

*Spectra and GPC Data for
Polyhydroxyurethanes Formation from
Bis(cyclic carbonate) Monomers in
Multicomponent Semi-IPN Hydrogels
Fabrication*

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Index and Keywords

Dataset language:
English

- NMR, ATR-FTIR and Mass Spectra of small molecules and monomers:
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Keywords: Cyclic carbonates, monomers, polyhydroxyurethanes, PHU, aminolysis, NIPU, non-isocyanate polyurethanes

Grant information

and

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Grant Number: US-1380587.
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1st Part:

Monomers and small molecules

- 1. {1-[3,5-bis(trifluoromethyl)phenyl]-3-cyclohexylthiourea} (TU)**
Pages [6-13]
 - ¹H NMR, COSY, ¹³C NMR, HSQC, ATR-FTIR, ESI-MS
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 - ¹H NMR, COSY, ¹³C NMR, HSQC, ATR-FTIR, ESI-MS, ESI-HRMS
- 4. Five-membered bis(cyclic carbonate) (Monomer A)**
Pages [28-38]
 - ¹H NMR, COSY, ¹³C NMR, HSQC, ATR-FTIR, ESI-HRMS
- 5. Five-membered bis(cyclic carbonate) (Monomer E)**
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 - ¹H NMR, COSY, ¹³C NMR, HSQC, ATR-FTIR, ESI-MS, ESI-HRMS

{1-[3,5-bis(trifluoromethyl)phenyl]-3-cyclohexylthiourea} (TU)

Spectrum $^1\text{H-RMN}$, 300 MHz, CDCl_3

— 8.131

— 7.761

— 7.707

— 6.074

— 4.190

— 2.105

— 2.094

— 2.063

— 2.052

— 1.738

— 1.725

— 1.706

— 1.693

— 1.679

— 1.647

— 1.631

— 1.618

— 1.606

— 1.494

— 1.482

— 1.472

— 1.455

— 1.444

— 1.433

— 1.400

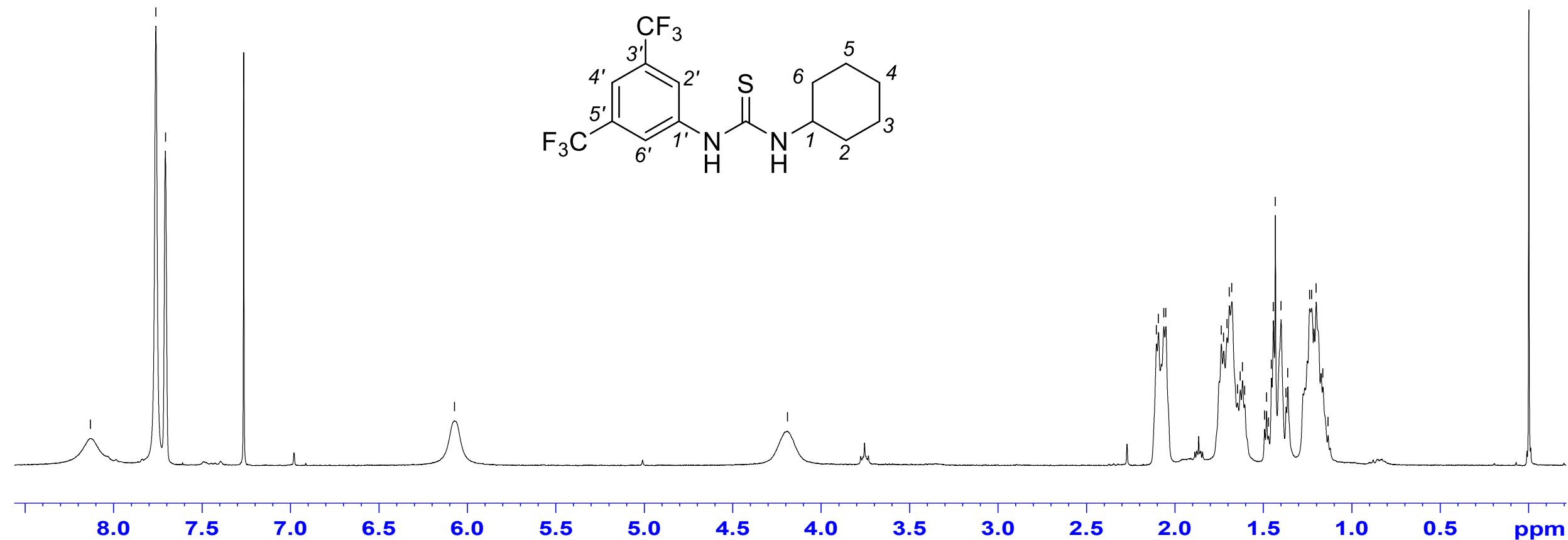
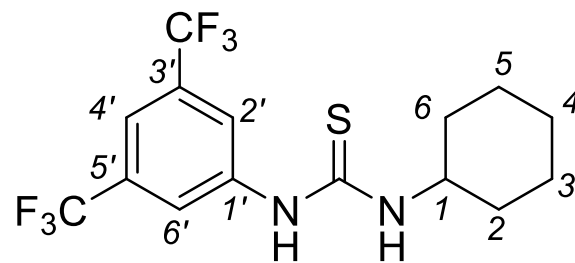
— 1.372

— 1.362

— 1.239

— 1.228

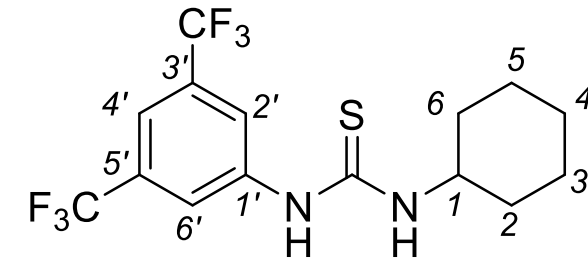
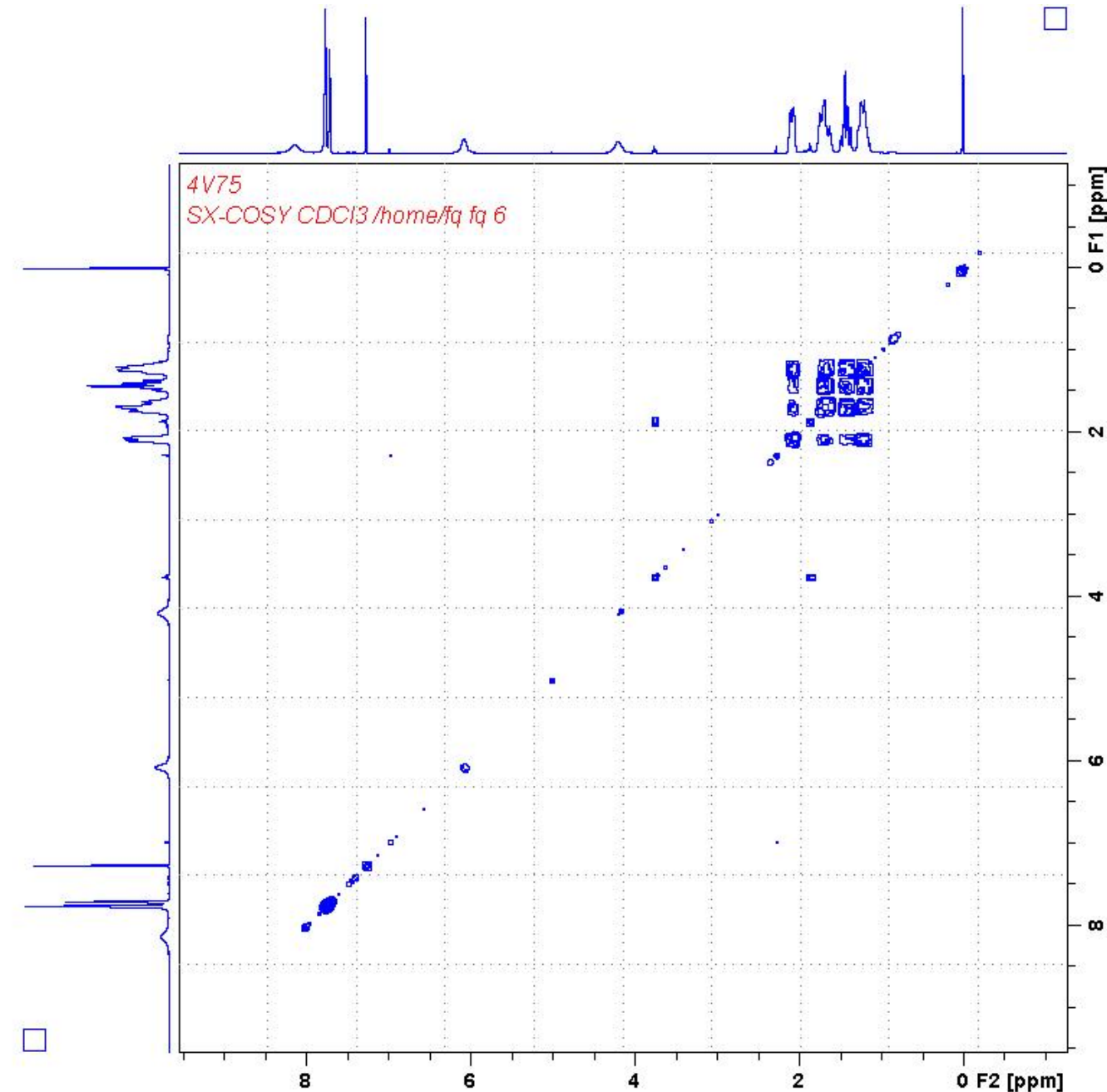
— 1.202



$^1\text{H-NMR}$ (300 MHz, CDCl_3 , δ ppm, J Hz) δ 8.13 (Bs, 1H, Ph-NH-), 7.76 (s, 2H, H-2', H-6'), 7.71 (s, 1H, H-4'), 6.07 (bs, 1H, -NH-cyclohexyle), 4.19 (bs, 1H, H-1), 2.07 (dd, H-2a, H-6a, $^2J_{2a,2b} = ^2J_{6a,6b} = 12.4$, $J_{2a,3a} = J_{6a,5a} = 3.3$), 1.70-1.10 (m, 8H, H-2b, H-3, H-4, H-5, H-6b).

{1-[3,5-bis(trifluoromethyl)phenyl]-3-cyclohexylthiourea} (TU)

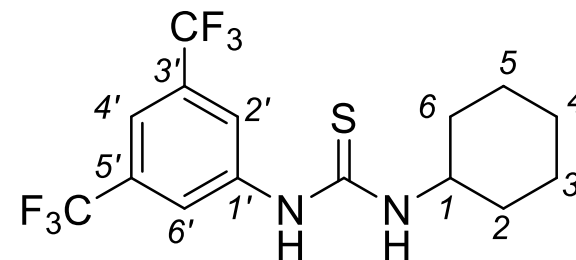
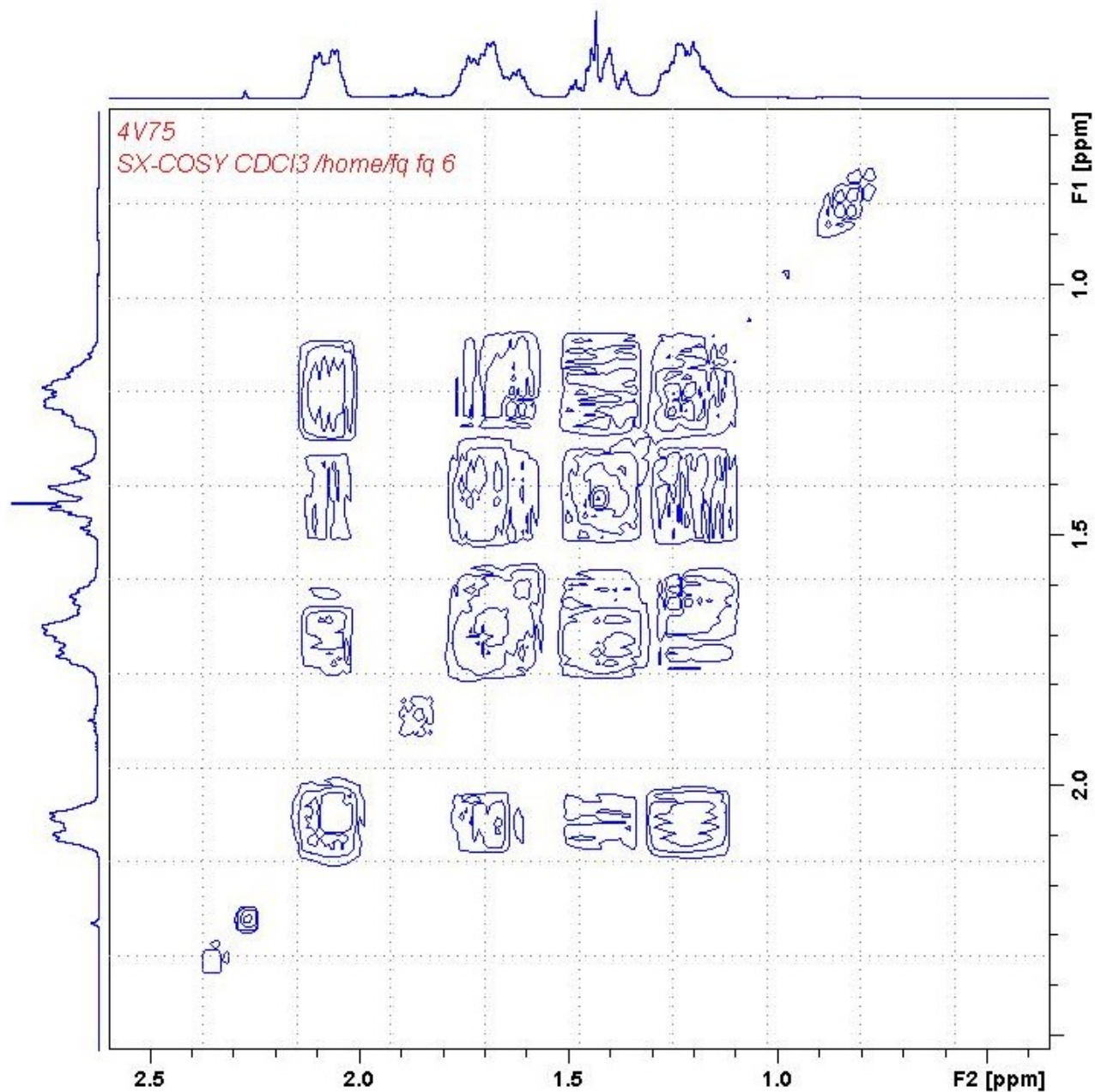
COSY (Bidimensional ^1H - ^1H)



^1H -NMR (300 MHz, CDCl₃, δ ppm, J Hz) δ 8.13 (Bs, 1H, Ph-NH-), 7.76 (s, 2H, H-2', H-6'), 7.71 (s, 1H, H-4'), 6.07 (bs, 1H, -NH-cyclohexyle), 4.19 (bs, 1H, H-1), 2.07 (dd, H-2a, H-6a, $^2J_{2a,2b} = ^2J_{6a,6b} = 12.4$, $J_{2a,3a} = J_{6a,5a} 3.3$), 1.70-1.10 (m, 8H, H-2b, H-3, H-4, H-5, H-6b).

{1-[3,5-bis(trifluoromethyl)phenyl]-3-cyclohexylthiourea} (TU)

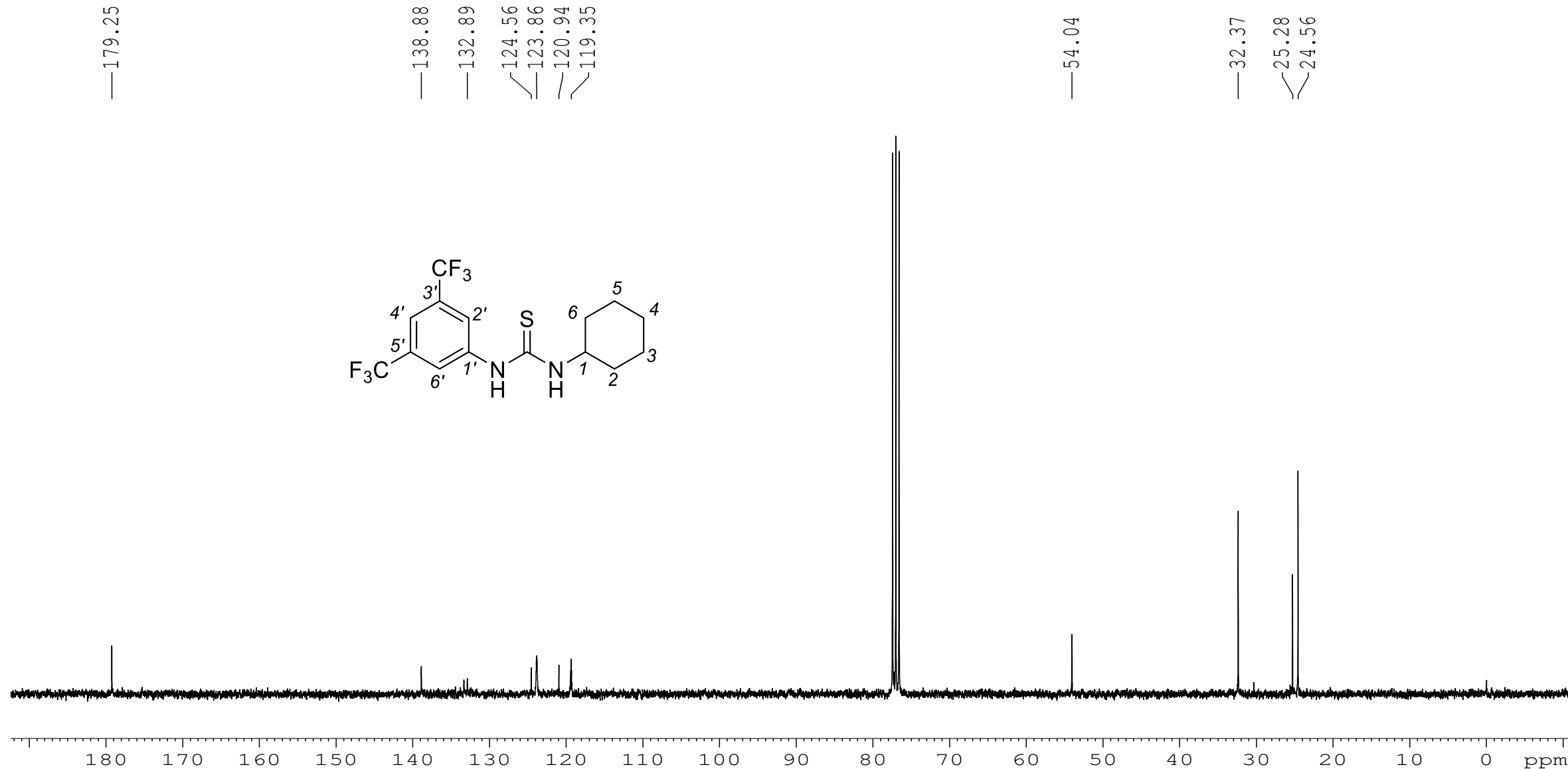
COSY (Bidimensional ^1H - ^1H)



^1H -NMR (300 MHz, CDCl_3 , δ ppm, J Hz) δ
8.13 (bs, 1H, Ph-NH-), 7.76 (s, 2H, H-2', H-6'), 7.71 (s, 1H, H-4'), 6.07 (bs, 1H, -NH-cyclohexyle), 4.19 (bs, 1H, H-1), 2.07 (dd, H-2a, H-6a, $^2J_{2a,2b} = ^2J_{6a,6b} = 12.4$, $J_{2a,3a} = J_{6a,5a} 3.3$), 1.70-1.10 (m, 8H, H-2b, H-3, H-4, H-5, H-6b).

{1-[3,5-bis(trifluoromethyl)phenyl]-3-cyclohexylthiourea} (TU)

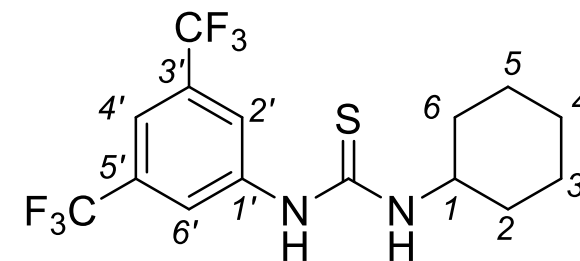
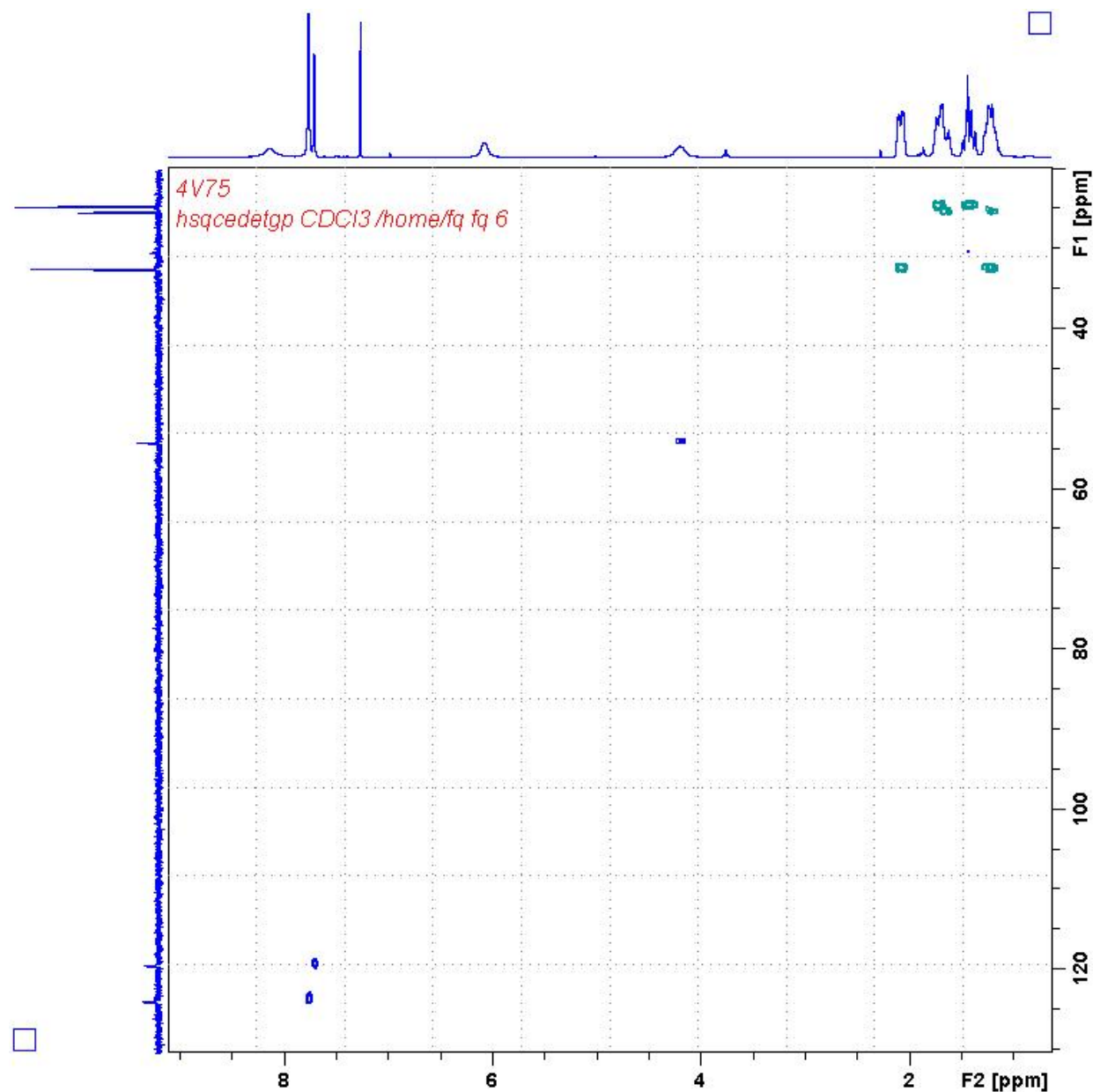
Spectrum ^{13}C -RMN, 75 MHz, CDCl_3



^{13}C -NMR (75 MHz, CDCl_3 , δ ppm) δ 179.3 (C=S), 138.9 (C-1'), 124.6 (C-2', C-6'), 123.9 (C-3', C-5'), 120.9 ($-\text{CF}_3$), 119.4 (C-4'), 54.0 (C-1), 32.4 (C-2, C-6), 35.3 (C-4), 24.6 (C-3, C-5).

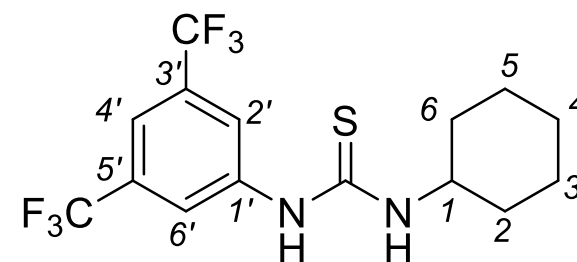
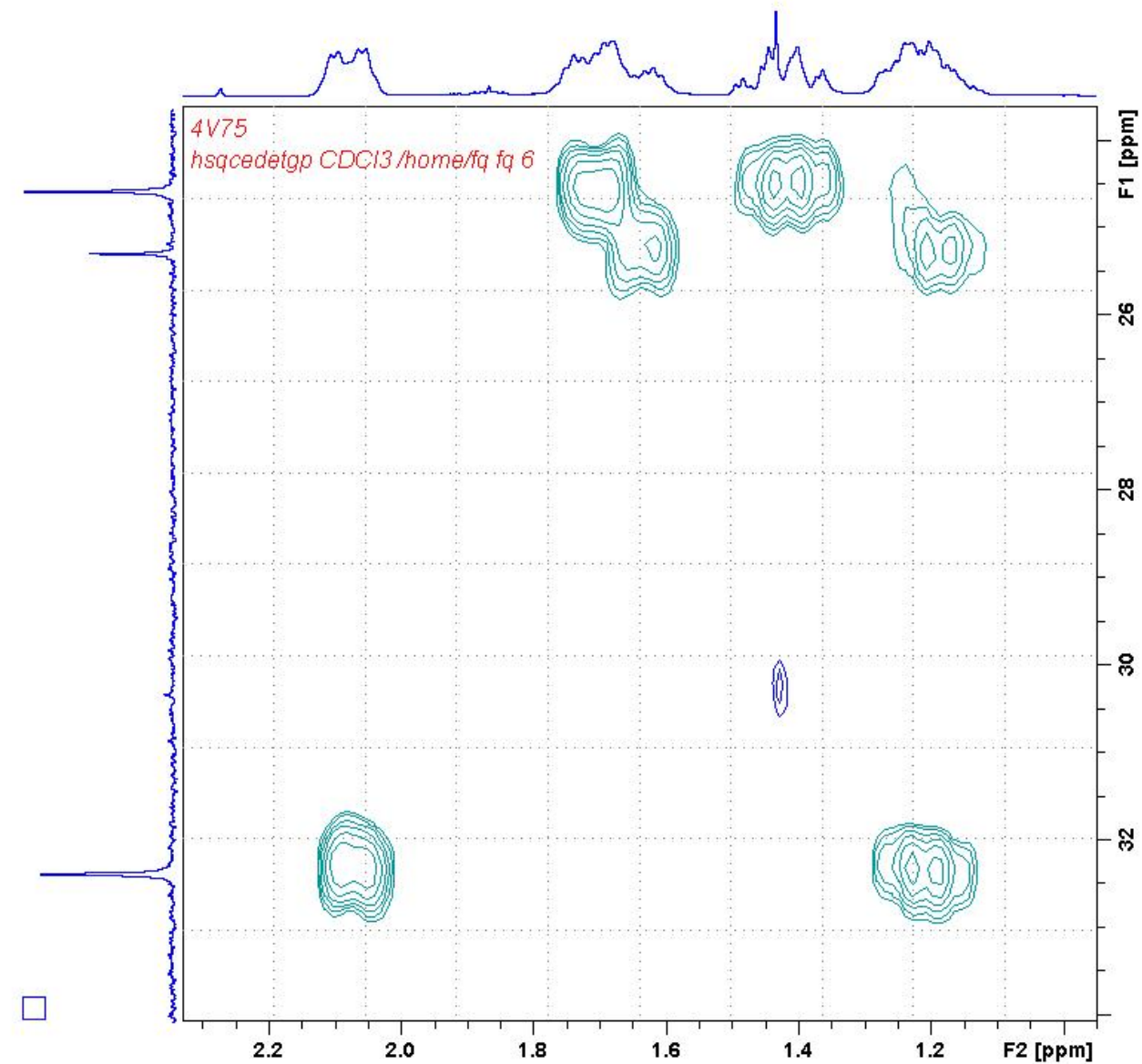
{1-[3,5-bis(trifluoromethyl)phenyl]-3-cyclohexylthiourea} (TU)

HSQC (Bidimensional ^1H - ^{13}C)



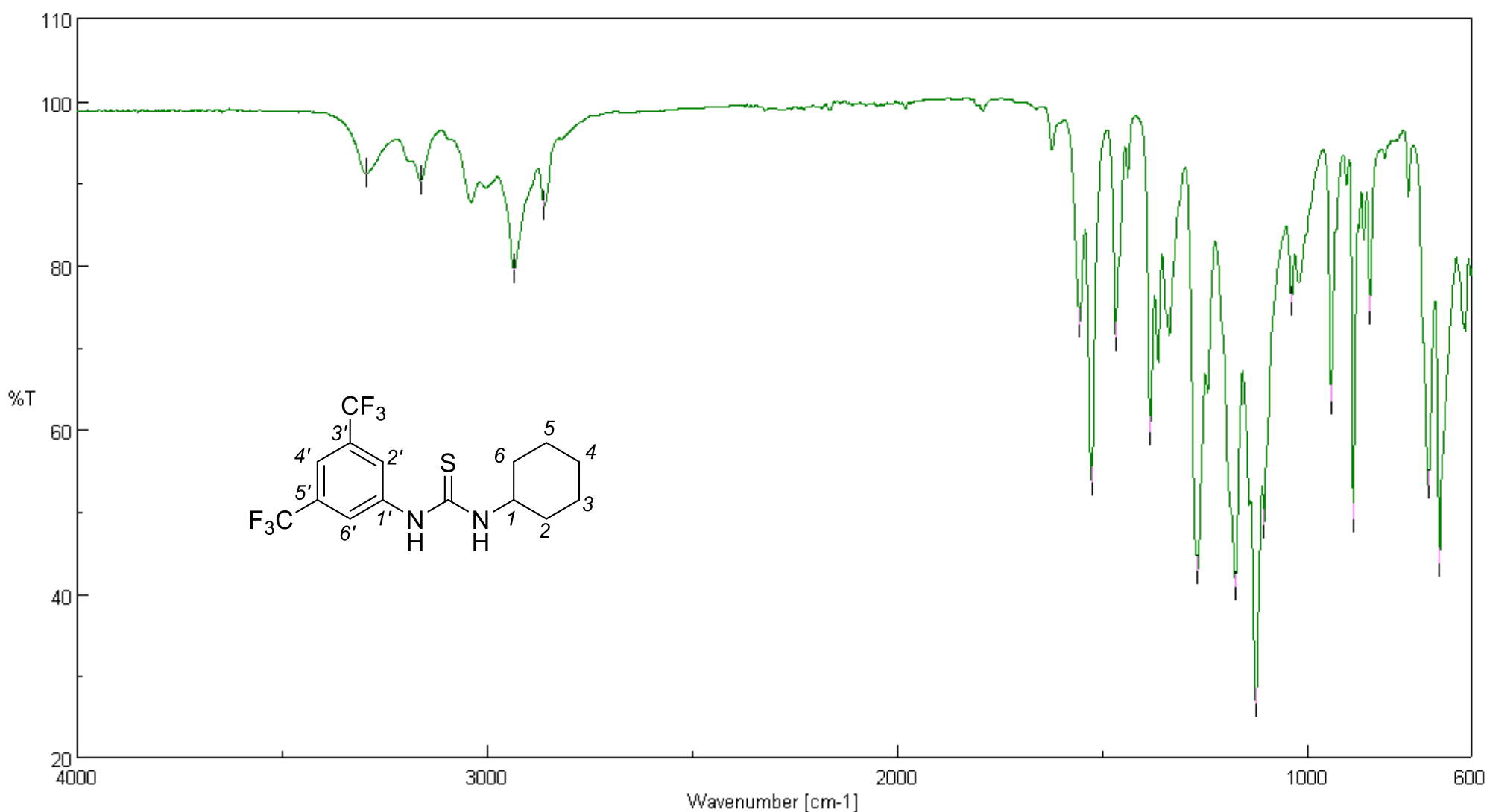
{1-[3,5-bis(trifluoromethyl)phenyl]-3-cyclohexylthiourea} (TU)

HSQC (Bidimensional ^1H - ^{13}C)



{1-[3,5-bis(trifluoromethyl)phenyl]-3-cyclohexylthiourea} (TU)

Spectrum ATR-FTIR



Wavenum...	%T
3293.82	91.1575
3162.69	90.187
2935.13	79.4663
2861.84	87.2686
1556.27	72.7857
1526.38	53.5249
1468.53	71.1762
1383.68	59.6547
1267.97	42.8543
1176.36	40.8769
1126.22	26.7318
1105.98	48.3029
1038.48	75.5616
942.056	63.4057
888.059	49.0884
847.561	74.4375
705.819	53.1968
678.82	43.7042

{1-[3,5-bis(trifluoromethyl)phenyl]-3-cyclohexylthiourea} (TU)

Spectrum ESI-MS

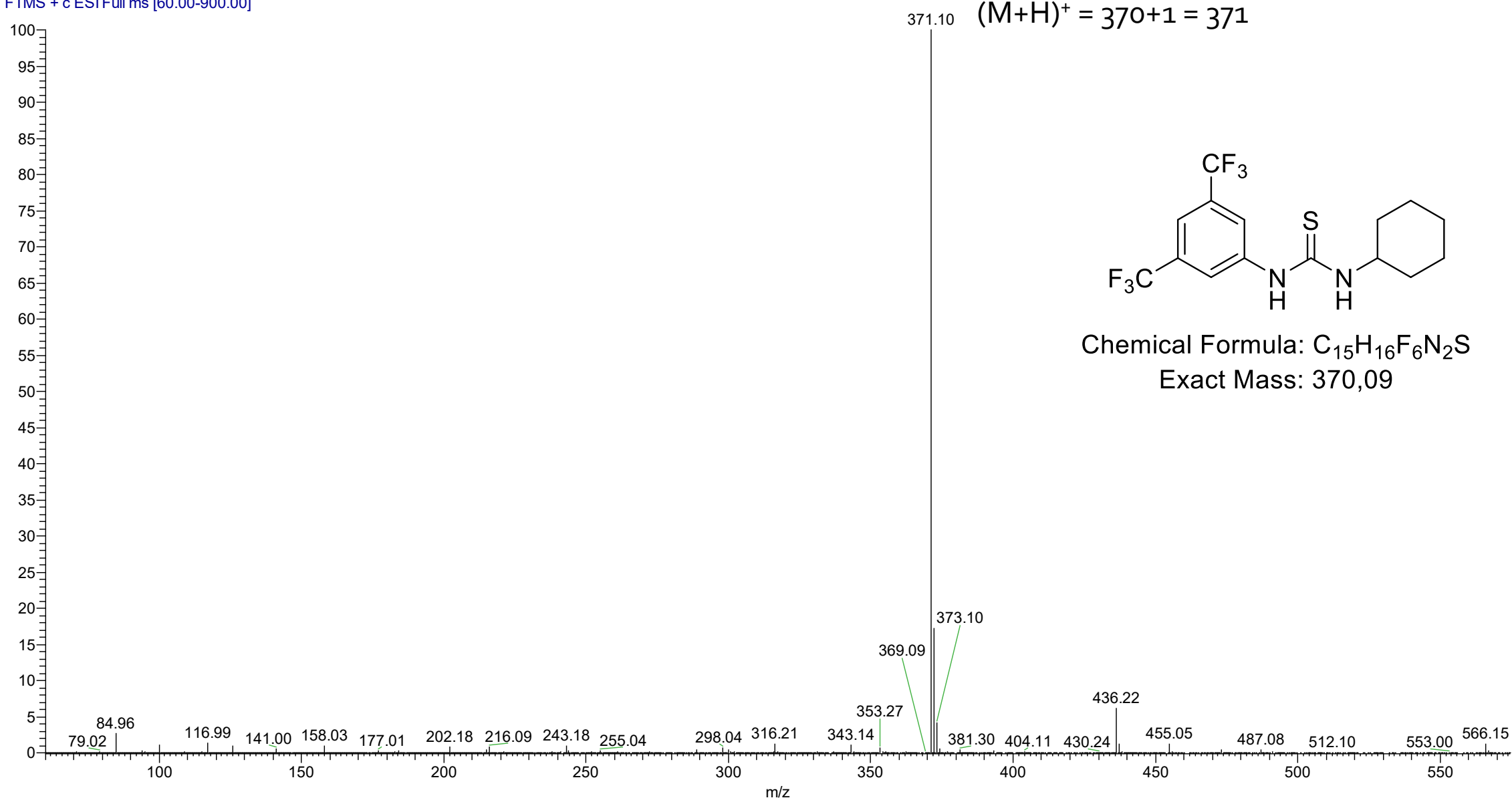
170628_4V75

06/28/17 12:08:39

4V75 PM=370 C15H16F6N2S

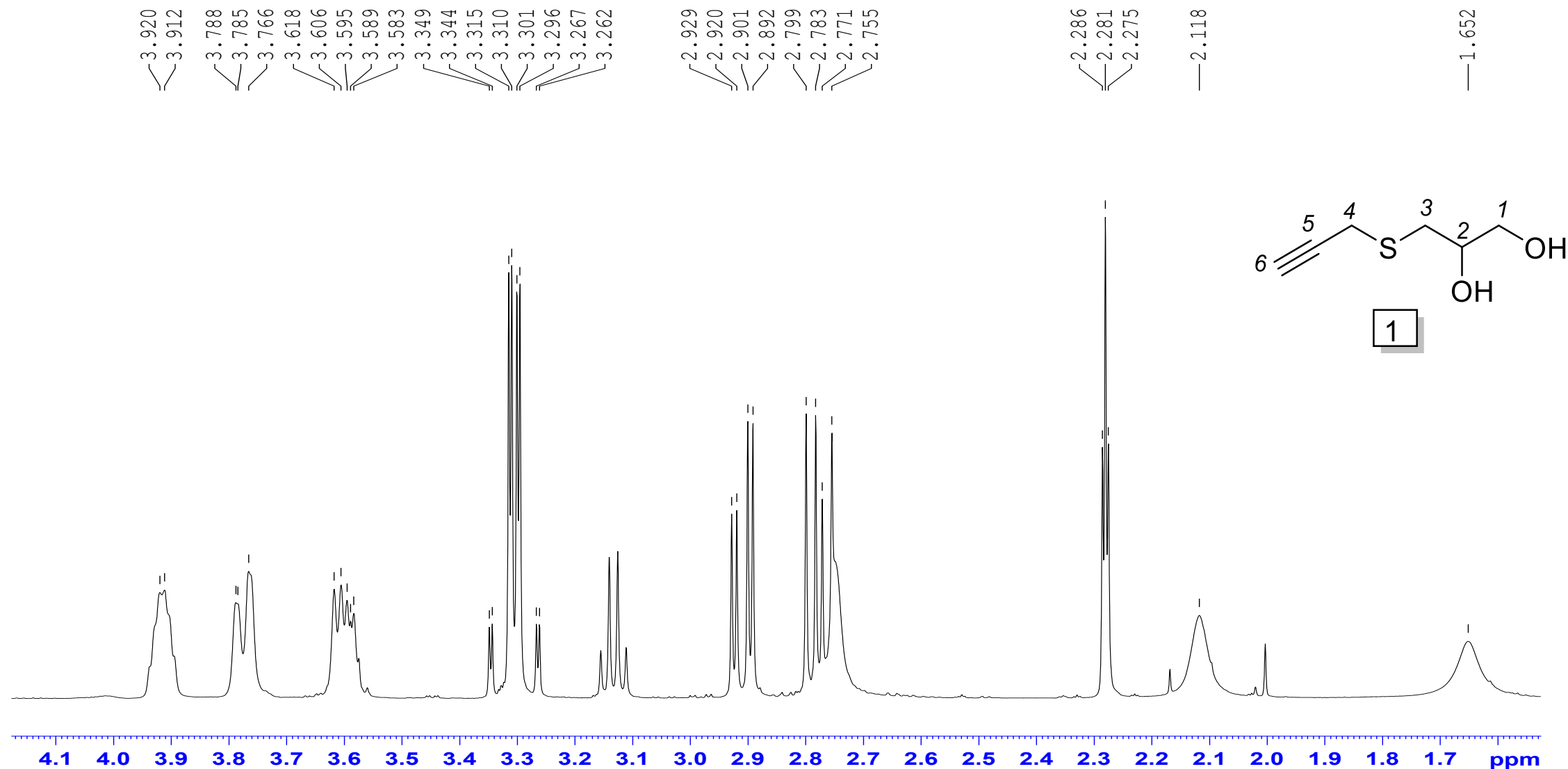
170628_4V75 #60-94 RT: 0.24-0.37 AV: 35 NL: 1.23E8

T: FTMS + c ESI Full ms [60.00-900.00]



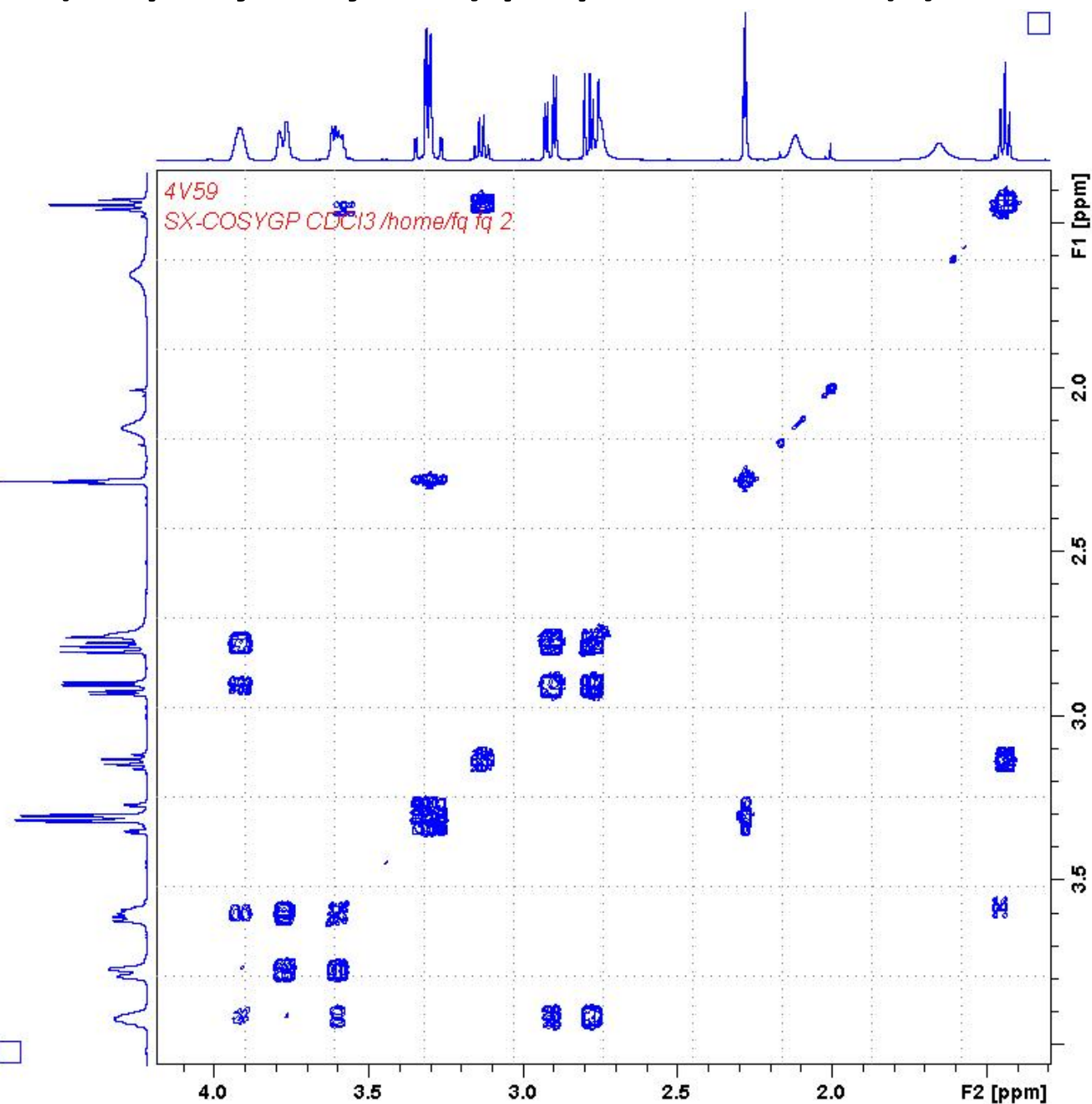
3-(Prop-2-yn-1-ylthio)propane-1,2-diol (1)

Spectrum ^1H -RMN, 500 MHz, CDCl_3

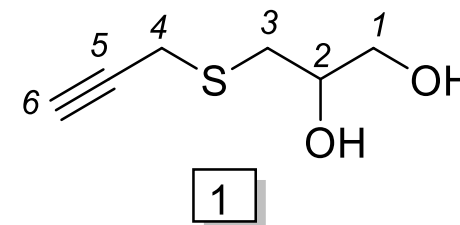


^1H -NMR (CDCl_3 , 500 MHz) δ (ppm) 3.93-3.89 (m, 1H, H-2), 3.79-3.75 (m, 1H, H-1a) 3.62-3.57 (m, 1H, H-1b), 3.33 (dd, 1H, H-1'a, $J_{1'a,3'} = 2.7$ Hz, $^2J_{1'a,1'b} = 17.0$ Hz), 3.28 (dd, 1H, H-1'b, $J_{1'b,3'} = 2.5$ Hz), 2.91 (dd, 1H, H-3a, $J_{3a,2} = 4.0$ Hz, $^2J_{3a,3b} = 13.9$ Hz), 2.78 (dd, 1H, H-3b, $J_{3b,2} = 8.0$ Hz), 2.28 (t, 1H, H-3'), 2.12, 1.65 (2 bs, 2H, OH).

