Supporting Information

Computation-guided rational design of a peptide motif that reacts with cyanobenzothiazoles via internal cysteine-lysine relay

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Contents

Table S1. List of sequences modeled using PEP-FOLD.[25-26] Bolded peptides in blue-shaded cells were subsequently made by SPPS.

AAAAAWGHGDGCKWGWGSGHGWAAAAA	AAAAAWGDGCKWGWGSGHGAAAAA
AAAAAHDGCKGDHAAAAA	PWGDGCKWGWGSGHGWP
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GGGGHGDGKCGGGGGG	GGGGGGGHDGKCGGGGGGGG
GGGGGHDGKCGGGGGG	GGGGGGGDHGKCGGGGGGGG
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GGDGHGCGKGG	GGKGDGHGCGG
GGKGDHGCGG	GGKGDHCGGG
GGDGHPCGKGG	GGDGHPCPKGG
GGDPHPCPKGG	GGKGHPCDGG
GGDPHPCKGGG	GGDGHPCKGGG
GGDPHPCKGGG	**GGHPDPCKGGG**
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GGFPCPKPHFGG	GGHPKPGCPFGG
GGHPKGPCPFGG	**GGHPKPGCGFGG**
GGHPKPGCFGG	**GGHPKPCGFGG**
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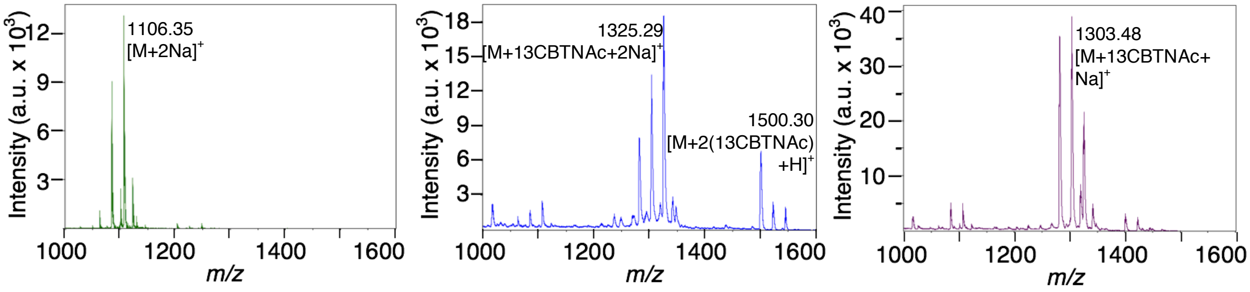
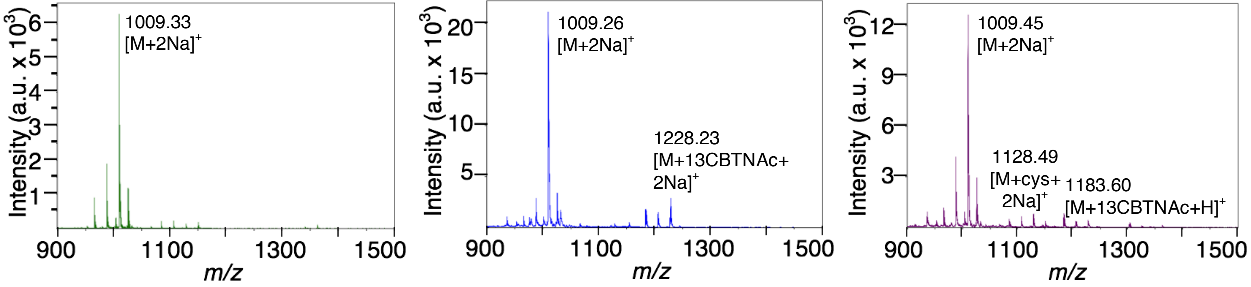
A. CBTag 1.0, Ac-GGHPDPCPKGG-NH_2 (**4**): 1061.47 g/mol



B. PEP-FOLD-4, Ac-GGDPHPCKGG-NH_2 (**5**): 964.42 g/mol



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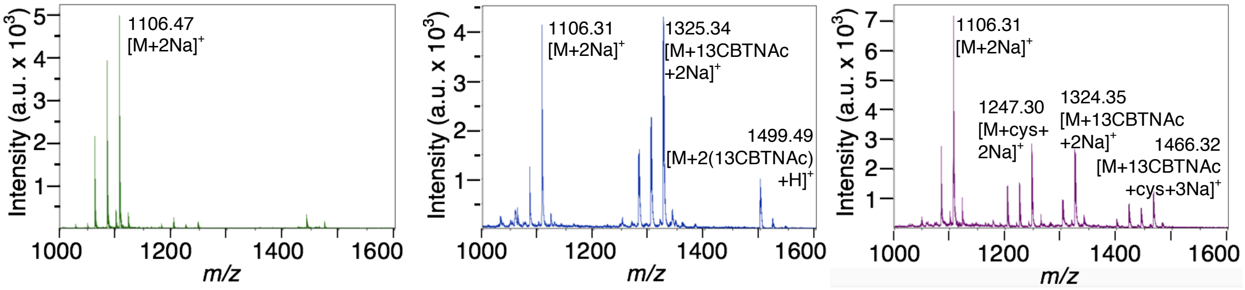

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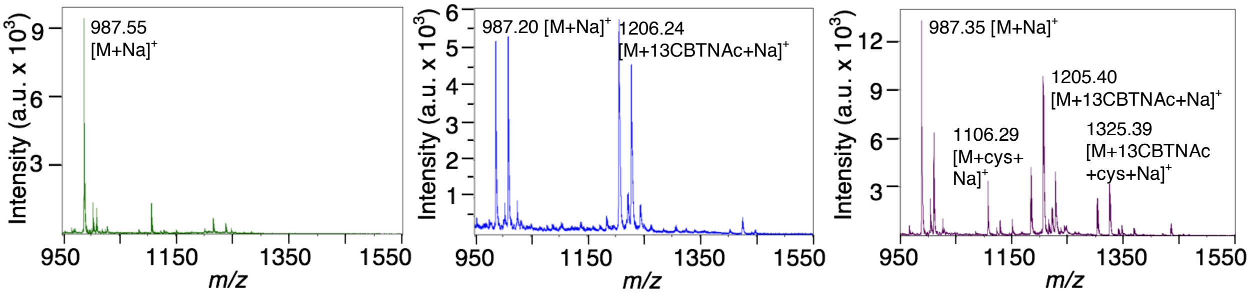
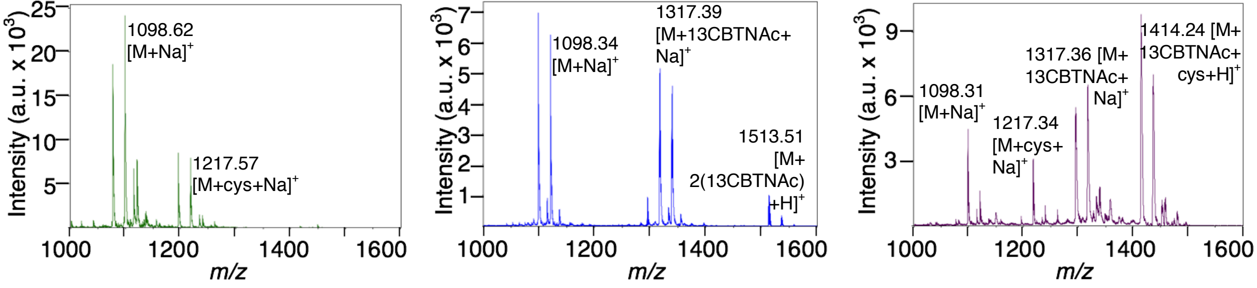
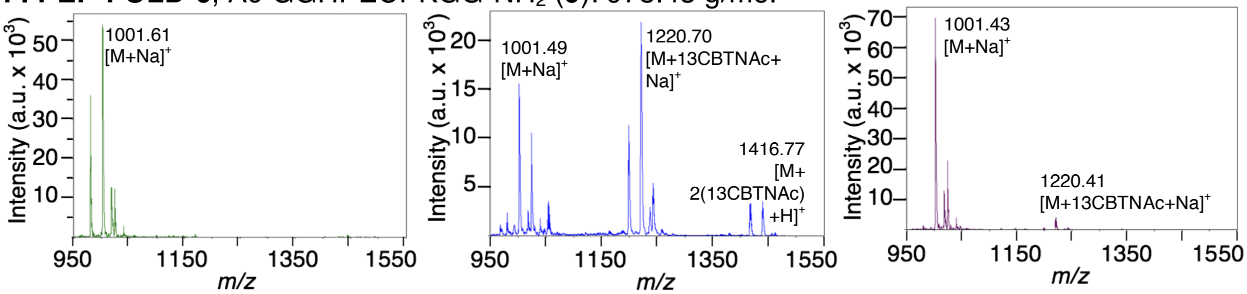


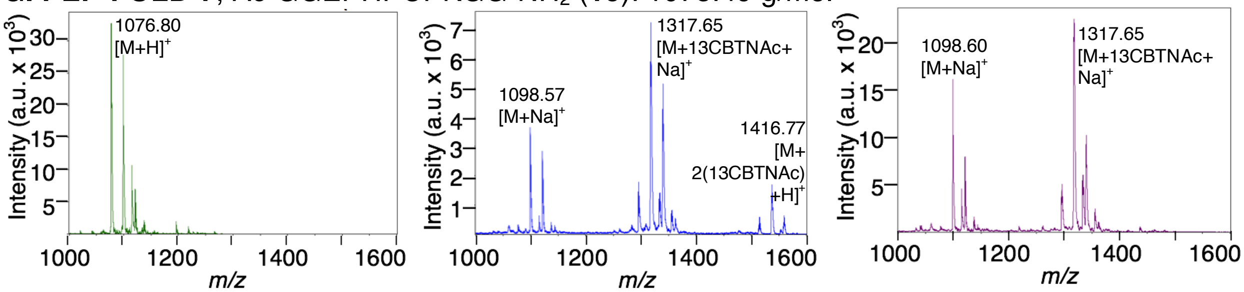
E. PEP-FOLD-5, Ac-GGHPEPCPKGG-NH_2 (**8**): 1075.49 g/mol



F. PEP-FOLD-6, Ac-GGHPECPKGG-NH_2 (**9**): 978.43 g/mol



G. PEP-FOLD-7, Ac-GGEPHPCPKGG-NH_2 (**10**): 1075.49 g/mol



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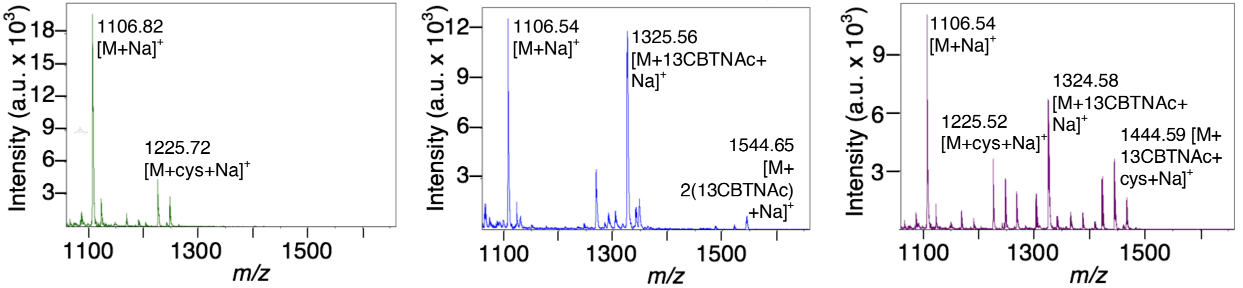
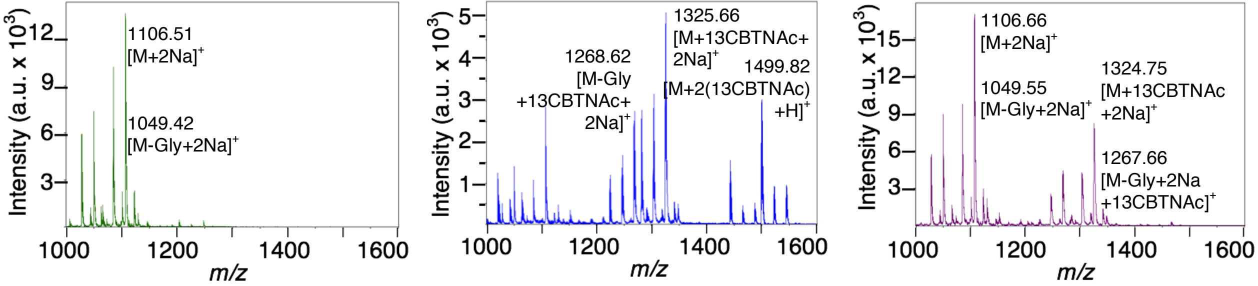
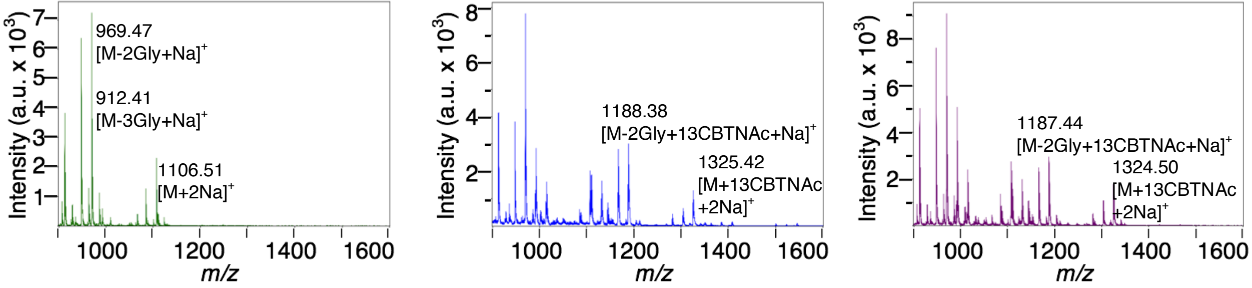


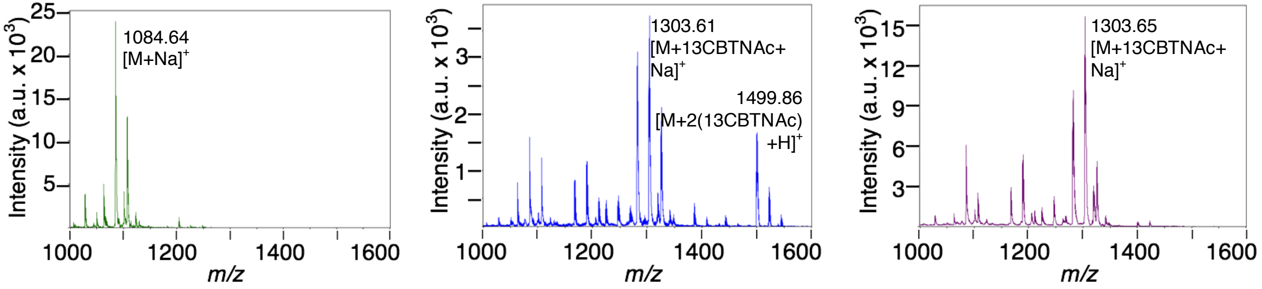
I. PEP-FOLD-9, Ac-GGCPKPDPHGG-NH_2 (**12**): 1061.47 g/mol (-Gly: 1004.45 g/mol)



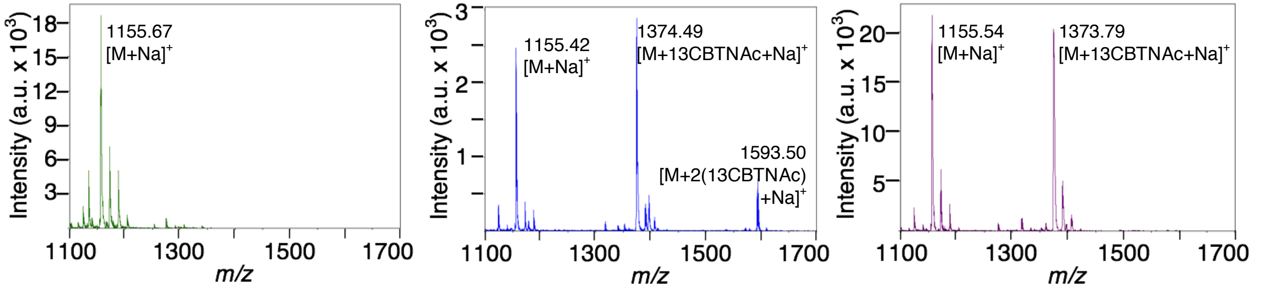
J. PEP-FOLD-11, Ac-GGCPDPHPKGG-NH_2 (**13**): 1061.47 g/mol (-2Gly: 947.43; -3Gly: 890.41)



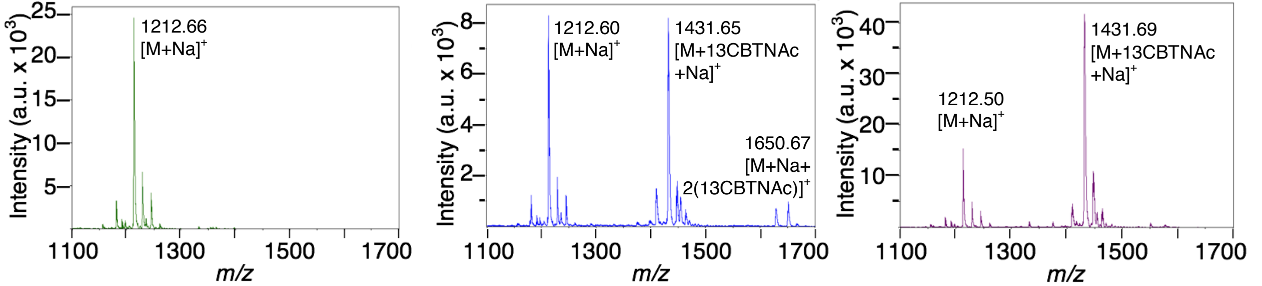
K. PEP-FOLD-12, Ac-GGKPCPHPDGG-NH_2 (**14**): 1061.47 g/mol



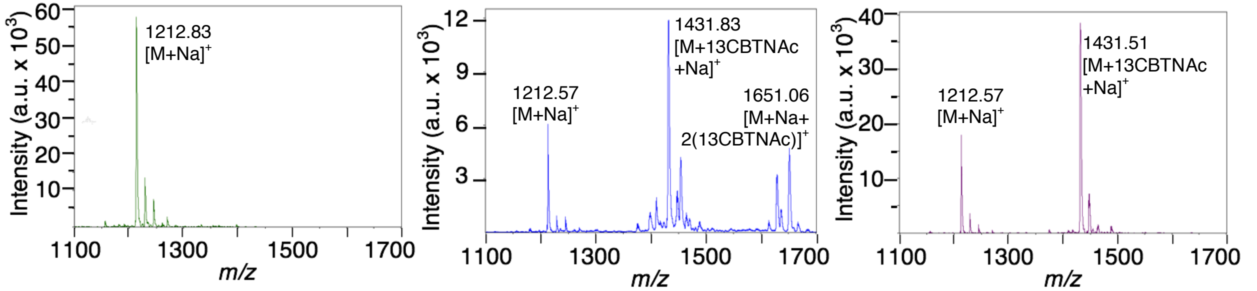
L. PEP-FOLD-13, Ac-GGWPHPCPKGG-NH_2 (**15**): 1132.52 g/mol



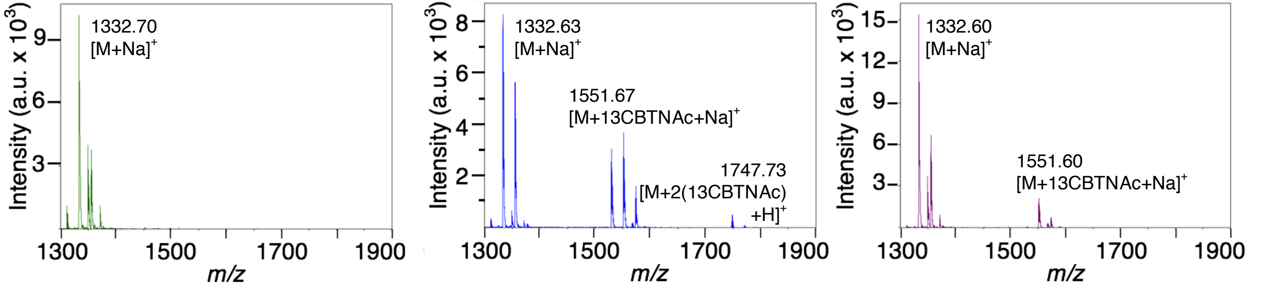
M. PEP-FOLD-14, Ac-GGWPHPGCPKGG-NH_2 (**16**): 1189.55 g/mol



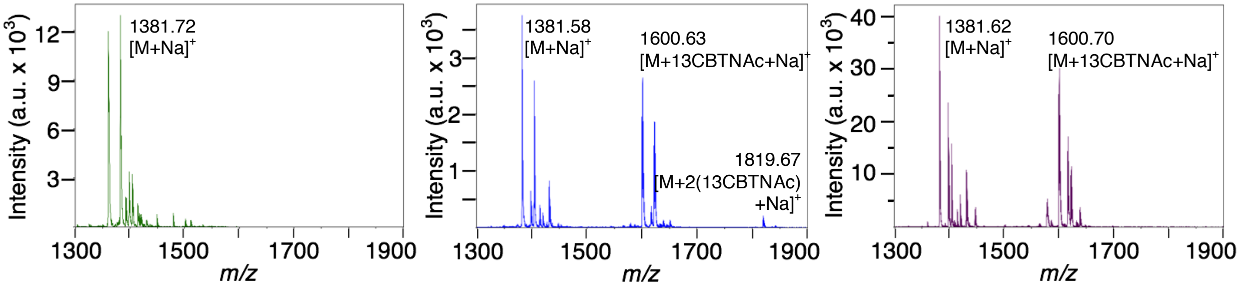
N. PEP-FOLD-15, Ac-GGKPCPGWPHGG-NH_2 (**17**): 1189.55 g/mol



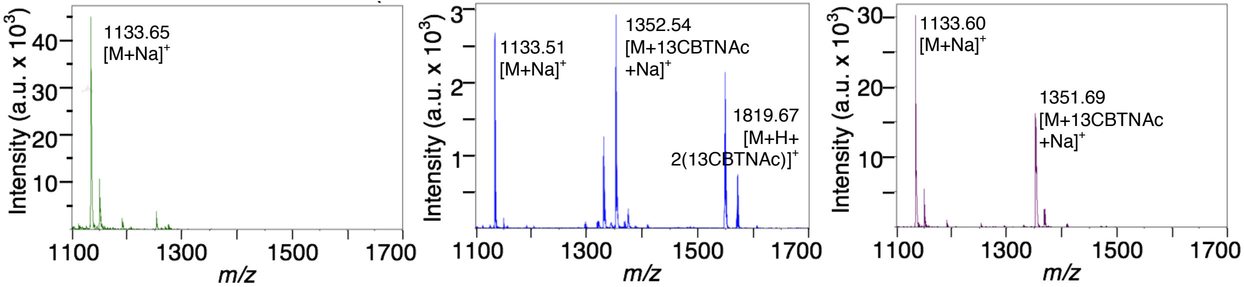
O. PEP-FOLD-16, Ac-GGHPHPKPCPEGG-NH_2 (**18**): 1309.60 g/mol



P. PEP-FOLD-17, Ac-GGHPWPKPCPEGG-NH_2 (**19**): 1358.62 g/mol



Q. PEP-FOLD-18, Ac-GGHPKPGCGFGG-NH_2 (**20**): 1110.50 g/mol



R. PEP-FOLD-19, Ac-GGHPKPCGFGG-NH_2 (**21**): 1053.48 g/mol (-Gly: 996.46 g/mol)

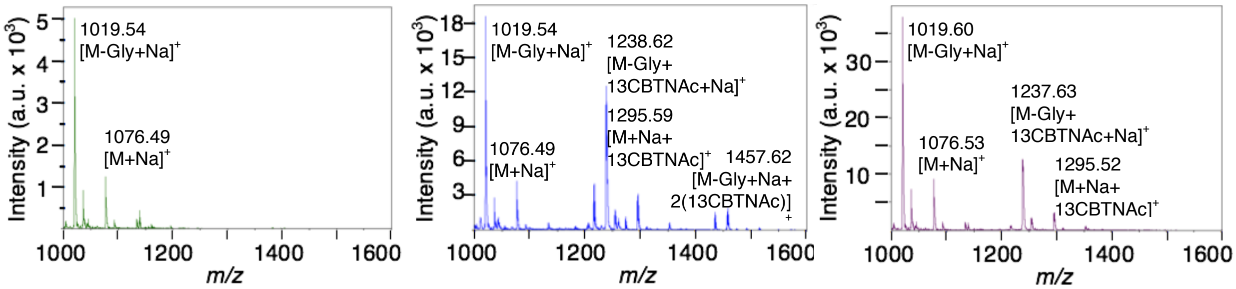


Figure S1. 13CBTNAc binding assay and cysteine competition MALDI-TOF-MS data for the eighteen peptides synthesized by SPPS. All peptides were re-purified by preparative RP-HPLC immediately prior to this experiment and all data in this figure were obtained in parallel in order to minimize sources of error. The binding assay and cysteine competition were as follows: 40 μL of a 10% DMF in PBS solution of peptide (0.9 mM) with or without 13CBTNAc (1 mM) was incubated 48 h at r.t. Then, the negative control (without 13CBTNAc) and half (20 μL) of the sample incubated with 13CBTNAc were each treated with an equal volume (20 μL) of a solution of cysteine and DTT (10 and 15 mM, respectively) in PBS. The other half of the sample incubated with 13CBTNAc was treated with an equal volume of a solution of DTT (15 mM) in PBS. After 48 h at r.t., MALDI-TOF MS was used to analyze the negative control (left column, green spectra), the sample incubated with 13CBTNAc then DTT alone (middle column, blue spectra), and the sample incubated with 13CBTNAc then cysteine and DTT (right column, purple spectra). Labels are in the format **Name of peptide**, Sequence (**Compound #)**: Calculated exact mass (identity of major impurity and calculated exact mass, where applicable). **A**) CBTag 1.0 (**4**), analogous to Figure 3B. **B**) PEP-FOLD-4, analogous to Figure 3C (**5**). **C-R**) Other peptides tested. Peptides in **I**, **J**, and **R** have additional peaks corresponding to glycine deletions, but the residues that confer reactivity (e.g., Cys, Lys) were not affected.

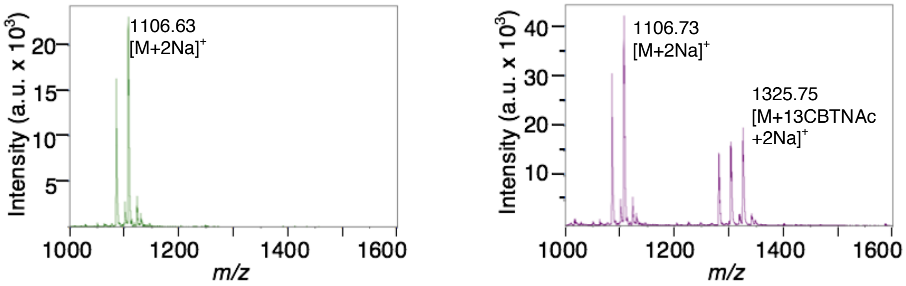


Figure S2. Results of the 13CBTNAc binding assay and cysteine treatment for CBTag 1.0 when conducted in the presence of 5 mM glutathione (reduced). Left (green spectrum), negative control after treatment with cysteine and DTT. Right (purple spectrum), CBTag 1.0 treated with 1.1 equiv. of 13CBTNAc then with 10 equiv. cysteine and 15 equiv. DTT relative to 13CBTNAc. CBTag 1.0-13CBTNAc adduct is observed, though less has formed than in the absence of glutathione.

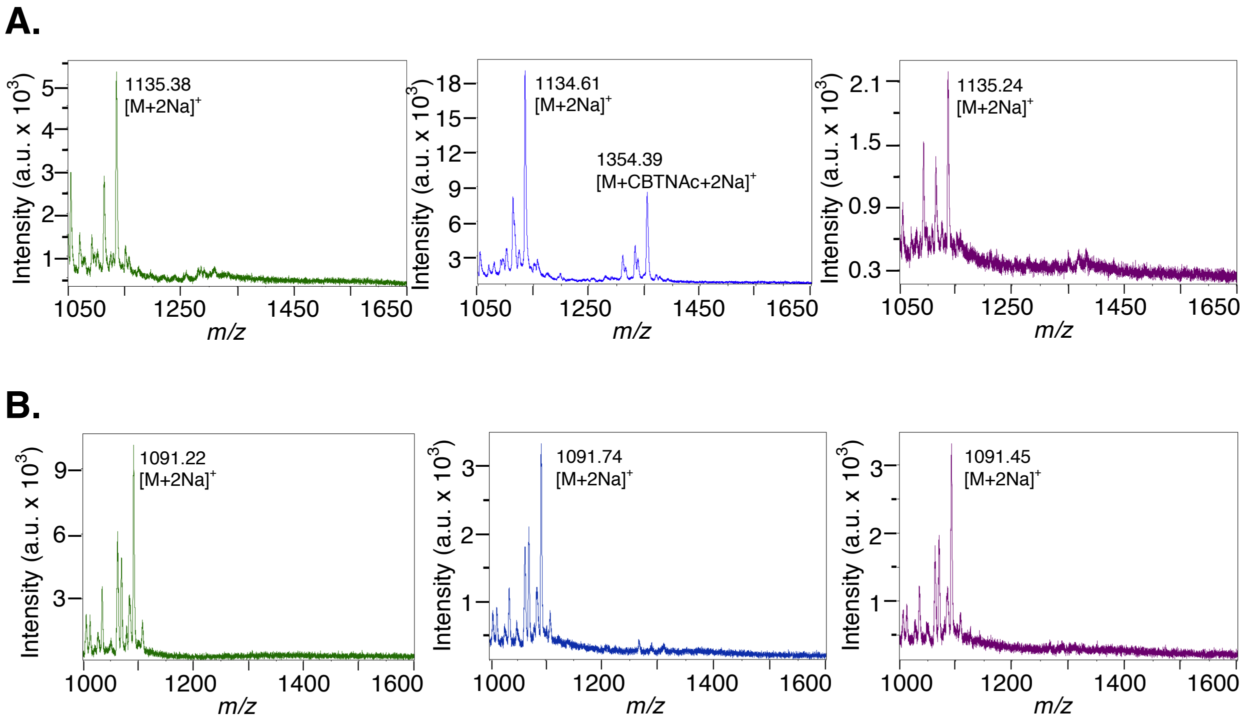
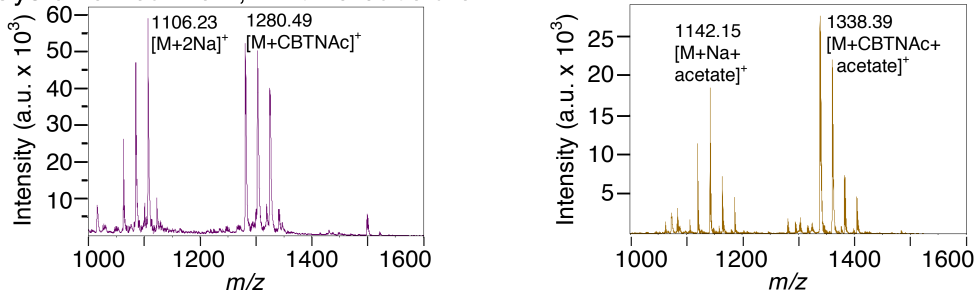
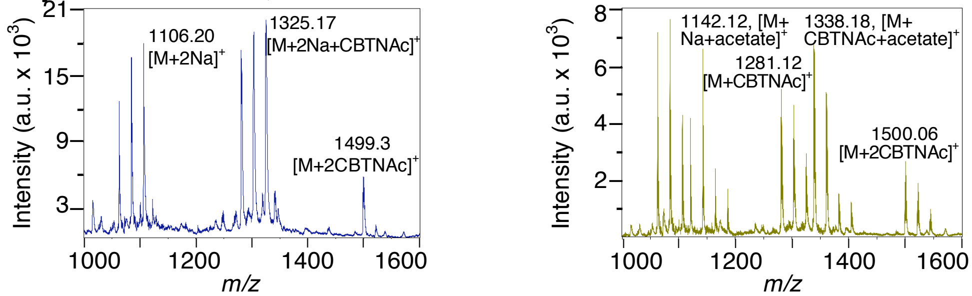


Figure S3. Results of binding experiment and cysteine competition assays for CBTag 1.0 (K9R) (**A.**) and CBTag 1.0 (C7S) (**B.**). Spectra are analogous to those in Figure 3. The first spectrum in each row corresponds to crude peptide, the second to the results of the binding assay, and the third to the results of the cysteine competition. In **A.**, CBTag 1.0 (K9R) is partially modified by one equivalent of CBTNAc, and that equivalent is removed by cysteine treatment, suggesting that, as expected, the modification is on the cysteine residue. In **B.**, CBTag 1.0 (C7S) is not at all modified by CBTNAc, implying that the cysteine residue is necessary for lysine modification.

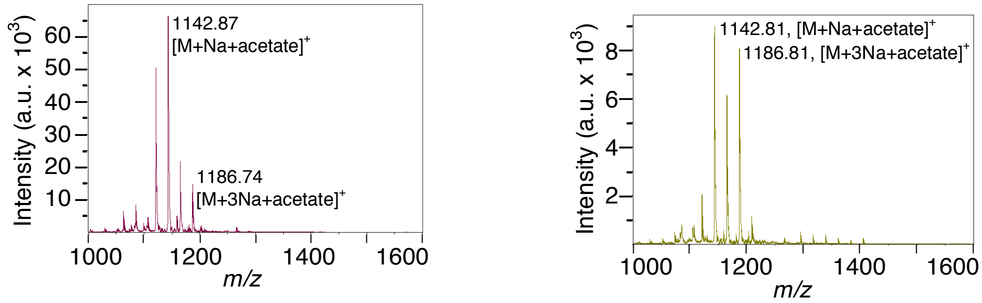
A. Cysteine treatment, -/+ chloroacetate



B. No cysteine treatment, -/+ chloroacetate

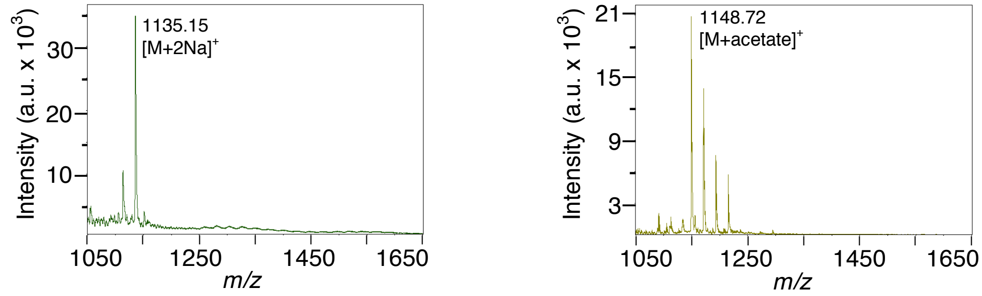


C. CBTag 1.0 pretreated with chloroacetate, -/+ CBTNAc



D.

CBTag 1.0 (K9R) -/+ chloroacetate



CBTag 1.0 (C7S) -/+ chloroacetate

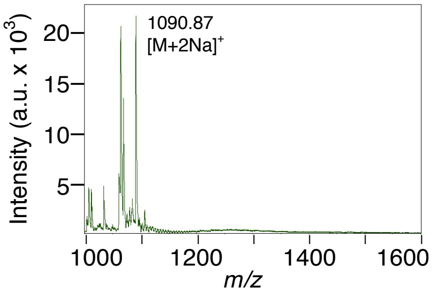
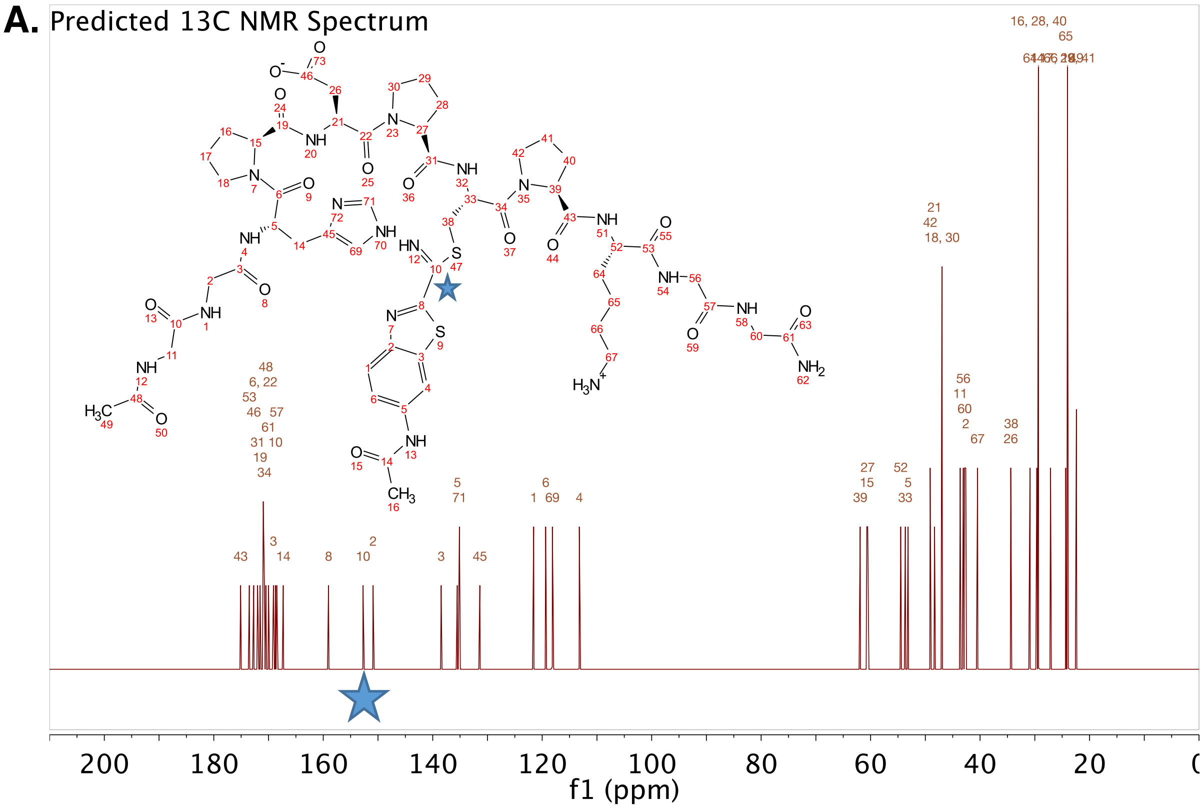
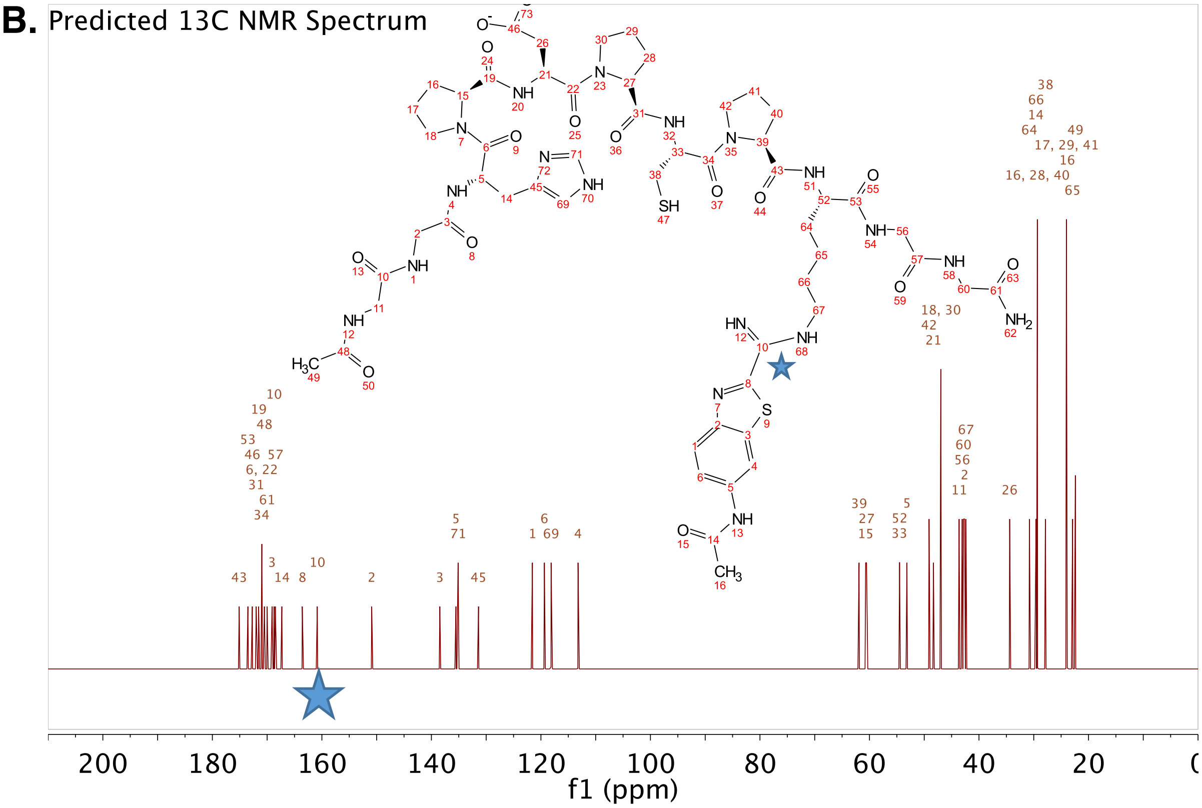


Figure S4. Results of chloroacetate labeling of thiols under various conditions. **A.** The left MALDI-TOF MS spectrum is after cysteine treatment of CBTag 1.0 that had been reacted with CBTNAc. The right spectrum are the results of treating the sample in the left spectrum with chloroacetate. The peaks shift by 57 *m/z*, indicating labeling of a thiol and suggesting CBTNAc is attached to the lysine residue. **B.** The left MALDI-TOF MS spectrum is after CBTag 1.0 was reacted with CBTNAc but before cysteine treatment. Chloroacetate treatment of this sample gave the spectrum on the right, where one population of the singly modified peptide was labeled (lysine adduct) and another was not (cysteine adduct). The peptide modified by two equivalents of CBTNAc was not labeled by chloroacetate. **C.** When CBTag 1.0 was pretreated with chloroacetate (left), no CBTNAc reacted with the resulting peptide (right). **D.** As a control to confirm chloroacetate thiol specificity, CBTag 1.0 (K9R) (top left) and CBTag 1.0 (C7S) (bottom left) were treated with chloroacetate. Only CBTag 1.0 (K9R) (top right) was labeled, confirming that lysine residues are not modified by chloroacetate.

