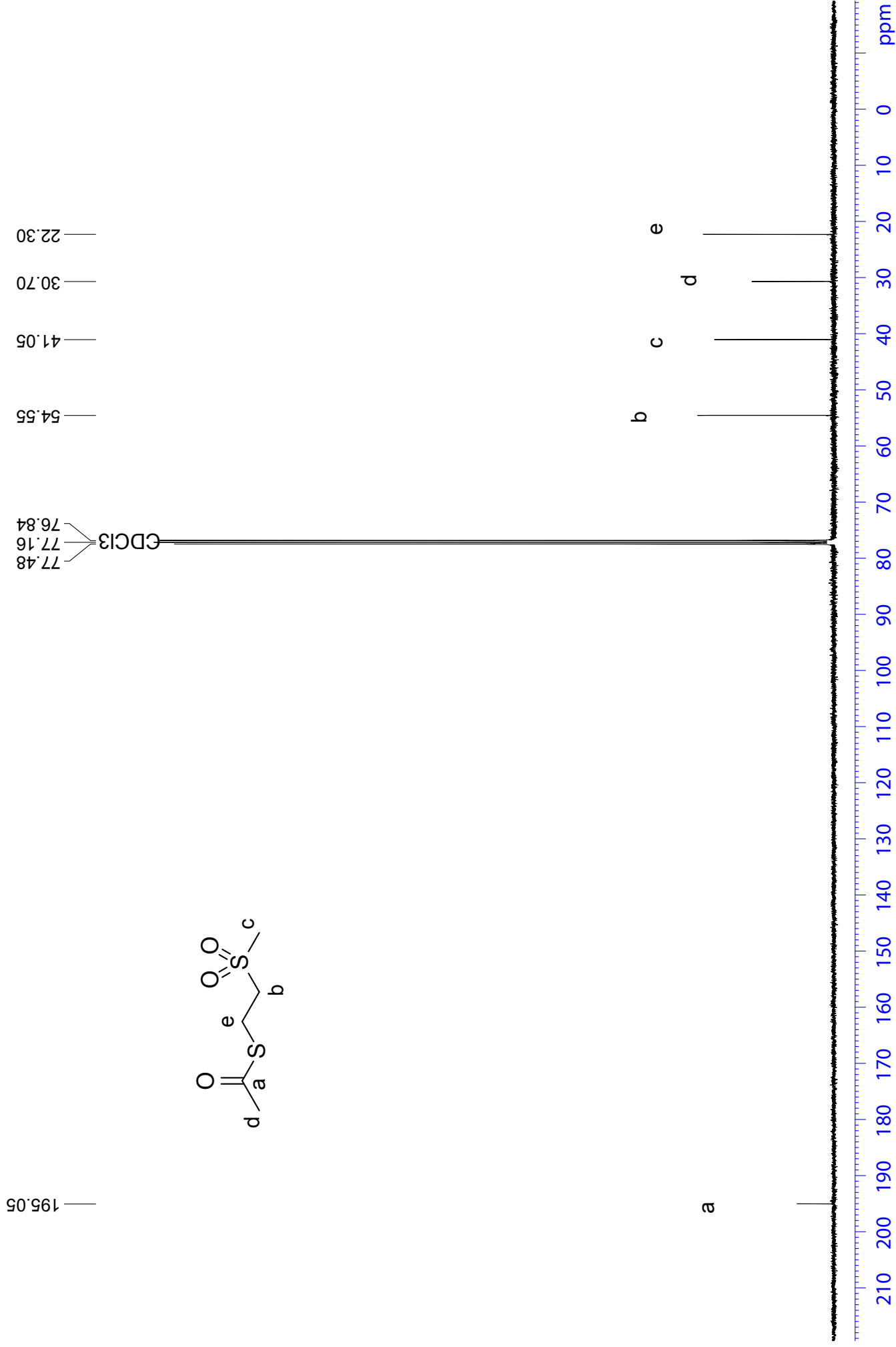
16.06.16

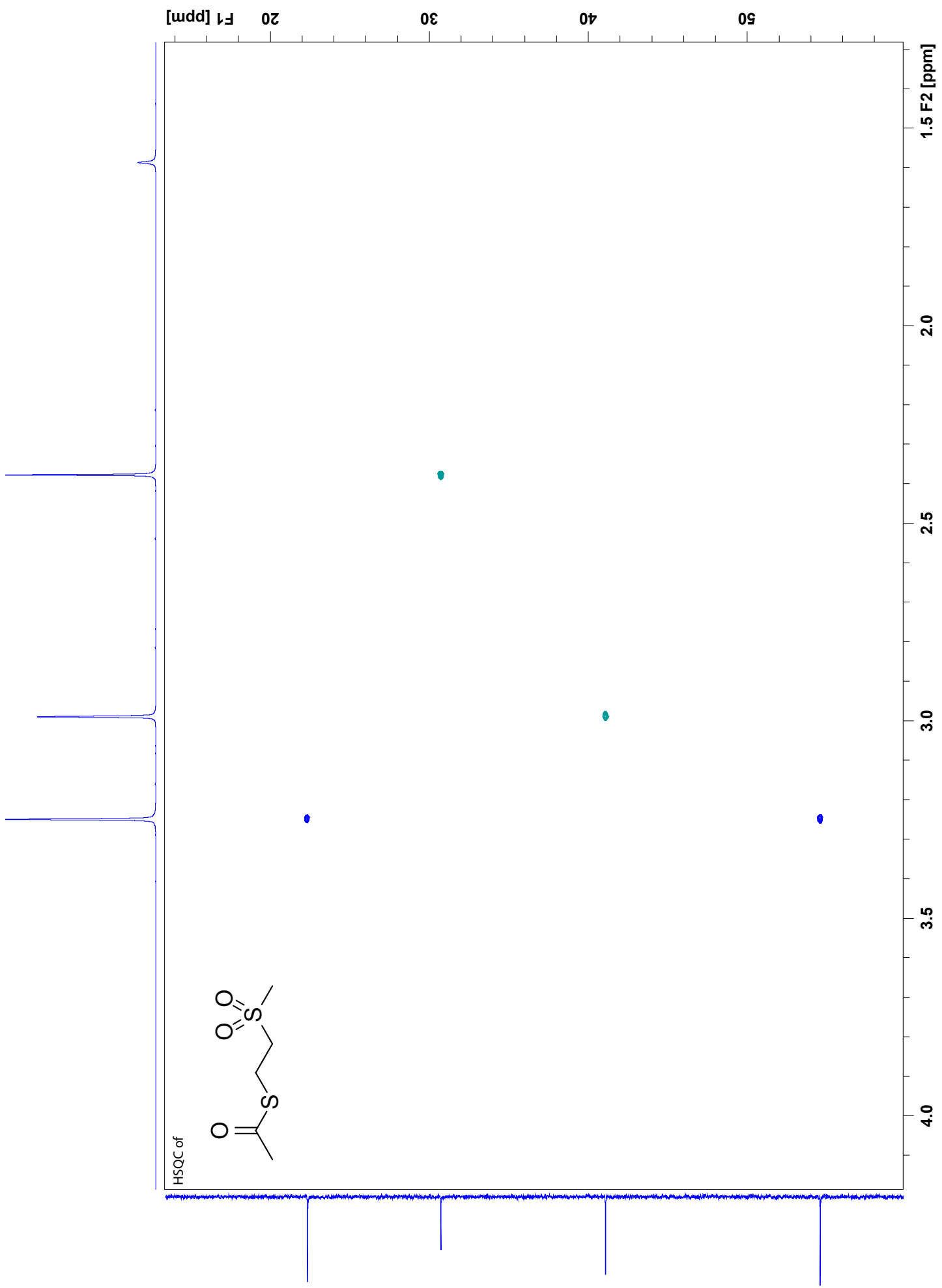
[S] 29.67%

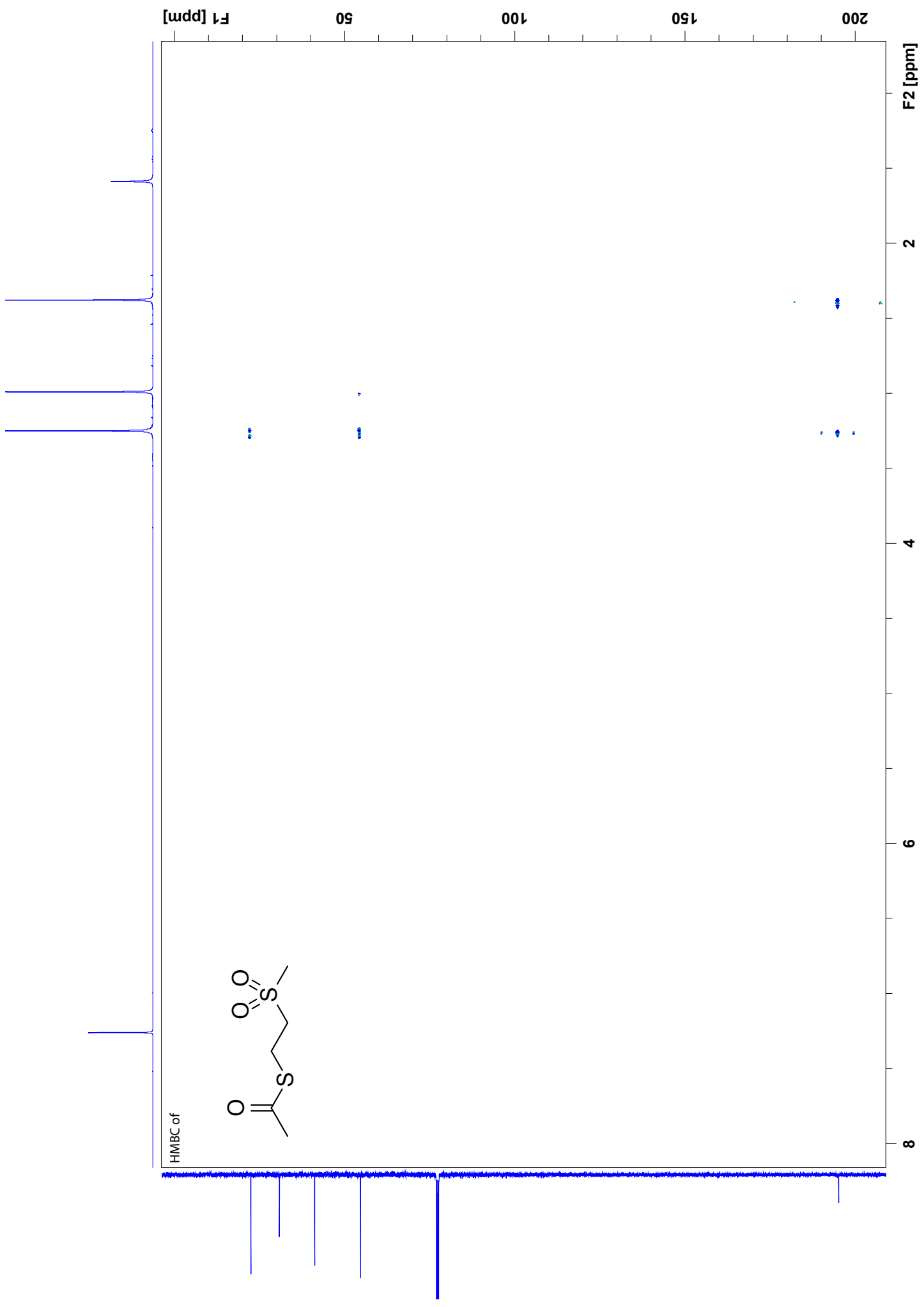
¹H NMR of

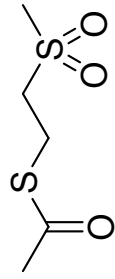


¹³C NMR of

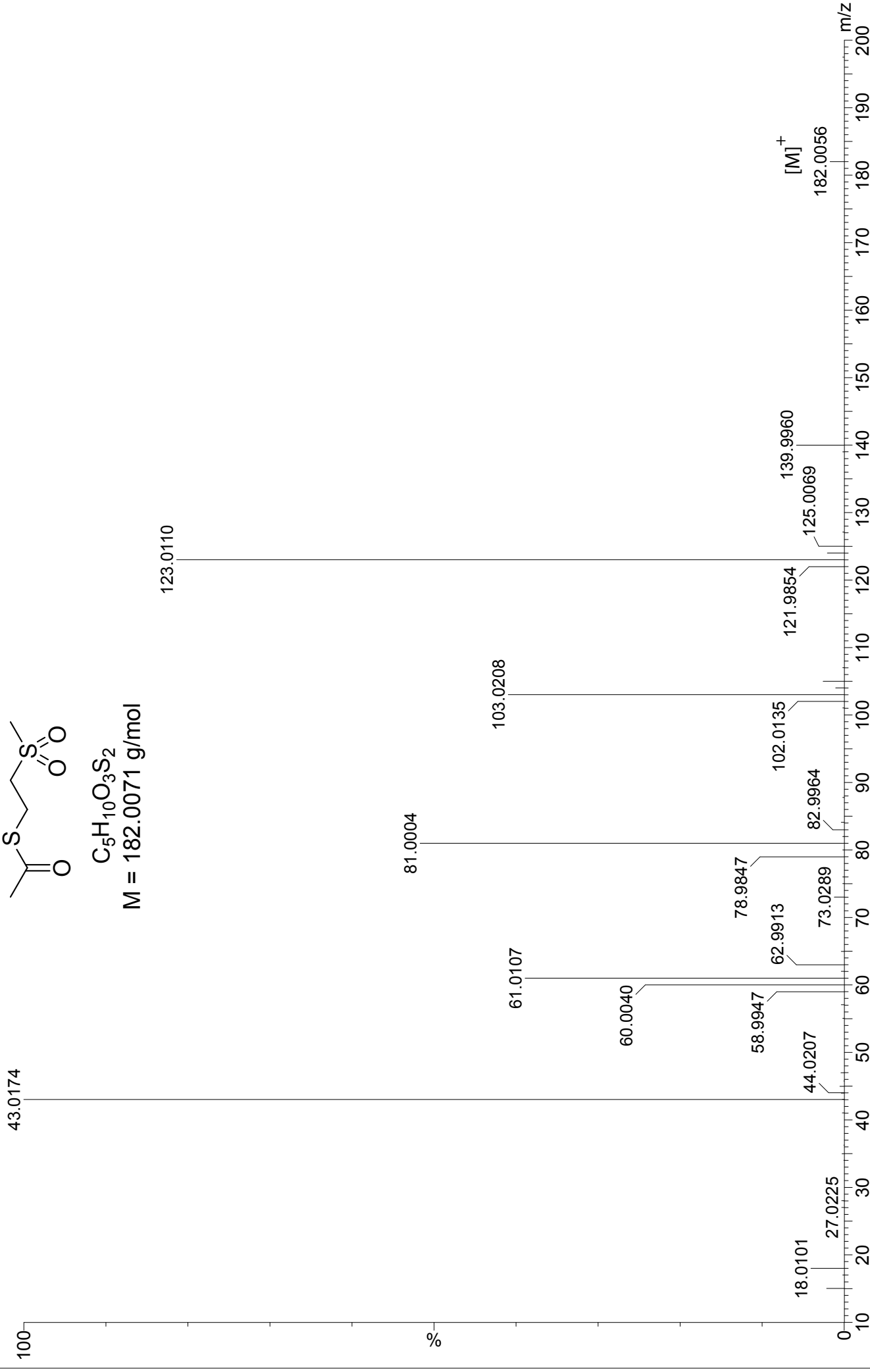


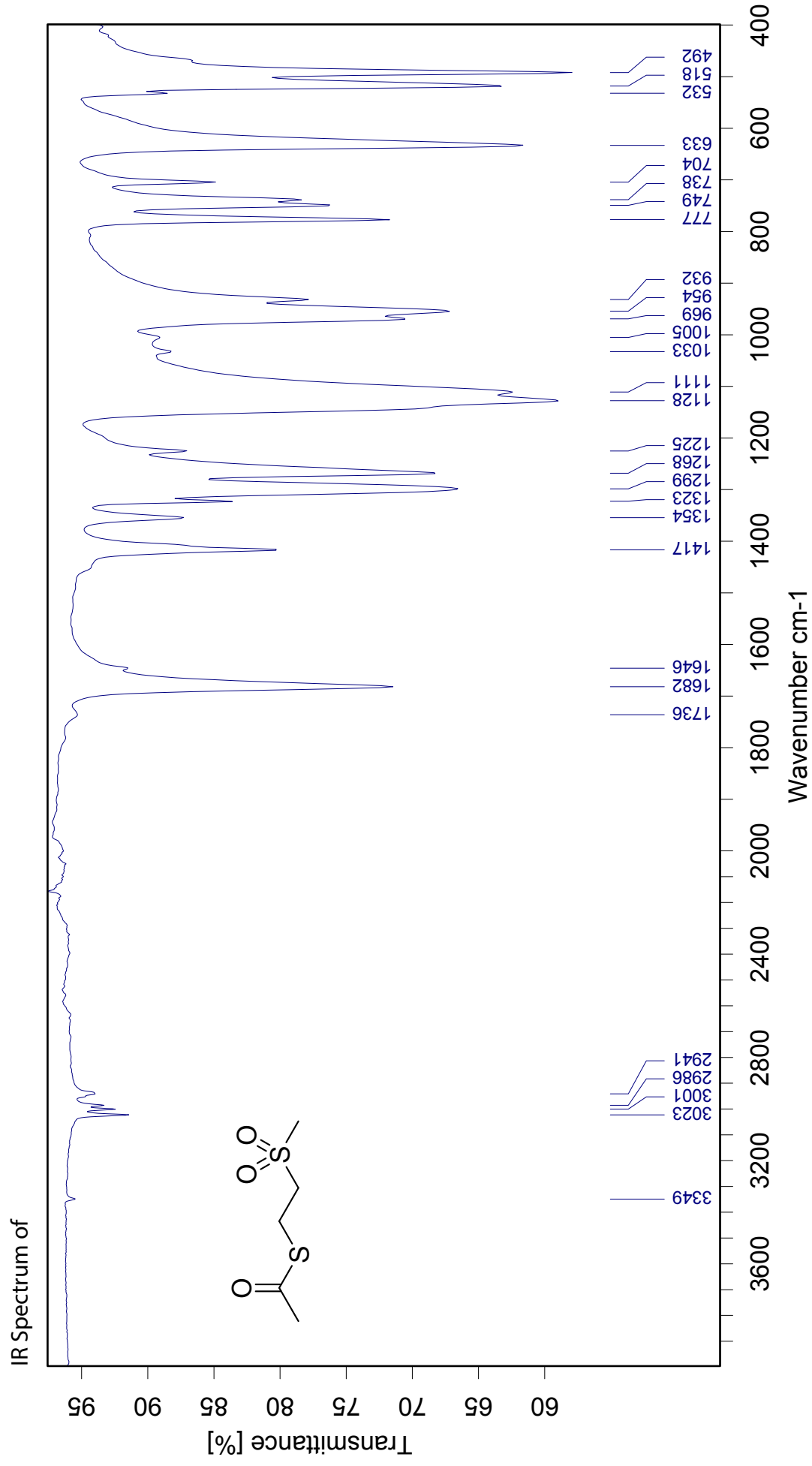


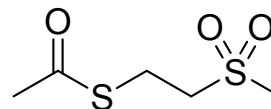




$\text{C}_5\text{H}_{10}\text{O}_3\text{S}_2$
 $M = 182.0071 \text{ g/mol}$







Molekularformel: C5 H10 O3 S2

Mr = 182.26g/mol

Schmelzpunkt: ?

gereinigt: chromat., UK

getrocknet: 18h HV

Bestimmungen: C H O S

Eingang: 14.06.16

Ausgang: 22.06.16

M-162428

Operator: PK

Berechnete Gewichtsanteile:

[C]	32.95%	[H]	5.53%	[O]	26.33%	[S]	35.19%
-----	--------	-----	-------	-----	--------	-----	--------

Gefundene Gewichtsanteile:

Einwaage: 0.938mg

LECO TruSpec Micro

[C] 32.81% [H] 5.42%

15.06.16

Einwaage: 1.983mg

LECO RO-478

[O] 26.54%

22.06.16

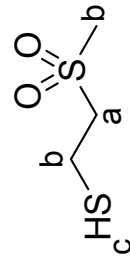
Einwaage: 1.657mg

LECO CHNS-932

[S] 34.89%

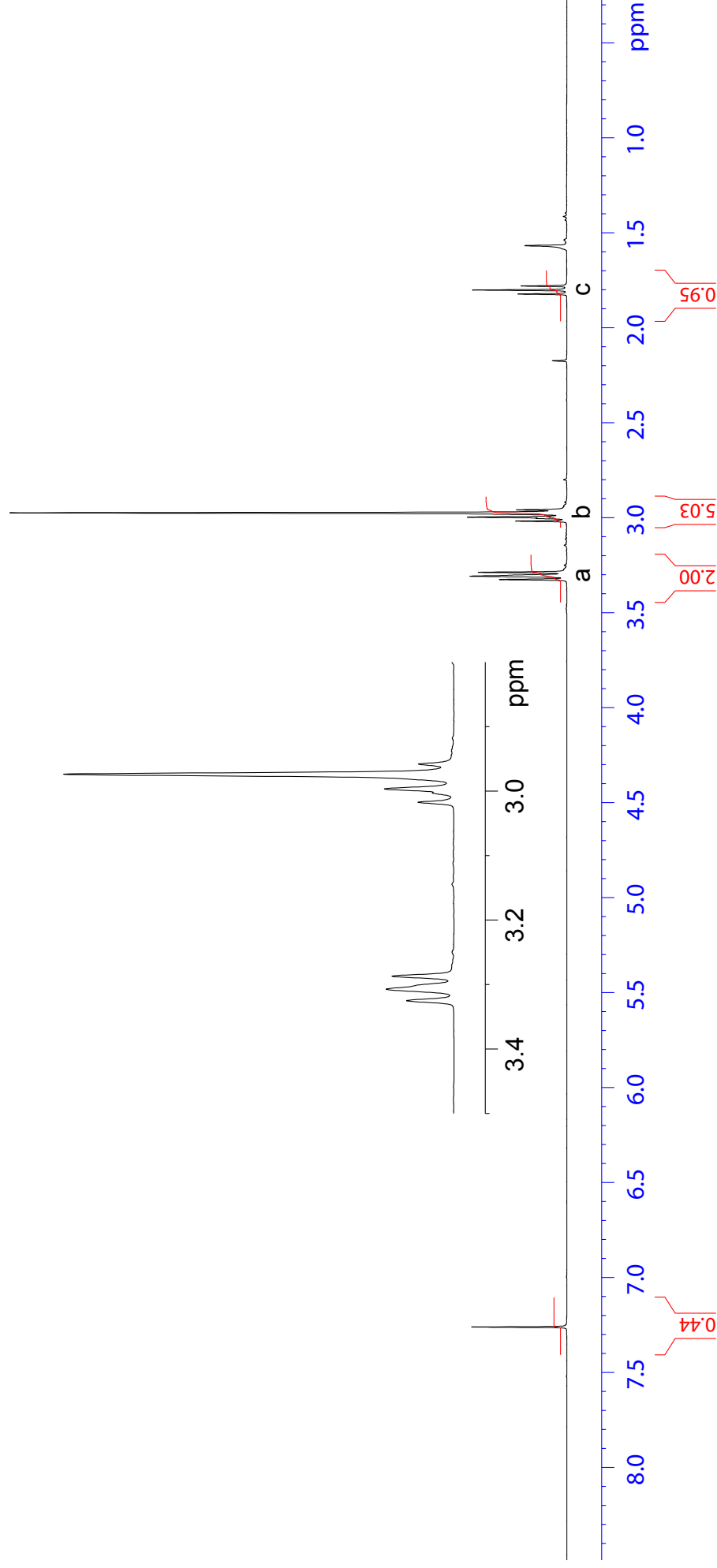
16.06.16

¹H NMR of

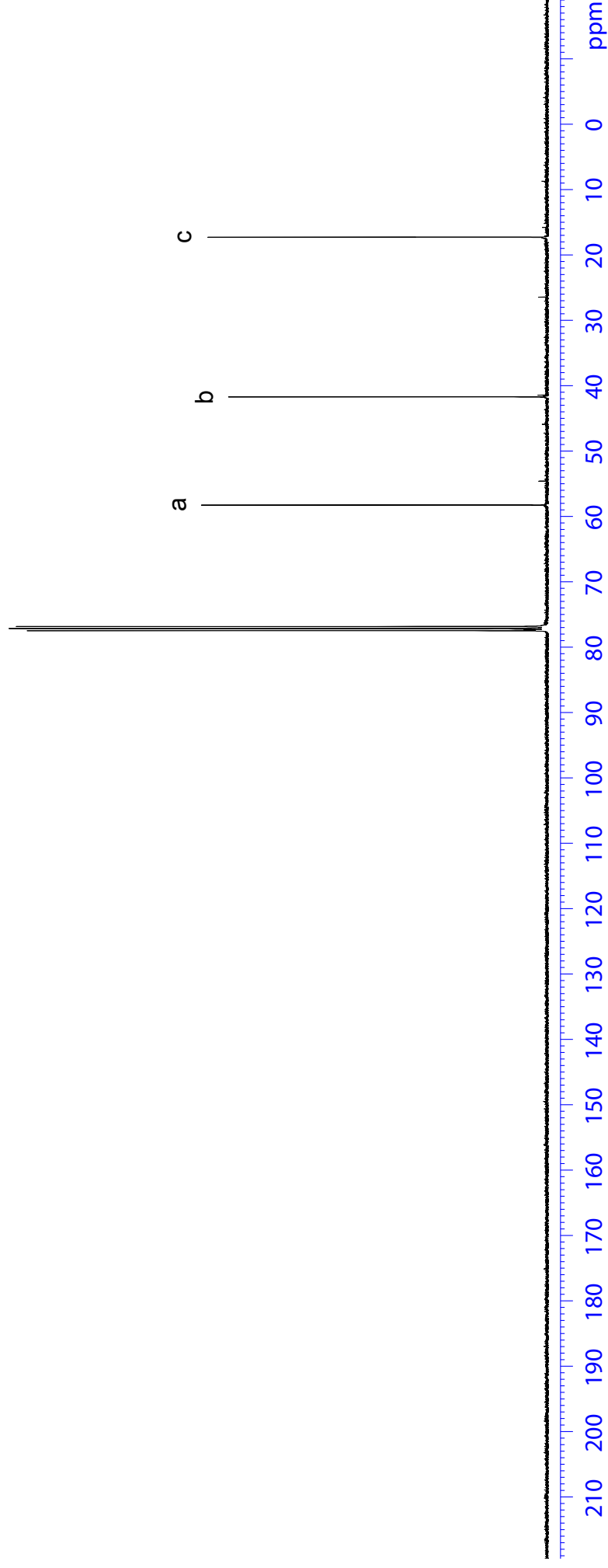
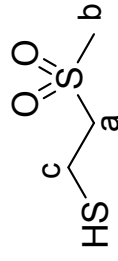