3-(Prop-2-yn-1-ylthio)propane-1,2-diol (1)



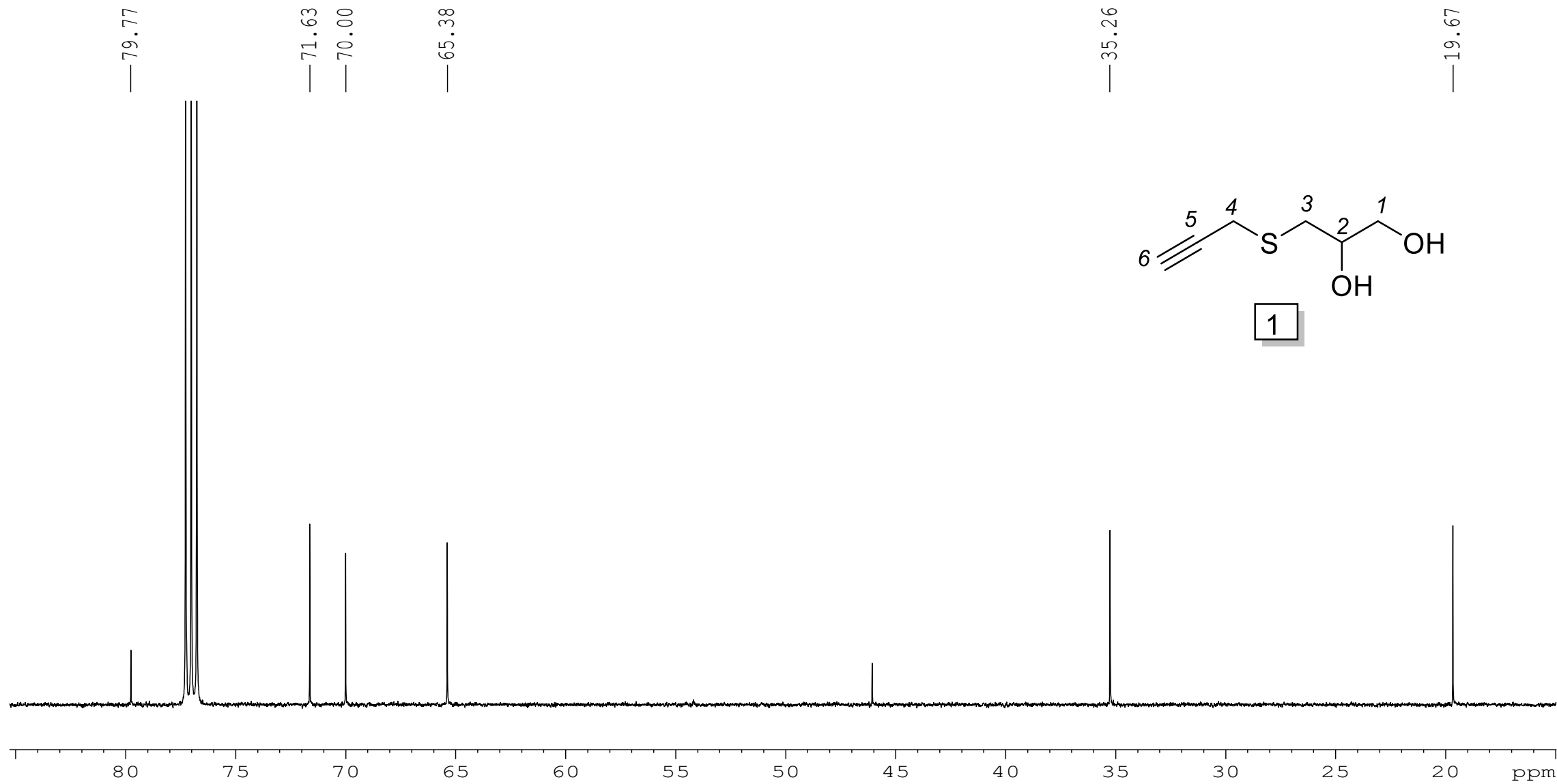
COSY (Bidimensional ^1H - ^1H)



^1H -NMR (CDCl_3 , 500 MHz) δ (ppm) 3.93-3.89 (m, 1H, H-2), 3.79-3.75 (m, 1H, H-1a) 3.62-3.57 (m, 1H, H-1b), 3.33 (dd, 1H, H-1'a, $J_{1'a,3'} = 2.7$ Hz, $^2J_{1'a,1'b} = 17.0$ Hz), 3.28 (dd, 1H, H-1'b, $J_{1'b,3'} = 2.5$ Hz), 2.91 (dd, 1H, H-3a, $J_{3a,2} = 4.0$ Hz, $^2J_{3a,3b} = 13.9$ Hz), 2.78 (dd, 1H, H-3b, $J_{3b,2} = 8.0$ Hz), 2.28 (t, 1H, H-3'), 2.12, 1.65 (2 bs, 2H, OH).

3-(Prop-2-yn-1-ylthio)propane-1,2-diol (1)

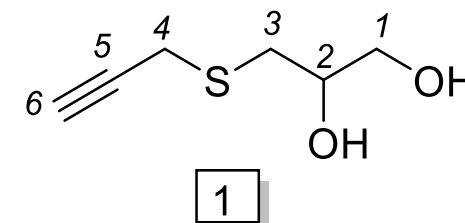
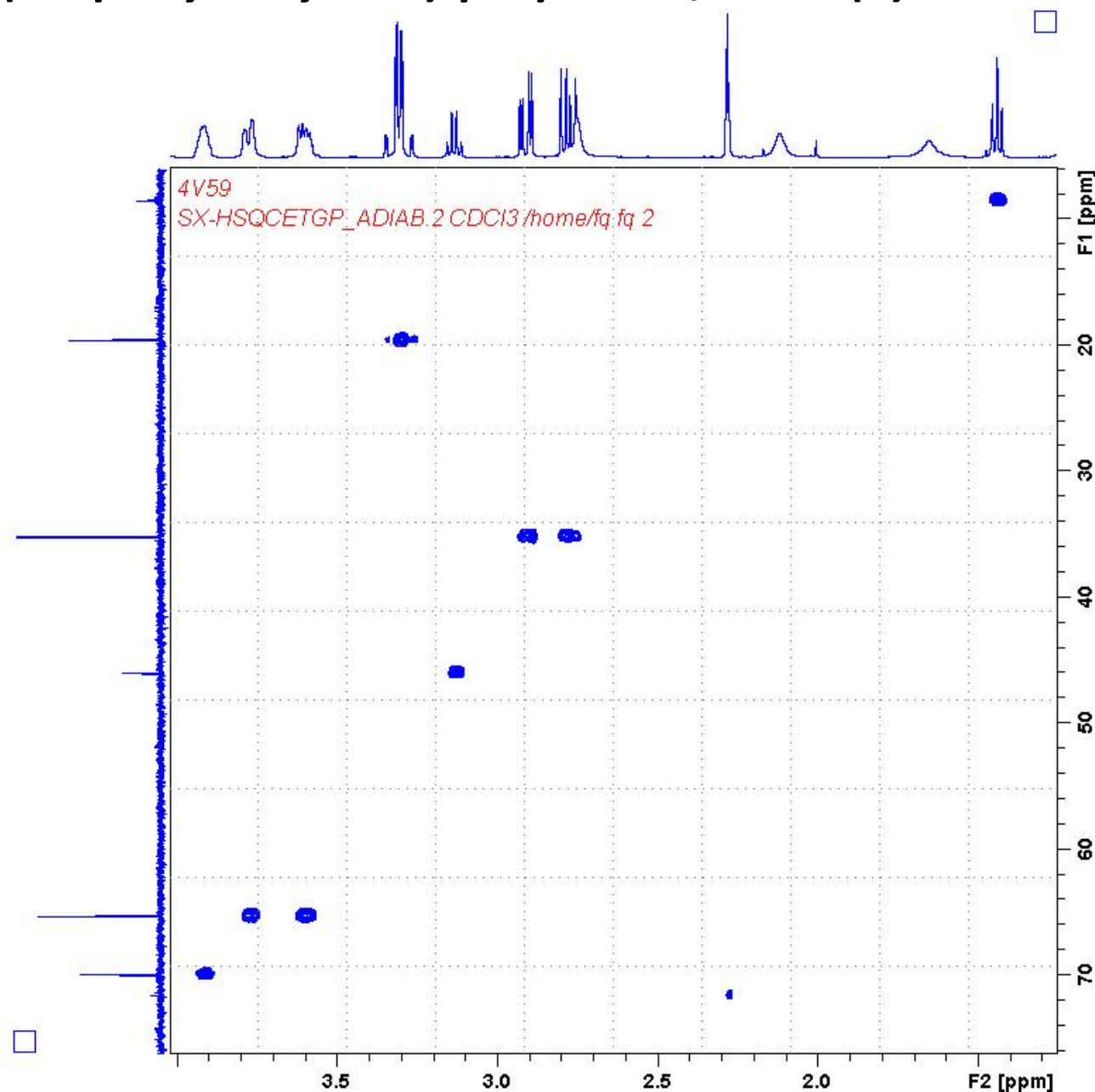
Spectrum ^{13}C -RMN, 125 MHz, CDCl_3



^{13}C -NMR (CDCl_3 , 125 MHz) δ (ppm) 79.7 (C-2'), 71.6 (C-3'), 70.0 (C-2), 65.3 (C-1), 35.4 (C-3), 19.7 (C-1').

3-(Prop-2-yn-1-ylthio)-propane-1,2-diol (1)

HSQC (Bidimensional ^1H - ^{13}C)

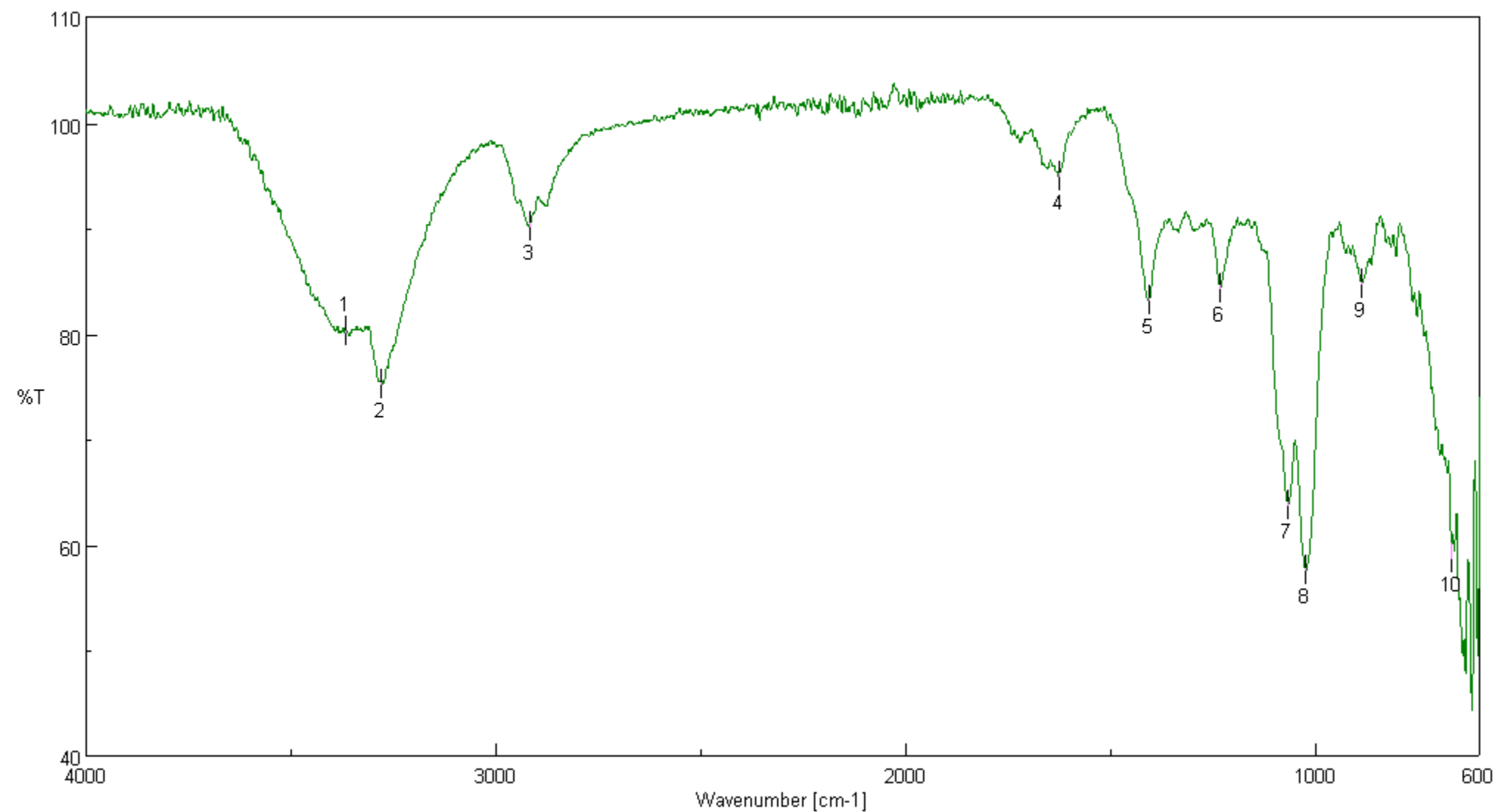
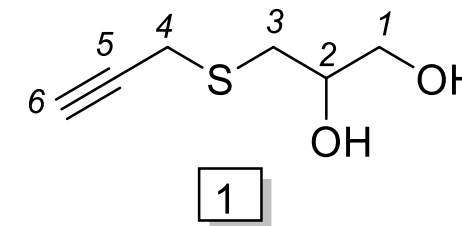


^1H -NMR (CDCl_3 , 500 MHz) δ (ppm) 3.93-3.89 (m, 1H, H-2), 3.79-3.75 (m, 1H, H-1a) 3.62-3.57 (m, 1H, H-1b), 3.33 (dd, 1H, H-1'a, $J_{1'a,3'} = 2.7$ Hz, $^2J_{1'a,1'b} = 17.0$ Hz), 3.28 (dd, 1H, H-1'b, $J_{1'b,3'} = 2.5$ Hz), 2.91 (dd, 1H, H-3a, $J_{3a,2} = 4.0$ Hz, $^2J_{3a,3b} = 13.9$ Hz), 2.78 (dd, 1H, H-3b, $J_{3b,2} = 8.0$ Hz), 2.28 (t, 1H, H-3'), 2.12, 1.65 (2 bs, 2H, OH).

^{13}C -NMR (CDCl_3 , 125 MHz) δ (ppm) 79.7 (C-2'), 71.6 (C-3'), 70.0 (C-2), 65.3 (C-1), 35.4 (C-3), 19.7 (C-1').

3-(Prop-2-yn-1-ylthio)propane-1,2-diol (1)

Spectrum ATR-FTIR



Wavenumber

[cm⁻¹]

%T

1	3365.17	80.1709
2	3279.36	75.2066
3	2918.73	90.1671
4	1626.66	94.8913
5	1406.82	83.1675
6	1232.29	84.3515
7	1066.44	63.7818
8	1024.02	57.5546
9	887.095	84.7066
10	668.214	58.7689

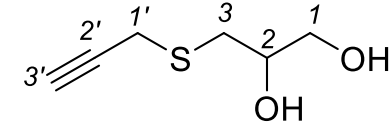
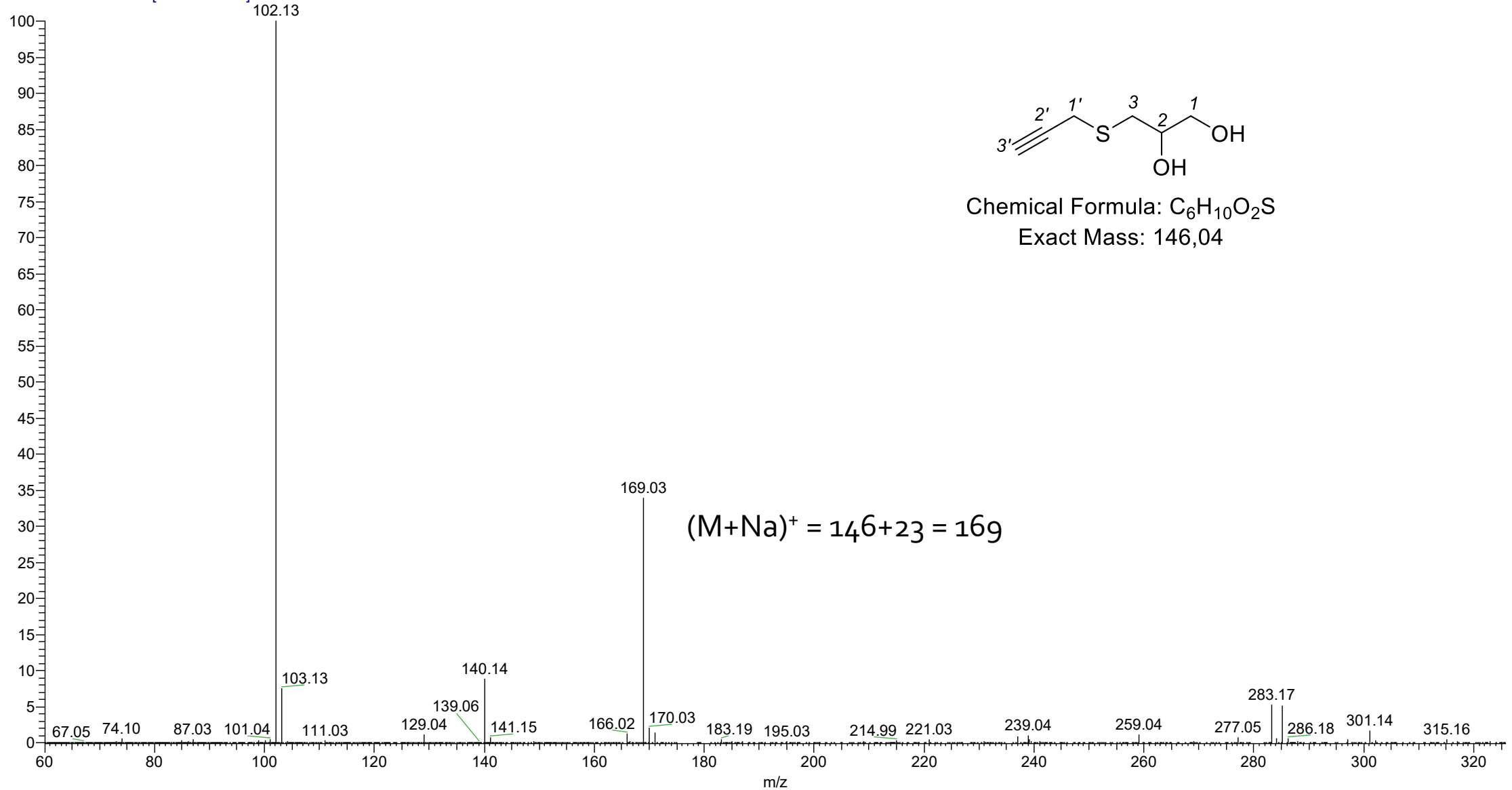
3-(Prop-2-yn-1-ylthio)propane-1,2-diol (1)

Spectrum ESI-MS

170303_4V59

4V59 PM=146 C6H10O2S

170303_4V59 #54-67 RT: 0.22-0.27 AV: 14 SB: 89 1.05-1.41 NL: 1.5
T: FTMS + c ESI Full ms [60.00-900.00]



Chemical Formula: C₆H₁₀O₂S
Exact Mass: 146,04

$$(M+Na)^+ = 146 + 23 = 169$$

3-(Prop-2-yn-1-ylthio)propane-1,2-diol (1)

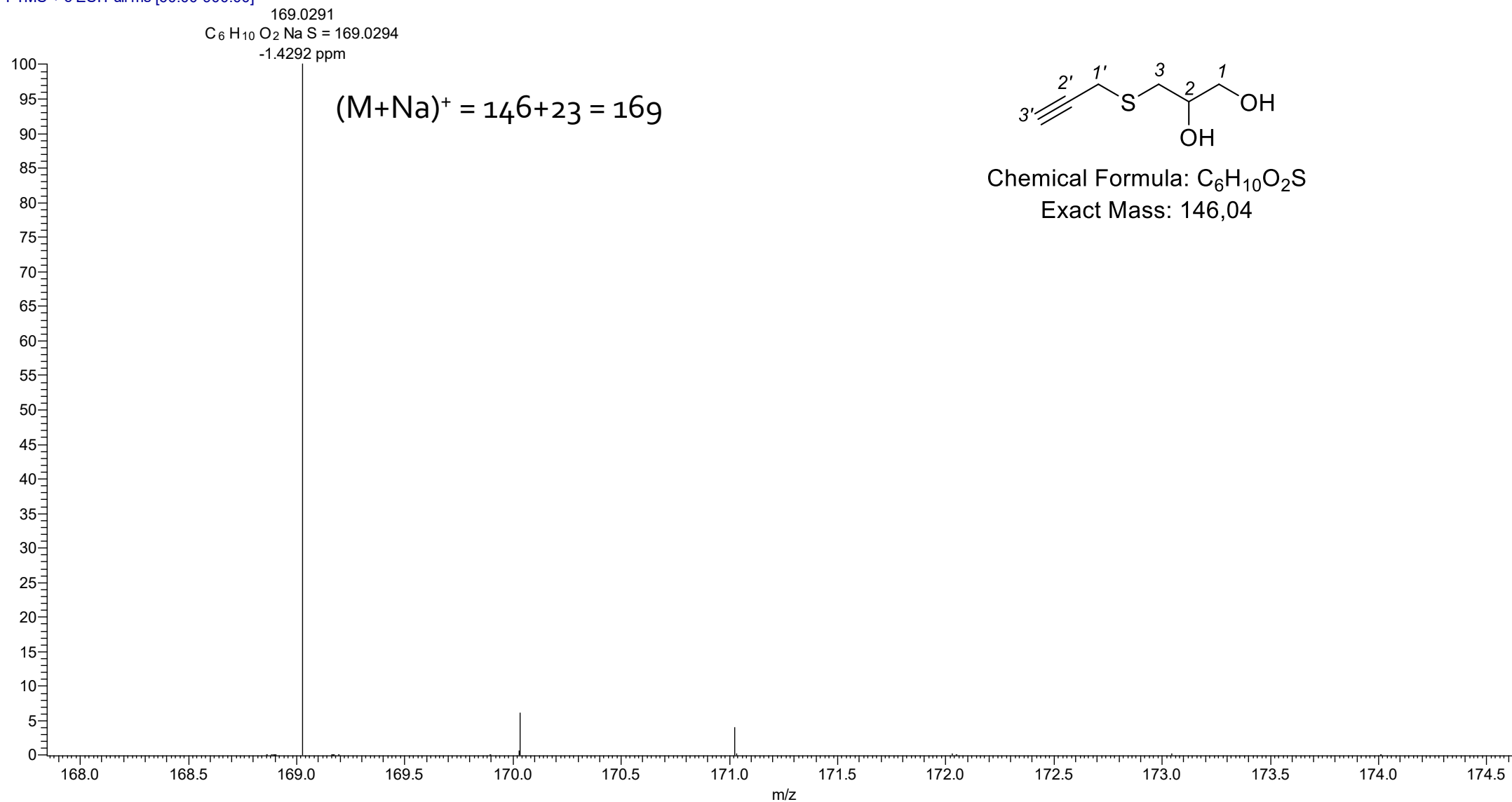
Spectrum ESI-HRMS

170303_4V59

03/03/17 13:43:07

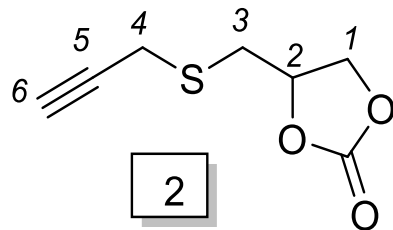
4V59 PM=146 C6H10O2S

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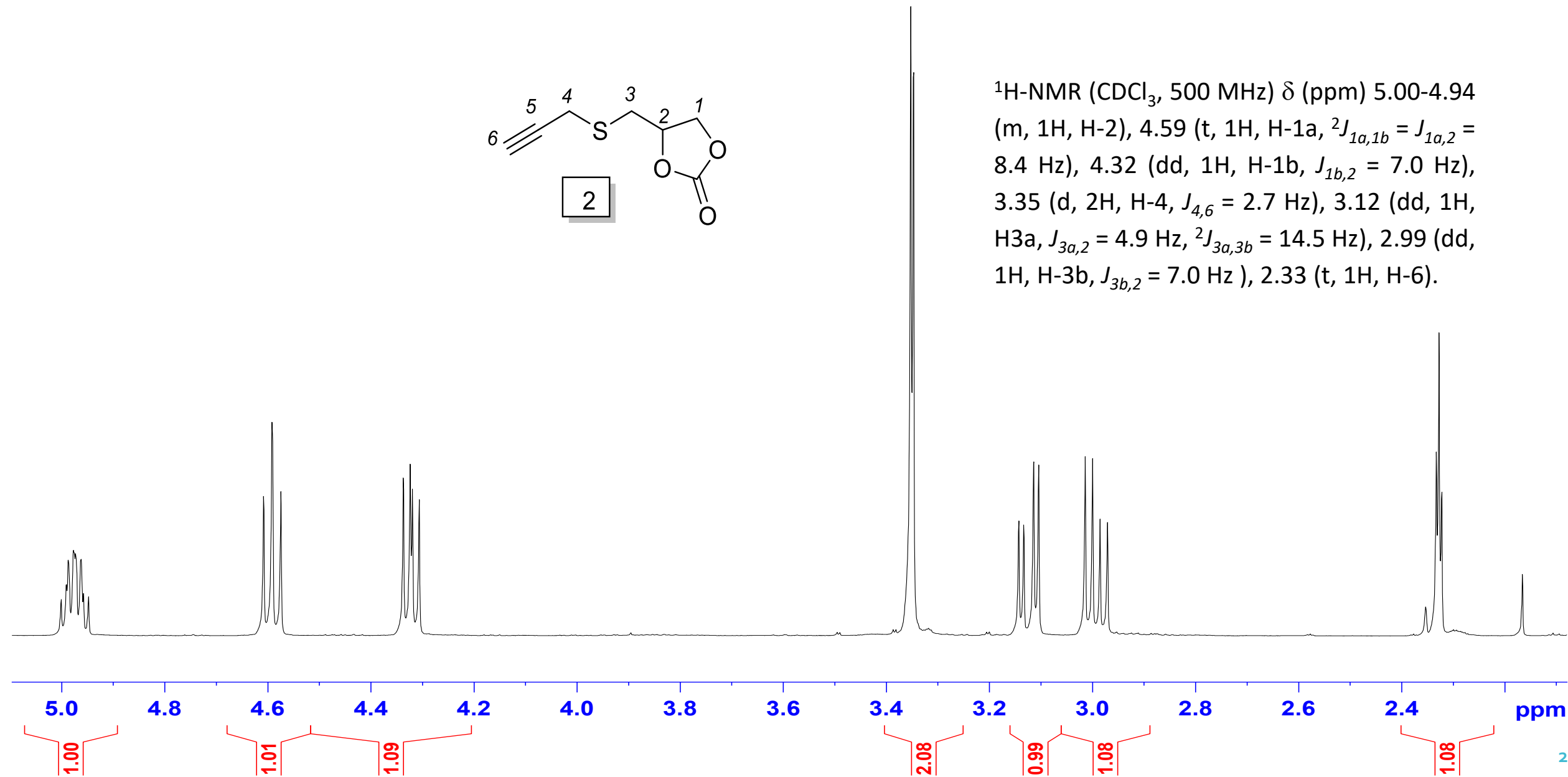


4-[(Prop-2-yn-1-ylthio)methyl]-1,3-dioxolan-2-one (2)

Spectrum ^1H -RMN, 500 MHz, CDCl_3

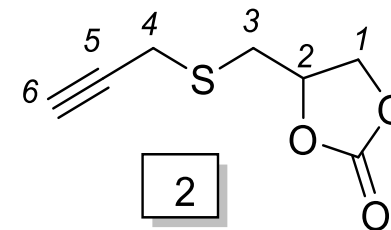
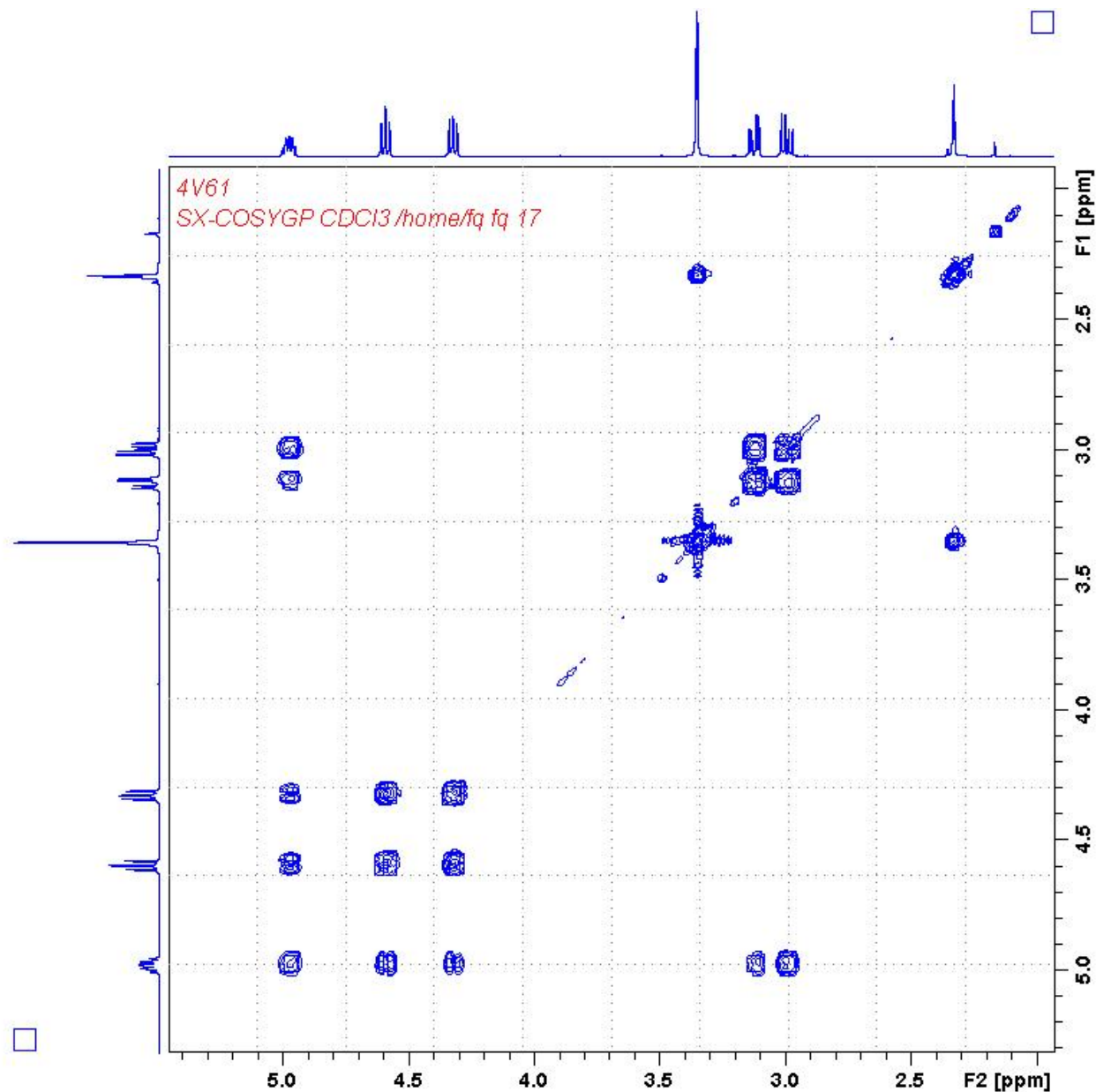


^1H -NMR (CDCl_3 , 500 MHz) δ (ppm) 5.00-4.94 (m, 1H, H-2), 4.59 (t, 1H, H-1a, $^2J_{1a,1b} = J_{1a,2} = 8.4$ Hz), 4.32 (dd, 1H, H-1b, $J_{1b,2} = 7.0$ Hz), 3.35 (d, 2H, H-4, $J_{4,6} = 2.7$ Hz), 3.12 (dd, 1H, H3a, $J_{3a,2} = 4.9$ Hz, $^2J_{3a,3b} = 14.5$ Hz), 2.99 (dd, 1H, H-3b, $J_{3b,2} = 7.0$ Hz), 2.33 (t, 1H, H-6).



4-[(Prop-2-yn-1-ylthio)methyl]-1,3-dioxolan-2-one (2)

COSY (Bidimensional ^1H - ^1H)



^1H -NMR (CDCl_3 , 500 MHz) δ (ppm) 5.00-4.94 (m, 1H, H-2), 4.59 (t, 1H, H-1a, $^2J_{1a,1b} = J_{1a,2} = 8.4$ Hz), 4.32 (dd, 1H, H-1b, $J_{1b,2} = 7.0$ Hz), 3.35 (d, 2H, H-4, $J_{4,6} = 2.7$ Hz), 3.12 (dd, 1H, H3a, $J_{3a,2} = 4.9$ Hz, $^2J_{3a,3b} = 14.5$ Hz), 2.99 (dd, 1H, H-3b, $J_{3b,2} = 7.0$ Hz), 2.33 (t, 1H, H-6).

4-[(Prop-2-yn-1-ylthio)methyl]-1,3-dioxolan-2-one (2)

Spectrum ^{13}C -RMN, 125 MHz, CDCl_3

—154.41

—79.02

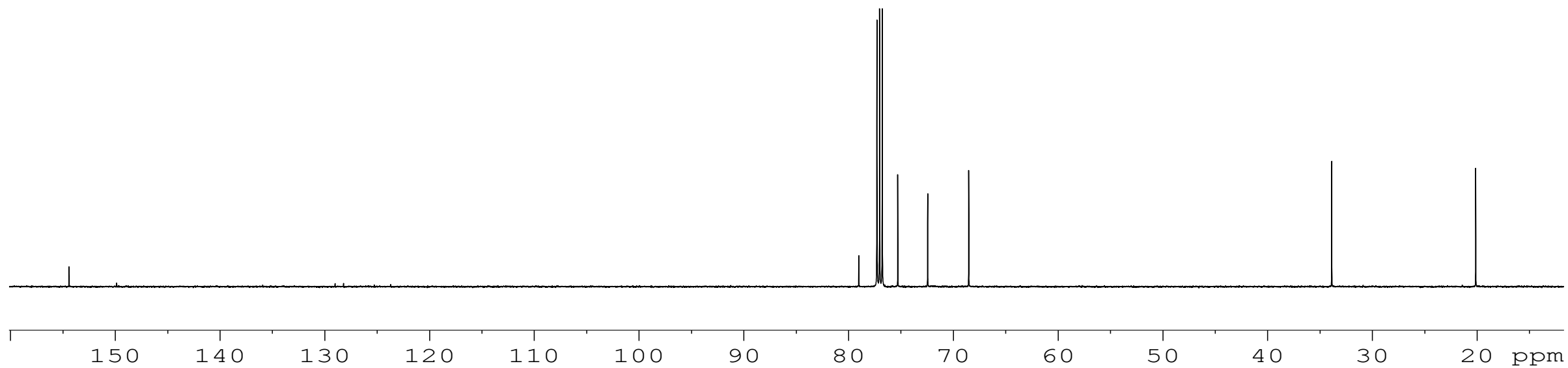
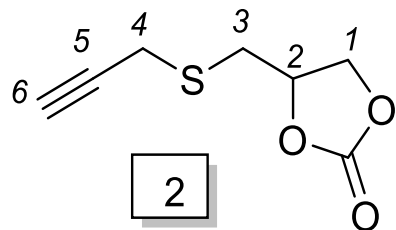
—75.31

—72.45

—68.54

—33.91

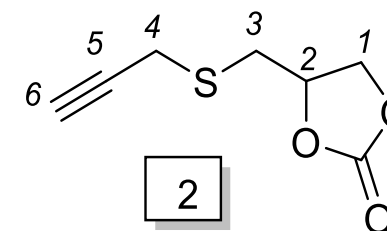
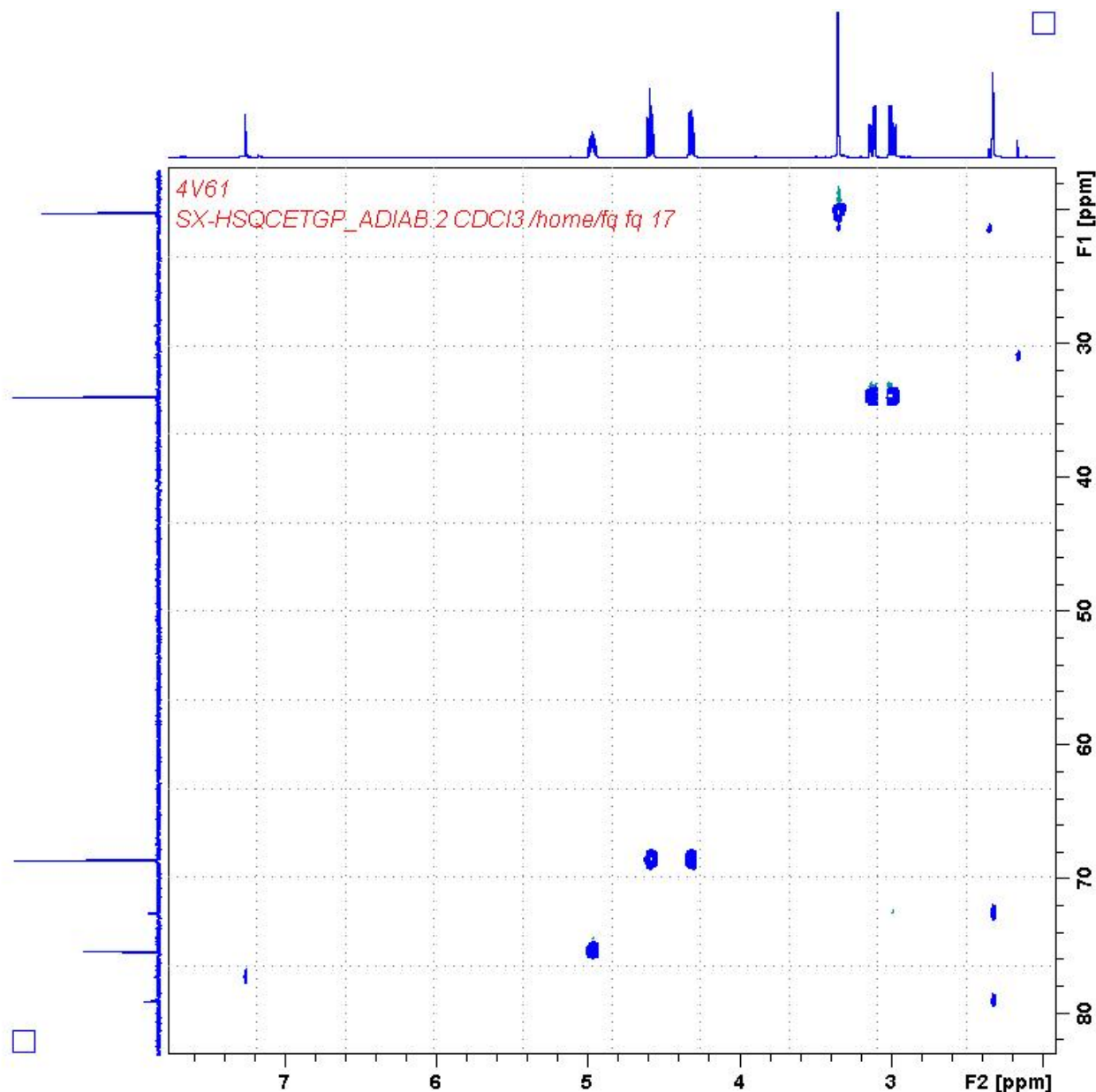
—20.16



^{13}C -NMR (CDCl_3 , 125 MHz) δ (ppm) 154.4 (C=O), 79.0 (C5), 75.3 (C-2), 72.5 (C-6), 68.6 (C-1), 33.9 (C-3), 20.2 (C-4).