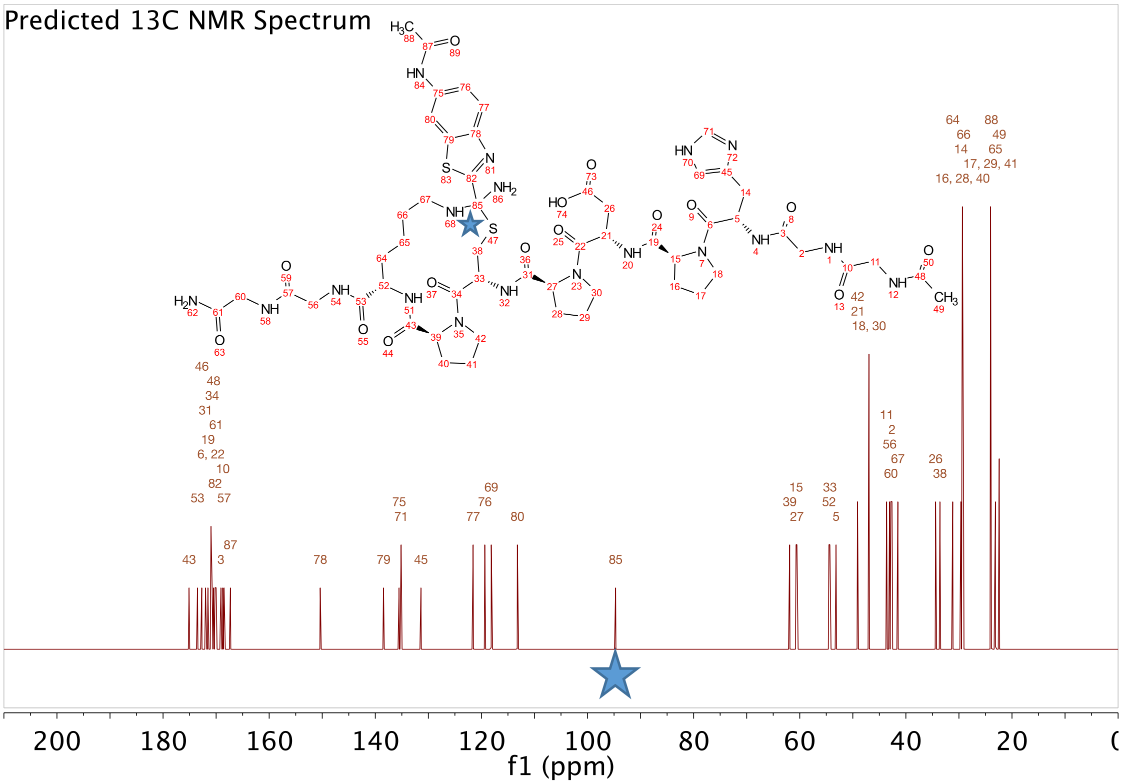


A. Predicted 13C NMR Spectrum



B. Predicted 13C NMR Spectrum

C.


Predicted 13C NMR Spectrum
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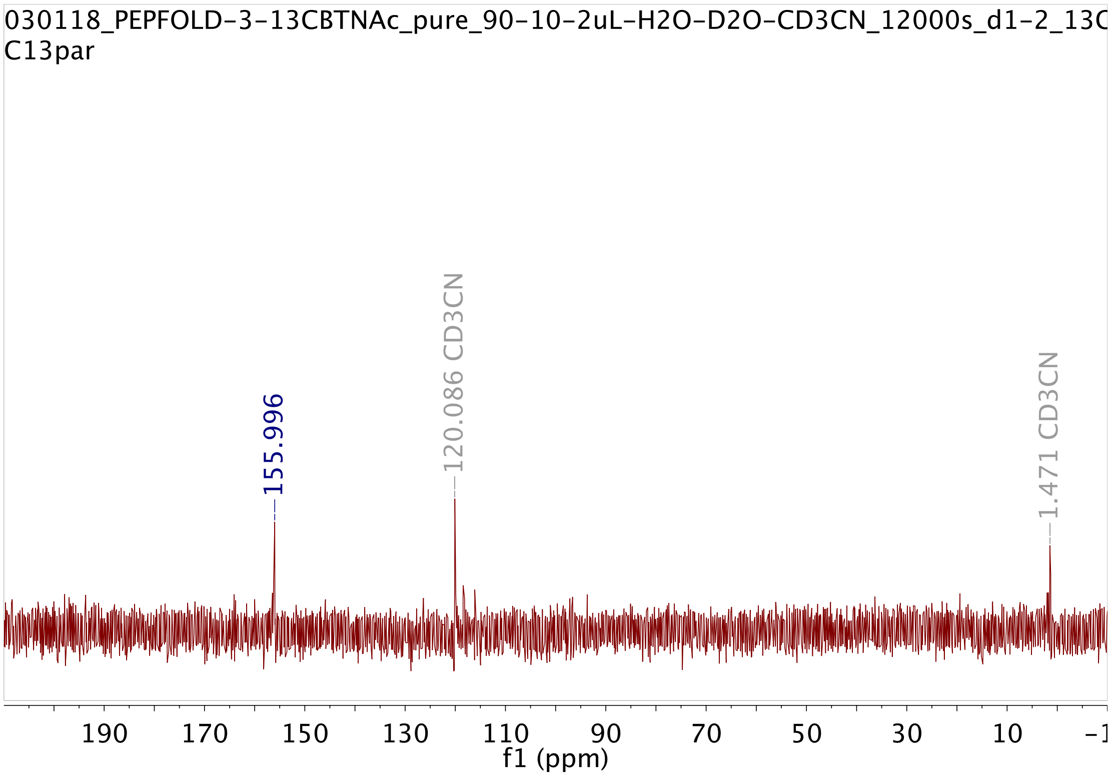
40
20
f1 (ppm)

D.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1.471 CD3CN
190
170
150
130
110
90
70
50
30
10
f1 (ppm)

Figure S5.^{13}C NMR confirms that the final CBTag 1.0-CBTNAc adduct is not the tetrahedral intermediate. **A.-C.**, Predicted spectra (MestreNova) for the cysteine adduct, the lysine adduct, and the tetrahedral intermediate. α-Carbon and corresponding peak are labelled with a blue star. **D.** ^{13}C NMR spectrum of (dilute) purified CBTag 1.0-13CBTNAc shows that the peak corresponding to the ^{13}C-labelled α-carbon is at 156 ppm (referenced to acetonitrile-d_3 methyl peak), which is similar to the predicted values for the lysine and cysteine adducts but significantly different from the predicted value for the tetrahedral intermediate.

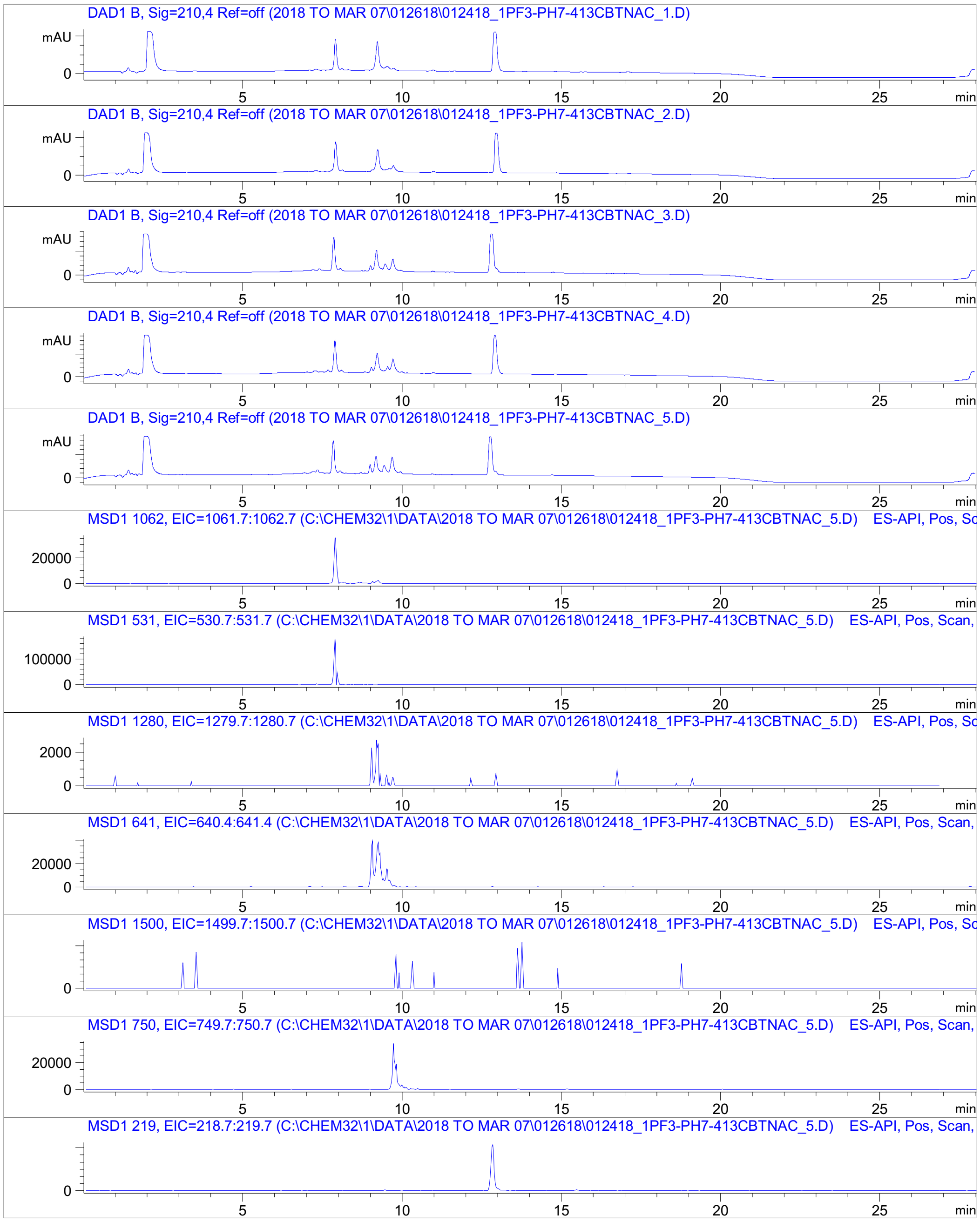

Figure S6. Overlay of LC-MS chromatographs for 1:4 CBTag 1.0/13CBTNAc over the time-course experiment and extracted mass ions. Identities of extracted mass ions: 1062 m/z, minute 7.9 – [CBTag 1.0 + H]$^{+}$; 531 m/z, minute 7.9 – [CBTag 1.0 + 2H]$^{2+}$; 1280 m/z, minutes 9 and 9.2 – [CBTag 1.0-13CBTNAc + H]$^{+}$; 641 m/z, minutes 9 and 9.2 – [CBTag 1.0-13CBTNAc + 2H]$^{2+}$; 1500 m/z, insignificant signal – [CBTag 1.0-2(13CBTNAc) + H]$^{+}$; 750 m/z, minute 9.7 – [CBTag 1.0-2(13CBTNAc) + 2H]$^{2+}$; 219 m/z, minute 12.9 – [13CBTNAc + H]$^{+}$

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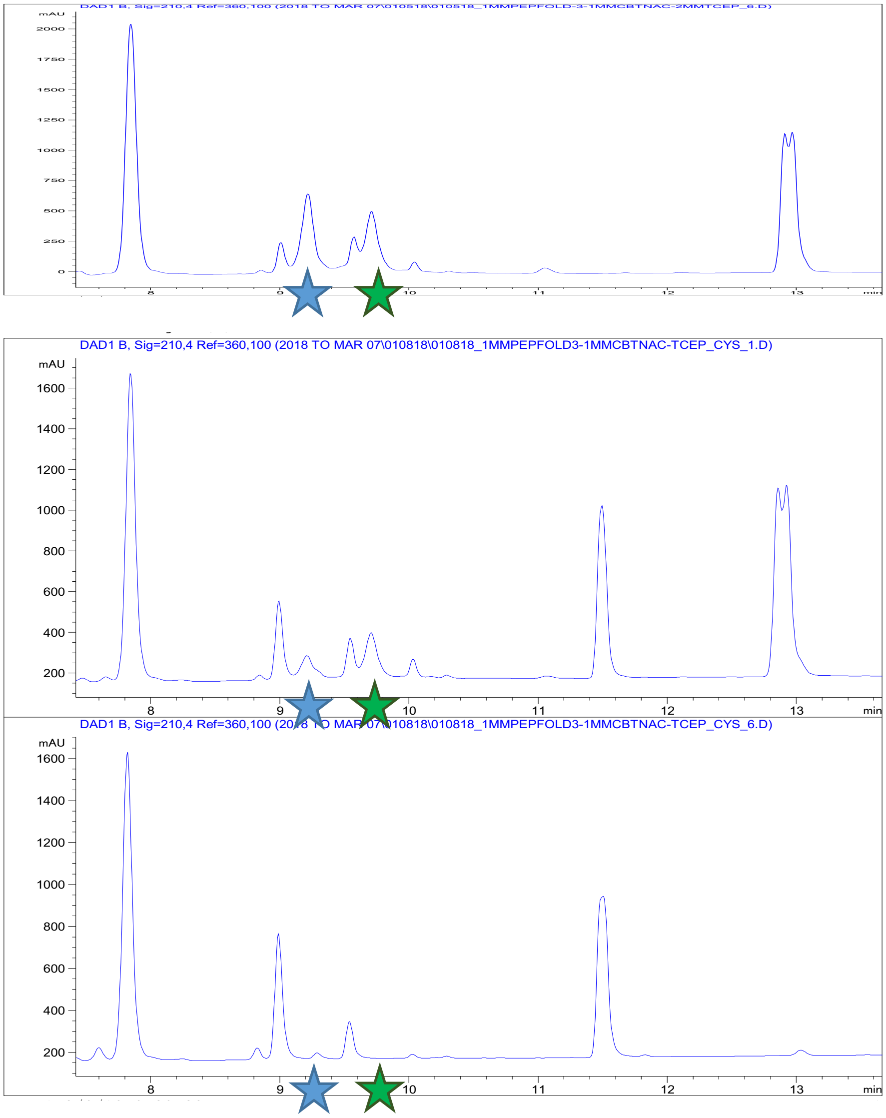

Figure S7. Cysteine treatment identifies peaks that contain cysteine adducts. Top spectrum was before cysteine treatment, middle was from an early time point during cysteine treatment, and bottom spectrum was at the end of the time-course assay. Based on these results and the mass spectrum in Figure S6, the blue star (minute 9.2) indicates the cysteine adduct, while the green star (minute 9.7) indicates the doubly modified peptide; the peak at minute 9 is the lysine adduct.

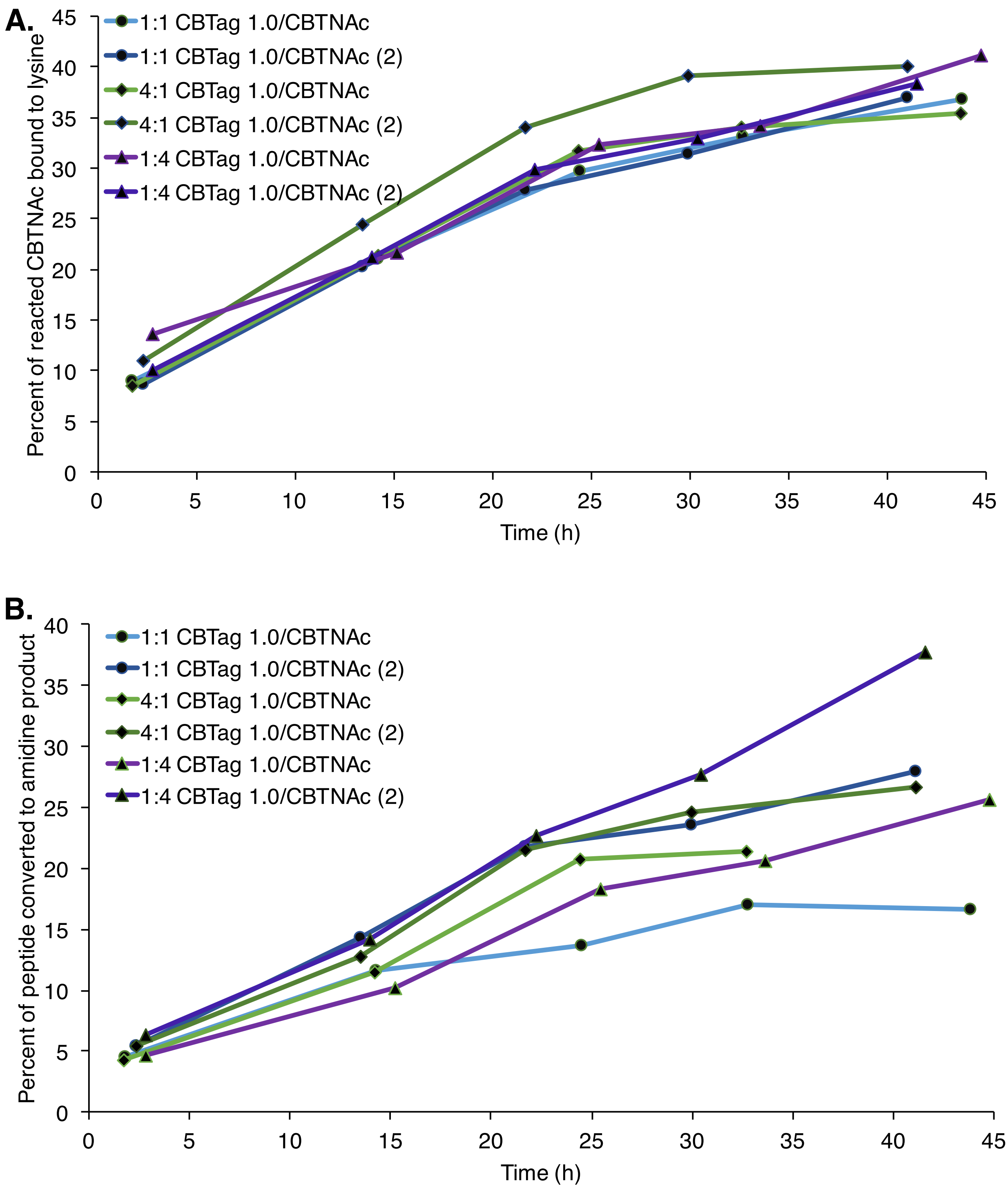

Figure S8. LC-MS-based time-course data for the reaction between CBTag 1.0 and CBTNAc. **A)** Percent of the CBTNAc bound to a peptide that is ligated through an amidine bond over time. **B)** Percent of the peptide that was converted to the amidine product over time. Blue lines and circular markers represent two replicates of the reaction between CBTag 1.0 (22.5 mM) and CBTNAc (22.5 mM). Green lines and diamond markers represent two replicates of the reaction between CBTag 1.0 (22.5 mM) and CBTNAc (5.63 mM). The last time point of the first replicate is not shown because an instrument error during injection resulted in overall lower-than-expected signal. Purple lines and triangular markers represent two replicates of the reaction between CBTag 1.0 (5.63 mM) and CBTNAc (22.5 mM). Spreadsheets containing the corresponding calculations, LC-MS spectra, and LC-MS integration results are in Tables S2-S4 and the section following Figure S13.

```
Data File   : C:\CHEM32\...TA\2018 TO MAR 07\010518\010518_1MMPEPFOLD-3R-1MM13CBTNAC-2MMTCEP.D
Sample Name : 010518_1mMpepfold-3R-1mMcbtnac_6
=====================================================================
Acq. Operator   : sglk                            Seq. Line : 107
Acq. Instrument : Instrument 1                     Location : Vial 30
Injection Date  : 1/7/18 8:15:04 PM                     Inj :   1
                                                 Inj Volume : 15.000 µl
Different Inj Volume from Sequence !      Actual Inj Volume : 10.000 µl
Acq. Method     : D:\CHEM32\1\METHODS\AP_C18_INSERT.M
Last changed    : 11/10/17 3:07:57 PM by Mason
Analysis Method : Z:\DESKTOP\BERTOZZI LAB\LCMS INFO\LCMS METHODS TO 112917\SGLK_BERTOZZIBP_
                  WITHINSERT.M
Last changed    : 3/8/18 8:51:08 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```

Current Chromatogram(s)

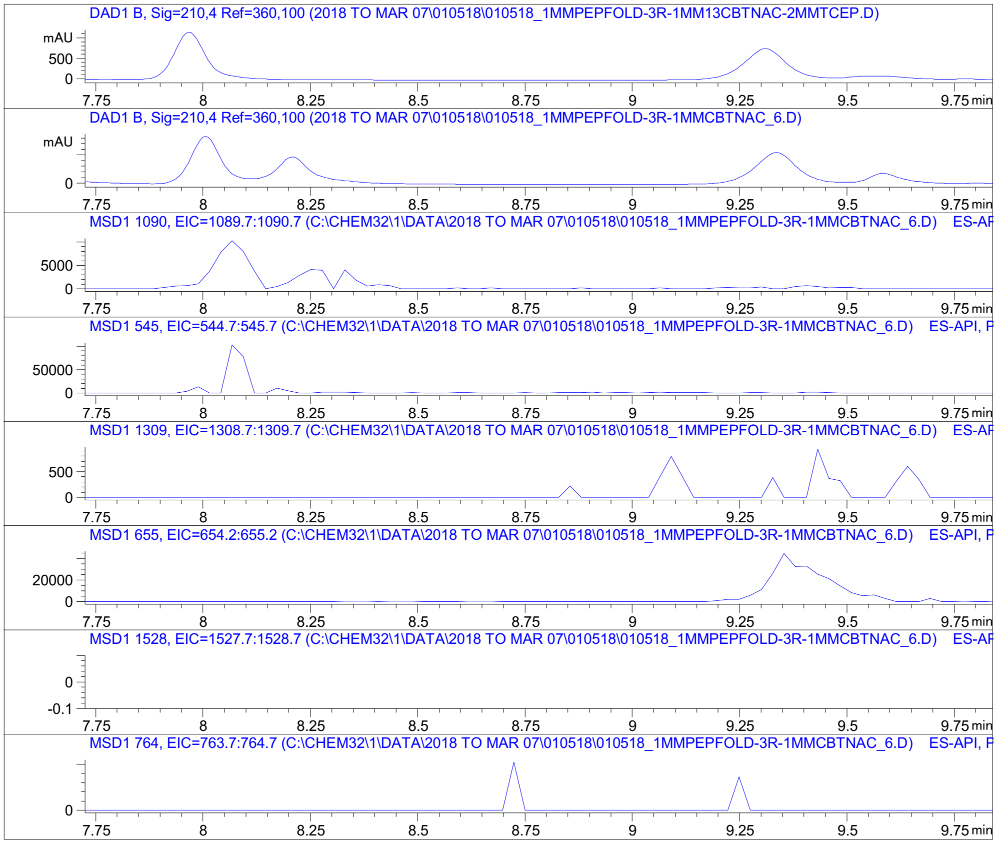

Figure S9. Extraction of relevant mass ions from the LC-MS spectrum of the reaction between CBTag 1.0 (K9R) and 13CBTNAc shows that the peptide is only modified by one equivalent of 13CBTNAc at the final time point of the assay. 1090 m/z, minute 8 – [CBTag 1.0(K9R) + H]$^{+}$; 545 m/z, minute 8 – [CBTag 1.0(K9R) + 2H]$^{2+}$; 1309 m/z, no signal – [CBTag 1.0(K9R)-13CBTNAc + H]$^{+}$; 655 m/z, minute 9.3 – [CBTag 1.0(K9R)-13CBTNAc + 2H]$^{2+}$; 1528 m/z, 764 m/z, no signal – [CBTag 1.0(K9R)-2(13CBTNAc) + (2)H]$^{(2)+}$.

```
Print of window 38: Current Chromatogram(s)
Data File   : C:\CHEM32\...TA\2018 TO MAR 07\010518\010518_1MMPEPFOLD-3R-1MM13CBTNAC-2MMTCEP.D
Sample Name : 010518_1mMpepfold-3R-1mMcbtnac-2mMTCEP_1
=====================================================================
Acq. Operator   : sglk                           Seq. Line :  21
Acq. Instrument : Instrument 1                    Location : Vial 31
Injection Date  : 1/6/18 2:26:29 AM                    Inj :   1
                                                Inj Volume : 15.000 µl
Different Inj Volume from Sequence !      Actual Inj Volume : 10.000 µl
Acq. Method     : D:\CHEM32\1\METHODS\AP_C18_INSERT.M
Last changed    : 11/10/17 3:07:57 PM by Mason
Analysis Method : Z:\DESKTOP\BERTOZZI LAB\LCMS INFO\LCMS METHODS TO 112917\SGLK_BERTOZZIBP_
                  WITHINSERT.M
Last changed    : 3/8/18 8:51:08 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```