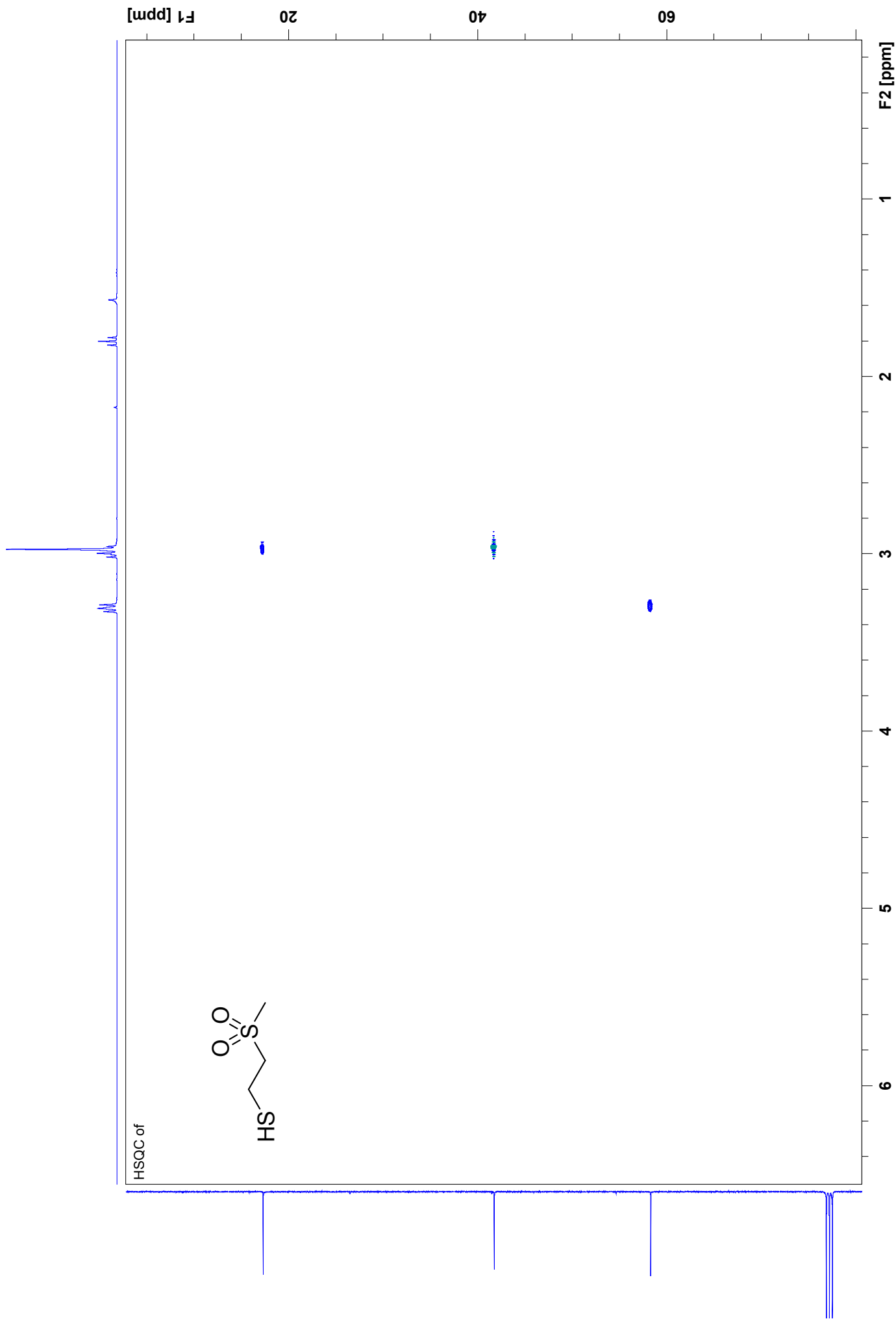
7.260

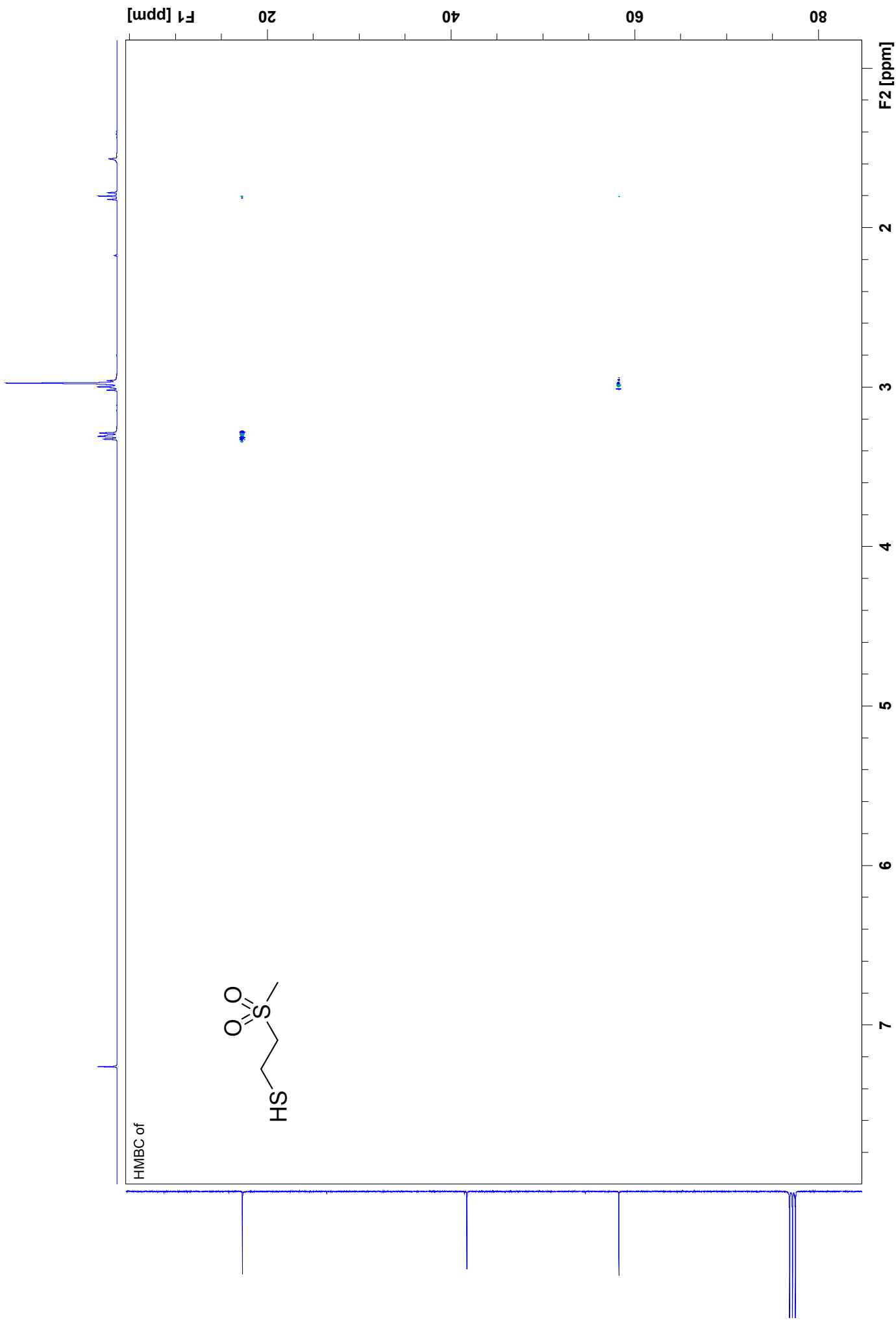
3.325
3.307
3.287
3.017
2.997
2.974
2.958
1.822
1.801
1.779



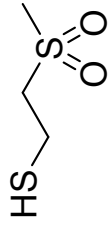
¹³C NMR of







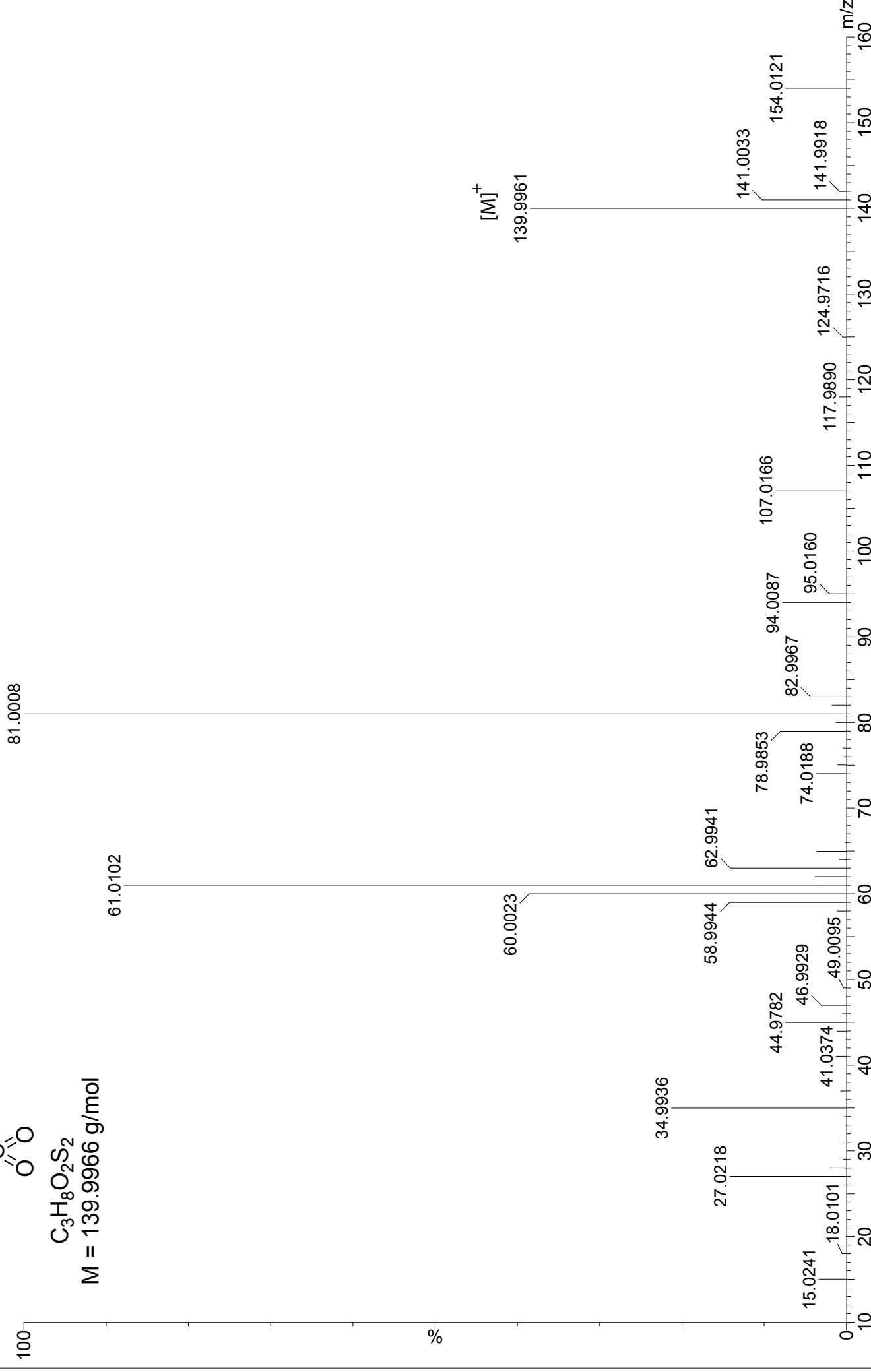
MS of

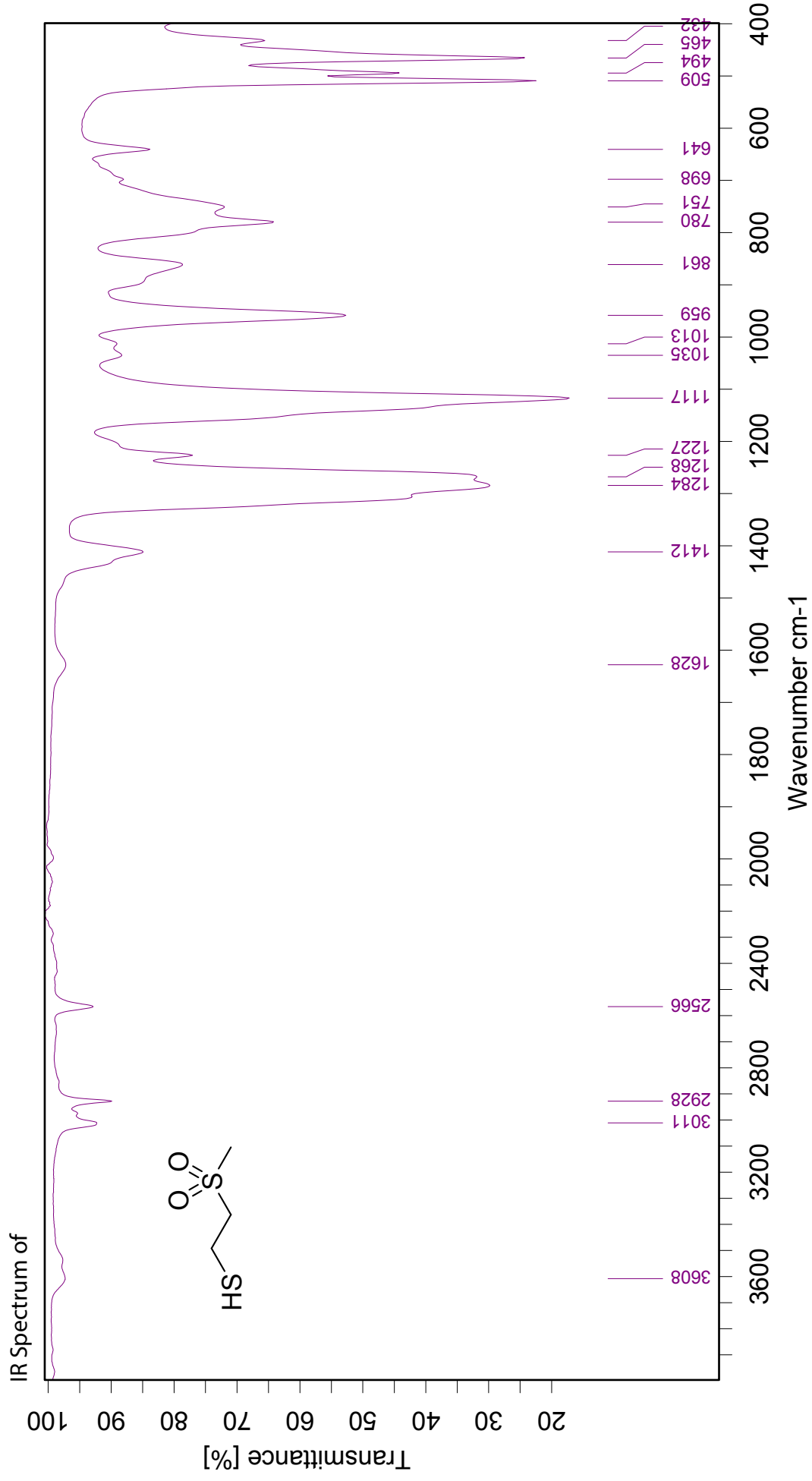


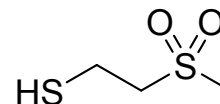
$\text{C}_3\text{H}_8\text{O}_2\text{S}_2$

$M = 139.9966 \text{ g/mol}$

Magnet EI+
4.89e3







Molekularformel: C₃ H₈ O₂ S₂

Mr = 140.23g/mol

Siedepunkt:

gereinigt: chromat.

getrocknet: 18h HV

Bestimmungen: C H O S

Eingang: 14.06.16

Ausgang: 22.06.16

M-162425

Operator: PK

Berechnete Gewichtsanteile:

[C]	25.70%	[H]	5.75%	[O]	22.82%	[S]	45.73%
-----	--------	-----	-------	-----	--------	-----	--------

Gefundene Gewichtsanteile:

Einwaage: 1.000mg

LECO TruSpec Micro

[C] 25.72% [H] 5.80%

14.06.15

Einwaage: 1.831mg

LECO RO-478

[O] 23.09%

22.06.16

Einwaage: 1.209mg

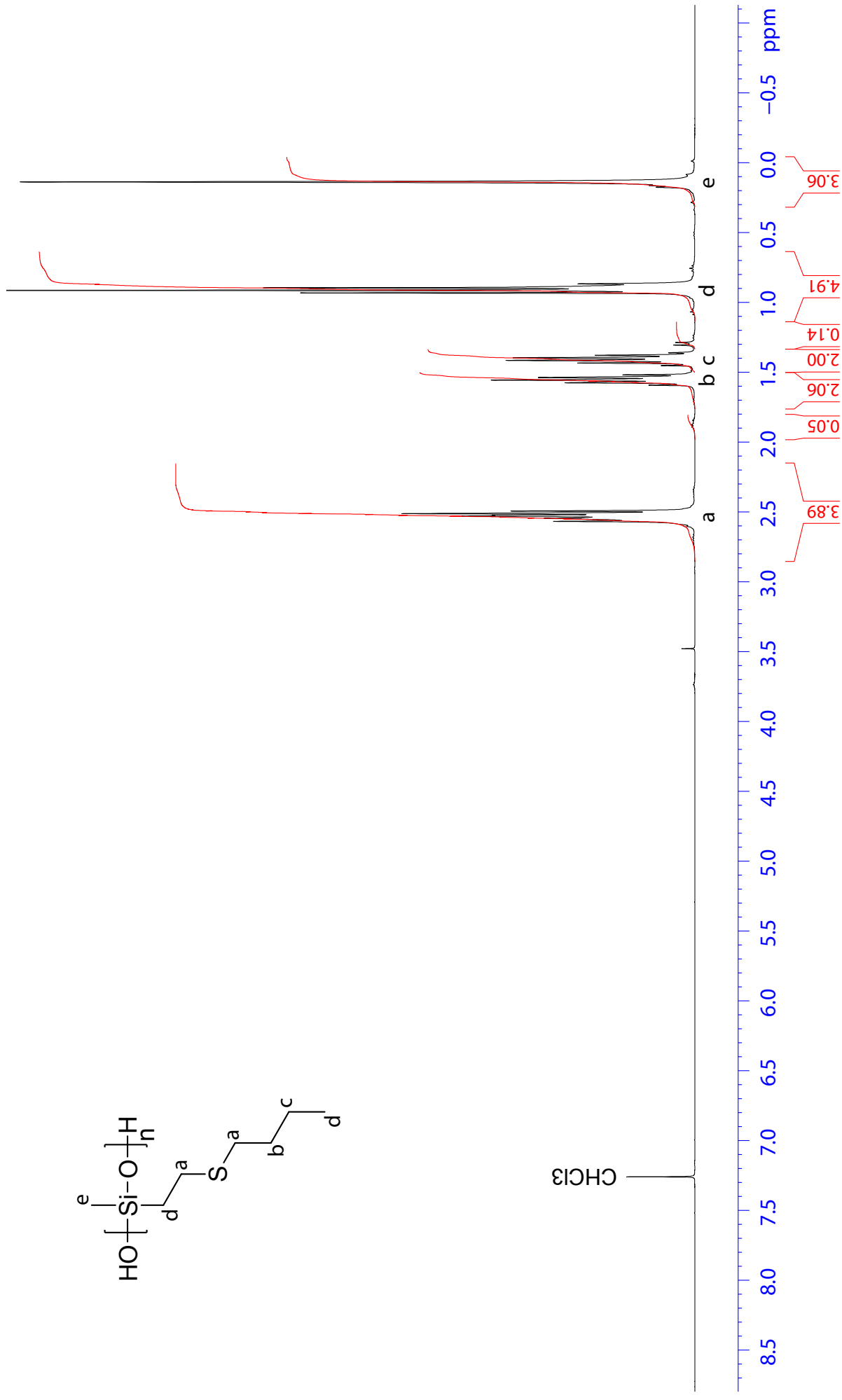
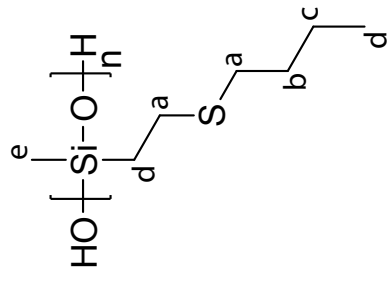
LECO CHNS-932

[S] 45.46%

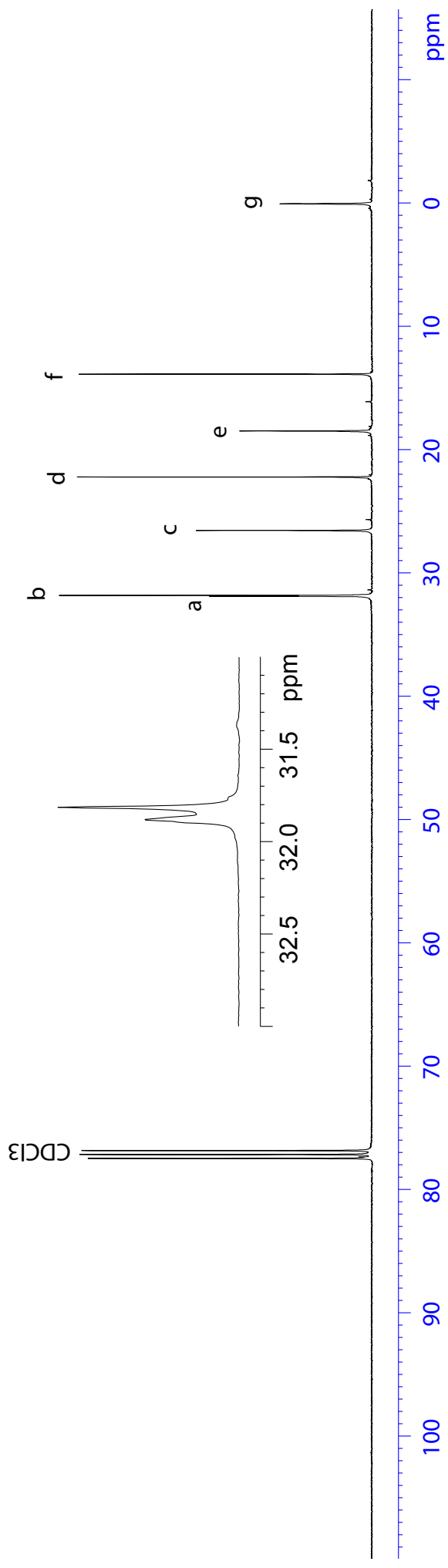
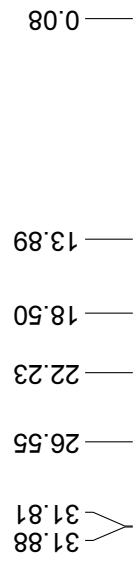
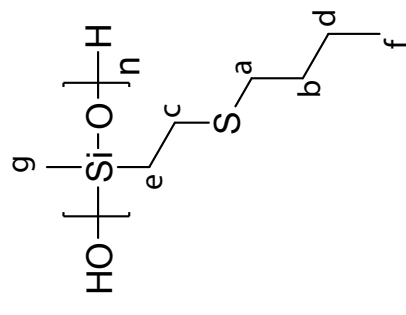
16.06.16

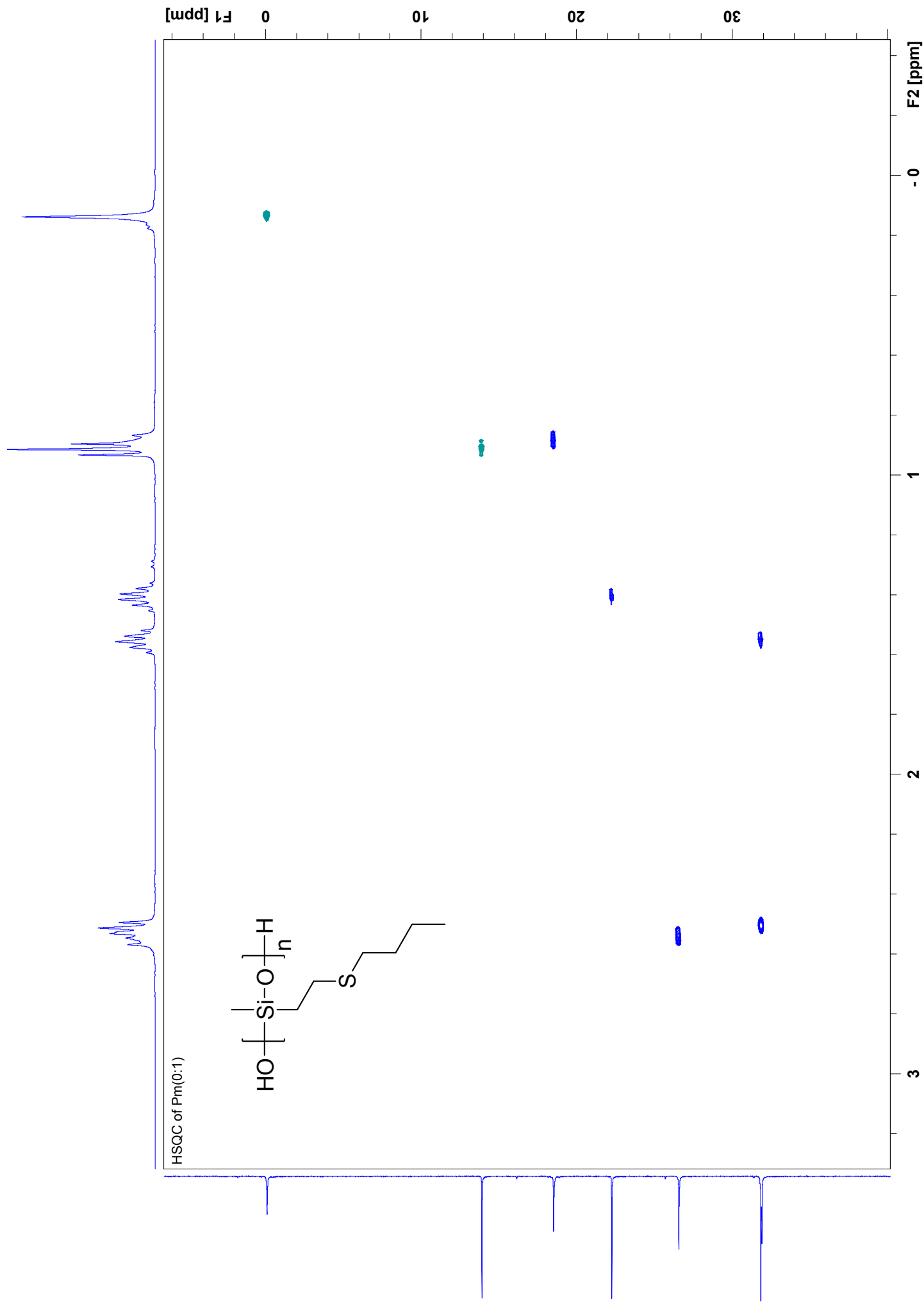
¹H NMR of Pm(0:1)