4-[(Prop-2-yn-1-ylthio)methyl]-1,3-dioxolan-2-one (2)

HSQC (Bidimensional ^1H - ^{13}C)

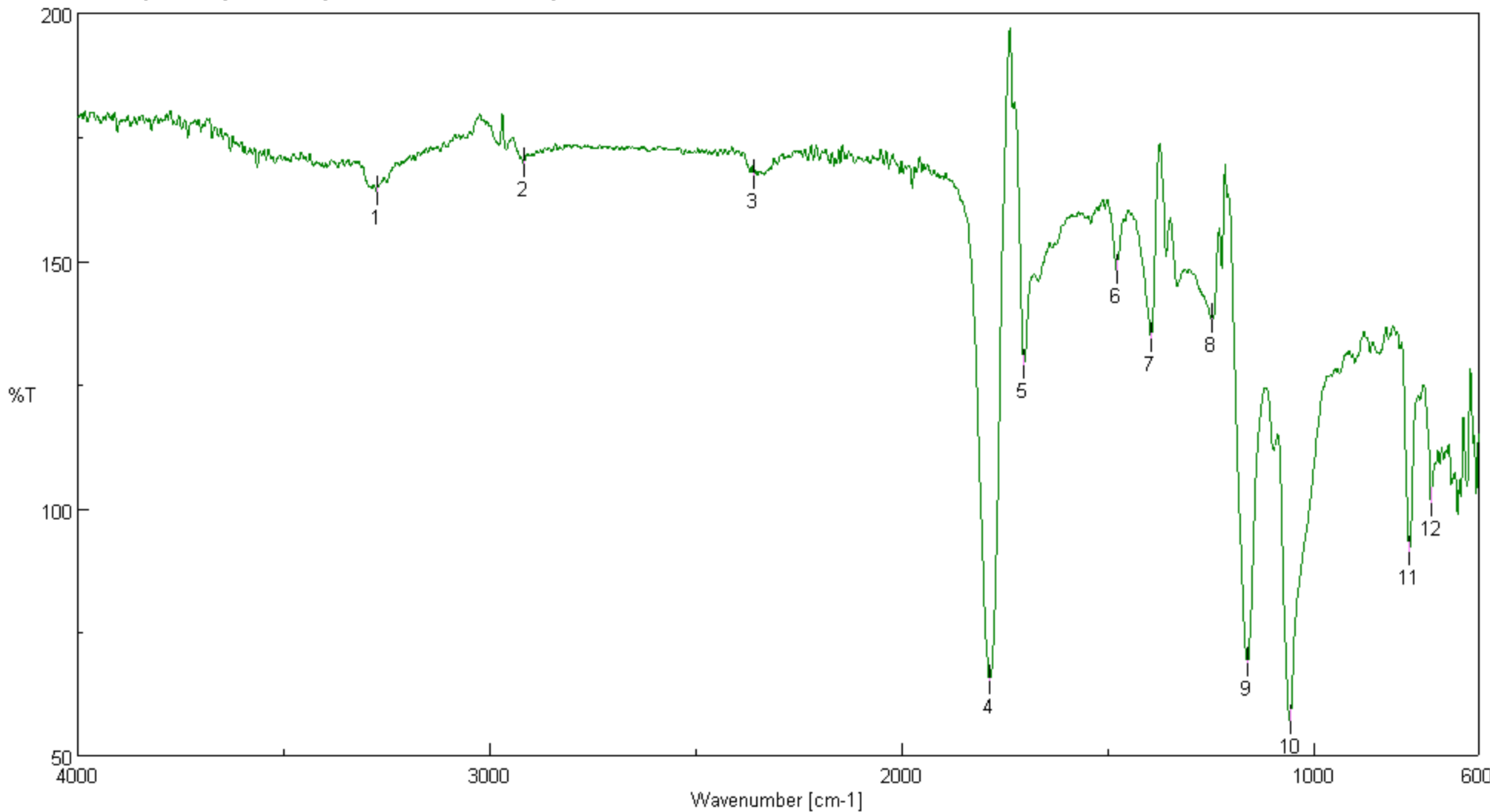
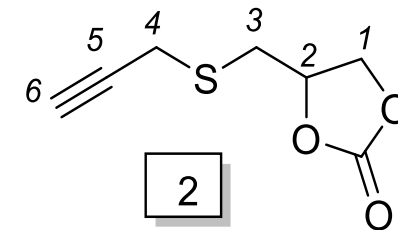


^1H -NMR (CDCl_3 , 500 MHz) δ (ppm) 5.00-4.94 (m, 1H, H-2), 4.59 (t, 1H, H-1a, $^2J_{1a,1b} = J_{1a,2} = 8.4$ Hz), 4.32 (dd, 1H, H-1b, $J_{1b,2} = 7.0$ Hz), 3.35 (d, 2H, H-4, $J_{4,6} = 2.7$ Hz), 3.12 (dd, 1H, H-3a, $J_{3a,2} = 4.9$ Hz, $^2J_{3a,3b} = 14.5$ Hz), 2.99 (dd, 1H, H-3b, $J_{3b,2} = 7.0$ Hz), 2.33 (t, 1H, H-6).

^{13}C -NMR (CDCl_3 , 125 MHz) δ (ppm) 154.4 (C=O), 79.0 (C5), 75.3 (C-2), 72.5 (C-6), 68.6 (C-1), 33.9 (C-3), 20.2 (C-4).

4-[(Prop-2-yn-1-ylthio)methyl]-1,3-dioxolan-2-one (2)

Spectrum ATR-FTIR



[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3274.54	164	2	2918.73	169.763	3	2358.52	167.399	4	1787.69	65.3931
5	1703.8	129.008	6	1479.13	148.18	7	1395.25	134.538	8	1247.72	138.294
9	1160.94	68.8097	10	1058.73	57.0412	11	768.494	91.3622	12	716.425	101.264

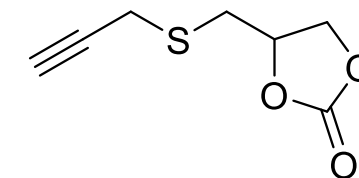
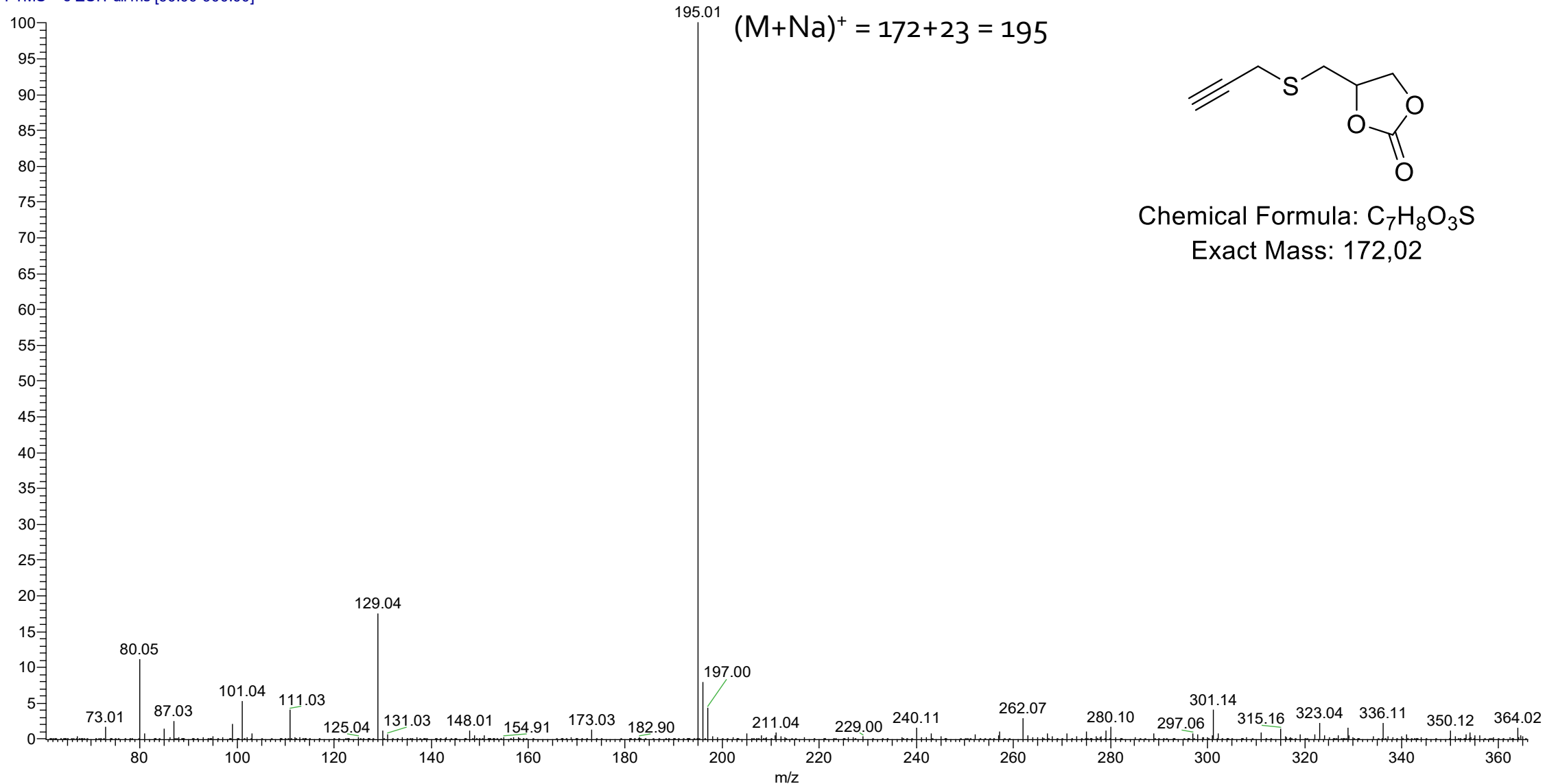
4-[(Prop-2-yn-1-ylthio)methyl]-1,3-dioxolan-2-one (2)

Spectrum ESI-MS

170314_4V61

4V61 PM=172 C7H8O3S

170314_4V61 #54 RT: 0.21 AV: 1 SB: 1 3.00 NL: 1.04E8
T: FTMS + c ESI Full ms [60.00-900.00]



Chemical Formula: C₇H₈O₃S

Exact Mass: 172,02

4-[(Prop-2-yn-1-ylthio)methyl]-1,3-dioxolan-2-one (2)

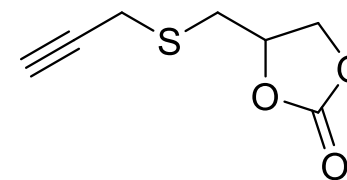
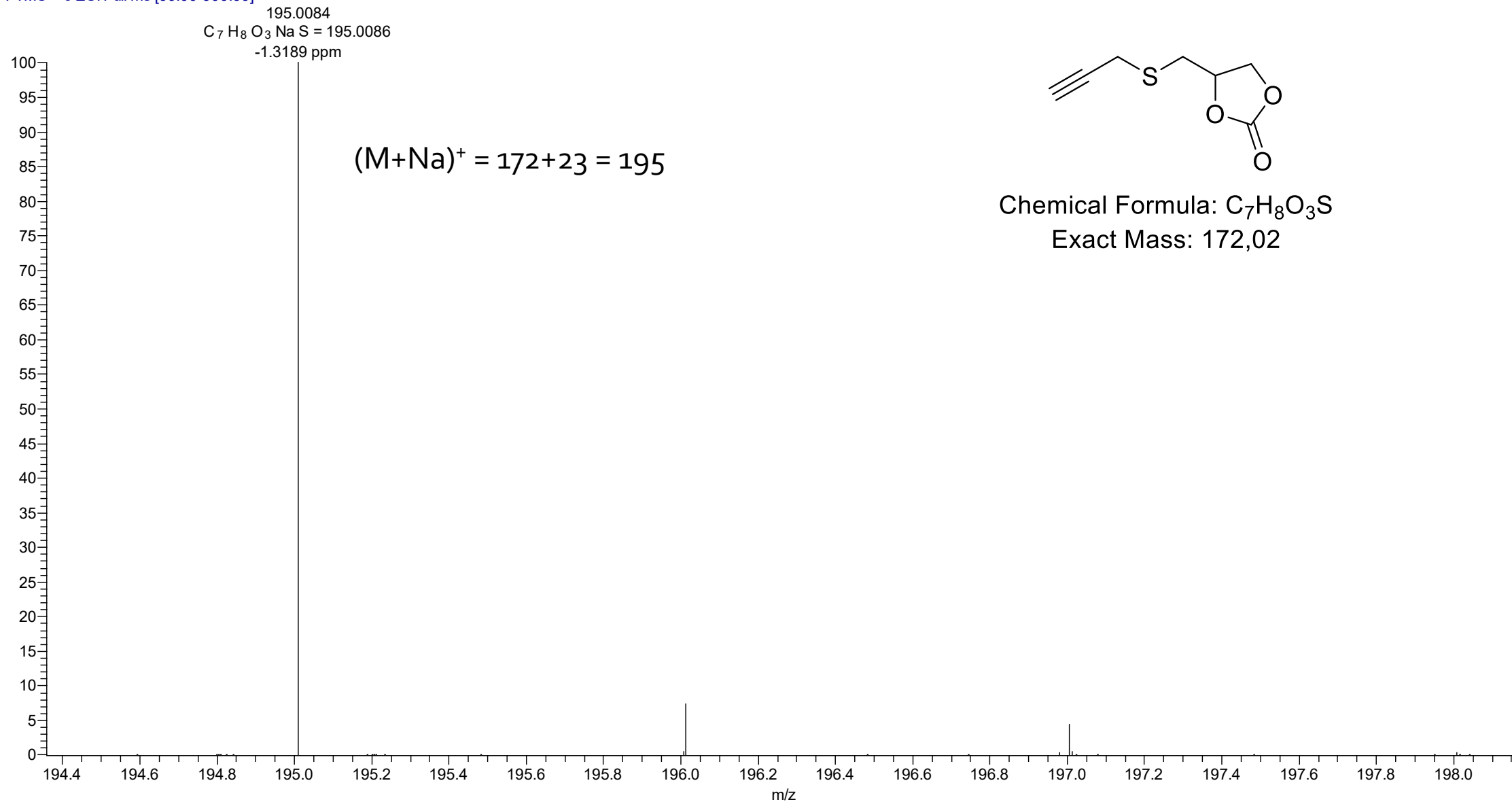
Spectrum ESI-MS

170314_4V61

03/14/17 12:22:58

4V61 PM=172 C7H8O3S

170314_4V61 #61 RT: 0.24 AV: 1 SB: 42 0.03-0.07, 1.25-1.37 NL: 9.94
T: FTMS + c ESI Full ms [60.00-900.00]



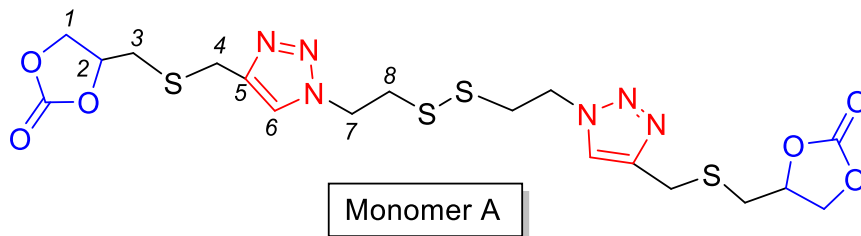
Chemical Formula: C₇H₈O₃S

Exact Mass: 172,02

Five-membered bis(cyclic carbonate) Monomer A

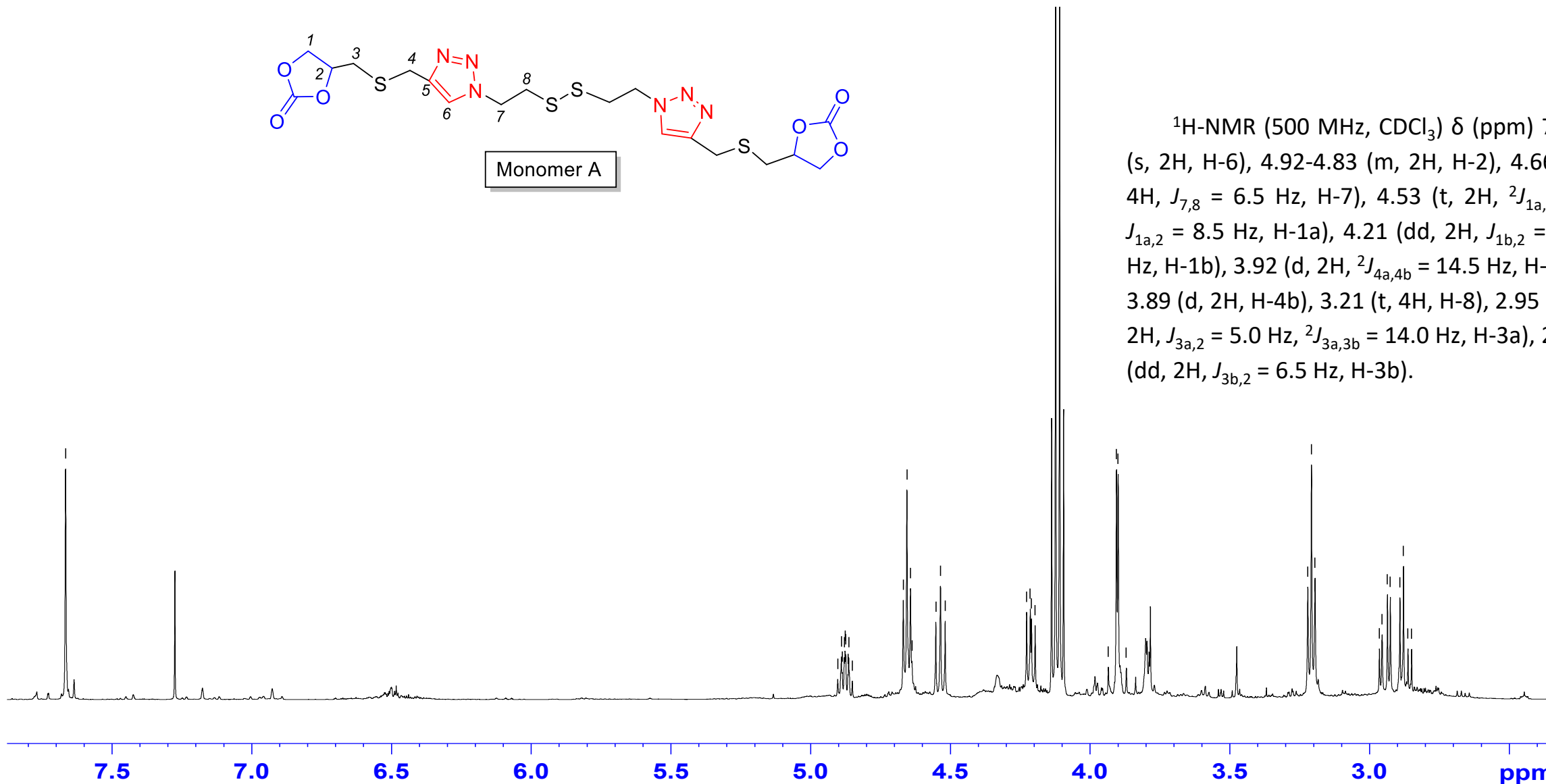
Spectrum $^1\text{H-RMN}$, 500 MHz, CDCl_3

— 7.666



4.903
4.890
4.887
4.879
4.877
4.874
4.866
4.864
4.851
4.668
4.655
4.642
4.637
4.552
4.535
4.518
4.228
4.215
4.210
4.197
3.935
3.906
3.900
3.871
3.221
3.208
3.196
2.965
2.955
2.936
2.926
2.892
2.879
2.863

$^1\text{H-NMR}$ (500 MHz, CDCl_3) δ (ppm) 7.65 (s, 2H, H-6), 4.92-4.83 (m, 2H, H-2), 4.66 (t, 4H, $J_{7,8} = 6.5$ Hz, H-7), 4.53 (t, 2H, $^2J_{1a,1b} = J_{1a,2} = 8.5$ Hz, H-1a), 4.21 (dd, 2H, $J_{1b,2} = 6.5$ Hz, H-1b), 3.92 (d, 2H, $^2J_{4a,4b} = 14.5$ Hz, H-4a), 3.89 (d, 2H, H-4b), 3.21 (t, 4H, H-8), 2.95 (dd, 2H, $J_{3a,2} = 5.0$ Hz, $^2J_{3a,3b} = 14.0$ Hz, H-3a), 2.87 (dd, 2H, $J_{3b,2} = 6.5$ Hz, H-3b).



Five-membered bis(cyclic carbonate) Monomer A

Spectrum $^1\text{H-RMN}$, 500 MHz, CDCl_3

4.903
4.890
4.887
4.879
4.877
4.874
4.866
4.864
4.851
4.668
4.655
4.642
4.637
4.552
4.535
4.518

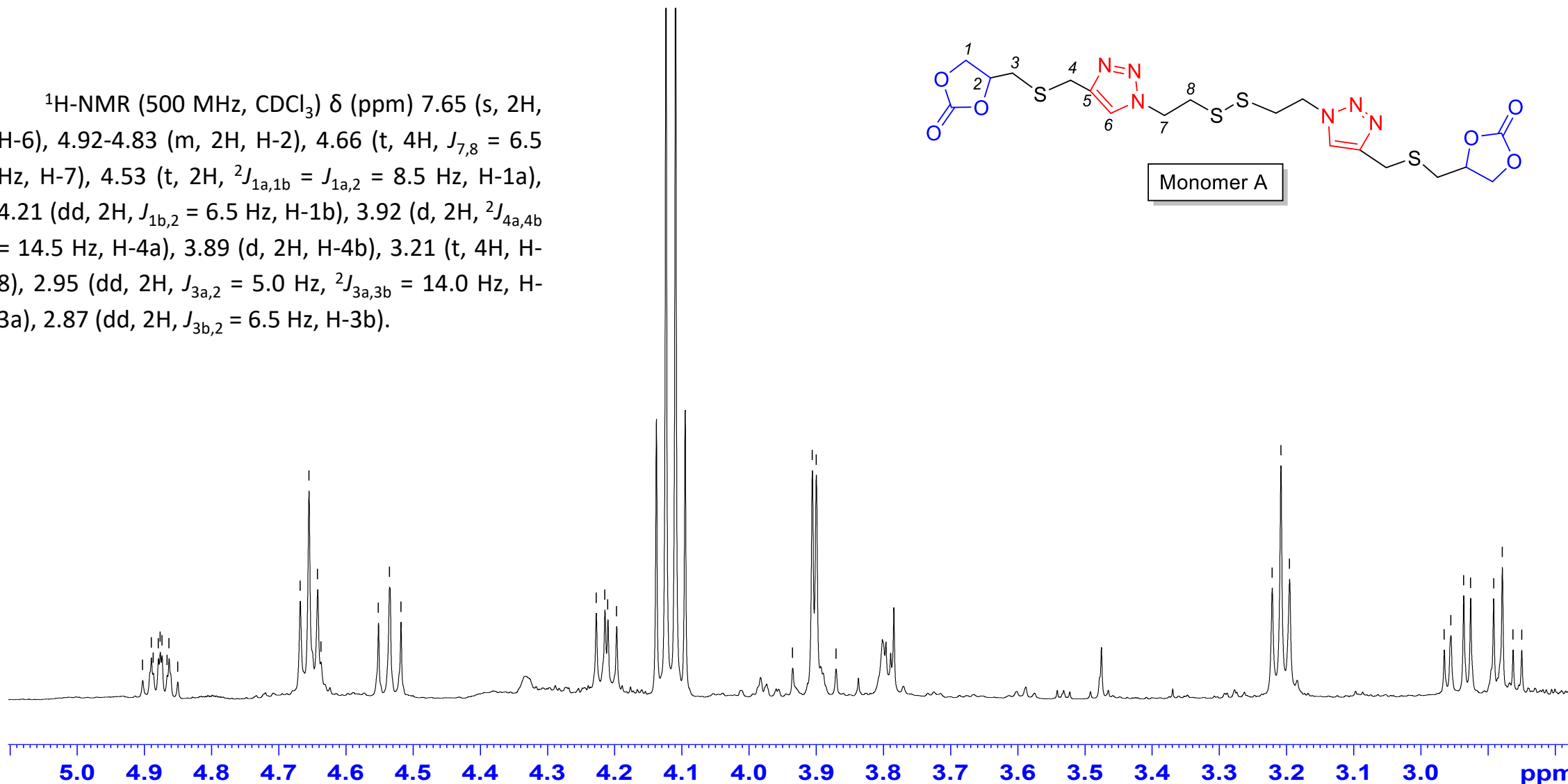
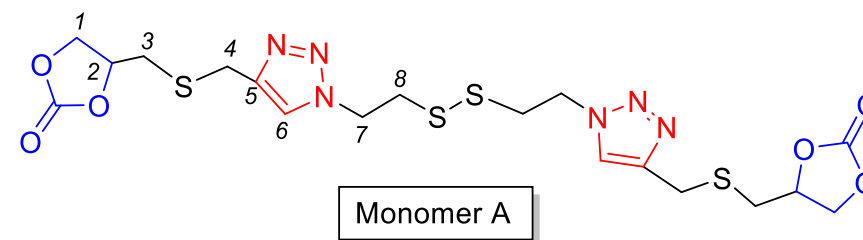
4.228
4.215
4.210
4.197

3.935
3.906
3.900
3.871

3.221
3.208
3.196

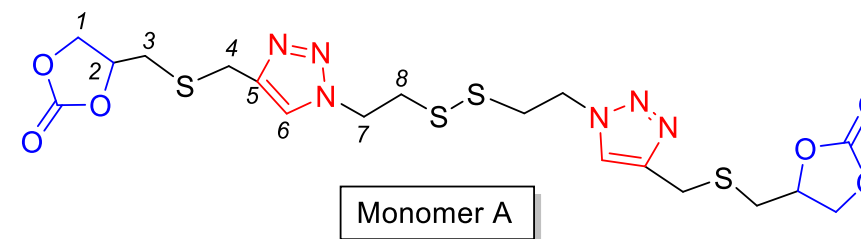
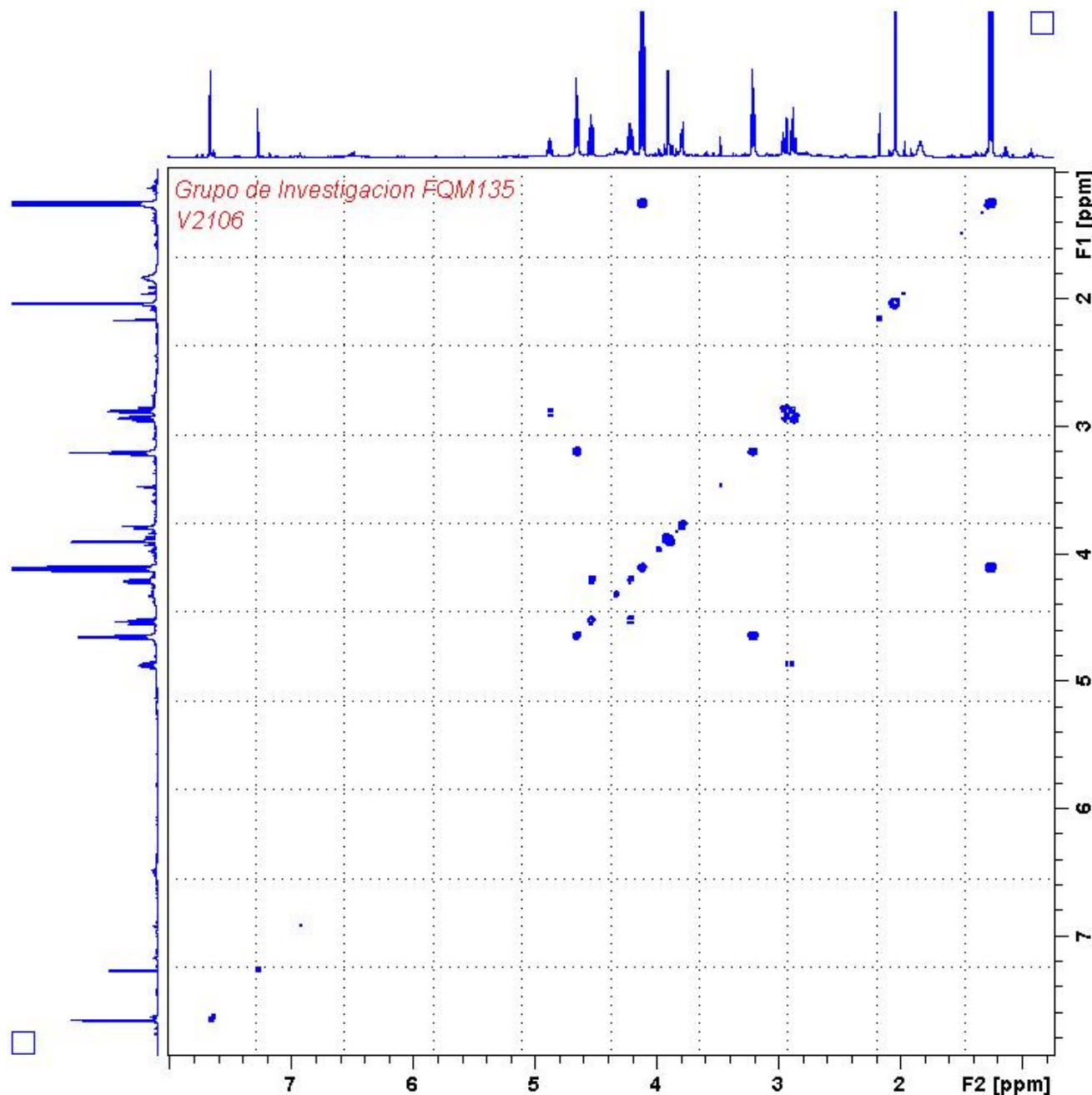
2.965
2.955
2.936
2.926
2.892
2.879

$^1\text{H-NMR}$ (500 MHz, CDCl_3) δ (ppm) 7.65 (s, 2H, H-6), 4.92-4.83 (m, 2H, H-2), 4.66 (t, 4H, $J_{7,8} = 6.5$ Hz, H-7), 4.53 (t, 2H, $^2J_{1a,1b} = J_{1a,2} = 8.5$ Hz, H-1a), 4.21 (dd, 2H, $J_{1b,2} = 6.5$ Hz, H-1b), 3.92 (d, 2H, $^2J_{4a,4b} = 14.5$ Hz, H-4a), 3.89 (d, 2H, H-4b), 3.21 (t, 4H, H-8), 2.95 (dd, 2H, $J_{3a,2} = 5.0$ Hz, $^2J_{3a,3b} = 14.0$ Hz, H-3a), 2.87 (dd, 2H, $J_{3b,2} = 6.5$ Hz, H-3b).



Five-membered bis(cyclic carbonate) Monomer A

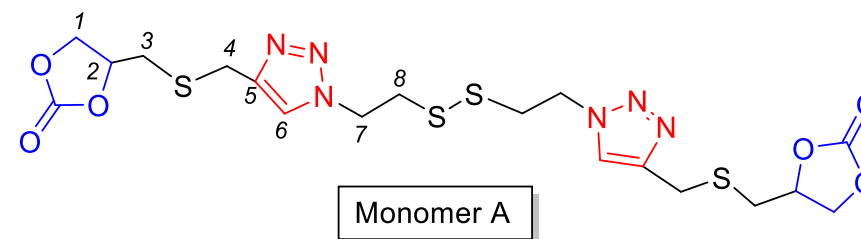
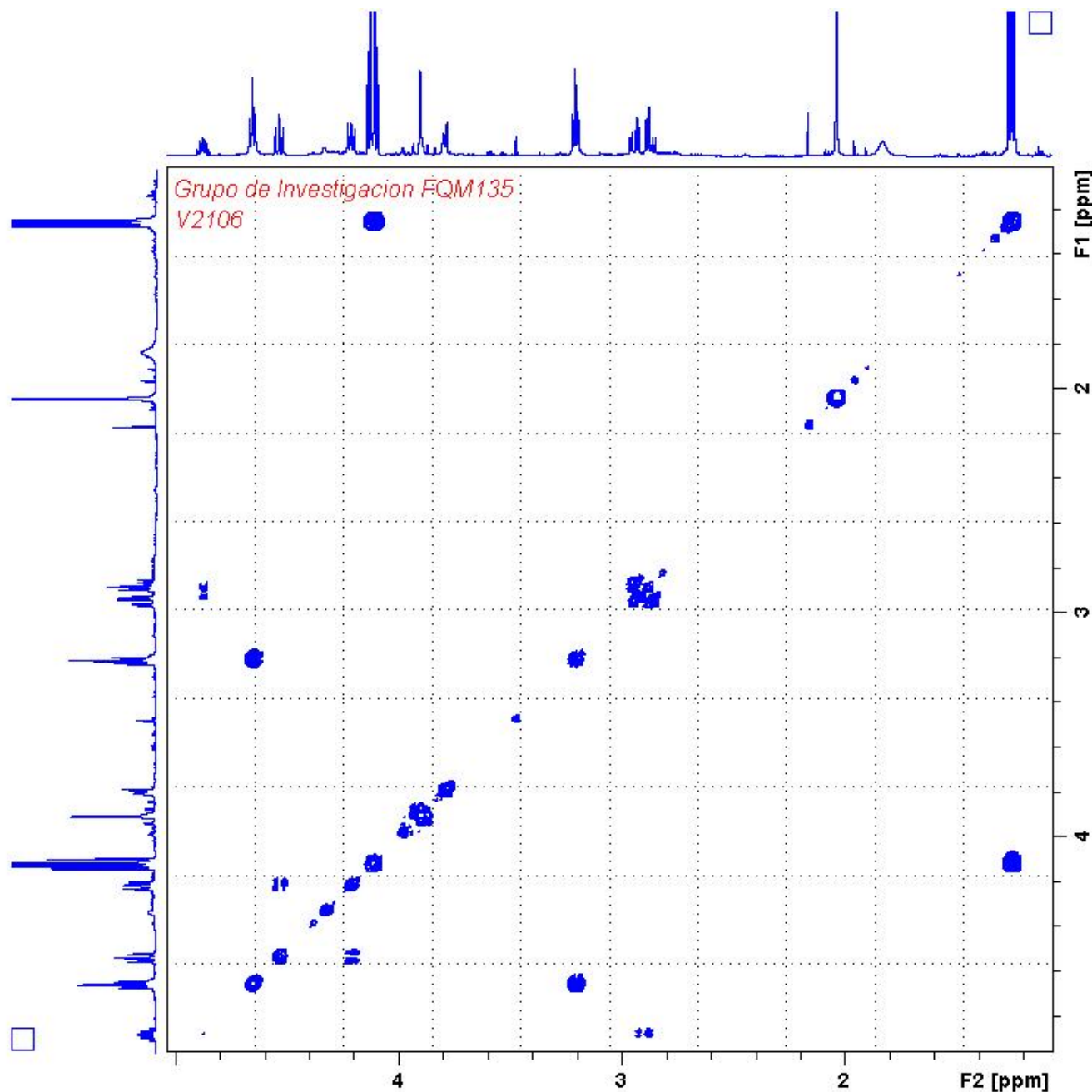
COSY (Bidimensional ^1H - ^1H)



^1H -NMR (500 MHz, CDCl_3) δ (ppm) 7.65 (s, 2H, H-6), 4.92-4.83 (m, 2H, H-2), 4.66 (t, 4H, $J_{7,8} = 6.5$ Hz, H-7), 4.53 (t, 2H, $^2J_{1a,1b} = J_{1a,2} = 8.5$ Hz, H-1a), 4.21 (dd, 2H, $J_{1b,2} = 6.5$ Hz, H-1b), 3.92 (d, 2H, $^2J_{4a,4b} = 14.5$ Hz, H-4a), 3.89 (d, 2H, H-4b), 3.21 (t, 4H, H-8), 2.95 (dd, 2H, $J_{3a,2} = 5.0$ Hz, $^2J_{3a,3b} = 14.0$ Hz, H-3a), 2.87 (dd, 2H, $J_{3b,2} = 6.5$ Hz, H-3b).

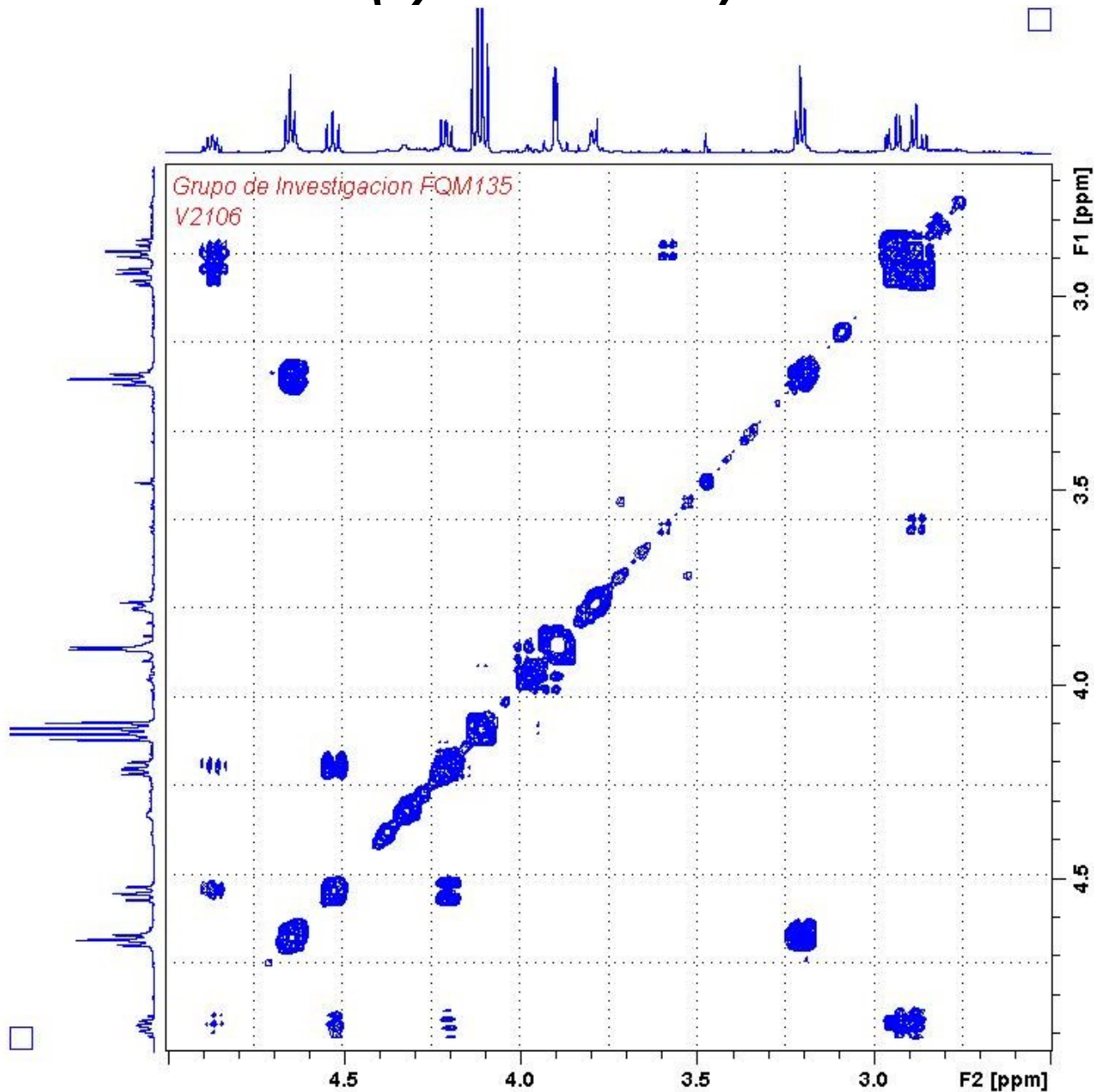
Five-membered bis(cyclic carbonate) Monomer A

COSY (Bidimensional ^1H - ^1H)

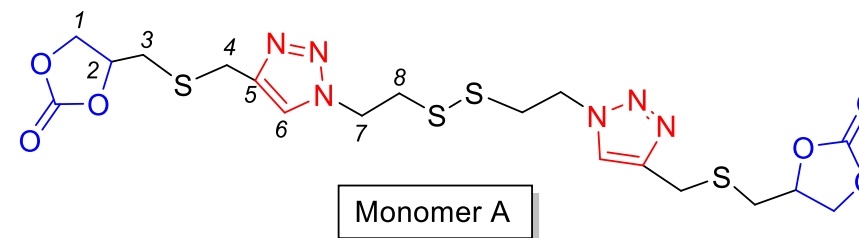


^1H -NMR (500 MHz, CDCl_3) δ (ppm) 7.65 (s, 2H, H-6), 4.92-4.83 (m, 2H, H-2), 4.66 (t, 4H, $J_{7,8} = 6.5$ Hz, H-7), 4.53 (t, 2H, $^2J_{1a,1b} = J_{1a,2} = 8.5$ Hz, H-1a), 4.21 (dd, 2H, $J_{1b,2} = 6.5$ Hz, H-1b), 3.92 (d, 2H, $^2J_{4a,4b} = 14.5$ Hz, H-4a), 3.89 (d, 2H, H-4b), 3.21 (t, 4H, H-8), 2.95 (dd, 2H, $J_{3a,2} = 5.0$ Hz, $^2J_{3a,3b} = 14.0$ Hz, H-3a), 2.87 (dd, 2H, $J_{3b,2} = 6.5$ Hz, H-3b).

Five-membered bis(cyclic carbonate) Monomer A



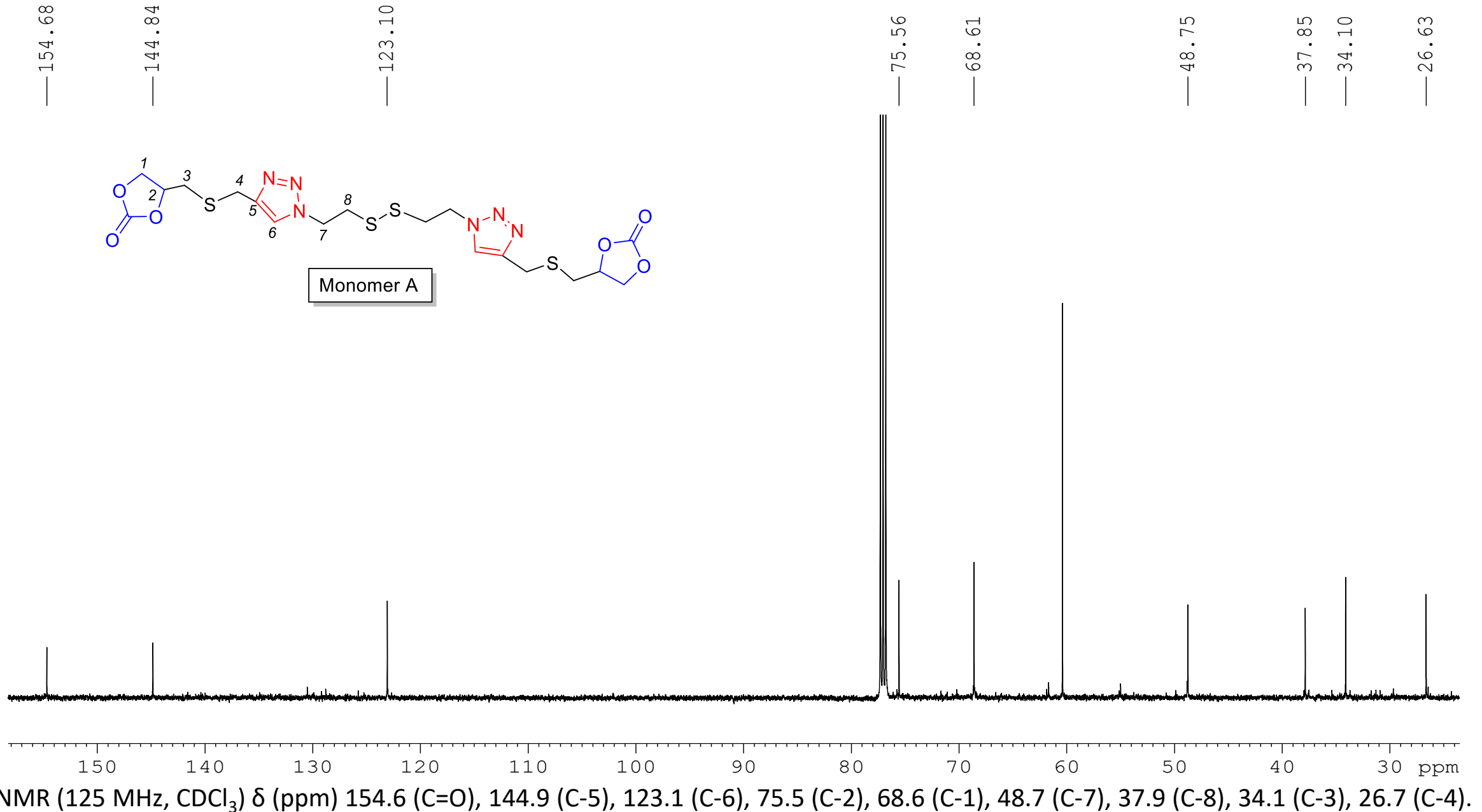
COSY (Bidimensional ^1H - ^1H)



^1H -NMR (500 MHz, CDCl_3) δ (ppm) 7.65 (s, 2H, H-6), 4.92-4.83 (m, 2H, H-2), 4.66 (t, 4H, $J_{7,8} = 6.5$ Hz, H-7), 4.53 (t, 2H, $^2J_{1a,1b} = J_{1a,2} = 8.5$ Hz, H-1a), 4.21 (dd, 2H, $J_{1b,2} = 6.5$ Hz, H-1b), 3.92 (d, 2H, $^2J_{4a,4b} = 14.5$ Hz, H-4a), 3.89 (d, 2H, H-4b), 3.21 (t, 4H, H-8), 2.95 (dd, 2H, $J_{3a,2} = 5.0$ Hz, $^2J_{3a,3b} = 14.0$ Hz, H-3a), 2.87 (dd, 2H, $J_{3b,2} = 6.5$ Hz, H-3b).