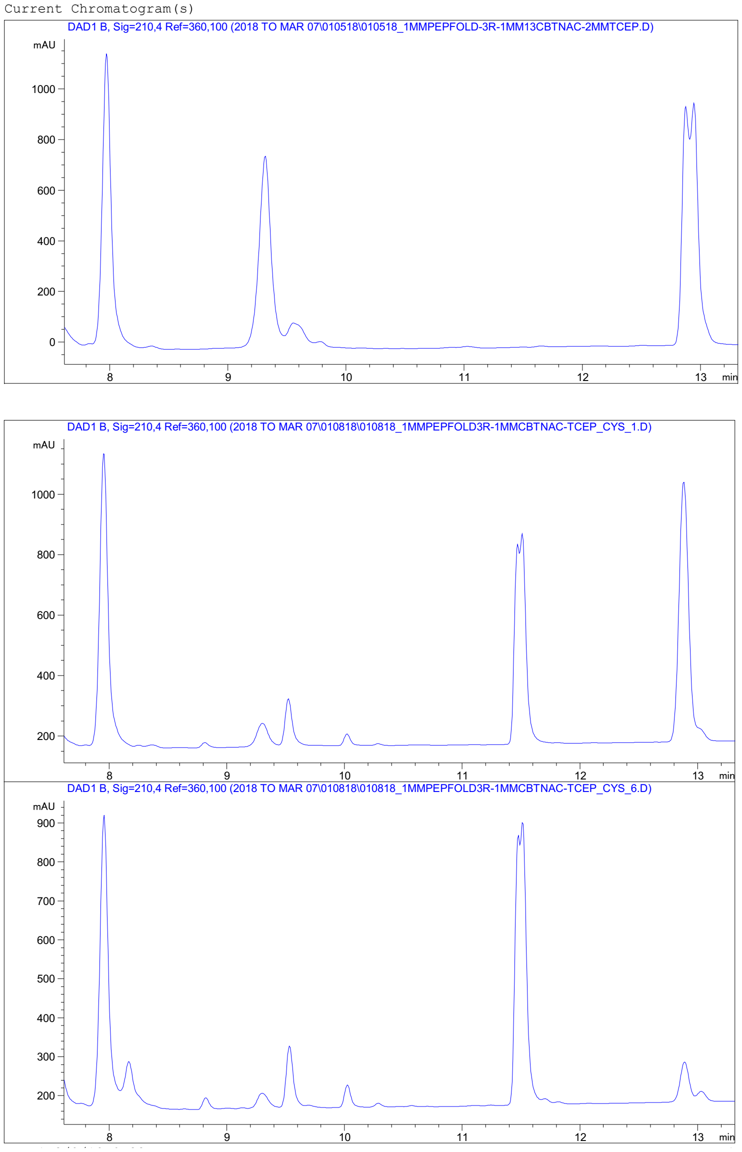

Figure S10. Cysteine treatment causes the minute 9.3 peak corresponding to the singly modified CBTag 1.0 (K9R) to disappear.

```
Print of window 38: Current Chromatogram(s)
Data File  : C:\CHEM32\...TA\2018 TO MAR 07\010518\010518_1MMPEPFOLD-3S-1MM13CBTNAC-2MMTCEP.D
Sample Name : 010518_1mMpepfold-3S-1mMcbtnac-2mMTCEP_6
=====================================================================
Acq. Operator   : sglk                              Seq. Line : 103
Acq. Instrument : Instrument 1                       Location : Vial 27
Injection Date  : 1/7/18 6:16:03 PM                       Inj :   1
                                                    Inj Volume : 15.000 µl
Different Inj Volume from Sequence !      Actual Inj Volume : 10.000 µl
Acq. Method     : D:\CHEM32\1\METHODS\AP_C18_INSERT.M
Last changed    : 11/10/17 3:07:57 PM by Mason
Analysis Method : Z:\DESKTOP\BERTOZZI LAB\LCMS INFO\LCMS METHODS TO 112917\SGLK_BERTOZZIBP_
                  WITHINSERT.M
Last changed    : 3/8/18 8:51:08 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```

Current Chromatogram(s)

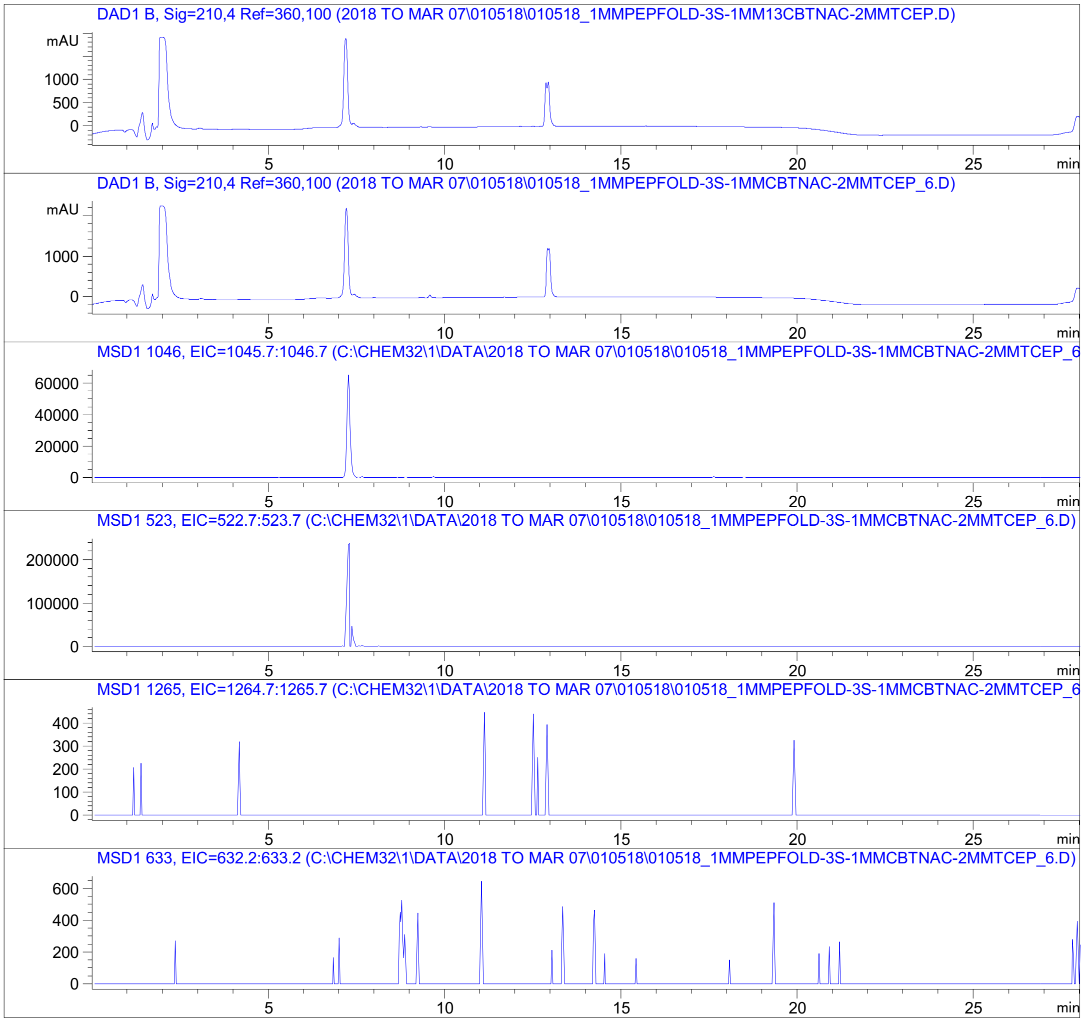

Figure S11. The LC-MS spectrum and the corresponding extracted mass ions at the final time point show that CBTag 1.0 (C7S) is not modified by 13CBTNAc. 1046 m/z, 523 m/z, minute 7 – [CBTag 1.0(C7S) + (2)H]$^{(2)+}$; 1265, 633 m/z, no signal – [CBTag 1.0(C7S)-13CBTNAc + (2)H]$^{(2)+}$

Table S2. Calculations for 1:1 CBTag 1.0/13CBTNAc LC-MS time-course assay (two replicates). Spectra and integration results used herein are included after Figure S13.

****Bolded columns were mentioned in text of paper or used in creation of graphs in Supporting Information**

26-Jan	Time 0 = 3:16 - 0:05:30 =	3:10:30

210 nm	Time of injection in file	**Actual time point (h)**	CBTag 1.0 (min 7.9)	CBTag 1.0-Lys-13CBTNAc (min 8.99)	CBTag 1.0-Cys-13CBTNAc (min 9.19)	CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc (min 9.7)	13CBTNAc (min 12.9)
012418_PF3-PH7-13CBTNAc_1	4:58:31 p.m.	**1.80**	19072.5	875.5	20975.8	2091.6	19164.1
012418_PF3-PH7-13CBTNAc_2	5:25:45 a.m.	**14.25**	21742.2	2265.4	20082	6531	16769.8
012418_PF3-PH7-13CBTNAc_3	3:39:38 p.m.	**24.48**	31604.91	2944.3	13766.1	8471.9	13473.4
012418_PF3-PH7-13CBTNAc_4	11:53:39 p.m.	**32.72**	28513.8	3432	13322.2	10263.3	14764.6
012418_PF3-PH7-13CBTNAc_5	11:01:48 a.m.	**43.85**	25995.5	2775.6	8668.3	8322.7	13238.1

26-Jan	Time 0 = 3:16 - 0:05:30 =	3:10:30

254 nm	Time of injection in file	**Actual time point (h)**	CBTag 1.0 (min 7.9)	CBTag 1.0-Lys-13CBTNAc (min 8.99)	CBTag 1.0-Cys-13CBTNAc (min 9.19)	CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc (min 9.7)	13CBTNAc (min 12.9)
012418_PF3-PH7-13CBTNAc_1	4:58:31 p.m.	**1.80**		138.3	4066.1	583	16074.4
012418_PF3-PH7-13CBTNAc_2	5:25:45 a.m.	**14.25**		365.8	3527.3	1575.1	11460.9
012418_PF3-PH7-13CBTNAc_3	3:39:38 p.m.	**24.48**		579.3	2843.1	2145.2	11569.5
012418_PF3-PH7-13CBTNAc_4	11:53:39 p.m.	**32.72**		561	2454	2562.6	12511.7
012418_PF3-PH7-13CBTNAc_5	11:01:48 a.m.	**43.85**		445.7	1461.1	1937.3	9349.3

Assumption: area under modified peptide peaks is proportional to number of modifications

210 nm

Lysine-modified: Sum CBTag 1.0-Lys-13CBTNAc and 1/2(CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc)	Any modification: Sum CBTag 1.0-Lys-13CBTNAc, CBTag 1.0-Cys-13CBTNAc, CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc	All peptide: Sum CBTag 1.0-Lys-13CBTNAc, CBTag 1.0-Cys-13CBTNAc, 1/2(CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc)	Percent of reacted 13CBTNAc bound to a lysine (Lysine-modified/Any modification)	**Percent of total peptide with a modification on lysine (Lysine-modified/All peptide)**	**Percent of total peptide that has any 13CBTNAc modification ((Any modification - 1/2(CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc))/All peptide)**
1921.3	23942.9	41969.6	8.024508309	**4.577837292**	**54.5563932**
5530.9	28878.4	47355.1	19.15237686	**11.67962902**	**54.08688821**
7180.25	25182.3	52551.26	28.5130826	**13.66332606**	**39.85889206**
8563.65	27017.5	50399.65	31.69667808	**16.99148704**	**43.42460712**
6936.95	19766.6	41600.75	35.09430049	**16.67505994**	**37.5119439**

254 nm

Lysine-modified: Sum CBTag 1.0-Lys-13CBTNAc and 1/2(CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc)	Any modification: Sum CBTag 1.0-Lys-13CBTNAc, CBTag 1.0-Cys-13CBTNAc, CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc	**Percent of reacted 13CBTNAc bound to a lysine (Lysine-modified/Any modification)**
429.8	4787.4	**8.977733216**
1153.35	5468.2	**21.09194982**
1651.9	5567.6	**29.66987571**
1842.3	5577.6	**33.03033563**
1414.35	3844.1	**36.79274733**

2-Feb	Time 0 = 5:02 - 0:05:30 =	4:56:30			*a lot of these peaks were saturated	using 280 nm as control		
210 nm	Time of injection in file	**Actual time point (h)**	CBTag 1.0 (min 7.9)	CBTag 1.0-Lys-13CBTNAc (min 8.99)	CBTag 1.0-Cys-13CBTNAc (min 9.19)	13CBTNAc 210 nm *(Ratio of CBTag 1.0-Cys 280 nm/13CBTNAc 280 nm)	CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc (min 9.7)	13CBTNAc (min 12.9)
020218_PF3-PH7-13CBTNAc_1	6:47:32 p.m.	**2.33**	14758.6	667.7	20164.3	21027.50305	2894.9	8795.9
020218_PF3-PH7-13CBTNAc_2	5:55:51 a.m.	**13.47**	15407.4	1732.7	24026.3	24579.91136	11859.8	11314.4
020218_PF3-PH7-13CBTNAc_3	2:09:56 p.m.	**21.71**	11620.8	2901.1	16445.3	18346.71955	15010.7	9674.1
020218_PF3-PH7-13CBTNAc_4	10:23:55 p.m.	**29.94**	11865.8	3692.2	17331.6	18916.25472	16845.4	4868.5
020218_PF3-PH7-13CBTNAc_5	9:32:20 a.m.	**41.08**	8382.1	3265.7	12603.9	10621.54062	13433.9	4078.5
280 nm				control for saturation	CBTag 1.0-Cys 280 nm	Ratio of CBTag 1.0-Cys 280 nm/13CBTNAc 280		13CBTNAc 280 nm
					4321.66	2.390602787		1807.77
					4781.66	2.172444969		2201.05
					4214.79	1.896478179		2222.43
					3953.2	3.885437962		1017.44
					1891.59	2.604276234		726.34

2-Feb	Time 0 = 5:02 - 0:05:30 =	4:56:30			*a lot of these peaks were saturated			
254 nm	Time of injection in file	**Actual time point (h)**	CBTag 1.0 (min 7.9)	CBTag 1.0-Lys-13CBTNAc (min 8.99)	CBTag 1.0-Cys-13CBTNAc (min 9.19)		CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc (min 9.7)	13CBTNAc (min 12.9)
020218_PF3-PH7-13CBTNAc_1	6:47:32 p.m.	2.33		167.6	6653.1		1016	4049.4
020218_PF3-PH7-13CBTNAc_2	5:55:51 a.m.	13.47		449.1	6981.6		3533.3	5390
020218_PF3-PH7-13CBTNAc_3	2:09:56 p.m.	21.71		668.3	5847.8		5163.1	5270.8
020218_PF3-PH7-13CBTNAc_4	10:23:55 p.m.	29.94		900.5	5806.4		6531.1	2182.5
020218_PF3-PH7-13CBTNAc_5	9:32:20 a.m.	41.08		765.4	3172		5281	1729

Assumption: area under modified peptide peaks is proportional to number of modifications

210 nm

Lysine-modified: Sum CBTag 1.0-Lys-13CBTNAc and 1/2(CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc)	Any modification: Sum CBTag 1.0-Lys-13CBTNAc, CBTag 1.0-Cys-13CBTNAc, CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc	All peptide: Sum CBTag 1.0-Lys-13CBTNAc, CBTag 1.0-Cys-13CBTNAc, 1/2(CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc)	Percent of reacted 13CBTNAc bound to a lysine (Lysine-modified/Any modification)	Percent of total peptide with a modification on lysine (Lysine-modified/All peptide)	Percent of total peptide that has any 13CBTNAc modification ((Any modification - 1/2(CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc))/All peptide)
2115.15	23726.9	37038.05	8.914565325	5.710748811	60.15286982
7662.6	37618.8	47096.3	20.36907078	16.27006792	67.28532815
10406.45	34357.1	38472.55	30.28908144	27.04902586	69.79456782
12114.9	37869.2	41312.3	31.99143367	29.32516466	71.27780346
9982.65	29303.5	30968.65	34.06640845	32.23469541	72.93359575

280 nm

Lysine-modified: Sum CBTag 1.0-Lys-13CBTNAc and 1/2(CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc)	Any modification (adjusted for saturation): Sum CBTag 1.0-Lys-13CBTNAc, CBTag 1.0-Cys-13CBTNAc, CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc	All peptide (adjusted for saturation): Sum CBTag 1.0-Lys-13CBTNAc, CBTag 1.0-Cys-13CBTNAc, 1/2(CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc)	Percent of reacted 13CBTNAc bound to a lysine (adjusted for saturation) (Lysine-modified/Any modification)	**Percent of total peptide with a modification on lysine (adjusted for saturation) (Lysine-modified/All peptide)**	**Percent of total peptide that has any 13CBTNAc modification (adjusted for saturation) ((Any modification - 1/2(CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc))/All peptide)**
2115.15	24590.10305	39348.70305	8.601631296	**5.375399533**	**58.81427152**
7662.6	38172.41136	53579.81136	20.07365981	**14.30128215**	**60.17660485**
10406.45	36258.51955	47879.31955	28.70070297	**21.73474915**	**60.05342144**
12114.9	39453.85472	51319.65472	30.70650533	**23.60674495**	**60.46641367**
9982.65	27321.14062	35703.24062	36.53818901	**27.960067**	**57.70958116**

254 nm

Lysine-modified: Sum CBTag 1.0-Lys-13CBTNAc and 1/2(CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc)	Any modification: Sum CBTag 1.0-Lys-13CBTNAc, CBTag 1.0-Cys-13CBTNAc, CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc	**Percent of reacted 13CBTNAc bound to a lysine (Lysine-modified/Any modification)**
675.6	7836.7	**8.620975666**
2215.75	10964	**20.20932142**
3249.85	11679.2	**27.82596411**
4166.05	13238	**31.47038828**
3405.9	9218.4	**36.94675866**

Table S3. Calculations for 1:4 CBTag 1.0/13CBTNAc LC-MS time-course assay (two replicates). Spectra and integration results used herein are included after Figure S13.

26-Jan	Time 0 = 3:20 - 0:05:30 =	3:14:30						
210 nm	Time of injection in file	**Actual time point (h)**	CBTag 1.0 (min 7.9)	CBTag 1.0-Lys-13CBTNAc (min 8.99)	CBTag 1.0-Cys-13CBTNAc (min 9.19)		CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc (min 9.7)	13CBTNAc (min 12.9)
012418_1PF3-PH7-413CBTNAc_1	6:02:03 p.m.	**2.81**	9417	487.3	12127.8		1118.1	19788.9
012418_1PF3-PH7-413CBTNAc_2	6:23:53 a.m.	**15.18**	9138.3	748.6	8372.4		2478	18214.2
012418_1PF3-PH7-413CBTNAc_3	4:37:48 p.m.	**25.41**	7891.2	1164.3	5924.5		3880.2	14152.5
012418_1PF3-PH7-413CBTNAc_4	12:51:47 a.m.	**33.64**	8335.7	1270.6	6181.5		4995.1	13985.1
012418_1PF3-PH7-413CBTNAc_5	12:00:02 p.m.	**44.78**	7711.9	1694.7	4647.7		5140.1	13714.5
254 nm	Time of injection in file	**Actual time point (h)**		CBTag 1.0-Lys-13CBTNAc (min 8.99)	CBTag 1.0-Cys-13CBTNAc (min 9.19)		CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc (min 9.7)	13CBTNAc (min 12.9)
012418_1PF3-PH7-413CBTNAc_1	6:02:03 p.m.	**2.81**		142.4	1966.5		394.1	17591.7
012418_1PF3-PH7-413CBTNAc_2	6:23:53 a.m.	**15.18**		161.1	1543.8		735.6	13625.9
012418_1PF3-PH7-413CBTNAc_3	4:37:48 p.m.	**25.41**		203.3	1016.1		1075.1	10742.7
012418_1PF3-PH7-413CBTNAc_4	12:51:47 a.m.	**33.64**		248.6	1101.1		1343.8	10660
012418_1PF3-PH7-413CBTNAc_5	12:00:02 p.m.	**44.78**		337.4	775.4		1352.4	9645.9
		Lysine-modified: Sum CBTag 1.0-Lys-13CBTNAc and 1/2(CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc)	Any modification: Sum CBTag 1.0-Lys-13CBTNAc, CBTag 1.0-Cys-13CBTNAc, CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc	All peptide: Sum CBTag 1.0-Lys-13CBTNAc, CBTag 1.0-Cys-13CBTNAc, 1/2(CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc)	**Percent of reacted 13CBTNAc bound to a lysine (Lysine-modified/Any modification)**	**Percent of total peptide with a modification on lysine (Lysine-modified/All peptide)**		**Percent of total peptide that has any 13CBTNAc modification ((Any modification - 1/2(CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc))/All peptide)**
		1046.35	13733.2	22591.15	7.61912737	4.63168099		58.31553507
		1987.6	11599	19498.3	17.13596	10.1937092		53.13283722
		3104.4	10969	16920.1	28.30157717	18.34740929		53.36197777
		3768.15	12447.2	18285.35	30.27307346	20.60748085		54.41323245
		4264.75	11482.5	16624.35	37.14130198	25.65363458		53.61081787
			8912.45	16624.35		25.65363458		53.61081787
		339.45	2503		**13.56172593**			
		528.9	2440.5		**21.67178857**			
		740.85	2294.5		**32.28808019**			
		920.5	2693.5		**34.17486542**			
		1013.6	2465.2		**41.11633945**			

2-Feb	Time 0 = 5:02 - 0:05:30 =	4:56:30						
210 nm	Time of injection in file	**Actual time point (h)**	CBTag 1.0 (min 7.9)	CBTag 1.0-Lys-13CBTNAc (min 8.99)	CBTag 1.0-Cys-13CBTNAc (min 9.19)		CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc (min 9.7)	13CBTNAc (min 12.9)
020218_1PF3-PH7-413CBTNAc_1	7:45:39 p.m.	**2.82**	4179.1	367.7	9649.2		1156.3	14850.1
020218_1PF3-PH7-413CBTNAc_2	6:54:01 a.m.	**13.96**	3660.3	461.7	9230.7		3333.8	14882.8
020218_1PF3-PH7-413CBTNAc_3	3:08:04 p.m.	**22.19**	3616.8	680.2	6993.7		4871.4	9454
020218_1PF3-PH7-413CBTNAc_4	11:22:05 p.m.	**30.42**	3166.8	877	7026.9		6074.1	15707.4
020218_1PF3-PH7-413CBTNAc_5	10:30:27 p.m.	**41.56**	2262.7	1027.3	4835.6		6570.6	11867
254 nm								
020218_1PF3-PH7-413CBTNAc_1	7:45:39 p.m.	**2.82**		55.9	1641.7		286.4	10866.8
020218_1PF3-PH7-413CBTNAc_2	6:54:01 a.m.	**13.96**		105.1	1616.7		902	8779.7
020218_1PF3-PH7-413CBTNAc_3	3:08:04 p.m.	**22.19**		152.1	1291.4		1378.6	4896.6
020218_1PF3-PH7-413CBTNAc_4	11:22:05 p.m.	**30.42**		196	1271.3		1673.5	14857.8
020218_1PF3-PH7-413CBTNAc_5	10:30:27 p.m.	**41.56**		190	791.4		1595.7	7938.7
		Lysine-modified: Sum CBTag 1.0-Lys-13CBTNAc and 1/2(CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc)	Any modification: Sum CBTag 1.0-Lys-13CBTNAc, CBTag 1.0-Cys-13CBTNAc, CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc	All peptide: Sum CBTag 1.0-Lys-13CBTNAc, CBTag 1.0-Cys-13CBTNAc, 1/2(CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc)	**Percent of reacted 13CBTNAc bound to a lysine (Lysine-modified/Any modification)**	**Percent of total peptide with a modification on lysine (Lysine-modified/All peptide)**		**Percent of total peptide that has any 13CBTNAc modification ((Any modification - 1/2(CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc))/All peptide)**
		945.85	11173.2	14774.15	8.465345649	6.402060355		71.71343191
		2128.6	13026.2	15019.6	16.34091293	14.17214839		75.62984367
		3115.9	12545.3	13726.4	24.83719002	22.70005245		73.65077515
		3914.05	13978	14107.75	28.00150236	27.74397051		77.55276355
		4312.6	12433.5	11410.9	34.68532593	37.79368849		80.17071397
			9148.2	11410.9		37.79368849		80.17071397
		199.1	1984		**10.03528226**			
		556.1	2623.8		**21.1944508**			
		841.4	2822.1		**29.81467701**			
		1032.75	3140.8		**32.88174987**			
		987.85	2577.1		**38.33184587**			

Table S4. Calculations for 4:1 CBTag 1.0/13CBTNAc LC-MS time-course assay (two replicates). Spectra and integration results used herein are included after Figure S13.

26-Jan	Time 0 = 3:18 - 0:05:30 =	3:12:30						
210 nm	Time of injection in file	**Actual time point (h)**	CBTag 1.0 (min 7.9)	CBTag 1.0-Lys-13CBTNAc (min 8.99)	CBTag 1.0-Cys-13CBTNAc (min 9.19)		CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc (min 9.7)	13CBTNAc (min 12.9)
012418_4PF3-PH7-13CBTNAc_1	5:27:34 p.m.	**1.75**	18495	642.7	18527.5		2025.3	1810.4
012418_4PF3-PH7-13CBTNAc_2	5:54:47 a.m.	**14.20**	20626.2	2080.7	18970.2		6051.6	1533.2
012418_4PF3-PH7-13CBTNAc_3	4:08:40 p.m.	**24.43**	14191.8	3157.1	12107.1		7429.6	1474.9
012418_4PF3-PH7-13CBTNAc_4	12:22:42 a.m.	**32.67**	15650.7	3078.2	12270.4		9018.7	1438.8
012418_4PF3-PH7-13CBTNAc_5	11:30:54 a.m.	**43.80**	666.5	50.9	199.5		196.9	74.8
254 nm								
012418_4PF3-PH7-13CBTNAc_1	5:27:34 p.m.	**1.75**		109.5	3892.3		554	767
012418_4PF3-PH7-13CBTNAc_2	5:54:47 a.m.	**14.20**		369.2	3423.6		1544.3	589.1
012418_4PF3-PH7-13CBTNAc_3	4:08:40 p.m.	**24.43**		556.6	2360.1		2024.4	596.6
012418_4PF3-PH7-13CBTNAc_4	12:22:42 a.m.	**32.67**		612.5	2387.1		2560	623.7
012418_4PF3-PH7-13CBTNAc_5	11:30:54 a.m.	**43.80**		10.7	38.9		46.6	33

Lysine-modified: Sum CBTag 1.0-Lys-13CBTNAc and 1/2(CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc)	Any modification: Sum CBTag 1.0-Lys-13CBTNAc, CBTag 1.0-Cys-13CBTNAc, CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc	All peptide: Sum CBTag 1.0-Lys-13CBTNAc, CBTag 1.0-Cys-13CBTNAc, 1/2(CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc)	**Percent of reacted 13CBTNAc bound to a lysine (Lysine-modified/Any modification)**	**Percent of total peptide with a modification on lysine (Lysine-modified/All peptide)**	**Percent of total peptide that has any 13CBTNAc modification ((Any modification - 1/2(CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc))/All peptide)**
1655.35	21195.5	38677.85	7.809912481	**4.279839753**	**52.18193359**
5106.5	27102.5	44702.9	18.84143529	**11.42319626**	**53.8593693**
6871.9	22693.8	33170.8	30.28095779	**20.7167147**	**57.21598514**
7587.55	24367.3	35508.65	31.13824675	**21.36817367**	**55.92426071**
149.35	447.3	1015.35	33.38922423	**14.70921357**	**34.35761068**
386.5	4555.8		**8.483691119**		
1141.35	5337.1		**21.3852092**		
1568.8	4941.1		**31.75001518**		
1892.5	5559.6		**34.04021872**		
34	96.2		**35.34303534**		

2-Feb	Time 0 = 5:02 - 0:05:30 =	4:56:30						
210 nm	Time of injection in file	**Actual time point (h)**	CBTag 1.0 (min 7.9)	CBTag 1.0-Lys-13CBTNAc (min 8.99)	CBTag 1.0-Cys-13CBTNAc (min 9.19)		CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc (min 9.7)	13CBTNAc (min 12.9)
020218_4PF3-PH7-13CBTNAc_1	7:16:34 p.m.	**2.33**	17726.9	919.9	17143.3		2137.4	1670
020218_4PF3-PH7-13CBTNAc_2	6:24:55 a.m.	**13.47**	20687.5	2669.5	17836.4		5985.9	1109.5
020218_4PF3-PH7-13CBTNAc_3	2:38:58 p.m.	**21.71**	15967.8	4050.5	12346.2		7415	1010.4
020218_4PF3-PH7-13CBTNAc_4	10:52:58 p.m.	**29.94**	16438.6	4837.6	11770.2		8735.1	863.5
020218_4PF3-PH7-13CBTNAc_5	10:01:22 a.m.	**41.08**	13302.2	4184.8	10201		8778.2	998.1
254 nm								
020218_4PF3-PH7-13CBTNAc_1	7:16:34 p.m.	**2.33**		200.3	4234.3		737	729.3
020218_4PF3-PH7-13CBTNAc_2	6:24:55 a.m.	**13.47**		572.6	3598.4		1752.5	474.2
020218_4PF3-PH7-13CBTNAc_3	2:38:58 p.m.	**21.71**		871.5	2728.3		2236.7	454
020218_4PF3-PH7-13CBTNAc_4	10:52:58 p.m.	**29.94**		1078.5	2427.3		2653.7	379.6
020218_4PF3-PH7-13CBTNAc_5	10:01:22 a.m.	**41.08**		886.4	1947.9		2469.6	429.6

Lysine-modified: Sum CBTag 1.0-Lys-13CBTNAc and 1/2(CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc)	Any modification: Sum CBTag 1.0-Lys-13CBTNAc, CBTag 1.0-Cys-13CBTNAc, CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc	All peptide: Sum CBTag 1.0-Lys-13CBTNAc, CBTag 1.0-Cys-13CBTNAc, 1/2(CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc)	**Percent of reacted 13CBTNAc bound to a lysine (Lysine-modified/Any modification)**	**Percent of total peptide with a modification on lysine (Lysine-modified/All peptide)**	**Percent of total peptide that has any 13CBTNAc modification ((Any modification - 1/2(CBTag 1.0-Cys-13CBTNAc-Lys-13CBTNAc))/All peptide)**
1988.6	20200.6	36858.8	9.844262052	**5.395183782**	**51.90592206**
5662.45	26491.8	44186.35	21.3743498	**12.8149304**	**53.18124262**
7758	23811.7	36072	32.58062213	**21.50698603**	**55.73353293**
9205.15	25342.9	37413.95	36.32240194	**24.60352355**	**56.06291236**
8573.9	23164	32077.1	37.01390088	**26.72903723**	**58.53054048**
568.8	5171.6		**10.99853044**		
1448.85	5923.5		**24.4593568**		
1989.85	5836.5		**34.09320655**		
2405.35	6159.5		**39.05105934**		
2121.2	5303.9		**39.99321254**		

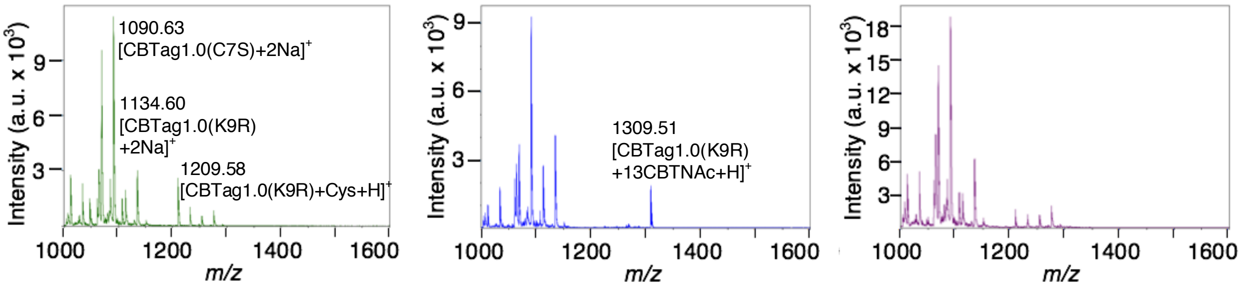

Figure S12. 13CBTNAc binding assay and cysteine treatment results for a 1:1 mixture of CBTag 1.0 (K9R) and CBTag 1.0 (C7S). The binding assay and cysteine competition were as follows: 40 μL of a 10% DMF in PBS solution of 1:1 CBTag 1.0 (K9R)/CBTag 1.0 (C7S) (0.9 mM total peptide) with or without 13CBTNAc (1 mM) was incubated 48 h at r.t. Then, the negative control (without 13CBTNAc) and half (20 μL) of the sample incubated with 13CBTNAc were each treated with an equal volume (20 μL) of a solution of cysteine and DTT (10 and 15 mM, respectively) in PBS. The other half of the sample incubated with 13CBTNAc was treated with an equal volume of a solution of DTT (15 mM) in PBS. After 48 h at r.t., MALDI-TOF MS was used to analyze the negative control (left column, green spectra), the sample incubated with 13CBTNAc then DTT alone (middle column, blue spectra), and the sample incubated with 13CBTNAc then cysteine and DTT (right column, purple spectra). The CBTag 1.0 (K9R)-13CBTNAc adduct disappears on cysteine treatment; no CBTag 1.0 (C7S)-13CBTNAc adduct is apparent under any of these conditions.

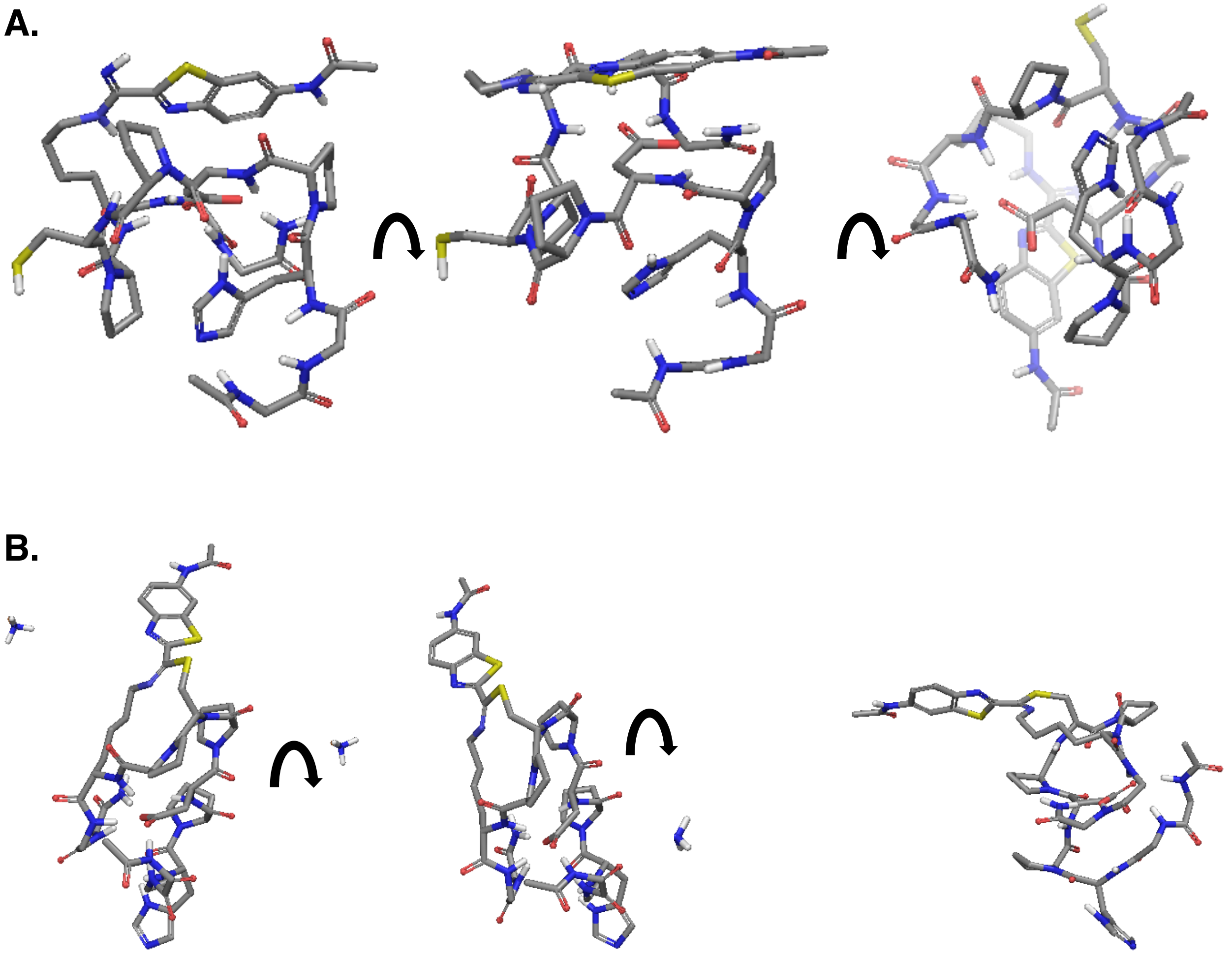

Figure S13. Lowest energy conformation of each potential final product (Maestro, Macromodel). **A.** Rotated views of the amidine product (observed). The energy of this conformer was found to be -488 kcal/mol. **B.** Rotated views of the condensation reaction product, including ammonia (not observed). The energy of this conformer was found to be -456 kcal/mol.

LC-MS time-course spectra and integration results

Peak identification based on Figures S6-7:

CBTag 1.0 – minute 7.9

CBTag 1.0-13CBTNAc, lysine adduct – minute 9

CBTag 1.0-13CBTNAc, cysteine adduct – minute 9.2

CBTag 1.0-2(13CBTNAc) – minute 9.7

13CBTNAc – minute 12.9

Integration results were consolidated previously in Tables S2-S4

```
Print of window 38: Current Chromatogram(s)
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Sample Name : 012218_PF3-ph7-13cbtnac_1
=====================================================================
Acq. Operator   : SGLK                            Seq. Line :   5
Acq. Instrument : Instrument 1                     Location : Vial 5
Injection Date  : 1/26/18 4:58:31 PM                    Inj :   1
                                                Inj Volume : 1.000 µl
Acq. Method     : D:\CHEM32\1\METHODS\AP_C18_INSERT.M
Last changed    : 1/22/18 3:04:38 PM by SGLK
Analysis Method : Z:\DESKTOP\BERTOZZI LAB\LCMS INFO\LCMS METHODS TO 112917\SGLK_BERTOZZIBP_
                  WITHINSERT.M
Last changed    : 3/8/18 8:51:08 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
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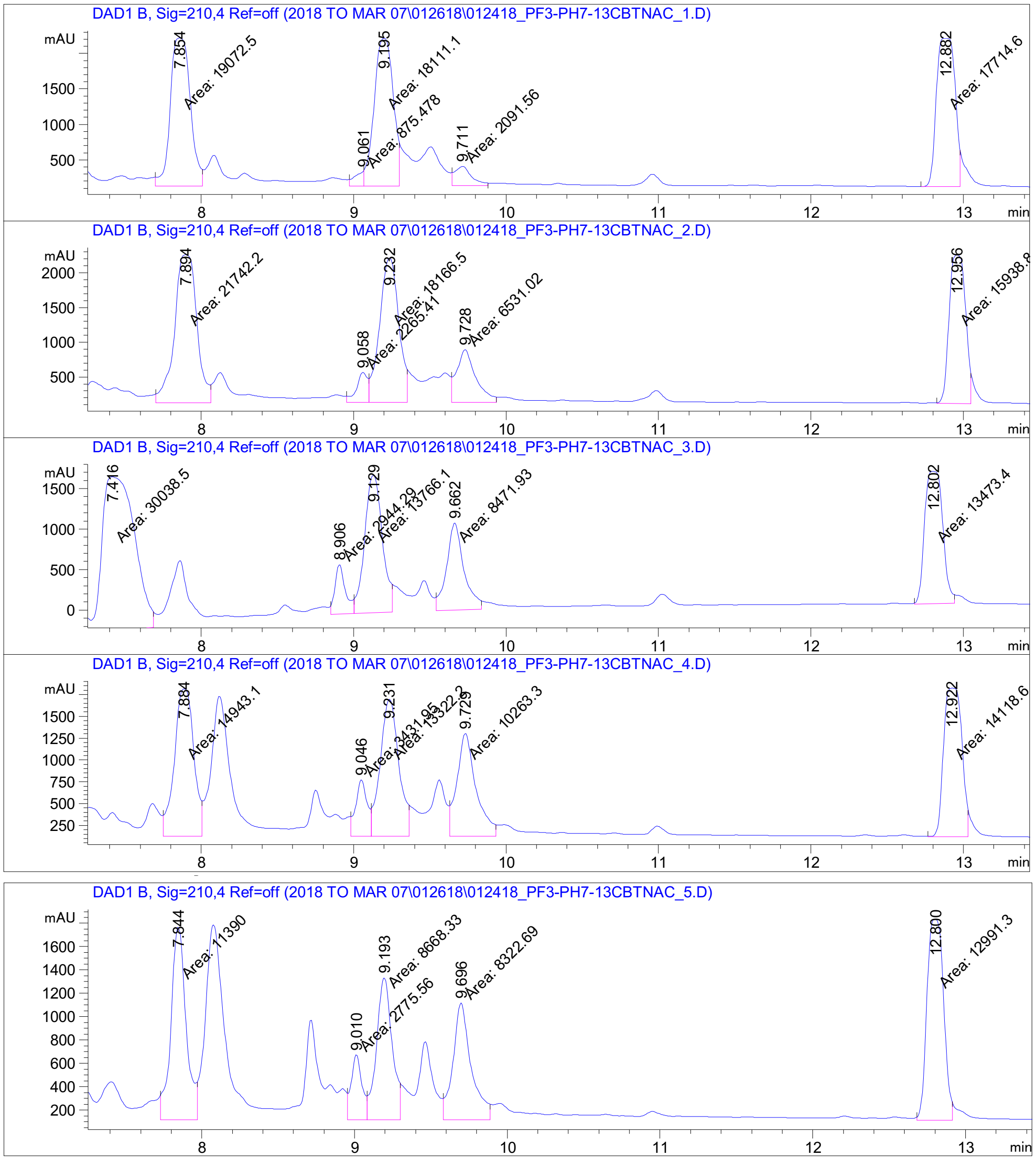
Current Chromatogram(s)



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Data File C:\CHEM32\1\DATA\2018 TO MAR 07\012618\012418_PF3-PH7-13CBTNAC_1.D
Sample Name: 012218_PF3-ph7-13cbtnac_1

    =====================================================================
                             Integration Results
    =====================================================================

    Signal 1: DAD1 B, Sig=210,4 Ref=off (2018 TO MAR 07\012618\012418_PF3-PH7-13CBTNAC_1.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]        [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    7.854 FM    1.90725e4   2084.91626  0.1525    7.697    8.004
       2    9.061 MF     875.47845   209.35365  0.0697    8.970    9.065
       3    9.195 MF    1.81111e4   2078.43286  0.1452    9.065    9.298
       4    9.711 FM    2091.56250   275.67270  0.1265    9.644    9.877
       5   12.882 MF    1.77146e4   2086.62402  0.1415   12.720   12.976


    Signal 2: DAD1 B, Sig=210,4 Ref=off (2018 TO MAR 07\012618\012418_PF3-PH7-13CBTNAC_2.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]        [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    7.894 FM    2.17422e4   2129.17847  0.1702    7.699    8.060
       2    9.058 FM    2265.41406   433.72296  0.0871    8.952    9.098
       3    9.232 MF    1.81665e4   2077.62915  0.1457    9.098    9.349
       4    9.728 FM    6531.01660   759.14935  0.1434    9.640    9.934
       5   12.956 MF    1.59388e4   2136.41089  0.1243   12.824   13.046


    Signal 3: DAD1 B, Sig=210,4 Ref=off (2018 TO MAR 07\012618\012418_PF3-PH7-13CBTNAC_3.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]        [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    7.416 FM    3.00385e4   1894.61292  0.2642    7.077    7.685
       2    8.906 MF    2944.28687   611.75421  0.0802    8.846    8.999
       3    9.129 MF    1.37661e4   1695.87073  0.1353    8.999    9.250
       4    9.662 MF    8471.92676  1076.19922  0.1312    9.538    9.835
       5   12.802 MF    1.34734e4   1632.25354  0.1376   12.676   12.937


    Signal 4: DAD1 B, Sig=210,4 Ref=off (2018 TO MAR 07\012618\012418_PF3-PH7-13CBTNAC_4.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]        [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    7.884 MF    1.49431e4   1688.32275  0.1475    7.747    8.001
       2    9.046 FM    3431.95166   649.64691  0.0880    8.979    9.113
       3    9.231 FM    1.33222e4   1571.53259  0.1413    9.113    9.360
       4    9.729 FM    1.02633e4   1182.65515  0.1446    9.627    9.932
       5   12.922 MF    1.41186e4   1700.74683  0.1384   12.764   13.027


    Signal 5: DAD1 B, Sig=210,4 Ref=off (2018 TO MAR 07\012618\012418_PF3-PH7-13CBTNAC_5.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]        [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    7.844 MF    1.13900e4   1649.19177  0.1151    7.726    7.969
       2    9.010 MF    2775.56274   557.69238  0.0829    8.951    9.081
       3    9.193 MF    8668.32715  1219.24573  0.1185    9.081    9.297
       4    9.696 MF    8322.69238  1001.90900  0.1384    9.578    9.886
       5   12.800 MF    1.29913e4   1721.24487  0.1258   12.678   12.910
```

```
Print of window 38: Current Chromatogram(s)
Data File  : C:\CHEM32\1\DATA\2018 TO MAR 07\012618\012418_PF3-PH7-13CBTNAC_1.D
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=====================================================================
Acq. Operator   : SGLK                              Seq. Line :    5
Acq. Instrument : Instrument 1                       Location : Vial 5
Injection Date  : 1/26/18 4:58:31 PM                      Inj :    1
                                                   Inj Volume : 1.000 µl
Acq. Method     : D:\CHEM32\1\METHODS\AP_C18_INSERT.M
Last changed    : 1/22/18 3:04:38 PM by SGLK
Analysis Method : Z:\DESKTOP\BERTOZZI LAB\LCMS INFO\LCMS METHODS TO 112917\SGLK_BERTOZZIBP_
                  WITHINSERT.M
Last changed    : 3/8/18 8:51:08 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
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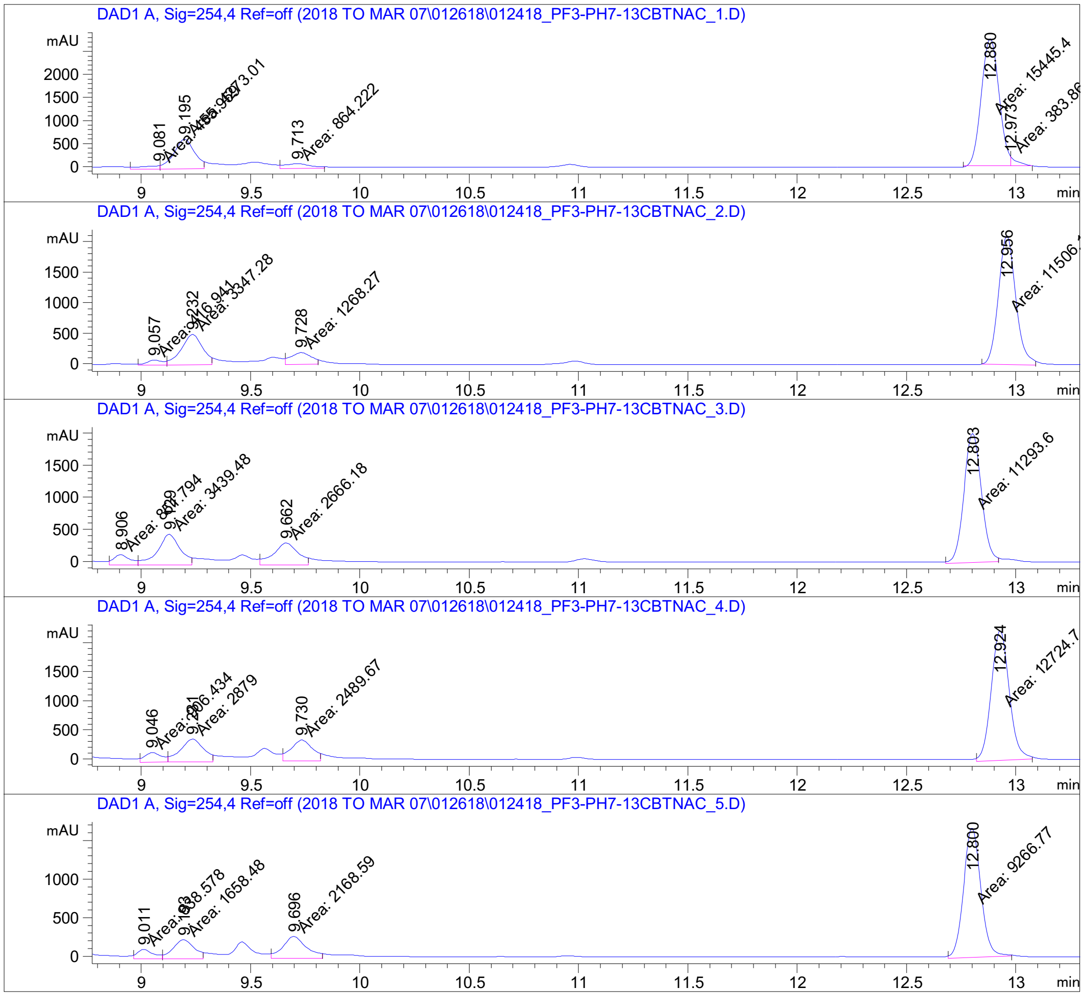
Current Chromatogram(s)



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Data File C:\CHEM32\1\DATA\2018 TO MAR 07\012618\012418_PF3-PH7-13CBTNAC_1.D
Sample Name: 012218_PF3-ph7-13cbtnac_1

    =====================================================================
                             Integration Results
    =====================================================================

    Signal 1: DAD1 A, Sig=254,4 Ref=off (2018 TO MAR 07\012618\012418_PF3-PH7-13CBTNAC_1.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]         [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    9.081 MF     455.95853    76.43199  0.0994    8.948    9.085
       2    9.195 MF    4273.00830   647.51642  0.1100    9.085    9.285
       3    9.713 FM     864.22162   103.05989  0.1398    9.631    9.836
       4   12.880 MF    1.54454e4   2768.33911  0.0930   12.757   12.973
       5   12.973 FM     383.86099   201.20613  0.0318   12.973   13.073


    Signal 2: DAD1 A, Sig=254,4 Ref=off (2018 TO MAR 07\012618\012418_PF3-PH7-13CBTNAC_2.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]         [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    9.057 MF     416.94113    78.41770  0.0886    8.983    9.115
       2    9.232 MF    3347.27686   497.54984  0.1121    9.115    9.320
       3    9.728 MF    1268.26978   193.05396  0.1095    9.657    9.807
       4   12.956 MM    1.15061e4   2109.27319  0.0909   12.842   13.088


    Signal 3: DAD1 A, Sig=254,4 Ref=off (2018 TO MAR 07\012618\012418_PF3-PH7-13CBTNAC_3.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]         [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    8.906 MF     851.79407   162.02739  0.0876    8.852    8.984
       2    9.129 FM    3439.48486   476.80533  0.1202    8.984    9.230
       3    9.662 FM    2666.17871   344.44800  0.1290    9.541    9.762
       4   12.803 MM    1.12936e4   2014.62061  0.0934   12.677   12.918


    Signal 4: DAD1 A, Sig=254,4 Ref=off (2018 TO MAR 07\012618\012418_PF3-PH7-13CBTNAC_4.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]         [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    9.046 MF     906.43396   164.82642  0.0917    8.992    9.120
       2    9.231 MF    2879.00098   392.18085  0.1224    9.120    9.325
       3    9.730 MF    2489.67114   360.50821  0.1151    9.647    9.817
       4   12.924 MM    1.27247e4   2235.55273  0.0949   12.818   13.074
    Signal 5: DAD1 A, Sig=254,4 Ref=off (2018 TO MAR 07\012618\012418_PF3-PH7-13CBTNAC_5.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]         [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    9.011 MF     638.57806   124.45227  0.0855    8.962    9.095
       2    9.193 FM    1658.48438   245.42241  0.1126    9.095    9.280
       3    9.696 FM    2168.59033   286.15845  0.1263    9.591    9.827
       4   12.800 MM    9266.77344  1678.98987  0.0920   12.687   12.978
```

```
Print of window 38: Current Chromatogram(s)
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======================================================================
Acq. Operator   : SGLK                            Seq. Line :    5
Acq. Instrument : Instrument 1                     Location : Vial 5
Injection Date  : 2/2/18 6:47:32 PM                     Inj :    1
                                                 Inj Volume : 1.000 µl
Acq. Method     : D:\CHEM32\1\METHODS\AP_C18_INSERT.M
Last changed    : 1/22/18 3:04:38 PM by SGLK
Analysis Method : Z:\DESKTOP\BERTOZZI LAB\LCMS INFO\LCMS METHODS TO 112917\SGLK_BERTOZZIBP_
                  WITHINSERT.M
Last changed    : 3/8/18 8:51:08 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```
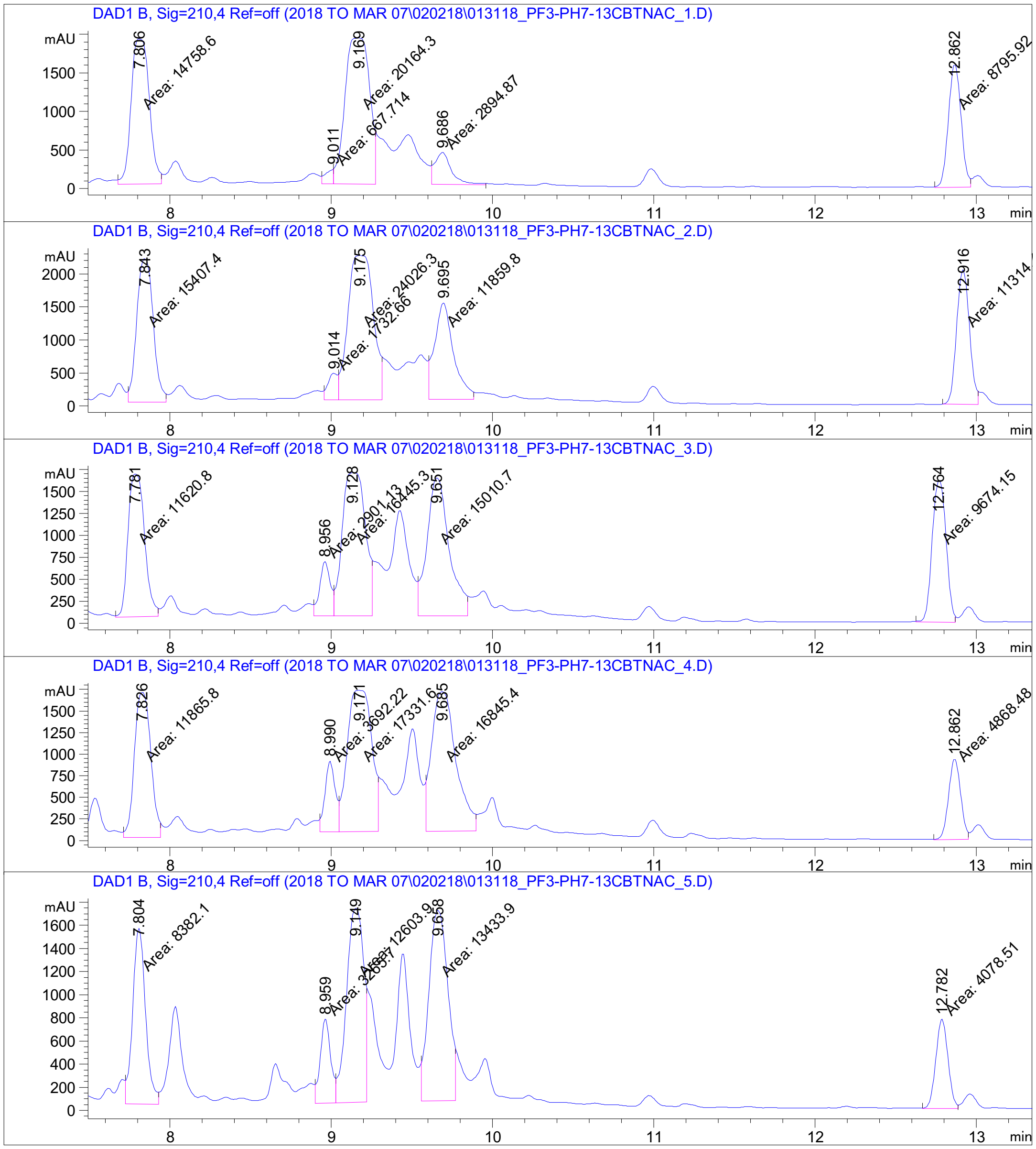
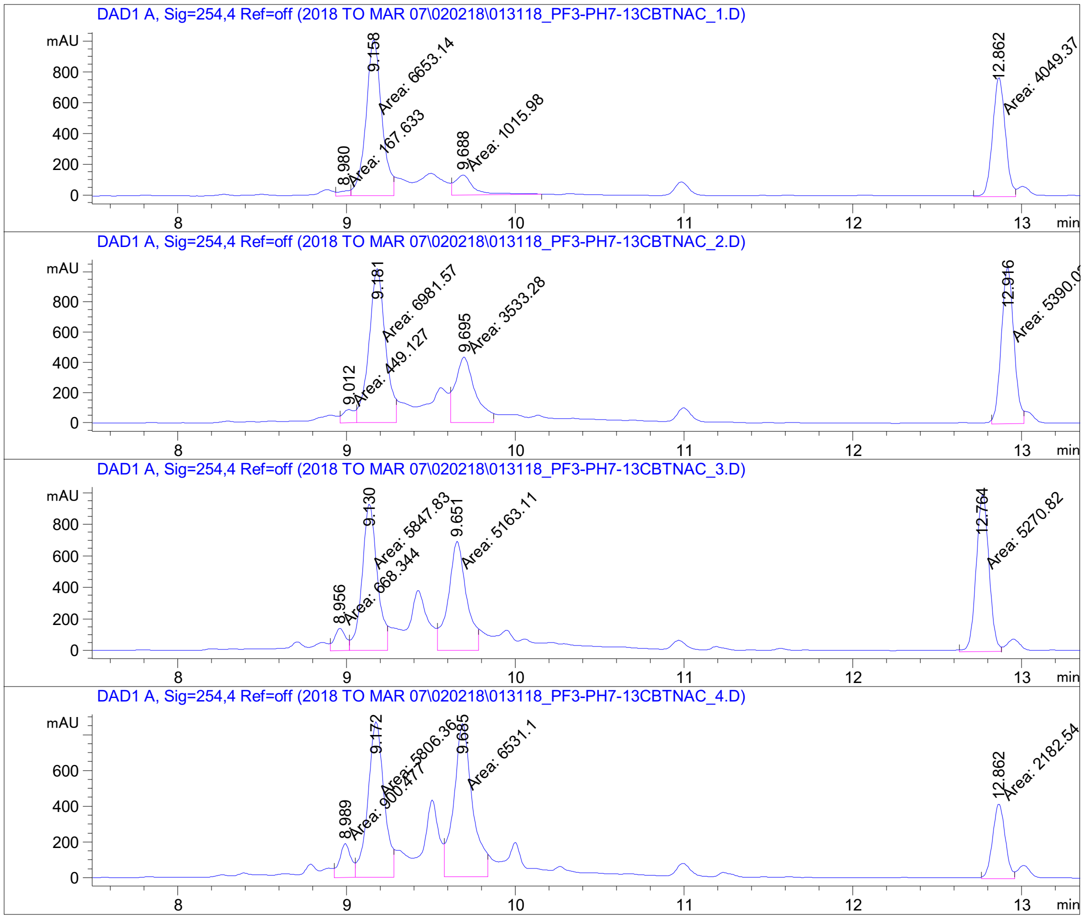

Current Chromatogram(s)