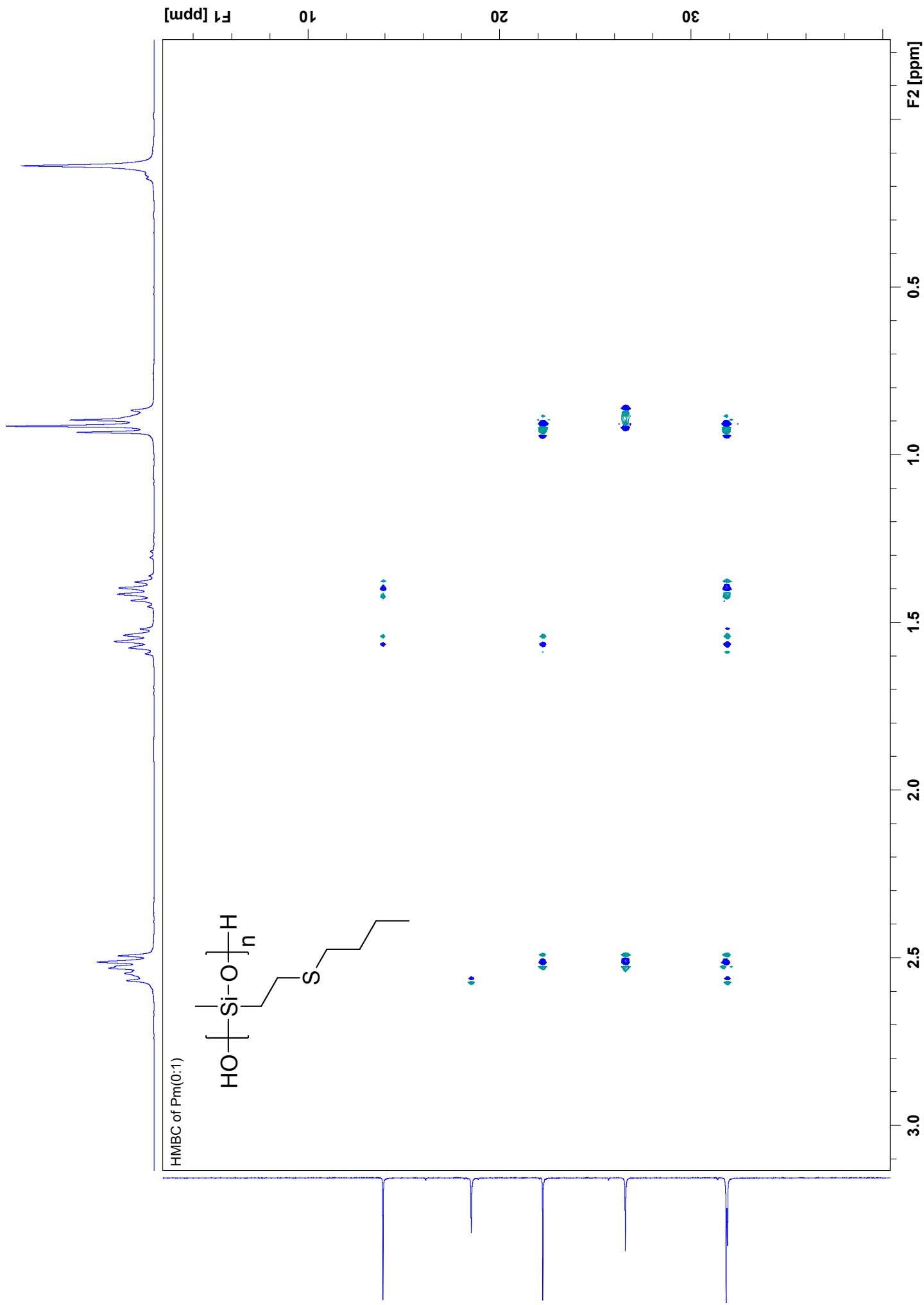
7.260

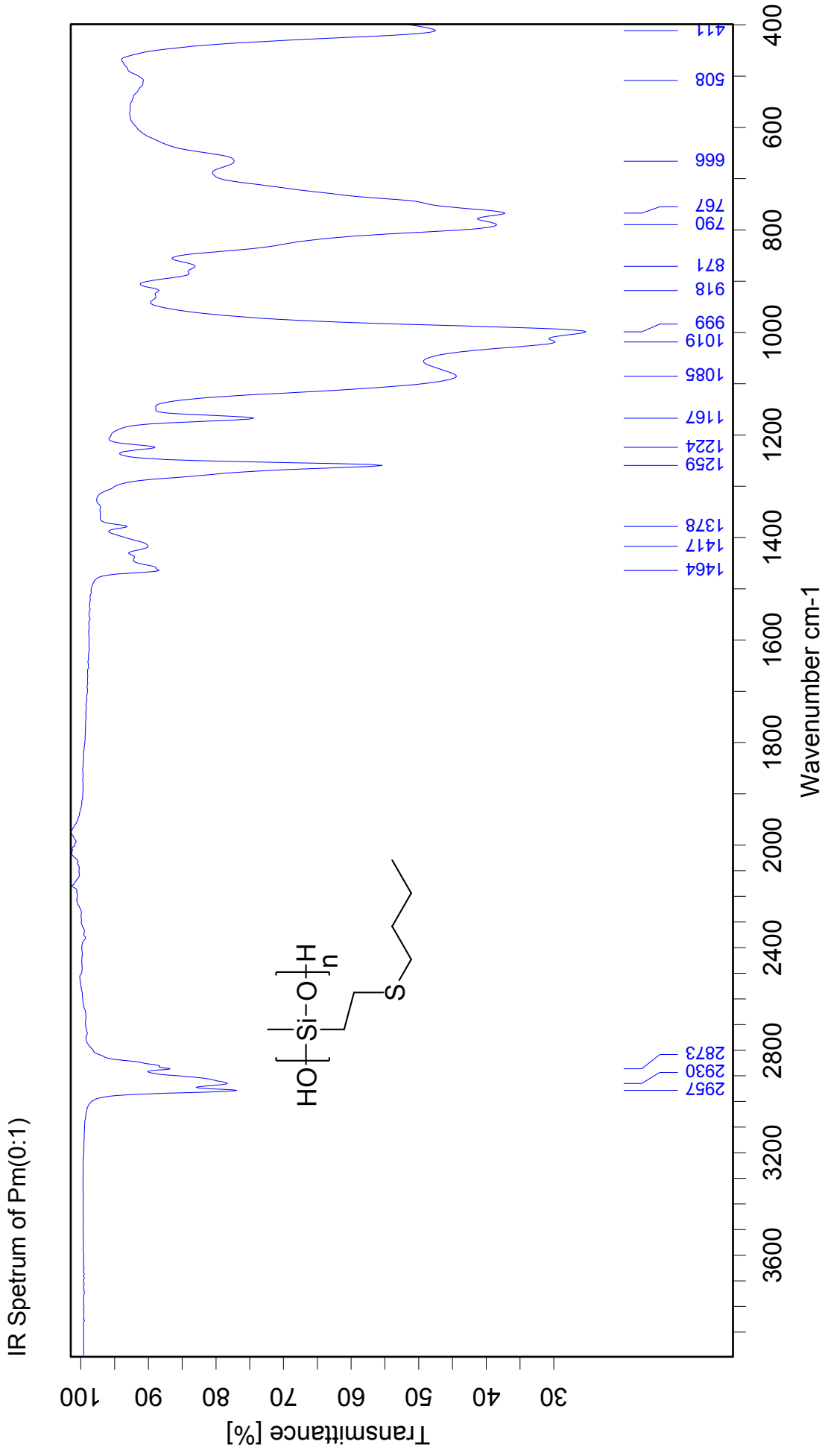


¹³C NMR of Pm(0:1)

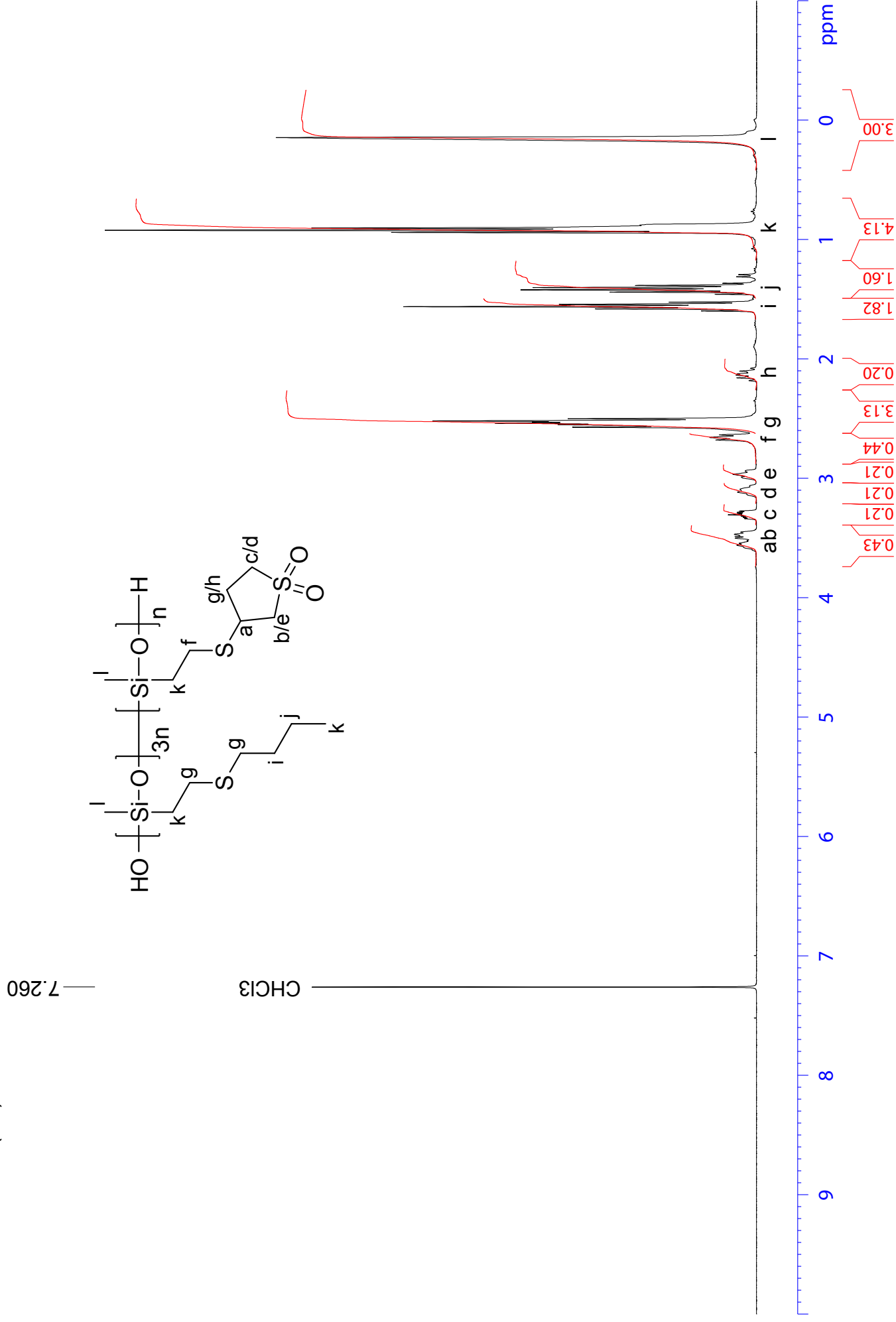




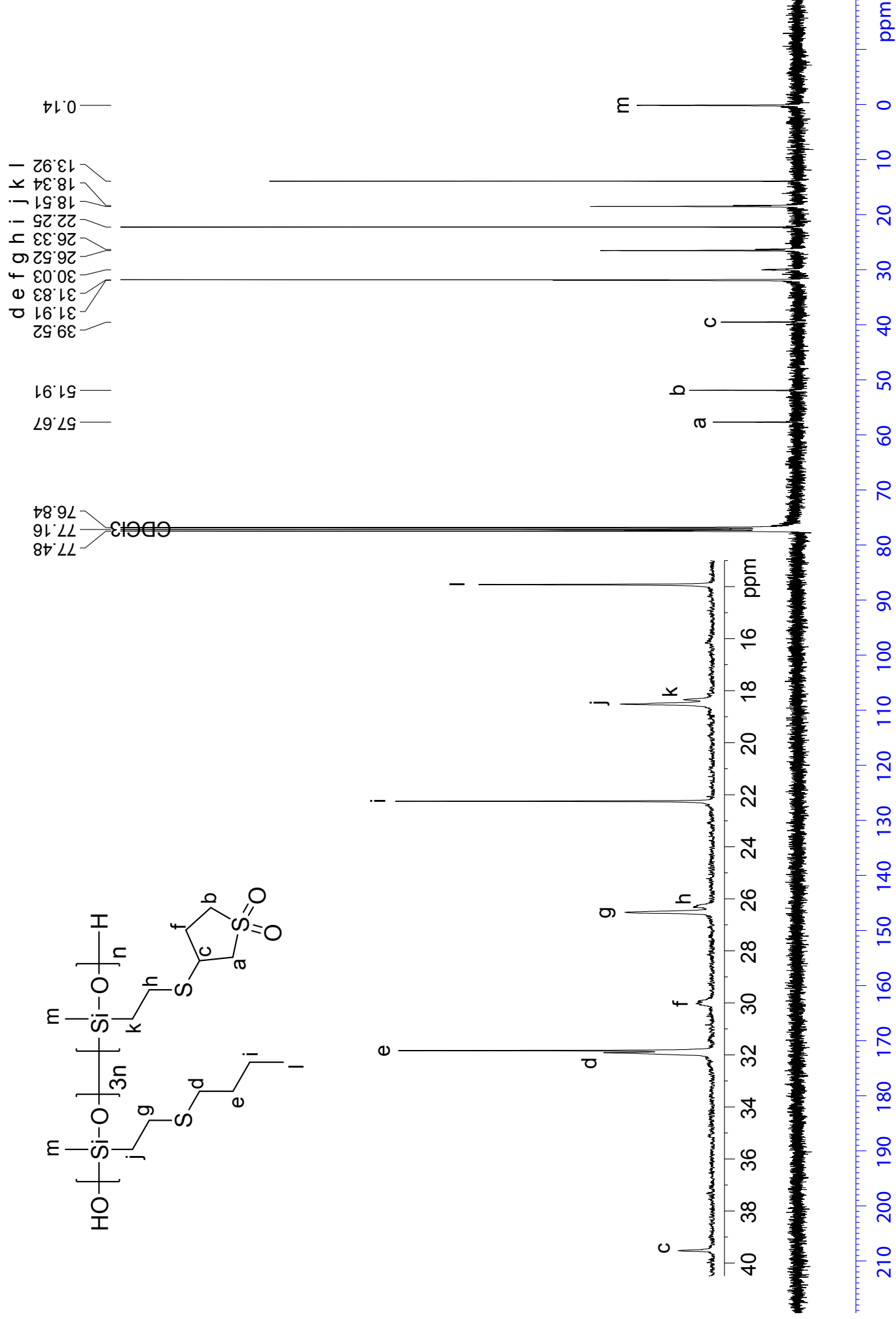
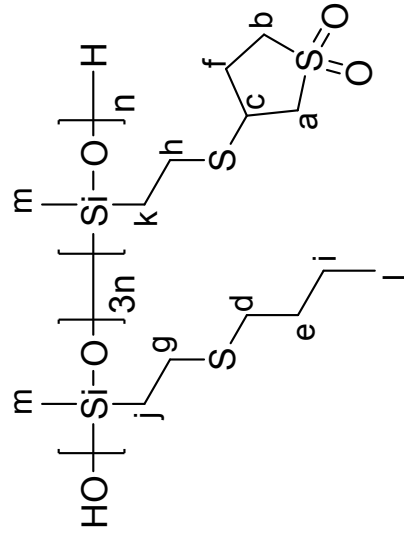




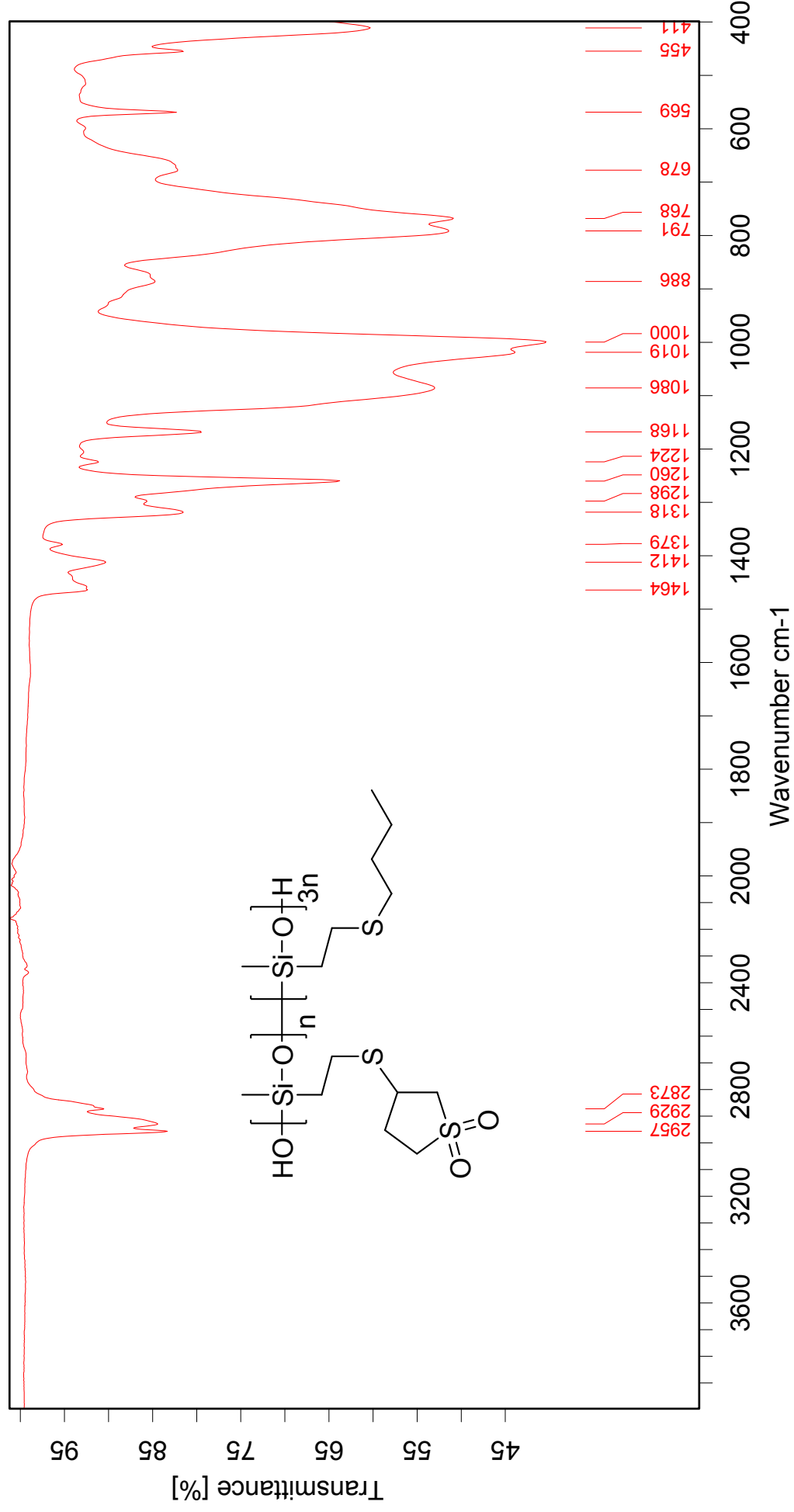
¹H NMR of Pm(1:3)



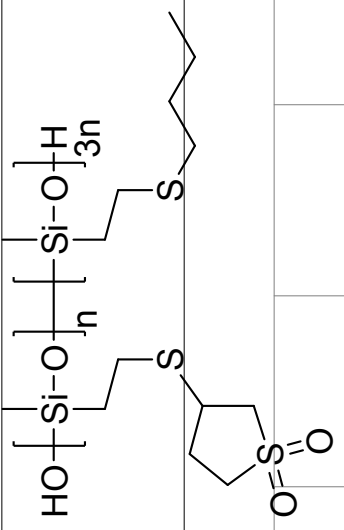
¹³C NMR of Pm(1:3)



IR Spectrum of Pm(1:3)

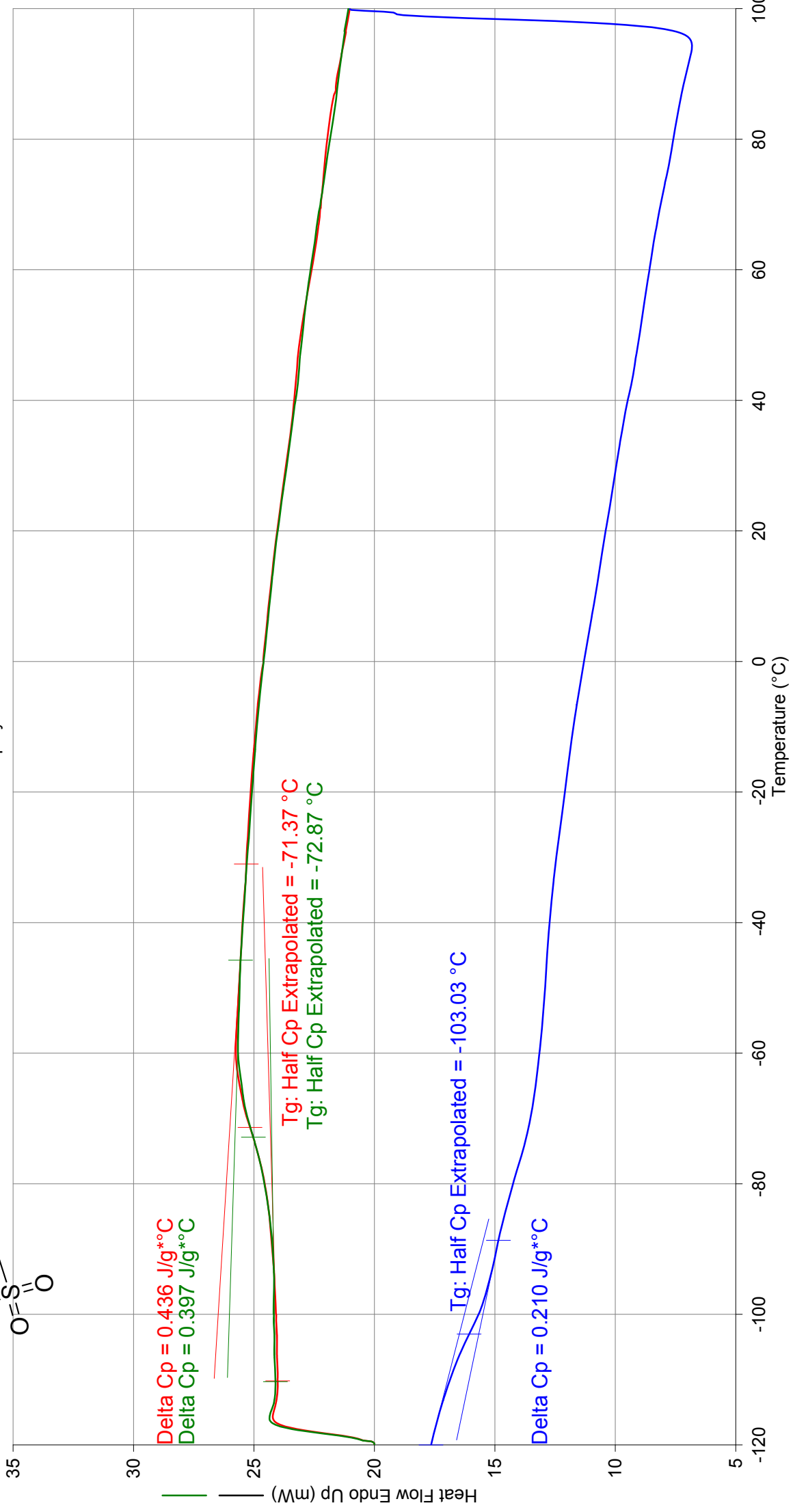


DSC of Pm(1:3)



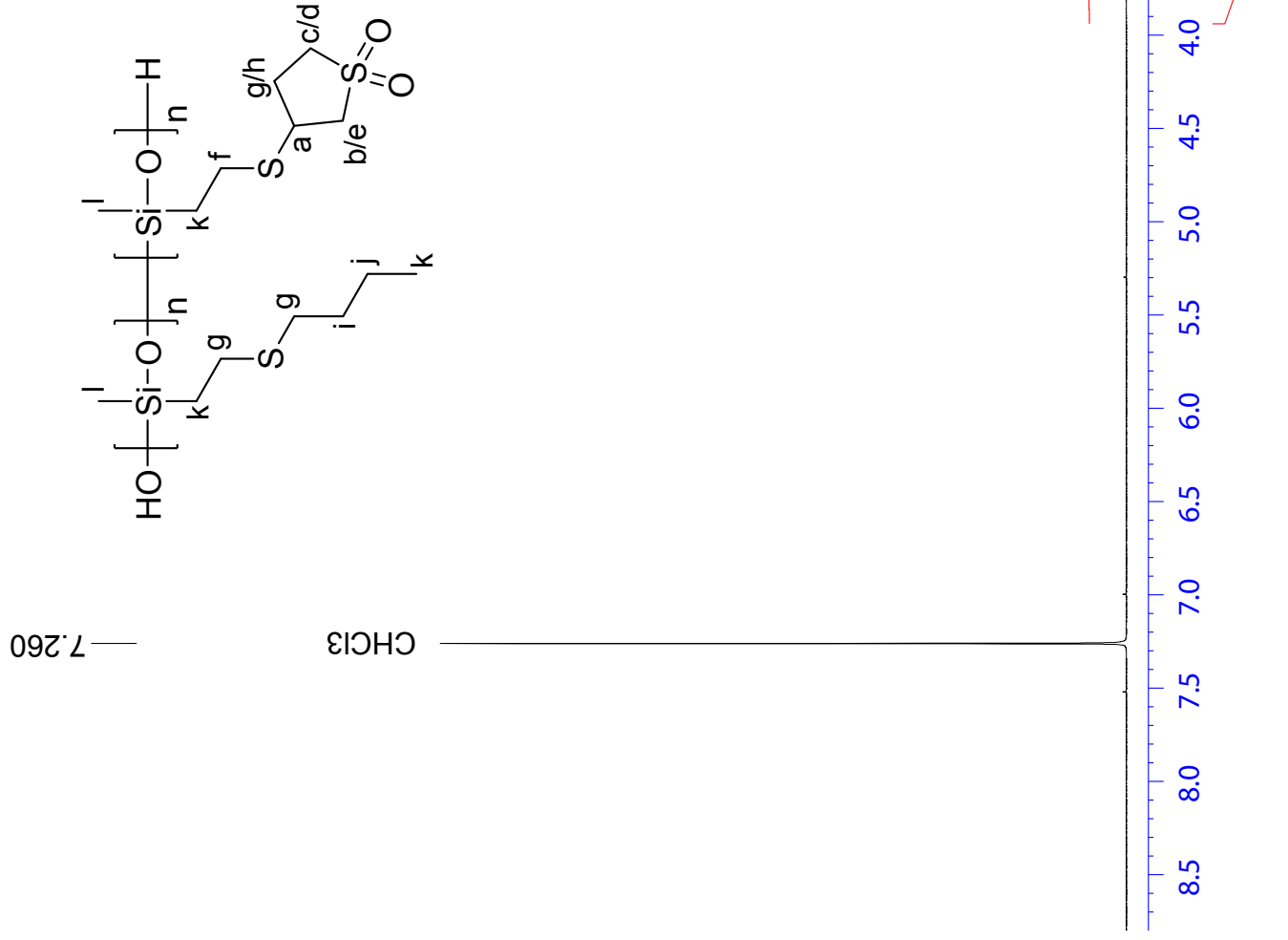
- Heat Flow Endo Up (mW) : Step: 1
- Heat Flow Endo Up (mW) : Step: 2
- Heat Flow Endo Up (mW) : Step: 1