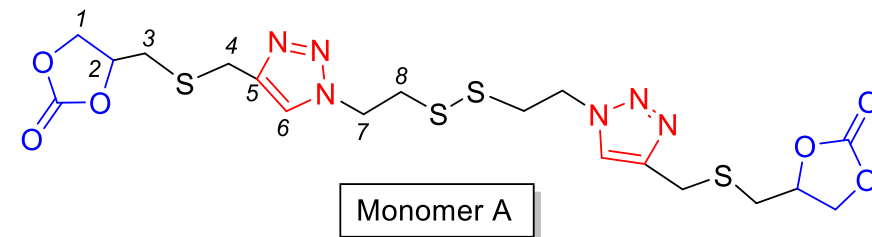
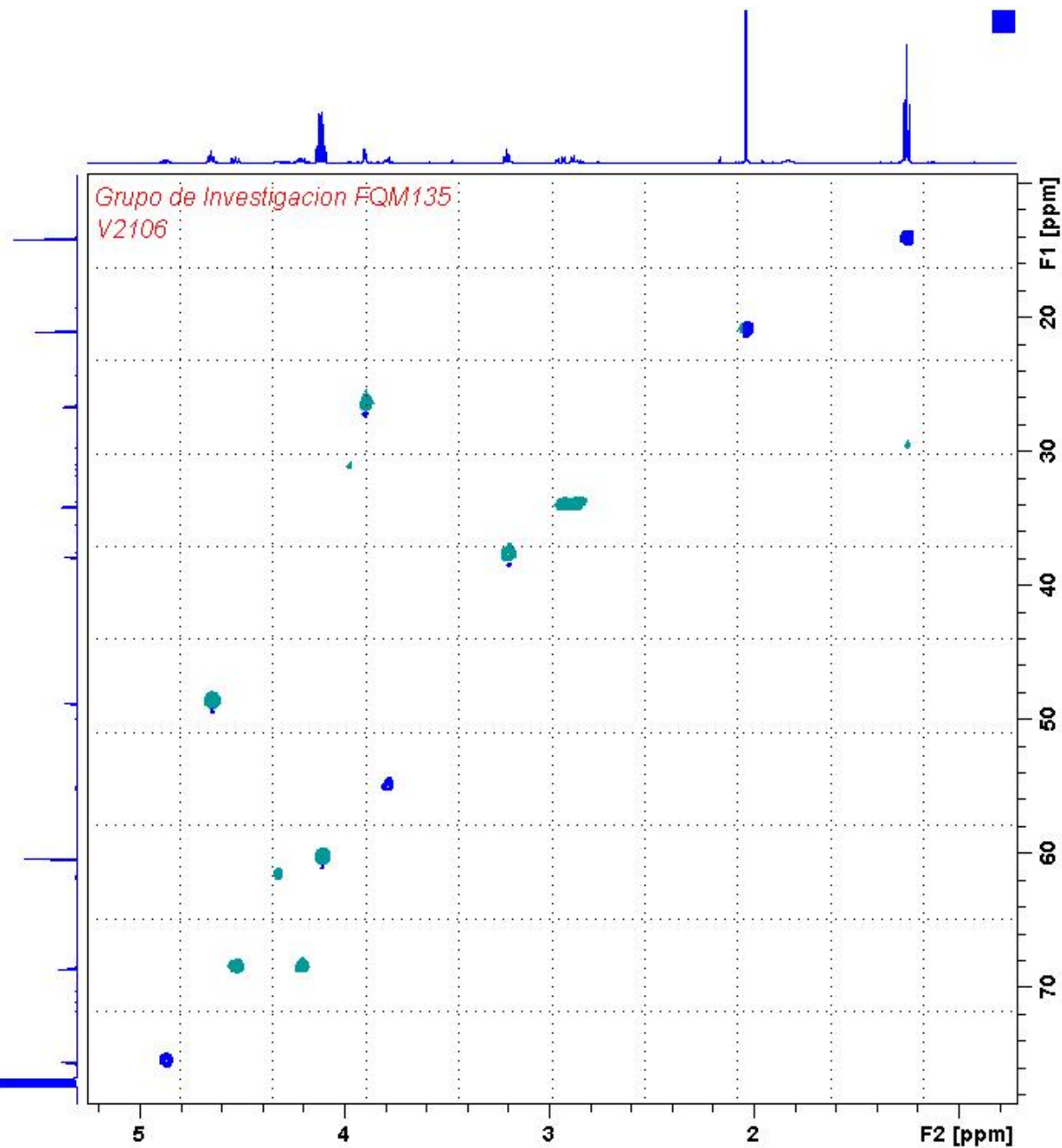
Five-membered bis(cyclic carbonate) Monomer A

Spectrum ^{13}C -RMN, 125 MHz, CDCl_3



Five-membered bis(cyclic carbonate) Monomer A

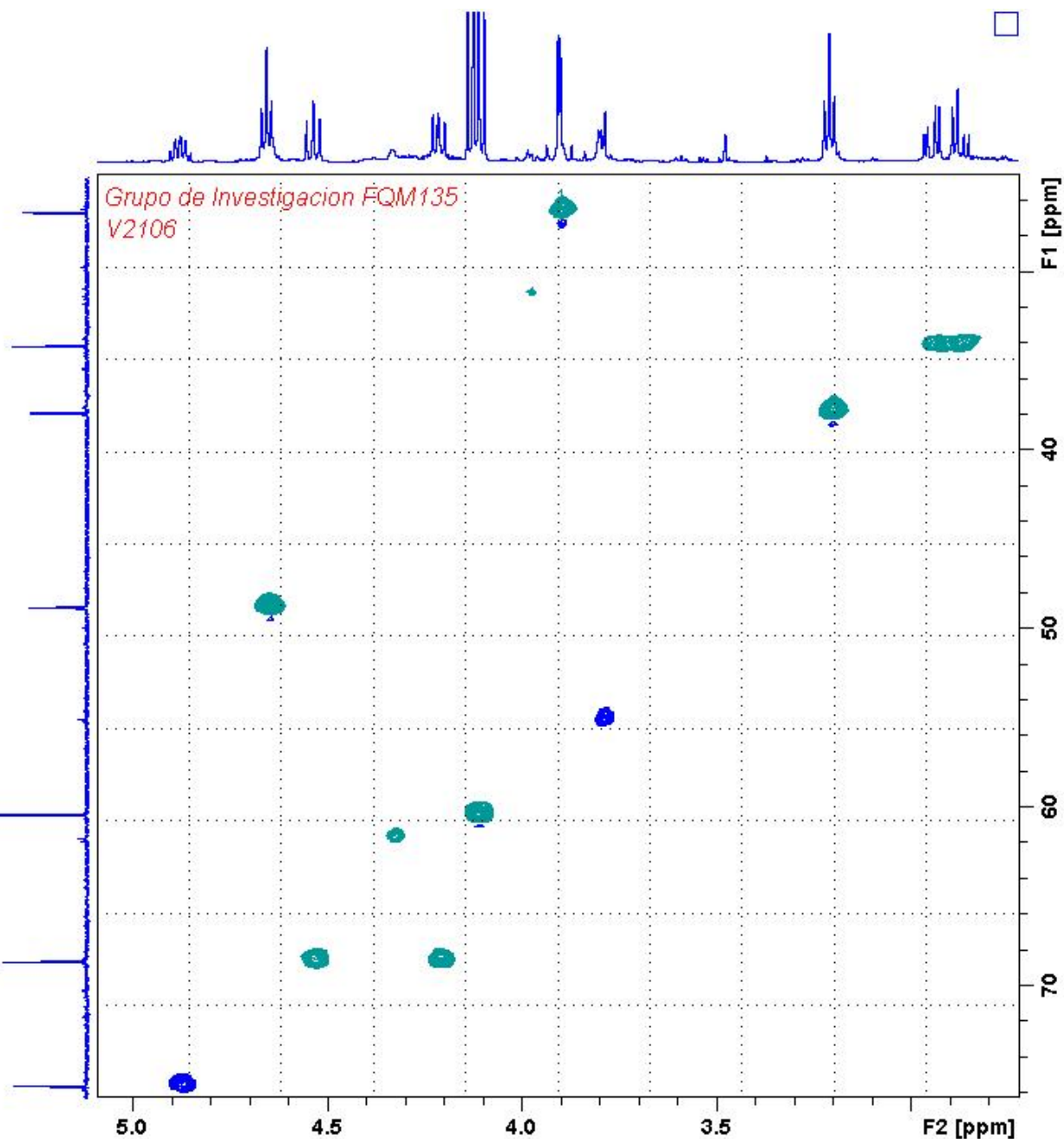
HSQC (Bidimensional ^1H - ^{13}C)



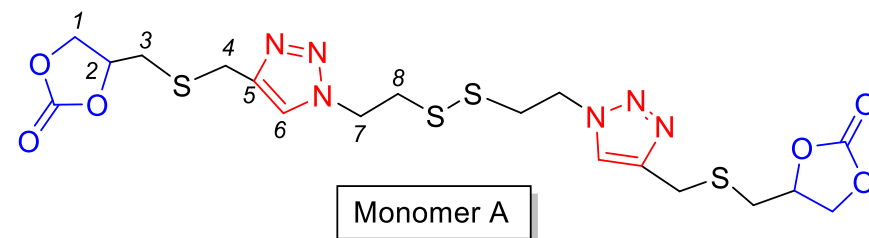
^1H -NMR (500 MHz, CDCl_3) δ (ppm) 7.65 (s, 2H, H-6), 4.92-4.83 (m, 2H, H-2), 4.66 (t, 4H, $J_{7,8} = 6.5$ Hz, H-7), 4.53 (t, 2H, $^2J_{1a,1b} = J_{1a,2} = 8.5$ Hz, H-1a), 4.21 (dd, 2H, $J_{1b,2} = 6.5$ Hz, H-1b), 3.92 (d, 2H, $^2J_{4a,4b} = 14.5$ Hz, H-4a), 3.89 (d, 2H, H-4b), 3.21 (t, 4H, H-8), 2.95 (dd, 2H, $J_{3a,2} = 5.0$ Hz, $^2J_{3a,3b} = 14.0$ Hz, H-3a), 2.87 (dd, 2H, $J_{3b,2} = 6.5$ Hz, H-3b).

^{13}C -NMR (125 MHz, CDCl_3) δ (ppm) 154.6 (C=O), 144.9 (C-5), 123.1 (C-6), 75.5 (C-2), 68.6 (C-1), 48.7 (C-7), 37.9 (C-8), 34.1 (C-3), 26.7 (C-4).

Five-membered bis(cyclic carbonate) Monomer A



HSQC (Bidimensional ^1H - ^{13}C)

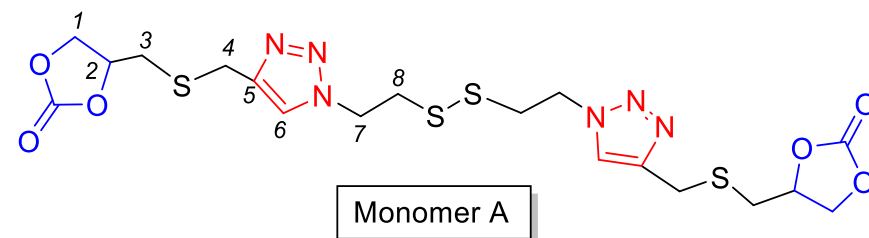
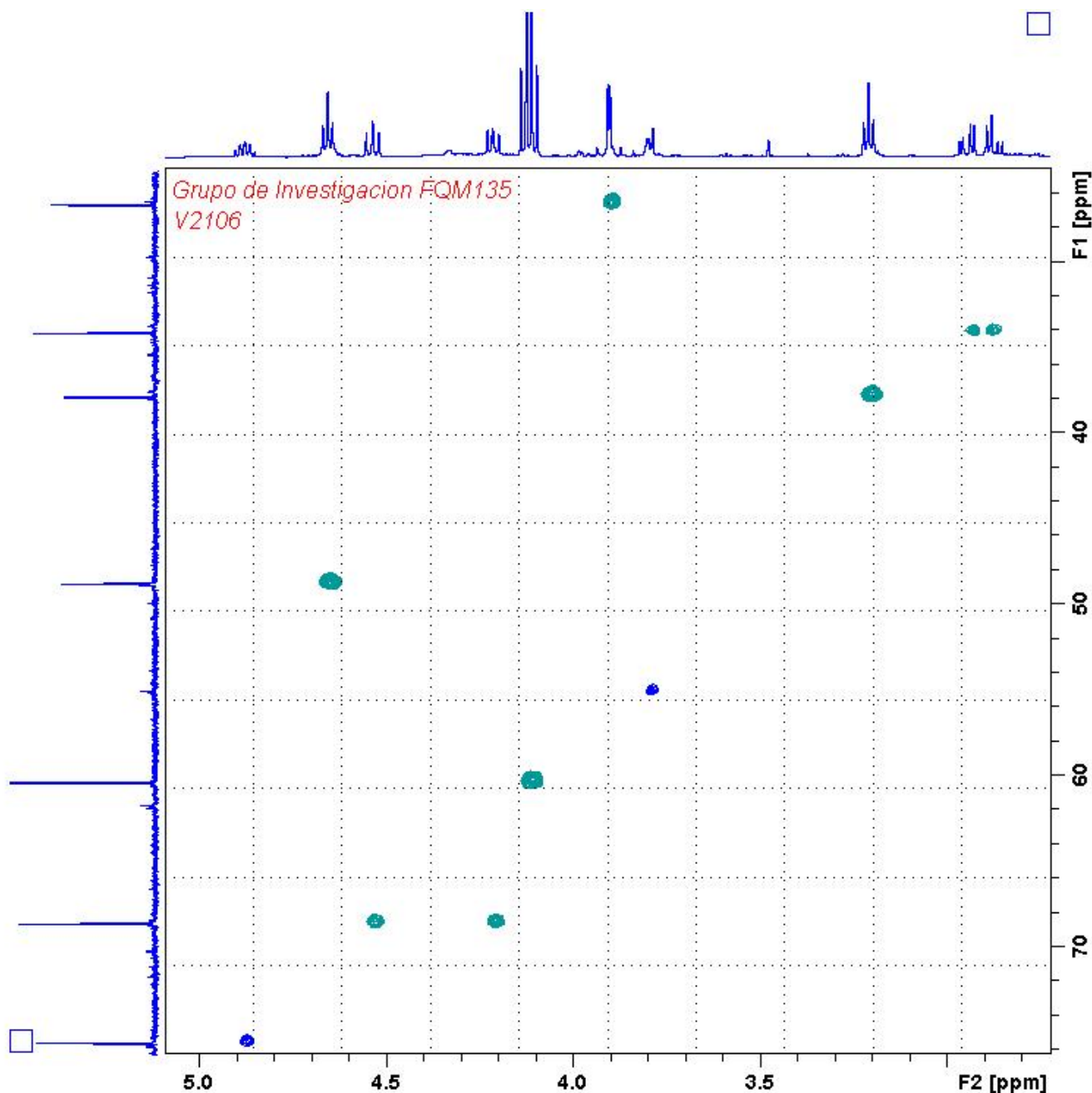


^1H -NMR (500 MHz, CDCl_3) δ (ppm) 7.65 (s, 2H, H-6), 4.92-4.83 (m, 2H, H-2), 4.66 (t, 4H, $J_{7,8} = 6.5$ Hz, H-7), 4.53 (t, 2H, $^2J_{1a,1b} = J_{1a,2} = 8.5$ Hz, H-1a), 4.21 (dd, 2H, $J_{1b,2} = 6.5$ Hz, H-1b), 3.92 (d, 2H, $^2J_{4a,4b} = 14.5$ Hz, H-4a), 3.89 (d, 2H, H-4b), 3.21 (t, 4H, H-8), 2.95 (dd, 2H, $J_{3a,2} = 5.0$ Hz, $^2J_{3a,3b} = 14.0$ Hz, H-3a), 2.87 (dd, 2H, $J_{3b,2} = 6.5$ Hz, H-3b).

^{13}C -NMR (125 MHz, CDCl_3) δ (ppm) 154.6 (C=O), 144.9 (C-5), 123.1 (C-6), 75.5 (C-2), 68.6 (C-1), 48.7 (C-7), 37.9 (C-8), 34.1 (C-3), 26.7 (C-4).

Five-membered bis(cyclic carbonate) Monomer A

HSQC (Bidimensional ^1H - ^{13}C)

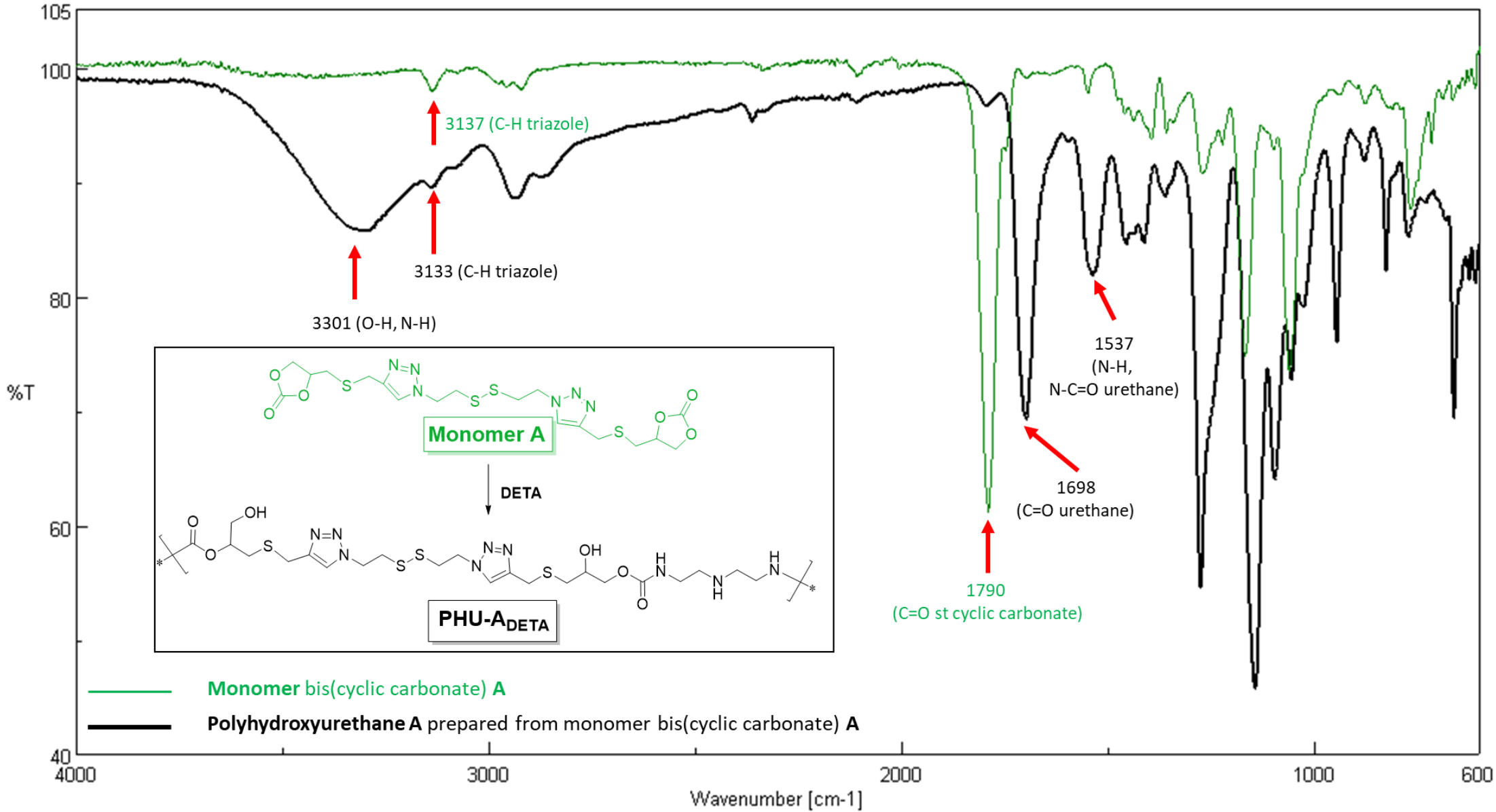


^1H -NMR (500 MHz, CDCl_3) δ (ppm) 7.65 (s, 2H, H-6), 4.92-4.83 (m, 2H, H-2), 4.66 (t, 4H, $J_{7,8} = 6.5$ Hz, H-7), 4.53 (t, 2H, $^2J_{1a,1b} = J_{1a,2} = 8.5$ Hz, H-1a), 4.21 (dd, 2H, $J_{1b,2} = 6.5$ Hz, H-1b), 3.92 (d, 2H, $^2J_{4a,4b} = 14.5$ Hz, H-4a), 3.89 (d, 2H, H-4b), 3.21 (t, 4H, H-8), 2.95 (dd, 2H, $J_{3a,2} = 5.0$ Hz, $^2J_{3a,3b} = 14.0$ Hz, H-3a), 2.87 (dd, 2H, $J_{3b,2} = 6.5$ Hz, H-3b).

^{13}C -NMR (125 MHz, CDCl_3) δ (ppm) 154.6 (C=O), 144.9 (C-5), 123.1 (C-6), 75.5 (C-2), 68.6 (C-1), 48.7 (C-7), 37.9 (C-8), 34.1 (C-3), 26.7 (C-4).

PHU MA-DETA (black) and Monomer A (green)

Spectra ATR-FTIR



Five-membered bis(cyclic carbonate) Monomer A

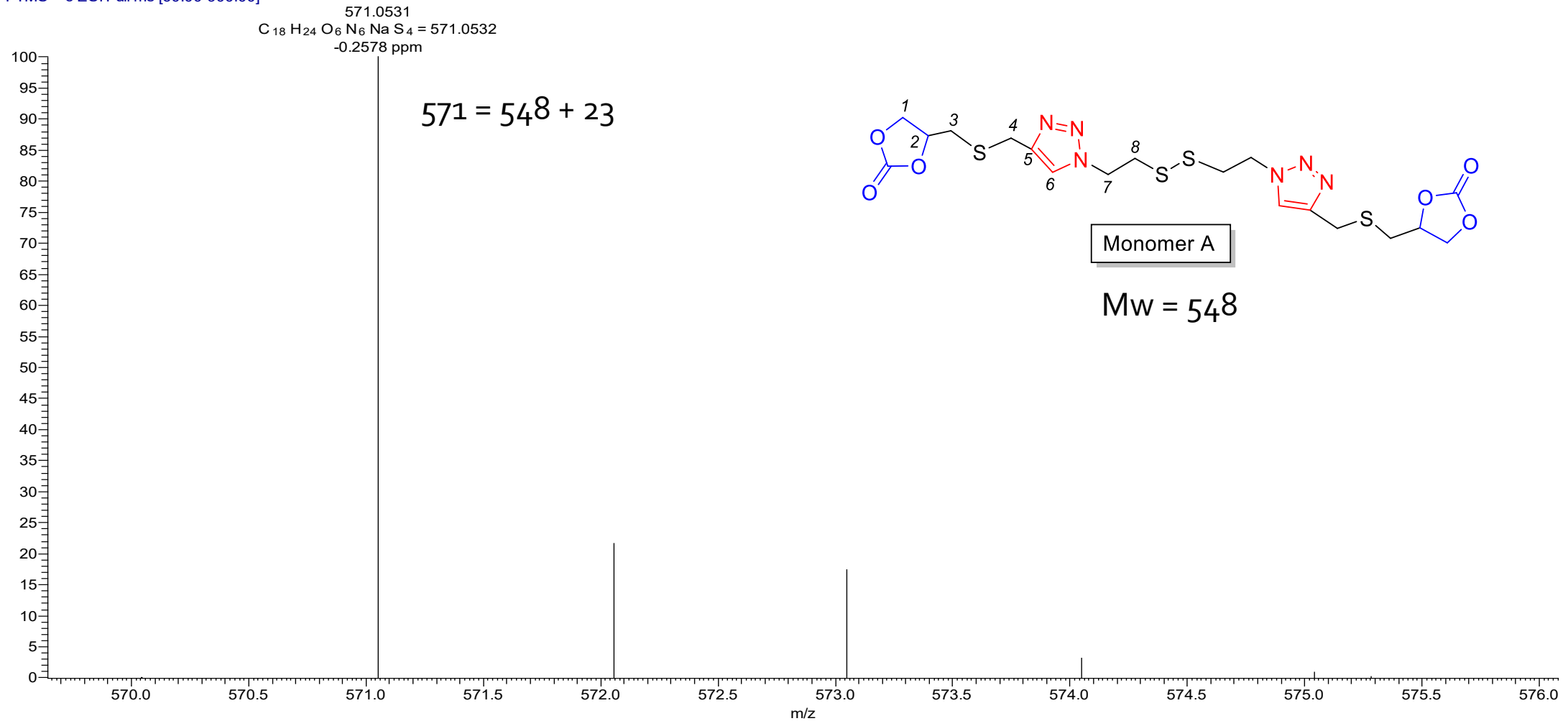
Spectrum ESI-HRMS

210219_V2003

02/19/21 14:14:44

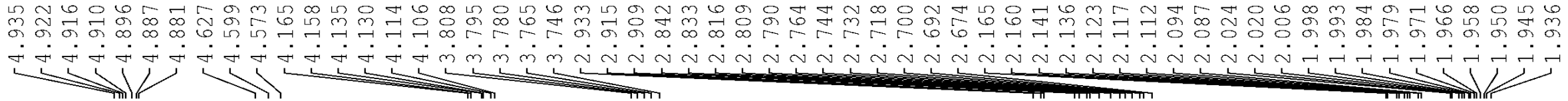
V2003 PM=548 C18H24N6O6S4

210219_V2003 #100 RT: 0.49 AV: 1 SB: 1 3.00 NL: 9.51E6
T: FTMS + c ESI Full ms [60.00-900.00]

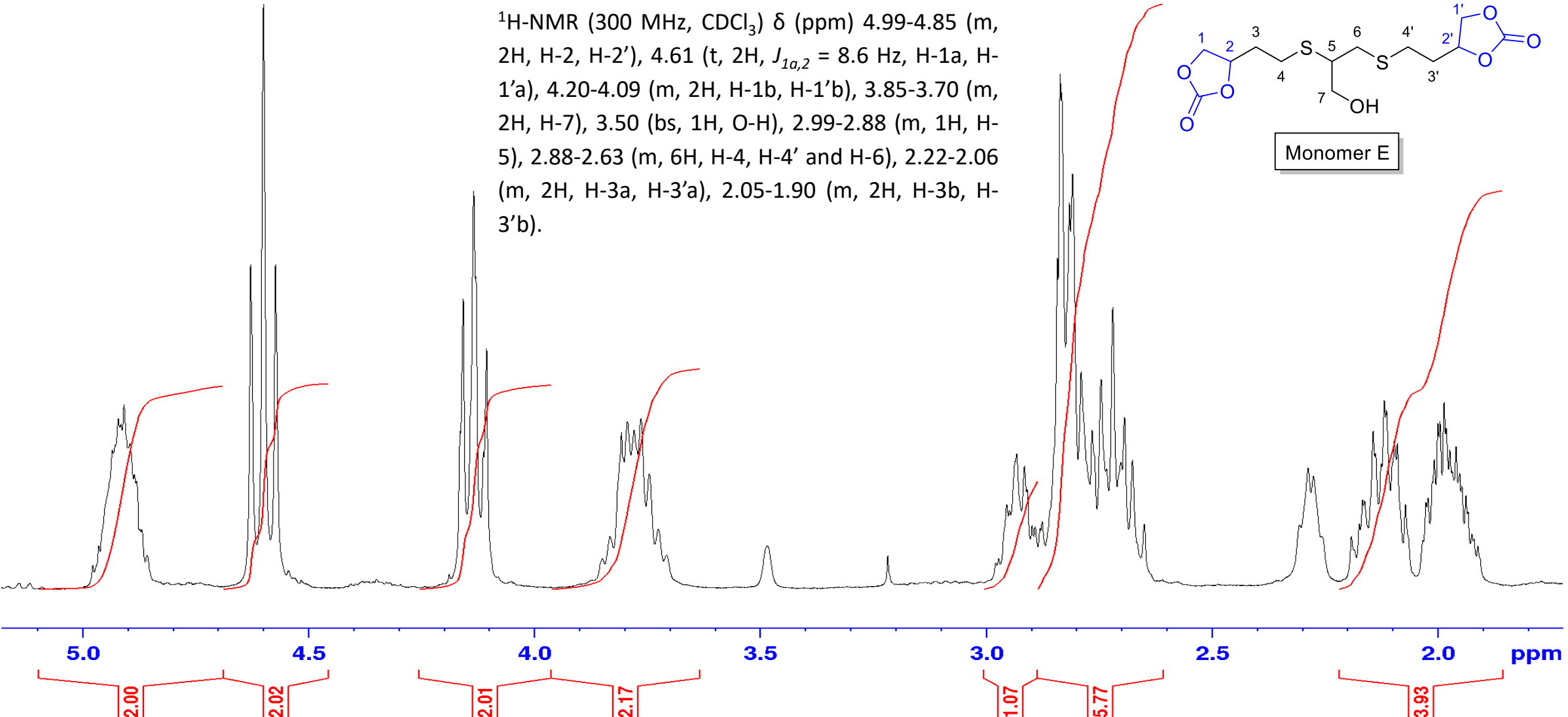
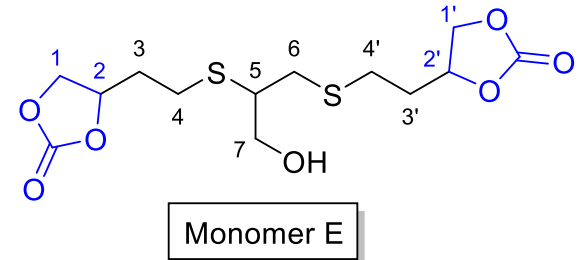


Five-membered bis(cyclic carbonate) Monomer E

Spectrum $^1\text{H-RMN}$, 300 MHz, CDCl_3

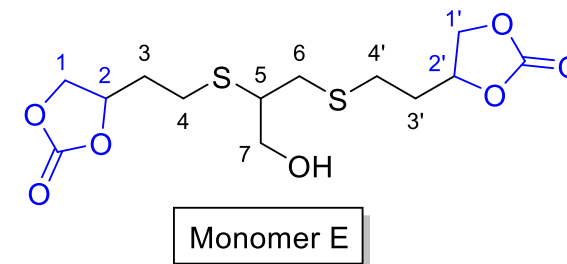
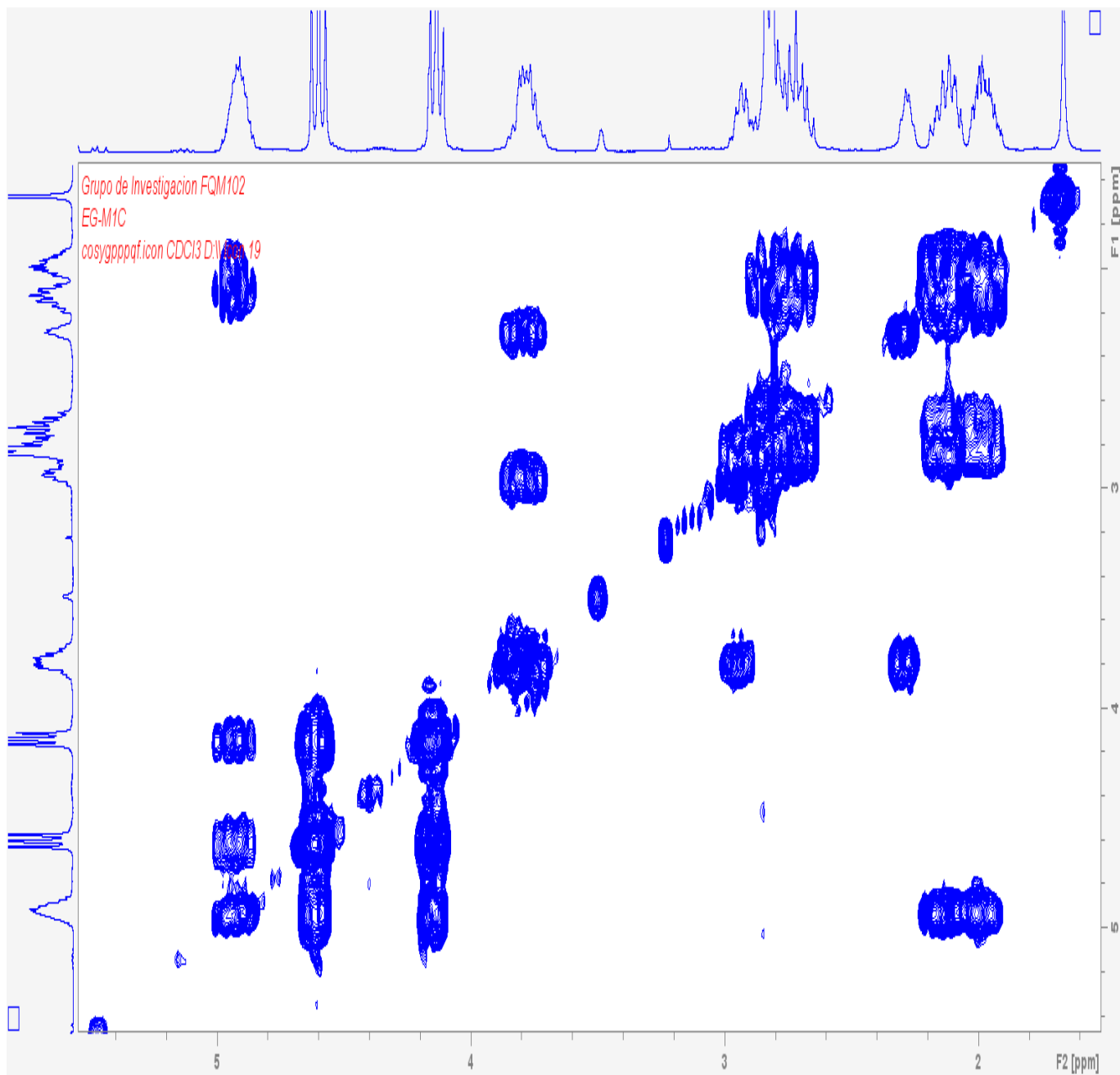


$^1\text{H-NMR}$ (300 MHz, CDCl_3) δ (ppm) 4.99-4.85 (m, 2H, H-2, H-2'), 4.61 (t, 2H, $J_{1a,2} = 8.6$ Hz, H-1a, H-1'a), 4.20-4.09 (m, 2H, H-1b, H-1'b), 3.85-3.70 (m, 2H, H-7), 3.50 (bs, 1H, O-H), 2.99-2.88 (m, 1H, H-5), 2.88-2.63 (m, 6H, H-4, H-4' and H-6), 2.22-2.06 (m, 2H, H-3a, H-3'a), 2.05-1.90 (m, 2H, H-3b, H-3'b).



Five-membered bis(cyclic carbonate) Monomer E

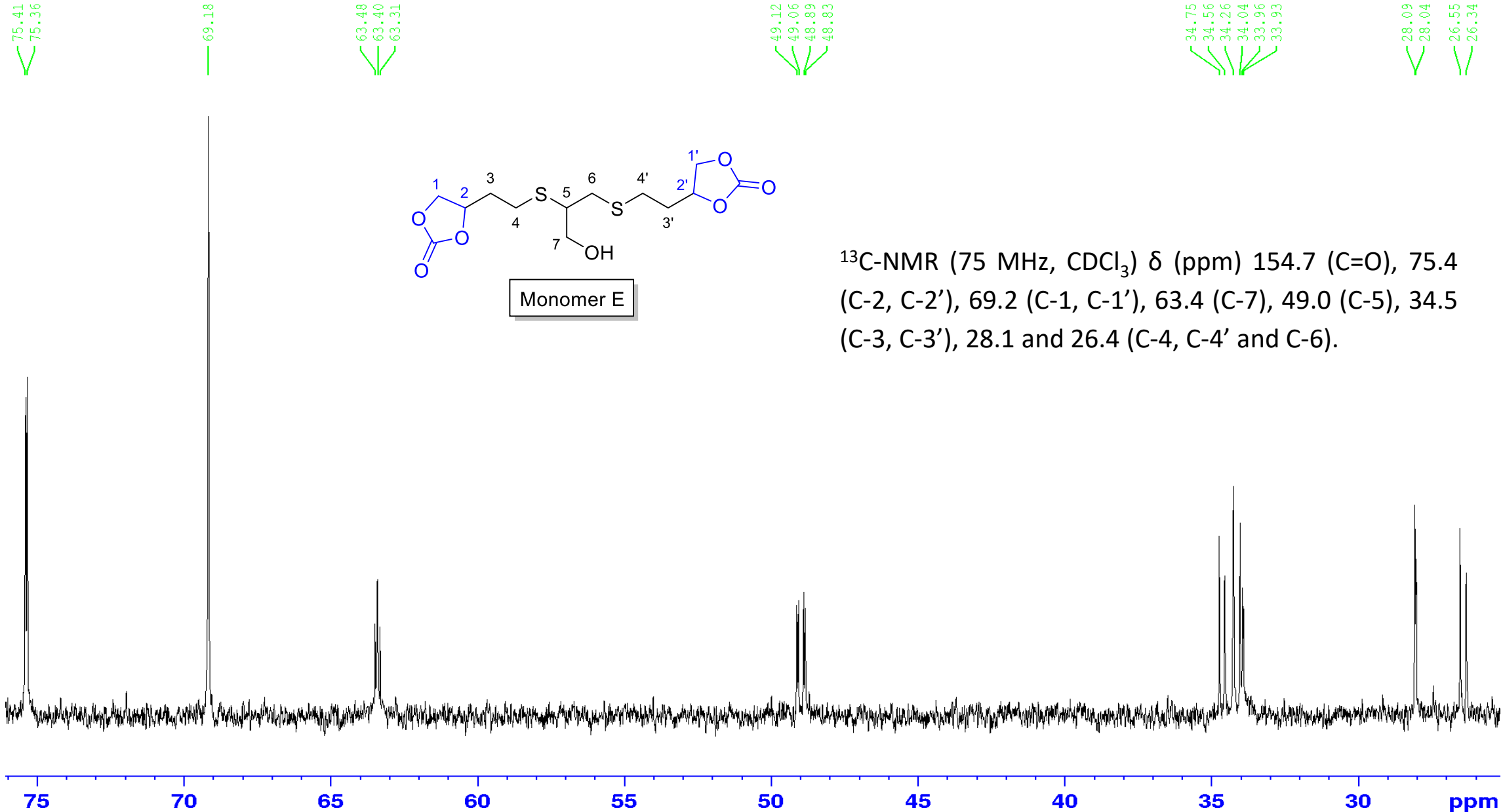
COSY (Bidimensional ^1H - ^1H)



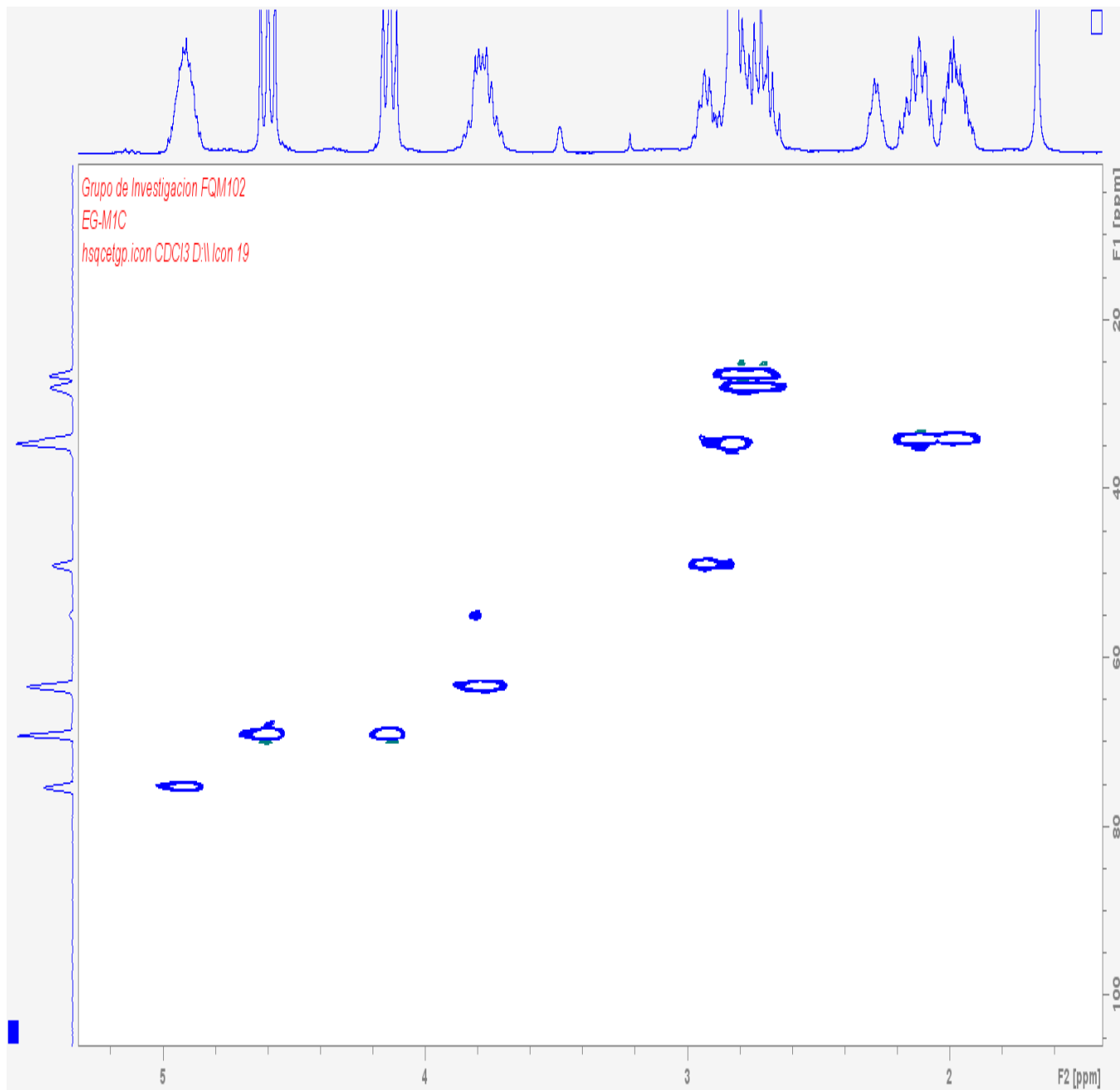
^1H -NMR (300 MHz, CDCl_3) δ (ppm) 4.99-4.85 (m, 2H, H-2, H-2'), 4.61 (t, 2H, $J_{1a,2} = 8.6$ Hz, H-1a, H-1'a), 4.20-4.09 (m, 2H, H-1b, H-1'b), 3.85-3.70 (m, 2H, H-7), 3.50 (bs, 1H, O-H), 2.99-2.88 (m, 1H, H-5), 2.88-2.63 (m, 6H, H-4, H-4' and H-6), 2.22-2.06 (m, 2H, H-3a, H-3'a), 2.05-1.90 (m, 2H, H-3b, H-3'b).