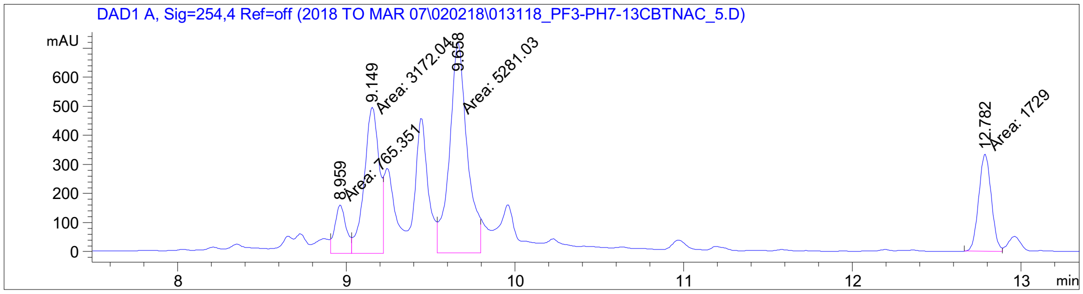


```
Data File C:\CHEM32\1\DATA\2018 TO MAR 07\020218\013118_PF3-PH7-13CBTNAC_1.D
Sample Name: 013118_PF3-ph7-13cbtnac_1

    =====================================================================
                             Integration Results
    =====================================================================

    Signal 1: DAD1 B, Sig=210,4 Ref=off (2018 TO MAR 07\020218\013118_PF3-PH7-13CBTNAC_1.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]         [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    7.806 MF    1.47586e4   1877.88623  0.1310    7.677    7.947
       2    9.011 MF     667.71442   192.94965  0.0577    8.939    9.012
       3    9.169 MF    2.01643e4   1890.88965  0.1777    9.012    9.273
       4    9.686 FM    2894.87231   414.46405  0.1164    9.622    9.956
       5   12.862 MF    8795.91797  1592.83997  0.0920   12.740   12.963


    Signal 2: DAD1 B, Sig=210,4 Ref=off (2018 TO MAR 07\020218\013118_PF3-PH7-13CBTNAC_2.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]         [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    7.843 FM    1.54074e4   2173.26514  0.1182    7.740    7.976
       2    9.014 MF    1732.66248   402.80444  0.0717    8.955    9.044
       3    9.175 MF    2.40263e4   2183.97681  0.1834    9.044    9.314
       4    9.695 MF    1.18598e4   1464.29858  0.1350    9.603    9.883
       5   12.916 MF    1.13144e4   2036.28650  0.0926   12.788   13.007


    Signal 3: DAD1 B, Sig=210,4 Ref=off (2018 TO MAR 07\020218\013118_PF3-PH7-13CBTNAC_3.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]         [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    7.781 MF    1.16208e4   1624.52429  0.1192    7.661    7.925
       2    8.956 MF    2901.13184   622.10889  0.0777    8.891    9.015
       3    9.128 MF    1.64453e4   1625.91223  0.1686    9.015    9.254
       4    9.651 MF    1.50107e4   1571.71680  0.1592    9.536    9.845
       5   12.764 MF    9674.14648  1609.95398  0.1001   12.623   12.868


    Signal 4: DAD1 B, Sig=210,4 Ref=off (2018 TO MAR 07\020218\013118_PF3-PH7-13CBTNAC_4.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]         [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    7.826 FM    1.18658e4   1681.22424  0.1176    7.712    7.941
       2    8.990 MF    3692.21680   820.23694  0.0750    8.929    9.047
       3    9.171 MF    1.73316e4   1636.02942  0.1766    9.047    9.292
       4    9.685 MF    1.68454e4   1617.40186  0.1736    9.587    9.896
       5   12.862 MF    4868.47998   934.37787  0.0868   12.734   12.947


    Signal 5: DAD1 B, Sig=210,4 Ref=off (2018 TO MAR 07\020218\013118_PF3-PH7-13CBTNAC_5.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]         [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    7.804 FM    8382.09668  1519.23242  0.0920    7.725    7.928
       2    8.959 MF    3265.69629   730.16943  0.0745    8.901    9.028
       3    9.149 MF    1.26039e4   1678.56458  0.1251    9.028    9.219
       4    9.658 MF    1.34339e4   1646.90576  0.1360    9.559    9.769
       5   12.782 MF    4078.51001   775.32263  0.0877   12.664   12.883
```

```
Print of window 38: Current Chromatogram(s)
Data File   : C:\CHEM32\1\DATA\2018 TO MAR 07\020218\013118_PF3-PH7-13CBTNAC_1.D
Sample Name : 013118_PF3-ph7-13cbtnac_1
======================================================================
Acq. Operator    : SGLK                             Seq. Line :    5
Acq. Instrument : Instrument 1                        Location : Vial 5
Injection Date   : 2/2/18 6:47:32 PM                       Inj :    1
                                                 Inj Volume : 1.000 µl
Acq. Method      : D:\CHEM32\1\METHODS\AP_C18_INSERT.M
Last changed     : 1/22/18 3:04:38 PM by SGLK
Analysis Method : Z:\DESKTOP\BERTOZZI LAB\LCMS INFO\LCMS METHODS TO 112917\SGLK_BERTOZZIBP_
                  WITHINSERT.M
Last changed     : 3/8/18 8:51:08 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```

Current Chromatogram(s)

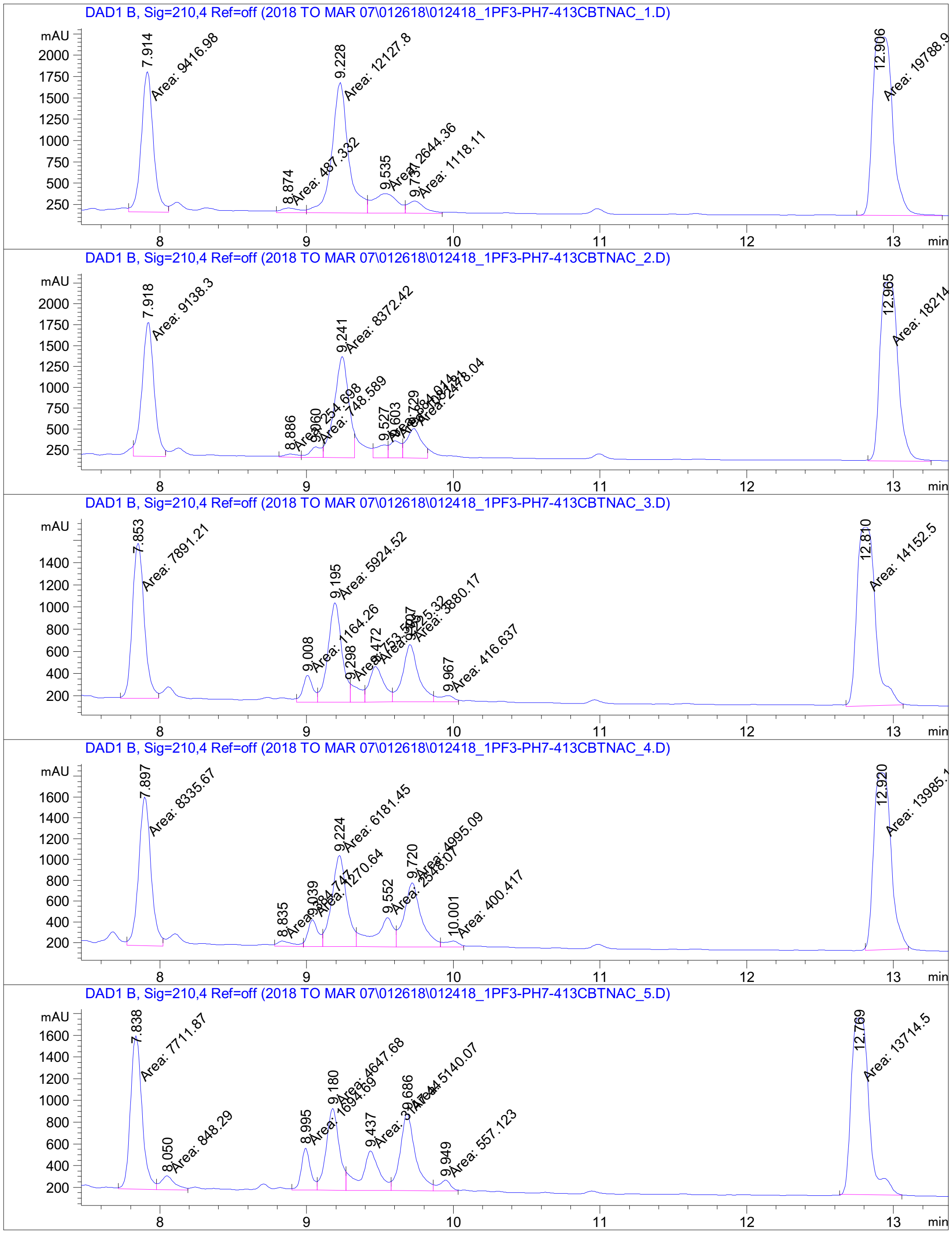




```
Data File C:\CHEM32\1\DATA\2018 TO MAR 07\020218\013118_PF3-PH7-13CBTNAC_1.D
Sample Name: 013118_PF3-ph7-13cbtnac_1

    =====================================================================
                             Integration Results
    =====================================================================

    Signal 1: DAD1 A, Sig=254,4 Ref=off (2018 TO MAR 07\020218\013118_PF3-PH7-13CBTNAC_1.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]        [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    8.980 MF     167.63275    40.41625  0.0691    8.935    9.025
       2    9.158 MF    6653.14258  1013.87598  0.1094    9.025    9.279
       3    9.688 FM    1015.97882   131.04523  0.1292    9.622   10.154
       4   12.862 MF    4049.37402   772.72168  0.0873   12.714   12.963


    Signal 2: DAD1 A, Sig=254,4 Ref=off (2018 TO MAR 07\020218\013118_PF3-PH7-13CBTNAC_2.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]        [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    9.012 FM     449.12659    88.06937  0.0850    8.959    9.058
       2    9.181 FM    6981.57227  1022.56451  0.1138    9.058    9.295
       3    9.695 FM    3533.27783   434.13306  0.1356    9.614    9.872
       4   12.916 FM    5390.01611  1040.12830  0.0864   12.820   13.013


    Signal 3: DAD1 A, Sig=254,4 Ref=off (2018 TO MAR 07\020218\013118_PF3-PH7-13CBTNAC_3.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]        [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    8.956 FM     668.34357   142.29138  0.0783    8.902    9.017
       2    9.130 FM    5847.83105   930.69971  0.1047    9.017    9.242
       3    9.651 FM    5163.11035   692.02686  0.1243    9.536    9.782
       4   12.764 MF    5270.82471   997.93738  0.0880   12.628   12.878


    Signal 4: DAD1 A, Sig=254,4 Ref=off (2018 TO MAR 07\020218\013118_PF3-PH7-13CBTNAC_4.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]        [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    8.989 FM     900.47656   190.13754  0.0789    8.927    9.049
       2    9.172 FM    5806.35840   870.80627  0.1111    9.049    9.279
       3    9.685 FM    6531.10059   858.56616  0.1268    9.577    9.835
       4   12.862 FM    2182.54004   418.45169  0.0869   12.759   12.955


    Signal 5: DAD1 A, Sig=254,4 Ref=off (2018 TO MAR 07\020218\013118_PF3-PH7-13CBTNAC_5.D)

    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]        [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    8.959 FM     765.35132   166.98950  0.0764    8.906    9.029
       2    9.149 FM    3172.03857   503.40402  0.1050    9.029    9.217
       3    9.658 FM    5281.03174   725.90582  0.1213    9.536    9.794
       4   12.782 MF    1728.99561   334.71692  0.0861   12.661   12.886
```

Print of window 38: Current Chromatogram(s)

Current Chromatogram(s)



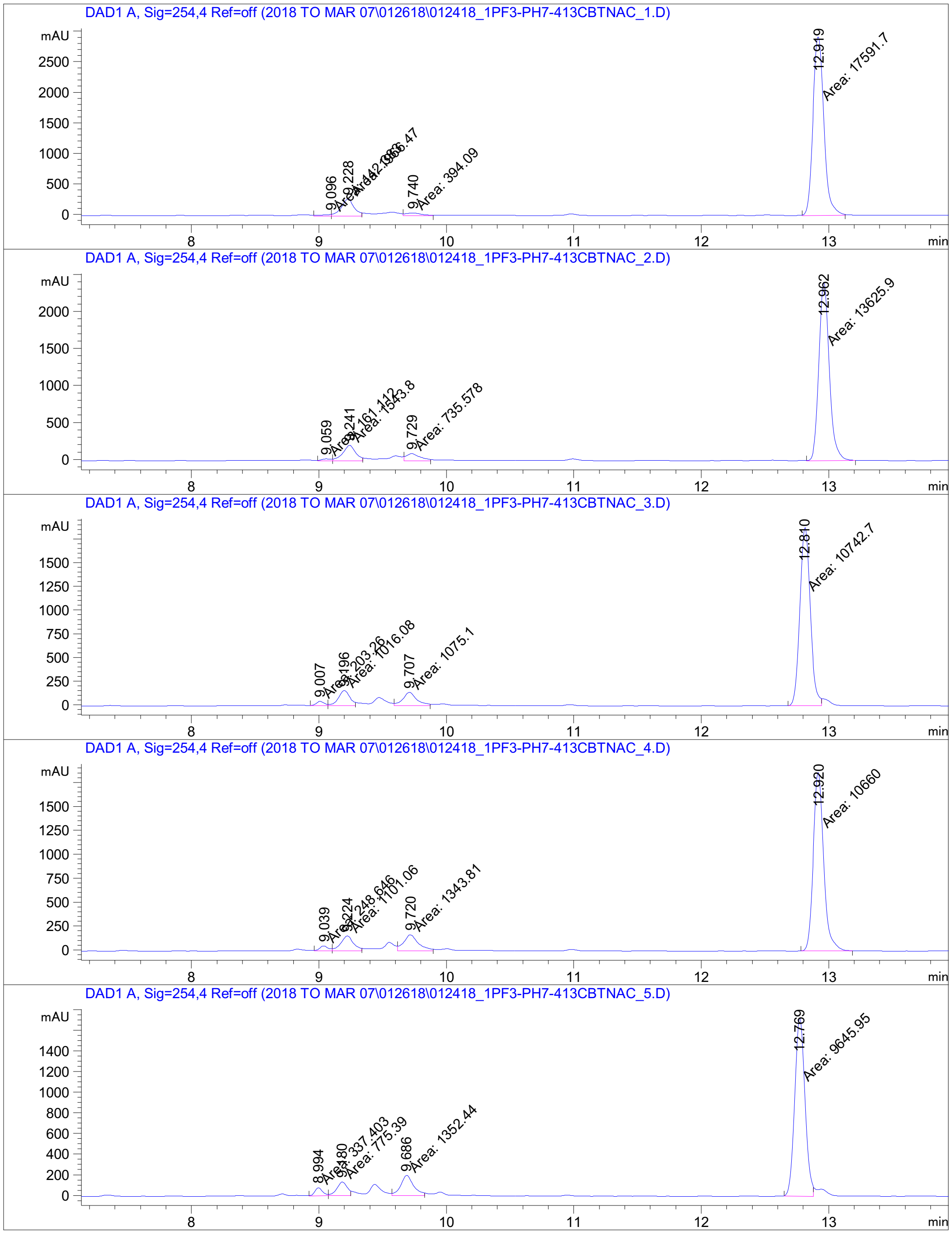
Instrument 1 3/8/18 8:48:54 AM

```
=====================================================================
                         Integration Results
=====================================================================

Signal 1: DAD1 B, Sig=210,4 Ref=off (2018 TO MAR 07\012618\012418_1PF3-PH7-413CBTNAC_1.D)


Peak   Time   Type     Area       Height     Width    Start     End
  #    [min]        [mAU*s]       [mAU]      [min]    [min]    [min]
----|--------|----|-----------|-----------|-------|--------|--------|
   1    7.914 MF    9416.98242  1647.93689  0.0952    7.787    8.060
   2    8.874 FM     487.33218    54.21212  0.1498    8.795    8.999
   3    9.228 FM    1.21278e4   1529.12659  0.1322    8.999    9.416
   4    9.535 FM    2644.35767   228.19458  0.1931    9.416    9.674
   5    9.737 FM    1118.11084   142.95132  0.1304    9.674    9.924
   6   12.906 FM    1.97889e4   2092.50806  0.1576   12.750   13.333
   7   17.096 MM     341.25854    47.20979  0.1205   16.977   17.244


Signal 2: DAD1 B, Sig=210,4 Ref=off (2018 TO MAR 07\012618\012418_1PF3-PH7-413CBTNAC_2.D)


Peak   Time   Type     Area       Height     Width    Start     End
  #    [min]        [mAU*s]       [mAU]      [min]    [min]    [min]
----|--------|----|-----------|-----------|-------|--------|--------|
   1    7.918 FM    9138.29590  1610.67407  0.0946    7.820    8.038
   2    8.886 MF     254.69795    37.63269  0.1128    8.811    8.965
   3    9.060 FM     748.58875   126.74625  0.0984    8.965    9.112
   4    9.241 FM    8372.42285  1212.87939  0.1150    9.112    9.326
   5    9.527 FM     884.01447   154.15724  0.0956    9.452    9.556
   6    9.603 FM    1081.20557   205.80222  0.0876    9.556    9.654
   7    9.729 FM    2478.03564   353.92752  0.1167    9.654    9.825
   8   12.965 FM    1.82142e4   2143.19775  0.1416   12.826   13.256
   9   17.135 FM     137.25032    18.79482  0.1217   17.041   17.286


Signal 3: DAD1 B, Sig=210,4 Ref=off (2018 TO MAR 07\012618\012418_1PF3-PH7-413CBTNAC_3.D)


Peak   Time   Type     Area       Height     Width    Start     End
  #    [min]        [mAU*s]       [mAU]      [min]    [min]    [min]
----|--------|----|-----------|-----------|-------|--------|--------|
   1    7.853 MF    7891.20898  1398.38062  0.0941    7.731    7.992
   2    9.008 MF    1164.25757   244.43816  0.0794    8.933    9.075
   3    9.195 MF    5924.52051   898.11829  0.1099    9.075    9.298
   4    9.298 MF     753.59515   167.25101  0.0595    9.298    9.396
   5    9.472 MF    2225.31738   319.45935  0.1161    9.396    9.586
   6    9.707 MF    3880.17480   515.12500  0.1255    9.586    9.867
   7    9.967 FM     416.63672    54.89103  0.1050    9.867   10.036
   8   12.810 MM    1.41525e4   1605.68469  0.1469   12.676   13.068
   9   17.018 FM     103.15417    13.08915  0.1313   16.907   17.166
```

```
Data File C:\CHEM32\1\DATA\2018 TO MAR 07\012618\012418_1PF3-PH7-413CBTNAC_1.D
Sample Name: 012418_1PF3-ph7-413CBTNAc_1

    Signal 4: DAD1 B, Sig=210,4 Ref=off (2018 TO MAR 07\012618\012418_1PF3-PH7-413CBTNAC_4.D)


    Peak  Time   Type    Area       Height     Width    Start     End
      #   [min]        [mAU*s]      [mAU]      [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1   7.897 MF    8335.66602 1429.31128  0.0972    7.776    8.022
       2   8.835 MF     384.74734   50.63771  0.1266    8.782    8.979
       3   9.039 FM    1270.64465  258.62827  0.0819    8.979    9.111
       4   9.224 FM    6181.45459  876.76721  0.1175    9.111    9.339
       5   9.552 FM    2548.07251  281.66565  0.1508    9.339    9.610
       6   9.720 FM    4995.09375  616.77344  0.1350    9.610    9.914
       7  10.001 FM     400.41724   57.92731  0.1152    9.914   10.071
       8  12.920 MM    1.39851e4  1702.83252  0.1369   12.809   13.102
       9  17.103 FM      84.47837   10.66243  0.1320   16.993   17.267


    Signal 5: DAD1 B, Sig=210,4 Ref=off (2018 TO MAR 07\012618\012418_1PF3-PH7-413CBTNAC_5.D)


    Peak  Time   Type    Area       Height     Width    Start     End
      #   [min]        [mAU*s]      [mAU]      [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1   7.838 MF    7711.86670 1410.79956  0.0911    7.715    7.976
       2   8.050 FM     848.29047  127.37299  0.1110    7.976    8.190
       3   8.995 MF    1694.69202  389.25287  0.0726    8.900    9.071
       4   9.180 MF    4647.68359  753.63672  0.1028    9.071    9.268
       5   9.437 MF    3147.43799  364.28168  0.1440    9.268    9.575
       6   9.686 MF    5140.07275  710.37439  0.1206    9.575    9.864
       7   9.949 FM     557.12329   97.50262  0.0952    9.864   10.032
       8  12.769 MM    1.37145e4  1626.81152  0.1405   12.634   13.059
       9  16.978 FM      75.99796    9.27865  0.1365   16.875   17.135

    ======================================================================
```

Print of window 38: Current Chromatogram(s)

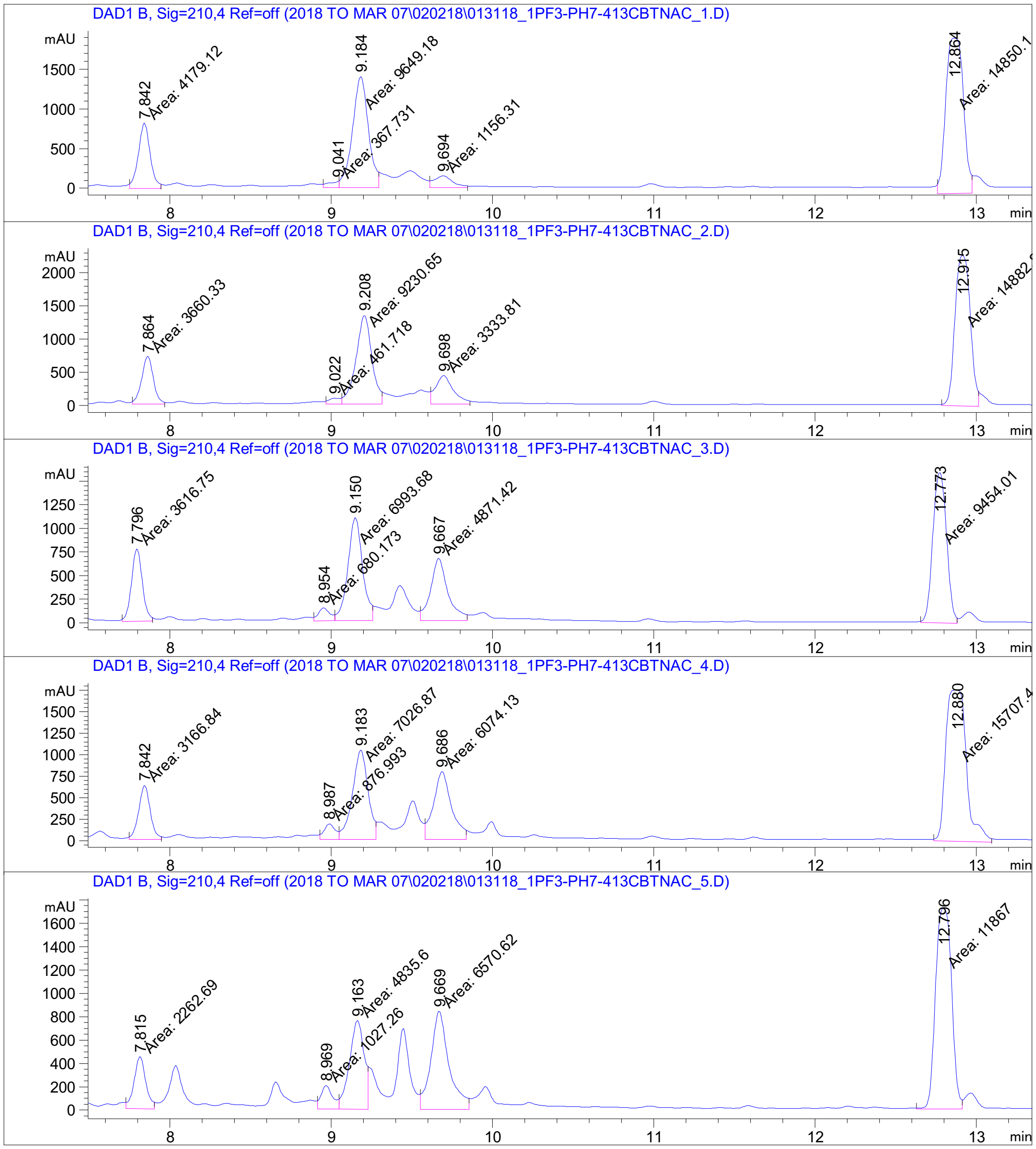
Current Chromatogram(s)



```
Data File C:\CHEM32\1\DATA\2018 TO MAR 07\012618\012418_1PF3-PH7-413CBTNAC_1.D
Sample Name: 012418_1PF3-ph7-413CBTNAc_1

    =====================================================================
                             Integration Results
    =====================================================================

    Signal 1: DAD1 A, Sig=254,4 Ref=off (2018 TO MAR 07\012618\012418_1PF3-PH7-413CBTNAC_1.D)


    Peak   Time   Type     Area       Height    Width     Start     End
      #    [min]         [mAU*s]      [mAU]     [min]     [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    9.096 MF     142.38287    26.04919  0.0911    8.961    9.097
       2    9.228 FM    1966.46570   281.31848  0.1165    9.097    9.336
       3    9.740 FM     394.09006    45.81873  0.1434    9.662    9.896
       4   12.919 MM    1.75917e4   2931.18726  0.1000   12.792   13.128


    Signal 2: DAD1 A, Sig=254,4 Ref=off (2018 TO MAR 07\012618\012418_1PF3-PH7-413CBTNAC_2.D)


    Peak   Time   Type     Area       Height    Width     Start     End
      #    [min]         [mAU*s]      [mAU]     [min]     [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    9.059 FM     161.11209    28.80318  0.0932    8.991    9.109
       2    9.241 FM    1543.80066   213.12289  0.1207    9.109    9.346
       3    9.729 FM     735.57843    97.84830  0.1253    9.668    9.876
       4   12.962 MM    1.36259e4   2410.98779  0.0942   12.827   13.210


    Signal 3: DAD1 A, Sig=254,4 Ref=off (2018 TO MAR 07\012618\012418_1PF3-PH7-413CBTNAC_3.D)


    Peak   Time   Type     Area       Height    Width     Start     End
      #    [min]         [mAU*s]      [mAU]     [min]     [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    9.007 FM     203.26022    46.58055  0.0727    8.934    9.072
       2    9.196 FM    1016.08386   161.26431  0.1050    9.072    9.288
       3    9.707 FM    1075.09631   142.35010  0.1259    9.590    9.875
       4   12.810 MF    1.07427e4   1886.81433  0.0949   12.681   12.946


    Signal 4: DAD1 A, Sig=254,4 Ref=off (2018 TO MAR 07\012618\012418_1PF3-PH7-413CBTNAC_4.D)


    Peak   Time   Type     Area       Height    Width     Start     End
      #    [min]         [mAU*s]      [mAU]     [min]     [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    9.039 FM     248.64555    52.22098  0.0794    8.962    9.105
       2    9.224 FM    1101.06201   155.99211  0.1176    9.105    9.337
       3    9.720 FM    1343.80579   168.67032  0.1328    9.618    9.895
       4   12.920 MM    1.06600e4   1872.36560  0.0949   12.783   13.186


    Signal 5: DAD1 A, Sig=254,4 Ref=off (2018 TO MAR 07\012618\012418_1PF3-PH7-413CBTNAC_5.D)


       1    8.994 MF     337.40302    79.62730  0.0706    8.922    9.075
       2    9.180 MF     775.38977   133.16174  0.0970    9.075    9.250
       3    9.686 MF    1352.44153   195.07692  0.1155    9.573    9.831
       4   12.769 MF    9645.94922  1733.51257  0.0927   12.652   12.880
```

```
Print of window 38: Current Chromatogram(s)
Data File   : C:\CHEM32\1\DATA\2018 TO MAR 07\020218\013118_1PF3-PH7-413CBTNAC_1.D
Sample Name : 013118_1PF3-ph7-413CBTNAc_1
======================================================================
Acq. Operator    : SGLK                              Seq. Line :    7
Acq. Instrument : Instrument 1                        Location : Vial 7
Injection Date   : 2/2/18 7:45:39 PM                       Inj :    1
                                                   Inj Volume : 1.000 µl
Acq. Method      : D:\CHEM32\1\METHODS\AP_C18_INSERT.M
Last changed     : 1/22/18 3:04:38 PM by SGLK
Analysis Method : Z:\DESKTOP\BERTOZZI LAB\LCMS INFO\LCMS METHODS TO 112917\SGLK_BERTOZZIBP_
                  WITHINSERT.M
Last changed     : 3/8/18 8:51:08 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```

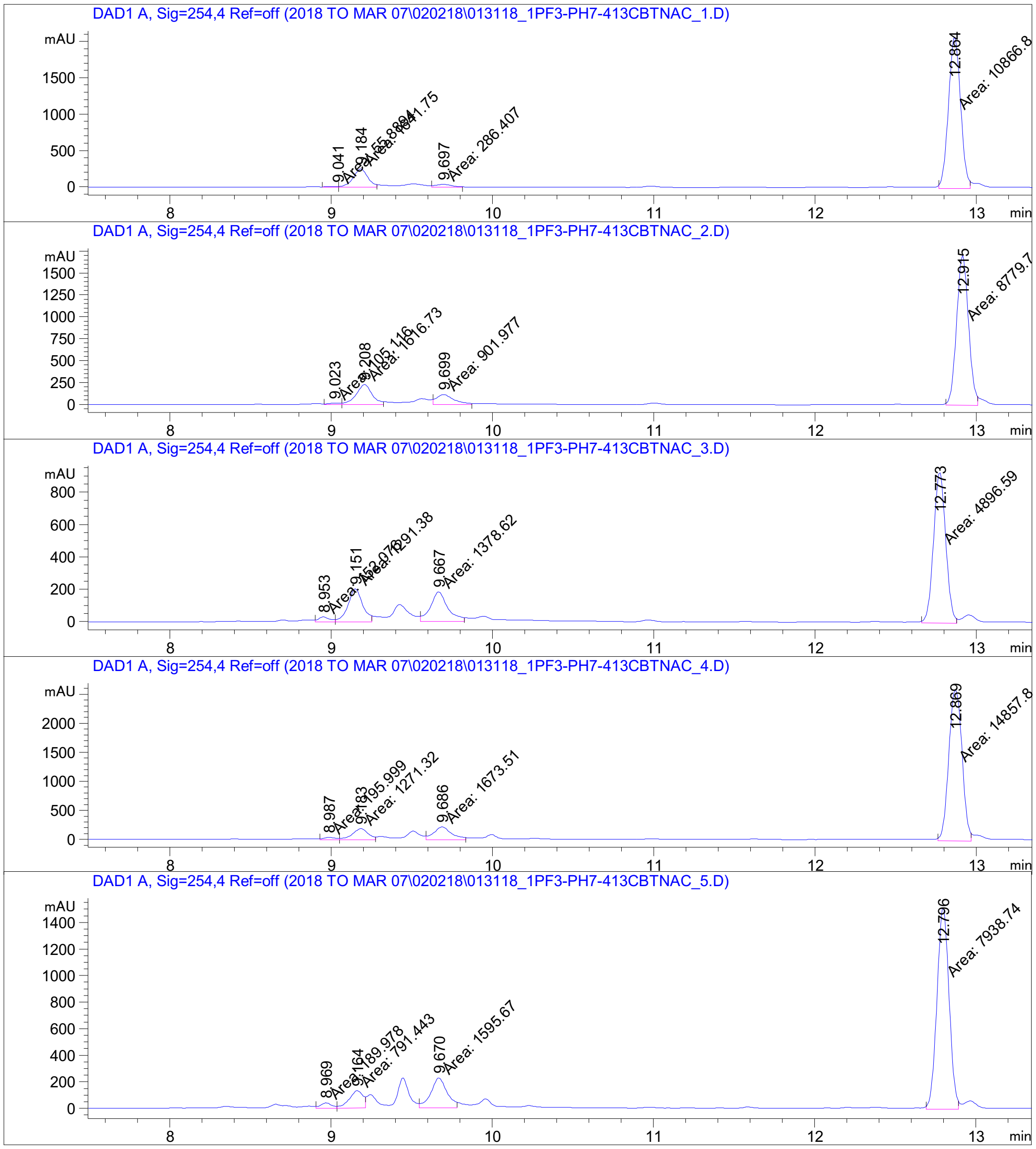
Current Chromatogram(s)



```
Data File C:\CHEM32\1\DATA\2018 TO MAR 07\020218\013118_1PF3-PH7-413CBTNAC_1.D
Sample Name: 013118_1PF3-ph7-413CBTNAc_1

    =====================================================================
                             Integration Results
    =====================================================================

    Signal 1: DAD1 B, Sig=210,4 Ref=off (2018 TO MAR 07\020218\013118_1PF3-PH7-413CBTNAC_1.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]        [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    7.842 FM    4179.11914   821.41675  0.0848    7.749    7.942
       2    9.041 FM     367.73087    78.21339  0.0784    8.950    9.047
       3    9.184 FM    9649.18066  1400.78040  0.1148    9.047    9.293
       4    9.694 FM    1156.30530   145.55722  0.1324    9.609    9.843
       5   12.864 FM    1.48501e4   1956.26233  0.1265   12.758   12.970


    Signal 2: DAD1 B, Sig=210,4 Ref=off (2018 TO MAR 07\020218\013118_1PF3-PH7-413CBTNAC_2.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]        [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    7.864 FM    3660.32935   723.93250  0.0843    7.767    7.966
       2    9.022 FM     461.71805    91.62712  0.0840    8.968    9.064
       3    9.208 FM    9230.65137  1339.48608  0.1149    9.064    9.313
       4    9.698 FM    3333.80762   432.63248  0.1284    9.615    9.858
       5   12.915 MF    1.48828e4   2264.37549  0.1095   12.782   13.012


    Signal 3: DAD1 B, Sig=210,4 Ref=off (2018 TO MAR 07\020218\013118_1PF3-PH7-413CBTNAC_3.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]        [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    7.796 FM    3616.75317   768.20435  0.0785    7.702    7.893
       2    8.954 FM     680.17310   138.71642  0.0817    8.891    9.020
       3    9.150 FM    6993.68018  1092.80615  0.1067    9.020    9.257
       4    9.667 FM    4871.42480   657.31110  0.1235    9.550    9.840
       5   12.773 FM    9454.00977  1592.20349  0.0990   12.652   12.879


    Signal 4: DAD1 B, Sig=210,4 Ref=off (2018 TO MAR 07\020218\013118_1PF3-PH7-413CBTNAC_4.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]        [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    7.842 FM    3166.83960   631.48499  0.0836    7.746    7.945
       2    8.987 FM     876.99335   181.88477  0.0804    8.929    9.047
       3    9.183 FM    7026.86963  1040.78650  0.1125    9.047    9.275
       4    9.686 FM    6074.12842   789.74097  0.1282    9.580    9.835
       5   12.880 MM    1.57074e4   1758.29065  0.1489   12.735   13.092


    Signal 5: DAD1 B, Sig=210,4 Ref=off (2018 TO MAR 07\020218\013118_1PF3-PH7-413CBTNAC_5.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]        [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    7.815 FM    2262.69141   448.04358  0.0842    7.726    7.901
       2    8.969 FM    1027.25977   204.35941  0.0838    8.915    9.047
       3    9.163 FM    4835.60400   760.72070  0.1059    9.047    9.228
       4    9.669 FM    6570.62402   840.52429  0.1303    9.550    9.852
       5   12.796 MF    1.18670e4   1718.16589  0.1151   12.625   12.910
```

```
Print of window 38: Current Chromatogram(s)
Data File   : C:\CHEM32\1\DATA\2018 TO MAR 07\020218\013118_1PF3-PH7-413CBTNAC_1.D
Sample Name : 013118_1PF3-ph7-413CBTNAc_1
======================================================================
Acq. Operator    : SGLK                              Seq. Line :    7
Acq. Instrument : Instrument 1                        Location : Vial 7
Injection Date   : 2/2/18 7:45:39 PM                       Inj :    1
                                                   Inj Volume : 1.000 µl
Acq. Method      : D:\CHEM32\1\METHODS\AP_C18_INSERT.M
Last changed     : 1/22/18 3:04:38 PM by SGLK
Analysis Method : Z:\DESKTOP\BERTOZZI LAB\LCMS INFO\LCMS METHODS TO 112917\SGLK_BERTOZZIBP_
                  WITHINSERT.M
Last changed     : 3/8/18 8:51:08 AM
                   (modified after loading)
Additional Info : Peak(s) manually integrated
```

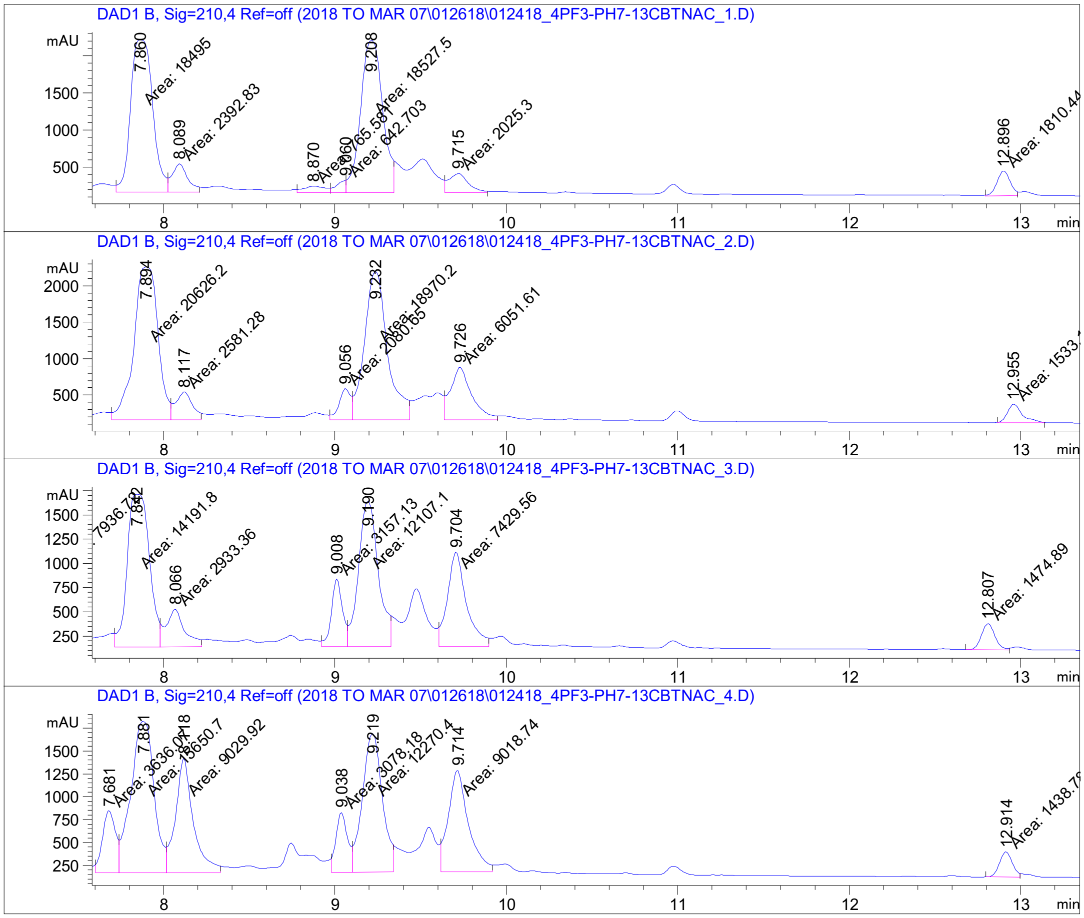
Current Chromatogram(s)



```
Data File C:\CHEM32\1\DATA\2018 TO MAR 07\020218\013118_1PF3-PH7-413CBTNAC_1.D
Sample Name: 013118_1PF3-ph7-413CBTNAc_1

    =====================================================================
                             Integration Results
    =====================================================================

    Signal 1: DAD1 A, Sig=254,4 Ref=off (2018 TO MAR 07\020218\013118_1PF3-PH7-413CBTNAC_1.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]        [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    9.041 FM      55.88944    11.06242  0.0842    8.942    9.044
       2    9.184 FM    1641.74548   253.71167  0.1078    9.044    9.283
       3    9.697 FM     286.40692    40.31698  0.1184    9.622    9.811
       4   12.864 FM    1.08668e4   2075.80518  0.0872   12.765   12.958


    Signal 2: DAD1 A, Sig=254,4 Ref=off (2018 TO MAR 07\020218\013118_1PF3-PH7-413CBTNAC_2.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]        [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    9.023 FM     105.11598    19.44548  0.0901    8.956    9.064
       2    9.208 FM    1616.72717   230.14301  0.1171    9.064    9.324
       3    9.699 FM     901.97675   117.54403  0.1279    9.631    9.870
       4   12.915 FM    8779.70313  1712.29663  0.0855   12.808   13.006


    Signal 3: DAD1 A, Sig=254,4 Ref=off (2018 TO MAR 07\020218\013118_1PF3-PH7-413CBTNAC_3.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]        [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    8.953 FM     152.07585    30.38887  0.0834    8.899    9.024
       2    9.151 FM    1291.37805   203.47014  0.1058    9.024    9.252
       3    9.667 FM    1378.61804   184.58427  0.1245    9.552    9.823
       4   12.773 FM    4896.59473   931.85321  0.0876   12.659   12.874


    Signal 4: DAD1 A, Sig=254,4 Ref=off (2018 TO MAR 07\020218\013118_1PF3-PH7-413CBTNAC_4.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]        [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    8.987 FM     195.99939    38.38641  0.0851    8.929    9.051
       2    9.183 FM    1271.32251   188.63309  0.1123    9.051    9.274
       3    9.686 FM    1673.51196   218.45514  0.1277    9.586    9.832
       4   12.869 MF    1.48578e4   2598.30322  0.0953   12.759   12.964


    Signal 5: DAD1 A, Sig=254,4 Ref=off (2018 TO MAR 07\020218\013118_1PF3-PH7-413CBTNAC_5.D)

    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]        [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    0.980 BB      31.18398  7.66578e-1  0.4986  1.45e-3    1.063
       2    8.969 FM     189.97842    40.02207  0.0791    8.906    9.035
       3    9.164 FM     791.44257   130.94086  0.1007    9.035    9.213
       4    9.670 FM    1595.67419   225.92827  0.1177    9.545    9.782
       5   12.796 FM    7938.74023  1519.81384  0.0871   12.690   12.891
```

```
Print of window 38: Current Chromatogram(s)
Data File  : C:\CHEM32\1\DATA\2018 TO MAR 07\012618\012418_4PF3-PH7-13CBTNAC_1.D
Sample Name : 012218_PF3-ph8-azidoCBTNAc_1
======================================================================
Acq. Operator   : SGLK                             Seq. Line :   6
Acq. Instrument : Instrument 1                      Location : Vial 6
Injection Date  : 1/26/18 5:27:34 PM                     Inj :   1
                                                 Inj Volume : 1.000 µl
Acq. Method     : D:\CHEM32\1\METHODS\AP_C18_INSERT.M
Last changed    : 1/22/18 3:04:38 PM by SGLK
Analysis Method : Z:\DESKTOP\BERTOZZI LAB\LCMS INFO\LCMS METHODS TO 112917\SGLK_BERTOZZIBP_
                  WITHINSERT.M
Last changed    : 3/8/18 8:51:08 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```

Current Chromatogram(s)

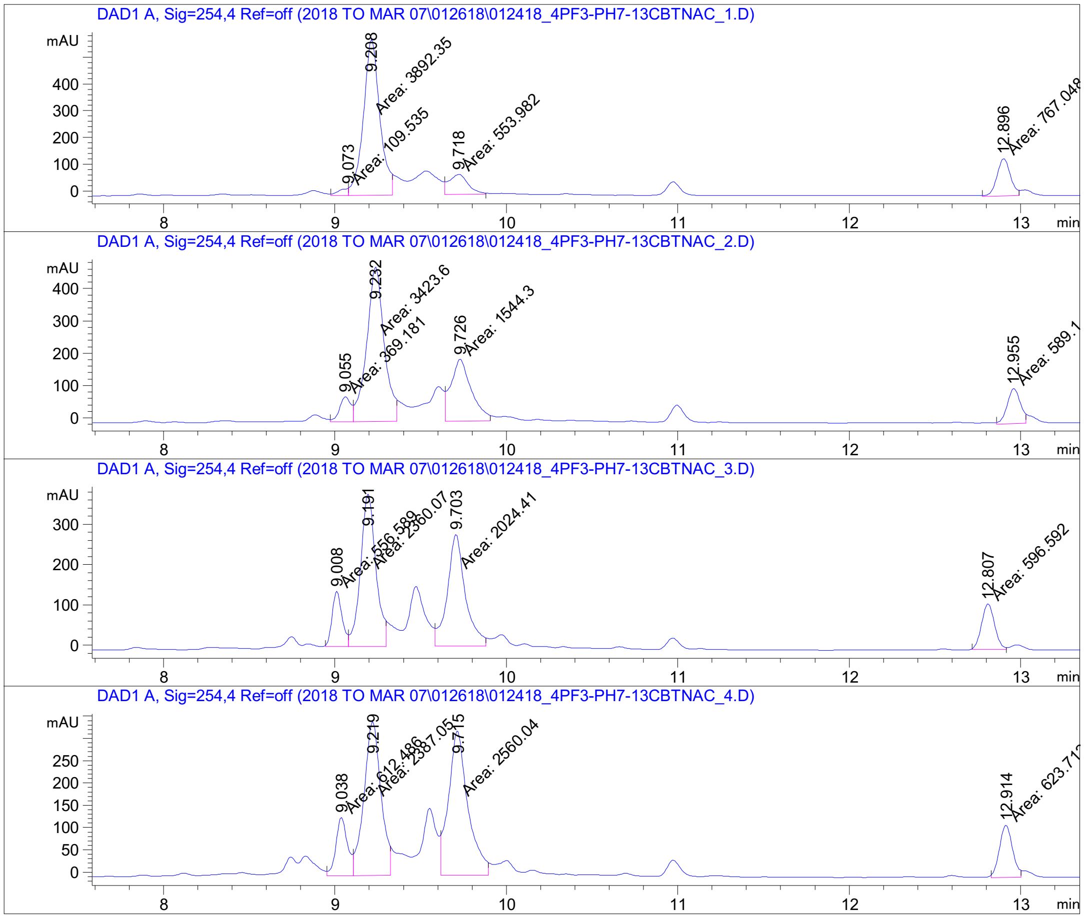