Funktionspolymere

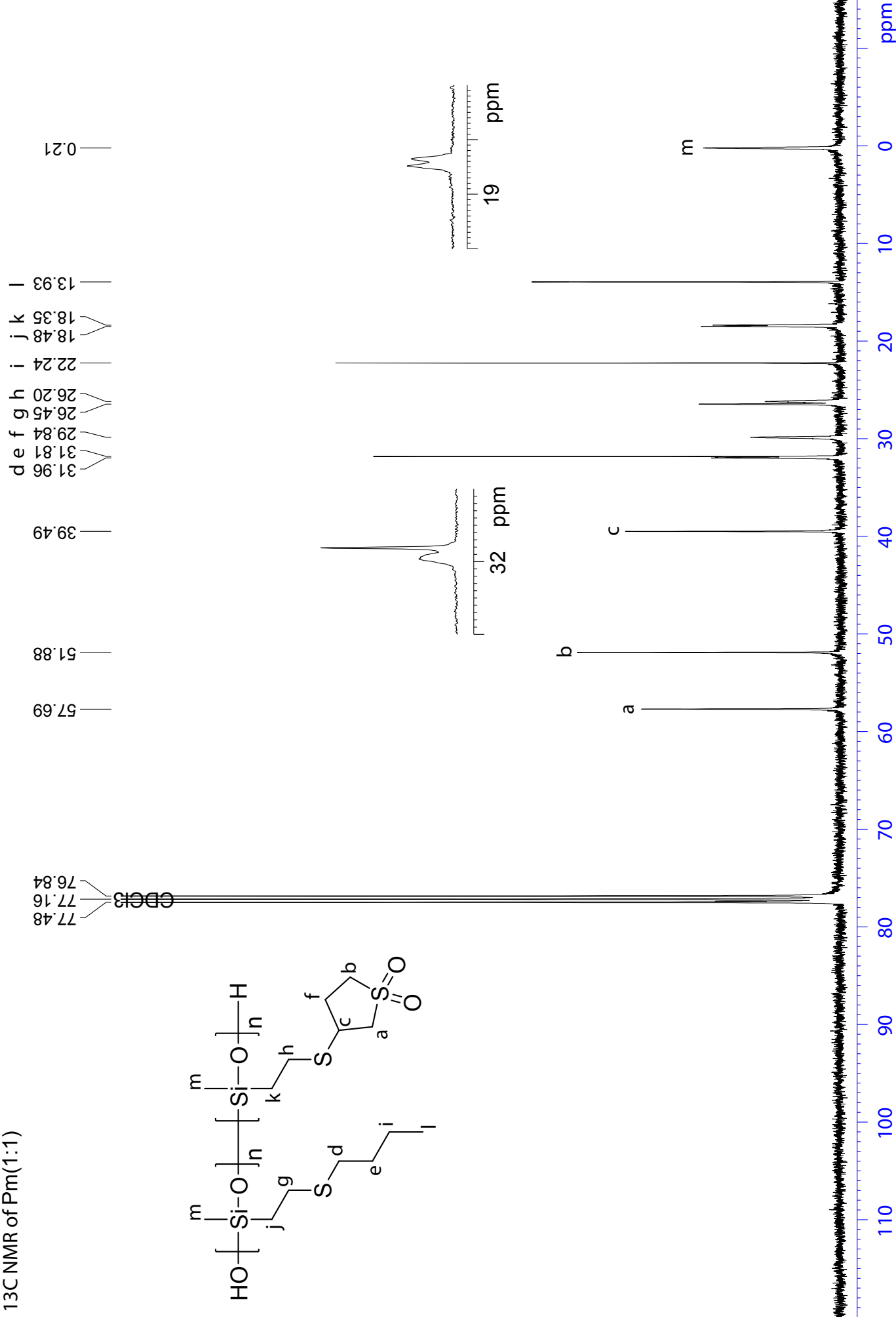
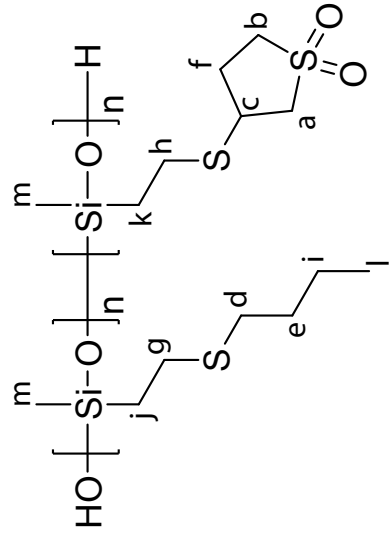


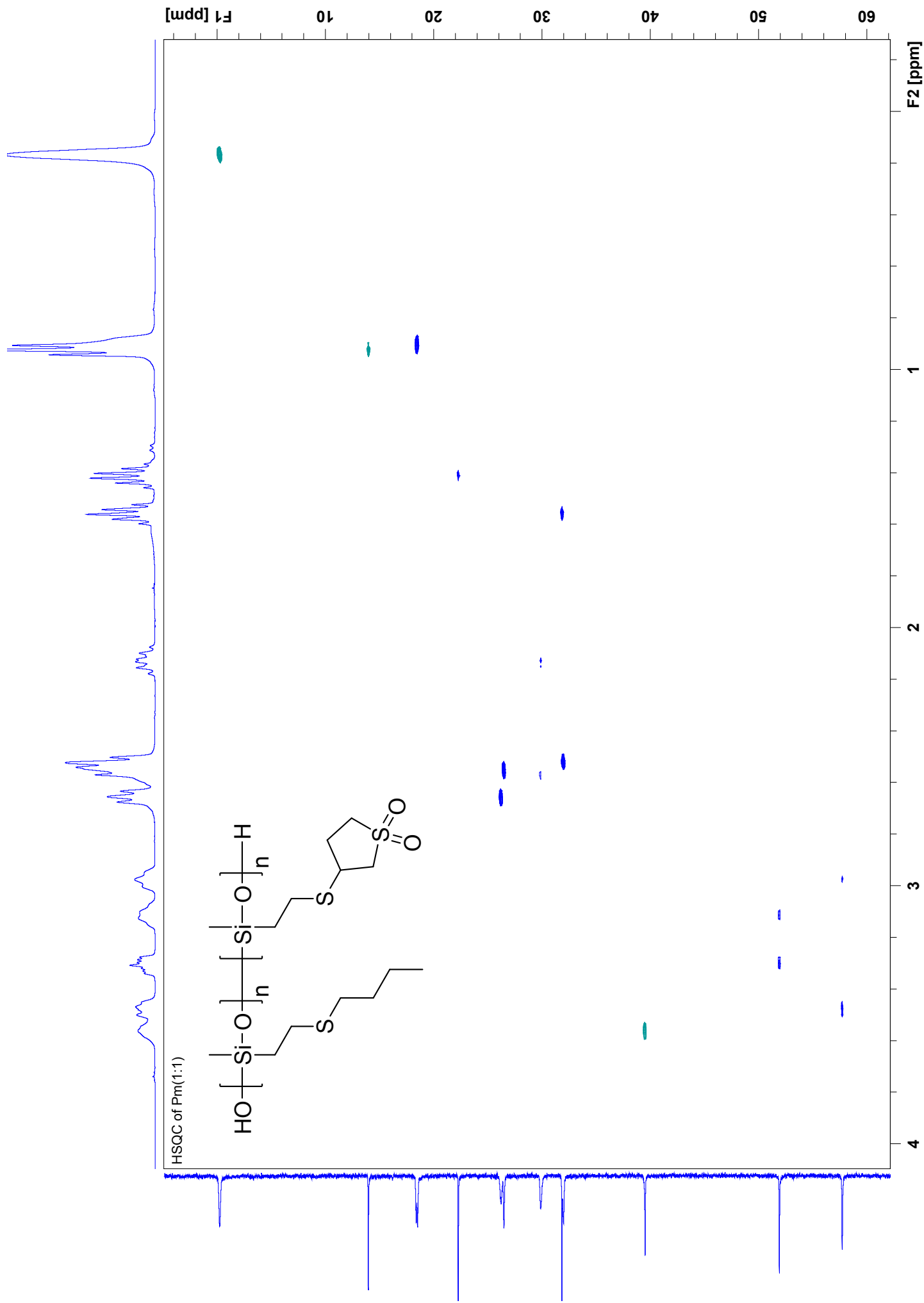
1) Heat from -120.00°C to 100.00°C at 20.00°C/min

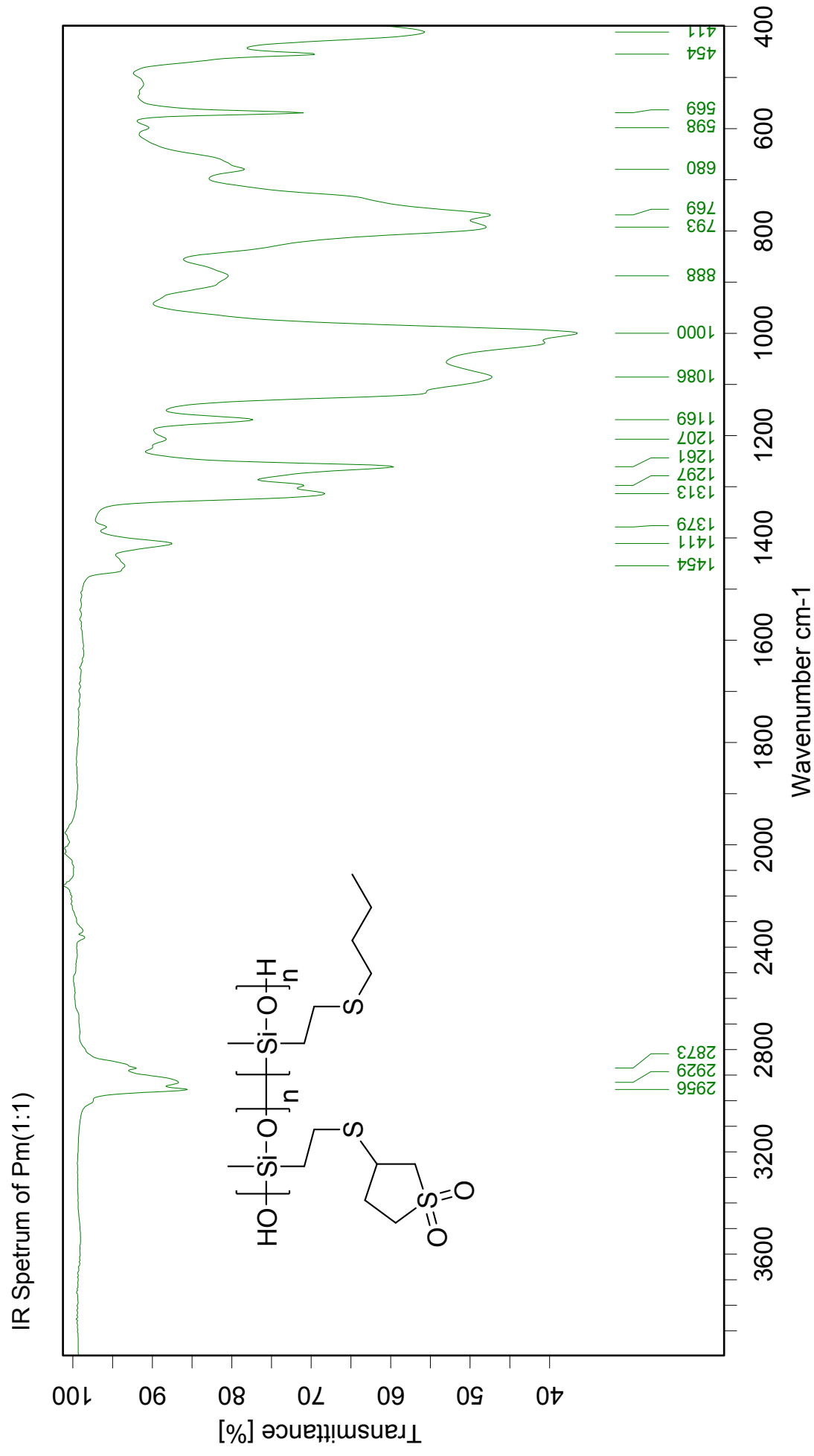
^1H NMR of Pm(1:1)



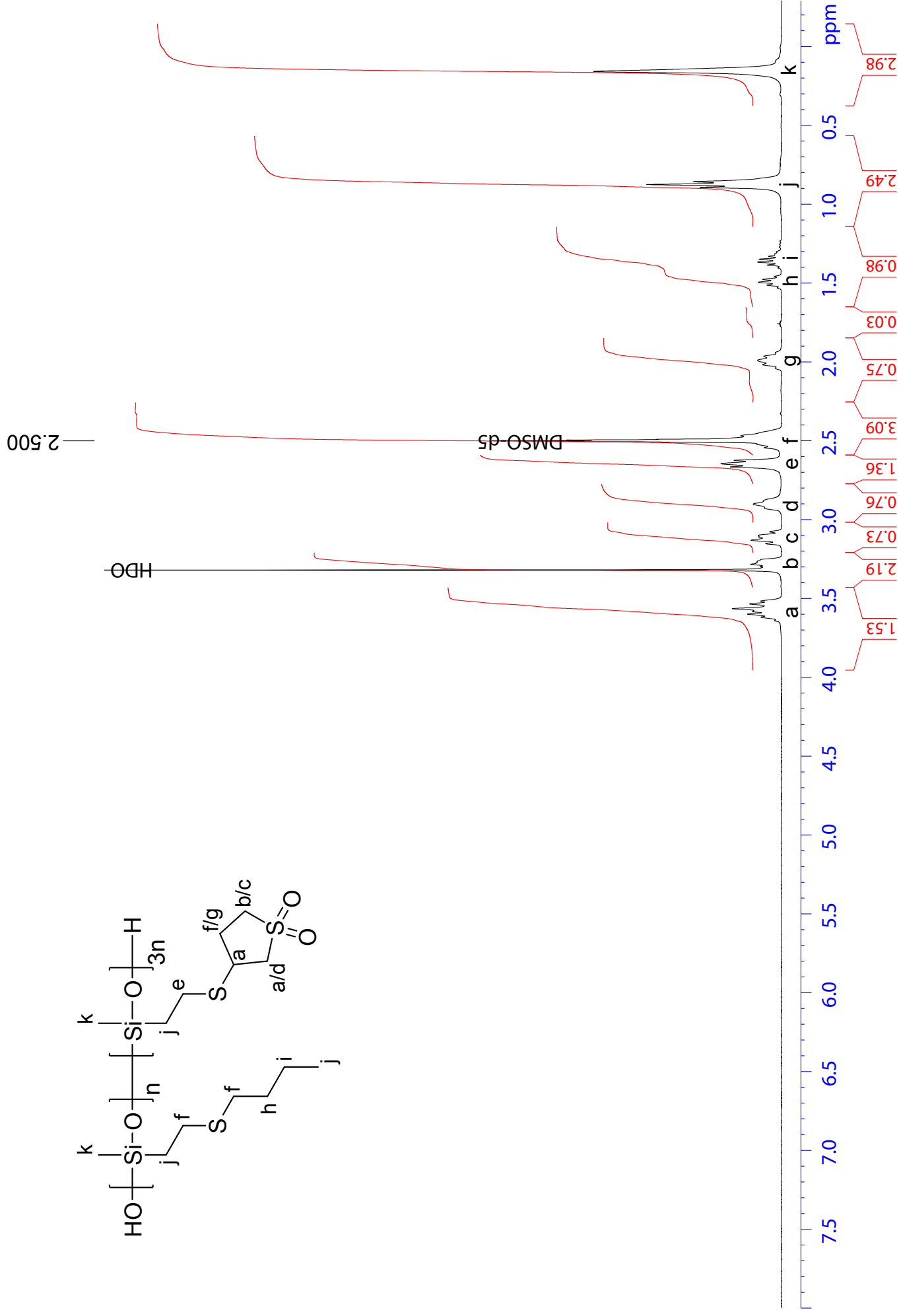
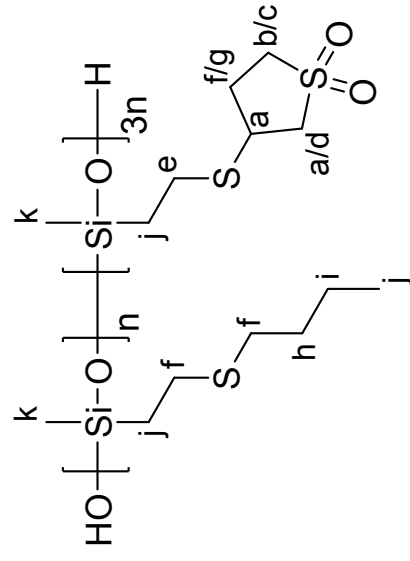
¹³C NMR of Pm(1:1)



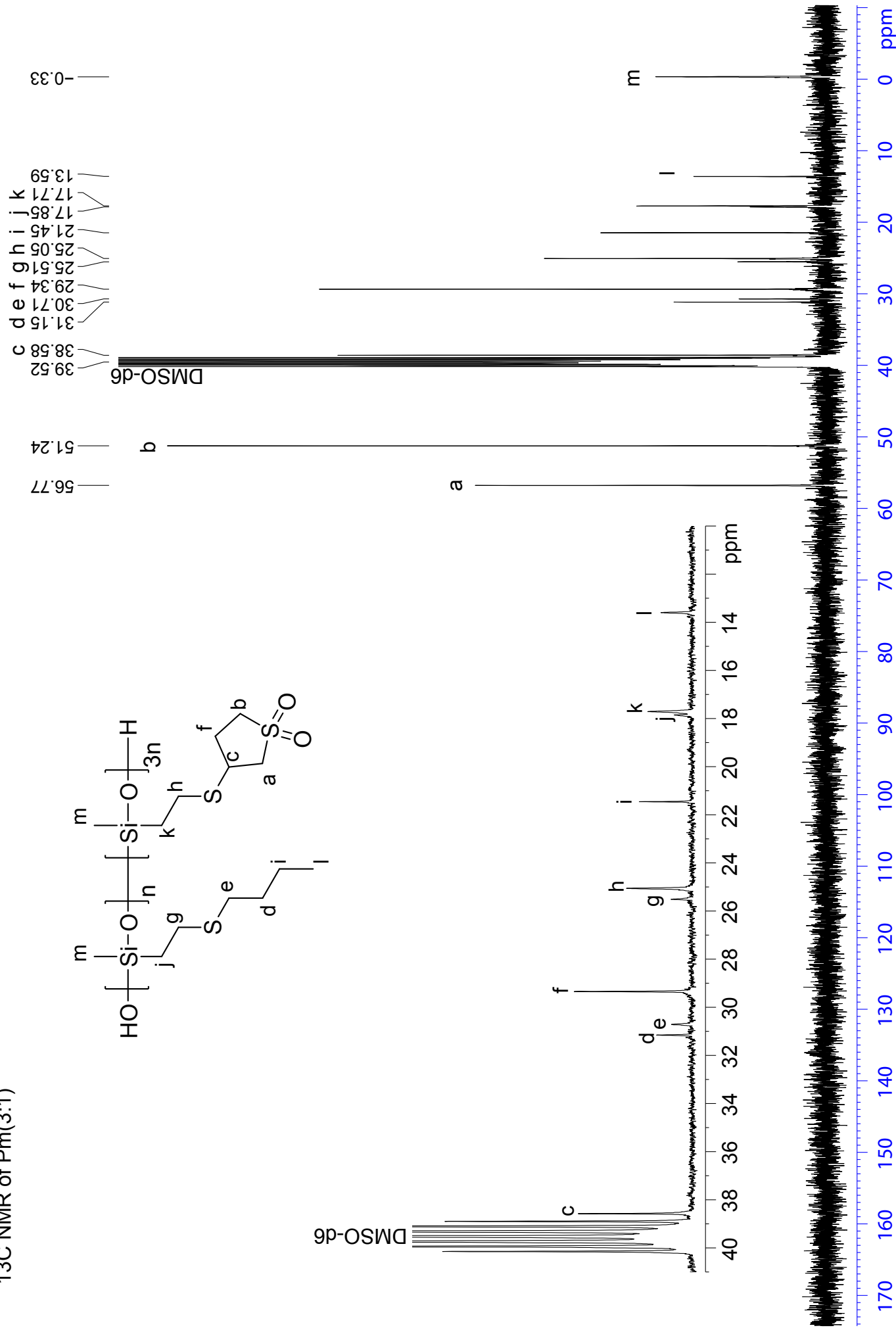


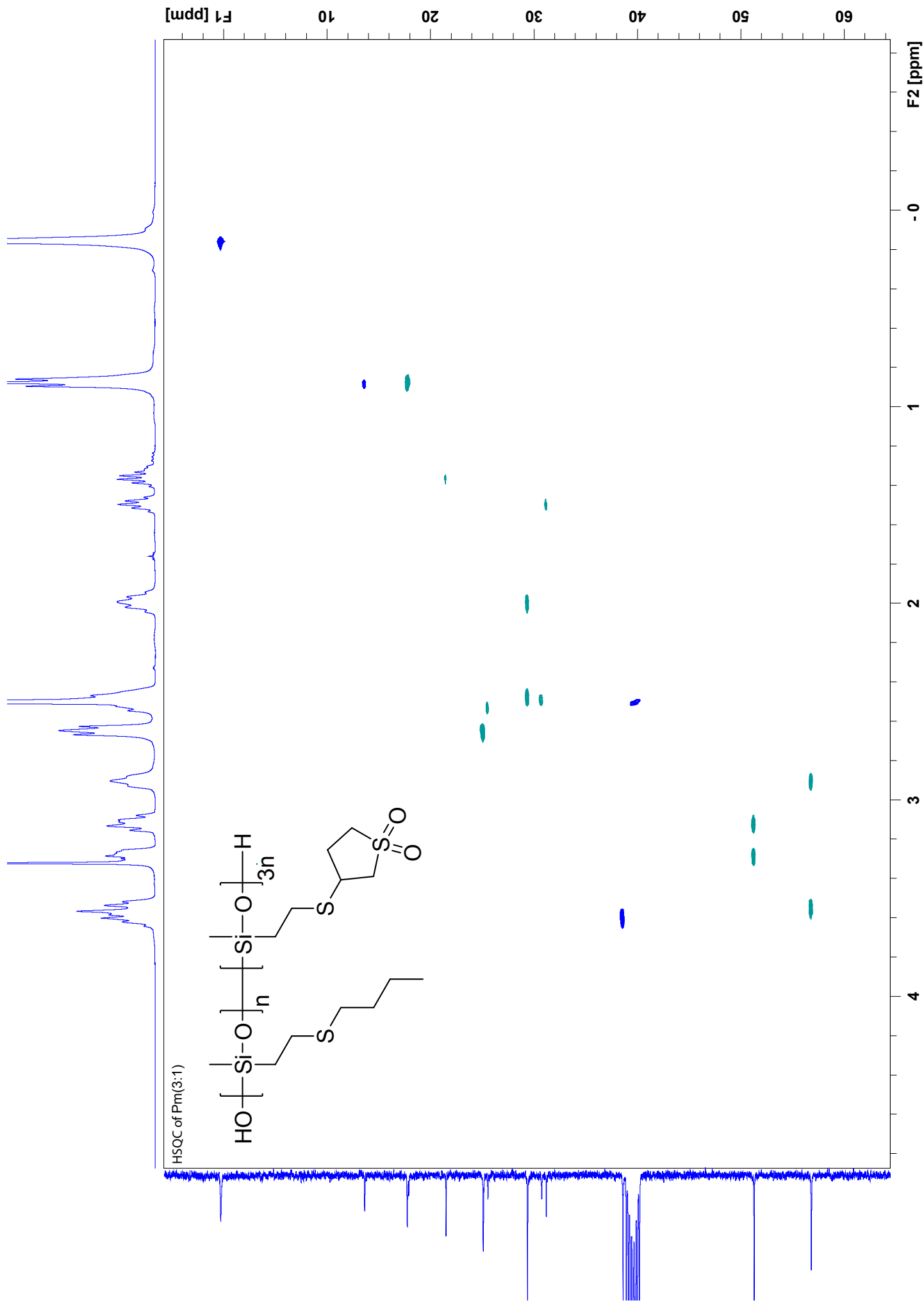


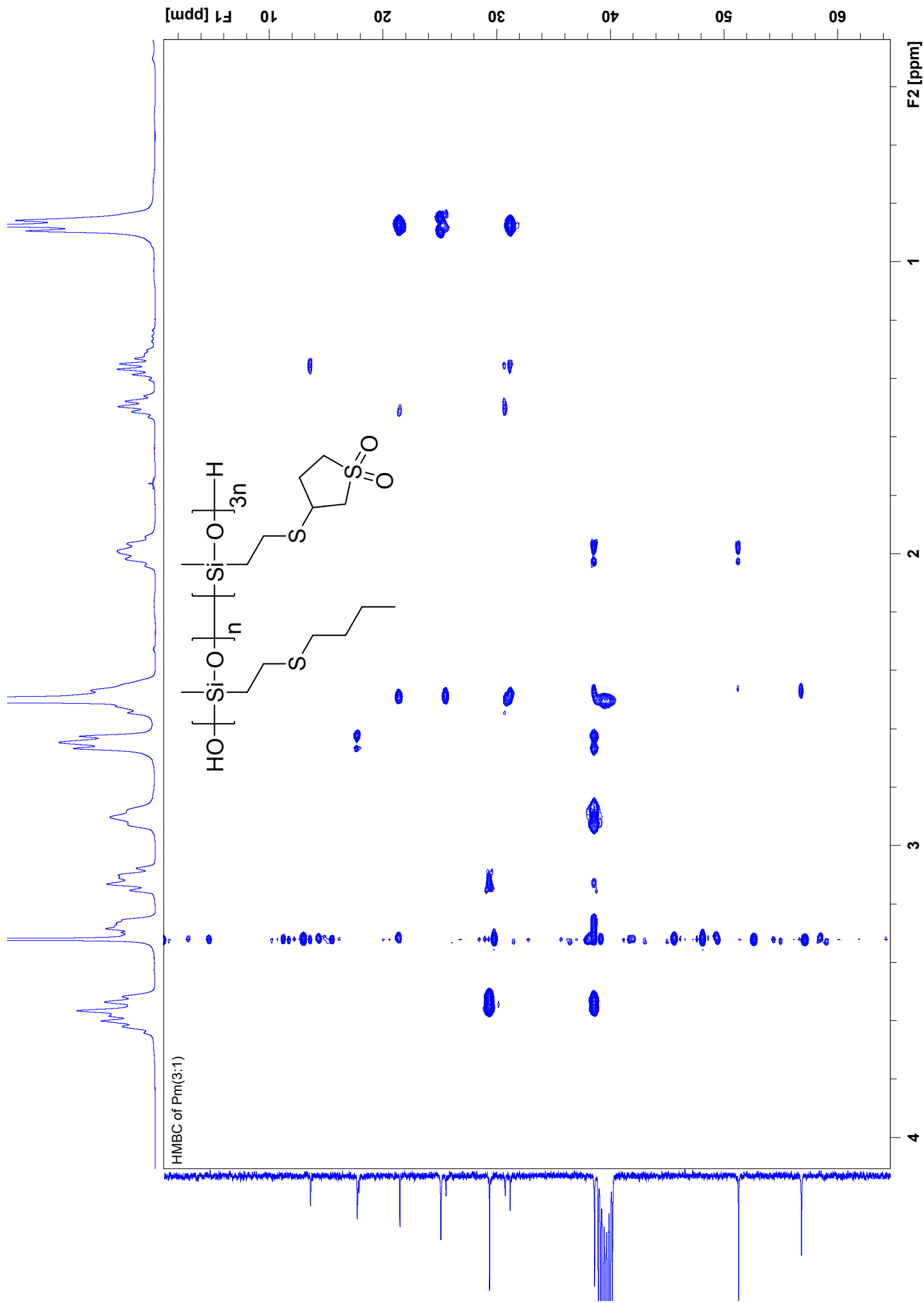
¹H NMR of Pm(3:1)