Five-membered bis(cyclic carbonate) Monomer E

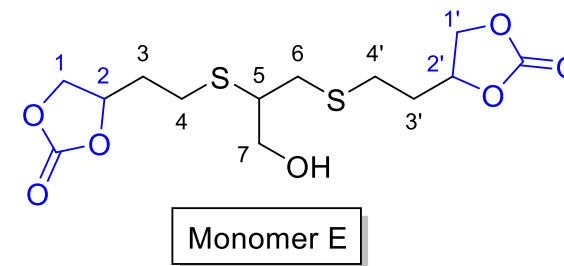
Spectrum ¹³C-RMN, 75 MHz, CDCl₃



Five-membered bis(cyclic carbonate) Monomer E



HSQC (Bidimensional ^1H - ^{13}C)

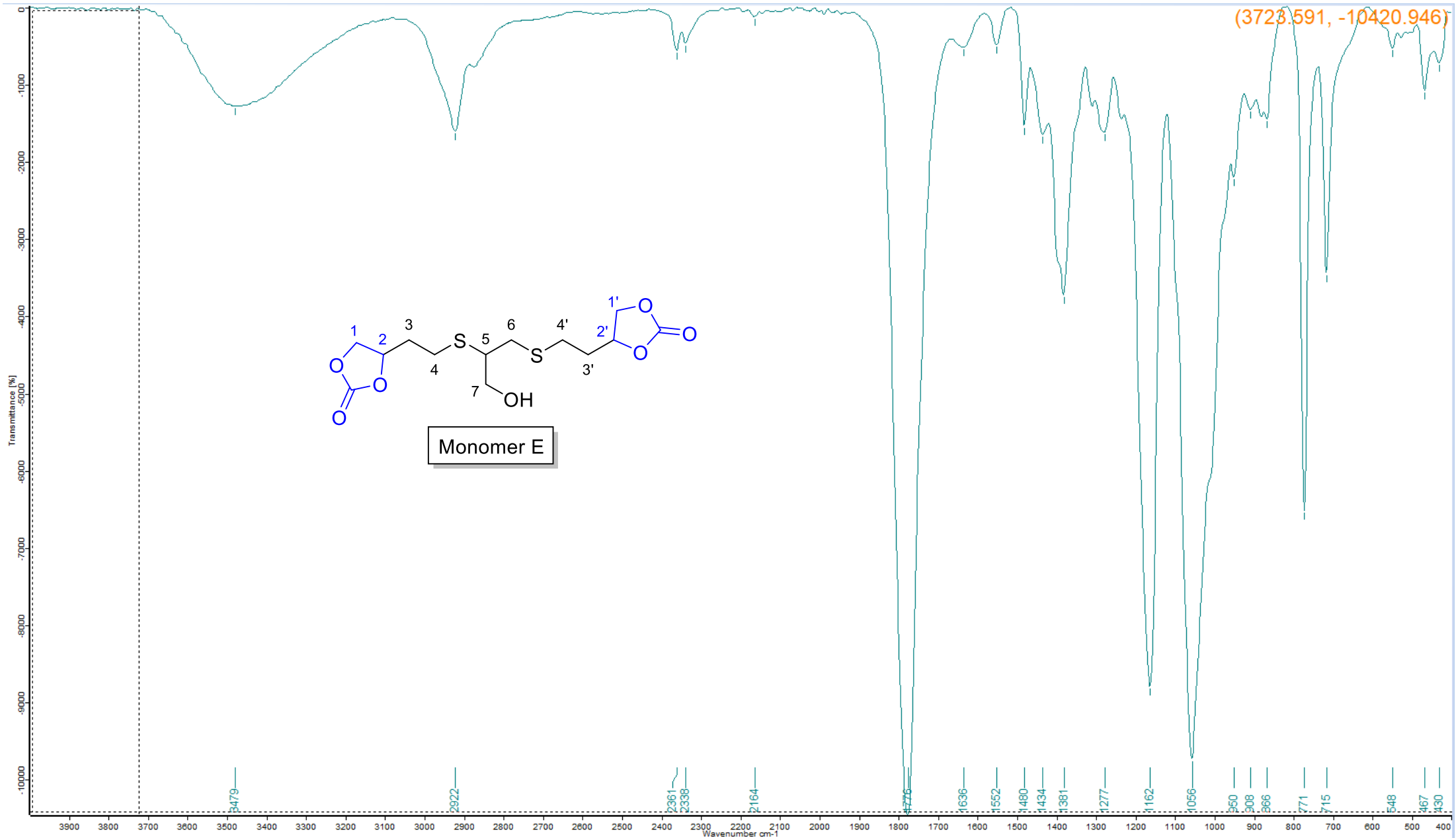


^1H -NMR (300 MHz, CDCl_3) δ (ppm) 4.99-4.85 (m, 2H, H-2, H-2'), 4.61 (t, 2H, $J_{1a,2} = 8.6$ Hz, H-1a, H-1'a), 4.20-4.09 (m, 2H, H-1b, H-1'b), 3.85-3.70 (m, 2H, H-7), 3.50 (bs, 1H, O-H), 2.99-2.88 (m, 1H, H-5), 2.88-2.63 (m, 6H, H-4, H-4' and H-6), 2.22-2.06 (m, 2H, H-3a, H-3'a), 2.05-1.90 (m, 2H, H-3b, H-3'b).

^{13}C -NMR (75 MHz, CDCl_3) δ (ppm) 154.7 (C=O), 75.4 (C-2, C-2'), 69.2 (C-1, C-1'), 63.4 (C-7), 49.0 (C-5), 34.5 (C-3, C-3'), 28.1 and 26.4 (C-4, C-4' and C-6).

Five-membered bis(cyclic carbonate) Monomer E

Spectrum ATR-FTIR



Five-membered bis(cyclic carbonate) Monomer E

Spectrum ESI-MS

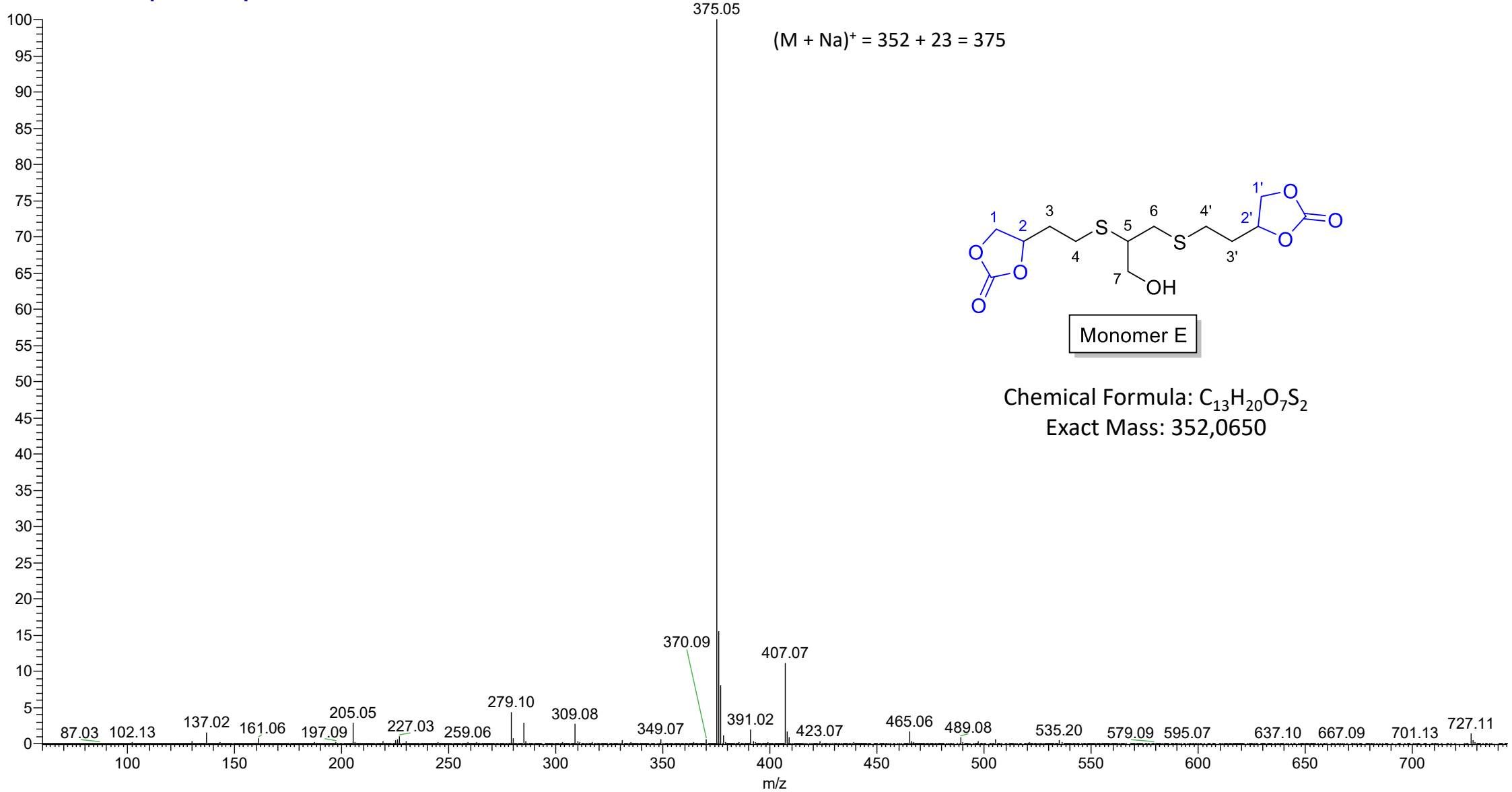
230322_EGM1

03/22/23 13:47:49

EG-M1 PM=352 C13H20O7S2

230322_EGM1 #34-66 RT: 0.17-0.34 AV: 33 SB: 242 1.39-2.67 NL: 1

T: FTMS + c ESI Full ms [60.00-900.00]



Five-membered bis(cyclic carbonate) Monomer E

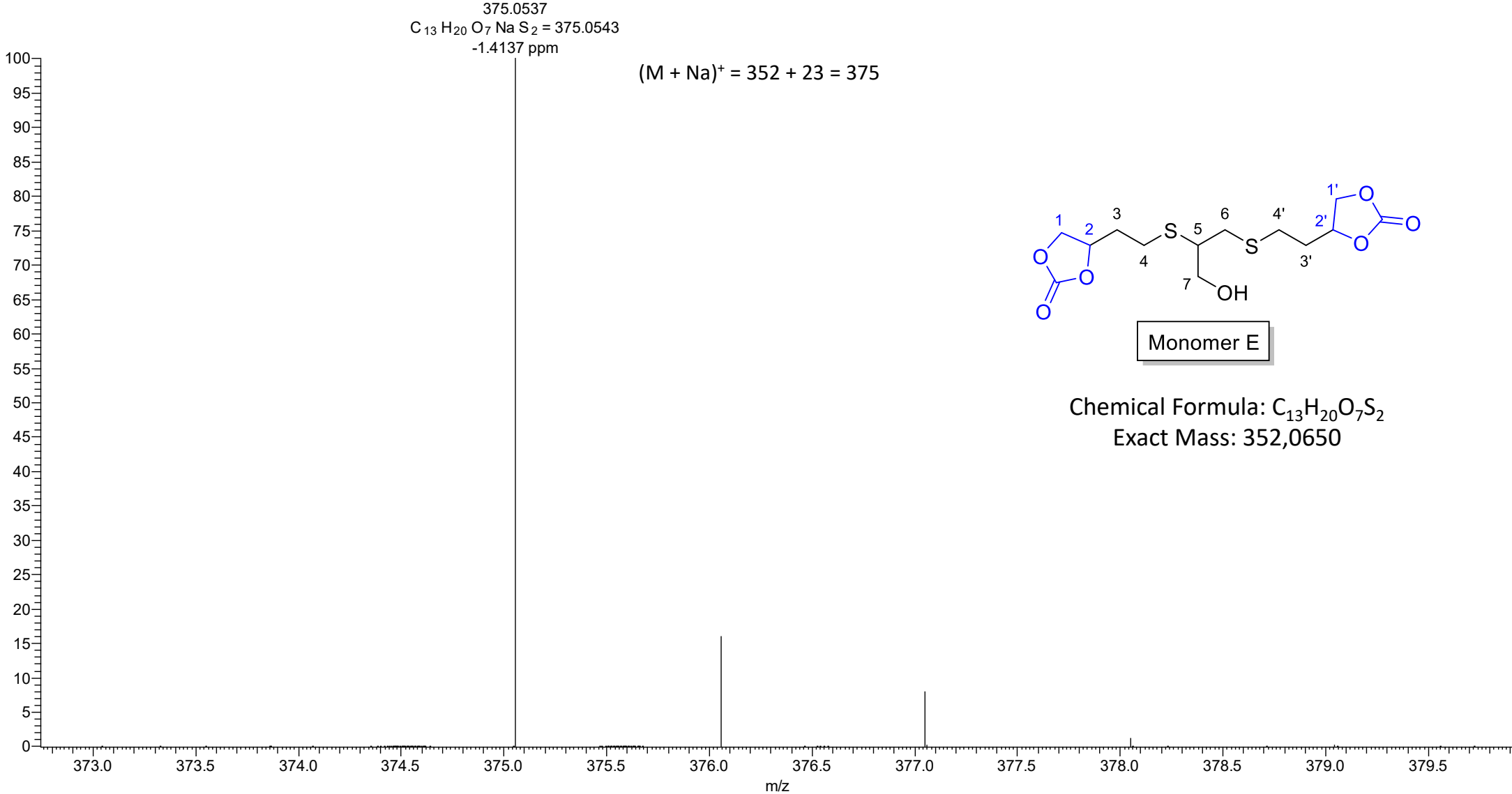
Spectrum ESI-HRMS

230328_EGM1

03/28/23 12:58:10

EG-M1 PM=352 C13H20O7S2

230328_EGM1 #72-94 RT: 0.28-0.37 AV: 23 NL: 1.07E8
T: FTMS + c ESI Full ms [60.00-900.00]



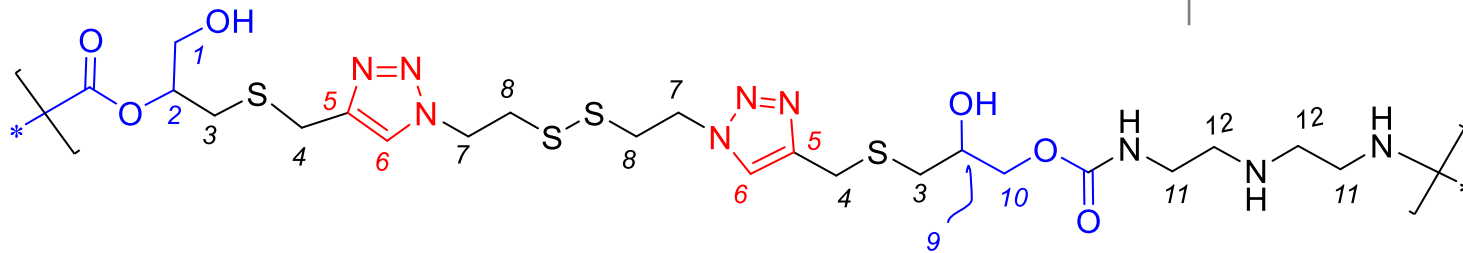
2nd Part:

Polyhydroxy-urethanes (PHU)

- 1. PHU A-DETA [monomer A + diethylenetriamine (DETA)]** **Pages [47-72]**
 - ¹H NMR, COSY, HSQC, ATR-FTIR, GPC (samples P2, P4-P20)
- 2. PHU E-DETA [monomer E + diethylenetriamine (DETA)]** **Pages [73-81]**
 - ¹H NMR, ¹³C NMR, ATR-FTIR, GPC (samples P1-P5)
- 3. PHU E-HMDA [monomer E + hexamethylenediamine (HMDA)]** **Pages [82-90]**
 - ¹H NMR, ¹³C NMR, ATR-FTIR, GPC (samples P1-P5)

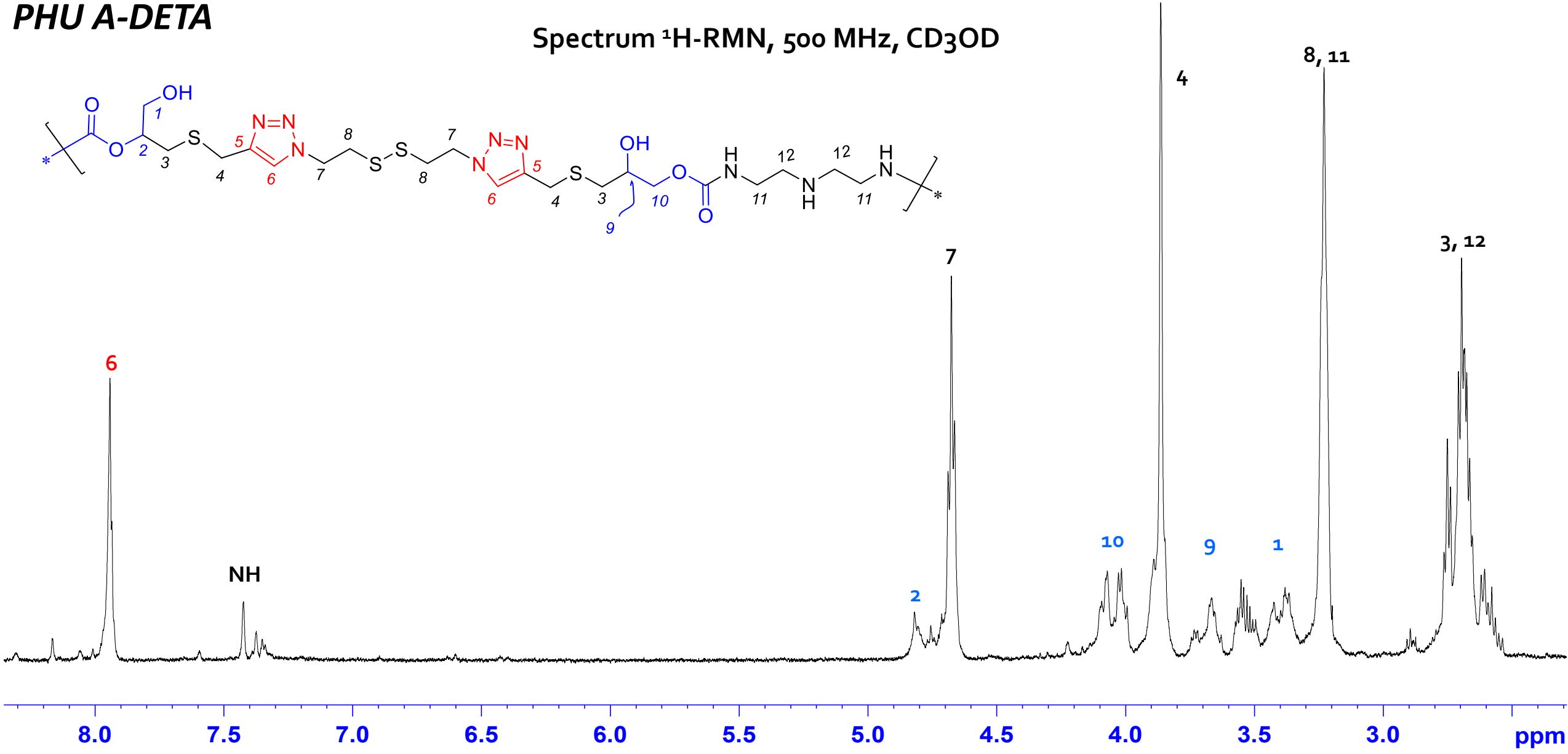
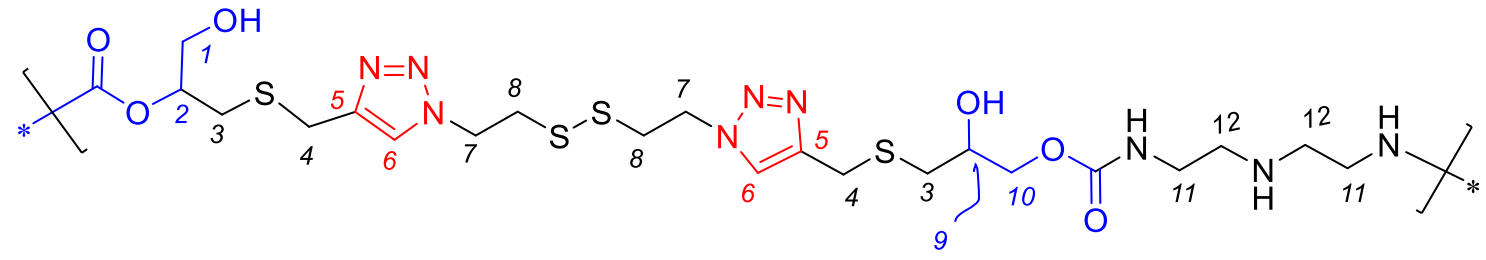
PHU A-DETA

*Monomer A +
diethylenetriamine
(DETA)]*

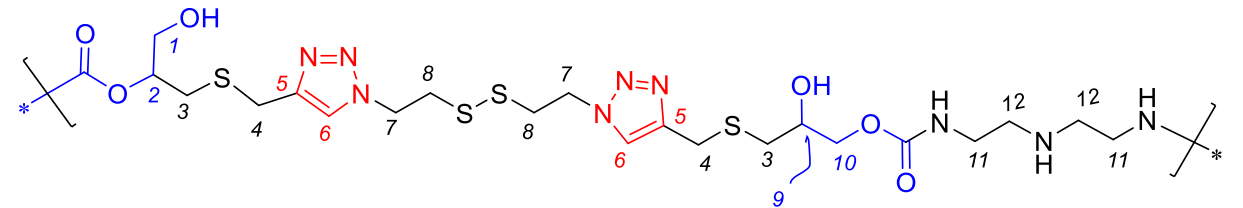
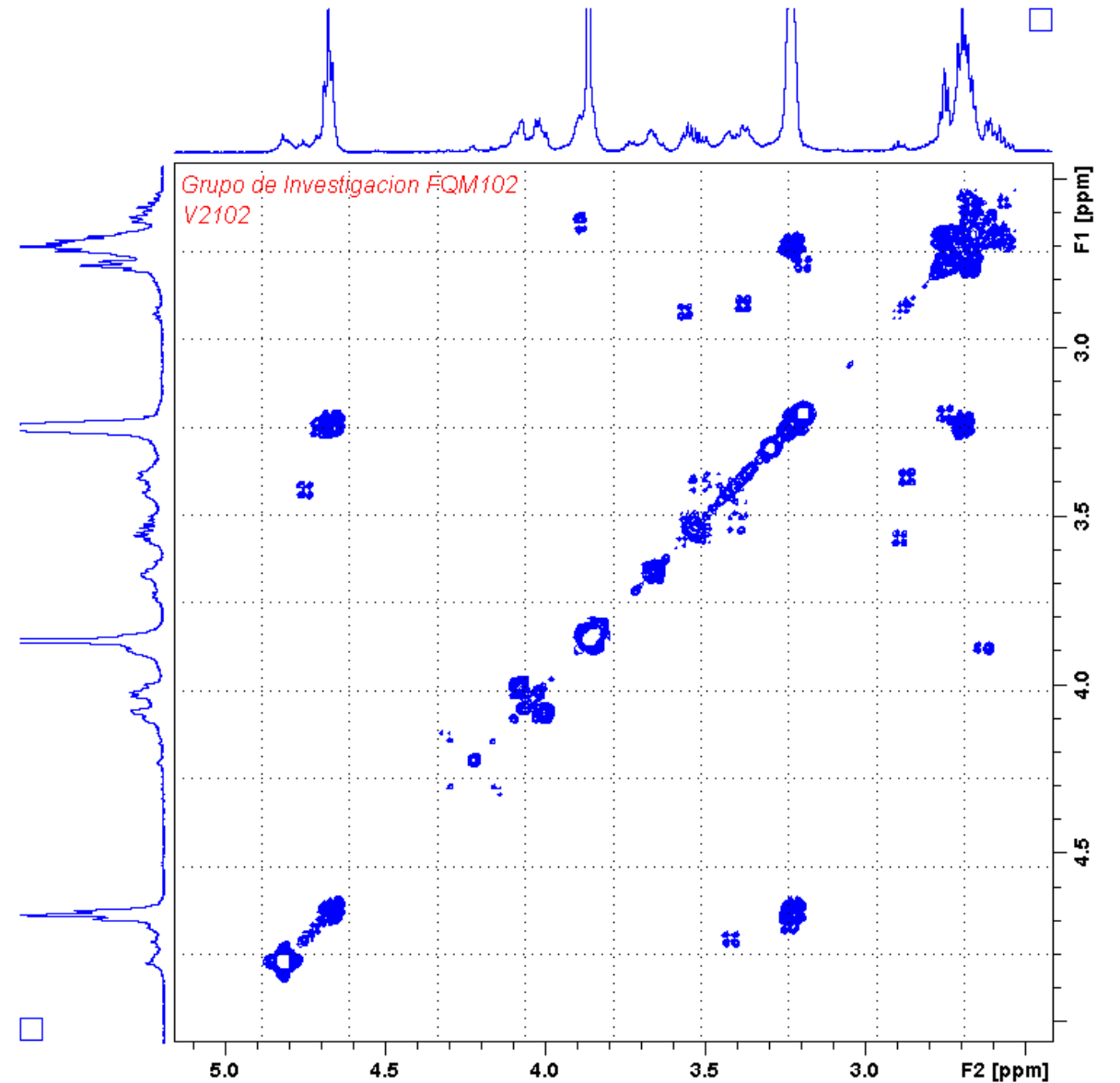


PHU A-DETA

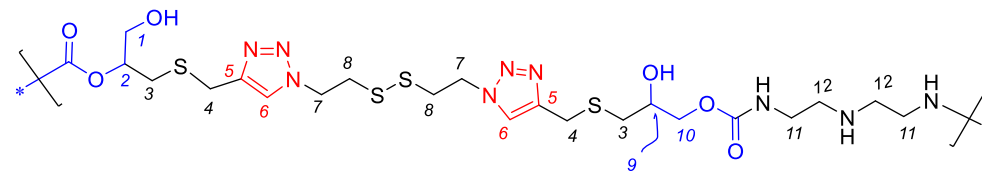
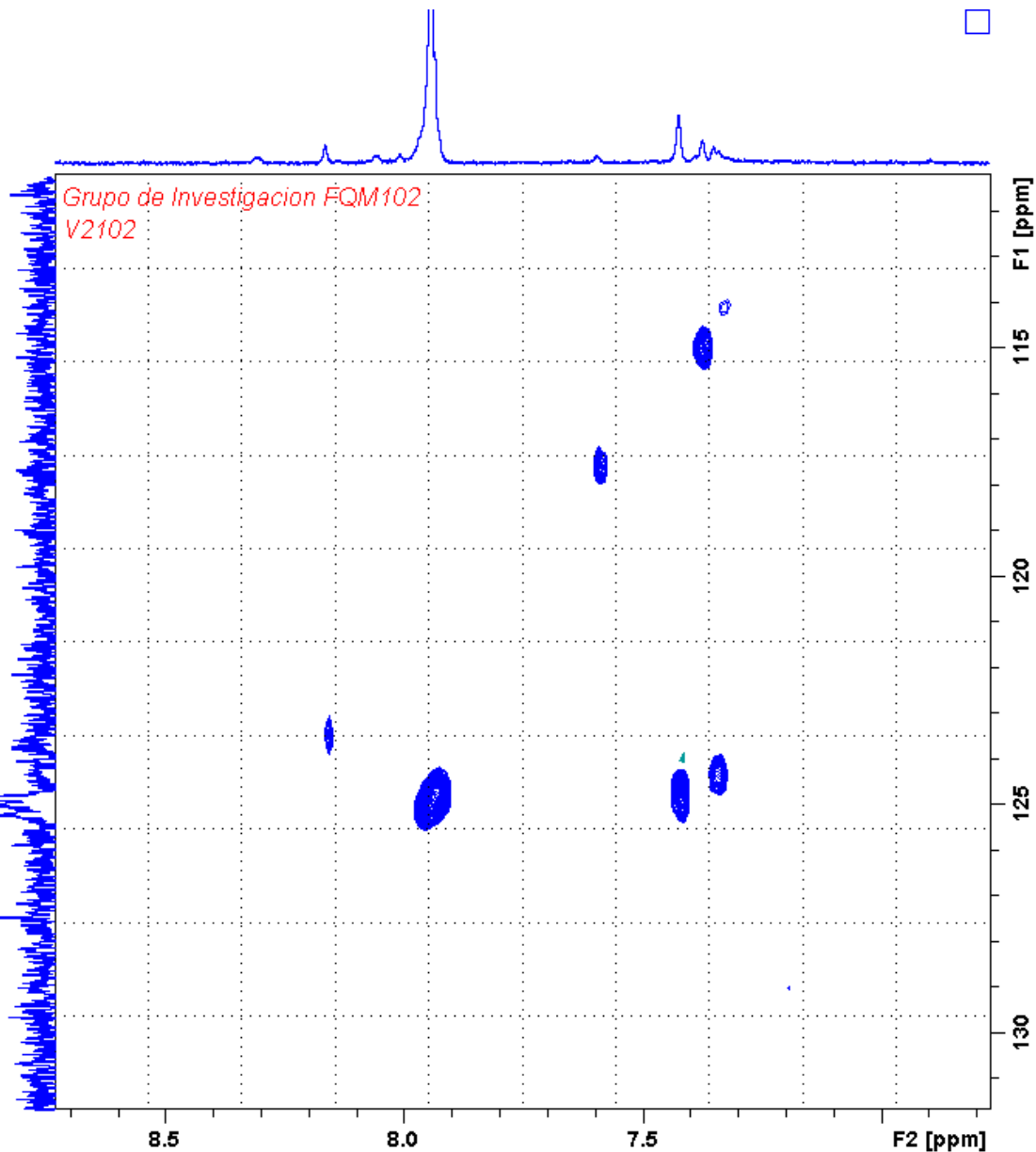
Spectrum ¹H-RMN, 500 MHz, CD₃OD



¹H-NMR (500 MHz, CD₃OD) δ (ppm) 7.94 (s, 2H, H-6), 7.34-7.11 (m, 2H, N-H urethane), 4.92 (bs, 1H, H-2), 4.68 (t, 4H, $J_{7,8} = 6.5$ Hz, H-7), 4.07, 4.02 (2 bs, 4H, H-10), 3.86 (bs, 4H, H-4), 3.77-3.31 (m, 2H, H-9, H-1), 3.24 (bs, 8H, H-8, H-11), 2.85-2.50 (m, 8H, H-3, H-12).

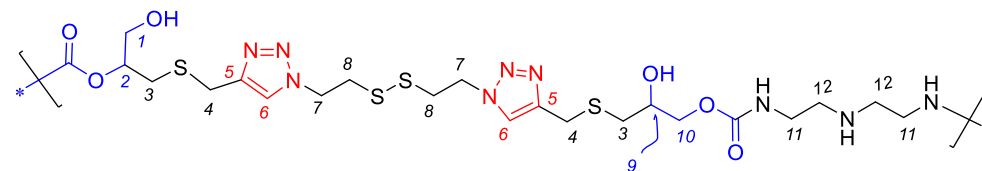
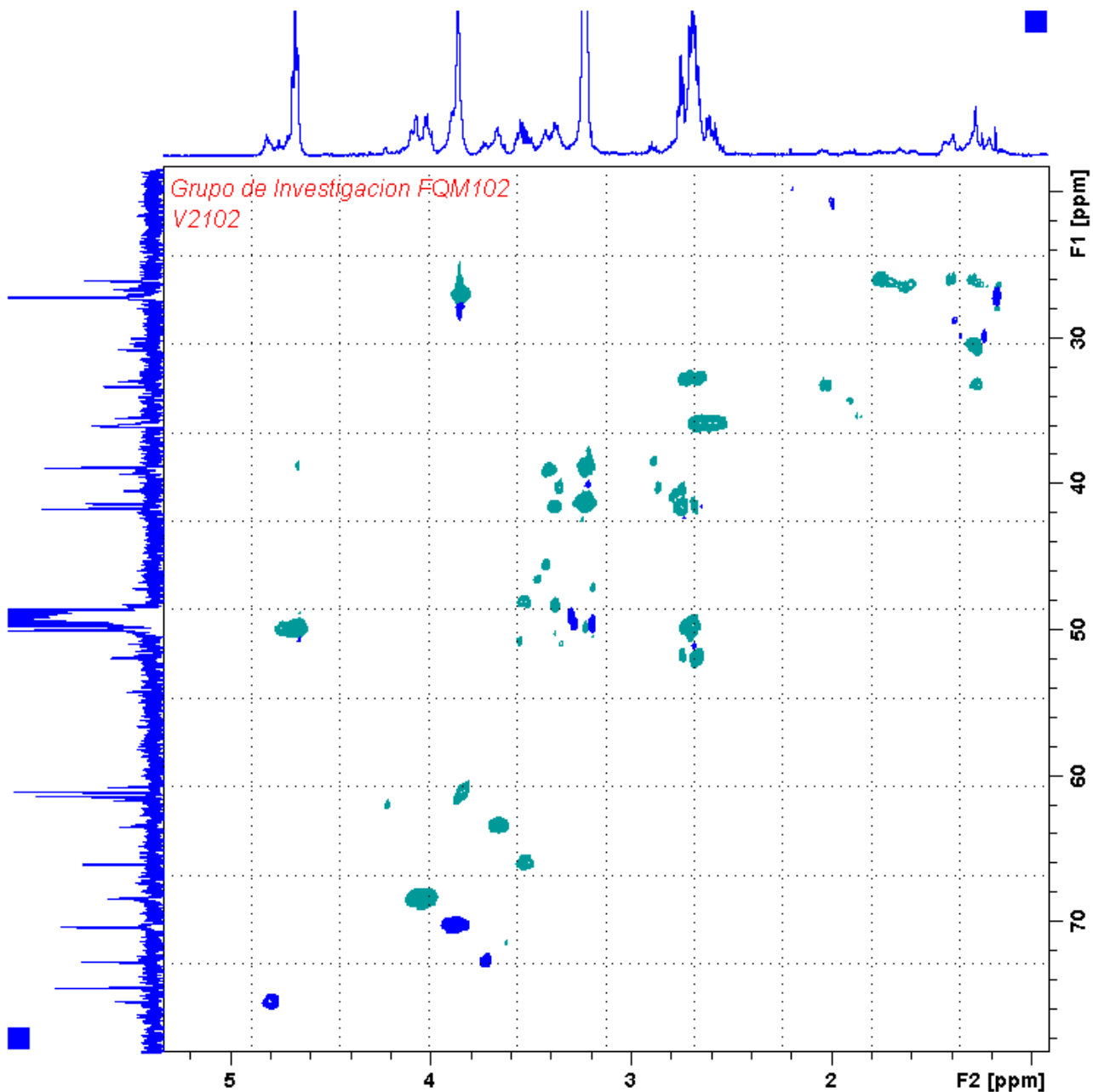


^1H -NMR (500 MHz, CD_3OD) δ (ppm) 7.94 (s, 2H, H-6), 7.34-7.11 (m, 2H, N-H urethane), 4.92 (bs, 1H, H-2), 4.68 (t, 4H, $J_{7,8} = 6.5$ Hz, H-7), 4.07, 4.02 (2 bs, 4H, H-10), 3.86 (bs, 4H, H-4), 3.77-3.31 (m, 2H, H-9, H-1), 3.24 (bs, 8H, H-8, H-11), 2.85-2.50 (m, 8H, H-3, H-12).



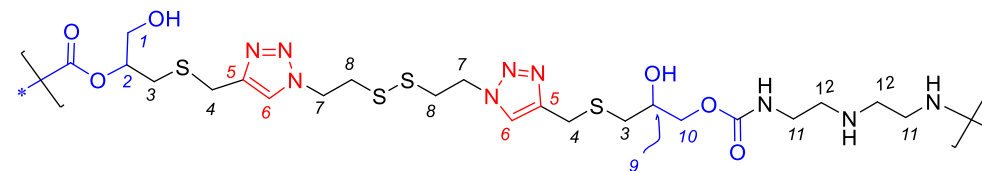
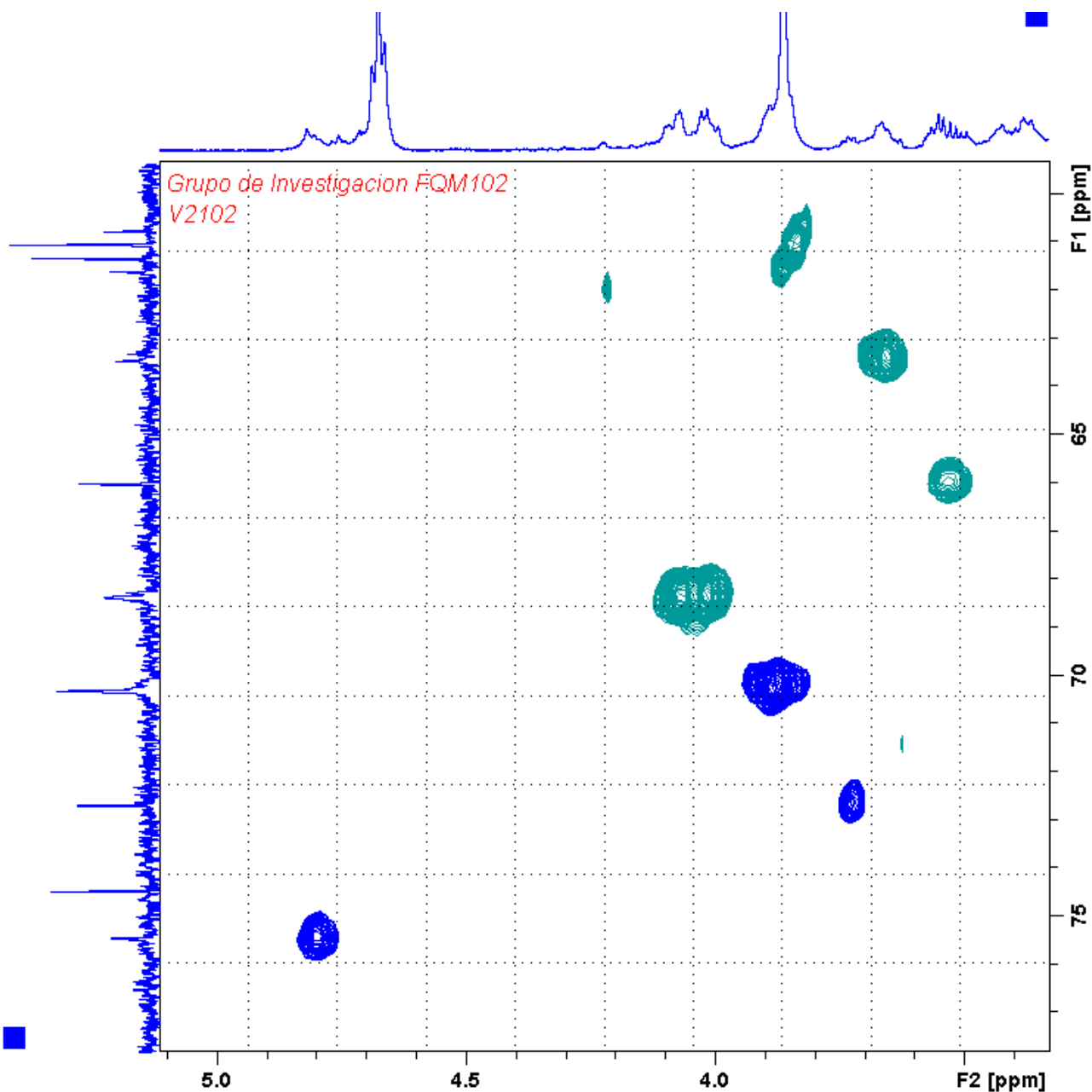
^1H -NMR (500 MHz, CD_3OD) δ (ppm) 7.94 (s, 2H, H-6), 7.34-7.11 (m, 2H, N-H urethane), 4.92 (bs, 1H, H-2), 4.68 (t, 4H, $J_{7,8} = 6.5$ Hz, H-7), 4.07, 4.02 (2 bs, 4H, H-10), 3.86 (bs, 4H, H-4), 3.77-3.31 (m, 2H, H-9, H-1), 3.24 (bs, 8H, H-8, H-11), 2.85-2.50 (m, 8H, H-3, H-12).

^{13}C -NMR (125 MHz, CD_3OD) δ (ppm) 159.1 (C=O), 143.7 (C-5), 125.0 (C-6), 75.6 (C-2), 70.5 (C-9), 68.5 (C-10), 63.6 (C-1), 50.1 (C-7), 41.5 (C-8), 39.0 (C-11), 36.1 (C-12) 33.1 (C-3), 27.4 (C-4).