```
Data File C:\CHEM32\1\DATA\2018 TO MAR 07\012618\012418_4PF3-PH7-13CBTNAC_1.D
Sample Name: 012218_PF3-ph8-azidoCBTNAc_1

    =====================================================================
                             Integration Results
    =====================================================================

    Signal 1: DAD1 B, Sig=210,4 Ref=off (2018 TO MAR 07\012618\012418_4PF3-PH7-13CBTNAC_1.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]        [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    7.860 MF    1.84950e4   2050.75513  0.1503    7.720    8.024
       2    8.089 MF    2392.83325   382.49109  0.1043    8.024    8.210
       3    8.870 MF     765.58057    85.67575  0.1489    8.776    8.971
       4    9.060 MF     642.70343   166.08194  0.0645    8.971    9.062
       5    9.208 MF    1.85275e4   2048.39893  0.1507    9.062    9.343
       6    9.715 MF    2025.30261   257.27994  0.1312    9.638    9.885
       7   12.896 MF    1810.43713   333.72260  0.0904   12.793   12.981
       8   17.091 MM    3022.47485   399.32254  0.1262   16.939   17.285


    Signal 2: DAD1 B, Sig=210,4 Ref=off (2018 TO MAR 07\012618\012418_4PF3-PH7-13CBTNAC_2.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]        [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    7.894 FM    2.06262e4   2095.16553  0.1641    7.694    8.040
       2    8.117 FM    2581.28320   382.76730  0.1124    8.040    8.218
       3    9.056 FM    2080.65186   425.99606  0.0814    8.969    9.100
       4    9.232 FM    1.89702e4   2035.62708  0.1553    9.100    9.433
       5    9.726 FM    6051.60547   719.79962  0.1401    9.636    9.945
       6   12.955 MM    1533.16333   254.23740  0.1005   12.864   13.138
       7   17.131 MM    1801.86560   237.32285  0.1265   16.935   17.304
       8   27.940 BBA   1001.94745   111.75077  0.1494   27.807   28.000


    Signal 3: DAD1 B, Sig=210,4 Ref=off (2018 TO MAR 07\012618\012418_4PF3-PH7-13CBTNAC_3.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]        [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    7.386 MF    7936.72314   765.12000  0.1729    7.089    7.572
       2    7.842 MF    1.41918e4   1574.01428  0.1503    7.712    7.979
       3    8.066 MF    2933.36401   388.90378  0.1257    7.979    8.220
       4    9.008 MF    3157.13452   698.73083  0.0753    8.918    9.071
       5    9.190 MF    1.21071e4   1499.39441  0.1346    9.071    9.325
       6    9.704 MF    7429.56299   972.61151  0.1273    9.604    9.896
       7   12.807 MF    1474.88635   268.96881  0.0914   12.678   12.932
       8   17.020 MM    1165.90271   149.83099  0.1297   16.844   17.177
       9   27.049 HH      38.29931     3.93957  0.1554   26.843   27.199
      10   27.931 BBA    964.60730    97.13586  0.1655   27.769   27.996
```

```
Data File C:\CHEM32\1\DATA\2018 TO MAR 07\012618\012418_4PF3-PH7-13CBTNAC_1.D
Sample Name: 012218_PF3-ph8-azidoCBTNAc_1

    Signal 4: DAD1 B, Sig=210,4 Ref=off (2018 TO MAR 07\012618\012418_4PF3-PH7-13CBTNAC_4.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]         [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    7.681 FM    3636.06616  680.77594  0.0890    7.600    7.738
       2    7.881 FM    1.56507e4  1654.62610  0.1576    7.738    8.014
       3    8.118 FM    9029.92383 1248.92078  0.1205    8.014    8.327
       4    9.038 FM    3078.17871  652.84564  0.0786    8.975    9.099
       5    9.219 FM    1.22704e4  1517.02673  0.1348    9.099    9.339
       6    9.714 FM    9018.74121 1109.87085  0.1354    9.616    9.914
       7   12.914 MF    1438.77722  274.10233  0.0875   12.795   12.995
       8   17.100 MM     878.28180  117.26001  0.1248   16.955   17.257
       9   27.939 HBA   5135.85693  416.95944  0.2053   27.132   27.999

    =====================================================================
```

```
Print of window 38: Current Chromatogram(s)
Data File  : C:\CHEM32\1\DATA\2018 TO MAR 07\012618\012418_4PF3-PH7-13CBTNAC_1.D
Sample Name : 012218_PF3-ph8-azidoCBTNAc_1
======================================================================
Acq. Operator    : SGLK                             Seq. Line :    6
Acq. Instrument : Instrument 1                       Location : Vial 6
Injection Date  : 1/26/18 5:27:34 PM                      Inj :    1
                                                   Inj Volume : 1.000 µl
Acq. Method      : D:\CHEM32\1\METHODS\AP_C18_INSERT.M
Last changed     : 1/22/18 3:04:38 PM by SGLK
Analysis Method : Z:\DESKTOP\BERTOZZI LAB\LCMS INFO\LCMS METHODS TO 112917\SGLK_BERTOZZIBP_
                  WITHINSERT.M
Last changed     : 3/8/18 8:51:08 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```

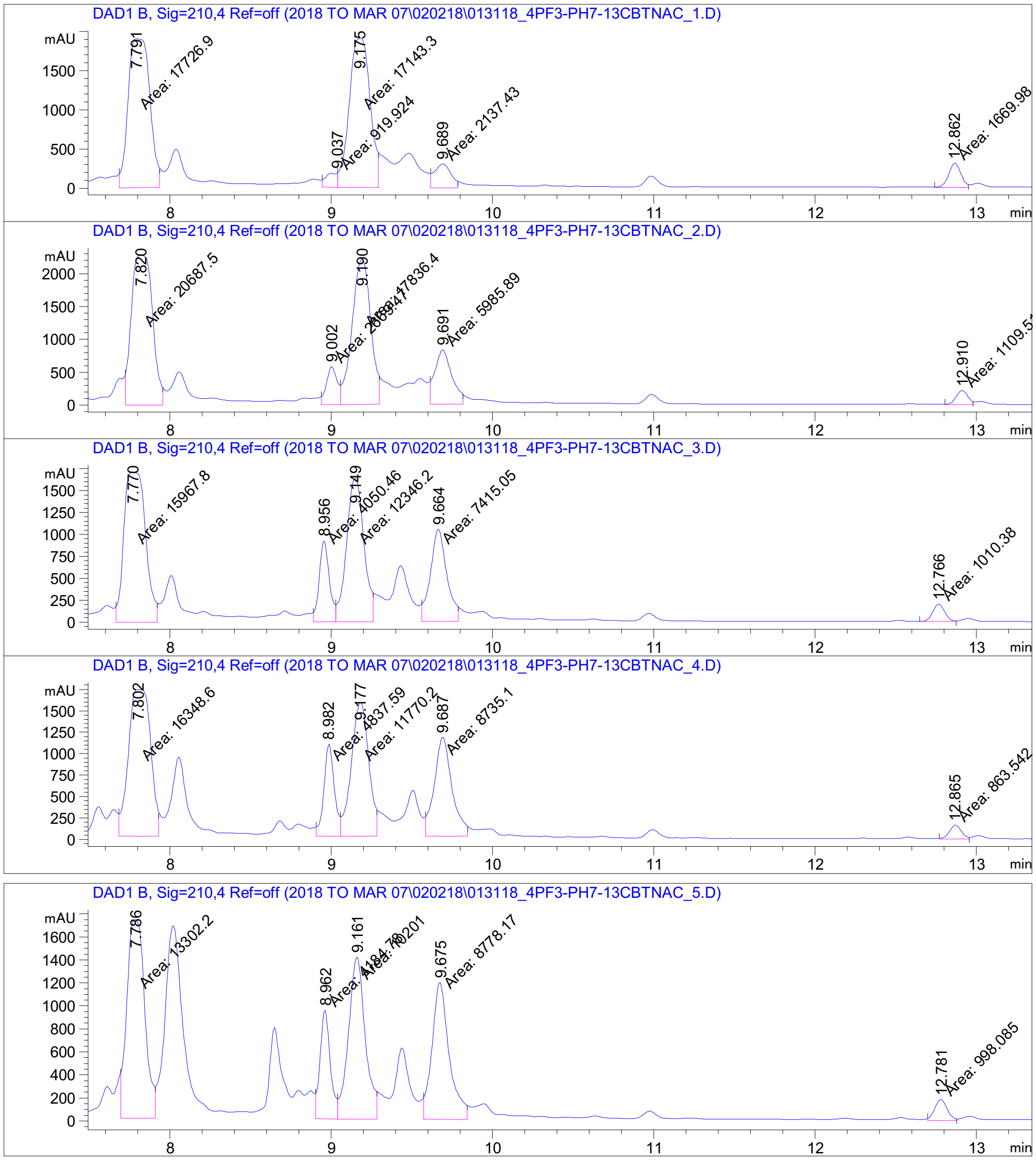
Current Chromatogram(s)



```
Data File C:\CHEM32\1\DATA\2018 TO MAR 07\012618\012418_4PF3-PH7-13CBTNAC_1.D
Sample Name: 012218_PF3-ph8-azidoCBTNAc_1

    =====================================================================
                             Integration Results
    =====================================================================

    Signal 1: DAD1 A, Sig=254,4 Ref=off (2018 TO MAR 07\012618\012418_4PF3-PH7-13CBTNAC_1.D)


    Peak   Time   Type     Area       Height     Width    Start     End
      #    [min]        [mAU*s]       [mAU]      [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    9.073 FM     109.53465    26.67127  0.0684    8.975    9.077
       2    9.208 FM    3892.34985   579.80493  0.1119    9.077    9.332
       3    9.718 FM     553.98206    74.16487  0.1245    9.638    9.879
       4   12.896 MF     767.04785   139.52420  0.0916   12.774   12.987


    Signal 2: DAD1 A, Sig=254,4 Ref=off (2018 TO MAR 07\012618\012418_4PF3-PH7-13CBTNAC_2.D)


    Peak   Time   Type     Area       Height     Width    Start     End
      #    [min]        [mAU*s]       [mAU]      [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    9.055 FM     369.18109    77.76151  0.0791    8.970    9.104
       2    9.232 FM    3423.59888   478.64450  0.1192    9.104    9.360
       3    9.726 FM    1544.29590   191.12616  0.1347    9.642    9.902
       4   12.955 MF     589.09991   108.67957  0.0903   12.857   13.029


    Signal 3: DAD1 A, Sig=254,4 Ref=off (2018 TO MAR 07\012618\012418_4PF3-PH7-13CBTNAC_3.D)


    Peak   Time   Type     Area       Height     Width    Start     End
      #    [min]        [mAU*s]       [mAU]      [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    9.008 MF     556.58862   136.95667  0.0677    8.942    9.077
       2    9.191 FM    2360.06812   378.14111  0.1040    9.077    9.295
       3    9.703 FM    2024.40527   277.56799  0.1216    9.582    9.879
       4   12.807 MF     596.59241   112.93456  0.0880   12.713   12.913


    Signal 4: DAD1 A, Sig=254,4 Ref=off (2018 TO MAR 07\012618\012418_4PF3-PH7-13CBTNAC_4.D)


    Peak   Time   Type     Area       Height     Width    Start     End
      #    [min]        [mAU*s]       [mAU]      [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    9.038 FM     612.48633   130.93390  0.0780    8.951    9.104
       2    9.219 FM    2387.05029   345.88968  0.1150    9.104    9.322
       3    9.715 FM    2560.03564   324.88141  0.1313    9.615    9.893
       4   12.914 MF     623.71161   117.50446  0.0885   12.825   13.001

    =====================================================================


Instrument 1 3/8/18 9:04:12 AM                                              Page   1 of 1
```

```
Print of window 38: Current Chromatogram(s)
Data File  : C:\CHEM32\1\DATA\2018 TO MAR 07\020218\013118_4PF3-PH7-13CBTNAC_1.D
Sample Name : 013118_4PF3-ph7-13CBTNAc_1
======================================================================
Acq. Operator   : SGLK                           Seq. Line :    6
Acq. Instrument : Instrument 1                    Location : Vial 6
Injection Date  : 2/2/18 7:16:34 PM                    Inj :    1
                                                Inj Volume : 1.000 µl
Acq. Method     : D:\CHEM32\1\METHODS\AP_C18_INSERT.M
Last changed    : 1/22/18 3:04:38 PM by SGLK
Analysis Method : Z:\DESKTOP\BERTOZZI LAB\LCMS INFO\LCMS METHODS TO 112917\SGLK_BERTOZZIBP_
                  WITHINSERT.M
Last changed    : 3/8/18 8:51:08 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```

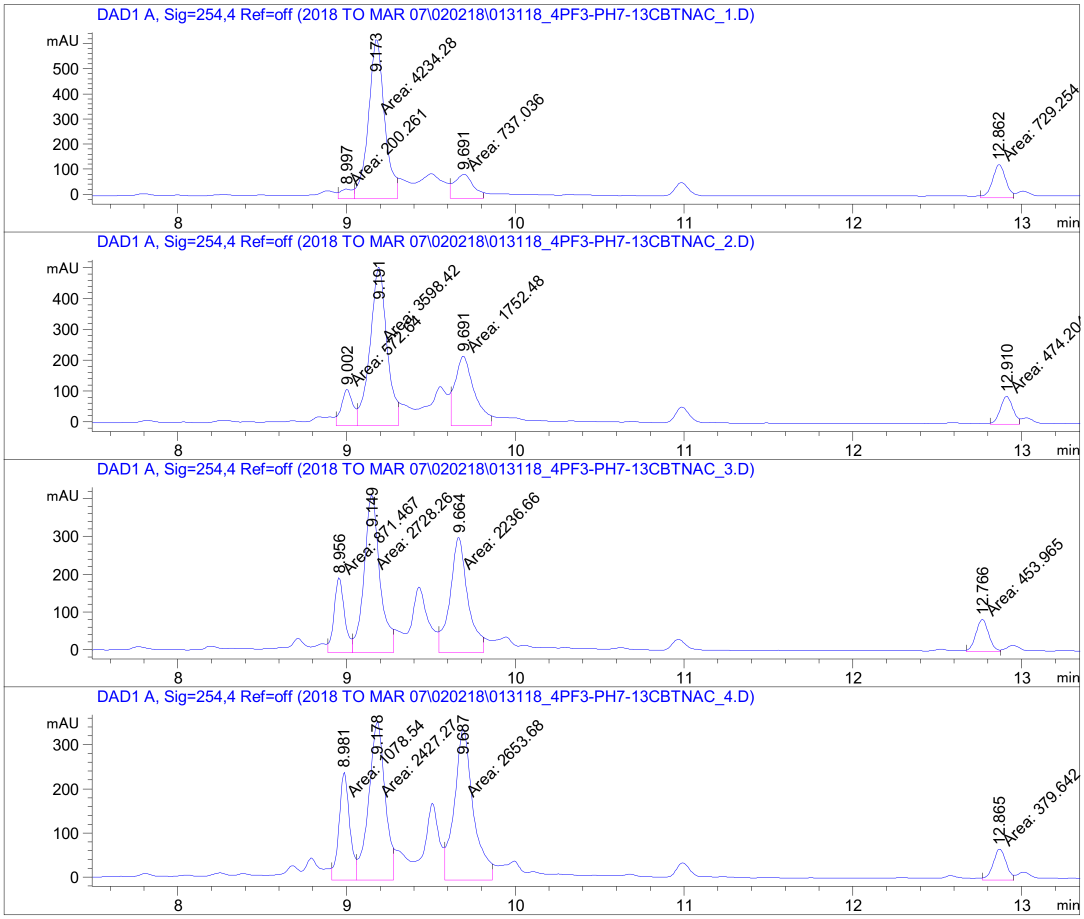
Current Chromatogram(s)

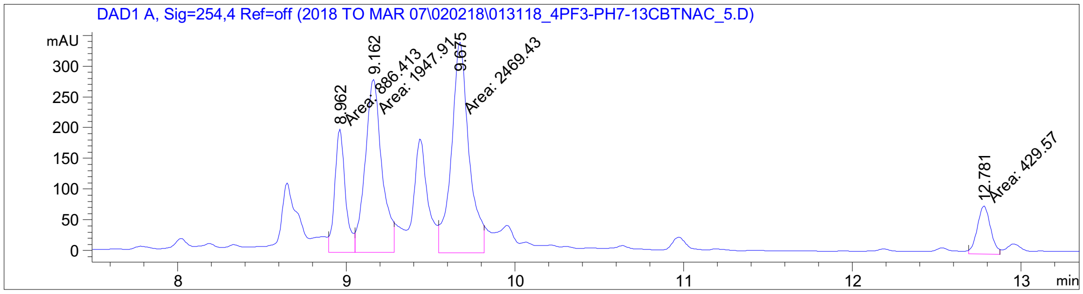


```
Data File C:\CHEM32\1\DATA\2018 TO MAR 07\020218\013118_4PF3-PH7-13CBTNAC_1.D
Sample Name: 013118_4PF3-ph7-13CBTNAc_1

    =====================================================================
                             Integration Results
    =====================================================================

    Signal 1: DAD1 B, Sig=210,4 Ref=off (2018 TO MAR 07\020218\013118_4PF3-PH7-13CBTNAC_1.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]        [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    7.791 FM    1.77269e4   1896.11926  0.1558    7.684    7.935
       2    9.037 FM     919.92407   184.64258  0.0830    8.943    9.039
       3    9.175 FM    1.71433e4   1902.55383  0.1502    9.039    9.290
       4    9.689 FM    2137.42554   306.13031  0.1164    9.615    9.783
       5   12.862 MF    1669.97876   311.27527  0.0894   12.740   12.947


    Signal 2: DAD1 B, Sig=210,4 Ref=off (2018 TO MAR 07\020218\013118_4PF3-PH7-13CBTNAC_2.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]        [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    7.820 MF    2.06875e4   2273.26367  0.1517    7.722    7.955
       2    9.002 MF    2669.47339   576.34473  0.0772    8.938    9.056
       3    9.190 MF    1.78364e4   2205.12256  0.1348    9.056    9.297
       4    9.691 MF    5985.88770   826.99255  0.1206    9.614    9.815
       5   12.910 MF    1109.50574   216.23482  0.0855   12.802   12.978


    Signal 3: DAD1 B, Sig=210,4 Ref=off (2018 TO MAR 07\020218\013118_4PF3-PH7-13CBTNAC_3.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]        [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    7.770 MF    1.59678e4   1708.92773  0.1557    7.666    7.921
       2    8.956 MF    4050.46216   925.19824  0.0730    8.888    9.028
       3    9.149 MF    1.23462e4   1635.00671  0.1259    9.028    9.260
       4    9.664 MF    7415.04932  1055.82605  0.1170    9.561    9.787
       5   12.766 MF    1010.38171   196.10500  0.0859   12.645   12.871


    Signal 4: DAD1 B, Sig=210,4 Ref=off (2018 TO MAR 07\020218\013118_4PF3-PH7-13CBTNAC_4.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]        [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    7.802 FM    1.63486e4   1706.57397  0.1597    7.682    7.930
       2    8.982 FM    4837.59375  1077.47766  0.0748    8.907    9.056
       3    9.177 FM    1.17702e4   1562.65039  0.1255    9.056    9.282
       4    9.687 FM    8735.09570  1156.13318  0.1259    9.583    9.843
       5   12.865 FM     863.54230   162.56932  0.0885   12.768   12.954


    Signal 5: DAD1 B, Sig=210,4 Ref=off (2018 TO MAR 07\020218\013118_4PF3-PH7-13CBTNAC_5.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]        [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    7.786 MF    1.33022e4   1725.83533  0.1285    7.694    7.908
       2    8.962 MF    4184.78467   947.06653  0.0736    8.904    9.040
       3    9.161 MF    1.02010e4   1408.12524  0.1207    9.040    9.282
       4    9.675 MF    8778.17090  1192.27075  0.1227    9.573    9.840
       5   12.781 MF     998.08514   184.60497  0.0901   12.695   12.875
```

```
Print of window 38: Current Chromatogram(s)
Data File  : C:\CHEM32\1\DATA\2018 TO MAR 07\020218\013118_4PF3-PH7-13CBTNAC_1.D
Sample Name : 013118_4PF3-ph7-13CBTNAc_1
======================================================================
Acq. Operator   : SGLK                          Seq. Line :   6
Acq. Instrument : Instrument 1                   Location : Vial 6
Injection Date  : 2/2/18 7:16:34 PM                   Inj :   1
                                               Inj Volume : 1.000 µl
Acq. Method     : D:\CHEM32\1\METHODS\AP_C18_INSERT.M
Last changed    : 1/22/18 3:04:38 PM by SGLK
Analysis Method : Z:\DESKTOP\BERTOZZI LAB\LCMS INFO\LCMS METHODS TO 112917\SGLK_BERTOZZIBP_
                  WITHINSERT.M
Last changed    : 3/8/18 8:51:08 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```

Current Chromatogram(s)





```
Data File C:\CHEM32\1\DATA\2018 TO MAR 07\020218\013118_4PF3-PH7-13CBTNAC_1.D
Sample Name: 013118_4PF3-ph7-13CBTNAc_1

    =====================================================================
                             Integration Results
    =====================================================================

    Signal 1: DAD1 A, Sig=254,4 Ref=off (2018 TO MAR 07\020218\013118_4PF3-PH7-13CBTNAC_1.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]         [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    8.997 MF     200.26137    38.45741  0.0868    8.950    9.045
       2    9.173 MF    4234.27588   634.43121  0.1112    9.045    9.299
       3    9.691 MF     737.03558    96.44783  0.1274    9.614    9.811
       4   12.862 MF     729.25427   132.65248  0.0916   12.754   12.951


    Signal 2: DAD1 A, Sig=254,4 Ref=off (2018 TO MAR 07\020218\013118_4PF3-PH7-13CBTNAC_2.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]         [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    9.002 FM     572.63983   118.38261  0.0806    8.938    9.062
       2    9.191 FM    3598.41650   516.68695  0.1161    9.062    9.304
       3    9.691 FM    1752.47876   226.24167  0.1291    9.619    9.856
       4   12.910 MF     474.20395    90.58943  0.0872   12.811   12.985


    Signal 3: DAD1 A, Sig=254,4 Ref=off (2018 TO MAR 07\020218\013118_4PF3-PH7-13CBTNAC_3.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]         [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    8.956 FM     871.46686   199.60472  0.0728    8.888    9.034
       2    9.149 FM    2728.26025   419.56812  0.1084    9.034    9.276
       3    9.664 FM    2236.65991   306.16095  0.1218    9.546    9.811
       4   12.766 FM     453.96454    85.18710  0.0888   12.670   12.873


    Signal 4: DAD1 A, Sig=254,4 Ref=off (2018 TO MAR 07\020218\013118_4PF3-PH7-13CBTNAC_4.D)


    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]         [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    8.981 FM    1078.54163   244.56328  0.0735    8.910    9.057
       2    9.178 FM    2427.26831   358.23096  0.1129    9.057    9.276
       3    9.687 FM    2653.67725   342.92633  0.1290    9.580    9.861
       4   12.865 FM     379.64224    70.02226  0.0904   12.766   12.951


    Signal 5: DAD1 A, Sig=254,4 Ref=off (2018 TO MAR 07\020218\013118_4PF3-PH7-13CBTNAC_5.D)
    Peak   Time   Type     Area       Height    Width    Start     End
      #    [min]         [mAU*s]       [mAU]     [min]    [min]    [min]
    ----|--------|----|-----------|-----------|-------|--------|--------|
       1    8.962 MF     886.41290   200.69423  0.0736    8.893    9.051
       2    9.162 MF    1947.91333   281.73981  0.1152    9.051    9.282
       3    9.675 MF    2469.42773   342.71152  0.1201    9.546    9.816
       4   12.781 MF     429.56952    78.42221  0.0913   12.687   12.873
```

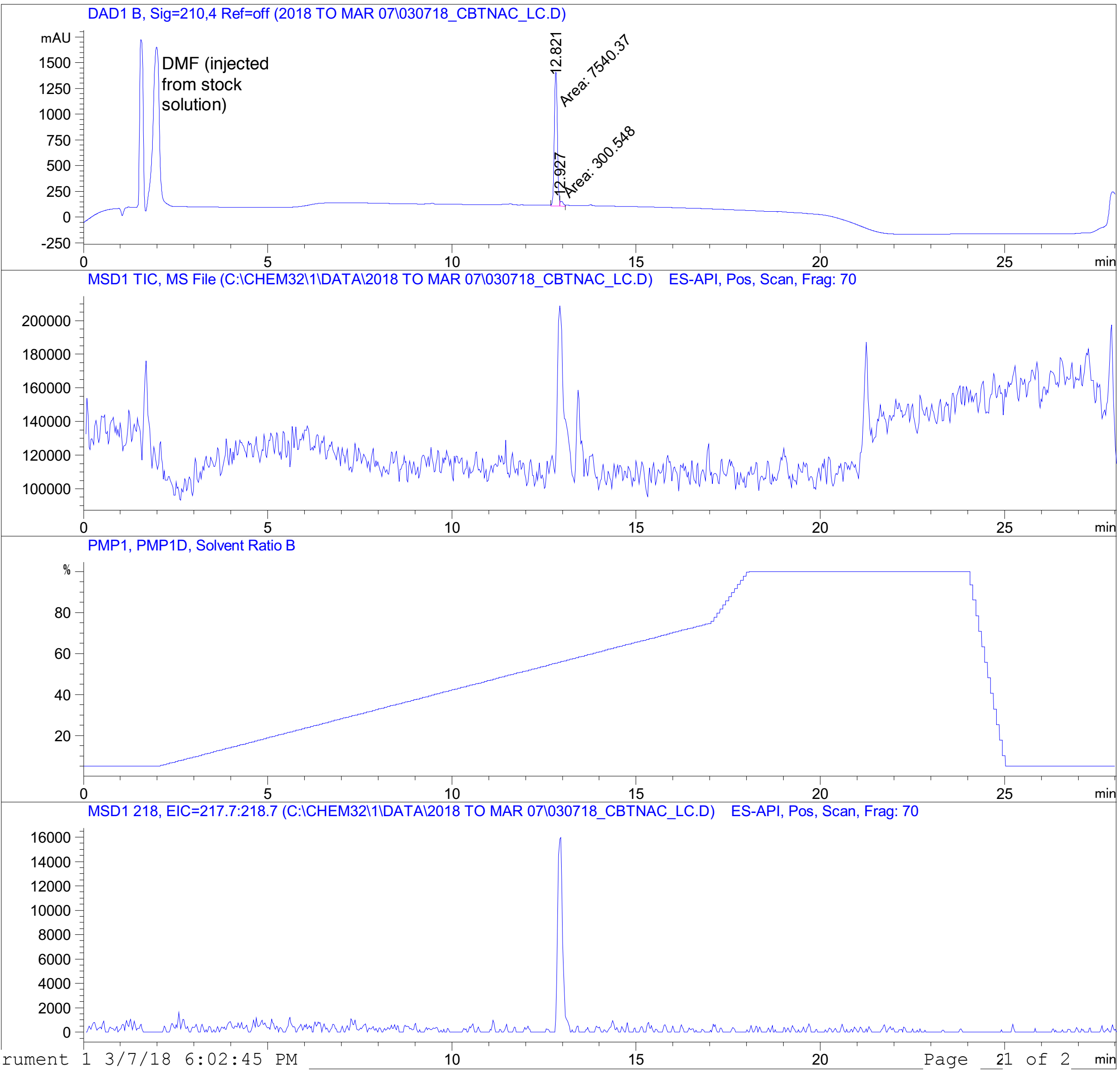
LC-MS spectra (compound purity)

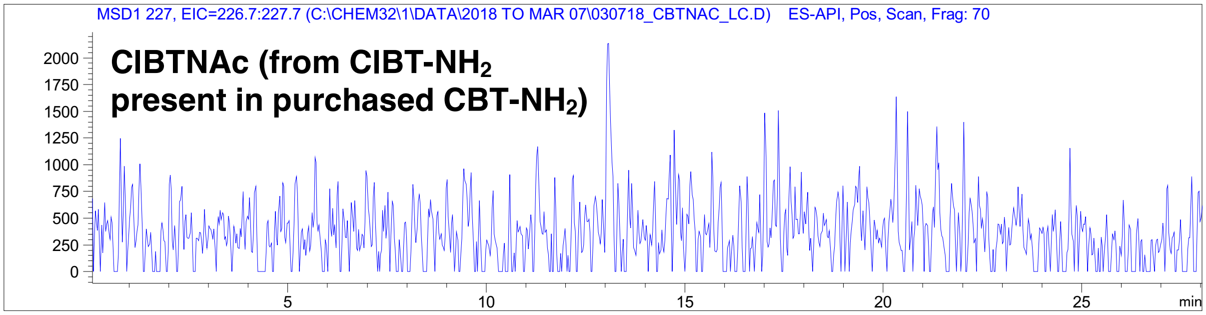
All extracted mass ions correspond to $[M + H]^+$ or $[M – H]^-$ for the given compound unless labeled otherwise.

S63-S64	CBTNAc (**1**)
S65-S66	ClBTNAc (**2**)
S67-S68	13CBTNAc (**3**)
S69-S70	CBTag 1.0 (**4**)
S71-S72	PEP-FOLD-4 (**5**)
S73	Blank (no injection) – background noise (MS+) in spectra for compounds 6-21
S74-S105	PEP-FOLD-1, -2, -5, -6, -7, -8, -9, -11, -12, -13, -14, -15, -16, -17, -18, -19 (**6-21**)
S106-S107	CBTag 1.0 (K9R) (**22**)
S108-S109	CBTag 1.0 (C7S) (**23**)
S110-S111	CBTag 1.0-13CBTNAc (amidine) (**24**)

CBTNAc (1)

```
Data File C:\CHEM32\1\DATA\2018 TO MAR 07\030718_CBTNAC_LC.D
Sample Name: 030718_CBTNAc_LC

    =====================================================================
    Acq. Operator   : SGLK                           Seq. Line :   5
    Acq. Instrument : Instrument 1                    Location : Vial 13
    Injection Date  : 3/7/18 3:16:46 PM                    Inj :   1
                                                    Inj Volume : 1.000 µl
    Different Inj Volume from Sequence !     Actual Inj Volume : 5.000 µl
    Acq. Method     : D:\CHEM32\1\METHODS\AP_C18_INSERT.M
    Last changed    : 3/2/18 3:32:17 PM by CLM
    Analysis Method : Z:\DESKTOP\BERTOZZI LAB\LCMS INFO\LCMS METHODS TO 112917\SGLK_BERTOZZIBP_
                      WITHINSERT.M
    Last changed    : 3/6/18 6:13:20 PM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

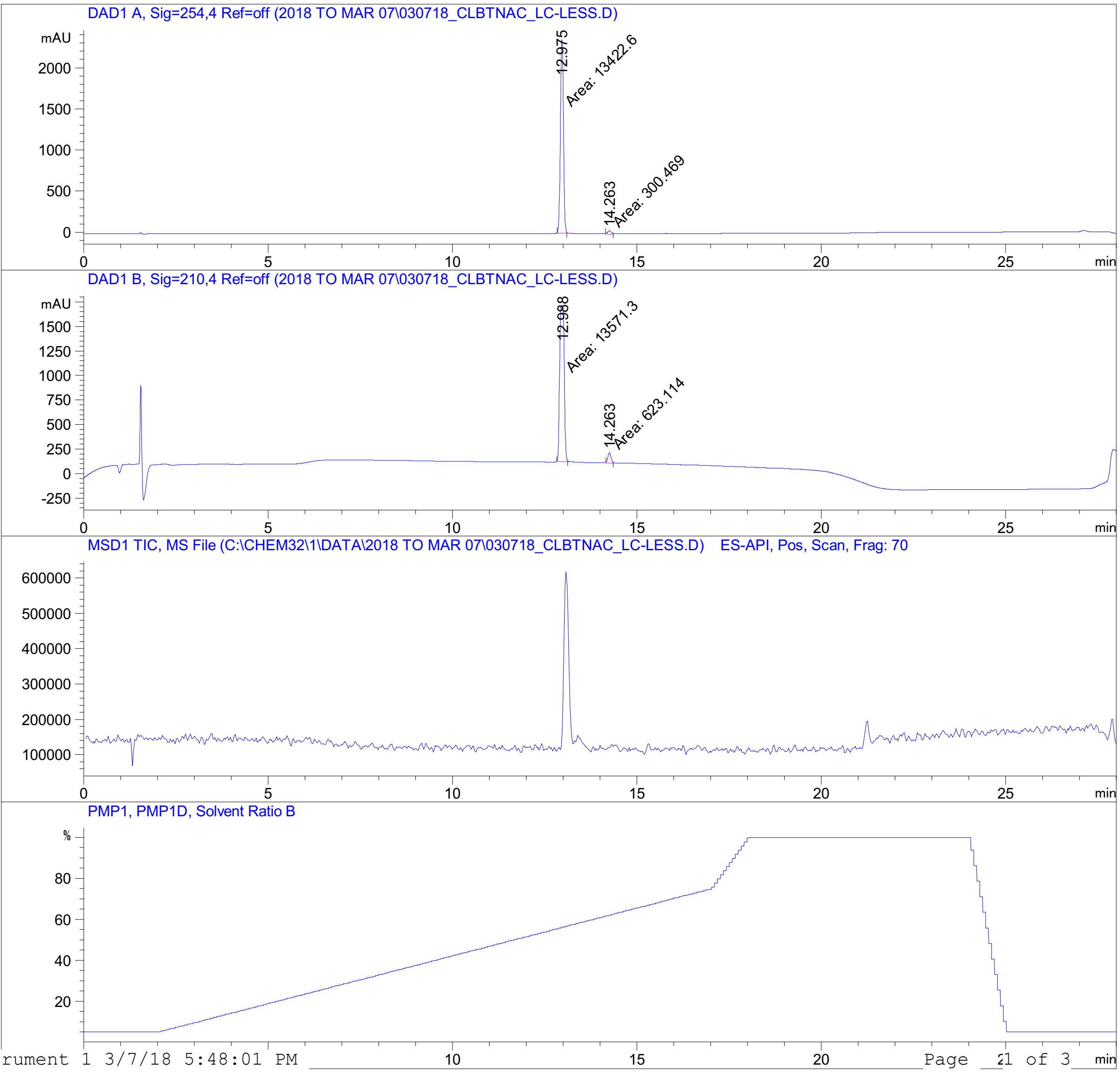


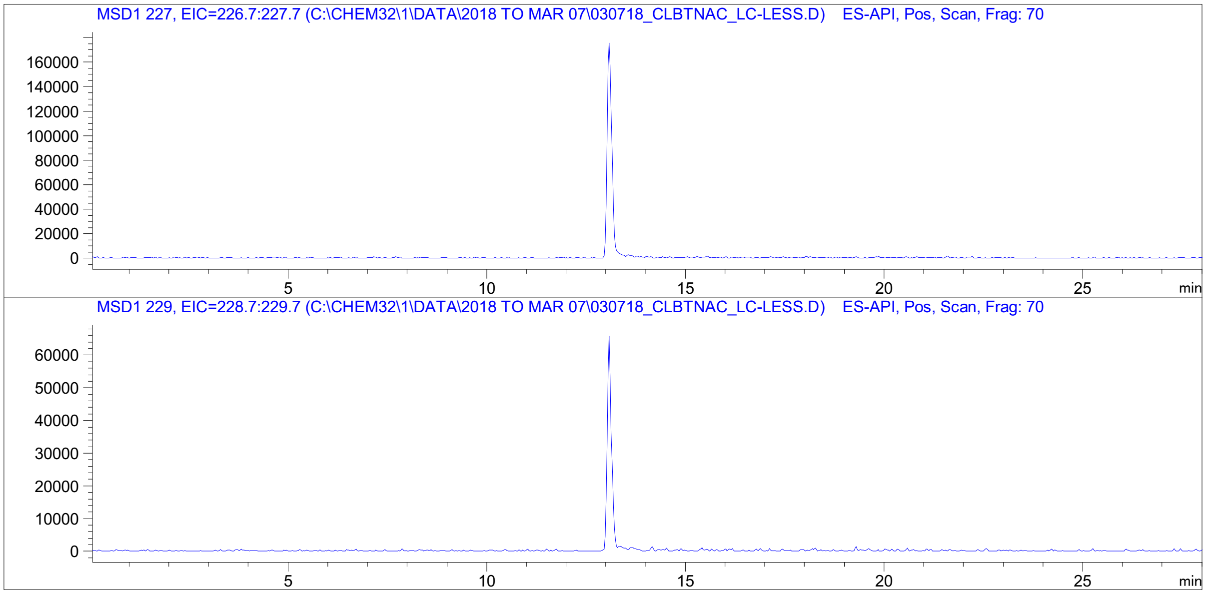


```
=====================================================================
                         Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 B, Sig=210,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]        %
----|-------|----|-------|----------|----------|--------|
   1  12.821 MF    0.0964 7540.36719 1303.94641  96.1669
   2  12.927 FM    0.0870  300.54807   49.86433   3.8331

Totals :                  7840.91525 1353.81074



Signal 2: MSD1 TIC, MS File

=====================================================================
                          *** End of Report ***
```

ClBTNAc (2)

```
Data File C:\CHEM32\1\DATA\2018 TO MAR 07\030718_CLBTNAC_LC-LESS.D
Sample Name: 030718_ClBTNAc_LC-less

    =====================================================================
    Acq. Operator   : SGLK                              Seq. Line :   4
    Acq. Instrument : Instrument 1                       Location : Vial 11
    Injection Date  : 3/7/18 2:47:36 PM                       Inj :   1
                                                       Inj Volume : 1.000 µl
    Different Inj Volume from Sequence !      Actual Inj Volume : 5.000 µl
    Acq. Method     : D:\CHEM32\1\METHODS\AP_C18_INSERT.M
    Last changed    : 3/2/18 3:32:17 PM by CLM
    Analysis Method : Z:\DESKTOP\BERTOZZI LAB\LCMS INFO\LCMS METHODS TO 112917\SGLK_BERTOZZIBP_
                      WITHINSERT.M
    Last changed    : 3/6/18 6:13:20 PM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

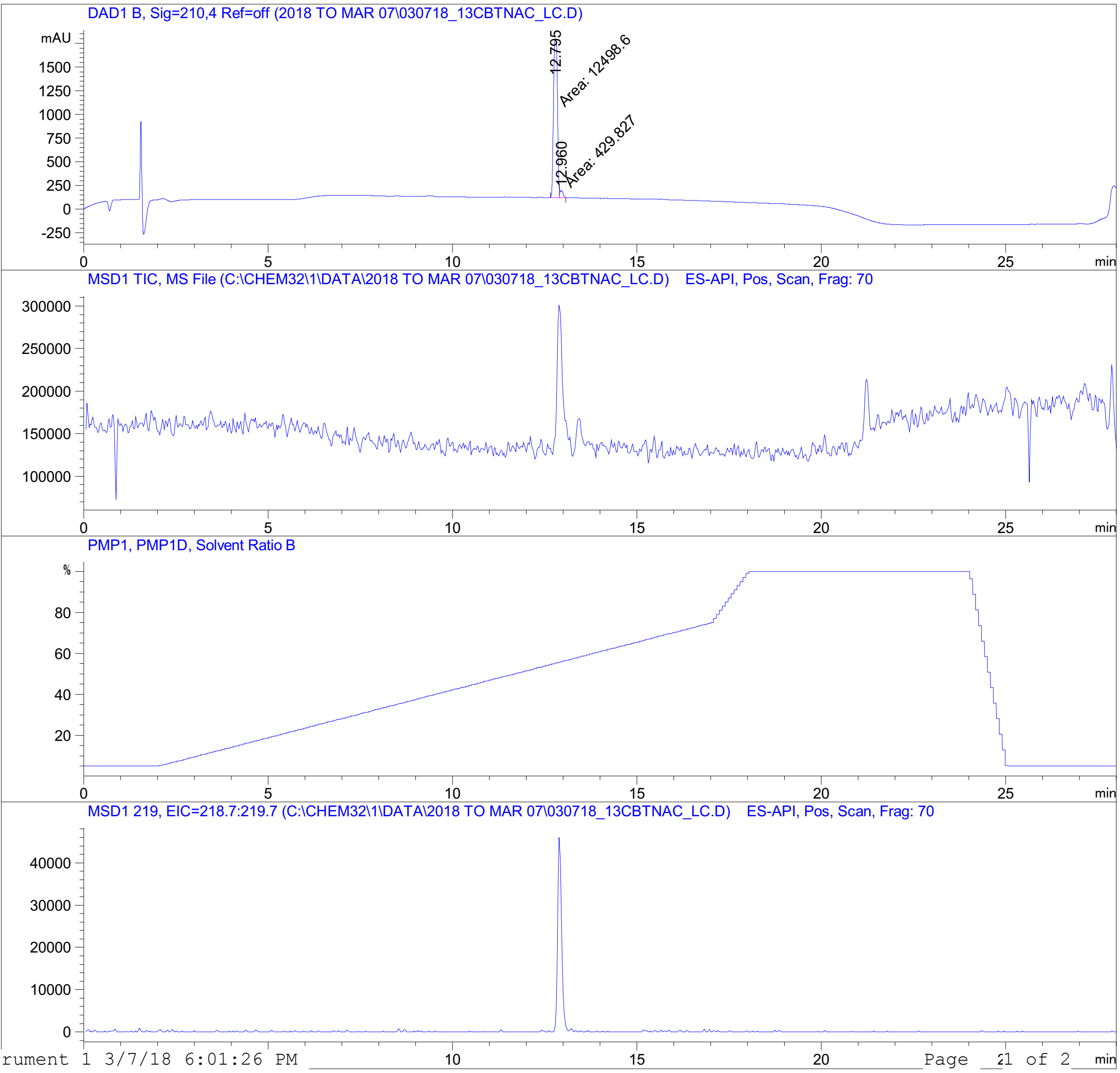


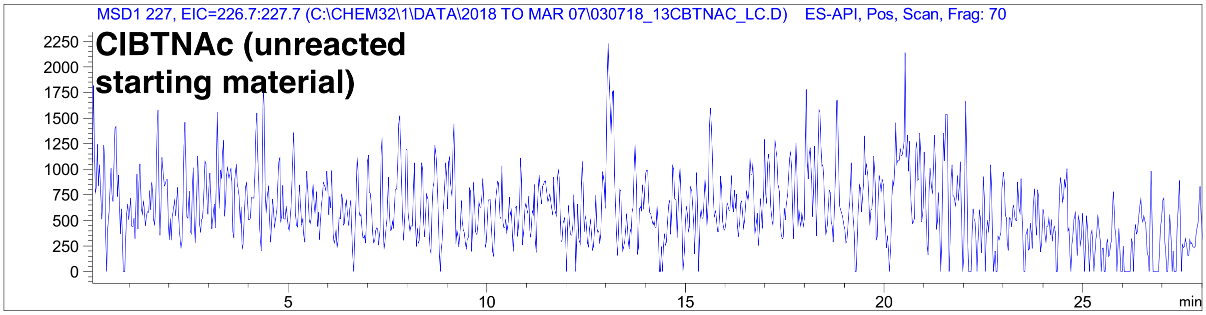


```
=====================================================================
                         Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #    [min]        [min]    [mAU*s]     [mAU]        %
----|-------|----|-------|----------|----------|--------|
   1  12.975 MM    0.0949 1.34226e4  2356.18262  97.8105
   2  14.263 MM    0.1172  300.46902   42.71576   2.1895

Totals :                  1.37231e4  2398.89838

Signal 2: DAD1 B, Sig=210,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #    [min]        [min]    [mAU*s]     [mAU]        %
----|-------|----|-------|----------|----------|--------|
   1  12.988 MM    0.1422 1.35713e4  1591.18579  95.6102
   2  14.263 MM    0.0988  623.11401  105.09184   4.3898

Totals :                  1.41944e4  1696.27763

Signal 3: MSD1 TIC, MS File
```