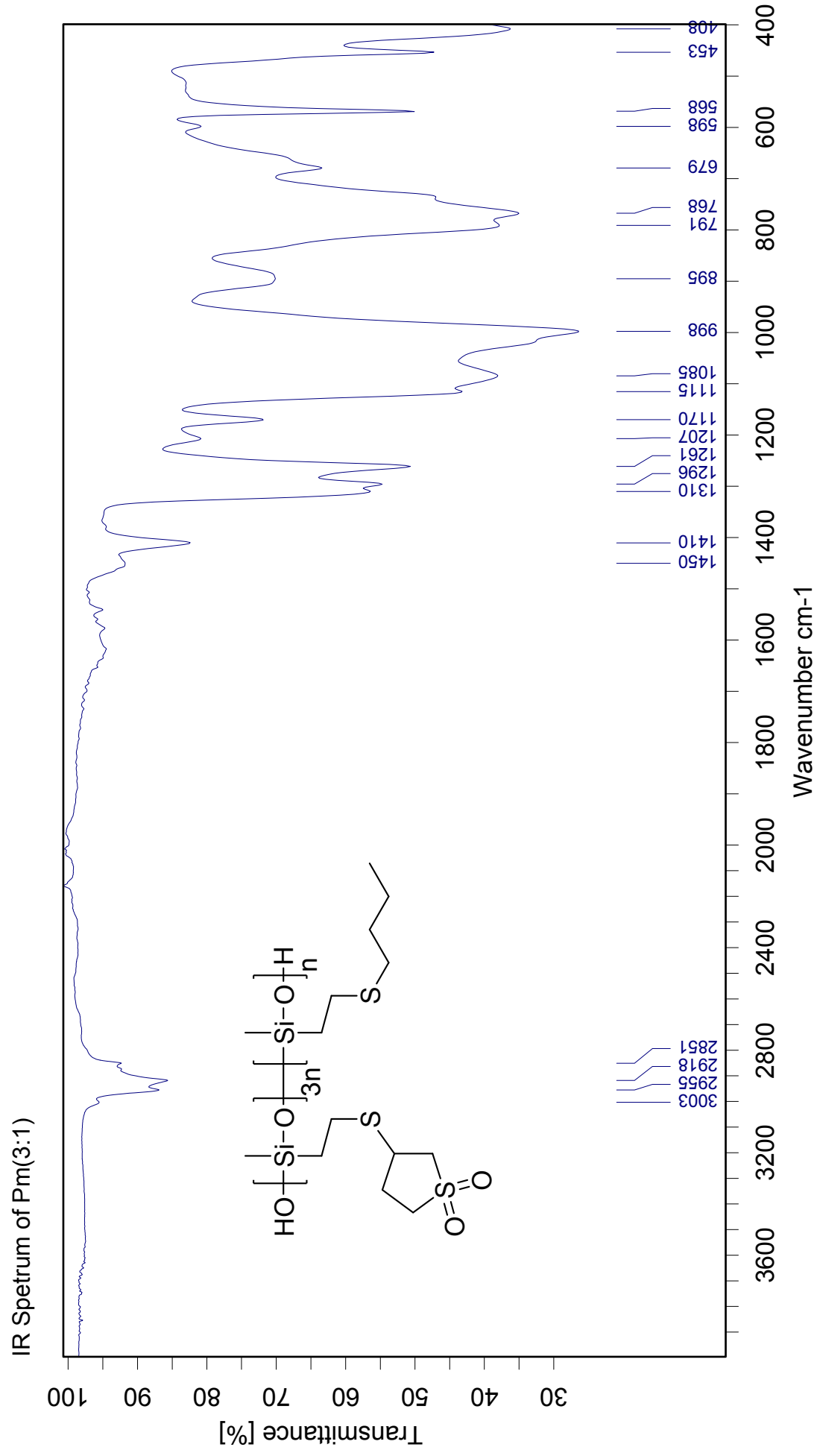


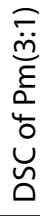
¹³C NMR of Pm(3:1)



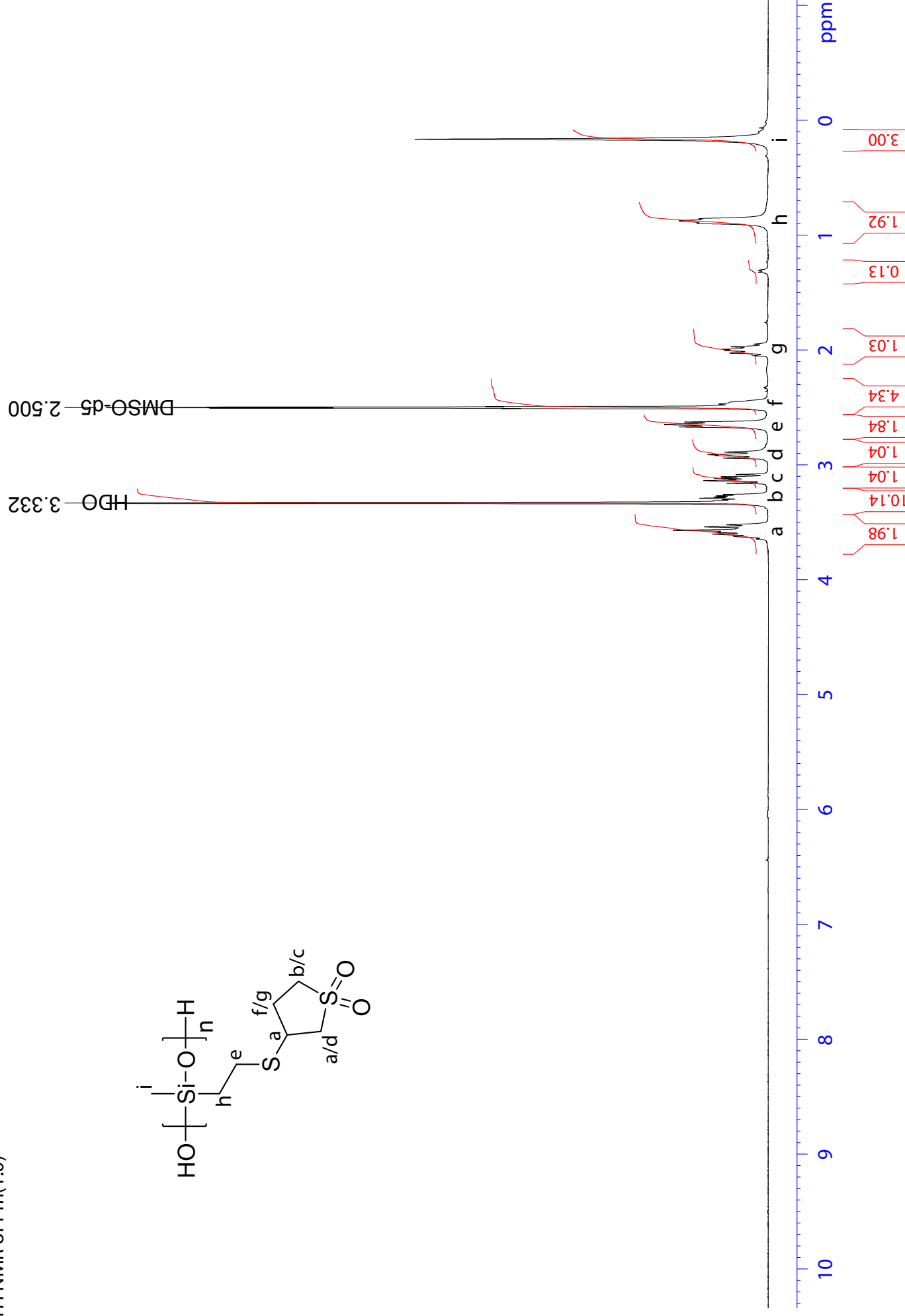
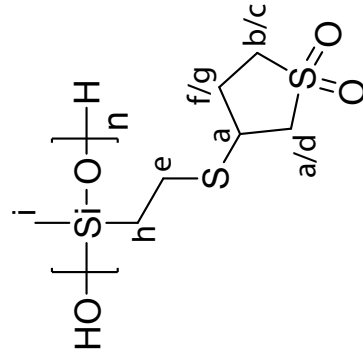




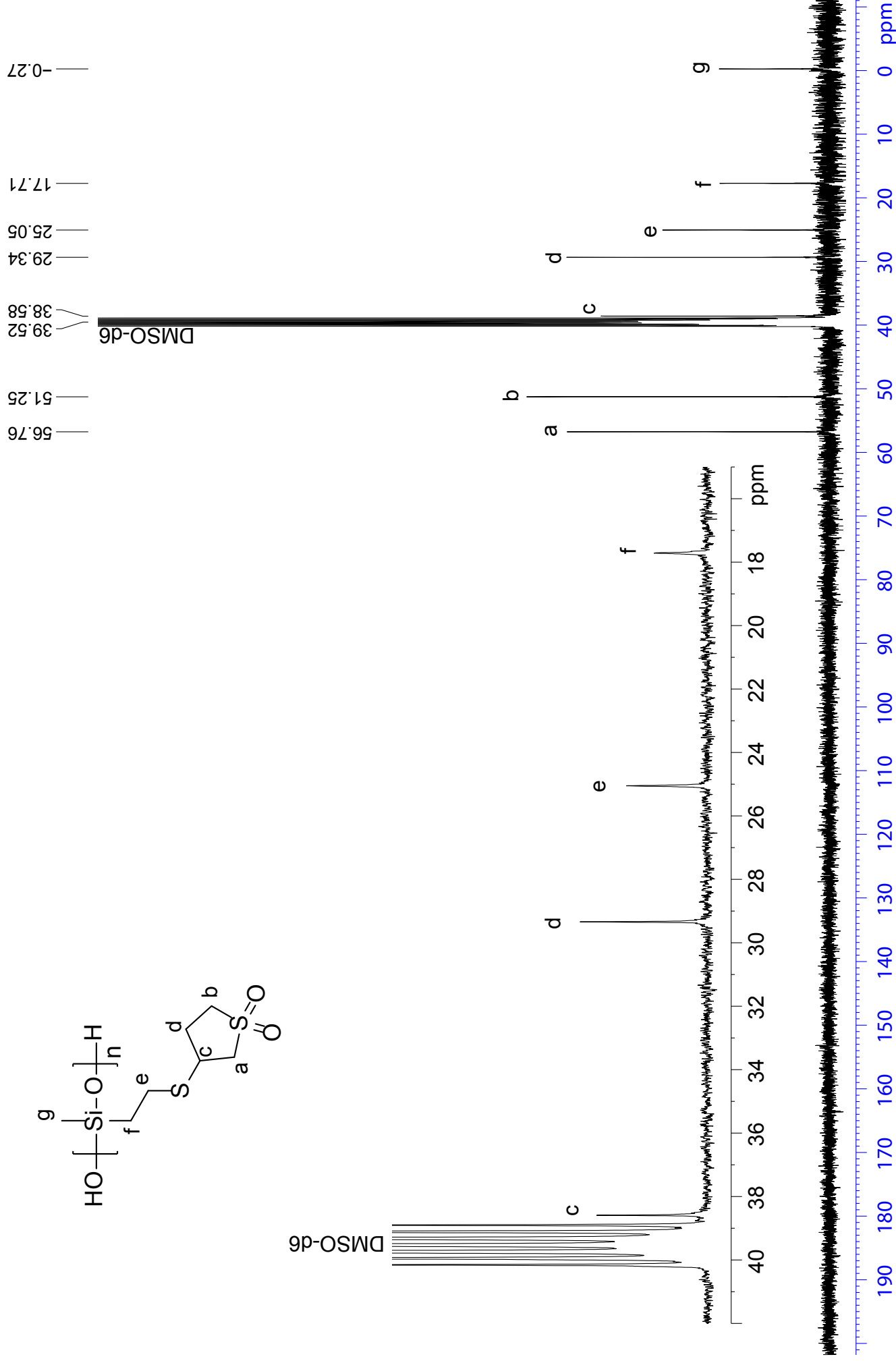
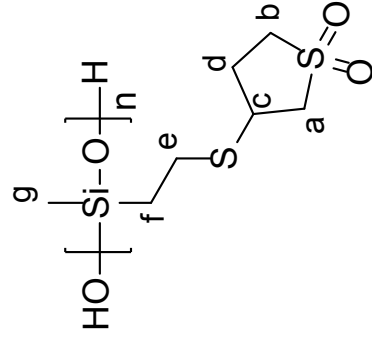


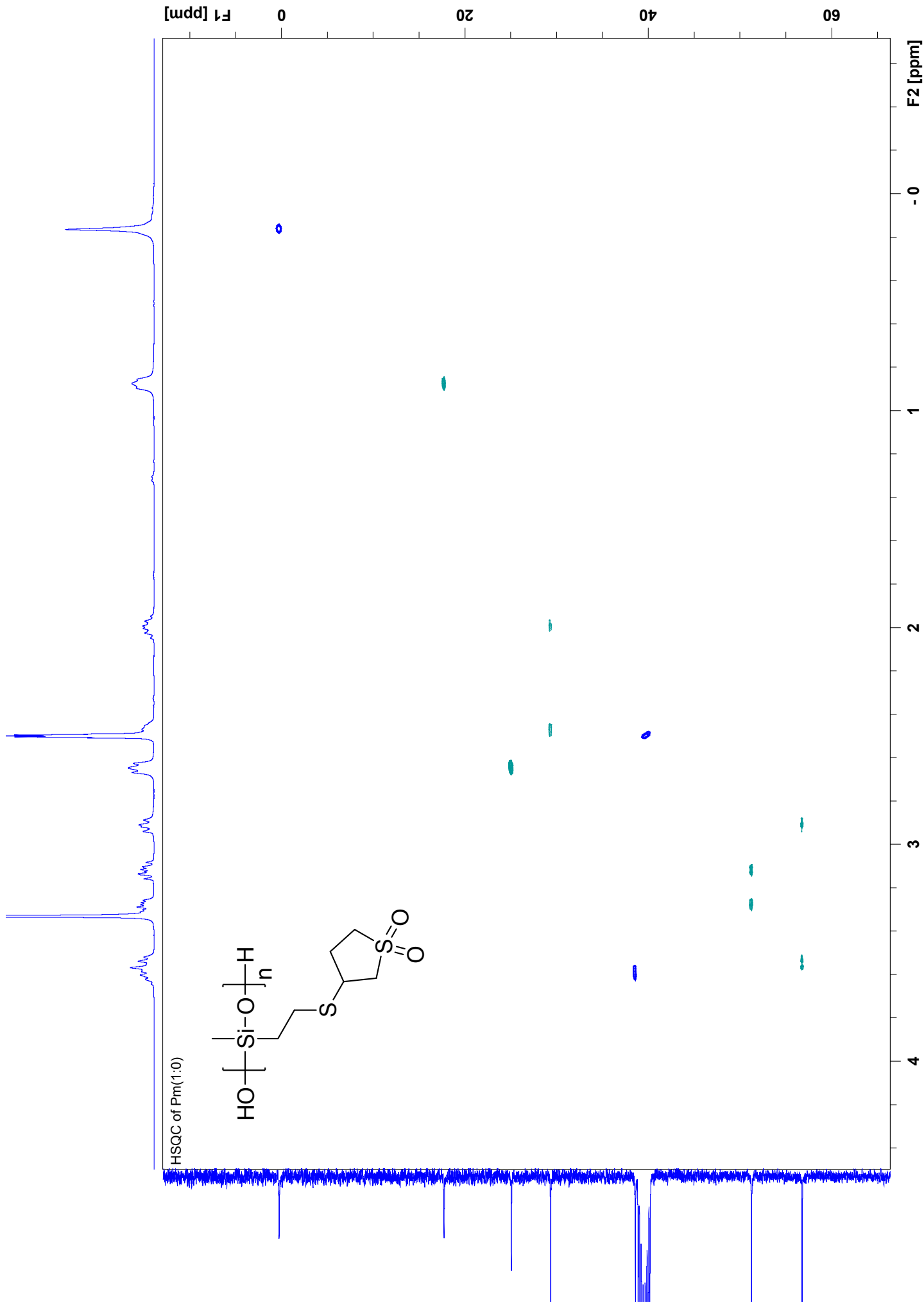


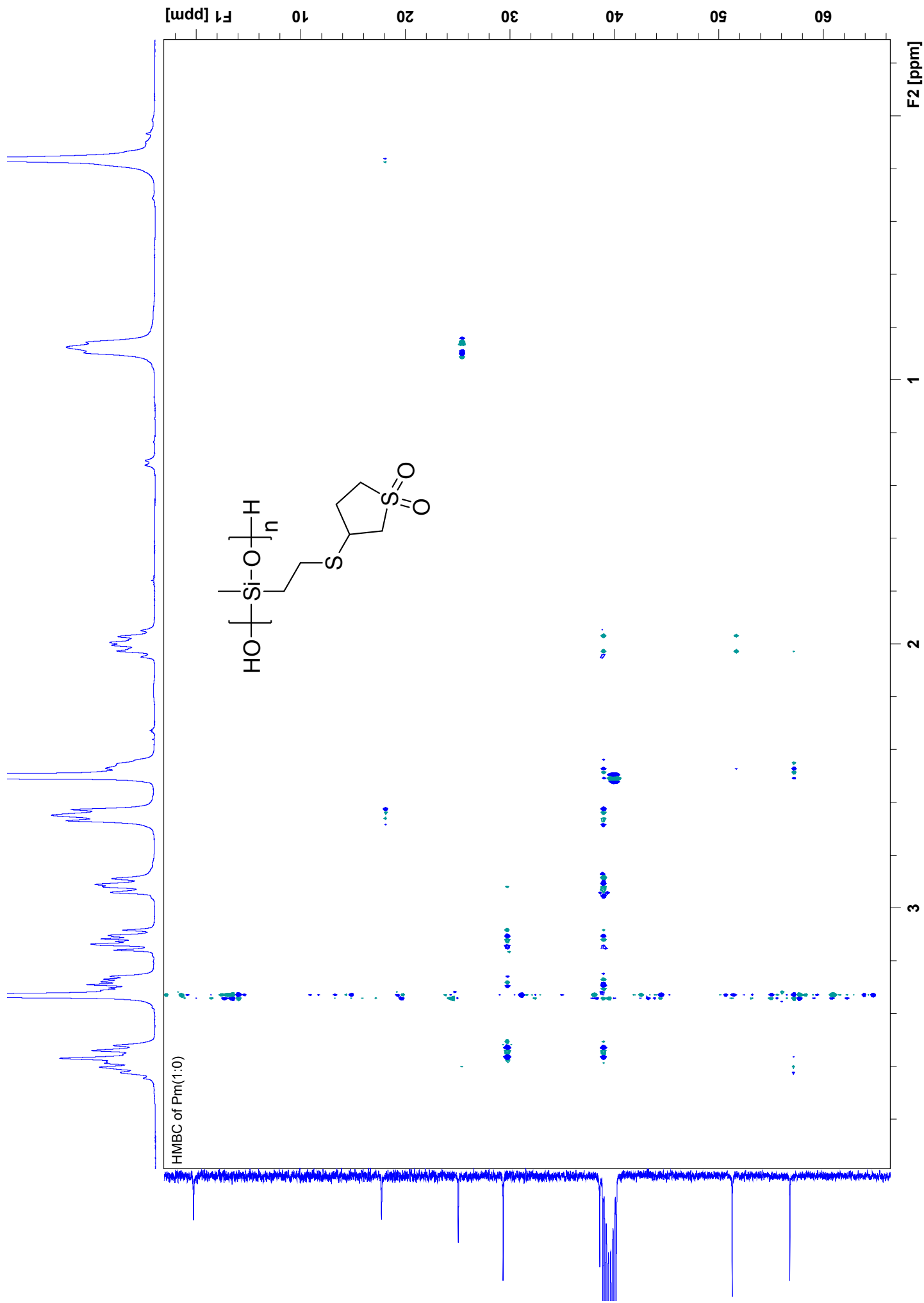
¹H NMR of Pm(1:0)



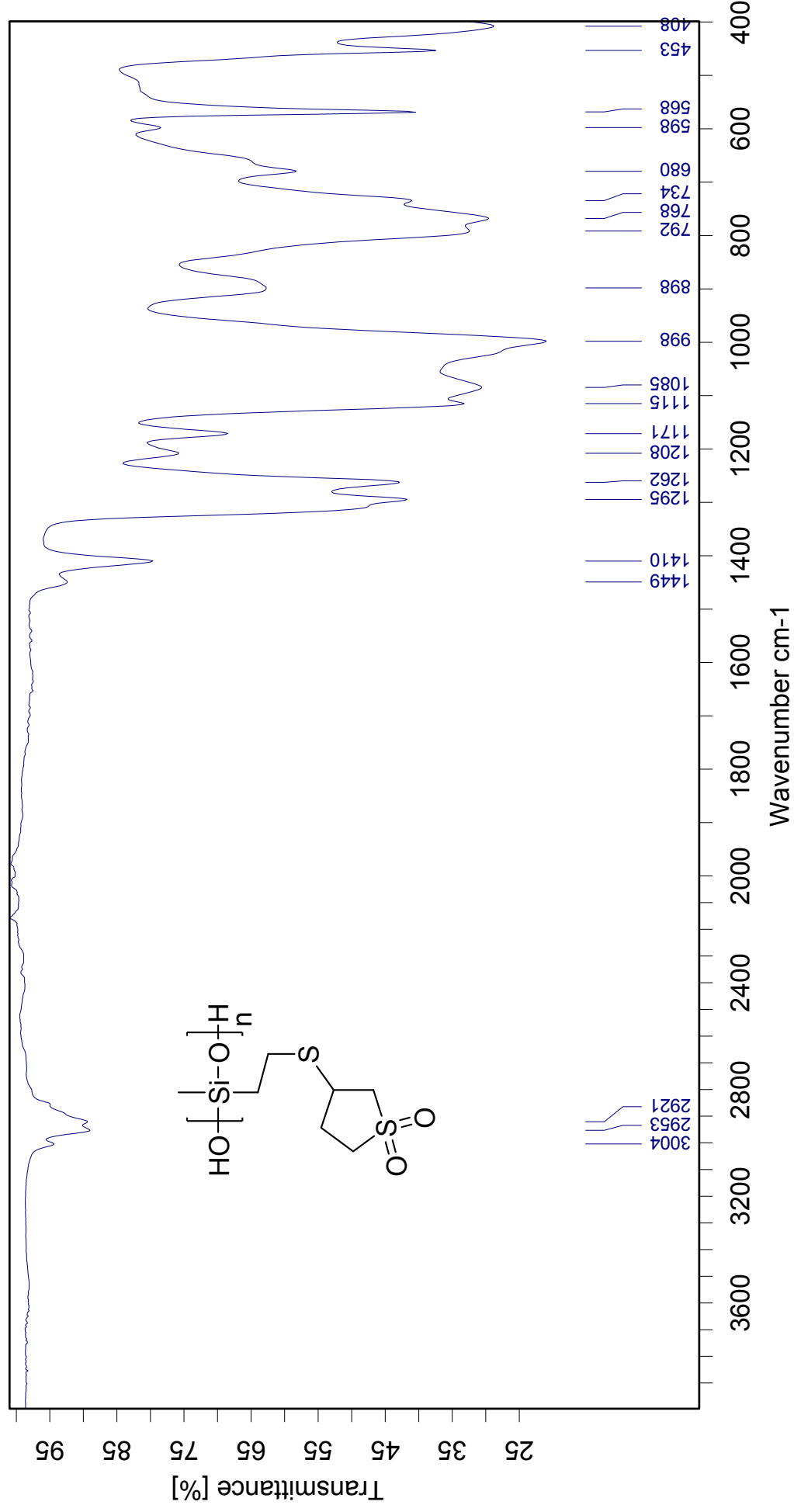
¹³C NMR of Pm(1:0)



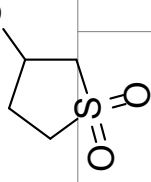
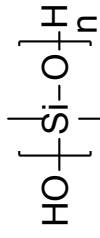




IR Spetrum of Pm(1:0)