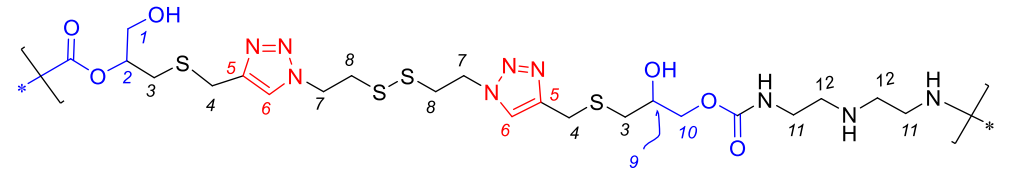
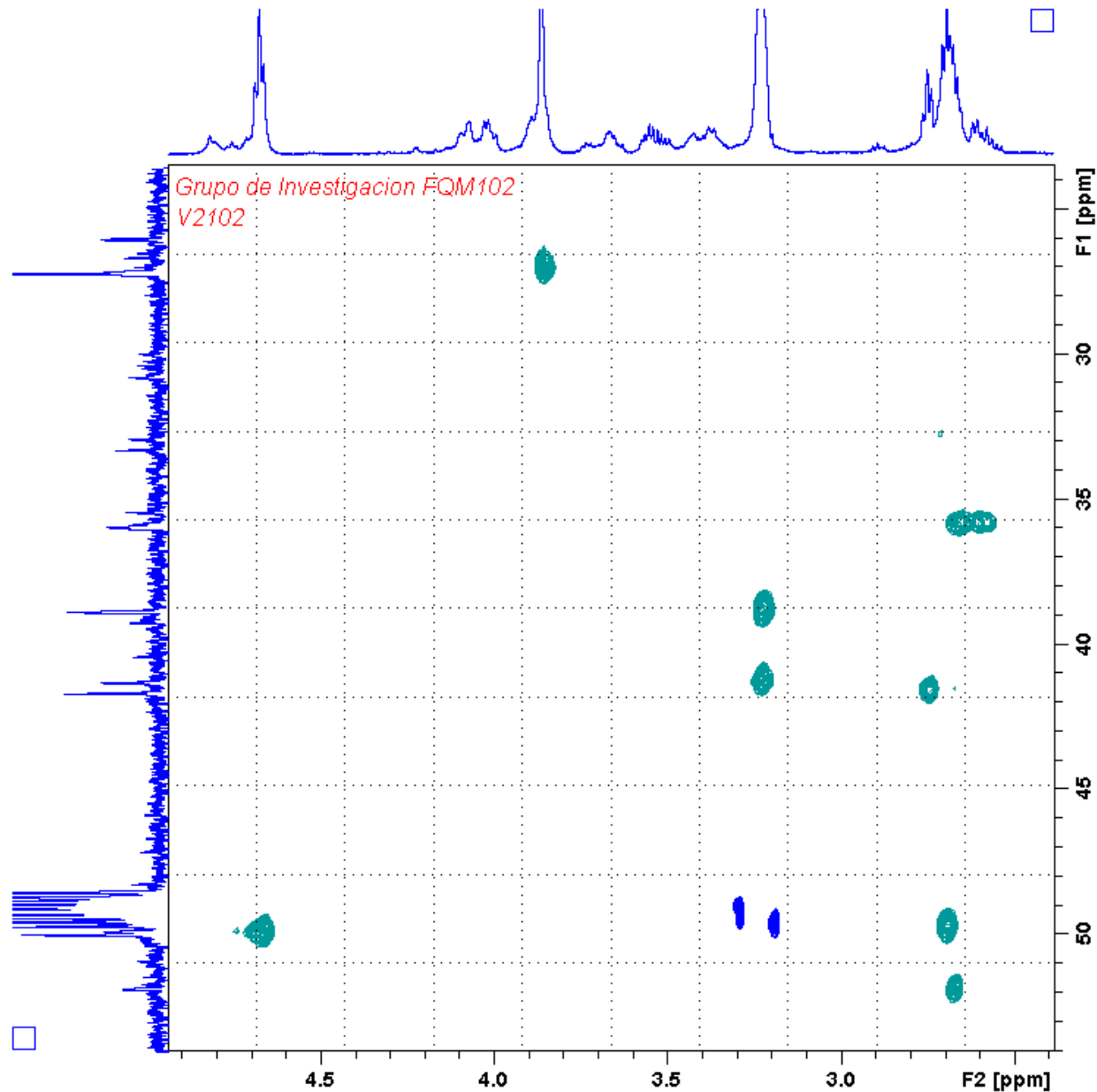
^1H -NMR (500 MHz, CD_3OD) δ (ppm) 7.94 (s, 2H, H-6), 7.34-7.11 (m, 2H, N-H urethane), 4.92 (bs, 1H, H-2), 4.68 (t, 4H, $J_{7,8} = 6.5$ Hz, H-7), 4.07, 4.02 (2 bs, 4H, H-10), 3.86 (bs, 4H, H-4), 3.77-3.31 (m, 2H, H-9, H-1), 3.24 (bs, 8H, H-8, H-11), 2.85-2.50 (m, 8H, H-3, H-12).

^{13}C -NMR (125 MHz, CD_3OD) δ (ppm) 159.1 (C=O), 143.7 (C-5), 125.0 (C-6), 75.6 (C-2), 70.5 (C-9), 68.5 (C-10), 63.6 (C-1), 50.1 (C-7), 41.5 (C-8), 39.0 (C-11), 36.1 (C-12) 33.1 (C-3), 27.4 (C-4).



^1H -NMR (500 MHz, CD_3OD) δ (ppm) 7.94 (s, 2H, H-6), 7.34-7.11 (m, 2H, N-H urethane), 4.92 (bs, 1H, H-2), 4.68 (t, 4H, $J_{7,8} = 6.5$ Hz, H-7), 4.07, 4.02 (2 bs, 4H, H-10), 3.86 (bs, 4H, H-4), 3.77-3.31 (m, 2H, H-9, H-1), 3.24 (bs, 8H, H-8, H-11), 2.85-2.50 (m, 8H, H-3, H-12).

^{13}C -NMR (125 MHz, CD_3OD) δ (ppm) 159.1 (C=O), 143.7 (C-5), 125.0 (C-6), 75.6 (C-2), 70.5 (C-9), 68.5 (C-10), 63.6 (C-1), 50.1 (C-7), 41.5 (C-8), 39.0 (C-11), 36.1 (C-12) 33.1 (C-3), 27.4 (C-4).

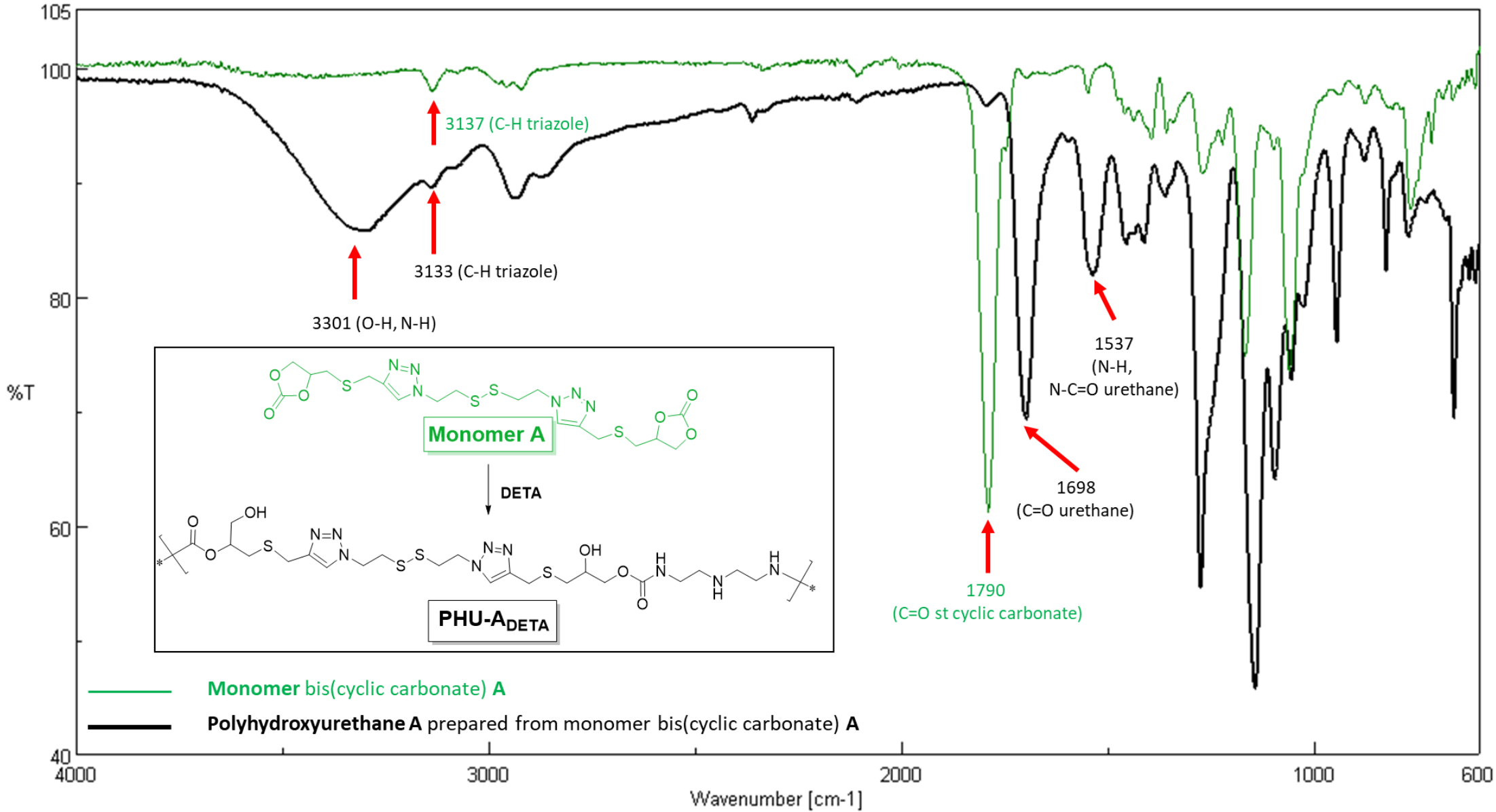


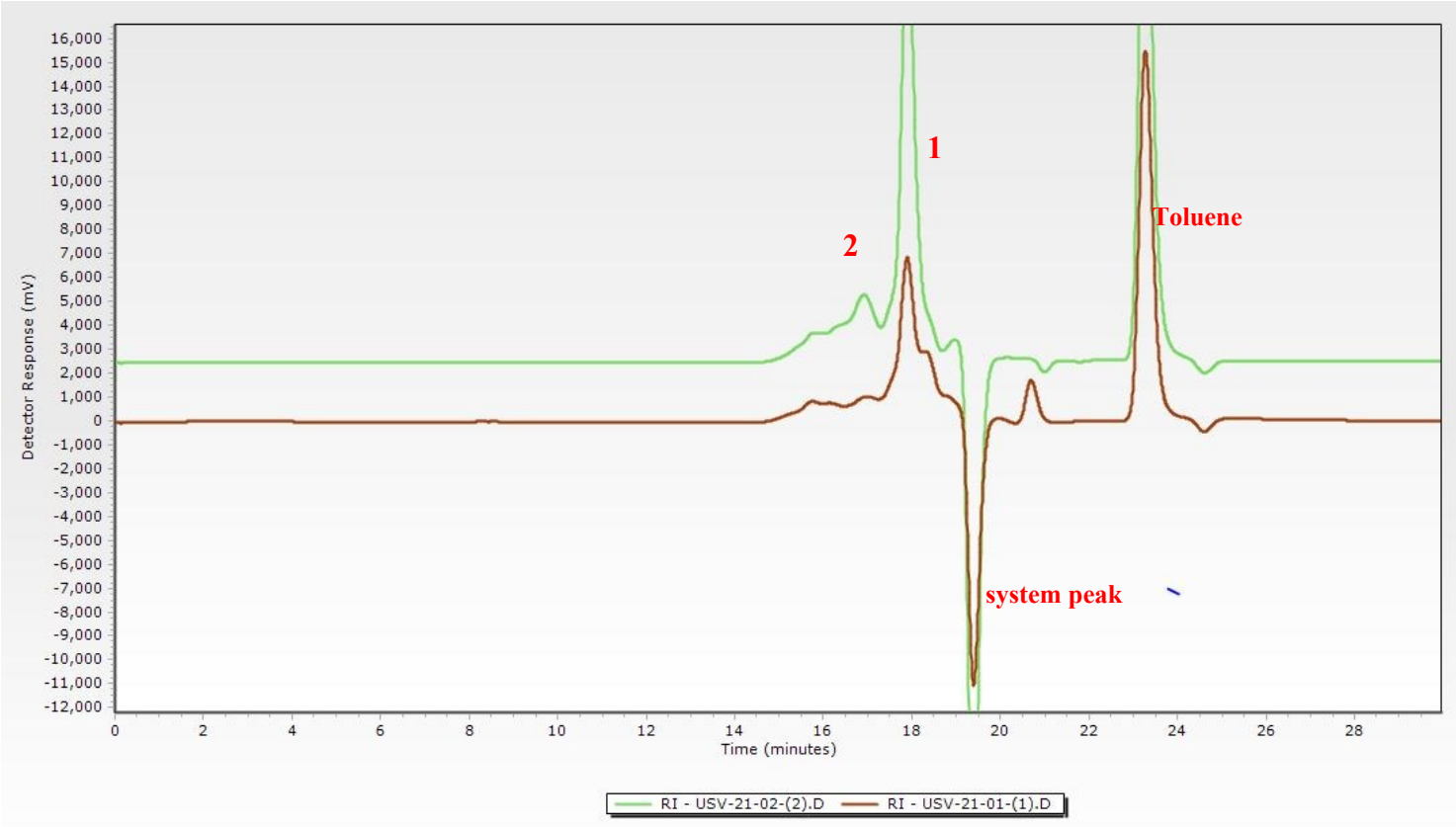
^1H -NMR (500 MHz, CD_3OD) δ (ppm) 7.94 (s, 2H, H-6), 7.34-7.11 (m, 2H, N-H urethane), 4.92 (bs, 1H, H-2), 4.68 (t, 4H, $J_{7,8} = 6.5$ Hz, H-7), 4.07, 4.02 (2 bs, 4H, H-10), 3.86 (bs, 4H, H-4), 3.77-3.31 (m, 2H, H-9, H-1), 3.24 (bs, 8H, H-8, H-11), 2.85-2.50 (m, 8H, H-3, H-12).

^{13}C -NMR (125 MHz, CD_3OD) δ (ppm) 159.1 (C=O), 143.7 (C-5), 125.0 (C-6), 75.6 (C-2), 70.5 (C-9), 68.5 (C-10), 63.6 (C-1), 50.1 (C-7), 41.5 (C-8), 39.0 (C-11), 36.1 (C-12) 33.1 (C-3), 27.4 (C-4).

PHU A-DETA (black) and Monomer A (green)

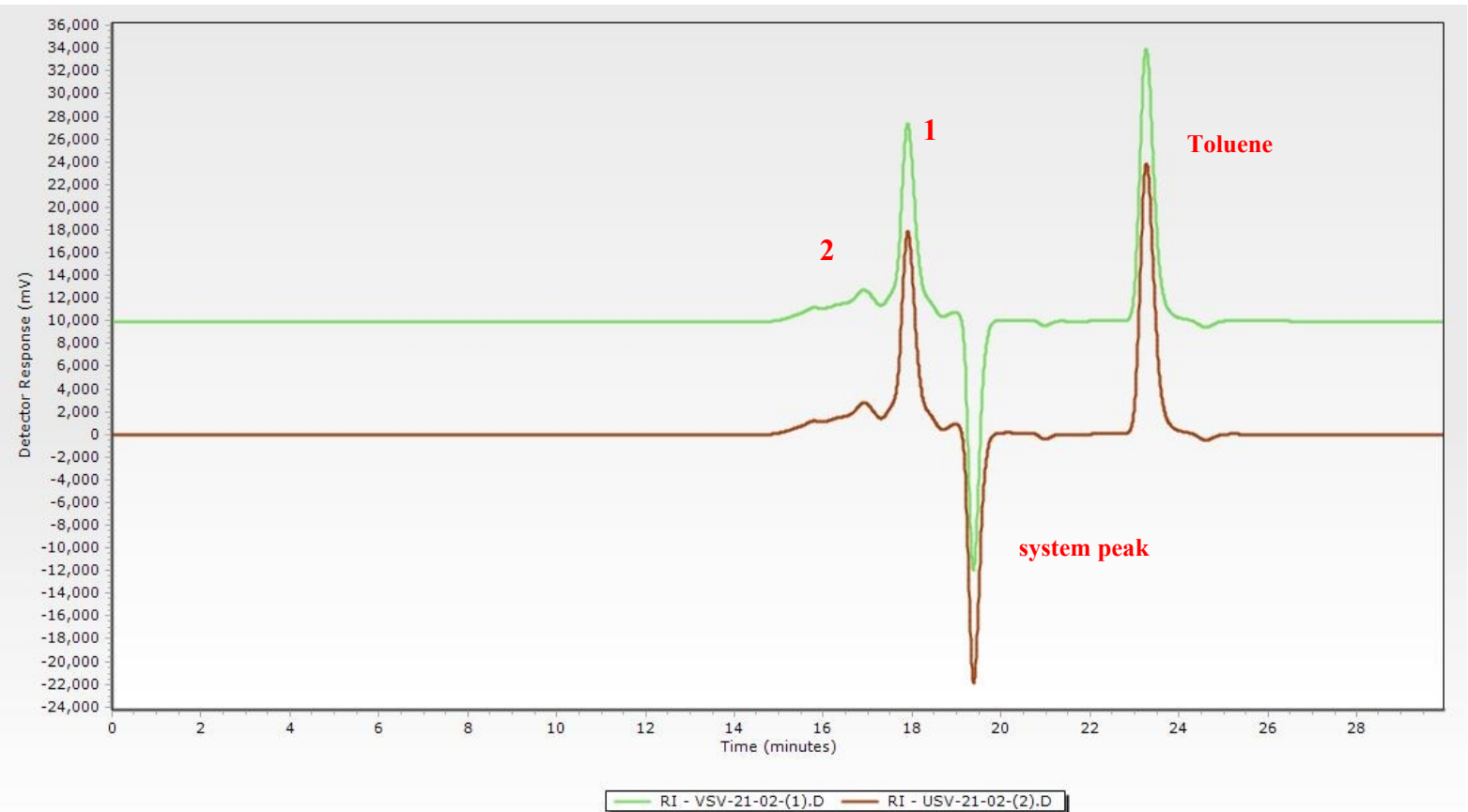
Spectra ATR-FTIR





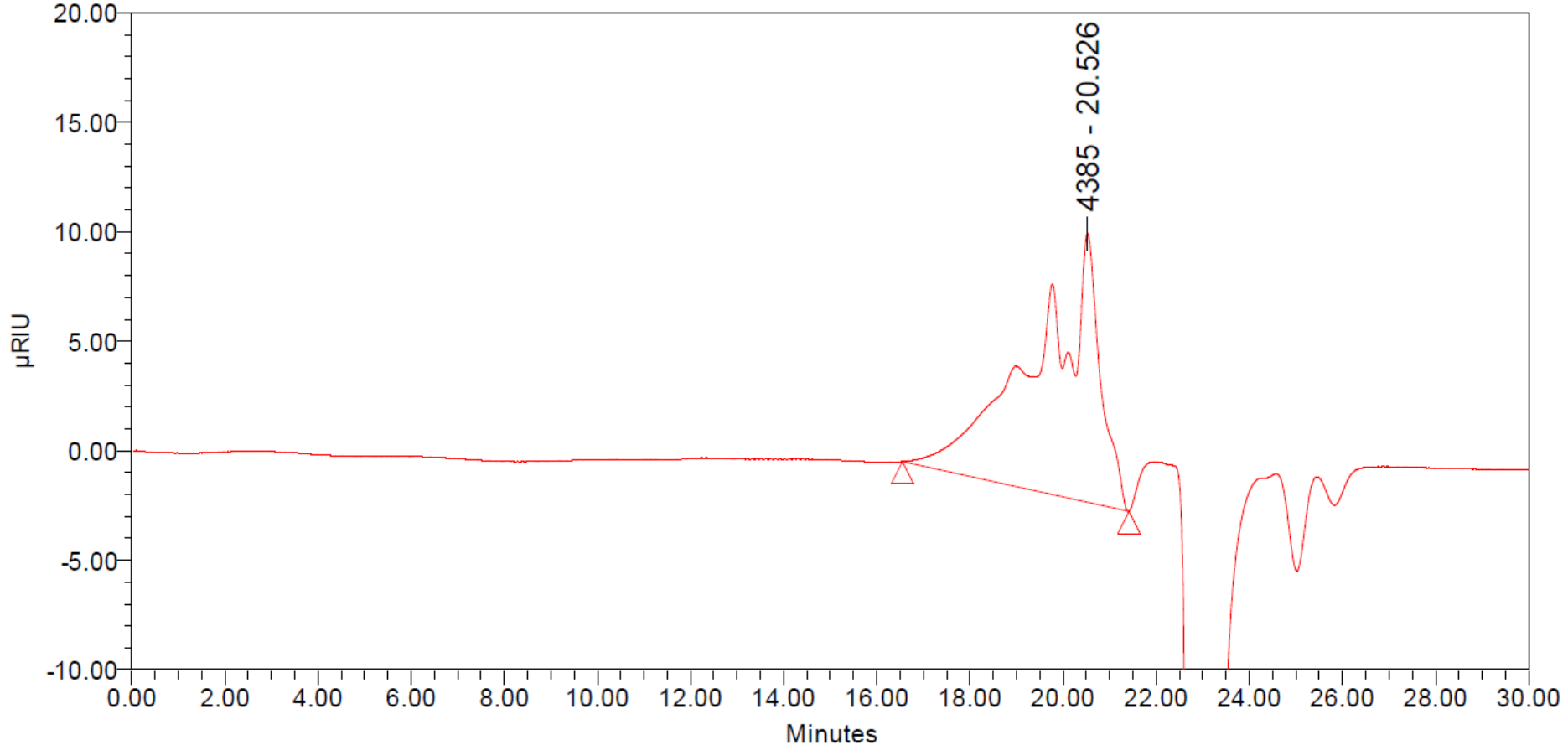
Injection	Peak	Mn	Mw	Mp	Mz	Đ
1	1	2787	3726	1889	4953	1.337
1	2	943	961	996	980	1.019
2	1	2565	3337	1984	4542	1.301
2	2	975	985	990	996	1.01

(*) Mn = number average molecular weight; Mw = weight average molecular weight; Mp = peak maximum molecular weight; Mz = Z average molecular weight



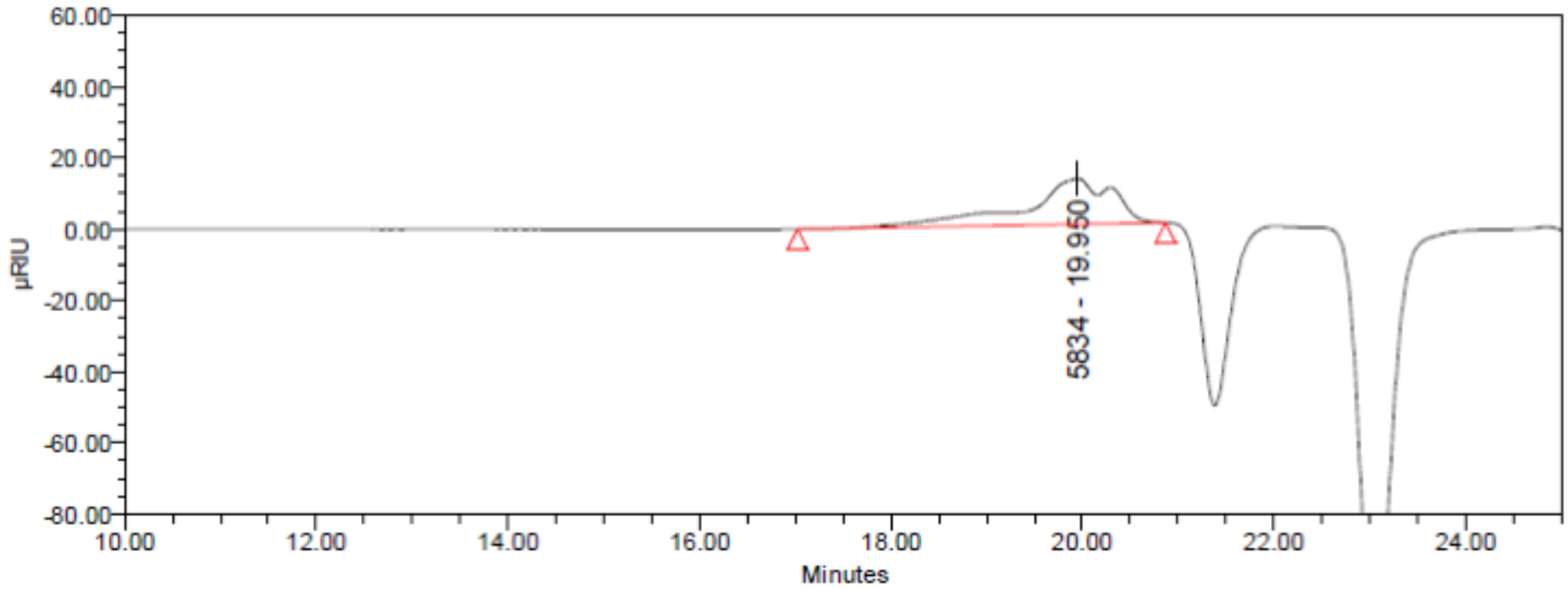
Injection	Peak	Mn	Mw	Mp	Mz	Đ
1	1	2576	3254	1975	4232	1.26
1	2	979	992	990	1006	1.01
2	1	2636	3382	1984	1014	1.28
2	2	987	1000	990	1014	1.01

(*) Mn = number average molecular weight; Mw = weight average molecular weight; Mp = peak maximum molecular weight; Mz = Z average molecular weight



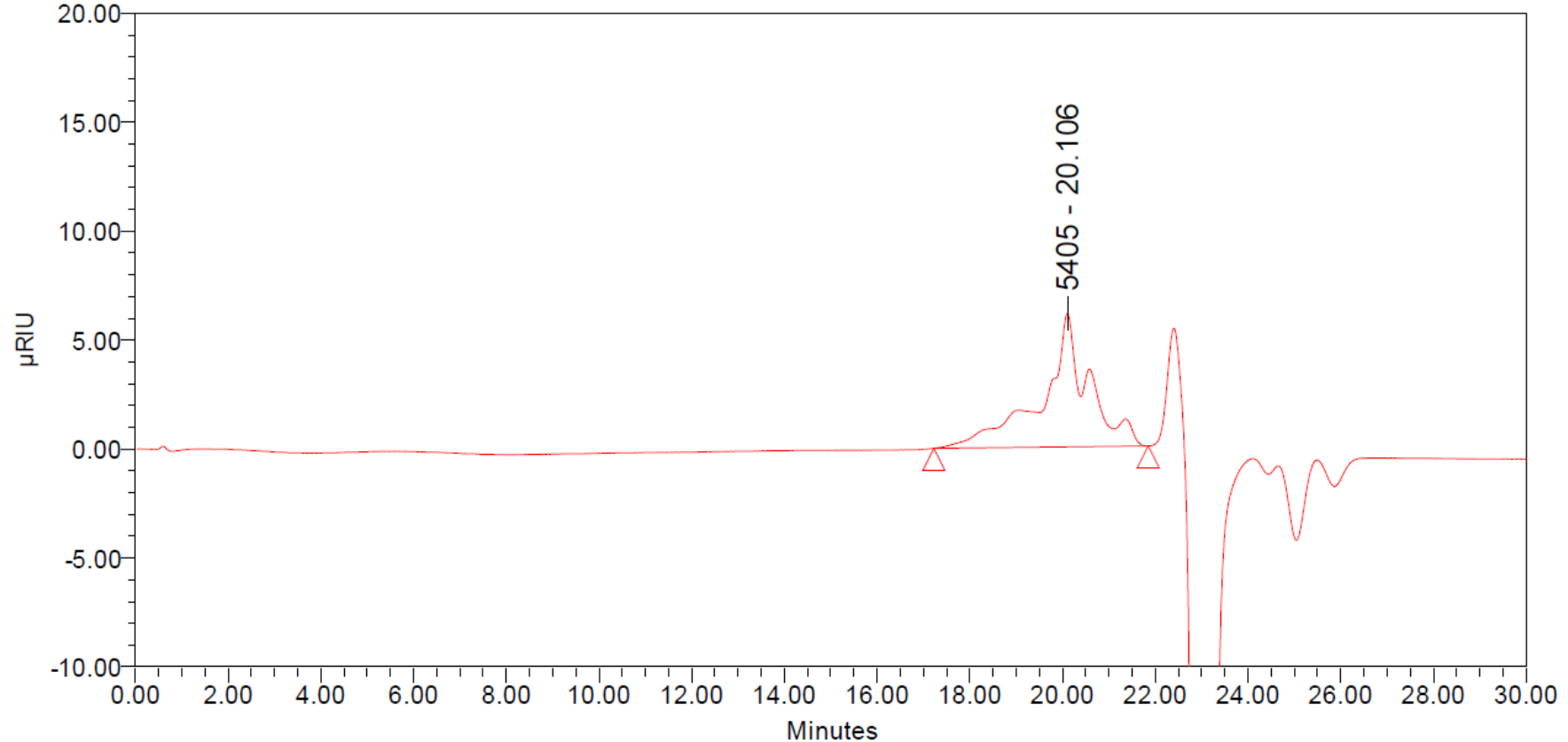
GPC Results

	Dist Name	Mn	Mw	MP	Mz	Mz+1	Mv	Polydispersity	MW Marker 1	MW Marker 2
1		6141	7702	4385	10054	12960		1.254299		



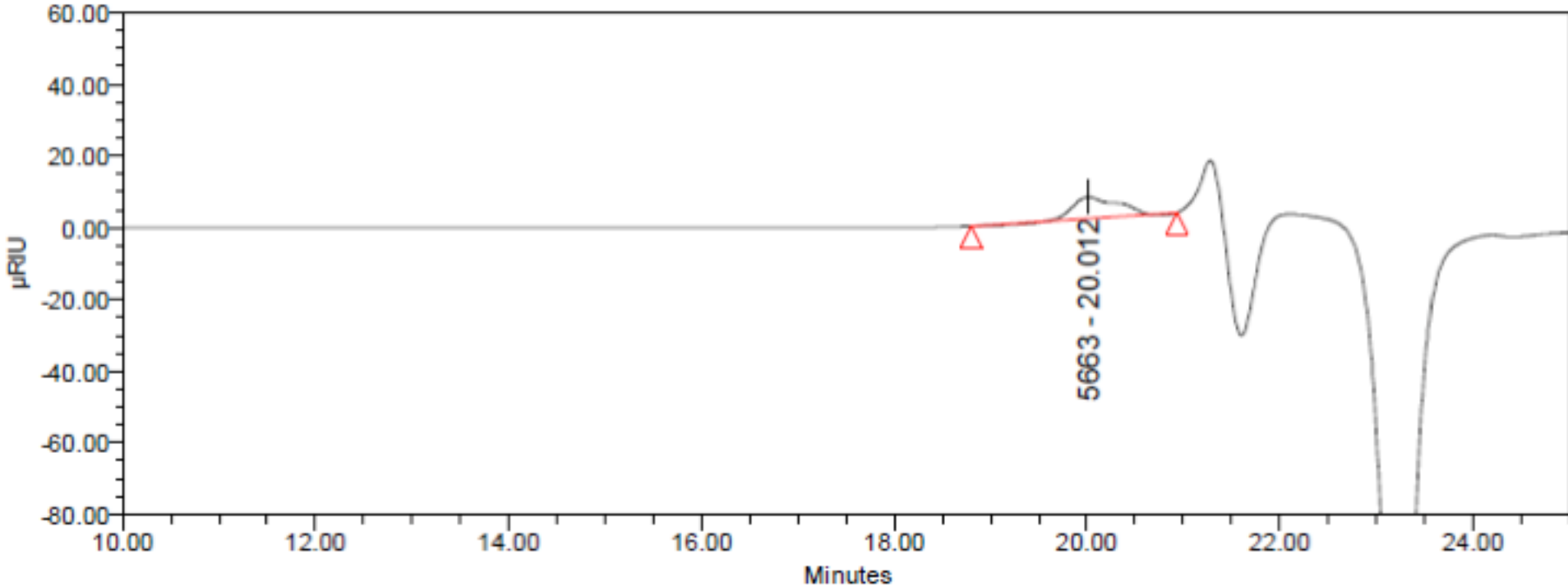
GPC Results

Dist Name	Mn	Mw	MP	Mz	Mz+1	Mv	Polydispersity	MW Marker 1	MW Marker 2
1	6368	6784	5834	7335	8026		1.065322		



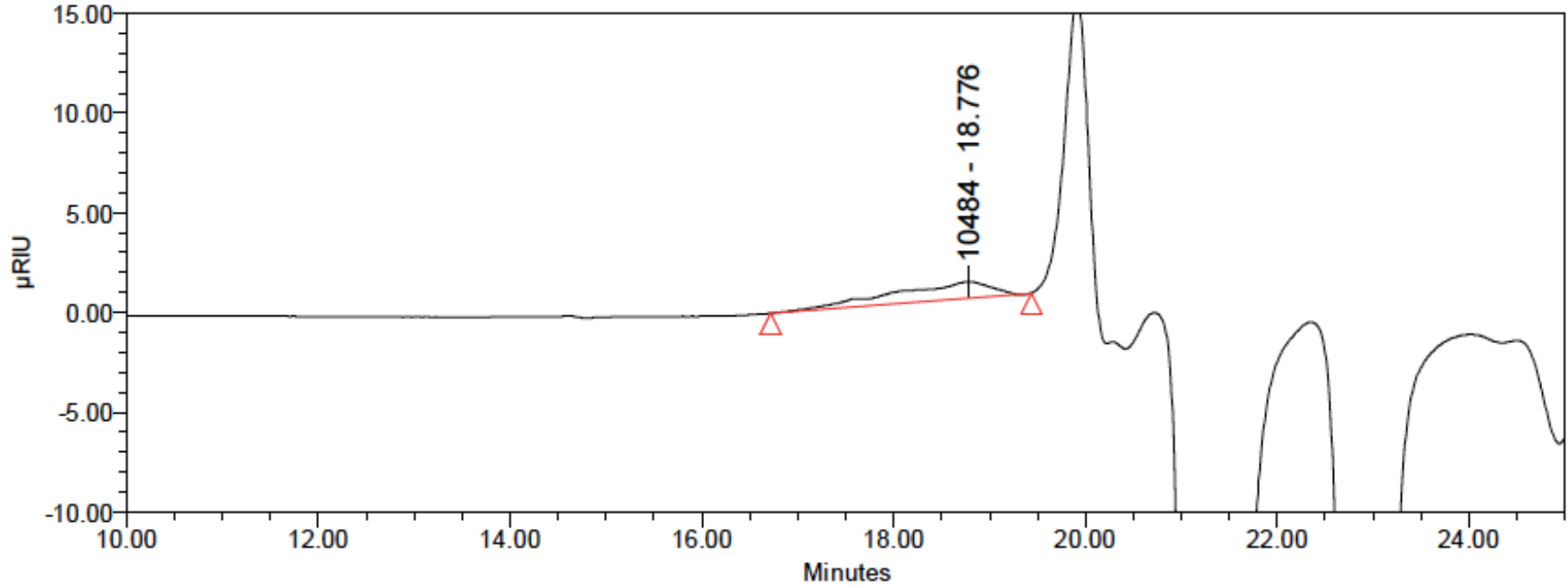
GPC Results

	Dist Name	Mn	Mw	MP	Mz	Mz+1	Mv	Polydispersity	MW Marker 1	MW Marker 2
1		5490	6507	5405	7925	9682		1.185260		



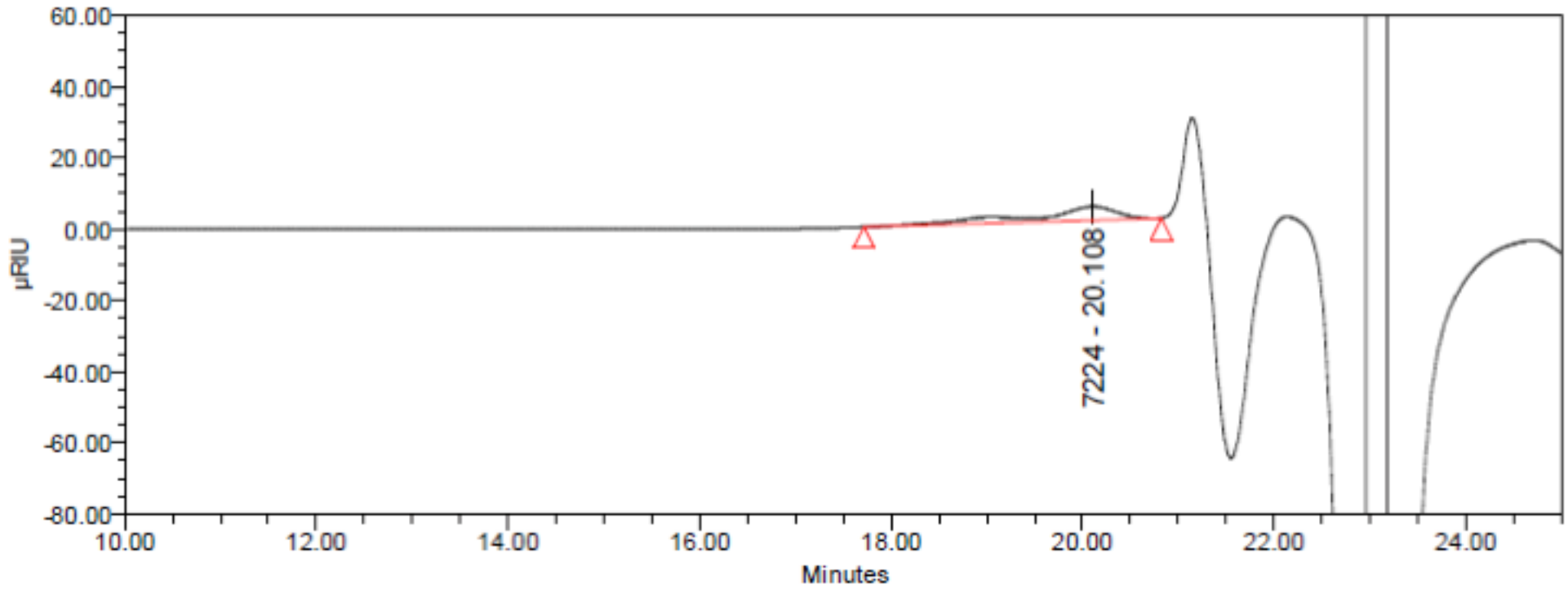
GPC Results

	Dist Name	Mn	Mw	MP	Mz	Mz+1	Mv	Polydispersity	MW Marker 1	MW Marker 2
1		5353	5413	5663	5472	5530		1.011196		



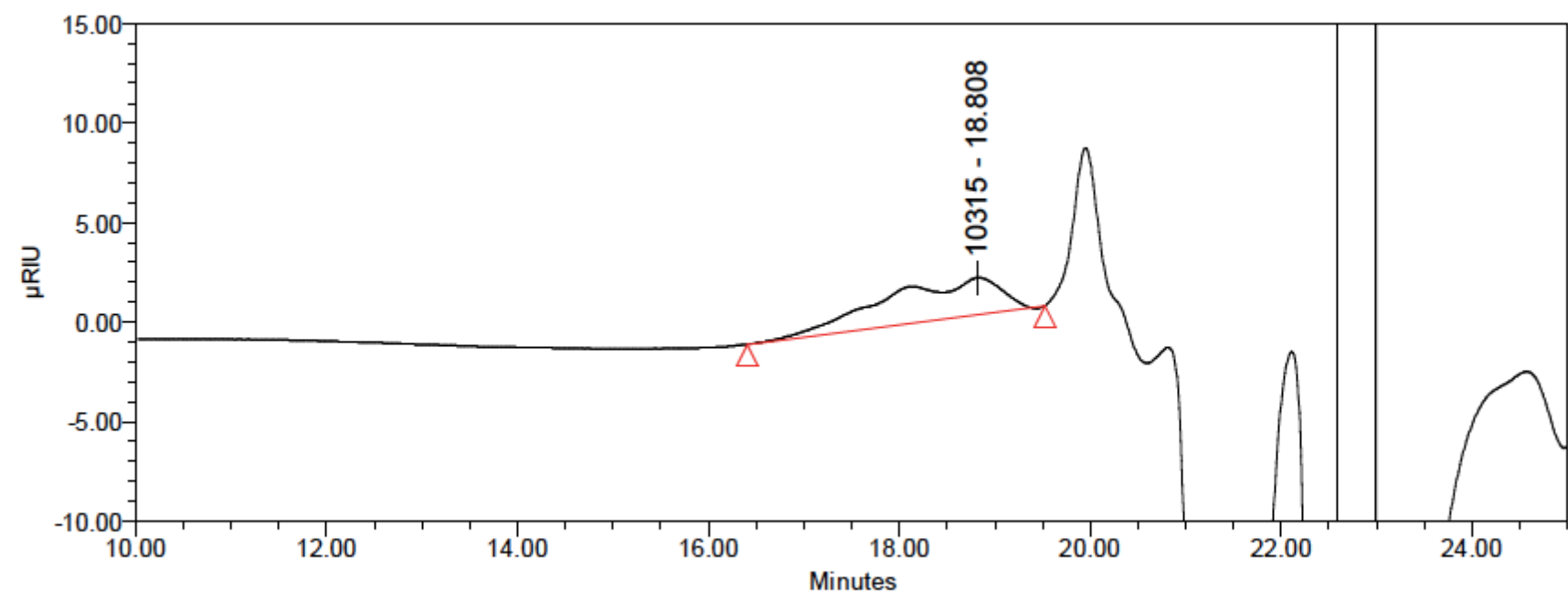
GPC Results

	Dist Name	Mn	Mw	MP	Mz	Mz+1	Mv	Polydispersity	MW Marker 1	MW Marker 2
1		12889	13804	10484	14864	16020		1.070925		



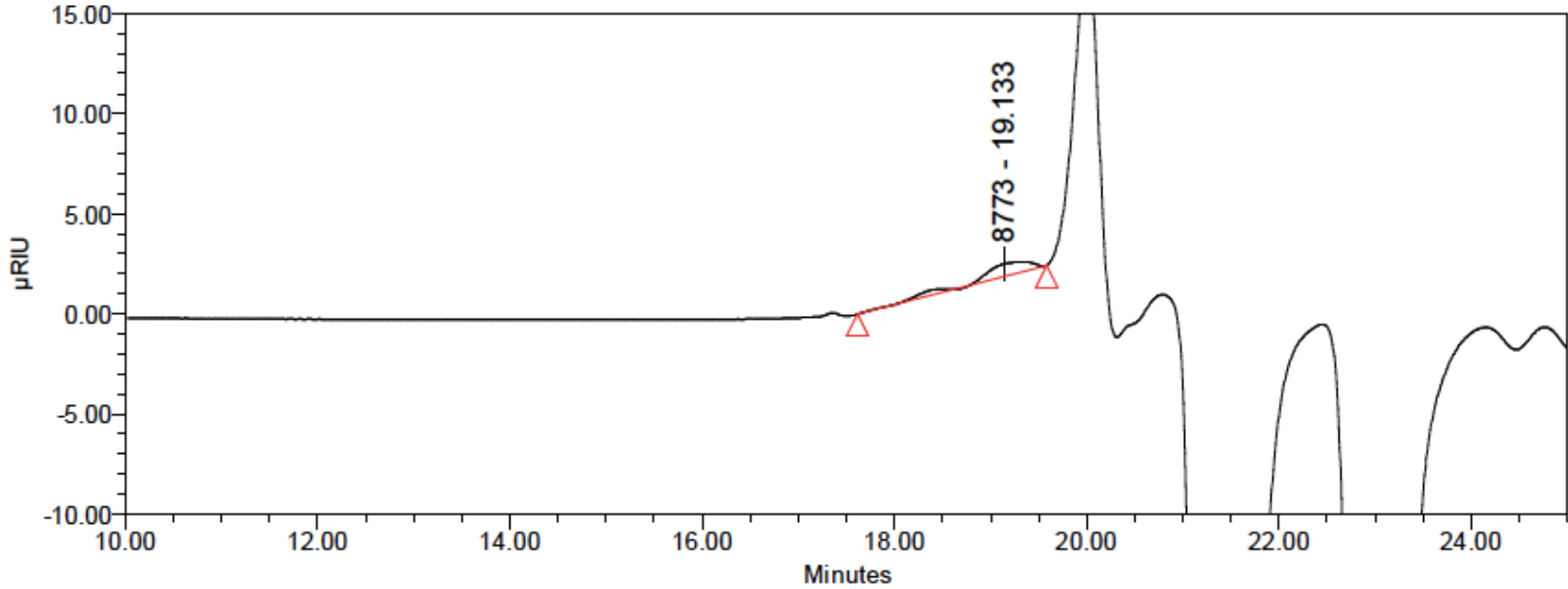
GPC Results

	Dist Name	Mn	Mw	MP	Mz	Mz+1	Mv	Polydispersity	MW Marker 1	MW Marker 2
1		8748	9589	7224	10630	11787		1.096097		