13CBTNAc (3)

```
Data File C:\CHEM32\1\DATA\2018 TO MAR 07\030718_13CBTNAC_LC.D
Sample Name: 030718_13CBTNAc_LC

    =====================================================================
    Acq. Operator   : SGLK                                Seq. Line :   2
    Acq. Instrument : Instrument 1                         Location : Vial 12
    Injection Date  : 3/7/18 1:49:08 PM                         Inj :   1
                                                         Inj Volume : 1.000 µl
    Different Inj Volume from Sequence !      Actual Inj Volume : 5.000 µl
    Acq. Method     : D:\CHEM32\1\METHODS\AP_C18_INSERT.M
    Last changed    : 3/2/18 3:32:17 PM by CLM
    Analysis Method : Z:\DESKTOP\BERTOZZI LAB\LCMS INFO\LCMS METHODS TO 112917\SGLK_BERTOZZIBP_
                      WITHINSERT.M
    Last changed    : 3/6/18 6:13:20 PM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```



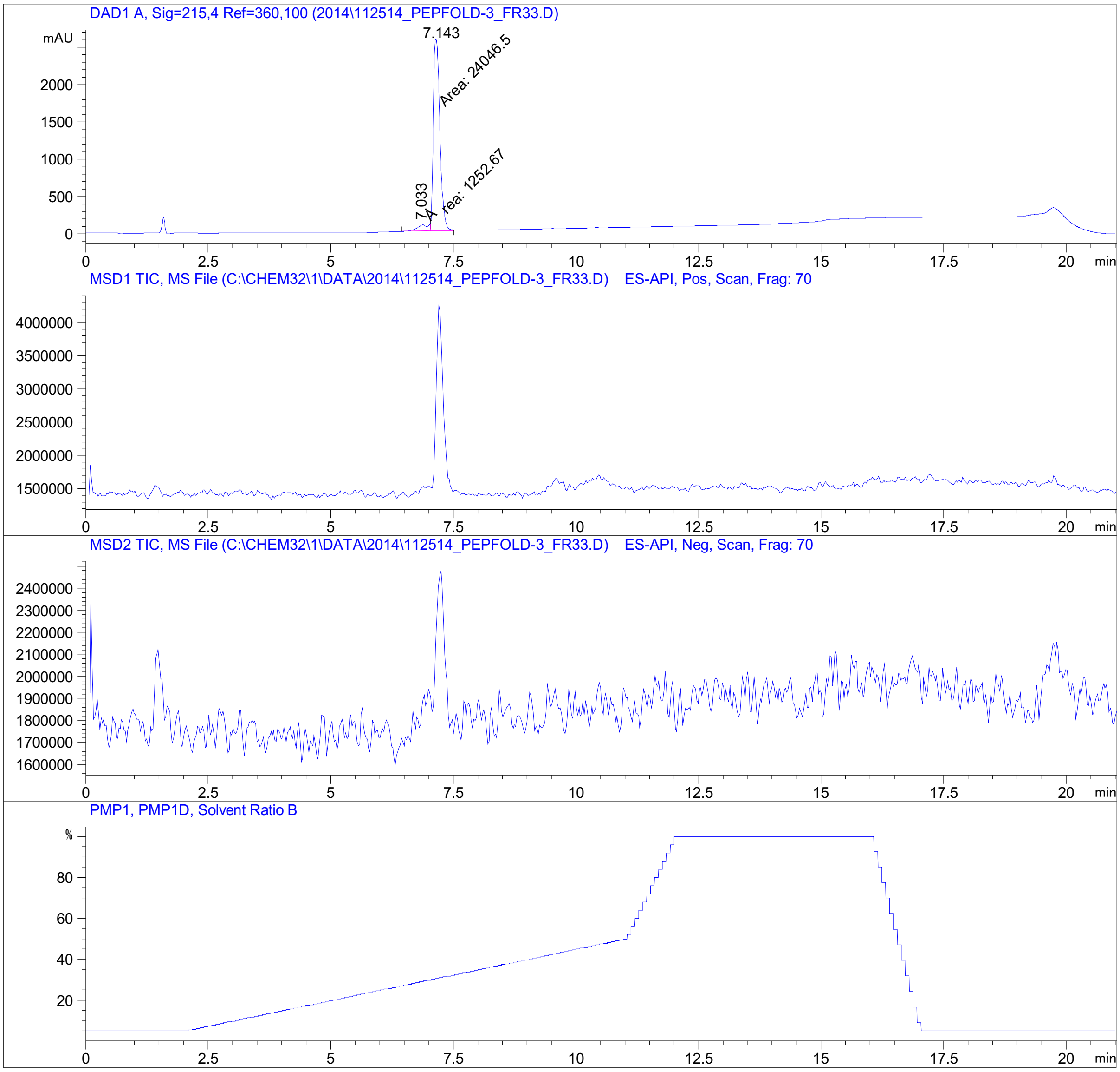


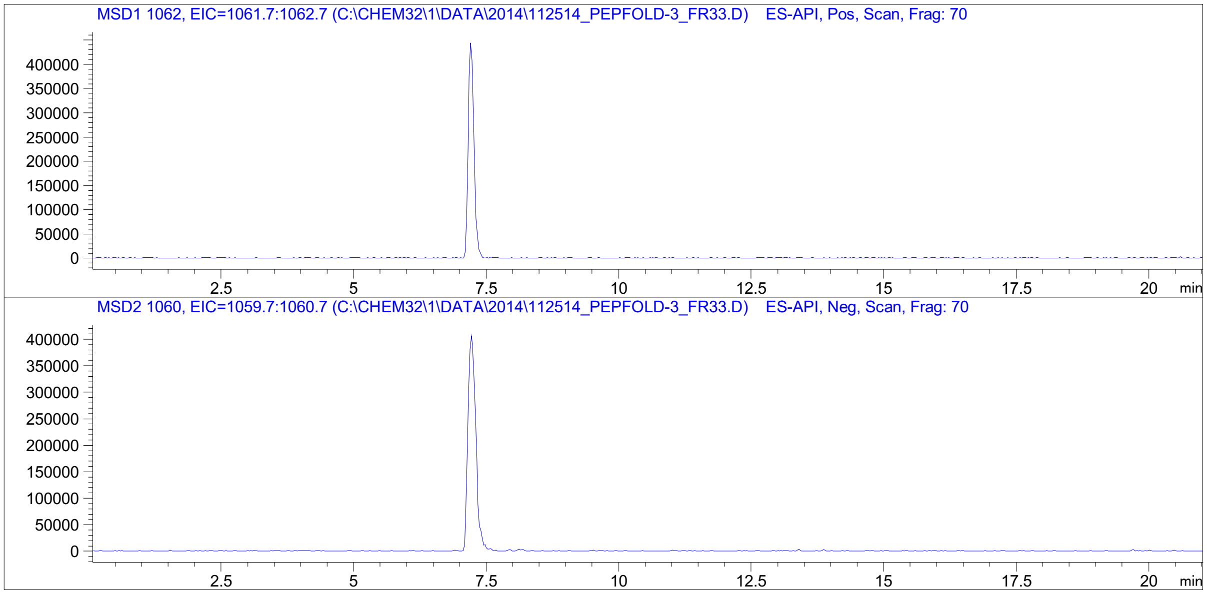
ClBTNAc (unreacted starting material)

```
=====================================================================
                         Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 B, Sig=210,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]        %
----|-------|----|-------|----------|----------|--------|
   1  12.795 MF    0.1249 1.24986e4  1667.93628  96.6753
   2  12.960 FM    0.0927  429.82697   77.28518   3.3247

Totals :                  1.29285e4  1745.22146



Signal 2: MSD1 TIC, MS File

=====================================================================
                          *** End of Report ***
```

CBTag 1.0, Ac-GGHPDPCPKGG-NH$_2$ **(4)**

```
Acq. Method : D:\CHEM32\1\METHODS\SGLK_BERTOZZILC_PEP
Inj Volume : 25.000 µl
Additional Info : Peak(s) manually integrated
```

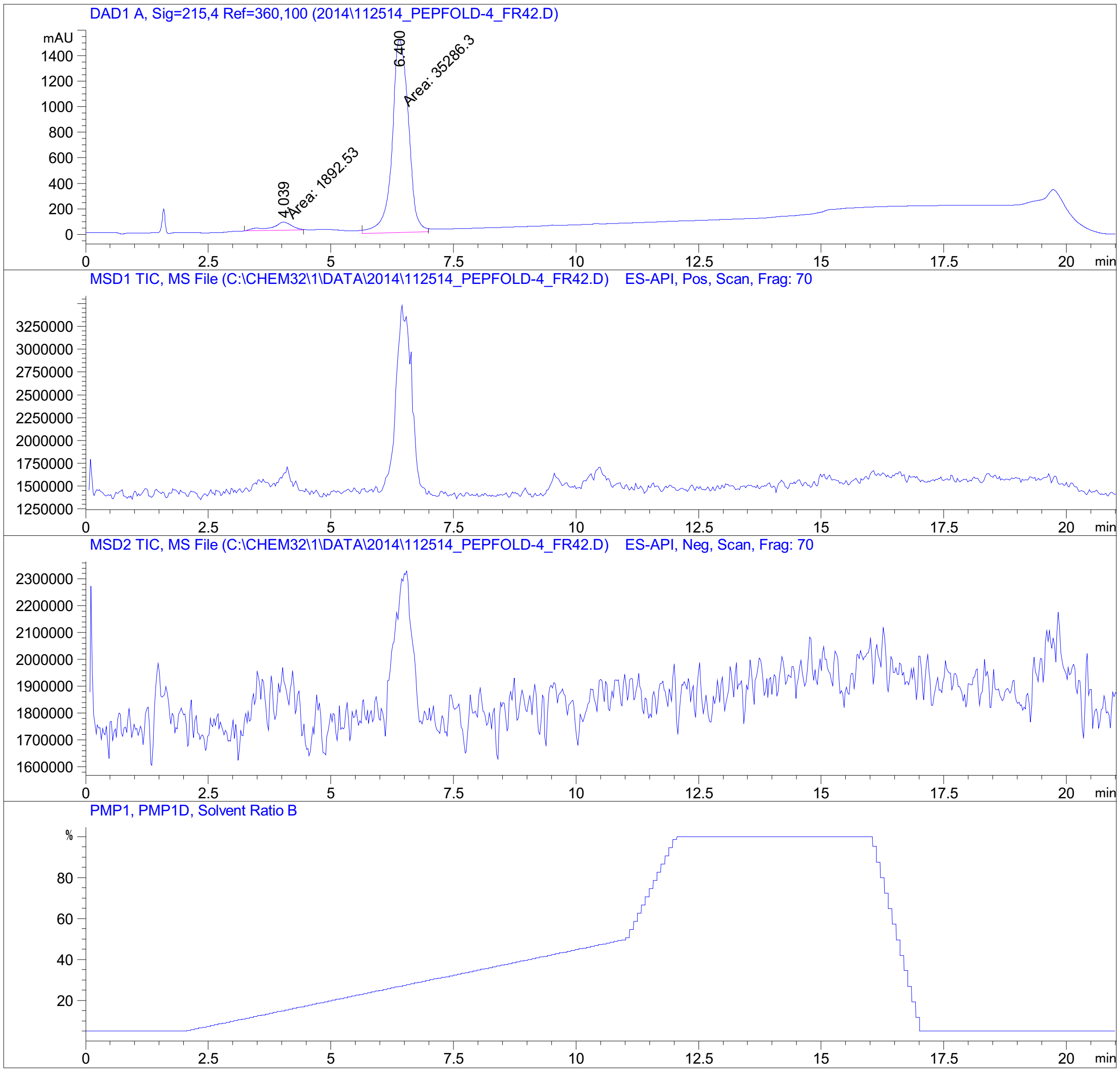


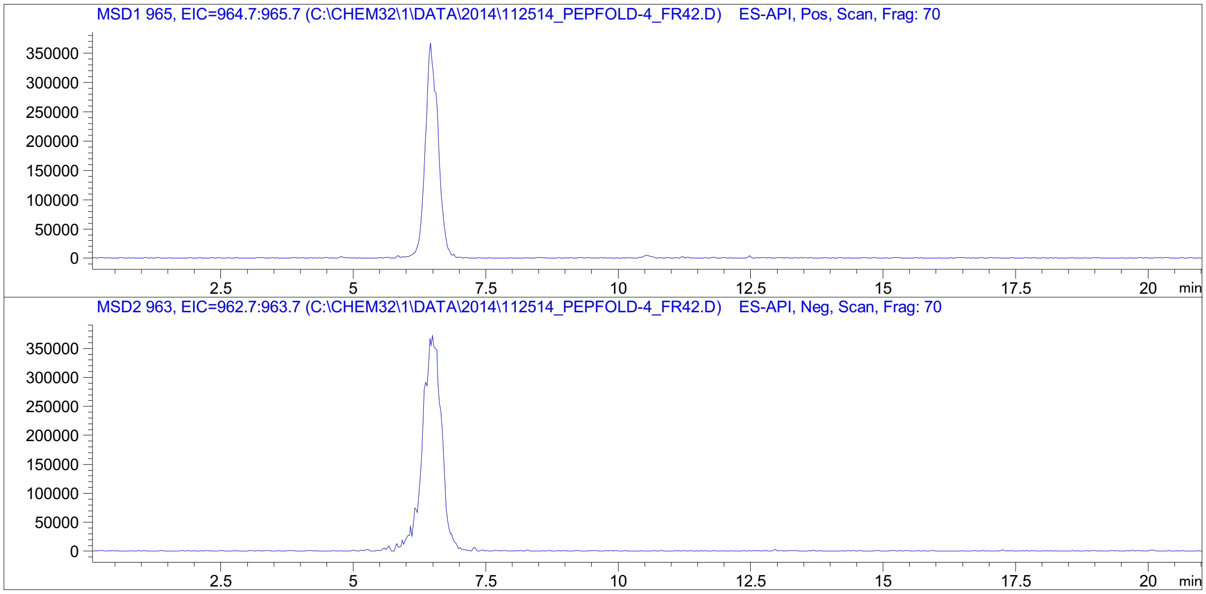


```
=====================================================================
                         Area Percent Report
=====================================================================

Signal 1: DAD1 A, Sig=215,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]        %
----|-------|----|-------|----------|----------|--------|
   1   7.033 MF    0.2265 1252.66980   92.18911   4.9514
   2   7.143 FM    0.1564 2.40465e4  2562.40234  95.0486

Totals :                  2.52992e4  2654.59145
```

PEP-FOLD-4, Ac-GGDPHPCKGG-NH$_2$ **(5)**

```
Data File C:\CHEM32\1\DATA\2014\112514_PEPFOLD-4_FR42.D
Sample Name: 112514_PEPFOLD-4_fr42

    =====================================================================
    Acq. Operator   : EM                               Seq. Line :   4
    Acq. Instrument : Instrument 1                      Location : Vial 77
    Injection Date  : 11/25/14 4:55:14 PM                    Inj :   1
                                                      Inj Volume : 25.000 µl
    Acq. Method     : D:\CHEM32\1\METHODS\SGLK_BERTOZZILC_PEP
    Last changed    : 11/25/14 3:41:49 PM by EM
    Analysis Method : Z:\DESKTOP\BERTOZZI LAB\LCMS INFO\LCMS METHODS TO 112917\SGLK_BERTOZZIBP_
                      WITHINSERT.M
    Last changed    : 2/7/18 7:43:15 PM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

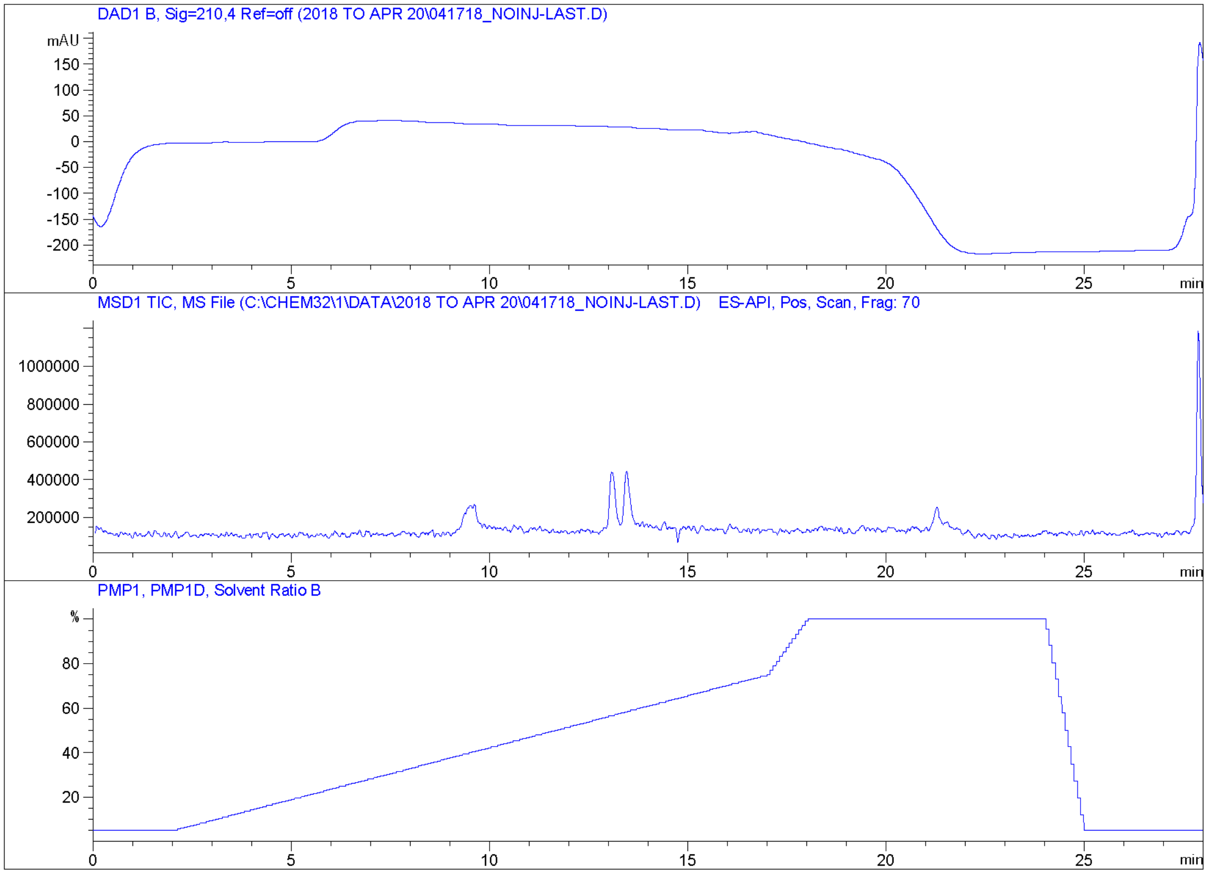




```
=====================================================================
                         Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                    :      1.0000
Dilution:                      :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=215,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]        %
----|-------|----|-------|----------|----------|--------|
   1   4.039 MM    0.4972 1892.52612   63.43561   5.0903
   2   6.400 MM    0.3892 3.52863e4  1511.20435  94.9097

Totals :                  3.71788e4  1574.63995



Signal 2: MSD1 TIC, MS File
```

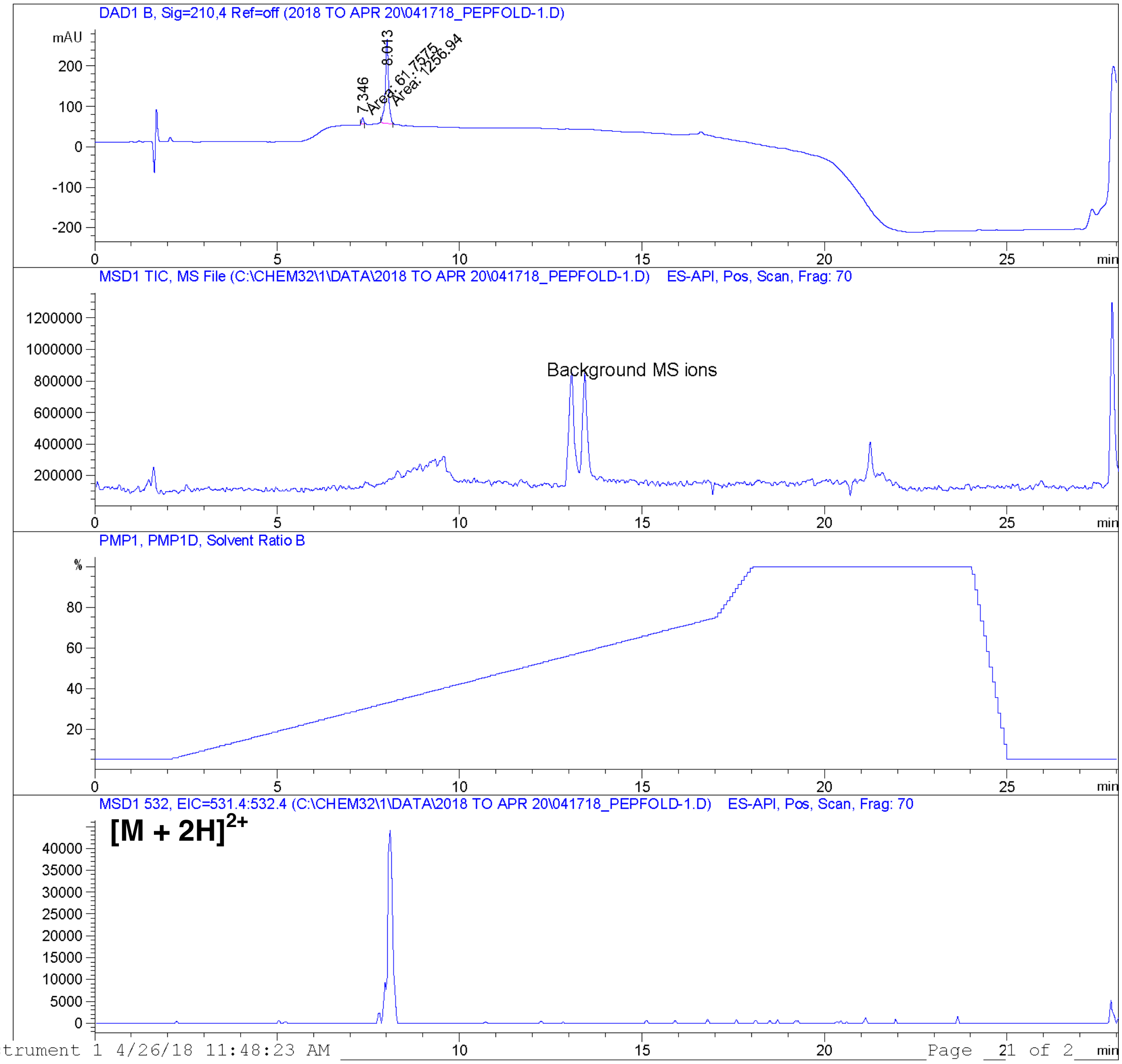
Blank (no injection) – background MS peaks for compounds 6-21

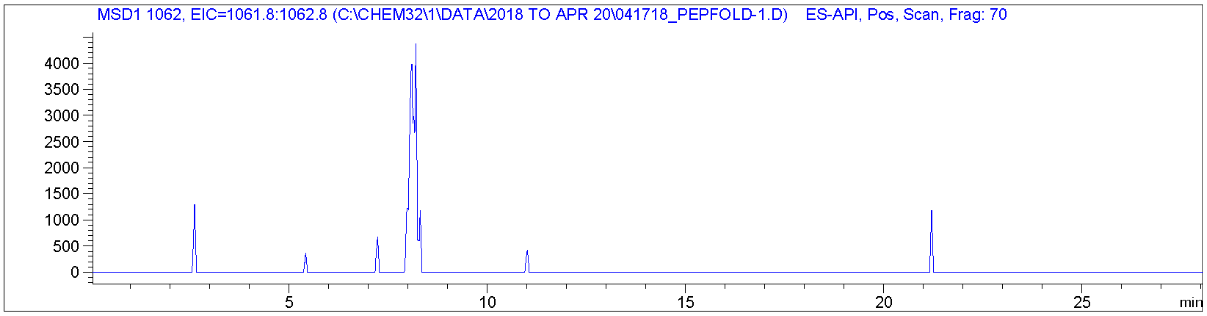
```
Data File C:\CHEM32\1\DATA\2018 TO APR 20\041718_NOINJ-LAST.D
Sample Name: 041718_noinj-last

    ======================================================================
    Acq. Operator   : SGLK                            Seq. Line :  21
    Acq. Instrument : Instrument 1                     Location : Vial 80
    Injection Date  : 4/17/18 9:15:18 PM                    Inj :   1
                                                     Inj Volume : 1.000 µl
    Different Inj Volume from Sequence !      Actual Inj Volume : 0.000 µl
    Acq. Method     : D:\CHEM32\1\METHODS\AP_C18_INSERT.M
    Last changed    : 4/17/18 11:25:09 AM by SGLK
    Analysis Method : Z:\DESKTOP\BERTOZZI LAB\LCMS INFO\LCMS METHODS TO 112917\SGLK_BERTOZZIBP_
                      WITHINSERT.M
    Last changed    : 4/26/18 12:19:51 PM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```



PEP-FOLD-1, Ac-GGDPCPHPKGG-NH$_2$ **(6)**

```
Data File C:\CHEM32\1\DATA\2018 TO APR 20\041718_PEPFOLD-1.D
Sample Name: 041718_pepfold-1

    =====================================================================
    Acq. Operator   : SGLK                            Seq. Line :   1
    Acq. Instrument : Instrument 1                     Location : Vial 61
    Injection Date  : 4/17/18 11:30:06 AM                   Inj :   1
                                                    Inj Volume : 1.000 µl
    Different Inj Volume from Sequence !     Actual Inj Volume : 2.000 µl
    Acq. Method     : D:\CHEM32\1\METHODS\AP_C18_INSERT.M
    Last changed    : 4/17/18 11:25:09 AM by SGLK
    Analysis Method : Z:\DESKTOP\BERTOZZI LAB\LCMS INFO\LCMS METHODS TO 112917\SGLK_BERTOZZIBP_
                      WITHINSERT.M
    Last changed    : 4/26/18 11:40:30 AM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

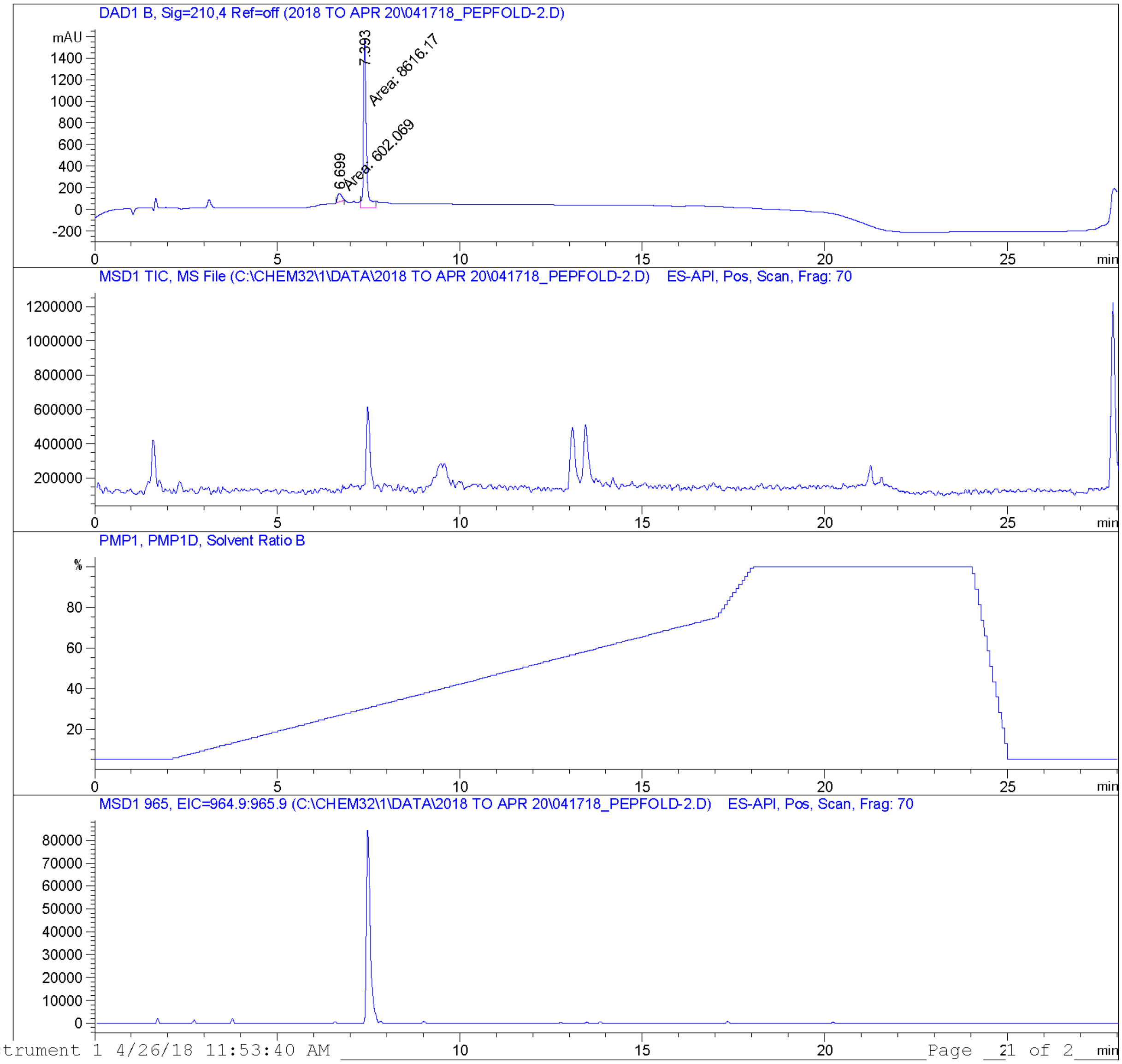




```
=====================================================================
                         Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 B, Sig=210,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]        %
----|-------|----|-------|----------|----------|--------|
   1   7.346 MM    0.0631   61.75753   16.30812   4.6832
   2   8.013 MM    0.1000 1256.93677  209.44200  95.3168

Totals :                  1318.69430  225.75012



Signal 2: MSD1 TIC, MS File


Signal 3: MSD1 532, EIC=531.4:532.4


Signal 4: MSD1 1062, EIC=1061.8:1062.8

=====================================================================
                          *** End of Report ***
```

PEP-FOLD-2, Ac-GGHPDCPKGG-NH_2 **(7)**

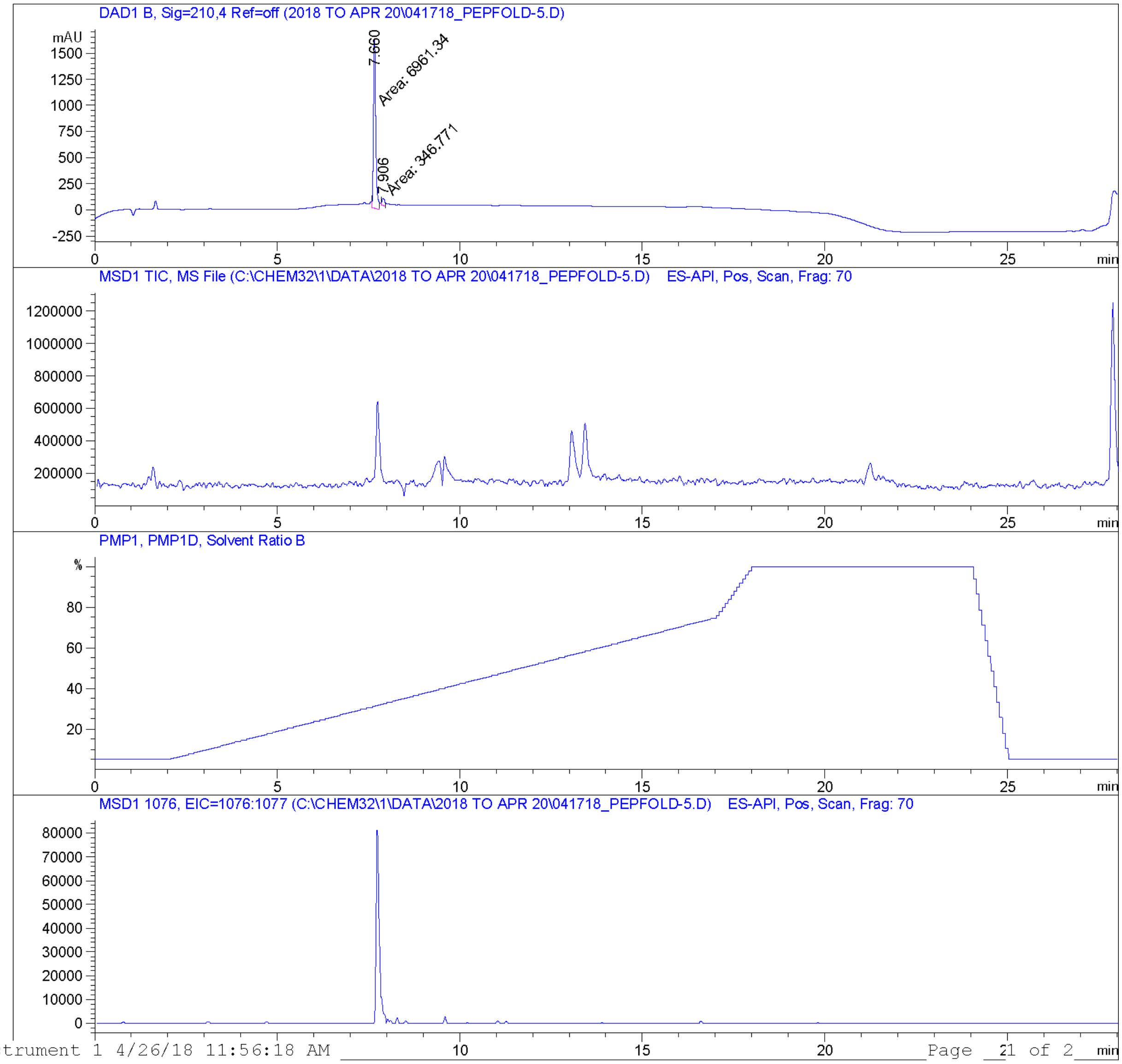
```
Data File C:\CHEM32\1\DATA\2018 TO APR 20\041718_PEPFOLD-2.D
Sample Name: 041718_pepfold-2

    ======================================================================
    Acq. Operator   : SGLK                               Seq. Line :    2
    Acq. Instrument : Instrument 1                        Location : Vial 62
    Injection Date  : 4/17/18 11:59:24 AM                      Inj :    1
                                                        Inj Volume : 1.000 µl
    Different Inj Volume from Sequence !     Actual Inj Volume : 2.000 µl
    Acq. Method     : D:\CHEM32\1\METHODS\AP_C18_INSERT.M
    Last changed    : 4/17/18 11:25:09 AM by SGLK
    Analysis Method : Z:\DESKTOP\BERTOZZI LAB\LCMS INFO\LCMS METHODS TO 112917\SGLK_BERTOZZIBP_
                      WITHINSERT.M
    Last changed    : 4/26/18 11:40:30 AM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```



```
Data File C:\CHEM32\1\DATA\2018 TO APR 20\041718_PEPFOLD-2.D
Sample Name: 041718_pepfold-2

    =====================================================================
                             Area Percent Report
    =====================================================================

    Sorted By             :      Signal
    Multiplier:                    :      1.0000
    Dilution:                      :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 B, Sig=210,4 Ref=off

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]        %
    ----|-------|----|-------|----------|----------|--------|
       1   6.699 MM    0.1309  602.06927   76.66061   6.5313
       2   7.393 MM    0.0916 8616.17383 1568.30005  93.4687

    Totals :                  9218.24310 1644.96066



    Signal 2: MSD1 TIC, MS File


    Signal 3: MSD1 965, EIC=964.9:965.9

    =====================================================================
                              *** End of Report ***
```

PEP-FOLD-5, Ac-GGHPEPCPKGG-NH_2 **(8)**

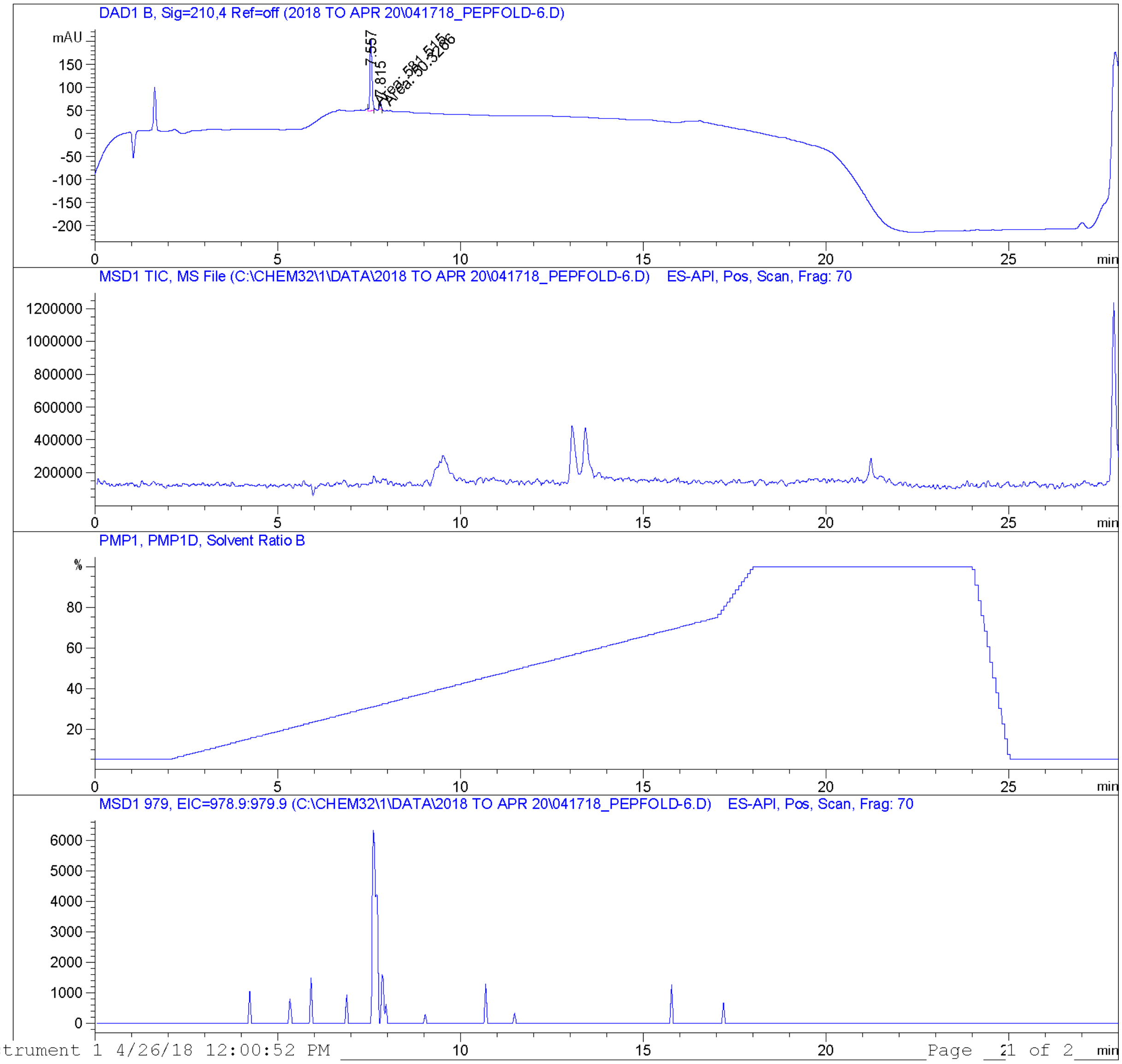
```
Data File C:\CHEM32\1\DATA\2018 TO APR 20\041718_PEPFOLD-5.D
Sample Name: 041718_pepfold-5

    =====================================================================
    Acq. Operator    : SGLK                            Seq. Line :   5
    Acq. Instrument : Instrument 1                      Location : Vial 65
    Injection Date   : 4/17/18 1:27:08 PM                    Inj :   1
                                                     Inj Volume : 1.000 µl
    Different Inj Volume from Sequence !     Actual Inj Volume : 2.000 µl
    Acq. Method      : D:\CHEM32\1\METHODS\AP_C18_INSERT.M
    Last changed     : 4/17/18 11:25:09 AM by SGLK
    Analysis Method : Z:\DESKTOP\BERTOZZI LAB\LCMS INFO\LCMS METHODS TO 112917\SGLK_BERTOZZIBP_
                      WITHINSERT.M
    Last changed     : 4/26/18 11:40:30 AM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```



```
Data File C:\CHEM32\1\DATA\2018 TO APR 20\041718_PEPFOLD-5.D
Sample Name: 041718_pepfold-5

    =====================================================================
                             Area Percent Report
    =====================================================================

    Sorted By             :      Signal
    Multiplier:                   :      1.0000
    Dilution:                     :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 B, Sig=210,4 Ref=off

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]        %
    ----|-------|----|-------|----------|----------|--------|
       1   7.660 MM    0.0715 6961.34277 1623.41699  95.2550
       2   7.906 MM    0.0808  346.77087   71.53614   4.7450

    Totals :                  7308.11365 1694.95313



    Signal 2: MSD1 TIC, MS File


    Signal 3: MSD1 1076, EIC=1076:1077

    =====================================================================
                              *** End of Report ***
```