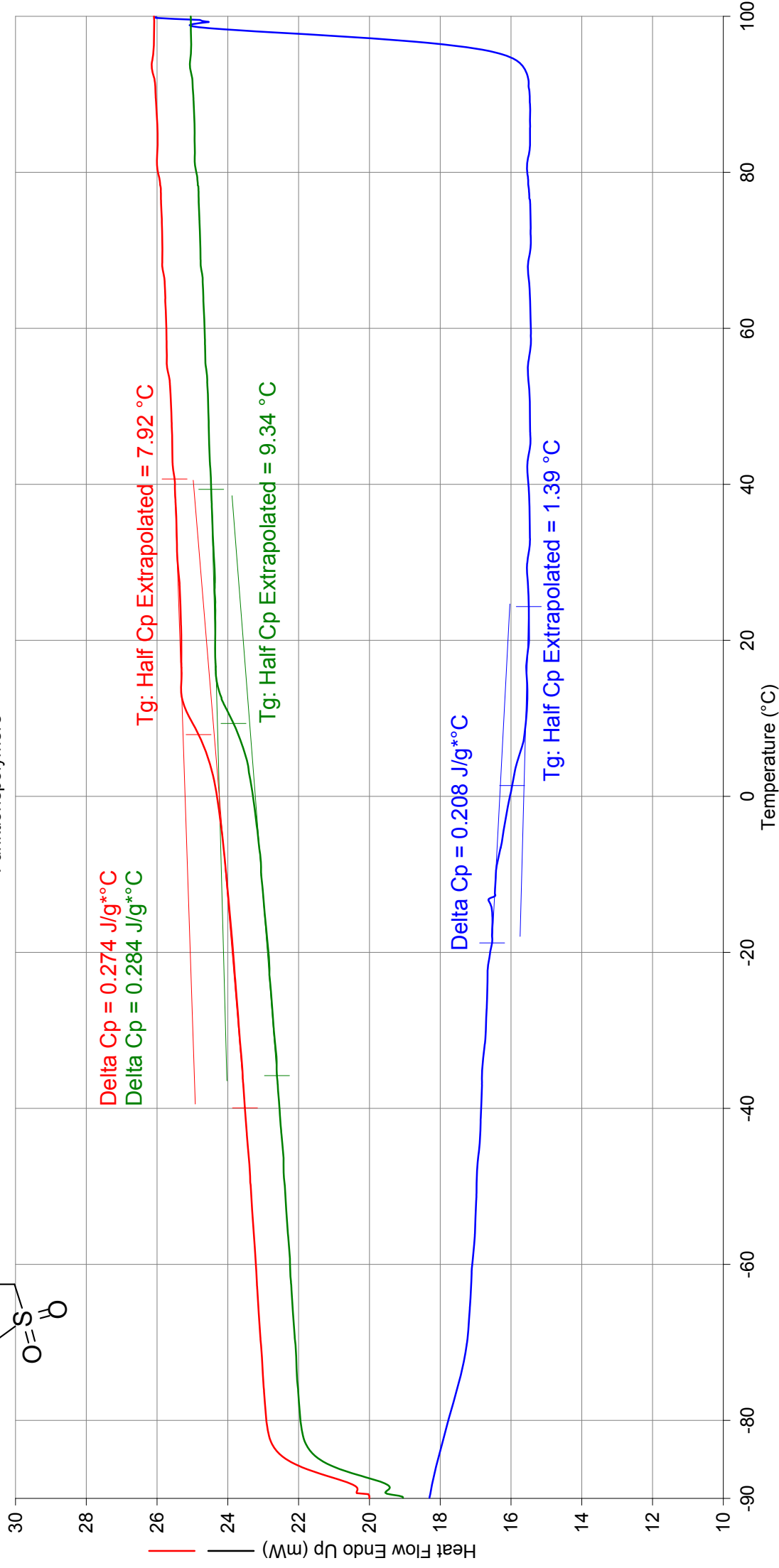


DSC of Pm(1:0)



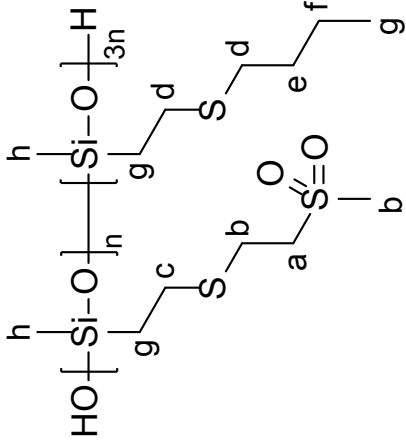
Funktionspolymere

- Heat Flow Endo Up (mW) : Step: 1
- Heat Flow Endo Up (mW) : Step: 2
- Heat Flow Endo Up (mW) : Step: 4

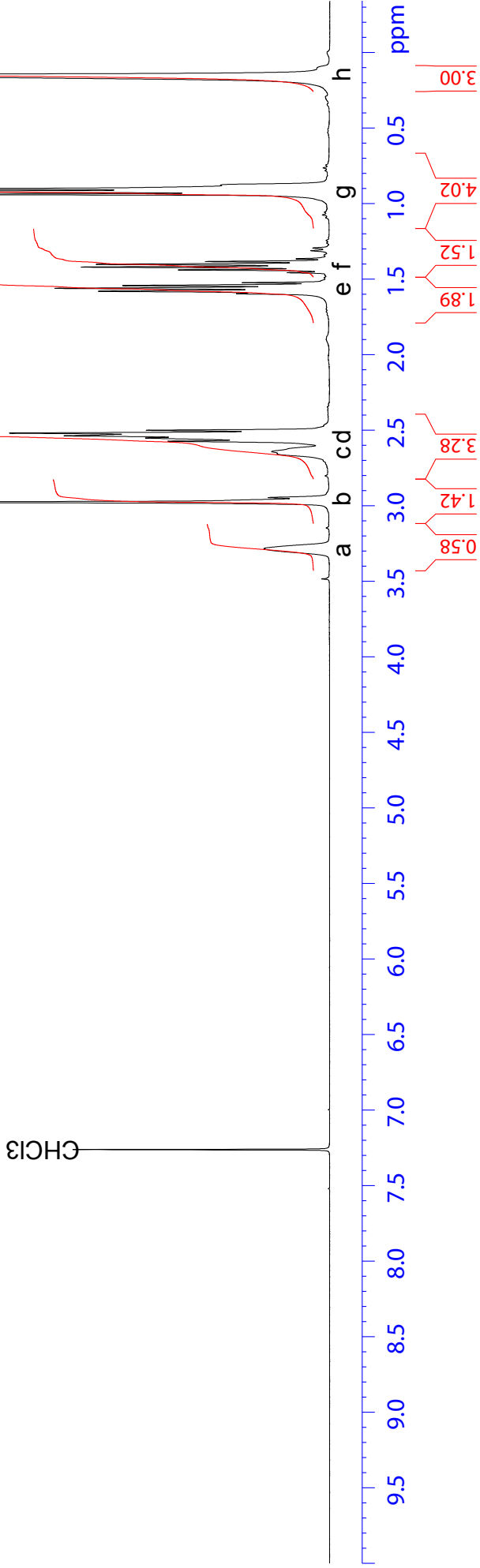


- Heat from -90.00°C to 100.00°C at 20.00°C/min
- Cool from 100.00°C to -90.00°C at 20.00°C/min

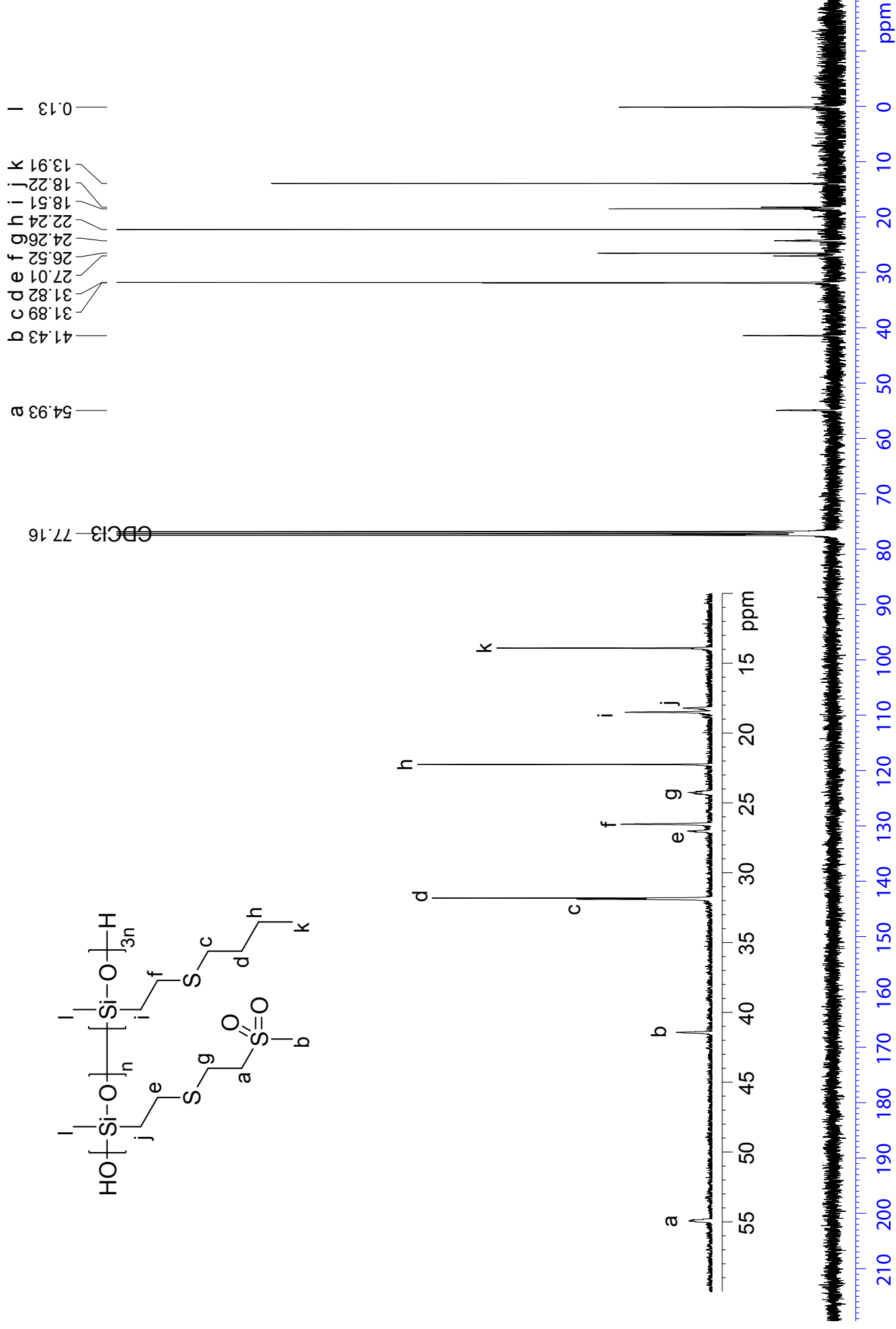
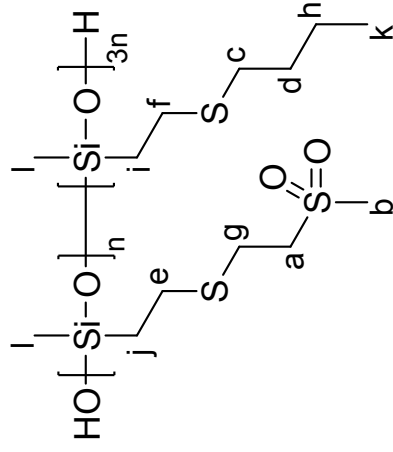
- Hold for 5.0 min at -90.00°C
- Heat from -90.00°C to 100.00°C at 20.00°C/min

¹H NMR of Pn(1:3)

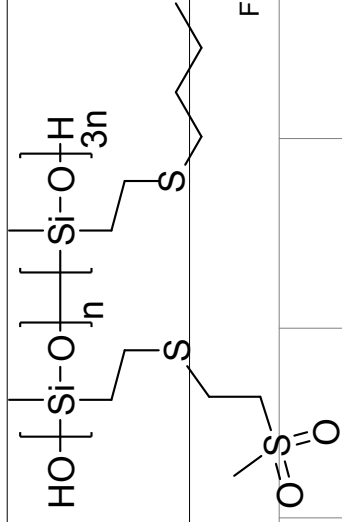
—7.260



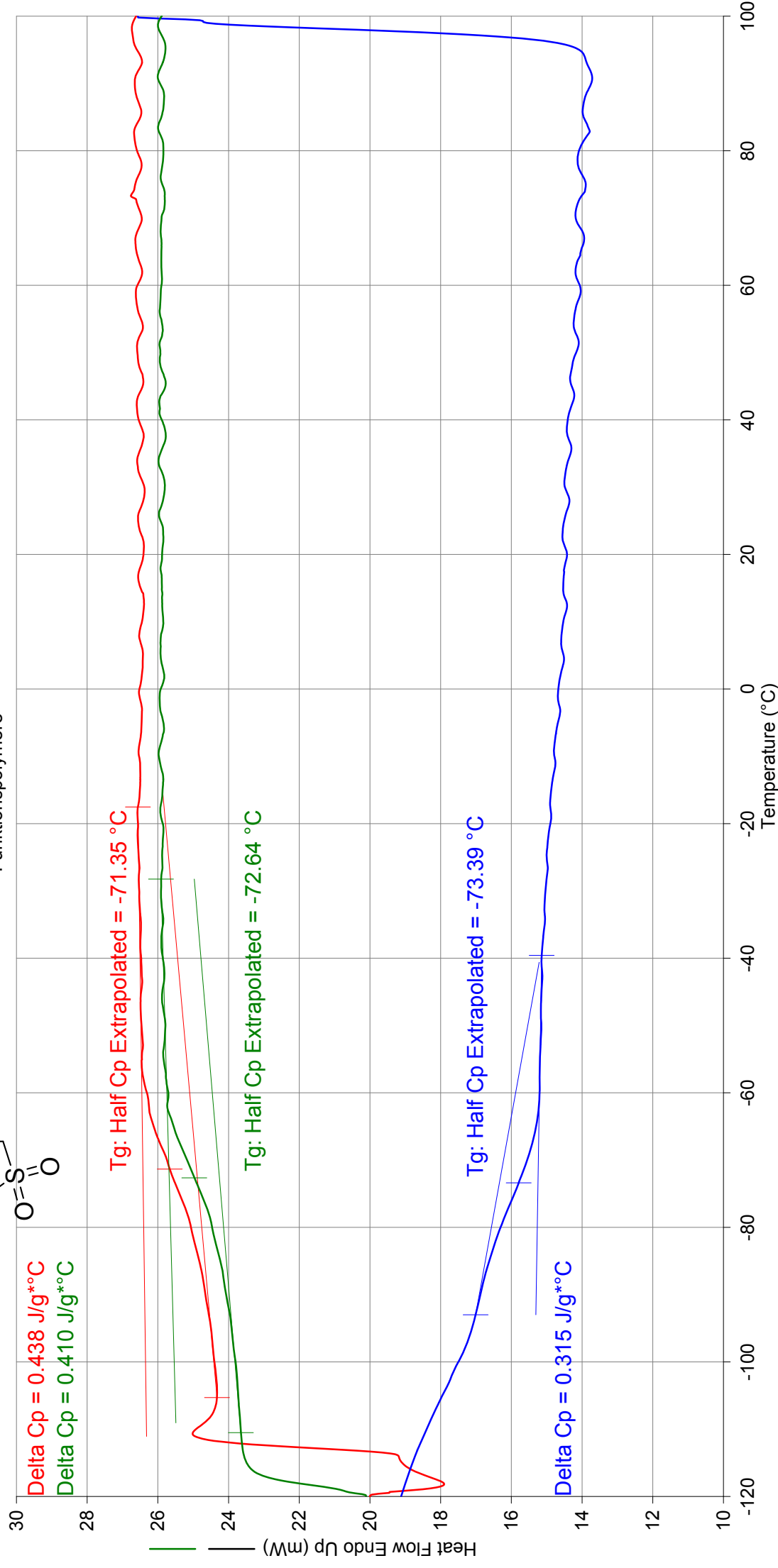
¹³C NMR of Pn(1:3)



DSC of Pn(1:3)

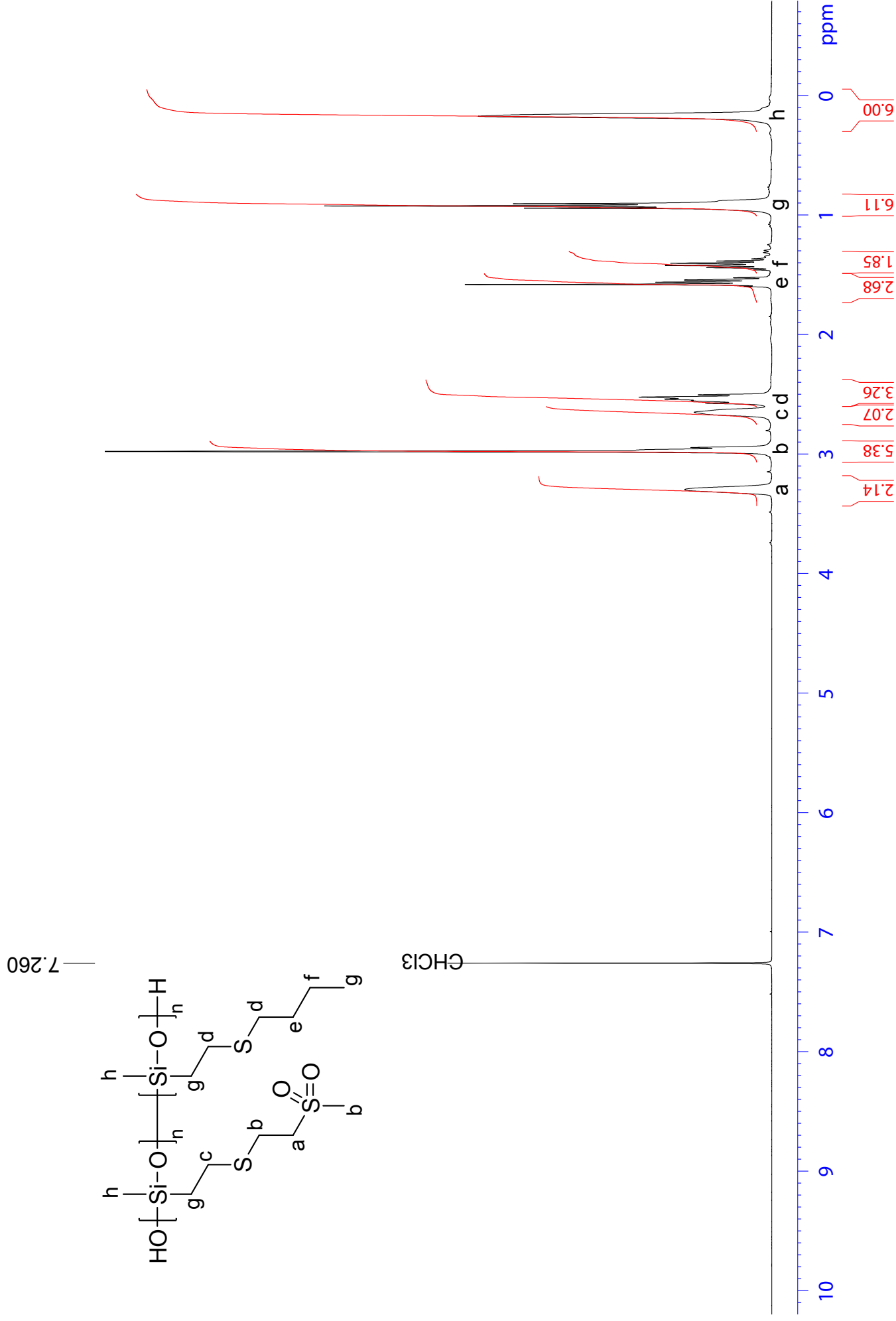


Funktionspolymere

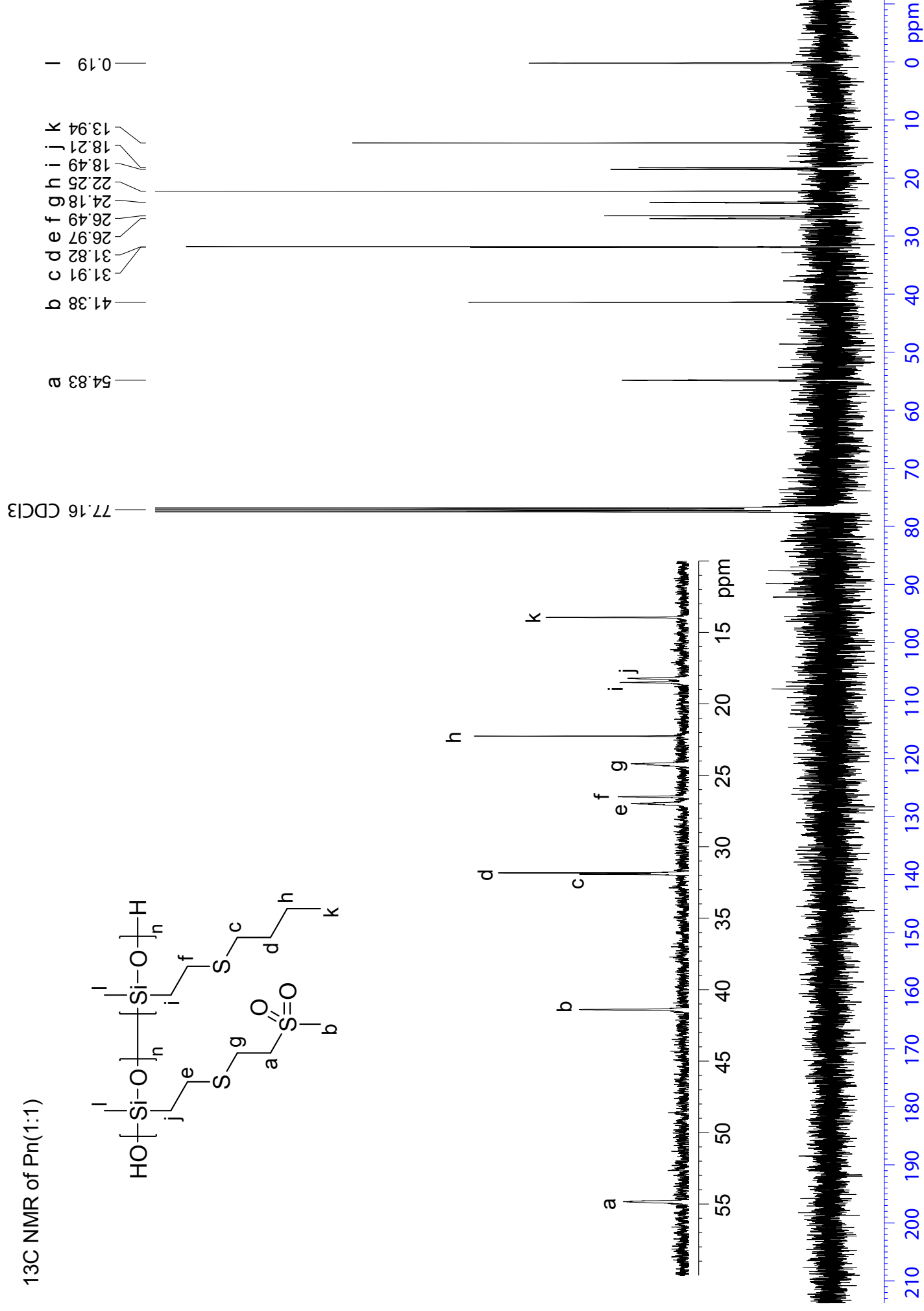
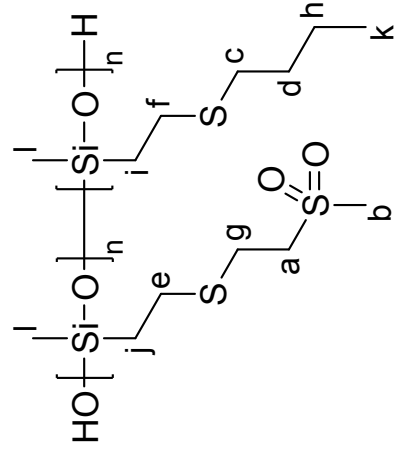


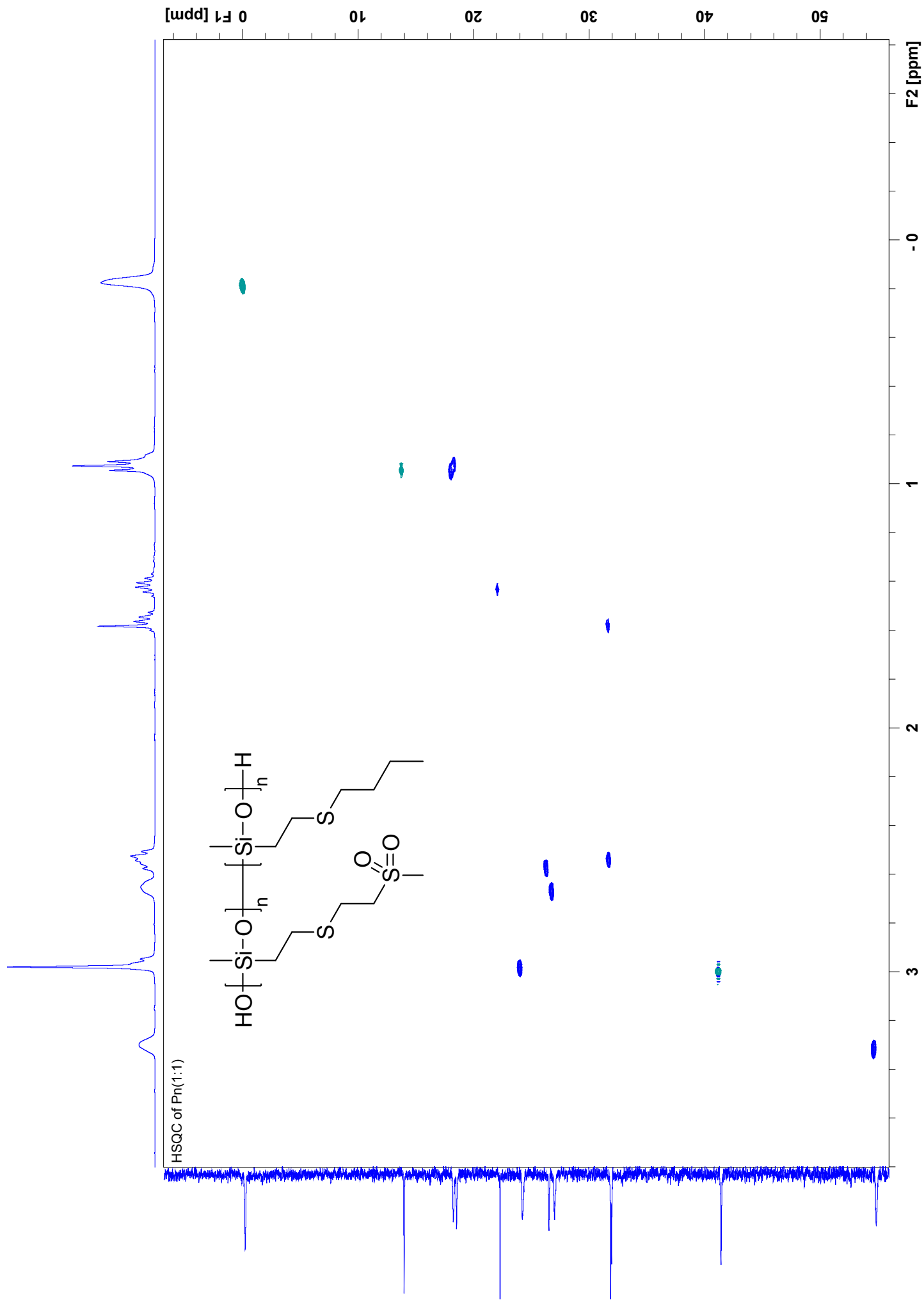
- | | |
|----|--|
| 1) | Heat from -120.00°C to 100.00°C at 20.00°C/min |
| 2) | Cool from 100.00°C to -120.00°C at 20.00°C/min |
| 3) | Hold for 5.0 min at -120.00°C |
| 4) | Heat from -120.00°C to 100.00°C at 20.00°C/min |