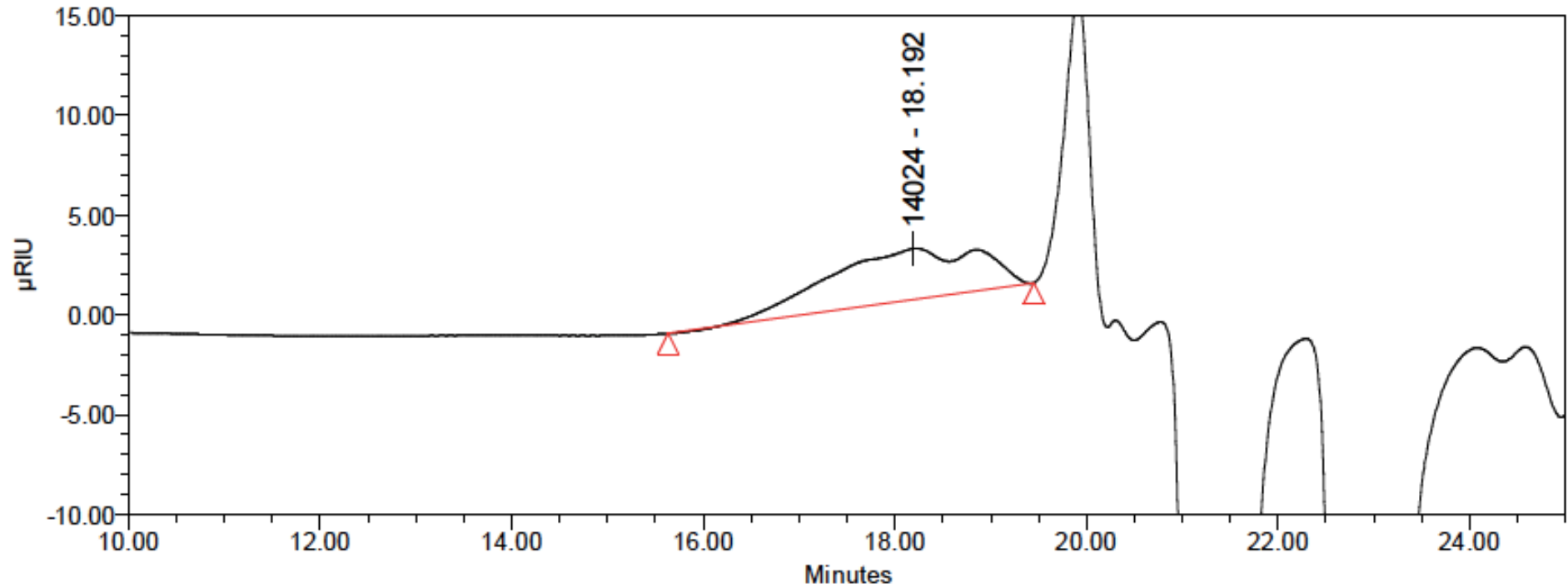
GPC Results

	Dist Name	Mn	Mw	MP	Mz	Mz+1	Mv	Polydispersity	MW Marker 1	MW Marker 2
1		13188	14326	10315	15634	17041		1.086360		



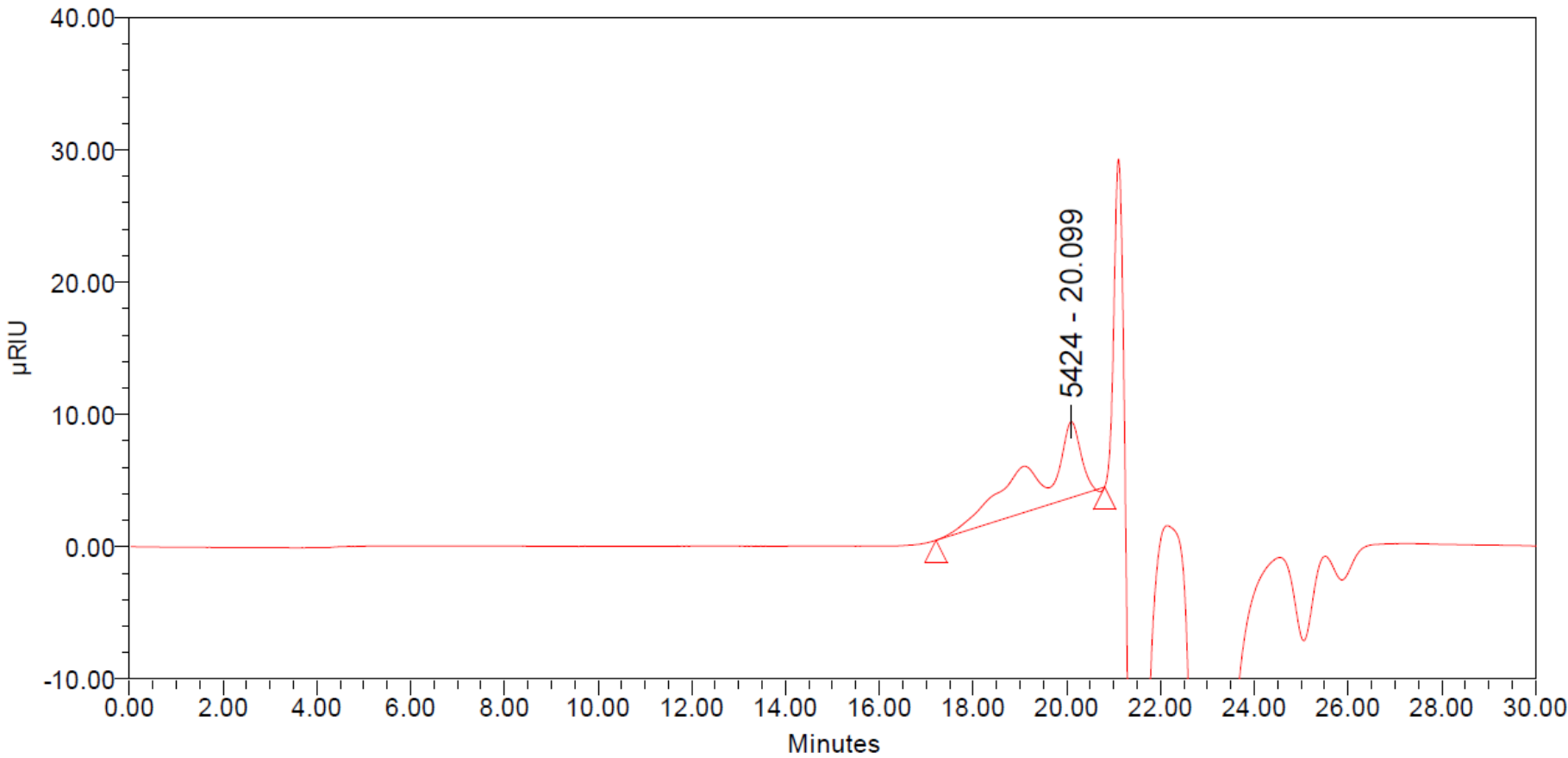
GPC Results

	Dist Name	Mn	Mw	MP	Mz	Mz+1	Mv	Polydispersity	MW Marker 1	MW Marker 2
1		8568	8624	8773	8680	8736		1.006530		



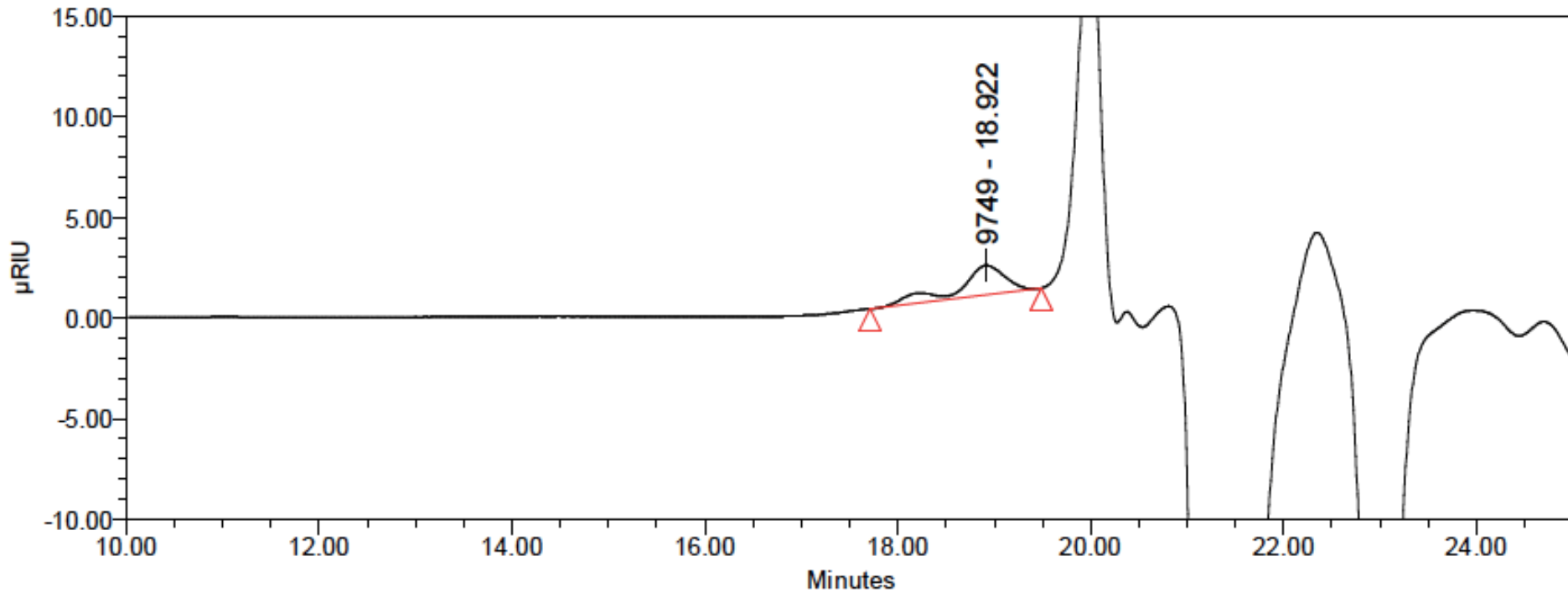
GPC Results

	Dist Name	Mn	Mw	MP	Mz	Mz+1	Mv	Polydispersity	MW Marker 1	MW Marker 2
1		14645	16409	14024	18407	20486		1.120469		



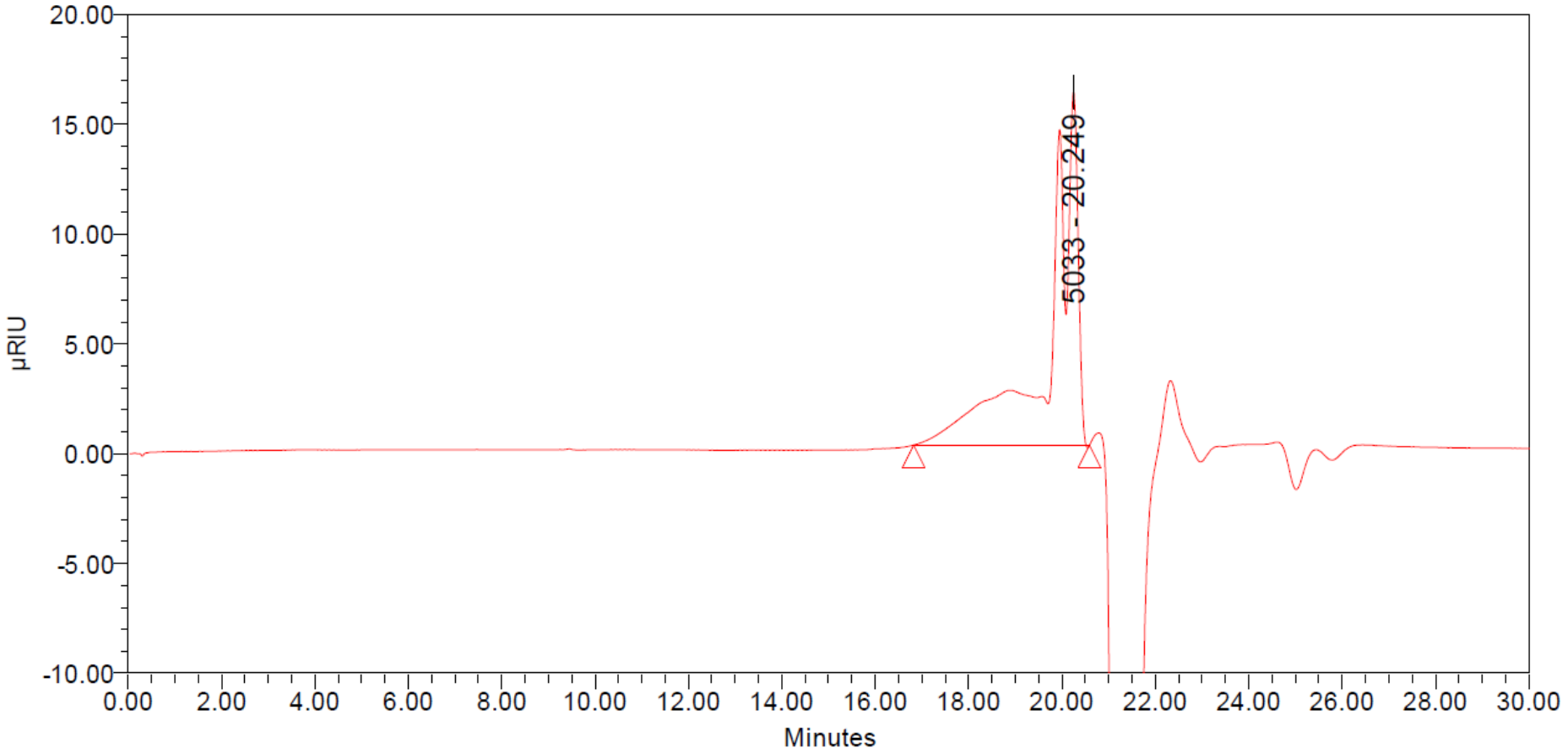
GPC Results

	Dist Name	Mn	Mw	MP	Mz	Mz+1	Mv	Polydispersity	MW Marker 1	MW Marker 2
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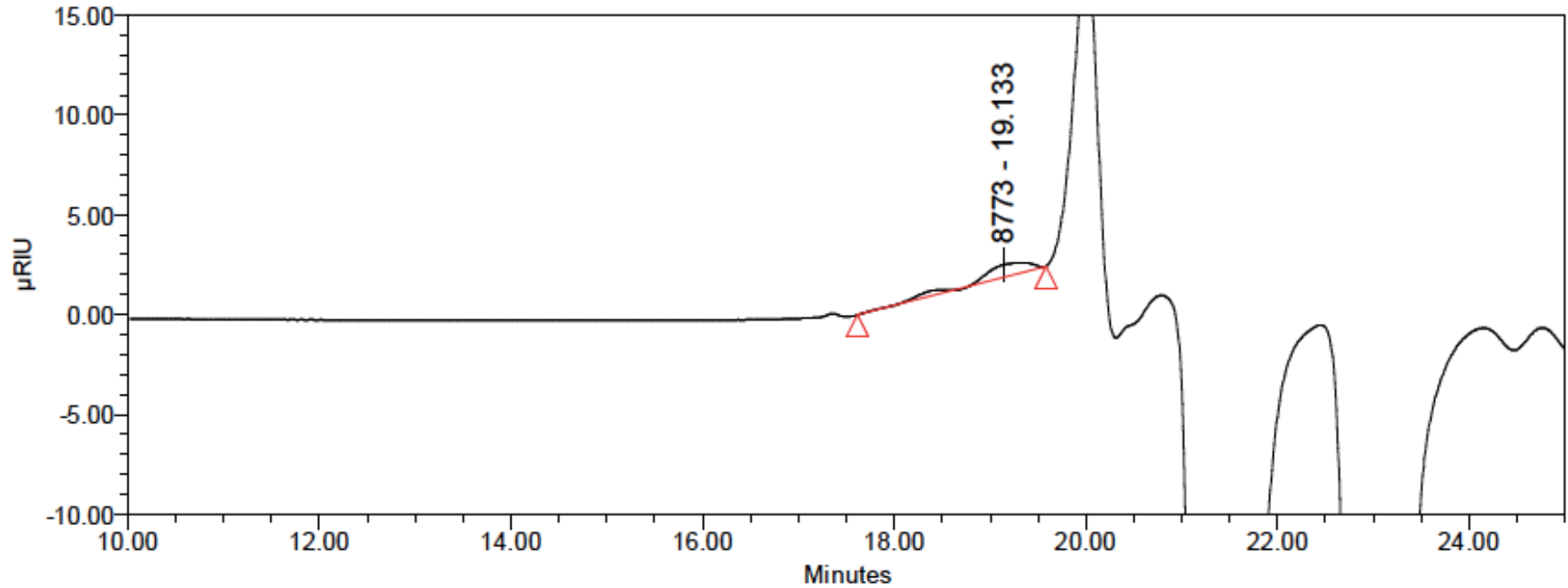
GPC Results

	Dist Name	Mn	Mw	MP	Mz	Mz+1	Mv	Polydispersity	MW Marker 1	MW Marker 2
1		10457	10769	9749	11130	11531		1.029884		



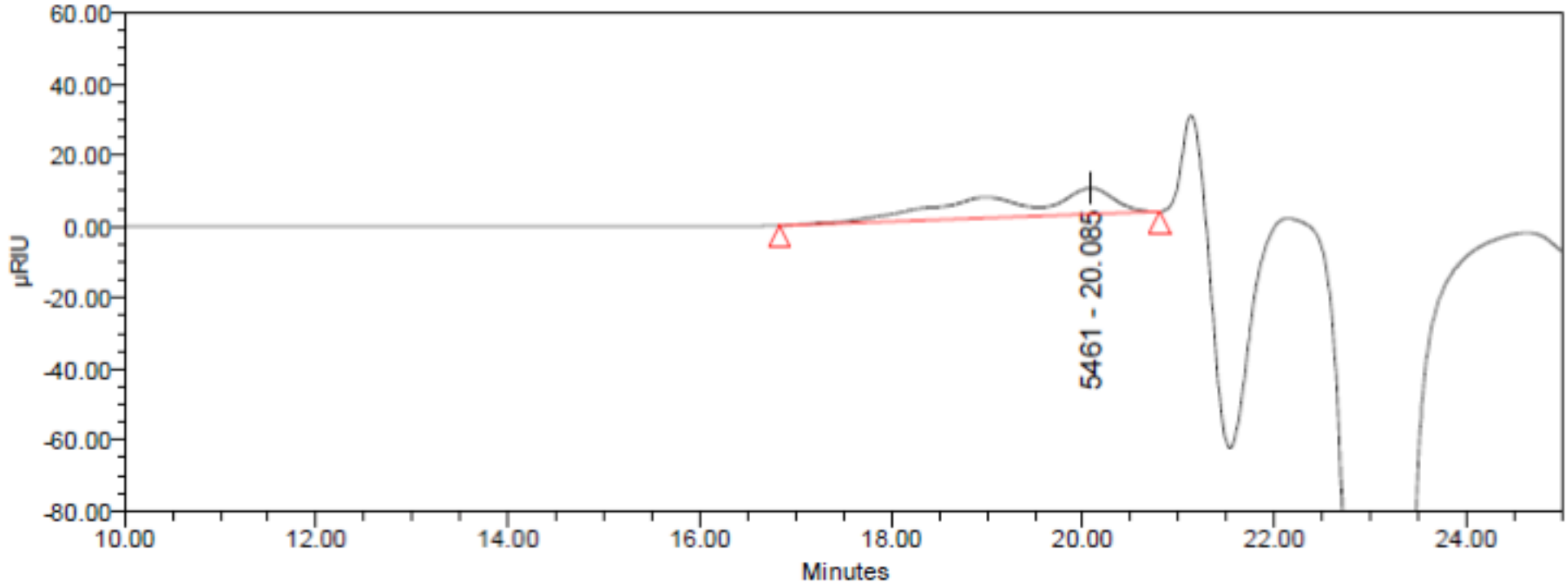
GPC Results

	Dist Name	Mn	Mw	MP	Mz	Mz+1	Mv	Polydispersity	MW Marker 1	MW Marker 2
1		6671	7883	5033	9855	12393		1.181585		



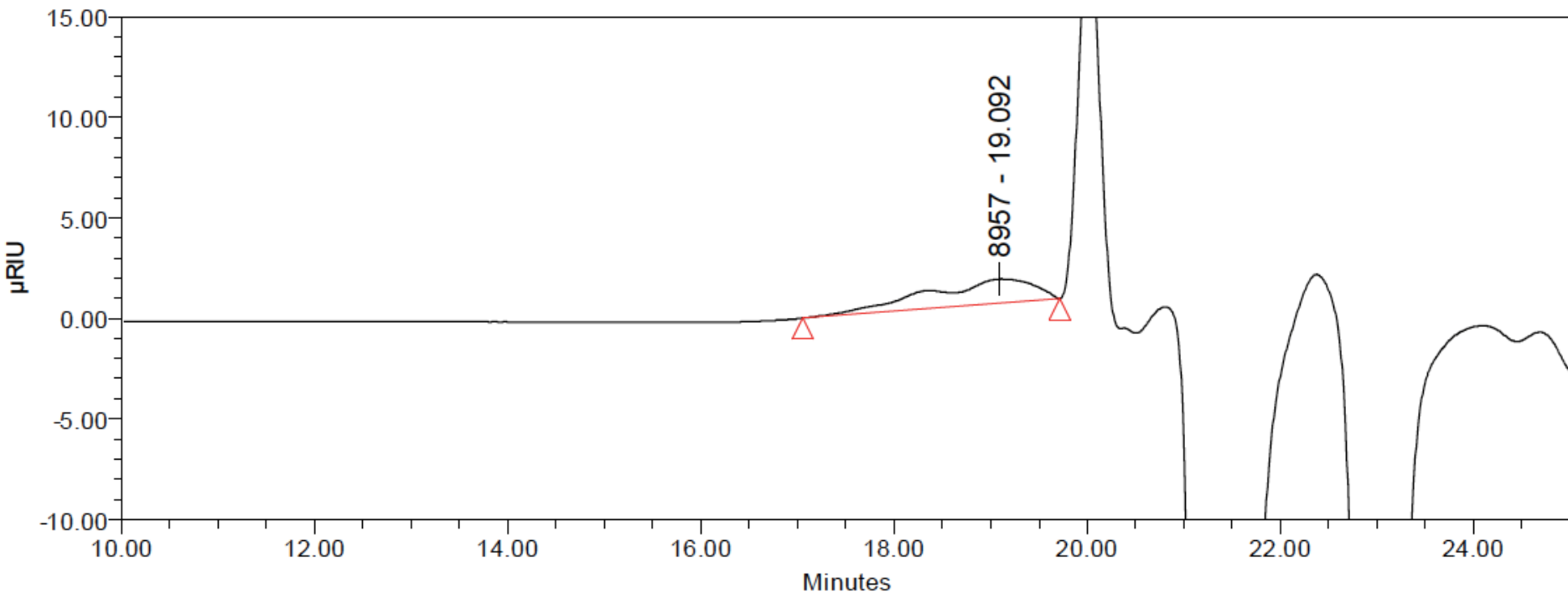
GPC Results

	Dist Name	Mn	Mw	MP	Mz	Mz+1	Mv	Polydispersity	MW Marker 1	MW Marker 2
1		8568	8624	8773	8680	8736		1.006530		



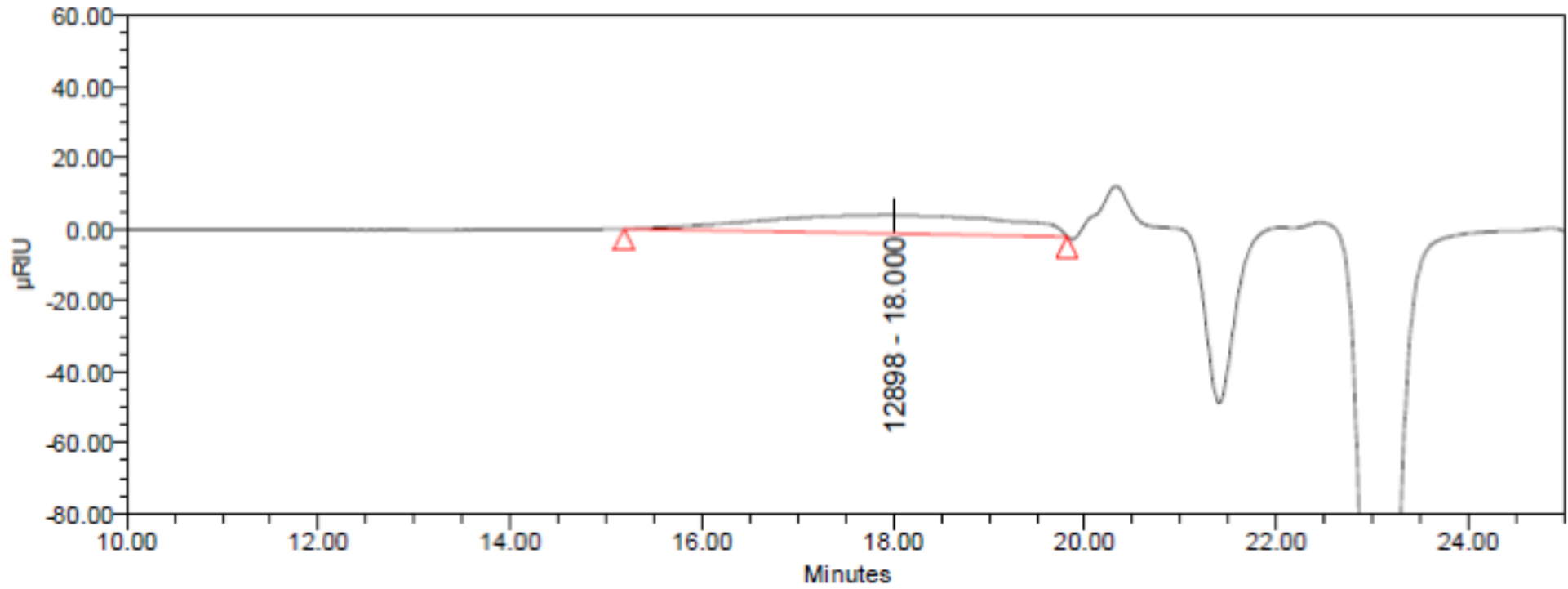
GPC Results

	Dist Name	Mn	Mw	MP	Mz	Mz+1	Mv	Polydispersity	MW Marker 1	MW Marker 2
1		7756	9018	5461	10524	12106		1.162762		



GPC Results

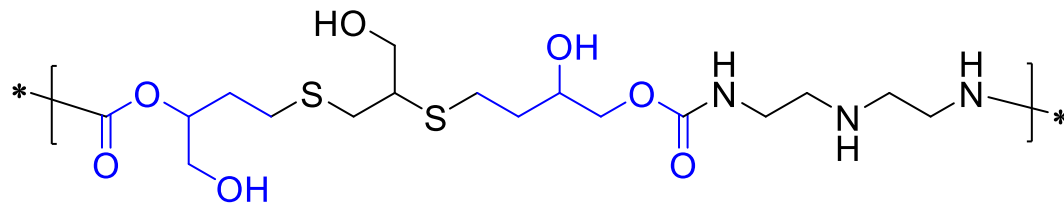
	Dist Name	Mn	Mw	MP	Mz	Mz+1	Mv	Polydispersity	MW Marker 1	MW Marker 2
1		10434	11245	8957	12198	13243		1.077784		



GPC Results

	Dist Name	Mn	Mw	MP	Mz	Mz+1	Mv	Polydispersity	MW Marker 1	MW Marker 2
1		12173	14705	12898	17932	21457		1.207967		

PHU E-DETA



***Monomer E +
diethylenetriamine
(DETA)***

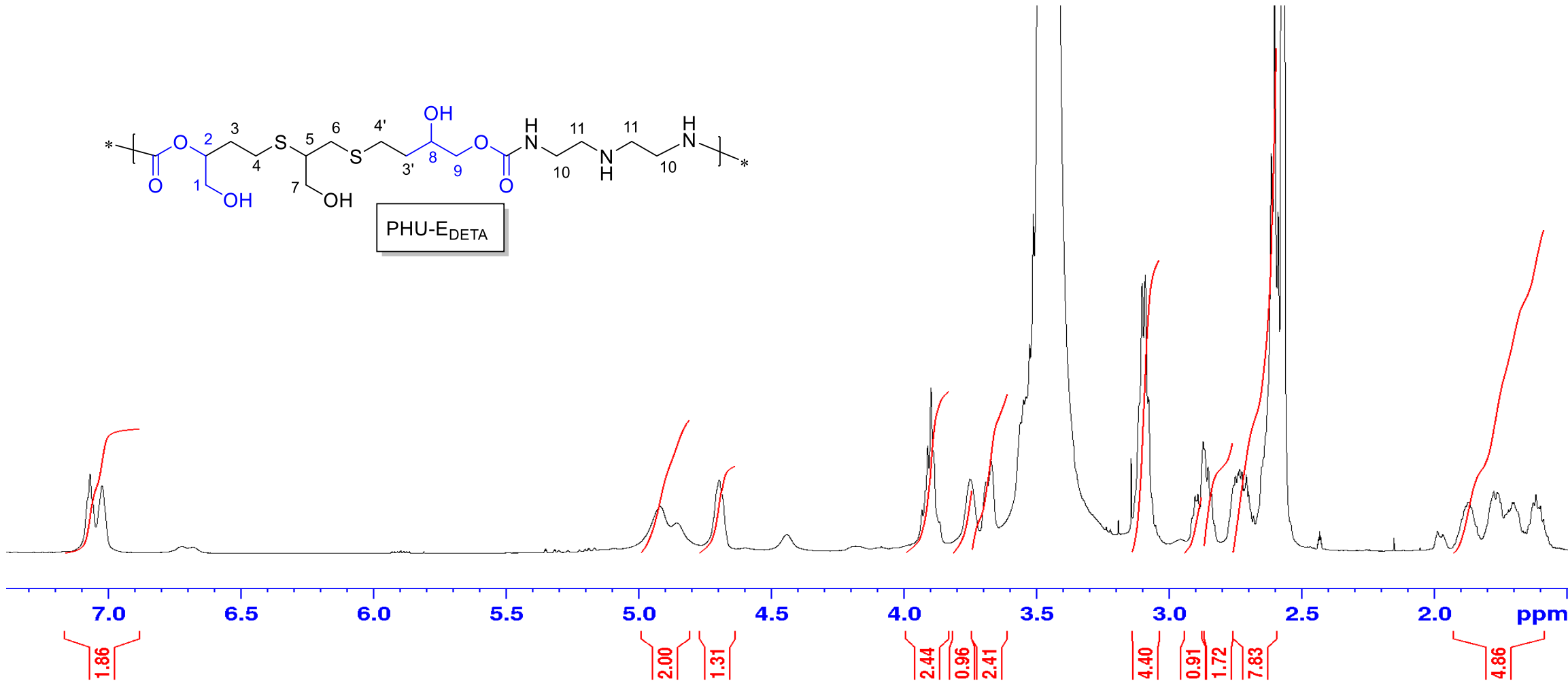
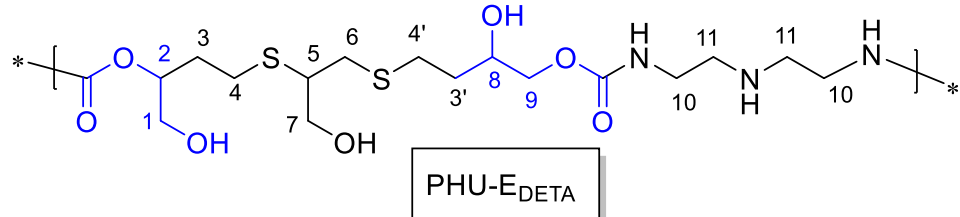
PHU E-DETA

Spectrum $^1\text{H-RMN}$, 500 MHz, $\text{DMSO-}d_6$

7.070
7.025

4.924
4.848
4.704
4.446

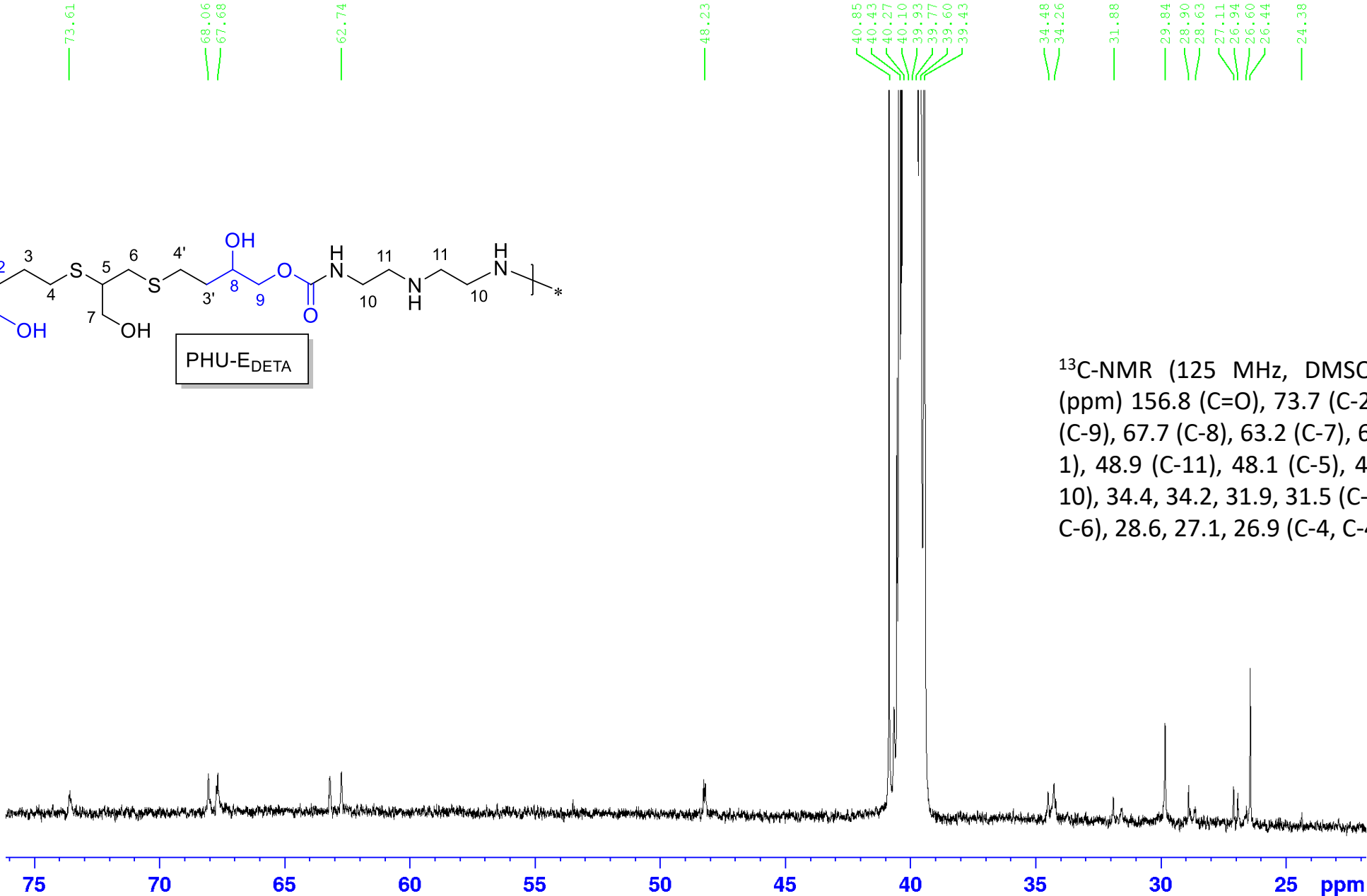
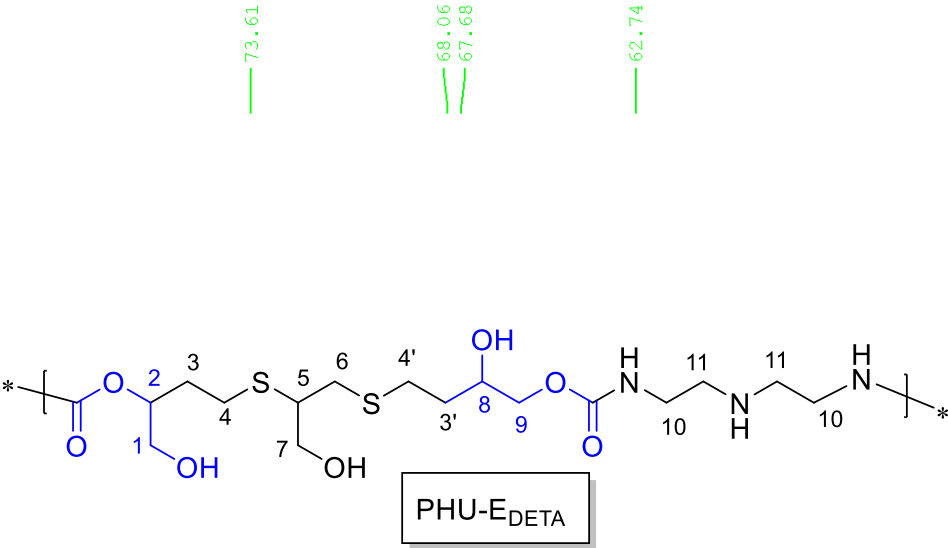
3.903
3.762
3.696
3.675
3.514
3.500
3.451
3.101
3.089
2.894
2.873
2.613
2.609
2.601
2.588
2.577
2.574
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2.567
2.563
1.984
1.870
1.768
1.699
1.615

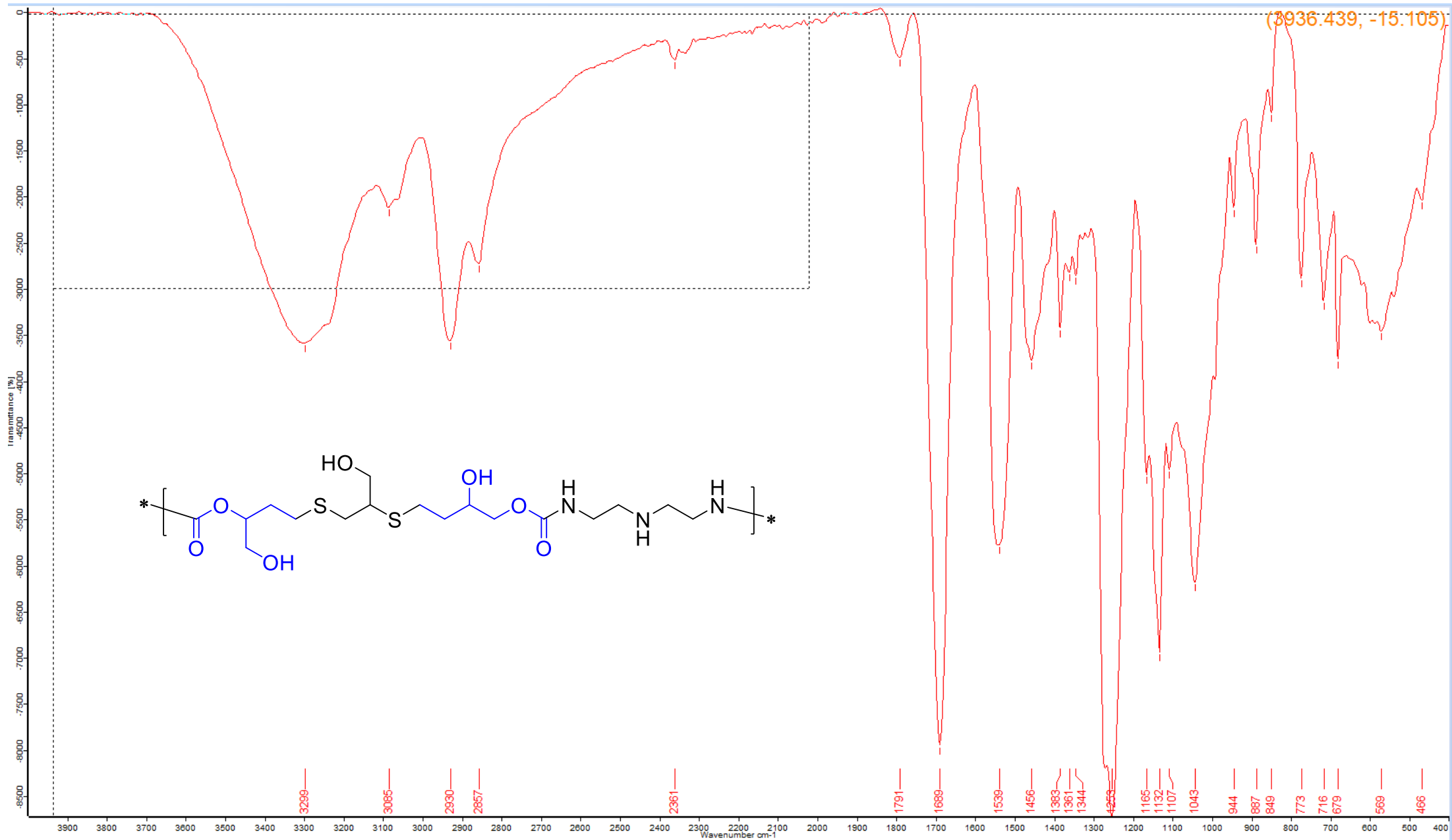


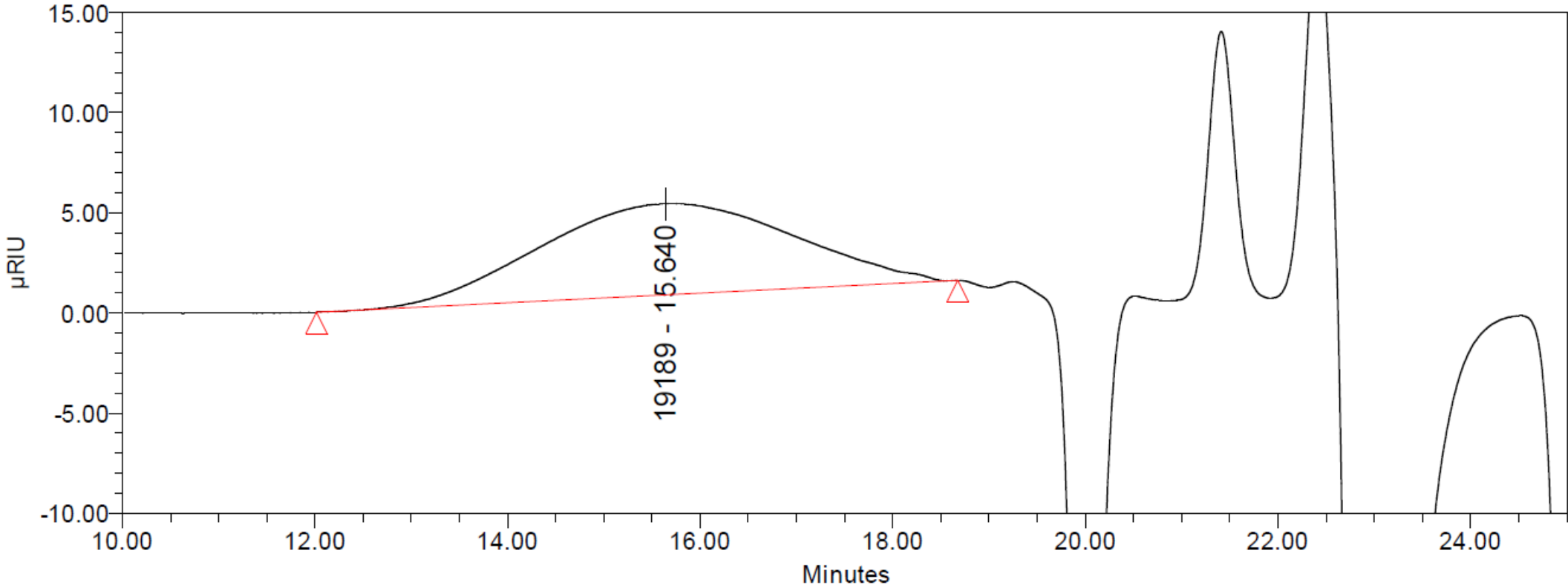
$^1\text{H-NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ (ppm) 7.07, 7.03 (2 bs, 2H, N-H), 4.99-4.81 (m, 3H, OH), 4.70 (bs, 1H, H-2), 3.99-3.83 (m, 2H, H-9), 3.76 (bs, 1H, H-8), 3.71-3.64 (m, 2H, H-7), 3.62-3.50 (m, H-1), 3.14-3.04 (m, 4H, H-10), 2.94-2.81 (m, 1H, H-5), 2.80-2.68 (m, 2H, H-6), 2.67-2.58 (m, 8H, H-4, H-4', H-11), 2.01-1.54 (m, 4H, H-3, H-3').