PEP-FOLD-6, Ac-GGHPECPKGG-NH_2 **(9)**

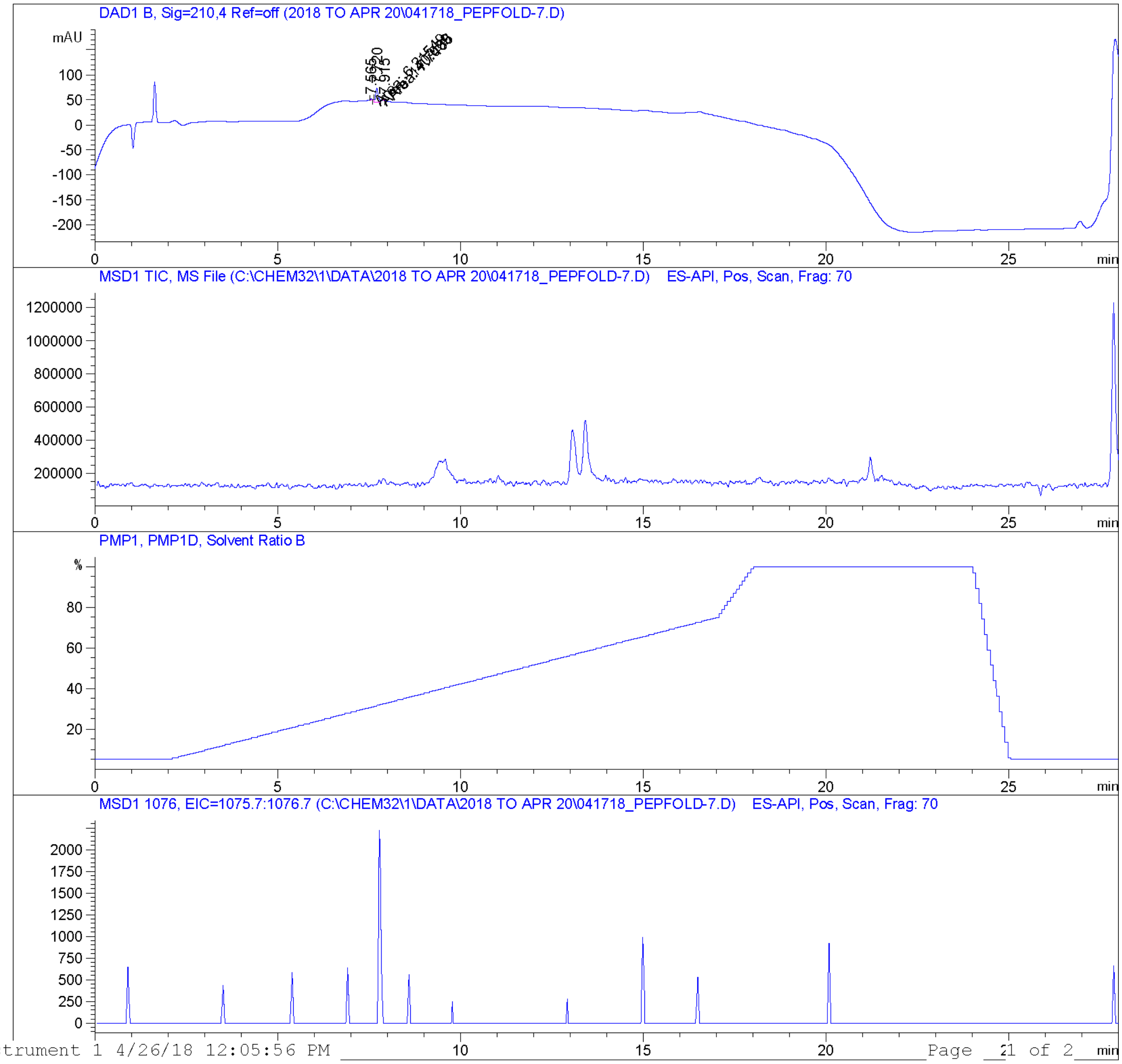
```
Data File C:\CHEM32\1\DATA\2018 TO APR 20\041718_PEPFOLD-6.D
Sample Name: 041718_pepfold-6

    =====================================================================
    Acq. Operator   : SGLK                            Seq. Line :   6
    Acq. Instrument : Instrument 1                     Location : Vial 66
    Injection Date  : 4/17/18 1:56:26 PM                    Inj :   1
                                                     Inj Volume : 1.000 µl
    Different Inj Volume from Sequence !      Actual Inj Volume : 2.000 µl
    Acq. Method     : D:\CHEM32\1\METHODS\AP_C18_INSERT.M
    Last changed    : 4/17/18 11:25:09 AM by SGLK
    Analysis Method : Z:\DESKTOP\BERTOZZI LAB\LCMS INFO\LCMS METHODS TO 112917\SGLK_BERTOZZIBP_
                      WITHINSERT.M
    Last changed    : 4/26/18 11:40:30 AM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

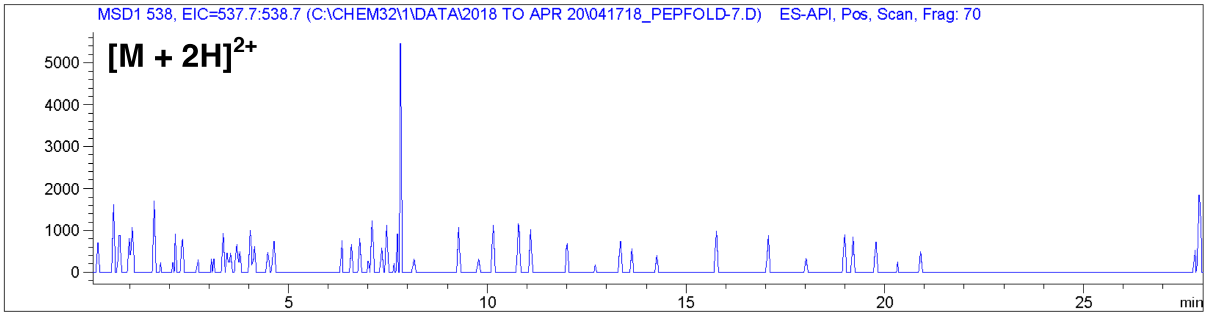


```
=====================================================================
                         Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 B, Sig=210,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]        %
----|-------|----|-------|----------|----------|--------|
   1   7.557 MM    0.0617  581.51514  157.19263  92.0349
   2   7.815 MM    0.0495   50.32655   16.94779   7.9651

Totals :                   631.84169  174.14042



Signal 2: MSD1 TIC, MS File

=====================================================================
                          *** End of Report ***
```

PEP-FOLD-7, Ac-GGEPHPCPKGG-NH_2 **(10)**

```
Data File C:\CHEM32\1\DATA\2018 TO APR 20\041718_PEPFOLD-7.D
Sample Name: 041718_pepfold-7

    =====================================================================
    Acq. Operator   : SGLK                            Seq. Line :   7
    Acq. Instrument : Instrument 1                     Location : Vial 67
    Injection Date  : 4/17/18 2:25:44 PM                    Inj :   1
                                                     Inj Volume : 1.000 µl
    Different Inj Volume from Sequence !      Actual Inj Volume : 2.000 µl
    Acq. Method     : D:\CHEM32\1\METHODS\AP_C18_INSERT.M
    Last changed    : 4/17/18 11:25:09 AM by SGLK
    Analysis Method : Z:\DESKTOP\BERTOZZI LAB\LCMS INFO\LCMS METHODS TO 112917\SGLK_BERTOZZIBP_
                      WITHINSERT.M
    Last changed    : 4/26/18 11:40:30 AM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

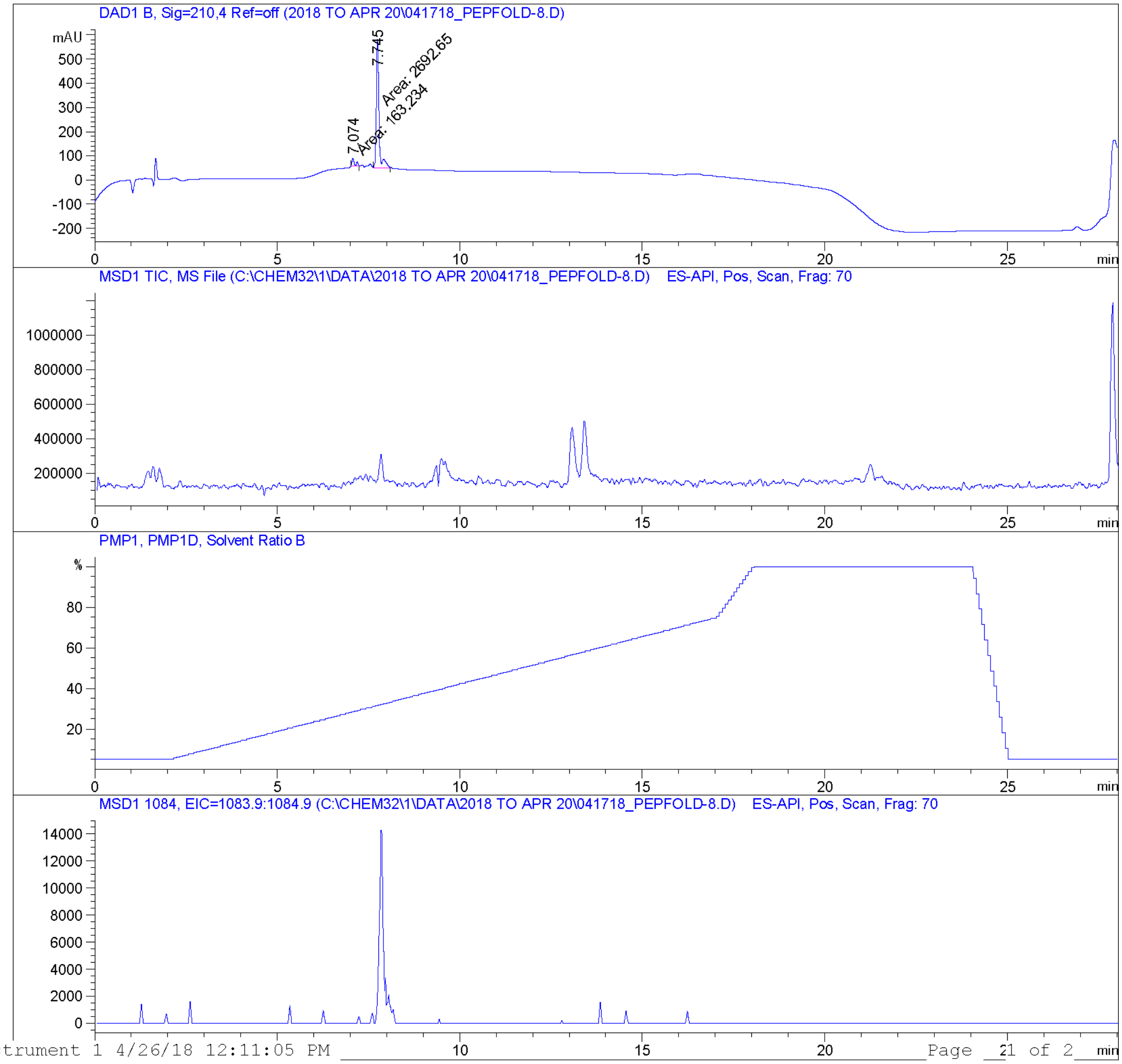




```
=====================================================================
                         Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 B, Sig=210,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]        %
----|-------|----|-------|----------|----------|--------|
   1   7.565 MM    0.0488    6.21549    2.12108    4.0360
   2   7.720 FM    0.0823  140.03857   28.36635   90.9326
   3   7.915 MM    0.0409    7.74860    3.15911    5.0315

Totals :                   154.00266   33.64654



Signal 2: MSD1 TIC, MS File


Signal 3: MSD1 1076, EIC=1075.7:1076.7


Signal 4: MSD1 538, EIC=537.7:538.7

=====================================================================
                          *** End of Report ***
```

PEP-FOLD-8, Ac-GGCPKPHPHGG-NH$_2$ **(11)**

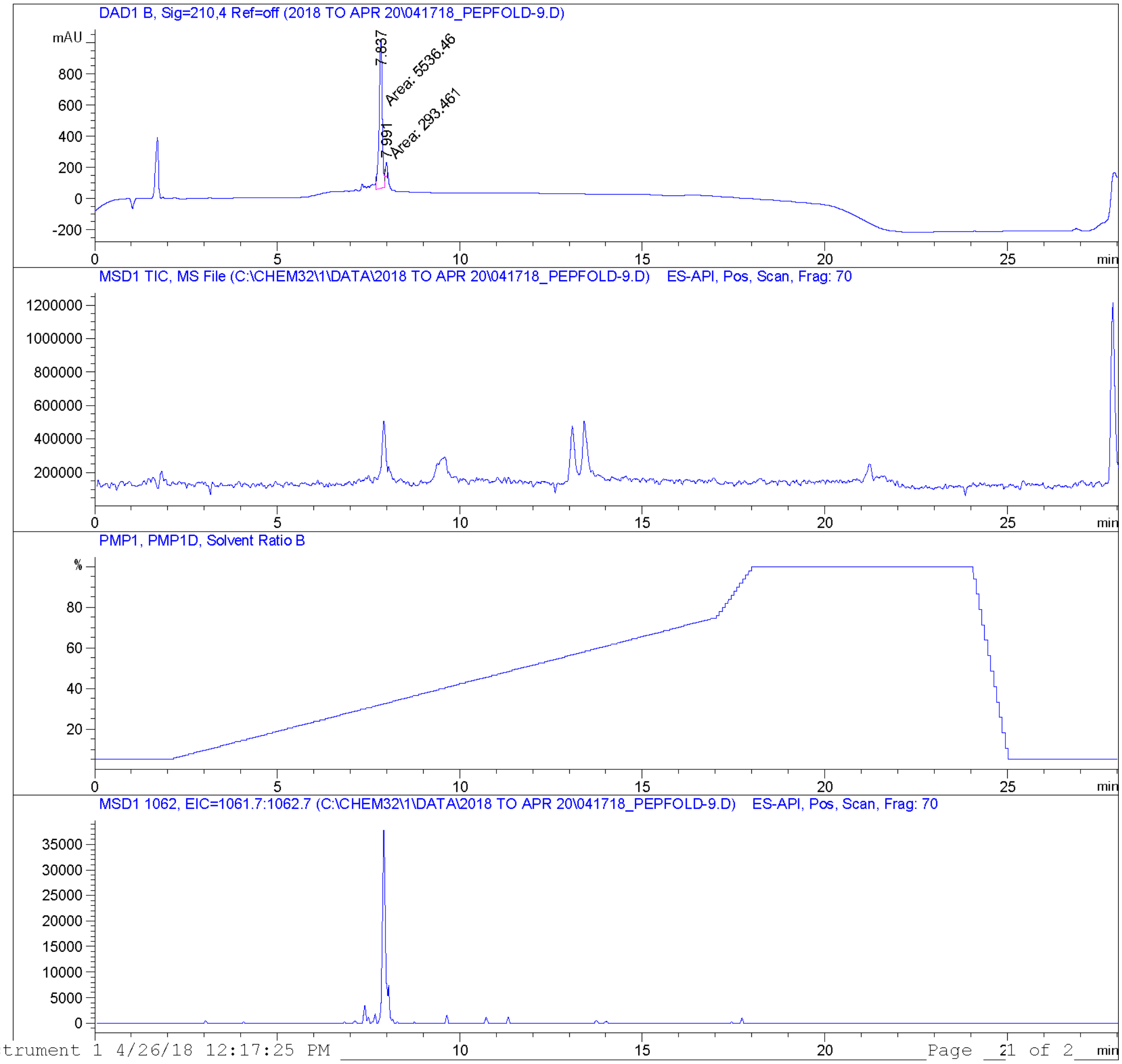
```
Data File C:\CHEM32\1\DATA\2018 TO APR 20\041718_PEPFOLD-8.D
Sample Name: 041718_pepfold-8

    =====================================================================
    Acq. Operator   : SGLK                          Seq. Line :   8
    Acq. Instrument : Instrument 1                   Location : Vial 68
    Injection Date  : 4/17/18 2:55:02 PM                  Inj :   1
                                                   Inj Volume : 1.000 µl
    Different Inj Volume from Sequence !     Actual Inj Volume : 2.000 µl
    Acq. Method     : D:\CHEM32\1\METHODS\AP_C18_INSERT.M
    Last changed    : 4/17/18 11:25:09 AM by SGLK
    Analysis Method : Z:\DESKTOP\BERTOZZI LAB\LCMS INFO\LCMS METHODS TO 112917\SGLK_BERTOZZIBP_
                      WITHINSERT.M
    Last changed    : 4/26/18 11:40:30 AM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

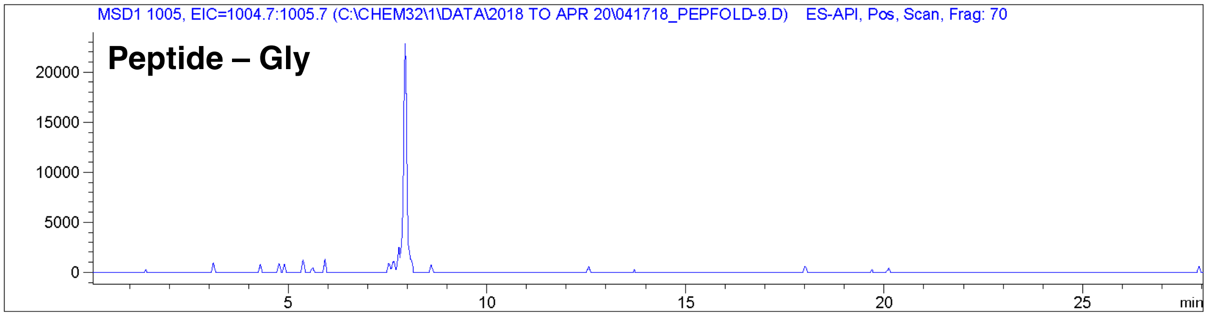


```
=====================================================================
                         Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 B, Sig=210,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]        %
----|-------|----|-------|----------|----------|--------|
   1   7.074 MM    0.0863  163.23375   31.52087   5.7157
   2   7.745 MM    0.0839 2692.64893  534.70697  94.2843

Totals :                  2855.88268  566.22784



Signal 2: MSD1 TIC, MS File


Signal 3: MSD1 1084, EIC=1083.9:1084.9

=====================================================================
                          *** End of Report ***
```

PEP-FOLD-9, Ac-GGCPKPDPHGG-NH$_2$ **(12)**

```
Data File C:\CHEM32\1\DATA\2018 TO APR 20\041718_PEPFOLD-9.D
Sample Name: 041718_pepfold-9

    ======================================================================
    Acq. Operator   : SGLK                              Seq. Line :   9
    Acq. Instrument : Instrument 1                       Location : Vial 69
    Injection Date  : 4/17/18 3:24:22 PM                      Inj :   1
                                                       Inj Volume : 1.000 µl
    Different Inj Volume from Sequence !      Actual Inj Volume : 2.000 µl
    Acq. Method     : D:\CHEM32\1\METHODS\AP_C18_INSERT.M
    Last changed    : 4/17/18 11:25:09 AM by SGLK
    Analysis Method : Z:\DESKTOP\BERTOZZI LAB\LCMS INFO\LCMS METHODS TO 112917\SGLK_BERTOZZIBP_
                      WITHINSERT.M
    Last changed    : 4/26/18 11:40:30 AM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

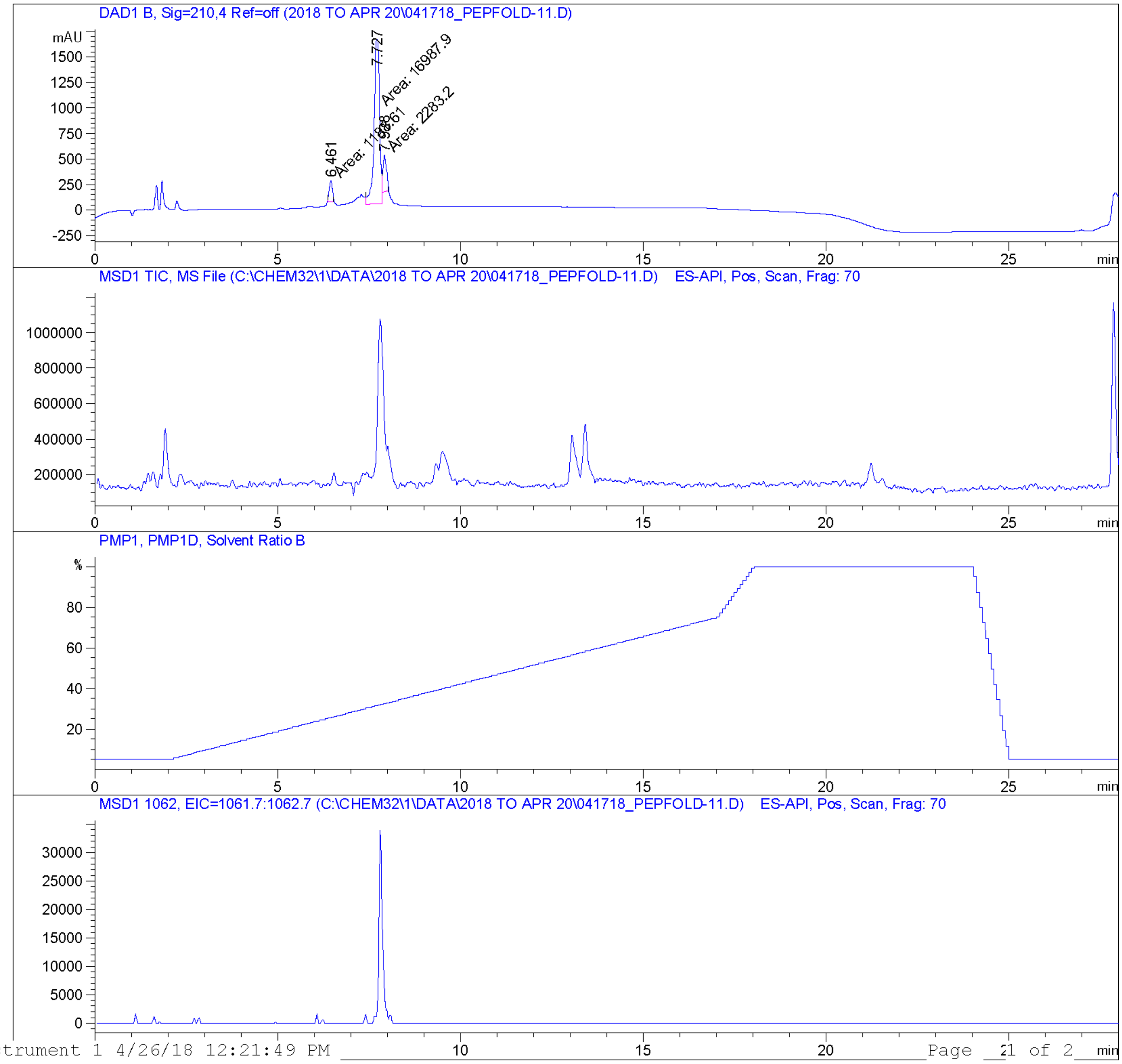


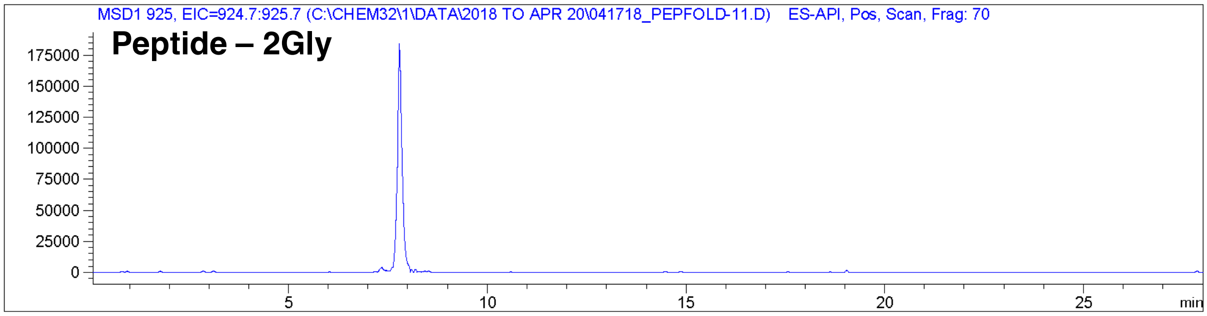


```
=====================================================================
                         Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 B, Sig=210,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]        %
----|-------|----|-------|----------|----------|--------|
   1   7.837 MM    0.0960 5536.45996  960.84705  94.9663
   2   7.991 MM    0.0538  293.46121   90.87576   5.0337

Totals :                  5829.92117 1051.72280



Signal 2: MSD1 TIC, MS File


Signal 3: MSD1 1062, EIC=1061.7:1062.7


Signal 4: MSD1 1005, EIC=1004.7:1005.7

=====================================================================
                          *** End of Report ***
```

PEP-FOLD-11, Ac-GGCPDPHPKGG-NH$_2$ **(13)**

```
Data File C:\CHEM32\1\DATA\2018 TO APR 20\041718_PEPFOLD-11.D
Sample Name: 041718_pepfold-11

    =====================================================================
    Acq. Operator   : SGLK                            Seq. Line :  10
    Acq. Instrument : Instrument 1                     Location : Vial 70
    Injection Date  : 4/17/18 3:53:42 PM                    Inj :   1
                                                     Inj Volume : 1.000 µl
    Different Inj Volume from Sequence !      Actual Inj Volume : 2.000 µl
    Acq. Method     : D:\CHEM32\1\METHODS\AP_C18_INSERT.M
    Last changed    : 4/17/18 11:25:09 AM by SGLK
    Analysis Method : Z:\DESKTOP\BERTOZZI LAB\LCMS INFO\LCMS METHODS TO 112917\SGLK_BERTOZZIBP_
                      WITHINSERT.M
    Last changed    : 4/26/18 12:19:51 PM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

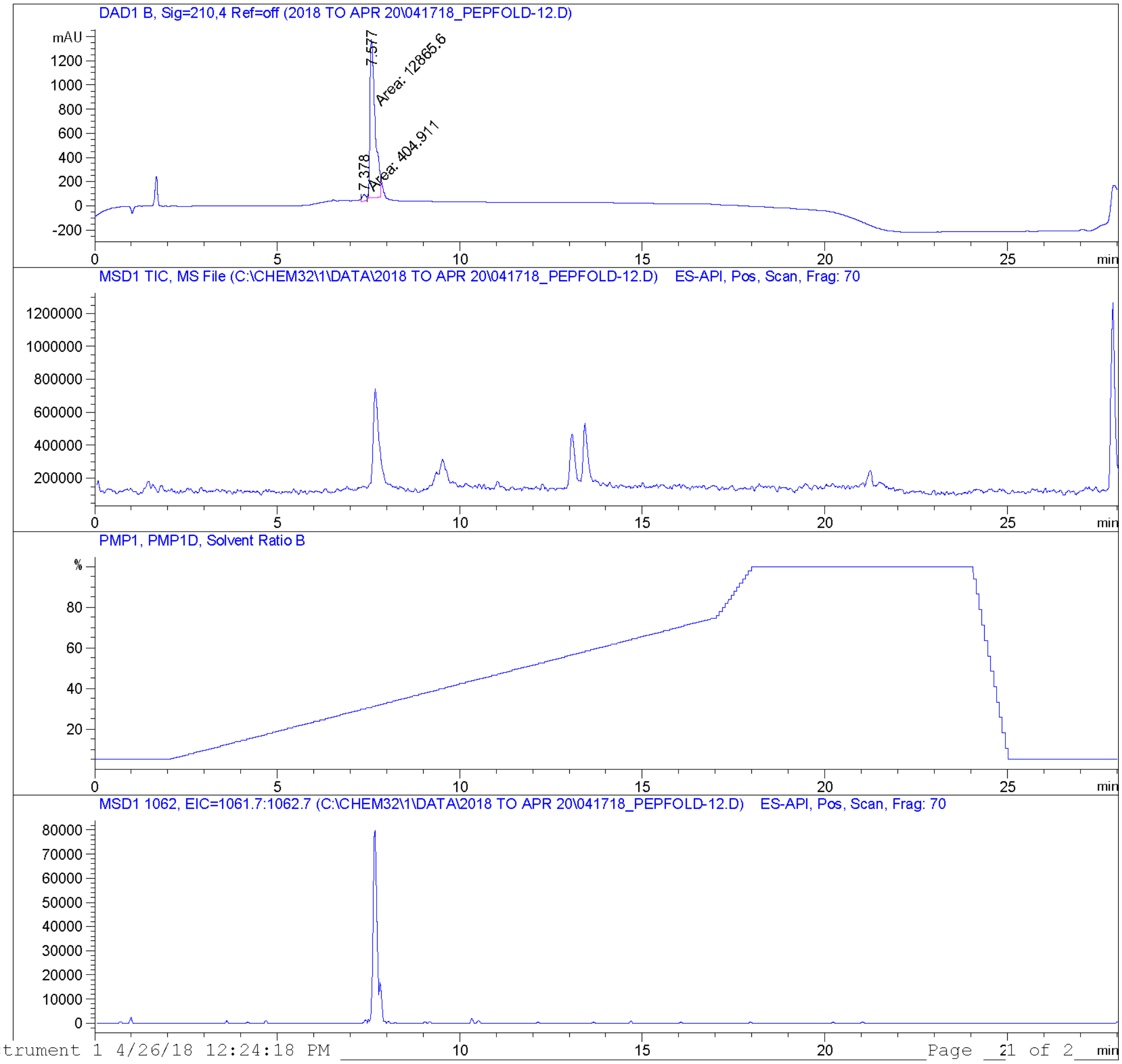




```
=====================================================================
                         Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 B, Sig=210,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #    [min]        [min]    [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.461 MM    0.0969 1188.60876  204.49396   5.8095
   2   7.727 MM    0.1756 1.69879e4  1612.37292  83.0310
   3   7.928 MM    0.1060 2283.19775  358.82666  11.1595

Totals :                  2.04597e4  2175.69354



Signal 2: MSD1 TIC, MS File


Signal 3: MSD1 1062, EIC=1061.7:1062.7


Signal 4: MSD1 925, EIC=924.7:925.7

=====================================================================
                          *** End of Report ***
```

PEP-FOLD-12, Ac-GGKPCPHPDGG-NH_2 **(14)**

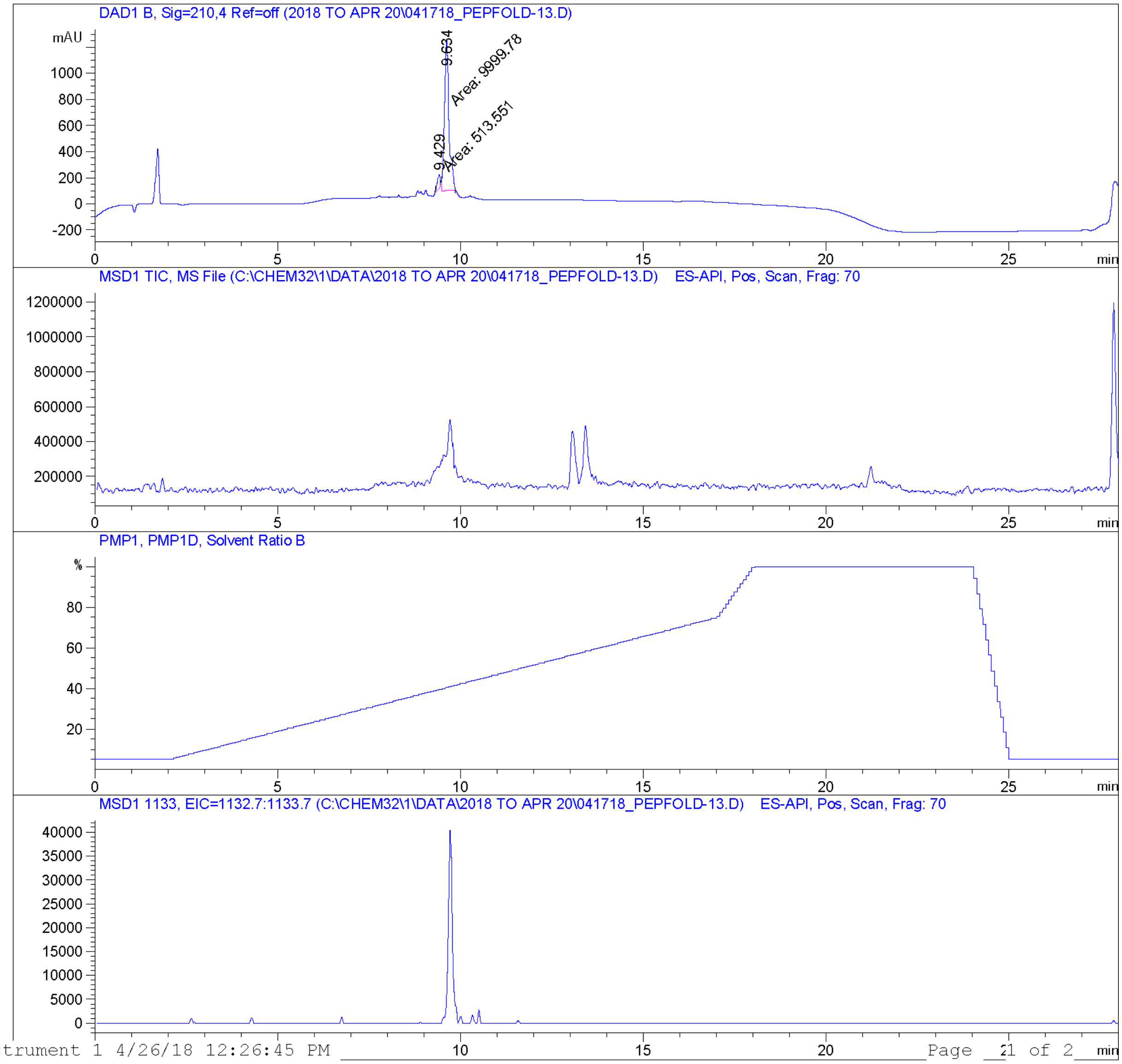
```
Data File C:\CHEM32\1\DATA\2018 TO APR 20\041718_PEPFOLD-12.D
Sample Name: 041718_pepfold-12

    =====================================================================
    Acq. Operator   : SGLK                                Seq. Line :  11
    Acq. Instrument : Instrument 1                         Location : Vial 71
    Injection Date  : 4/17/18 4:23:01 PM                        Inj :   1
                                                         Inj Volume : 1.000 µl
    Different Inj Volume from Sequence !      Actual Inj Volume : 2.000 µl
    Acq. Method     : D:\CHEM32\1\METHODS\AP_C18_INSERT.M
    Last changed    : 4/17/18 11:25:09 AM by SGLK
    Analysis Method : Z:\DESKTOP\BERTOZZI LAB\LCMS INFO\LCMS METHODS TO 112917\SGLK_BERTOZZIBP_
                      WITHINSERT.M
    Last changed    : 4/26/18 12:19:51 PM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```



```
=====================================================================
                          Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 B, Sig=210,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]        %
----|-------|----|-------|----------|----------|--------|
   1   7.378 MF    0.1246  404.91074   54.17891   3.0512
   2   7.577 MM    0.1629 1.28656e4  1316.29163  96.9488

Totals :                  1.32706e4  1370.47054



Signal 2: MSD1 TIC, MS File


Signal 3: MSD1 1062, EIC=1061.7:1062.7

=====================================================================
                            *** End of Report ***
```

PEP-FOLD-13, Ac-GGWPHPCPKGG-NH_2 **(15)**

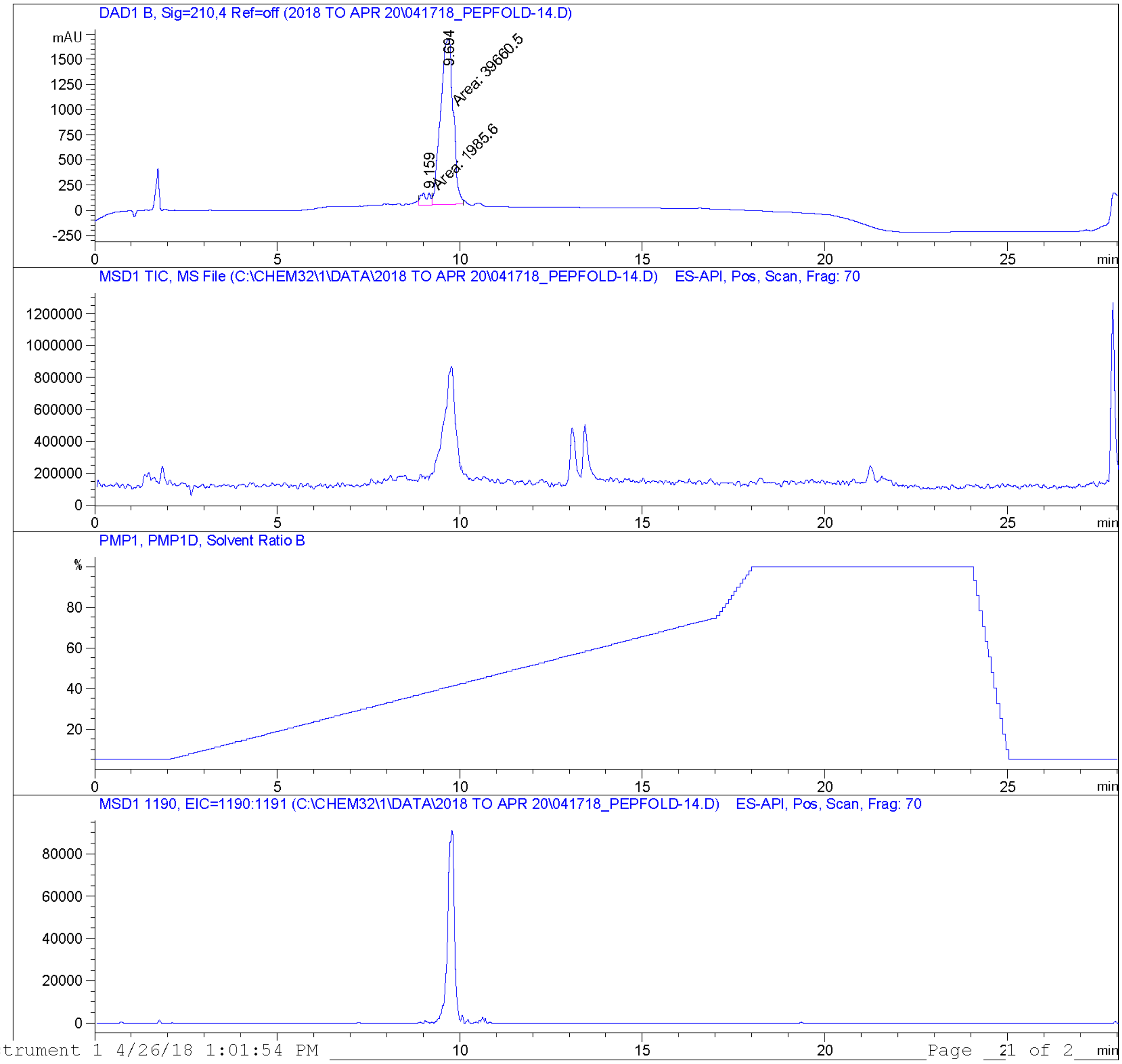
```
Data File C:\CHEM32\1\DATA\2018 TO APR 20\041718_PEPFOLD-13.D
Sample Name: 041718_pepfold-13

    =====================================================================
    Acq. Operator   : SGLK                            Seq. Line :  12
    Acq. Instrument : Instrument 1                     Location : Vial 72
    Injection Date  : 4/17/18 4:52:16 PM                    Inj :   1
                                                     Inj Volume : 1.000 µl
    Different Inj Volume from Sequence !      Actual Inj Volume : 2.000 µl
    Acq. Method     : D:\CHEM32\1\METHODS\AP_C18_INSERT.M
    Last changed    : 4/17/18 11:25:09 AM by SGLK
    Analysis Method : Z:\DESKTOP\BERTOZZI LAB\LCMS INFO\LCMS METHODS TO 112917\SGLK_BERTOZZIBP_
                      WITHINSERT.M
    Last changed    : 4/26/18 12:19:51 PM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```



```
Data File C:\CHEM32\1\DATA\2018 TO APR 20\041718_PEPFOLD-13.D
Sample Name: 041718_pepfold-13

    =====================================================================
                             Area Percent Report
    =====================================================================

    Sorted By             :      Signal
    Multiplier:                   :      1.0000
    Dilution:                     :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 B, Sig=210,4 Ref=off

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]        %
    ----|-------|----|-------|----------|----------|--------|
       1   9.429 MM    0.0862  513.55121   99.34387   4.8848
       2   9.634 FM    0.1434 9999.78418 1161.94617  95.1152

    Totals :                  1.05133e4  1261.29004



    Signal 2: MSD1 TIC, MS File


    Signal 3: MSD1 1133, EIC=1132.7:1133.7

    =====================================================================
                              *** End of Report ***
```

PEP-FOLD-14, Ac-GGWPHPGCPKGG-NH_2 **(16)**

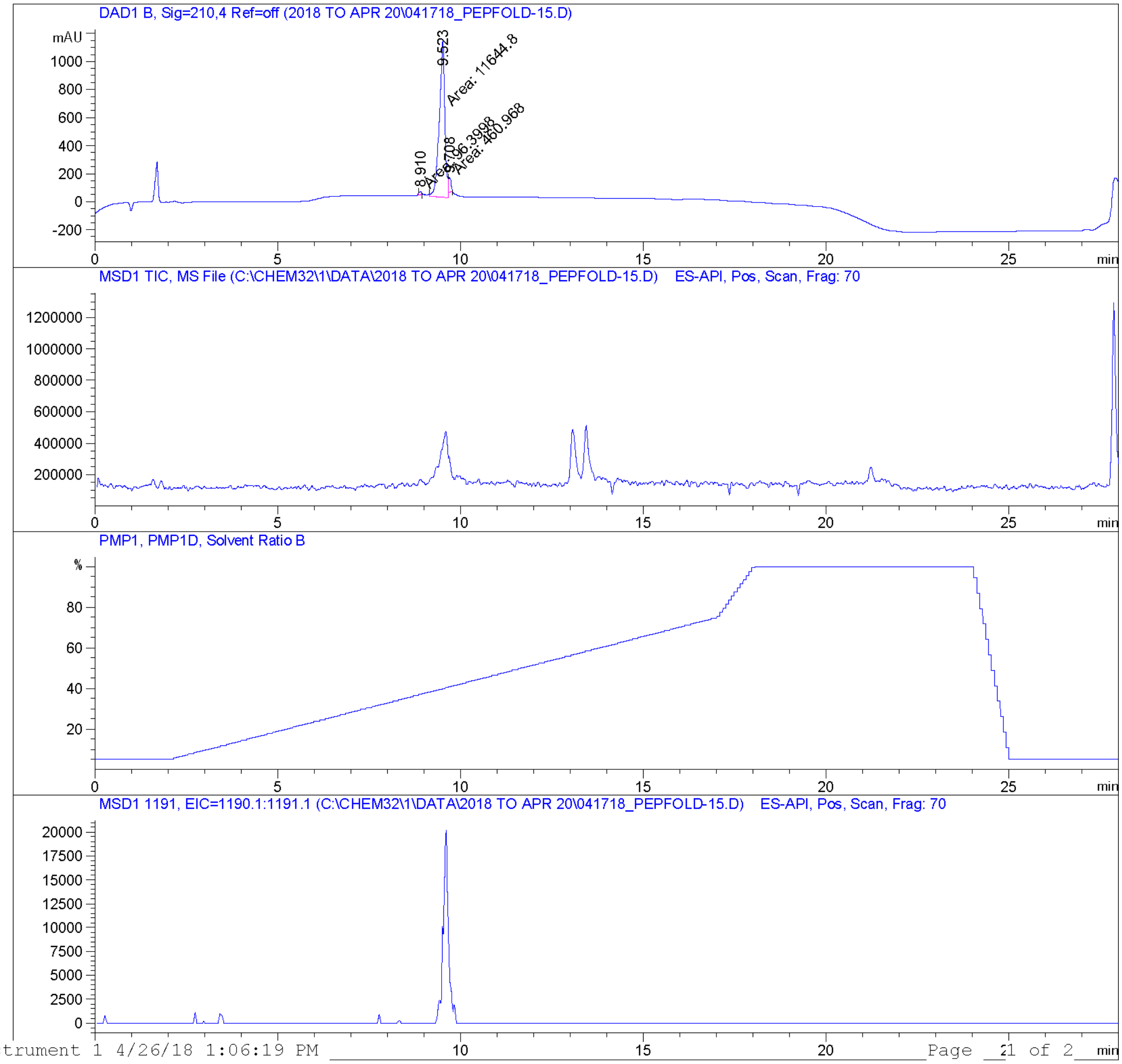
```
Data File C:\CHEM32\1\DATA\2018 TO APR 20\041718_PEPFOLD-14.D
Sample Name: 041718_pepfold-14