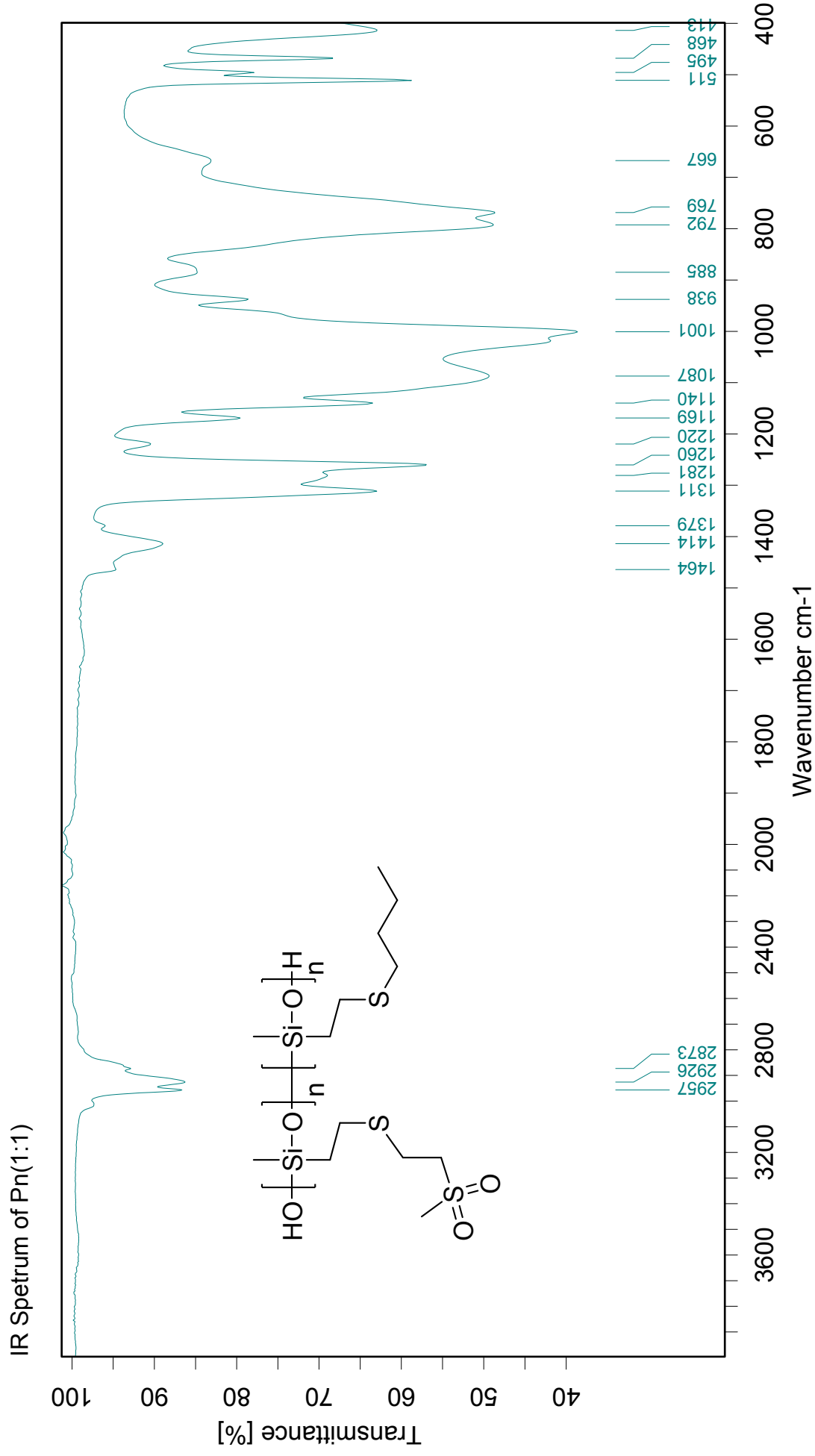
¹H NMR of Pn(1:1)



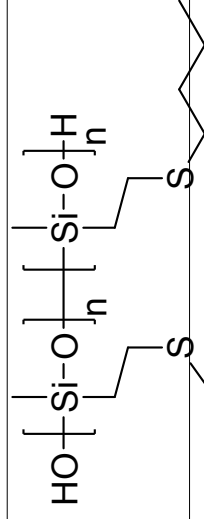
¹³C NMR of Pn(1:1)



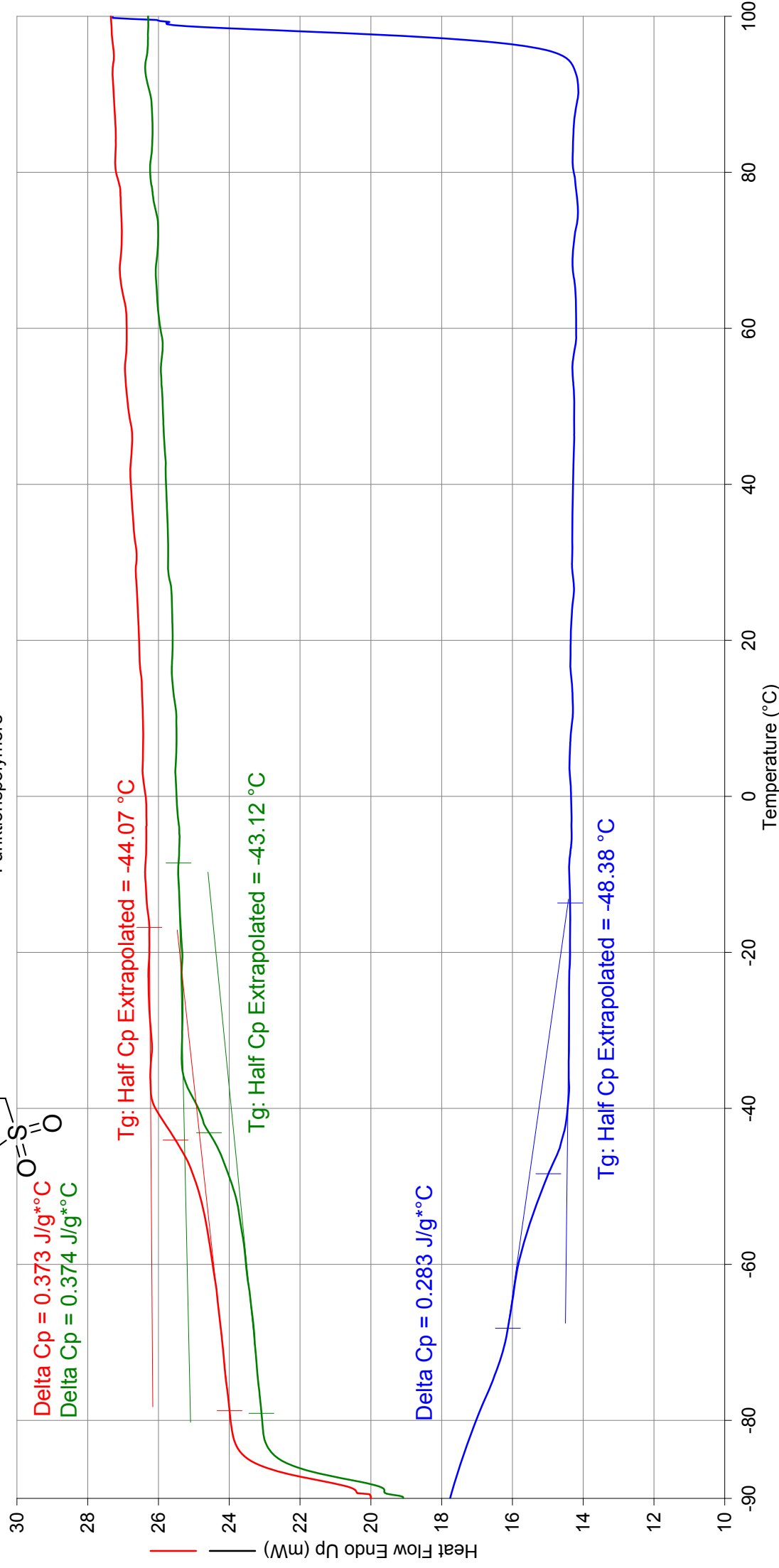




DSC of Pn(1:1)



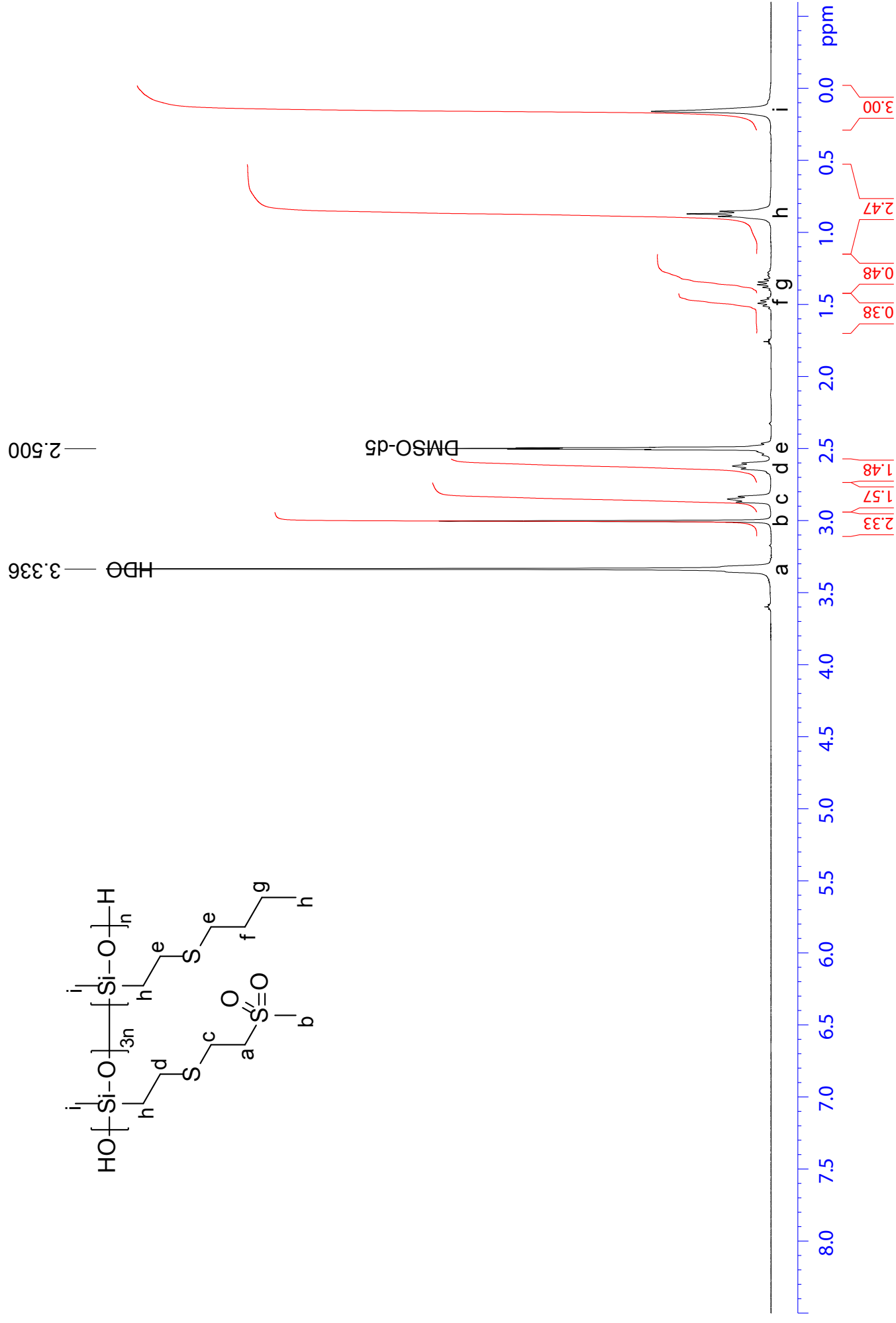
Funktionspolymere



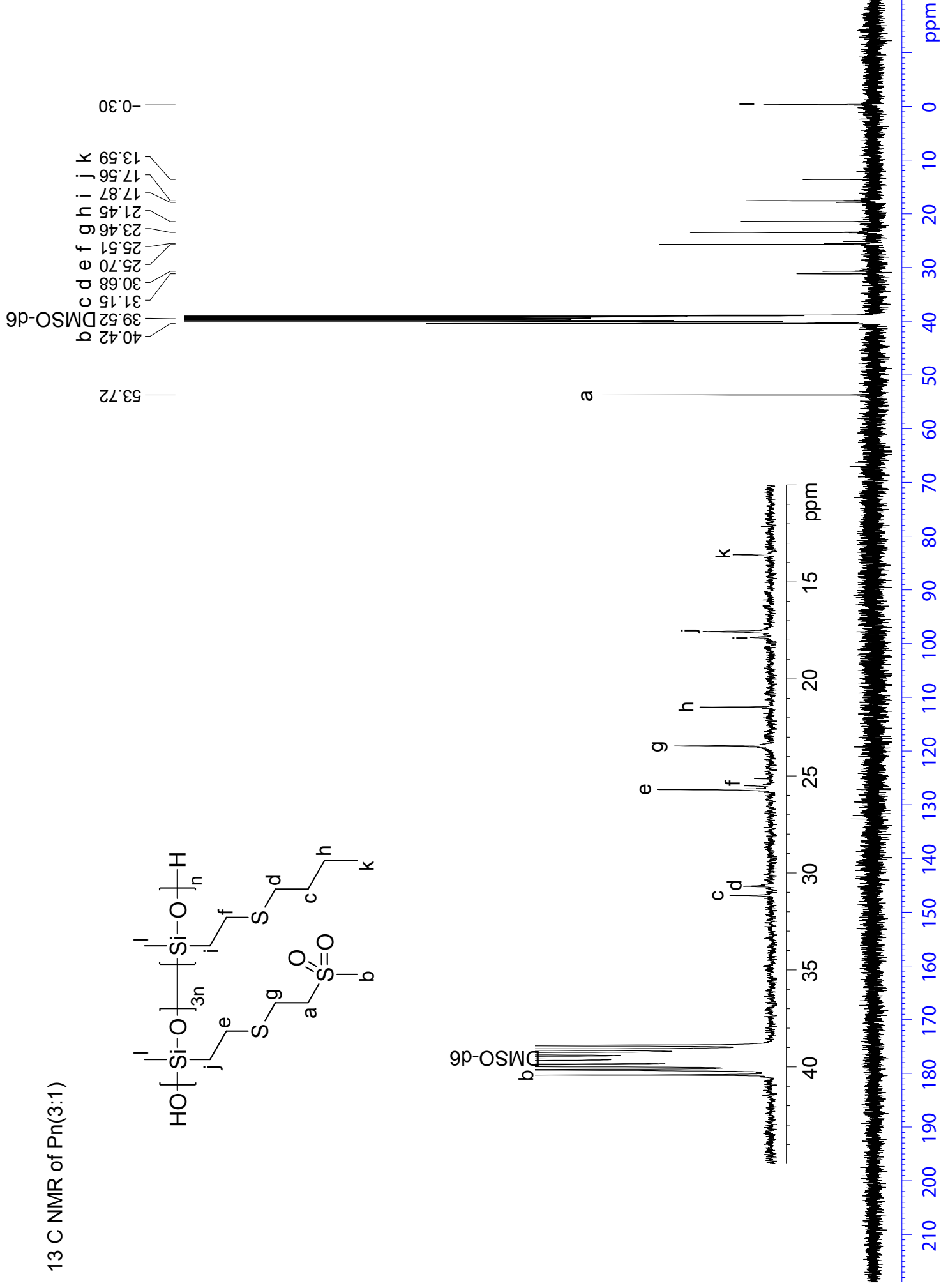
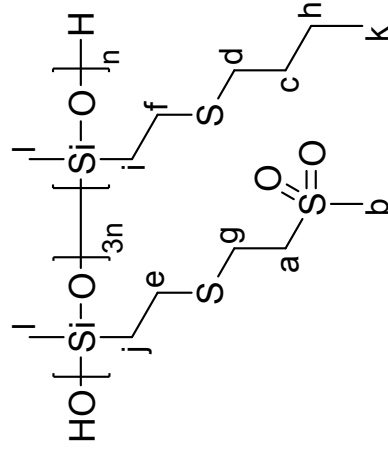
1) Heat from -90.00°C to 100.00°C at 20.00°C/min

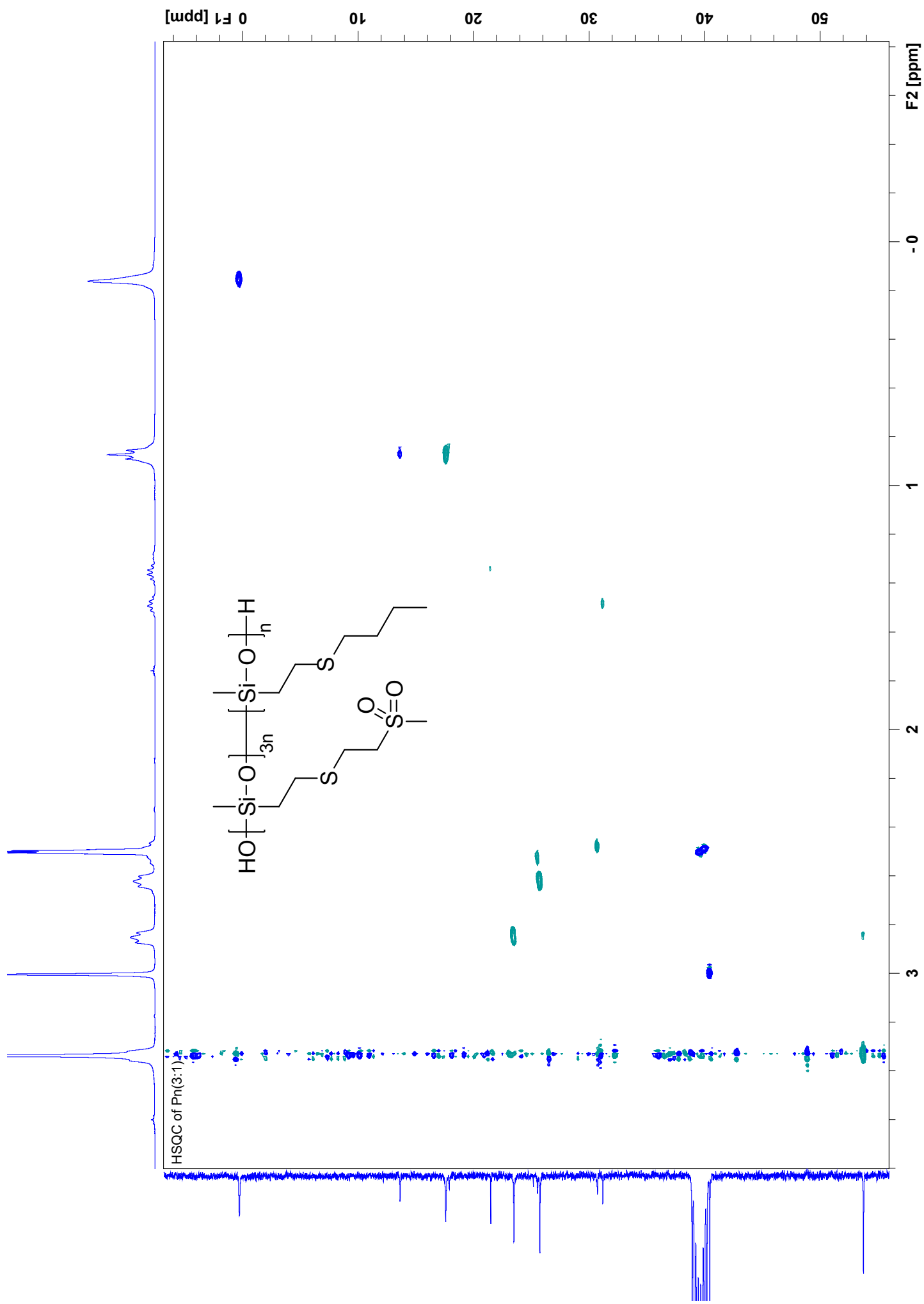
3)	Hold for 5.0 min at -90.00°C
4)	Heat from -90.00°C to 100.00°C at 20.00°C/min

¹H NMR of Pn(3:1)

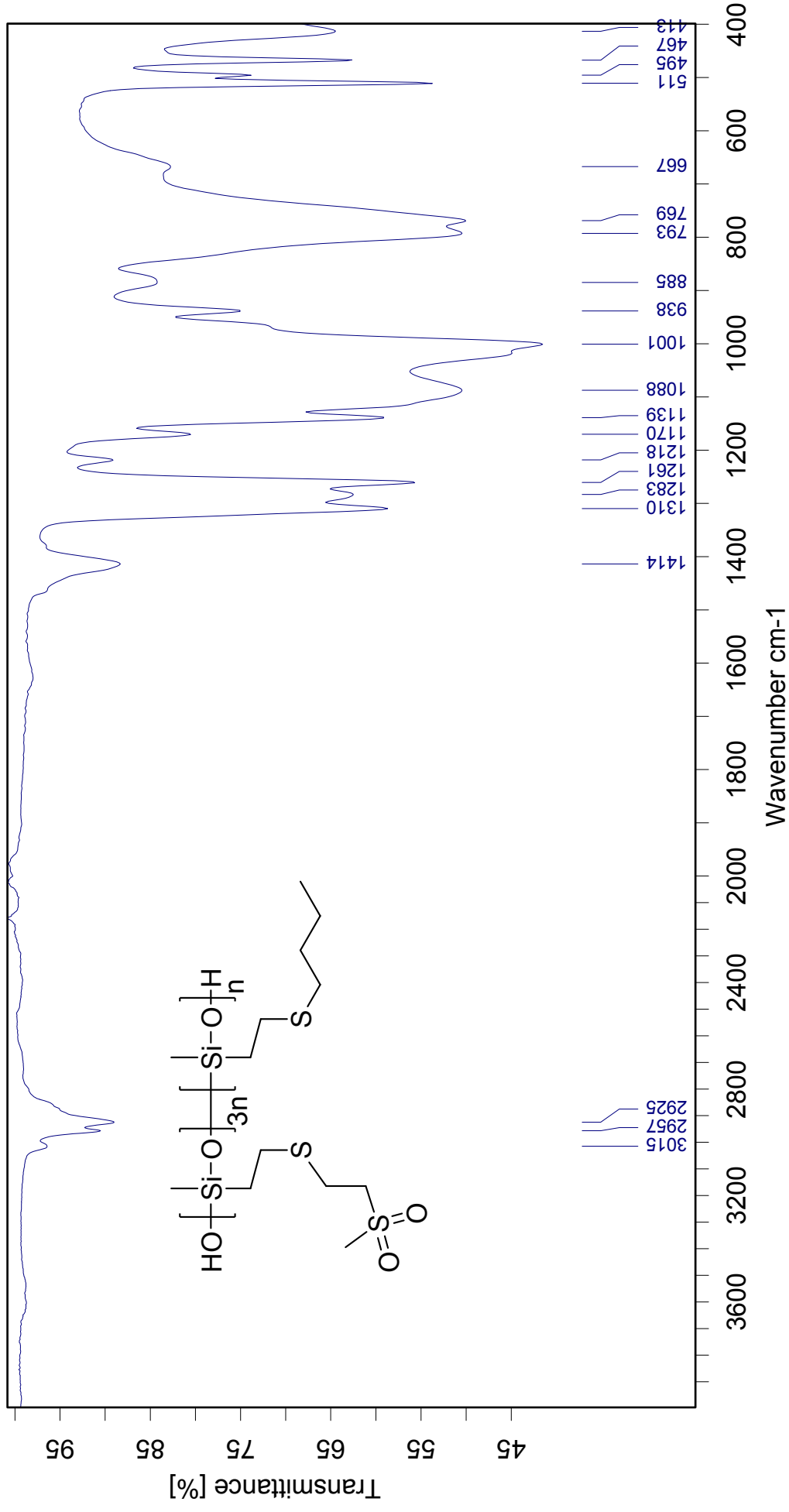


¹³C NMR of Pn(3:1)