PHU E-DETA

Spectrum ^{13}C -RMN, 125 MHz, DMSO- d_6

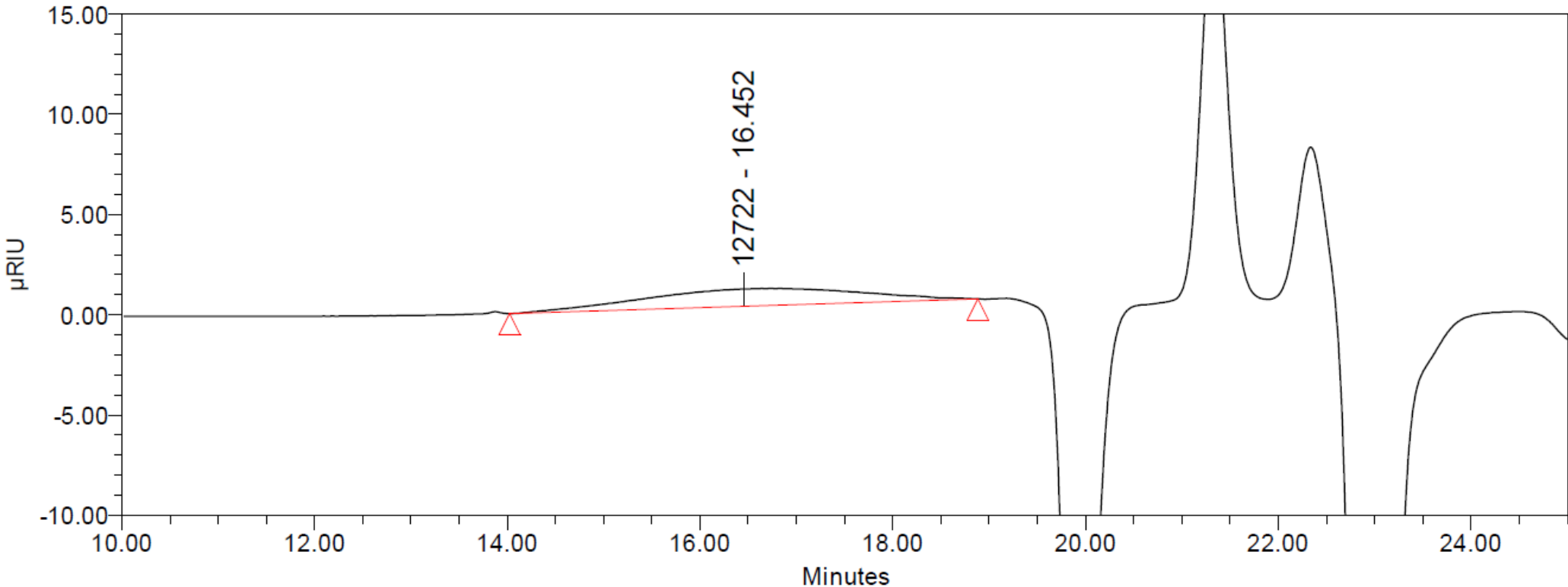






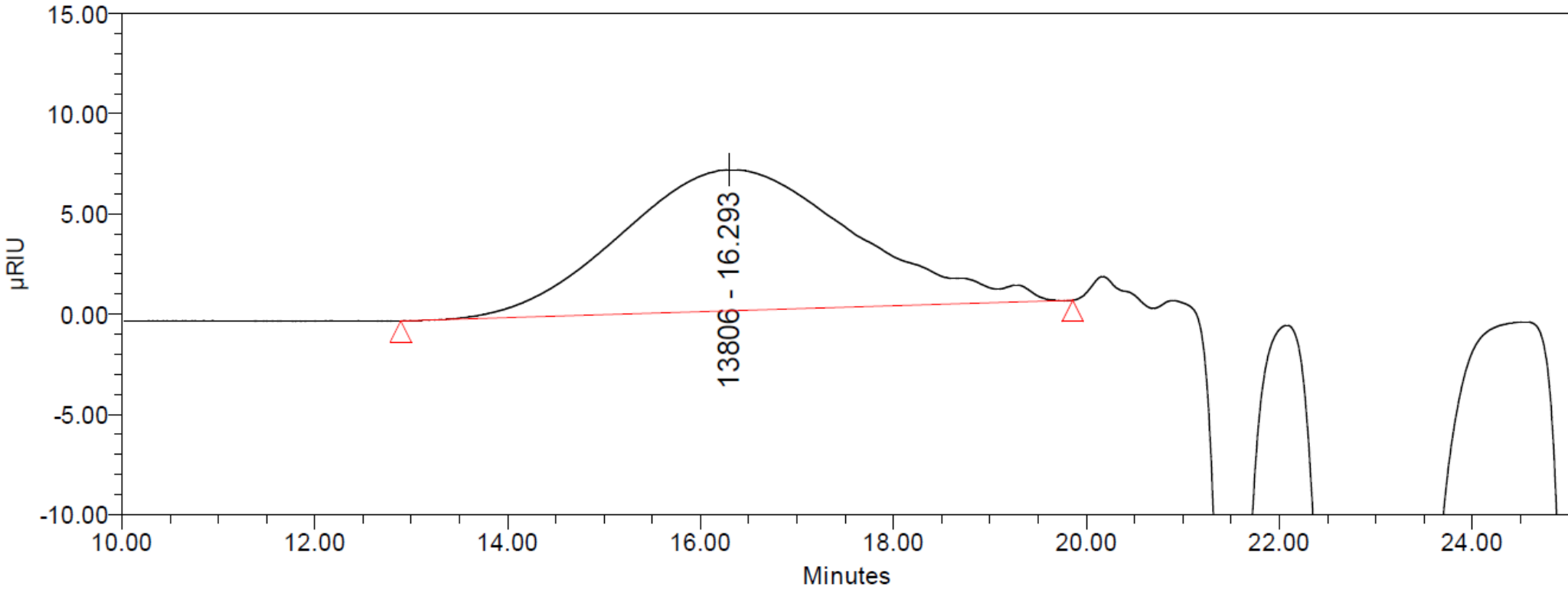
GPC Results

	Dist Name	Mn	Mw	MP	Mz	Mz+1	Mv	Polydispersity	MW Marker 1	MW Marker 2
1		15922	21841	19189	28842	36056		1.371764		



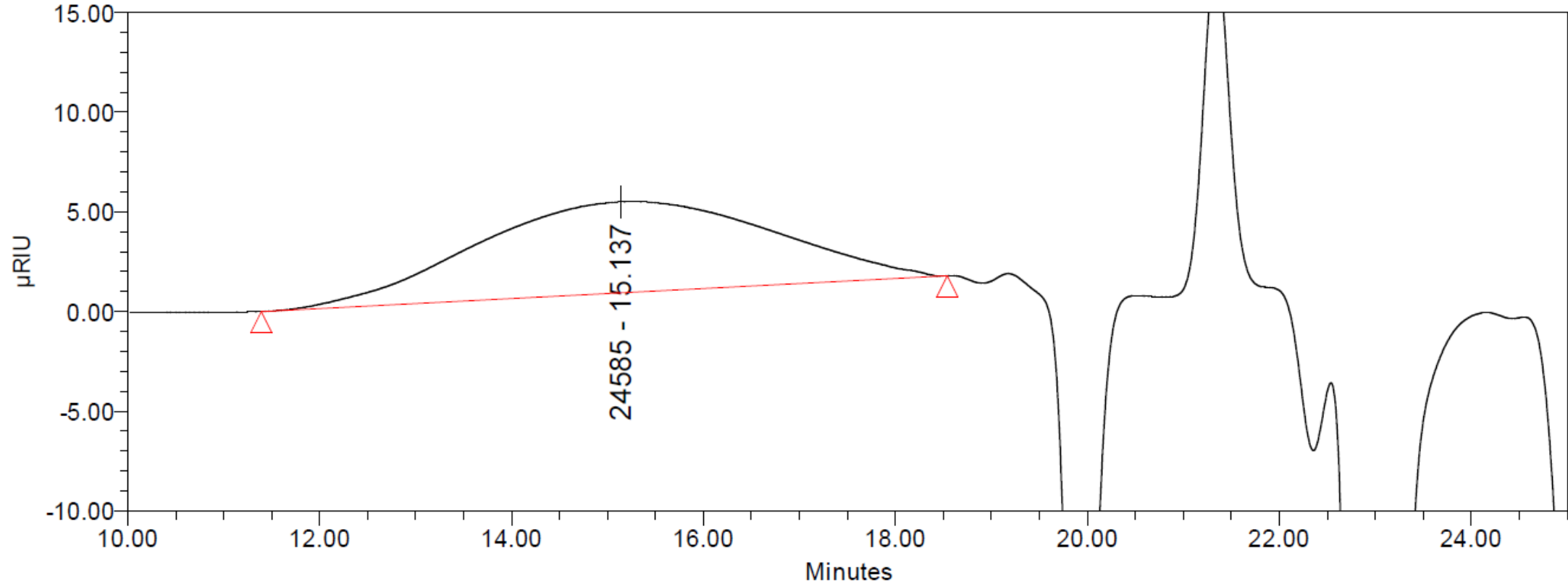
GPC Results

Dist Name	Mn	Mw	MP	Mz	Mz+1	Mv	Polydispersity	MW Marker 1	MW Marker 2
1	10717	13777	12722	17222	20609		1.285451		



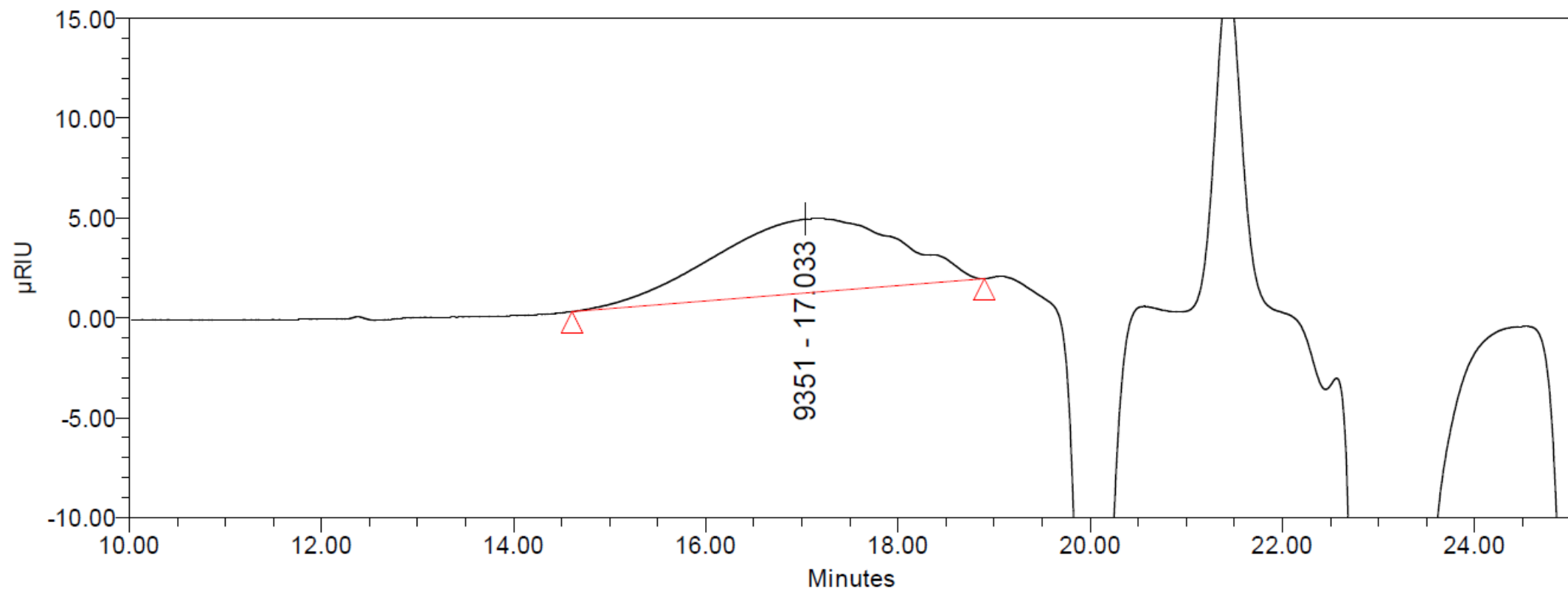
GPC Results

	Dist Name	Mn	Mw	MP	Mz	Mz+1	Mv	Polydispersity	MW Marker 1	MW Marker 2
1		10133	14518	13806	19080	23558		1.432751		



GPC Results

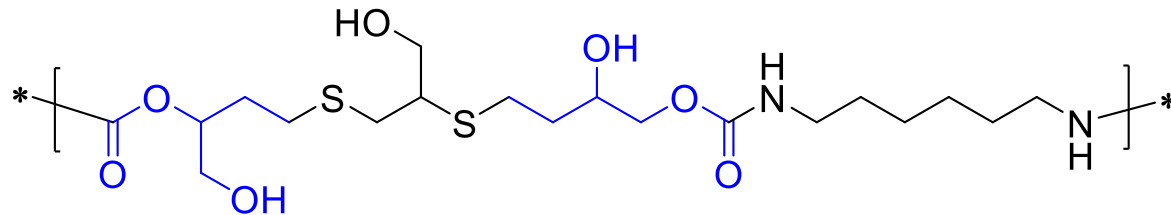
	Dist Name	Mn	Mw	MP	Mz	Mz+1	Mv	Polydispersity	MW Marker 1	MW Marker 2
1		19419	29629	24585	43185	58085		1.525796		



GPC Results

	Dist Name	Mn	Mw	MP	Mz	Mz+1	Mv	Polydispersity	MW Marker 1	MW Marker 2
1		8503	10316	9351	12396	14549		1.213128		

PHU E-HMDA



*Monomer E +
hexamethylenediamine
(HMDA)*

PHU E-HMDA

Spectrum $^1\text{H-RMN}$, 500 MHz, $\text{DMSO-}d_6$

7.109
7.064

4.898

4.681

3.898

3.735

3.670

3.446

3.011

2.850

2.724

2.603

2.572

2.568

2.564

2.561

2.557

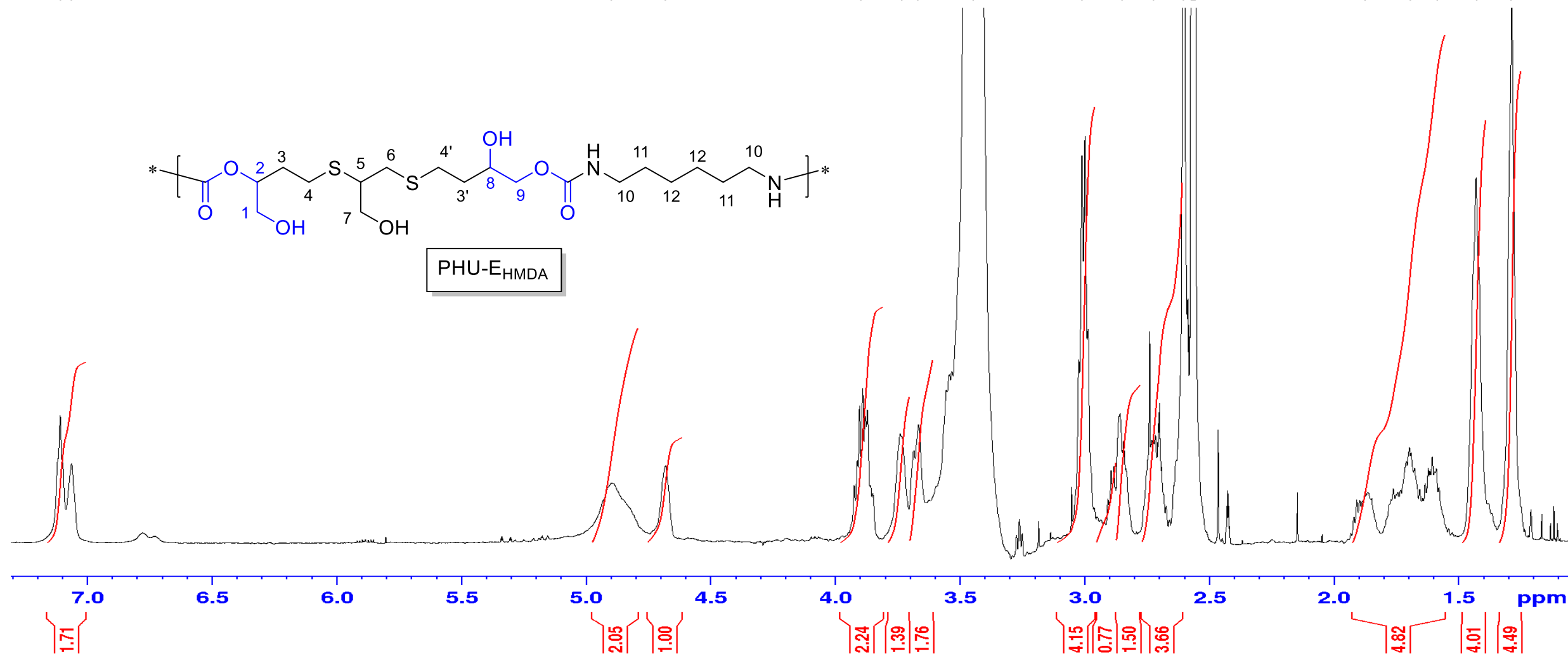
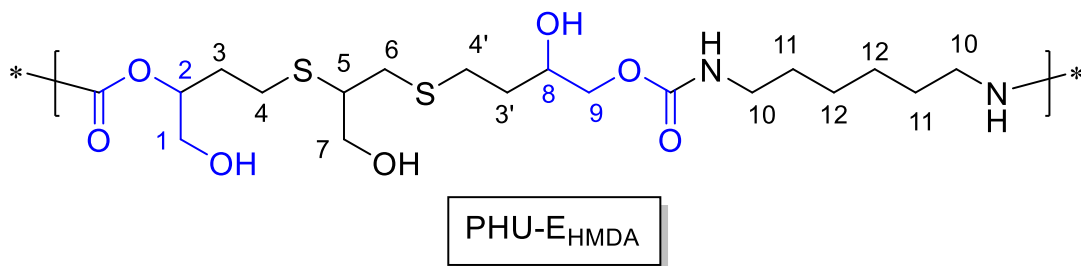
1.876

1.696

1.586

1.428

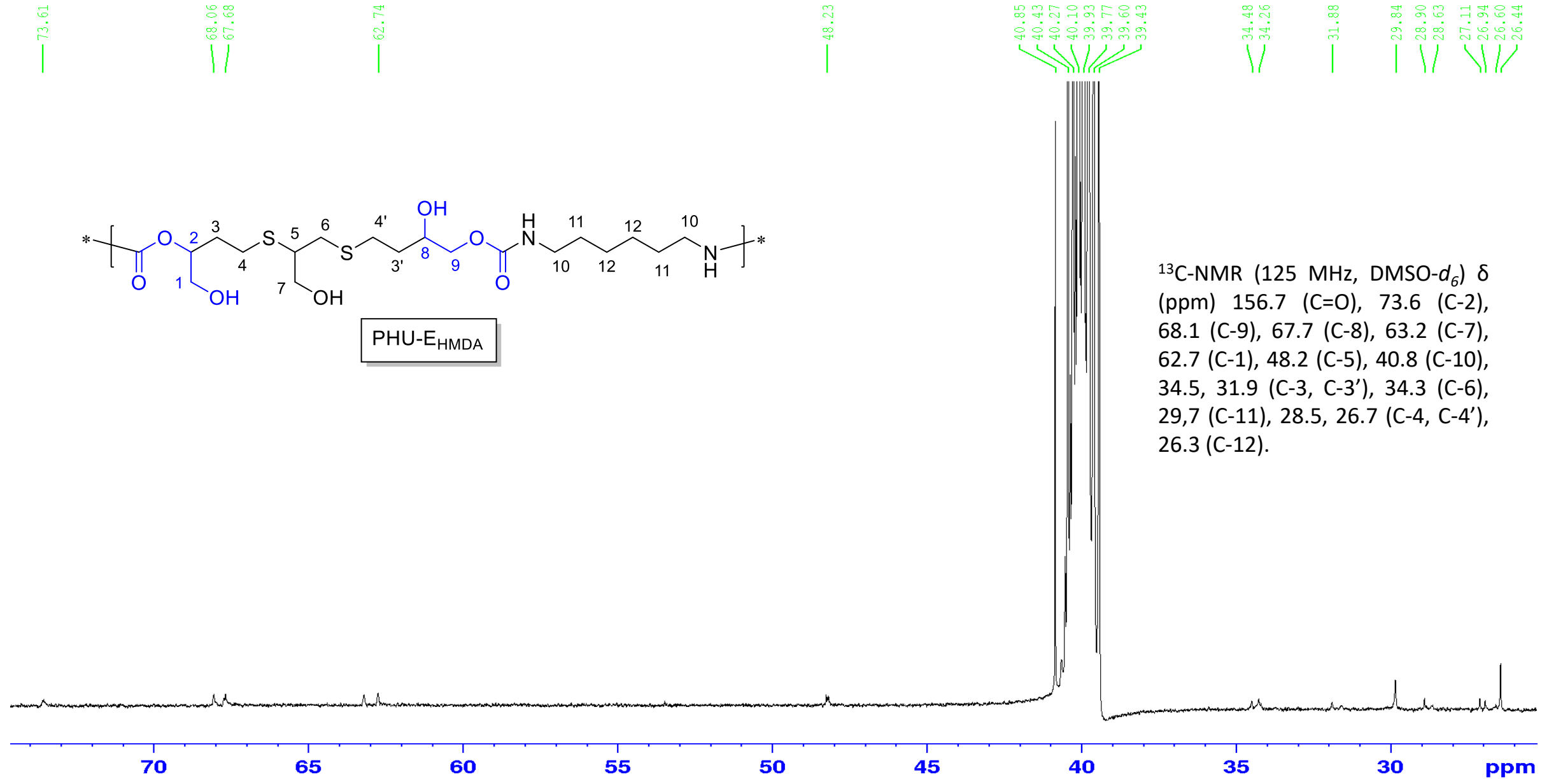
1.290



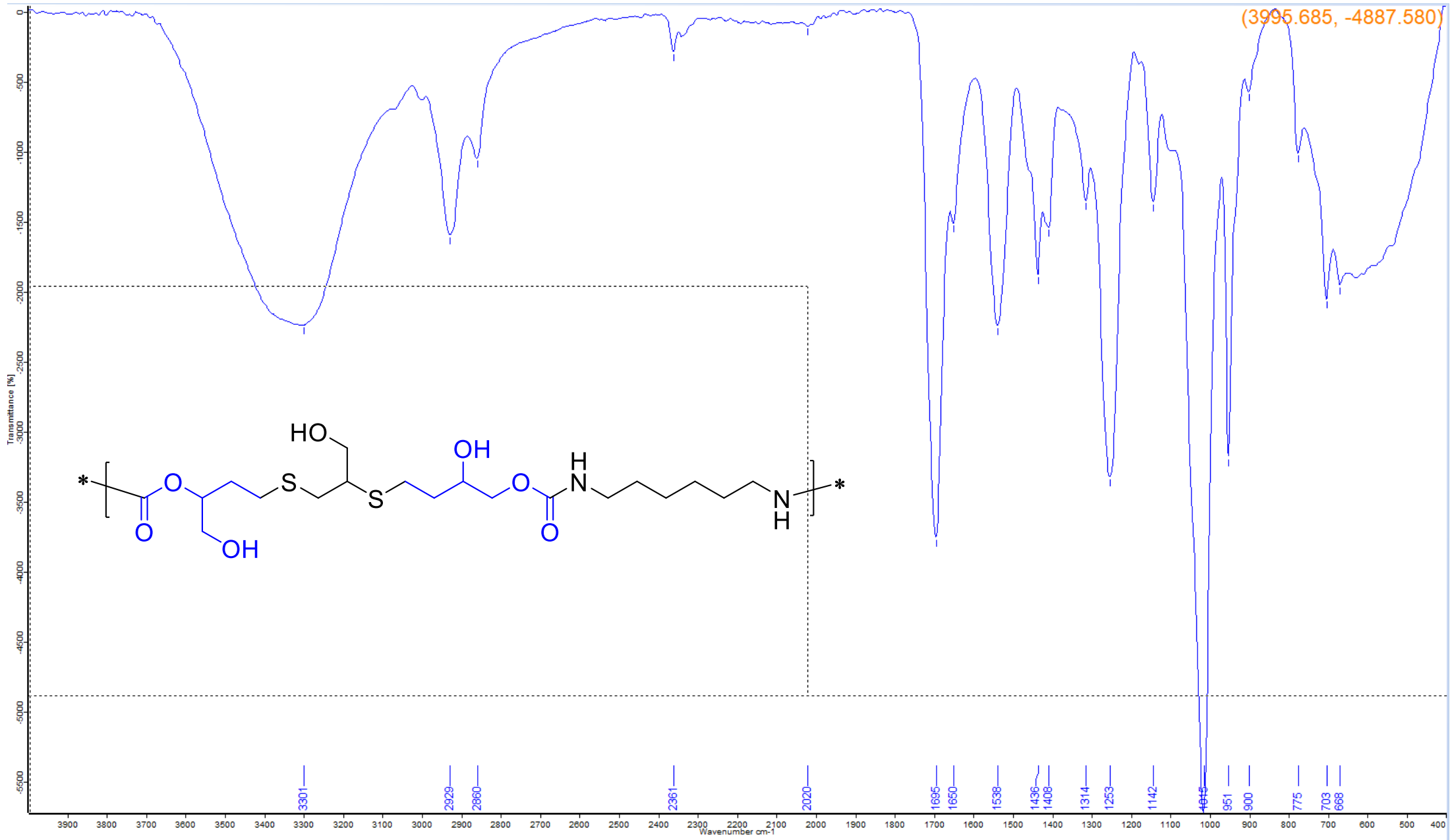
$^1\text{H-NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ (ppm) 7.11, 7.06 (2 bs, 2H, N-H), 4.97-4.79 (m, 2H, OH), 4.68 (bs, 1H, H-2), 3.97-3.81 (m, 2H, H-9), 3.73 (bs, 1H, H-8), 3.70-3.61 (m, 2H, H-7), 3.60-3.51 (m, 2H, H-1), 3.07-2.96 (m, 4H, H-10), 2.95-2.80 (m, 1H, H-5), 2.79-2.66 (m, 2H, H-6), 2.46-2.58 (m, 4H, H-4, H-4'), 1.95-1.52 (m, 4H, H-3, H-3'), 1.43 (bs, 4H, H-11), 1.29 (bs, 4H, H-12).

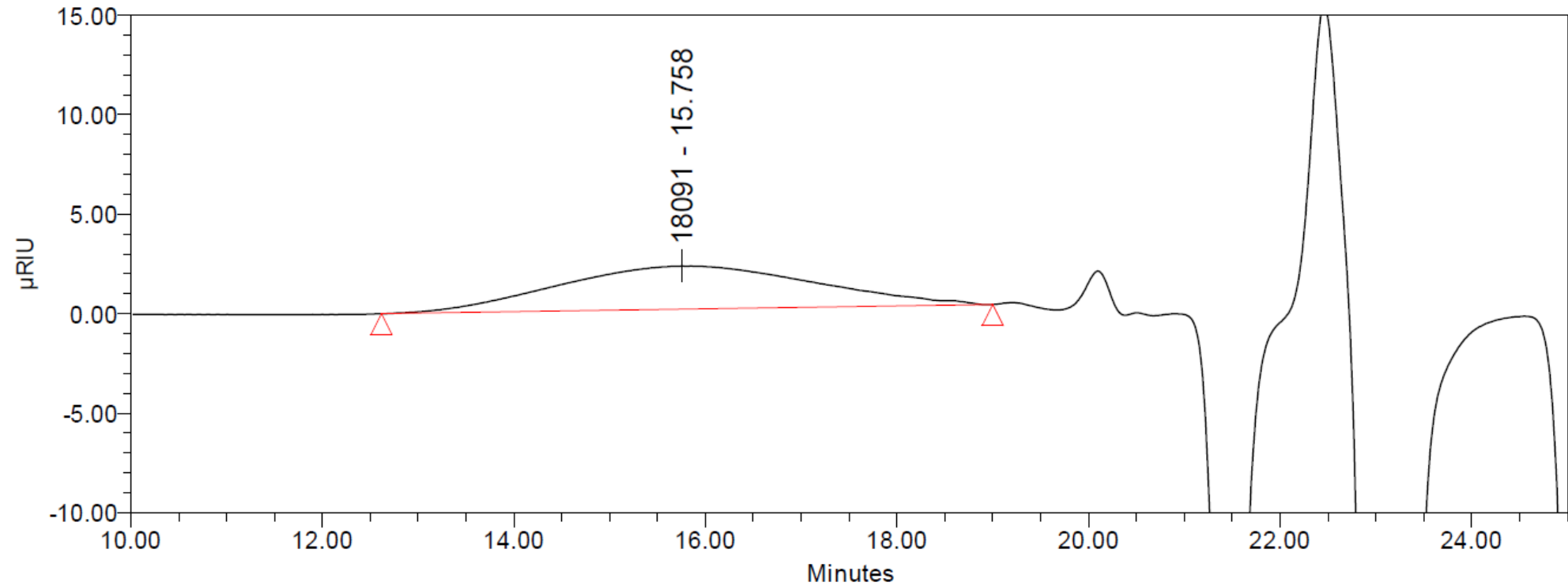
PHU E-HMDA

Spectrum ^{13}C -RMN, 125 MHz, DMSO- d_6



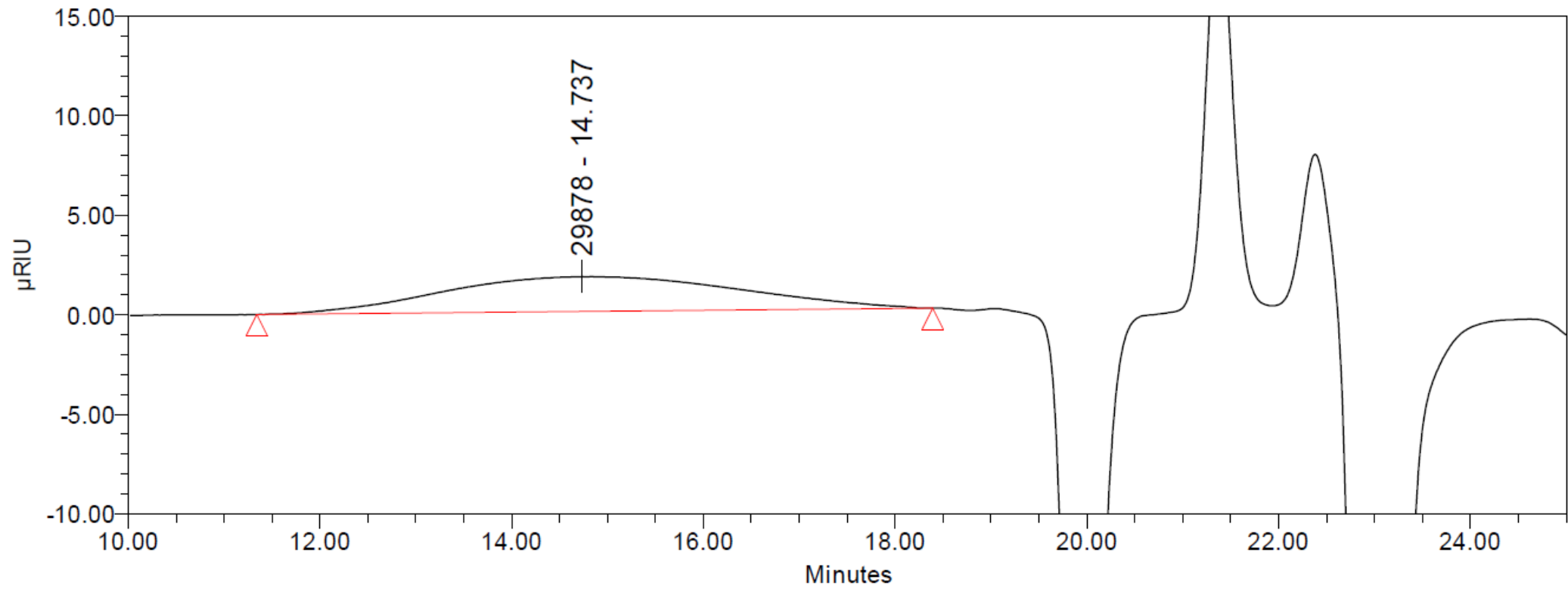
^{13}C -NMR (125 MHz, DMSO- d_6) δ (ppm) 156.7 (C=O), 73.6 (C-2), 68.1 (C-9), 67.7 (C-8), 63.2 (C-7), 62.7 (C-1), 48.2 (C-5), 40.8 (C-10), 34.5, 31.9 (C-3, C-3'), 34.3 (C-6), 29.7 (C-11), 28.5, 26.7 (C-4, C-4'), 26.3 (C-12).





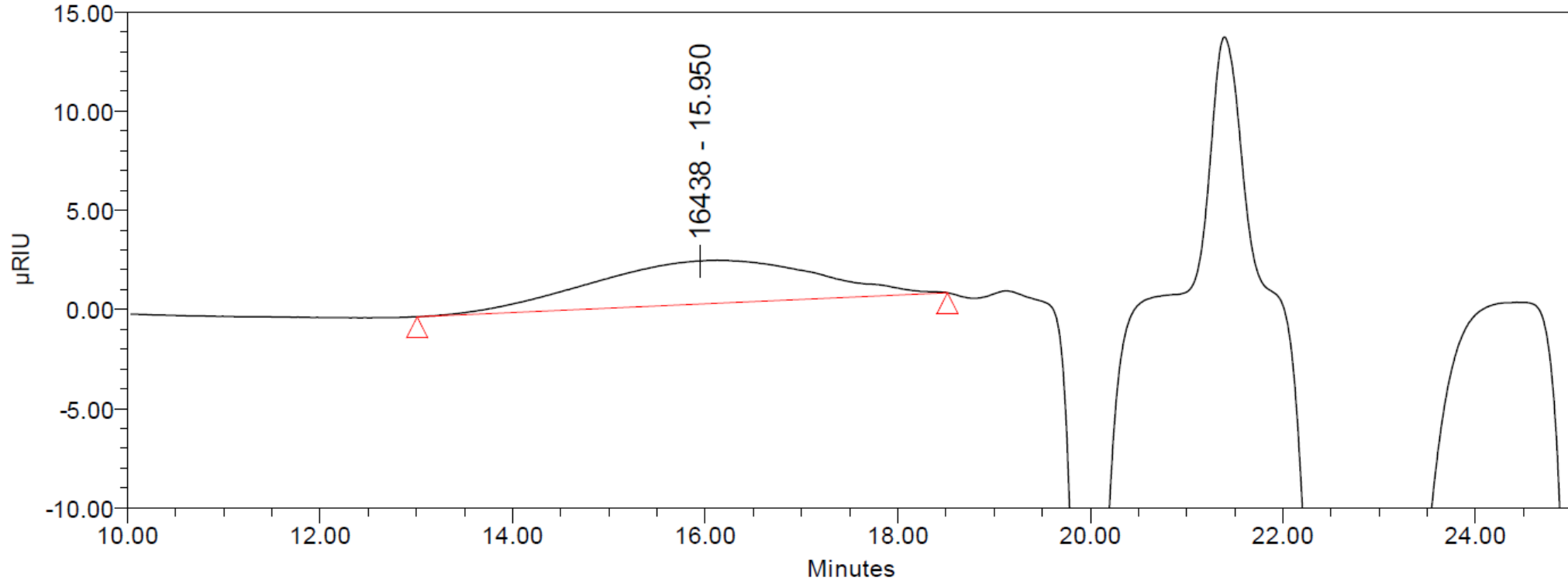
GPC Results

	Dist Name	Mn	Mw	MP	Mz	Mz+1	Mv	Polydispersity	MW Marker 1	MW Marker 2
1		14210	20262	18091	27264	34324		1.425931		



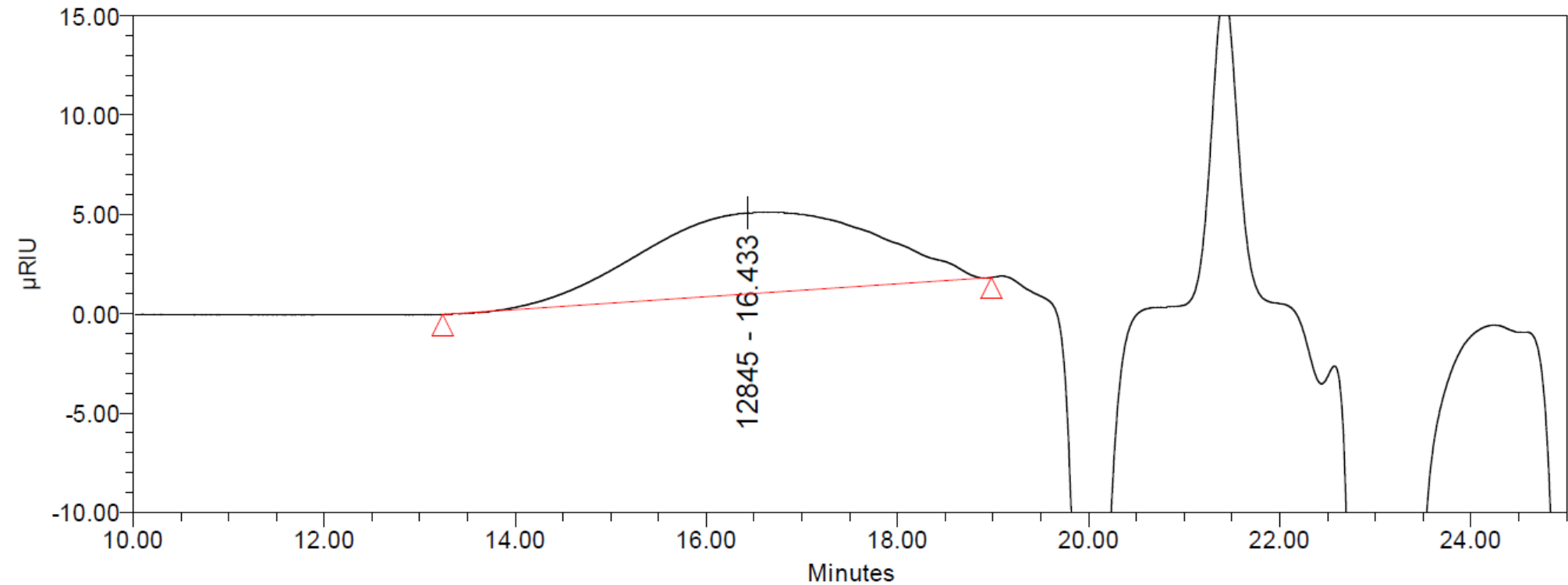
GPC Results

	Dist Name	Mn	Mw	MP	Mz	Mz+1	Mv	Polydispersity	MW Marker 1	MW Marker 2
1		22470	34055	29878	48802	64461		1.515543		



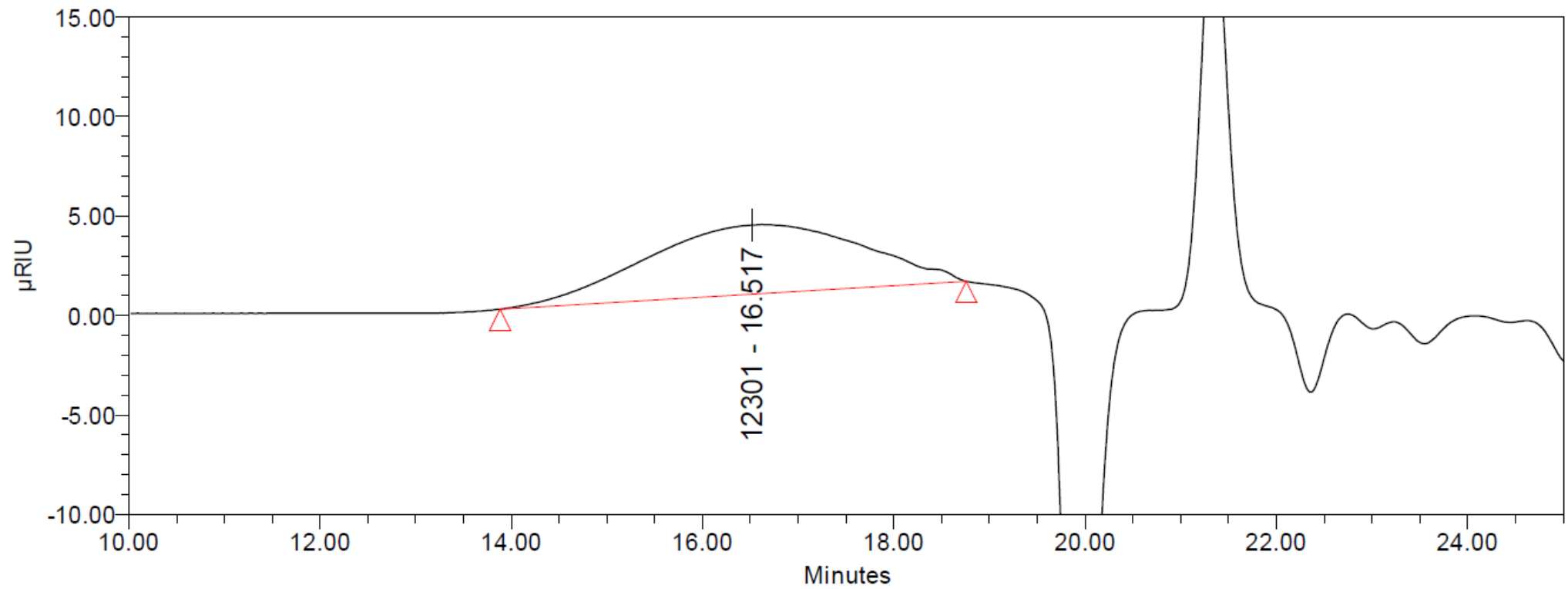
GPC Results

	Dist Name	Mn	Mw	MP	Mz	Mz+1	Mv	Polydispersity	MW Marker 1	MW Marker 2
1		14266	18476	16438	23445	28646		1.295087		



GPC Results

	Dist Name	Mn	Mw	MP	Mz	Mz+1	Mv	Polydispersity	MW Marker 1	MW Marker 2
1		10371	13639	12845	17415	21186		1.315142		



GPC Results

	Dist Name	Mn	Mw	MP	Mz	Mz+1	Mv	Polydispersity	MW Marker 1	MW Marker 2
1		10643	13657	12301	17107	20577		1.283156		