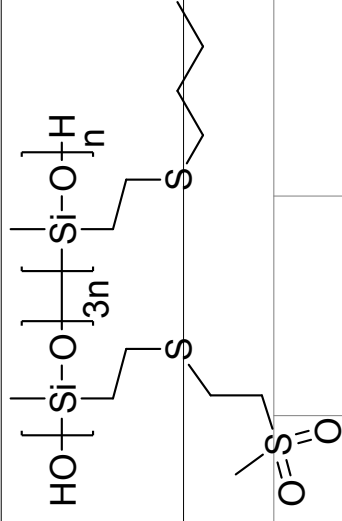




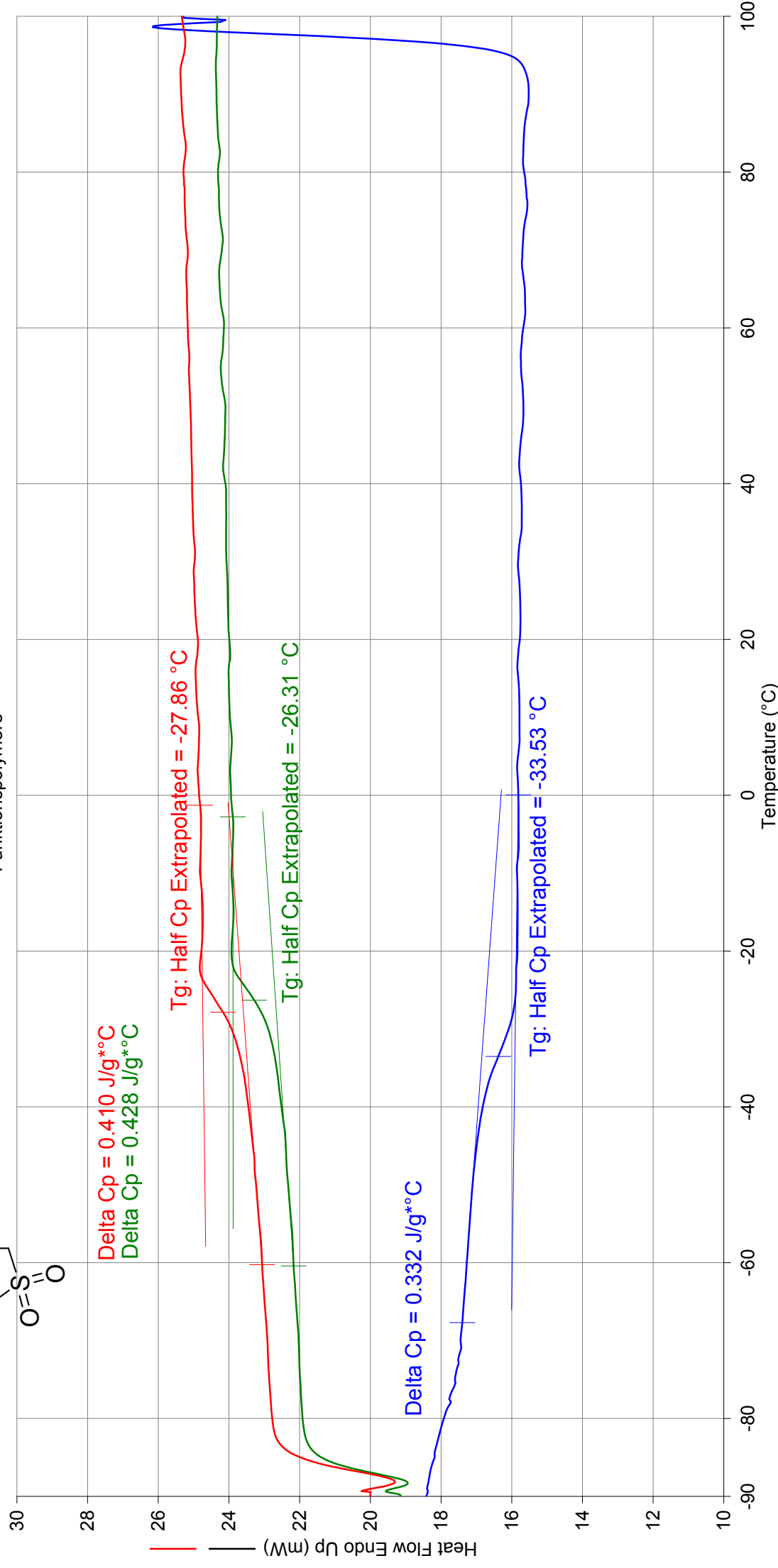
IR Spetrum of Pn(3:1)



DSC of Pn(3:1)



Funktionspolymere



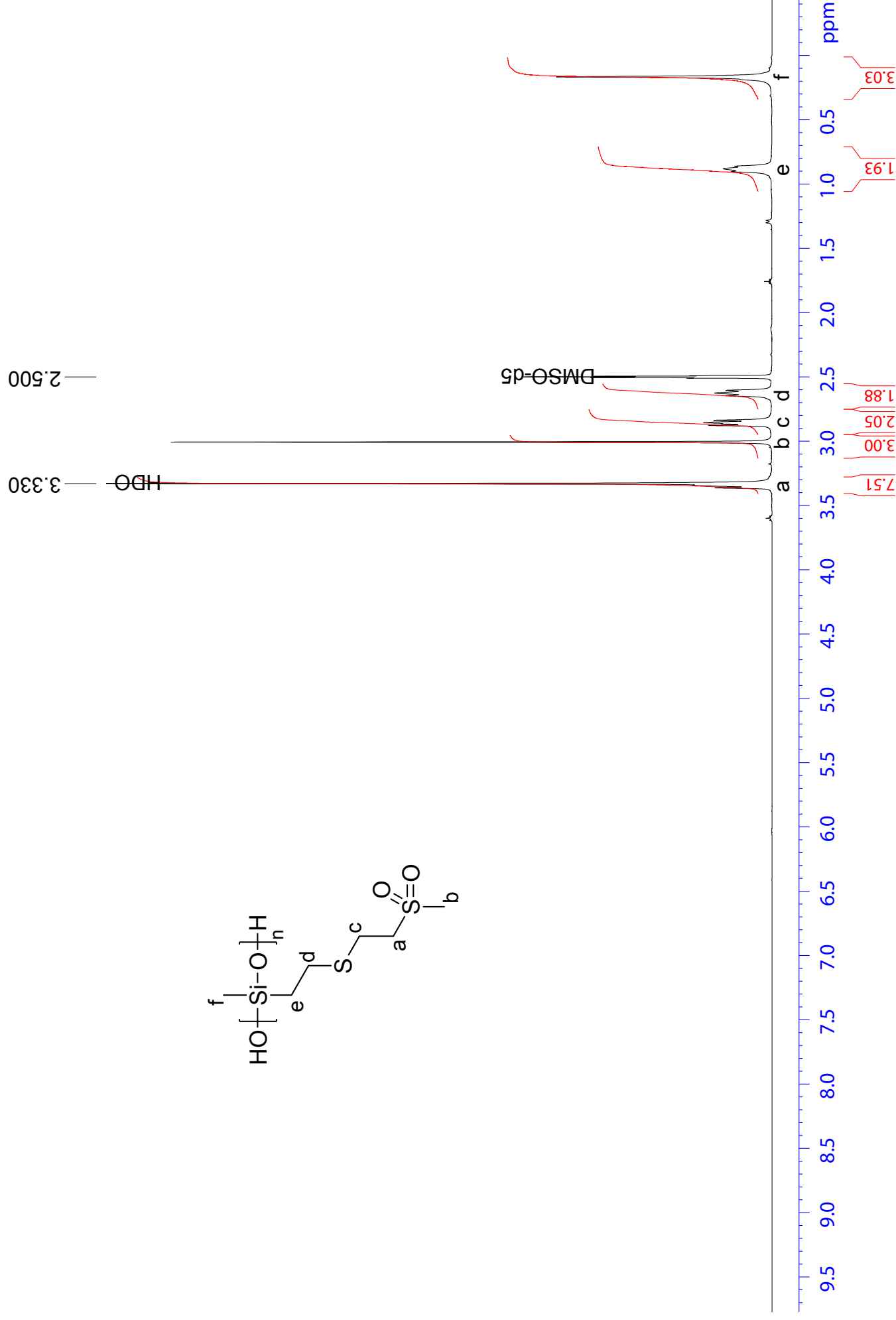
1) Heat from -90.00°C to 100.00°C at 20.00°C/min

3) Hold for 5.0 min at -90.00°C

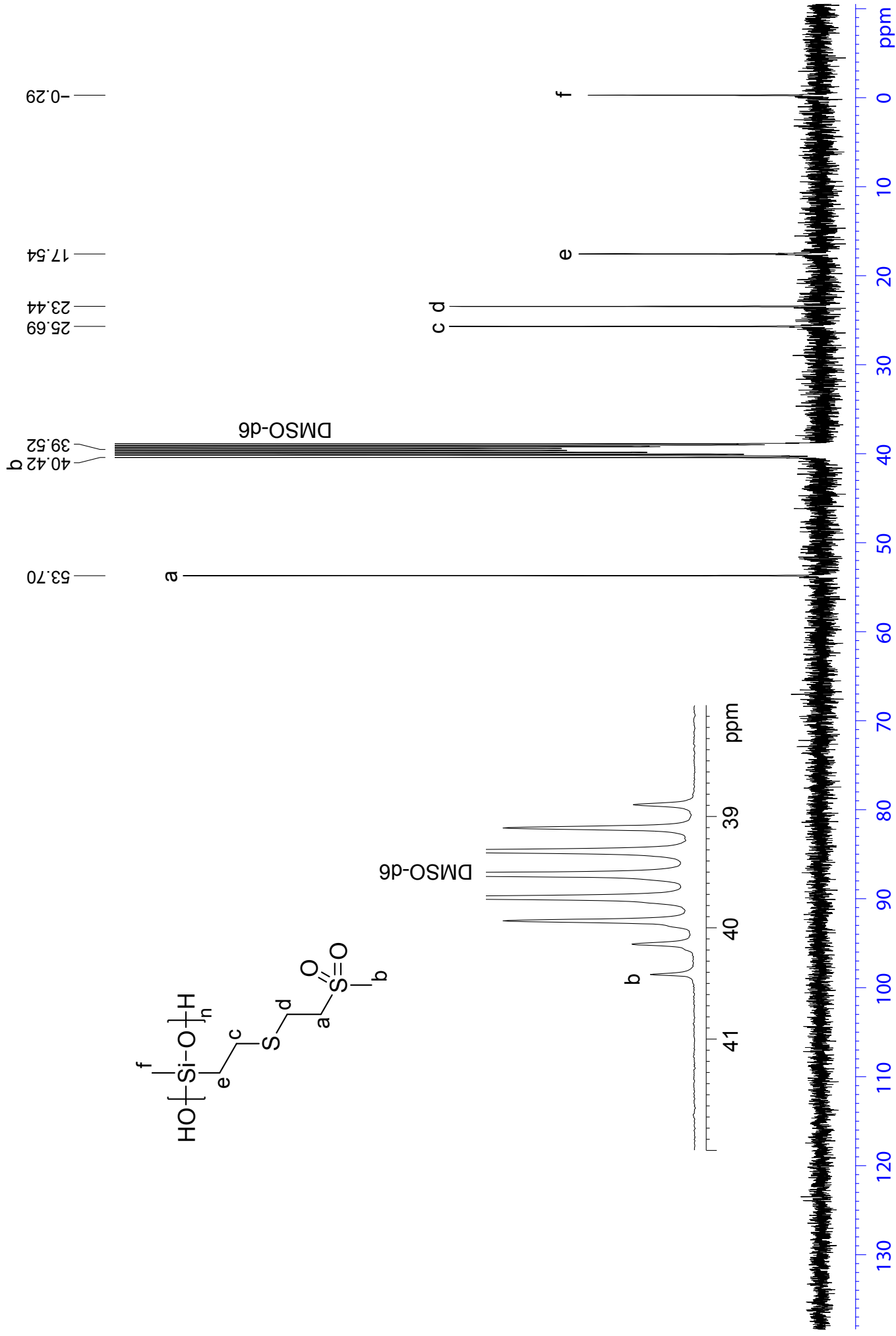
2) Cool from 100.00°C to -90.00°C at 20.00°C/min

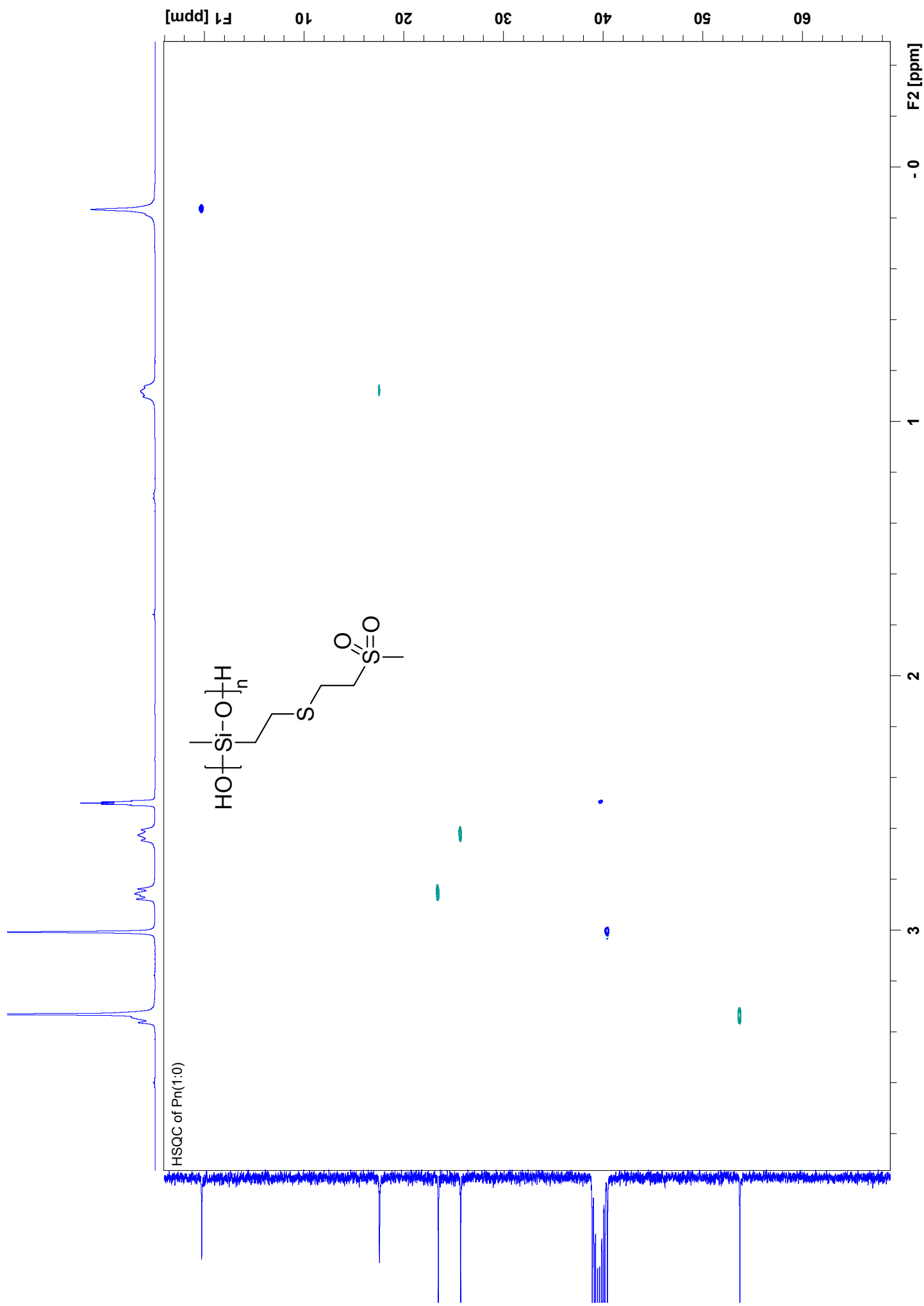
4) Heat from -90.00°C to 100.00°C at 20.00°C/min

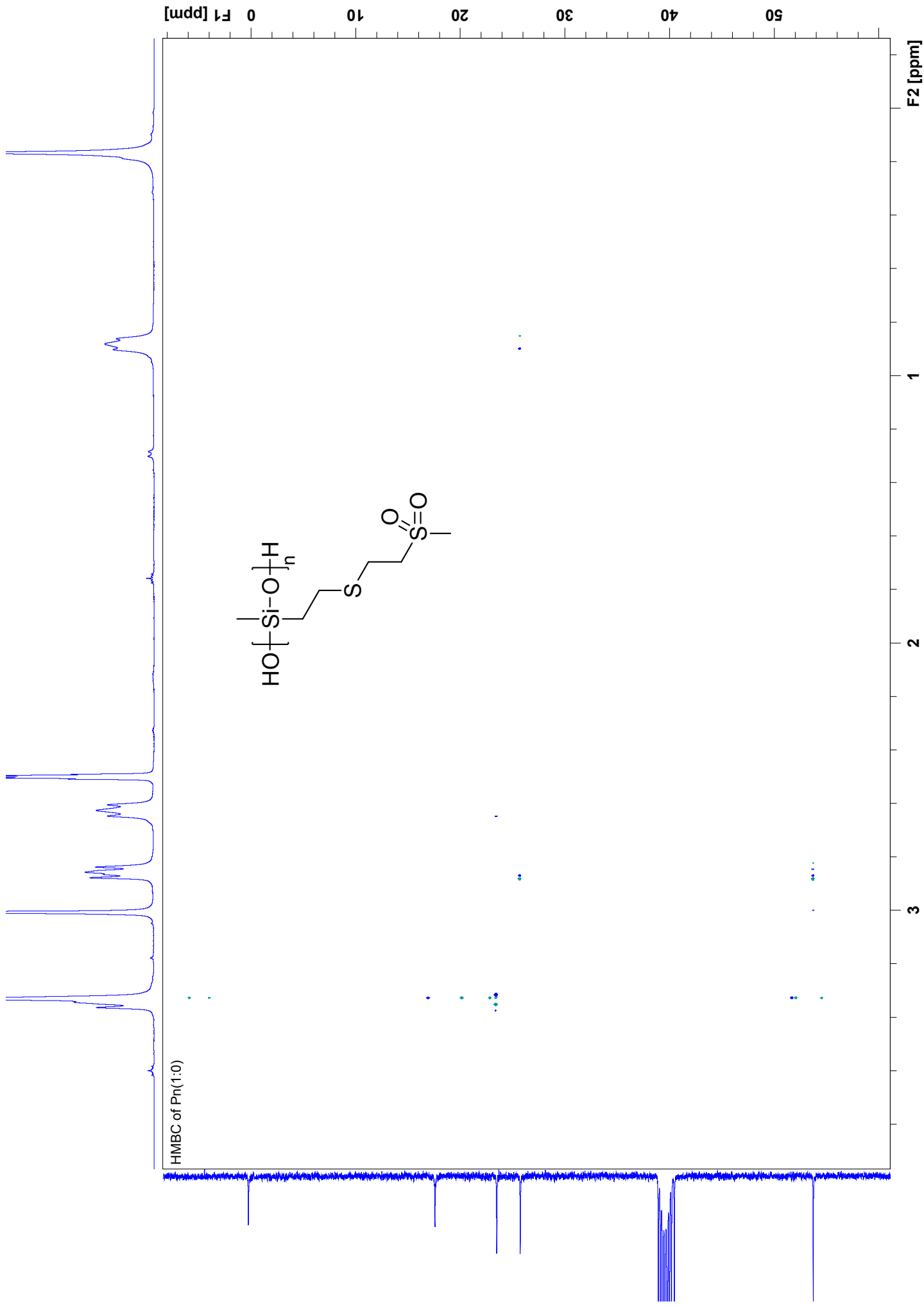
¹H NMR of Pn(1:0)



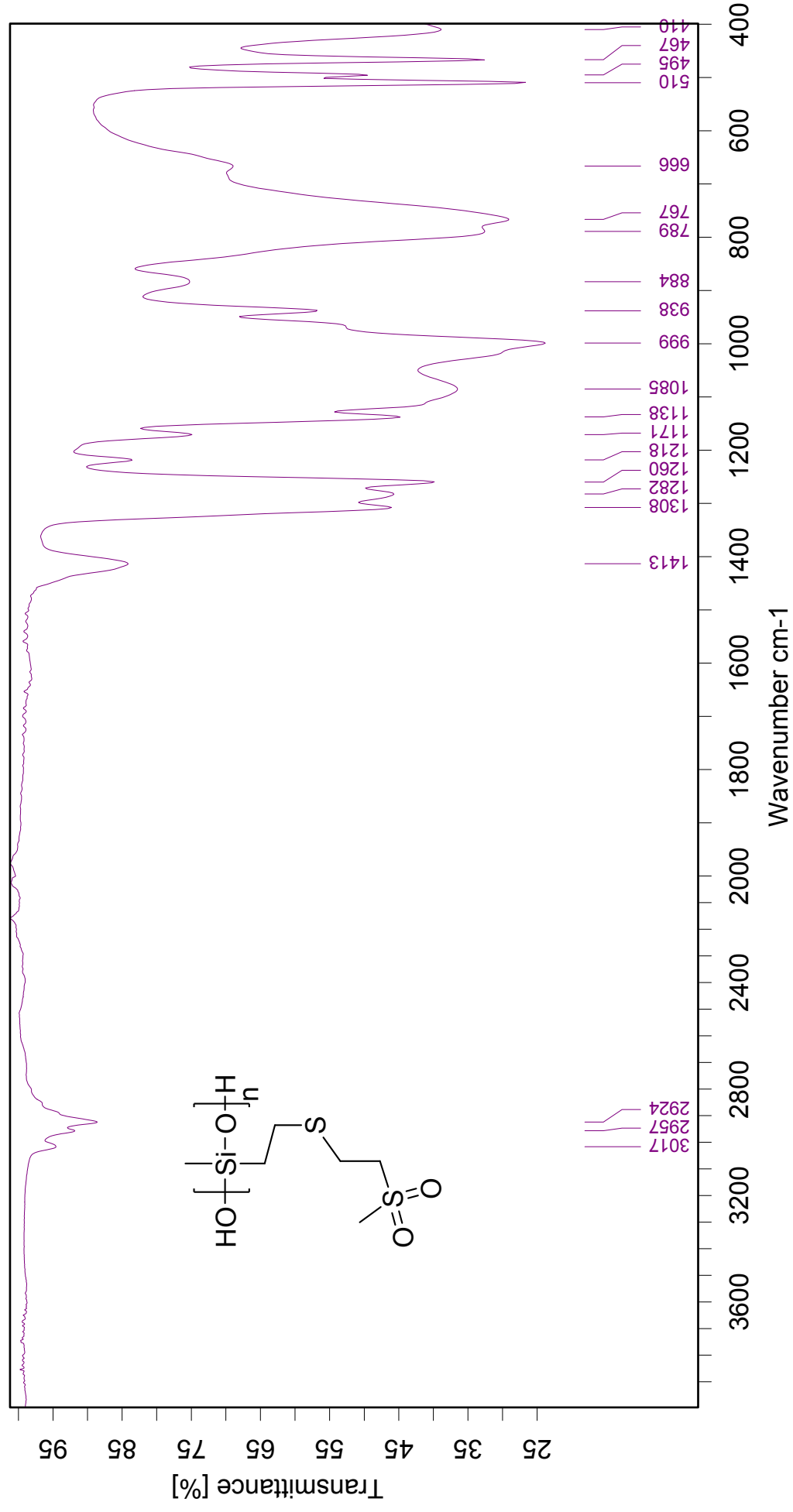
^{13}C NMR of Pn(1:0)

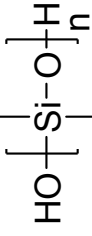






IR Spectrum of Pn(1:0)

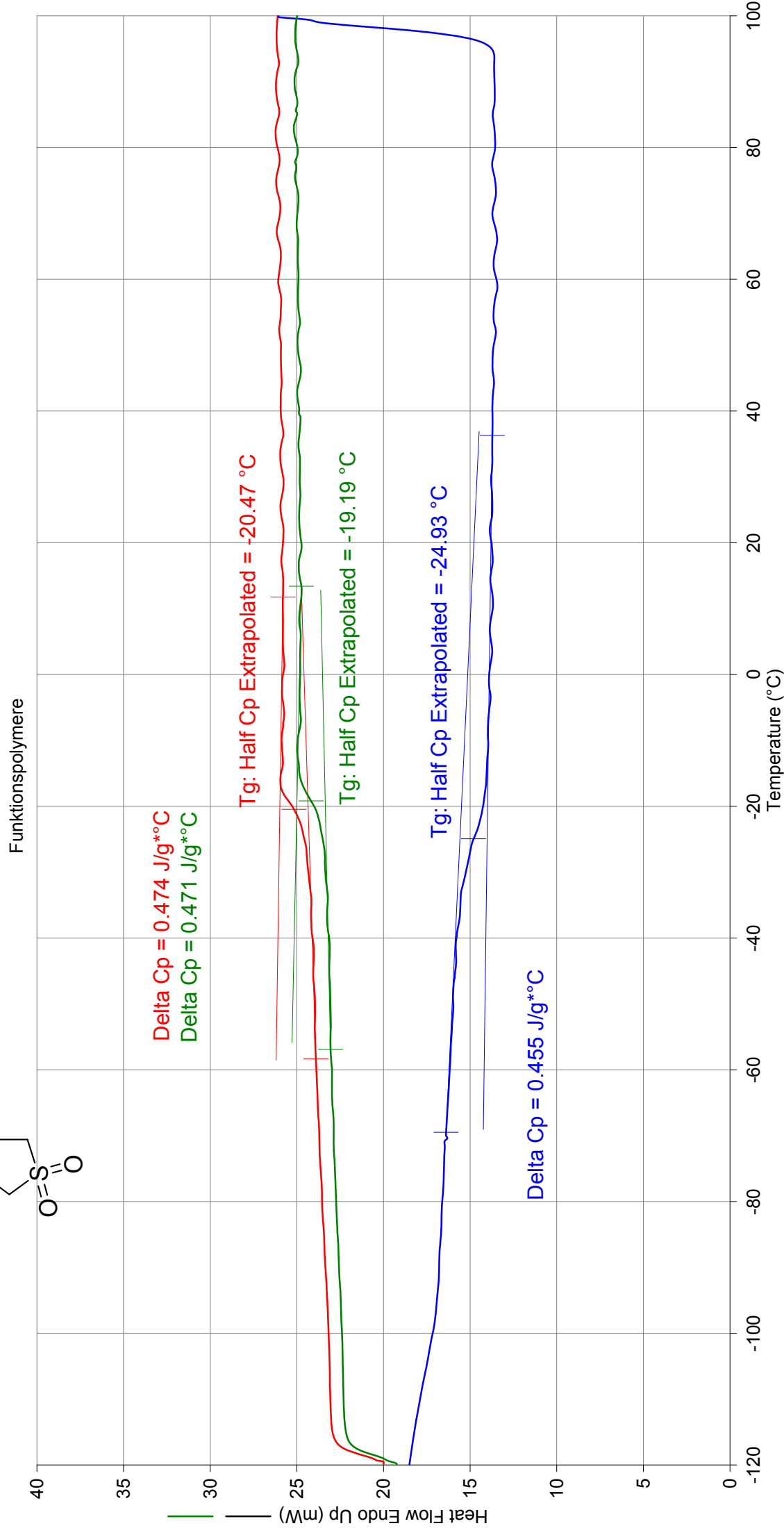




Heat Flow Endo Up (mW) : Step: 1

Heat Flow Endo Up (mW) : Step: 2

Heat Flow Endo Up (mW) : Step: 4



- | | | | |
|----|--|----|--|
| 1) | Heat from -120.00°C to 100.00°C at 20.00°C/min | 3) | Hold for 5.0 min at -120.00°C |
| 2) | Cool from 100.00°C to -120.00°C at 20.00°C/min | 4) | Heat from -120.00°C to 100.00°C at 20.00°C/min |