    =====================================================================
    Acq. Operator   : SGLK                            Seq. Line :  13
    Acq. Instrument : Instrument 1                     Location : Vial 73
    Injection Date  : 4/17/18 5:21:31 PM                    Inj :   1
                                                     Inj Volume : 1.000 µl
    Different Inj Volume from Sequence !      Actual Inj Volume : 2.000 µl
    Acq. Method     : D:\CHEM32\1\METHODS\AP_C18_INSERT.M
    Last changed    : 4/17/18 11:25:09 AM by SGLK
    Analysis Method : Z:\DESKTOP\BERTOZZI LAB\LCMS INFO\LCMS METHODS TO 112917\SGLK_BERTOZZIBP_
                      WITHINSERT.M
    Last changed    : 4/26/18 12:19:51 PM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```



```
Data File C:\CHEM32\1\DATA\2018 TO APR 20\041718_PEPFOLD-14.D
Sample Name: 041718_pepfold-14

    =====================================================================
                             Area Percent Report
    =====================================================================

    Sorted By             :      Signal
    Multiplier:                   :      1.0000
    Dilution:                     :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 B, Sig=210,4 Ref=off

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]        %
    ----|-------|----|-------|----------|----------|--------|
       1   9.159 MF    0.2637 1985.60120  125.47730   4.7678
       2   9.694 FM    0.4020 3.96605e4  1644.22729  95.2322

    Totals :                  4.16461e4  1769.70460



    Signal 2: MSD1 TIC, MS File

    =====================================================================
                              *** End of Report ***
```

PEP-FOLD-15, Ac-GGKPCPGWPHGG-NH_2 **(17)**

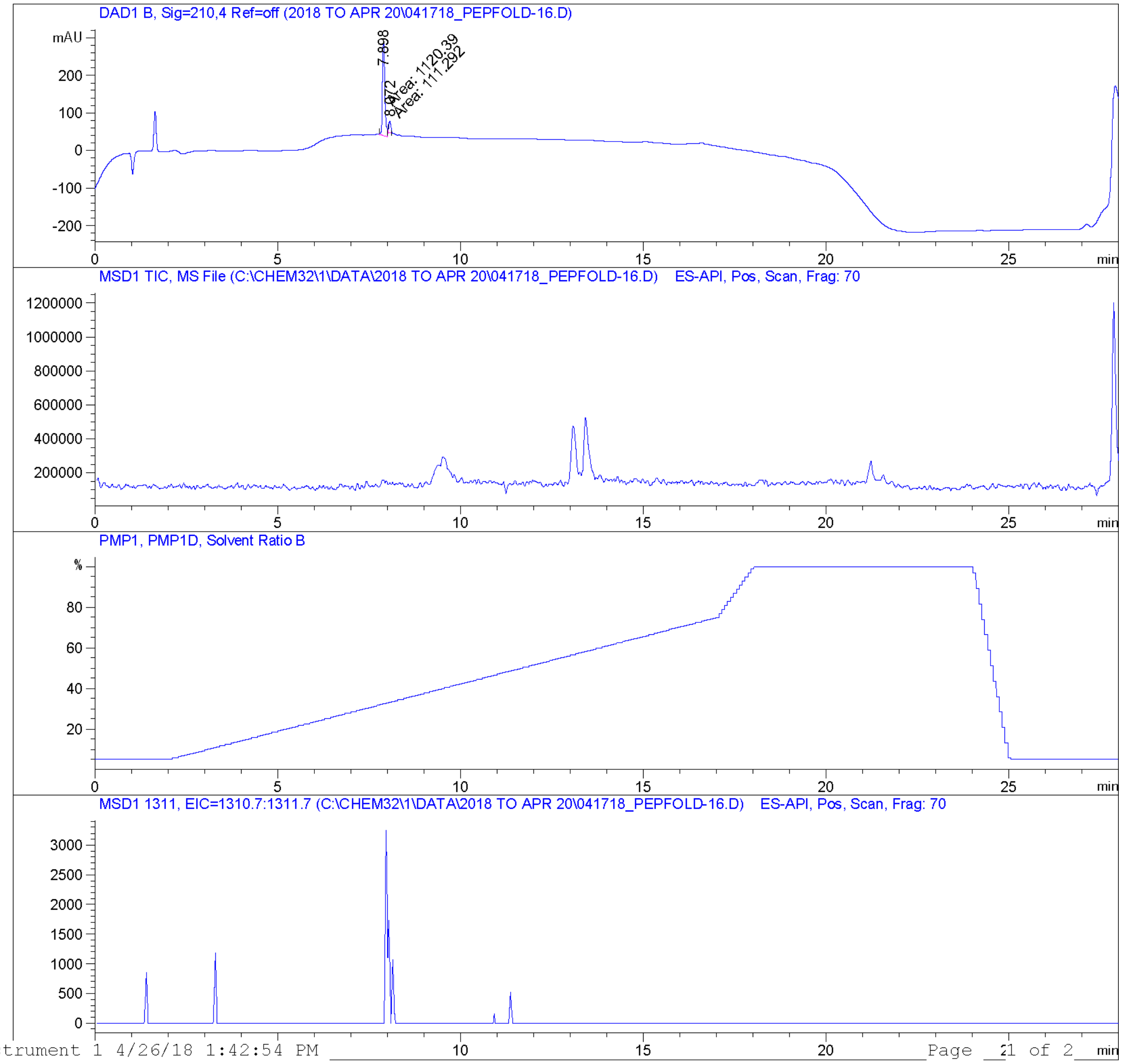
```
Data File C:\CHEM32\1\DATA\2018 TO APR 20\041718_PEPFOLD-15.D
Sample Name: 041718_pepfold-15

    =====================================================================
    Acq. Operator   : SGLK                           Seq. Line :  14
    Acq. Instrument : Instrument 1                    Location : Vial 74
    Injection Date  : 4/17/18 5:50:51 PM                   Inj :   1
                                                    Inj Volume : 1.000 µl
    Different Inj Volume from Sequence !     Actual Inj Volume : 2.000 µl
    Acq. Method     : D:\CHEM32\1\METHODS\AP_C18_INSERT.M
    Last changed    : 4/17/18 11:25:09 AM by SGLK
    Analysis Method : Z:\DESKTOP\BERTOZZI LAB\LCMS INFO\LCMS METHODS TO 112917\SGLK_BERTOZZIBP_
                      WITHINSERT.M
    Last changed    : 4/26/18 12:19:51 PM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

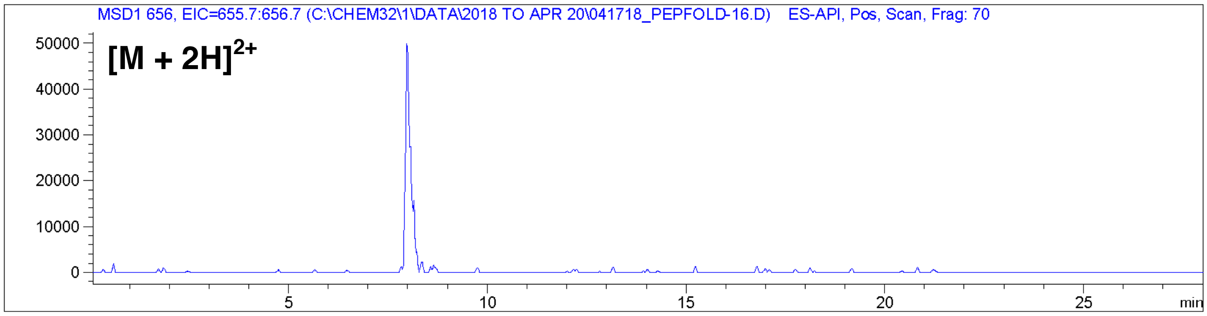


```
    =====================================================================
                             Area Percent Report
    =====================================================================

    Sorted By             :      Signal
    Multiplier:                   :      1.0000
    Dilution:                     :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 B, Sig=210,4 Ref=off

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]        %
    ----|-------|----|-------|----------|----------|--------|
       1   8.910 MM    0.0731   96.39982   21.96997   0.7900
       2   9.523 MM    0.1717 1.16448e4  1130.44336  95.4322
       3   9.708 MM    0.0727  460.96796  105.69280   3.7777

    Totals :                  1.22022e4  1258.10614



    Signal 2: MSD1 TIC, MS File

    =====================================================================
                              *** End of Report ***
```

PEP-FOLD-16, Ac-GGHPHPKPCPEGG-NH_2 **(18)**

```
Data File C:\CHEM32\1\DATA\2018 TO APR 20\041718_PEPFOLD-16.D
Sample Name: 041718_pepfold-16

    =====================================================================
    Acq. Operator   : SGLK                            Seq. Line :  15
    Acq. Instrument : Instrument 1                     Location : Vial 75
    Injection Date  : 4/17/18 6:20:08 PM                    Inj :   1
                                                     Inj Volume : 1.000 µl
    Different Inj Volume from Sequence !      Actual Inj Volume : 2.000 µl
    Acq. Method     : D:\CHEM32\1\METHODS\AP_C18_INSERT.M
    Last changed    : 4/17/18 11:25:09 AM by SGLK
    Analysis Method : Z:\DESKTOP\BERTOZZI LAB\LCMS INFO\LCMS METHODS TO 112917\SGLK_BERTOZZIBP_
                      WITHINSERT.M
    Last changed    : 4/26/18 12:19:51 PM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

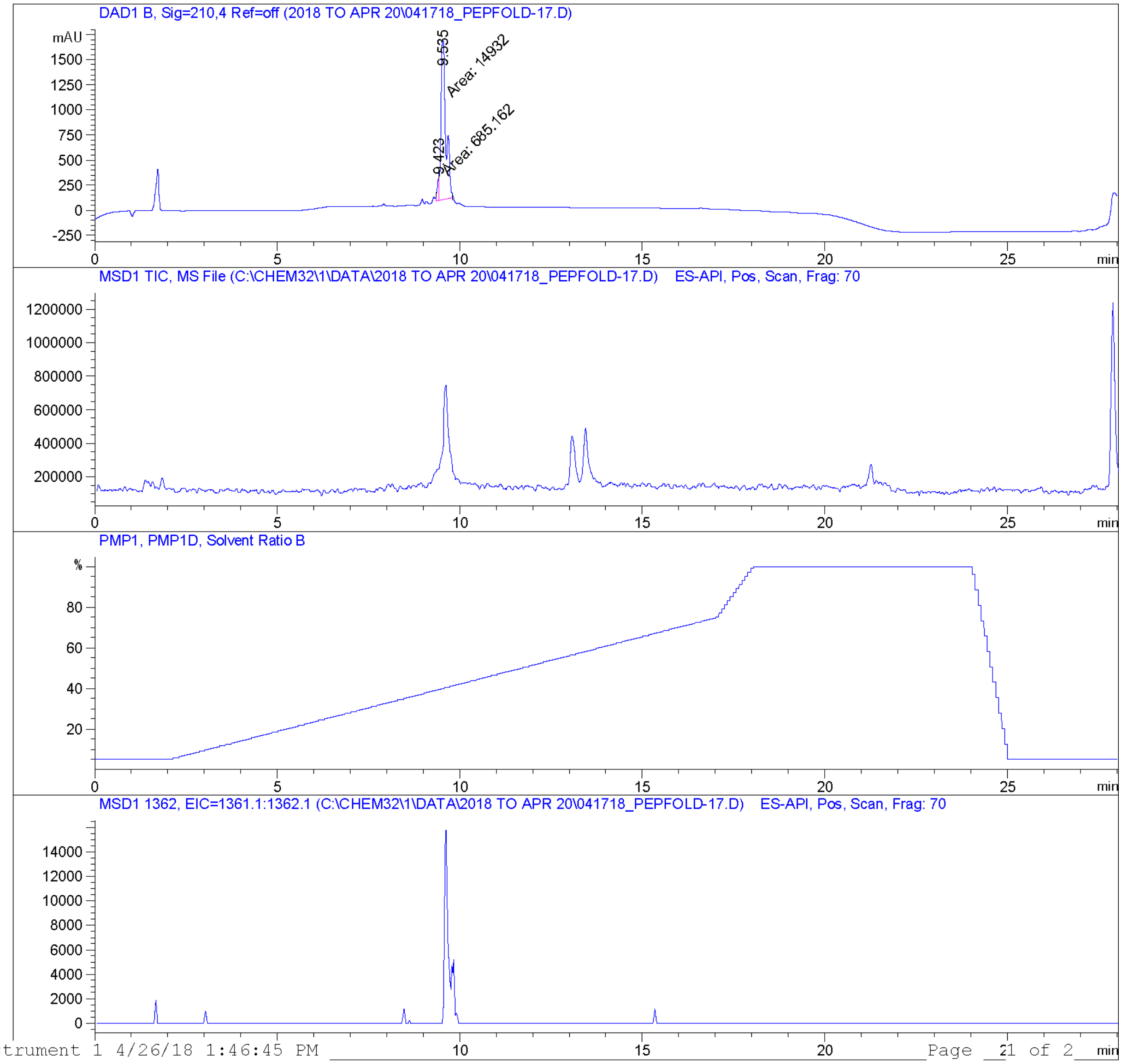




```
=====================================================================
                         Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                    :      1.0000
Dilution:                      :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 B, Sig=210,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]        %
----|-------|----|-------|----------|----------|--------|
   1   7.898 MM    0.0726 1120.38989  257.31540  90.9642
   2   8.072 MM    0.0570  111.29197   32.53252   9.0358

Totals :                  1231.68186  289.84792



Signal 2: MSD1 TIC, MS File

=====================================================================
                          *** End of Report ***
```

PEP-FOLD-17, Ac-GGHPWPKPCPEGG-NH_2 **(19)**

```
Data File C:\CHEM32\1\DATA\2018 TO APR 20\041718_PEPFOLD-17.D
Sample Name: 041718_pepfold-17

    =====================================================================
    Acq. Operator   : SGLK                            Seq. Line :  16
    Acq. Instrument : Instrument 1                     Location : Vial 76
    Injection Date  : 4/17/18 6:49:27 PM                    Inj :   1
                                                     Inj Volume : 1.000 µl
    Different Inj Volume from Sequence !      Actual Inj Volume : 2.000 µl
    Acq. Method     : D:\CHEM32\1\METHODS\AP_C18_INSERT.M
    Last changed    : 4/17/18 11:25:09 AM by SGLK
    Analysis Method : Z:\DESKTOP\BERTOZZI LAB\LCMS INFO\LCMS METHODS TO 112917\SGLK_BERTOZZIBP_
                      WITHINSERT.M
    Last changed    : 4/26/18 12:19:51 PM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

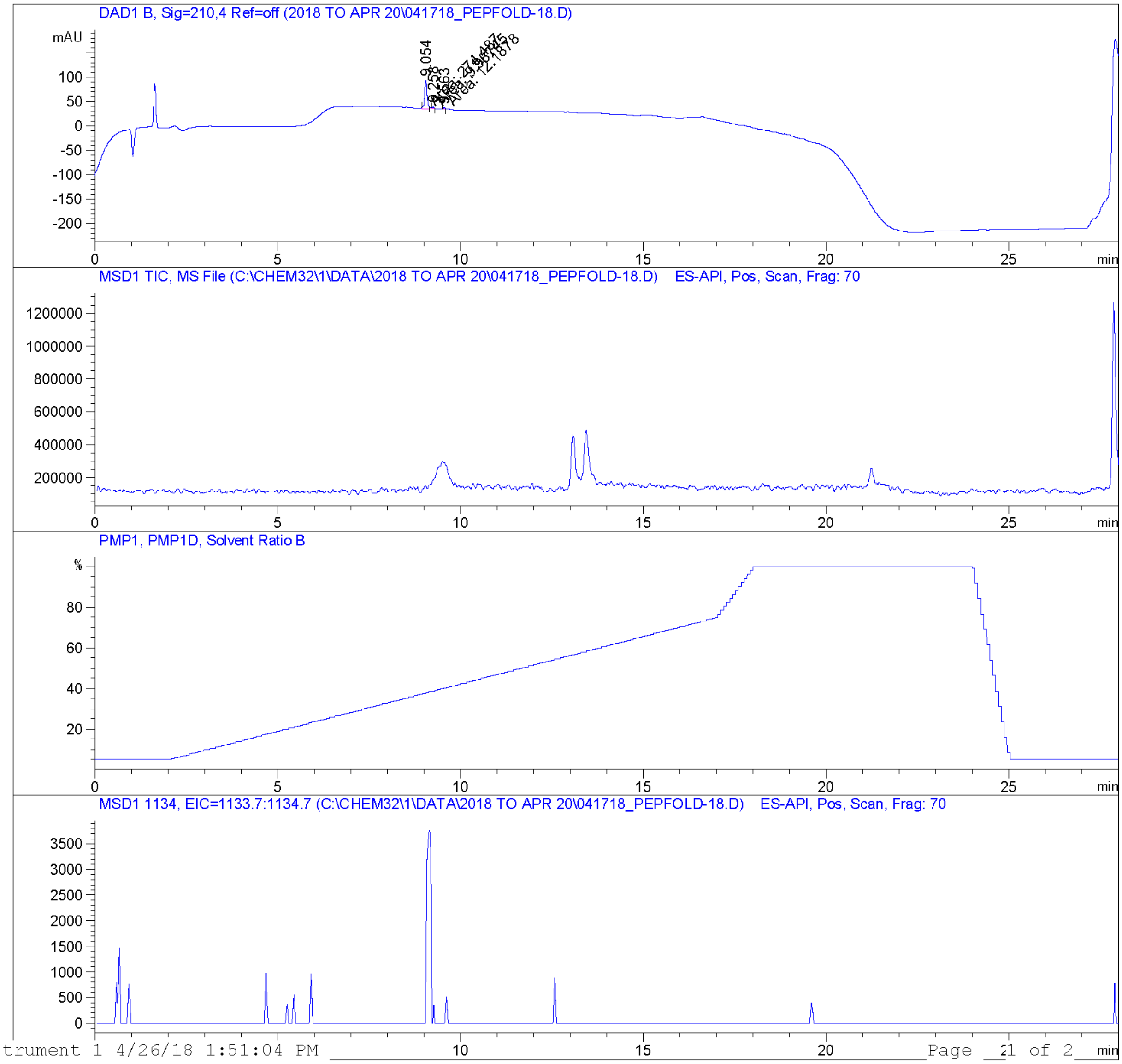


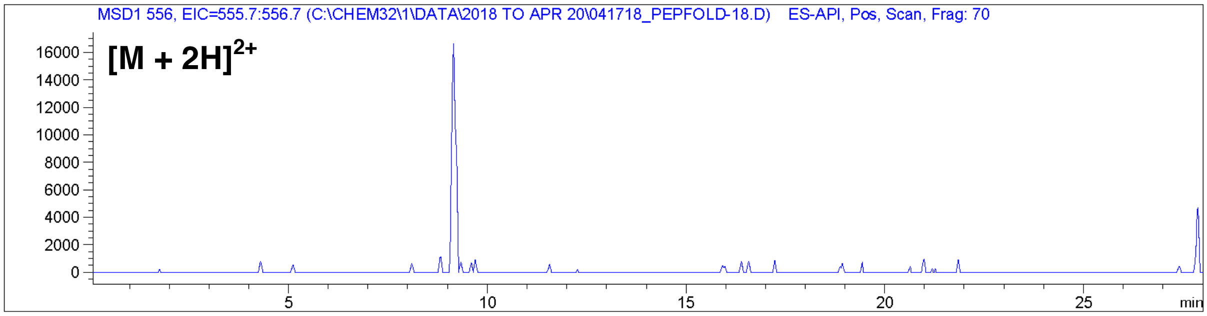
Instrument 1 4/26/18 1:46:45 PM Page 1 of 2

```
=====================================================================
                         Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                    :      1.0000
Dilution:                      :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 B, Sig=210,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]        %
----|-------|----|-------|----------|----------|--------|
   1   9.423 MF    0.0528  685.16229  216.40576   4.3872
   2   9.535 FM    0.1557 1.49320e4  1598.33960  95.6128

Totals :                  1.56172e4  1814.74536



Signal 2: MSD1 TIC, MS File


Signal 3: MSD1 1362, EIC=1361.1:1362.1

=====================================================================
                          *** End of Report ***
```

PEP-FOLD-18, Ac-GGHPKPGCGFGG-NH_2 **(20)**

```
Data File C:\CHEM32\1\DATA\2018 TO APR 20\041718_PEPFOLD-18.D
Sample Name: 041718_pepfold-18

    =====================================================================
    Acq. Operator   : SGLK                            Seq. Line :  17
    Acq. Instrument : Instrument 1                     Location : Vial 77
    Injection Date  : 4/17/18 7:18:44 PM                    Inj :   1
                                                     Inj Volume : 1.000 µl
    Different Inj Volume from Sequence !      Actual Inj Volume : 2.000 µl
    Acq. Method     : D:\CHEM32\1\METHODS\AP_C18_INSERT.M
    Last changed    : 4/17/18 11:25:09 AM by SGLK
    Analysis Method : Z:\DESKTOP\BERTOZZI LAB\LCMS INFO\LCMS METHODS TO 112917\SGLK_BERTOZZIBP_
                      WITHINSERT.M
    Last changed    : 4/26/18 12:19:51 PM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

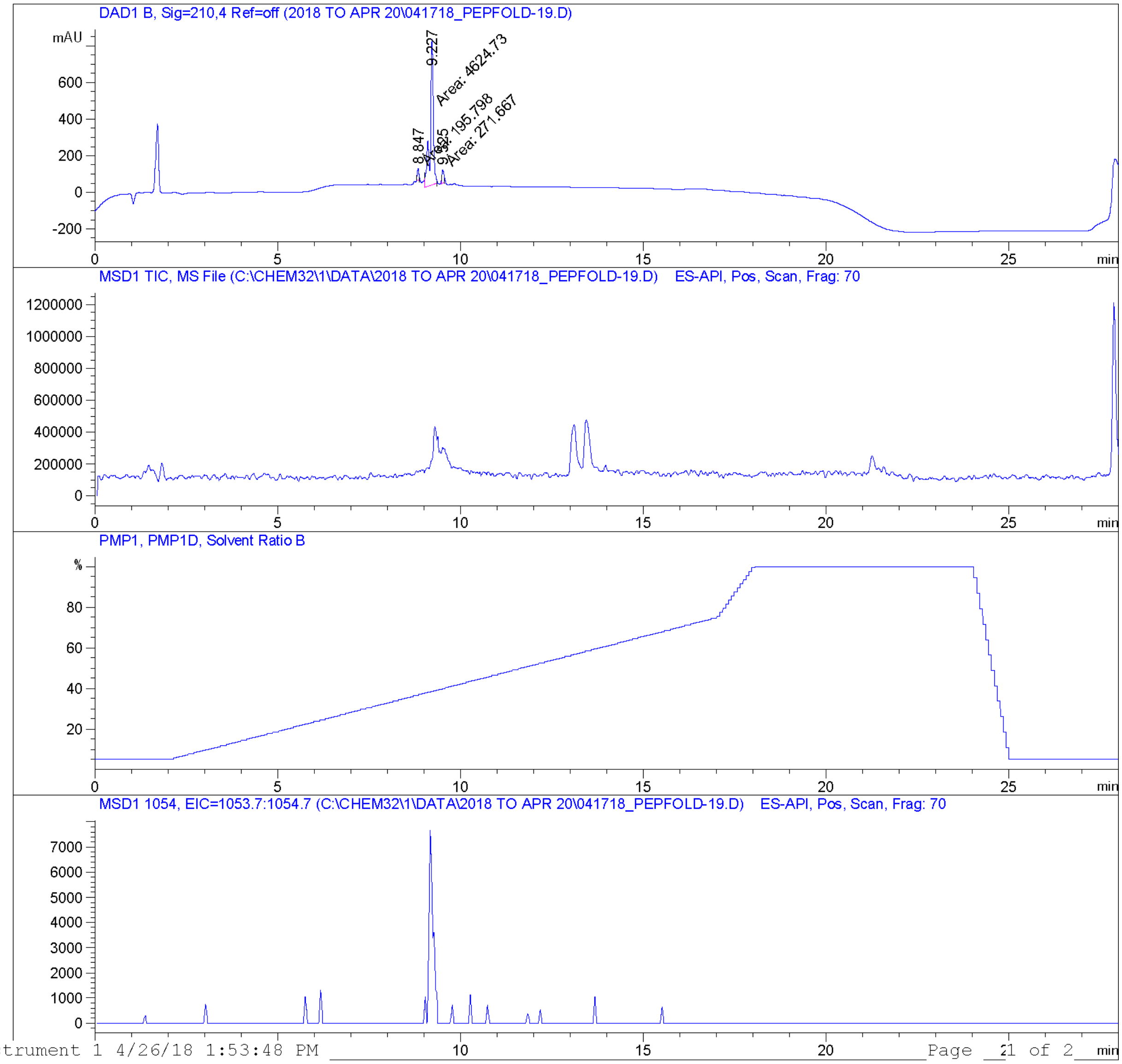


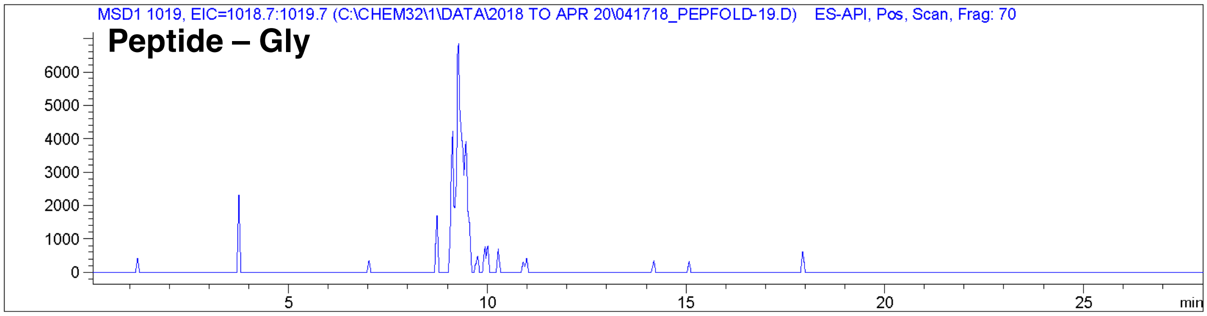


```
=====================================================================
                         Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 B, Sig=210,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]         [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.054 MM    0.0770  274.48676   59.39601  92.5251
   2   9.258 MM    0.0569    9.98745    2.92673   3.3666
   3   9.563 MM    0.0678   12.18780    2.99629   4.1083

Totals :                   296.66201   65.31904



Signal 2: MSD1 TIC, MS File

=====================================================================
                          *** End of Report ***
```

PEP-FOLD-19, Ac-GGHPKPCGFGG-NH_2 **(21)**

```
Data File C:\CHEM32\1\DATA\2018 TO APR 20\041718_PEPFOLD-19.D
Sample Name: 041718_pepfold-19

    =====================================================================
    Acq. Operator   : SGLK                              Seq. Line :  18
    Acq. Instrument : Instrument 1                       Location : Vial 78
    Injection Date  : 4/17/18 7:48:01 PM                      Inj :   1
                                                       Inj Volume : 1.000 µl
    Different Inj Volume from Sequence !        Actual Inj Volume : 2.000 µl
    Acq. Method     : D:\CHEM32\1\METHODS\AP_C18_INSERT.M
    Last changed    : 4/17/18 11:25:09 AM by SGLK
    Analysis Method : Z:\DESKTOP\BERTOZZI LAB\LCMS INFO\LCMS METHODS TO 112917\SGLK_BERTOZZIBP_
                      WITHINSERT.M
    Last changed    : 4/26/18 12:19:51 PM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

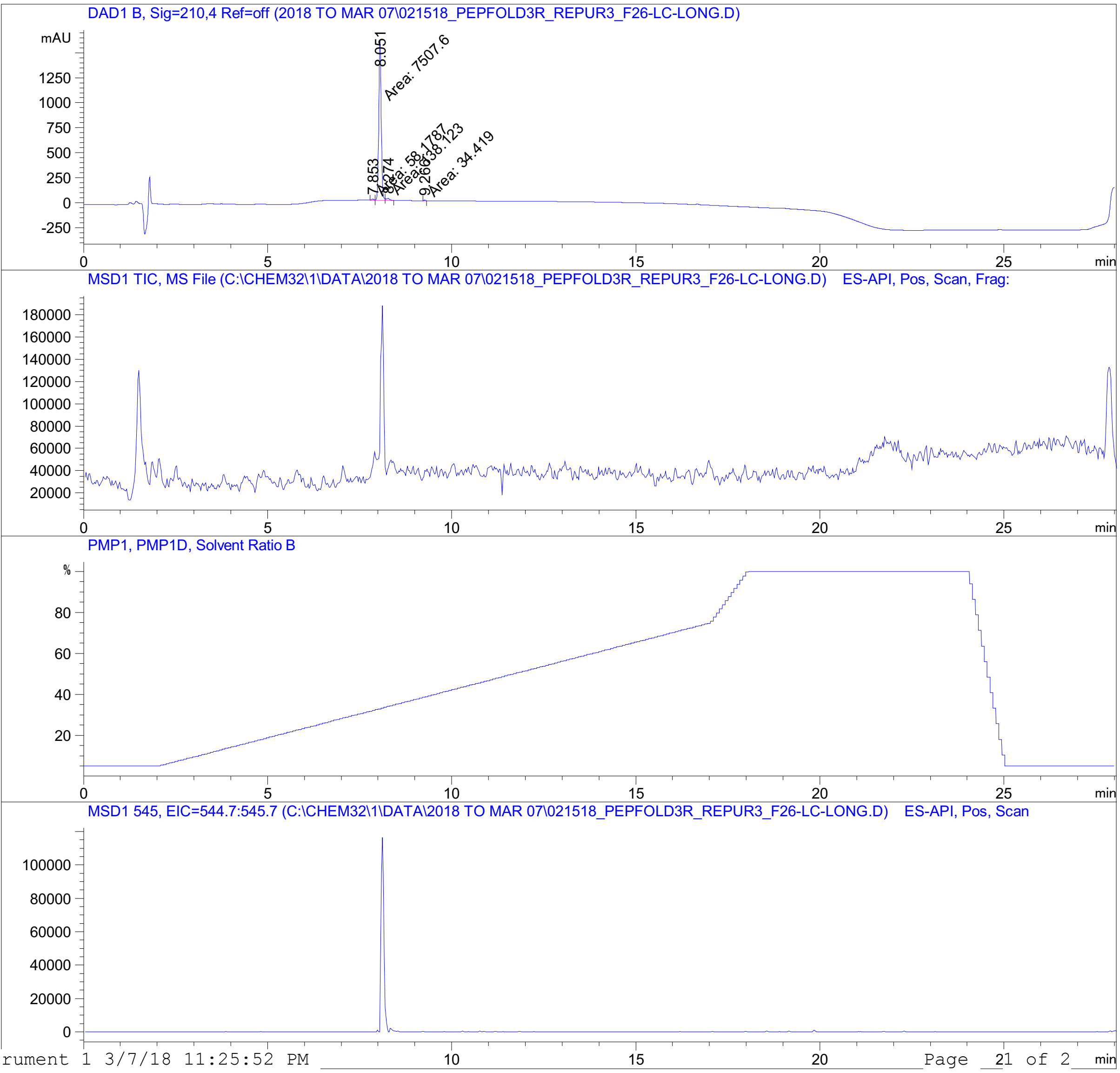


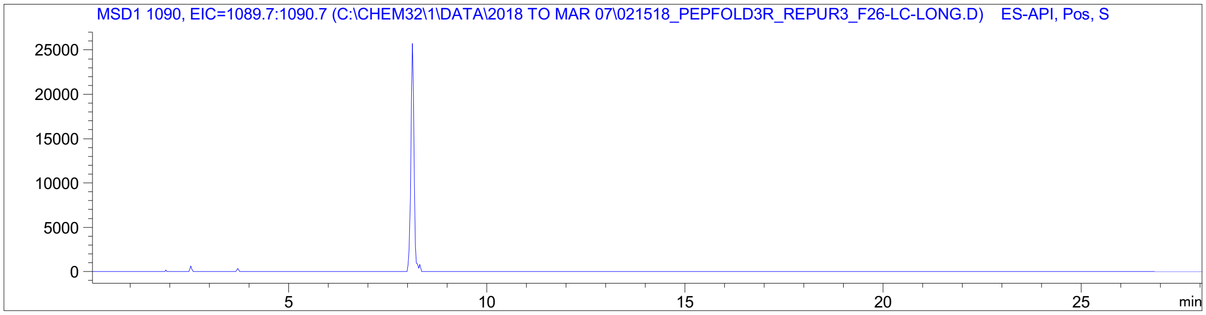


```
=====================================================================
                         Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 B, Sig=210,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #    [min]        [min]   [mAU*s]     [mAU]        %
----|-------|----|-------|----------|----------|--------|
   1   8.847 MM    0.0498  195.79842   65.58862   3.8451
   2   9.227 MM    0.0964 4624.72705  799.44141  90.8199
   3   9.525 MM    0.0609  271.66748   74.33782   5.3350

Totals :                  5092.19295  939.36784



Signal 2: MSD1 TIC, MS File


Signal 3: MSD1 1054, EIC=1053.7:1054.7


Signal 4: MSD1 1019, EIC=1018.7:1019.7

=====================================================================
                          *** End of Report ***
```

CBTag 1.0 (K9R), Ac-GGHPDPCPRGG-NH_2 (**22**)

```
Data File C:\CHEM32\1\DATA\2018 TO MAR 07\021518_PEPFOLD3R_REPUR3_F26-LC-LONG.D
Sample Name: 021518_pepfold3r_repur3_f26-lc-long

    =====================================================================
    Acq. Operator   : SGLK                           Seq. Line :   1
    Acq. Instrument : Instrument 1                    Location : Vial 21
    Injection Date  : 2/15/18 3:16:09 PM                   Inj :   1
                                                Inj Volume : 1.000 µl
    Different Inj Volume from Sequence !     Actual Inj Volume : 25.000 µl
    Acq. Method     : D:\CHEM32\1\METHODS\AP_C18_INSERT.M
    Last changed    : 2/14/18 7:50:15 PM by SGLK
    Analysis Method : Z:\DESKTOP\BERTOZZI LAB\LCMS INFO\LCMS METHODS TO 112917\SGLK_BERTOZZIBP_
                      WITHINSERT.M
    Last changed    : 3/6/18 6:13:20 PM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

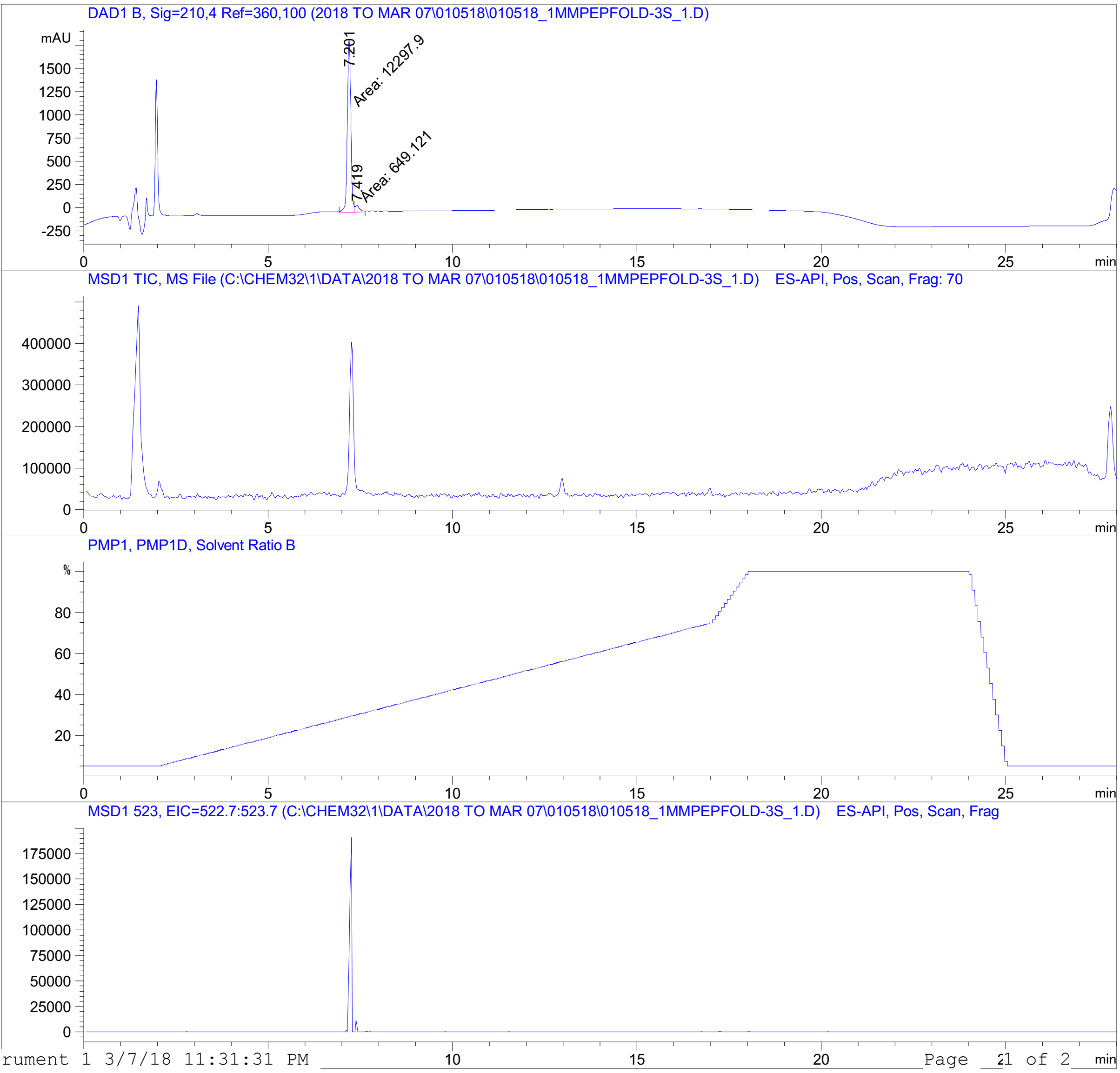




```
=====================================================================
                         Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 B, Sig=210,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]        %
----|-------|----|-------|----------|----------|--------|
   1   7.853 MF    0.0853   58.17865   11.36420   0.7518
   2   8.051 FM    0.0776 7507.59863 1611.58948  97.0185
   3   8.274 FM    0.1097  138.12289   20.97552   1.7849
   4   9.266 MM    0.0639   34.41899    8.97556   0.4448

Totals :                  7738.31917 1652.90476



Signal 2: MSD1 TIC, MS File

=====================================================================
                          *** End of Report ***
```

CBTag 1.0 (C7S), Ac-GGHPDPSPKGG-NH_2 **(23)**

```
Data File C:\CHEM32\1\DATA\2018 TO MAR 07\010518\010518_1MMPEPFOLD-3S_1.D
Sample Name: 010518_1mMpepfold-3S_1

     =====================================================================
     Acq. Operator   : sglk                              Seq. Line :  28
     Acq. Instrument : Instrument 1                       Location : Vial 38
     Injection Date  : 1/6/18 5:50:45 AM                       Inj :   1
                                                        Inj Volume : 15.000 µl
     Different Inj Volume from Sequence !       Actual Inj Volume : 10.000 µl
     Acq. Method     : D:\CHEM32\1\METHODS\AP_C18_INSERT.M
     Last changed    : 11/10/17 3:07:57 PM by Mason
     Analysis Method : Z:\DESKTOP\BERTOZZI LAB\LCMS INFO\LCMS METHODS TO 112917\SGLK_BERTOZZIBP_
                       WITHINSERT.M
     Last changed    : 3/6/18 6:13:20 PM
                       (modified after loading)
     Additional Info : Peak(s) manually integrated
```

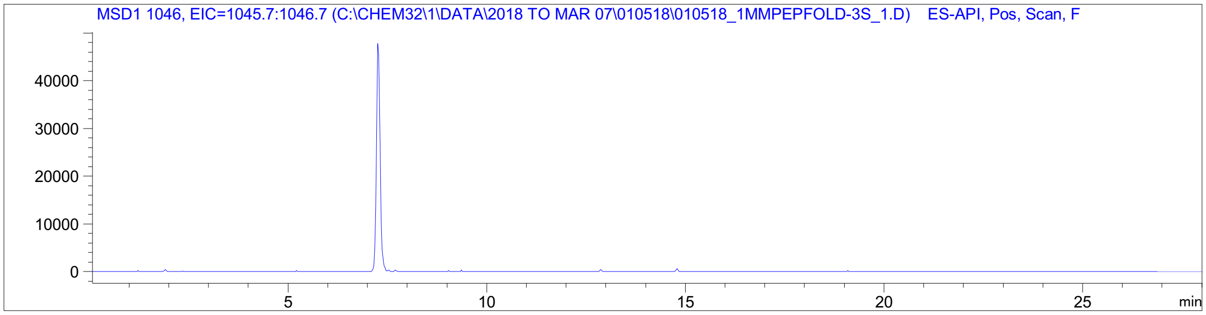


DAD1 B, Sig=210,4 Ref=360,100 (2018 TO MAR 07\010518\010518_1MMPEPFOLD-3S_1.D)

MSD1 TIC, MS File (C:\CHEM32\1\DATA\2018 TO MAR 07\010518\010518_1MMPEPFOLD-3S_1.D)   ES-API, Pos, Scan, Frag: 70

PMP1, PMP1D, Solvent Ratio B

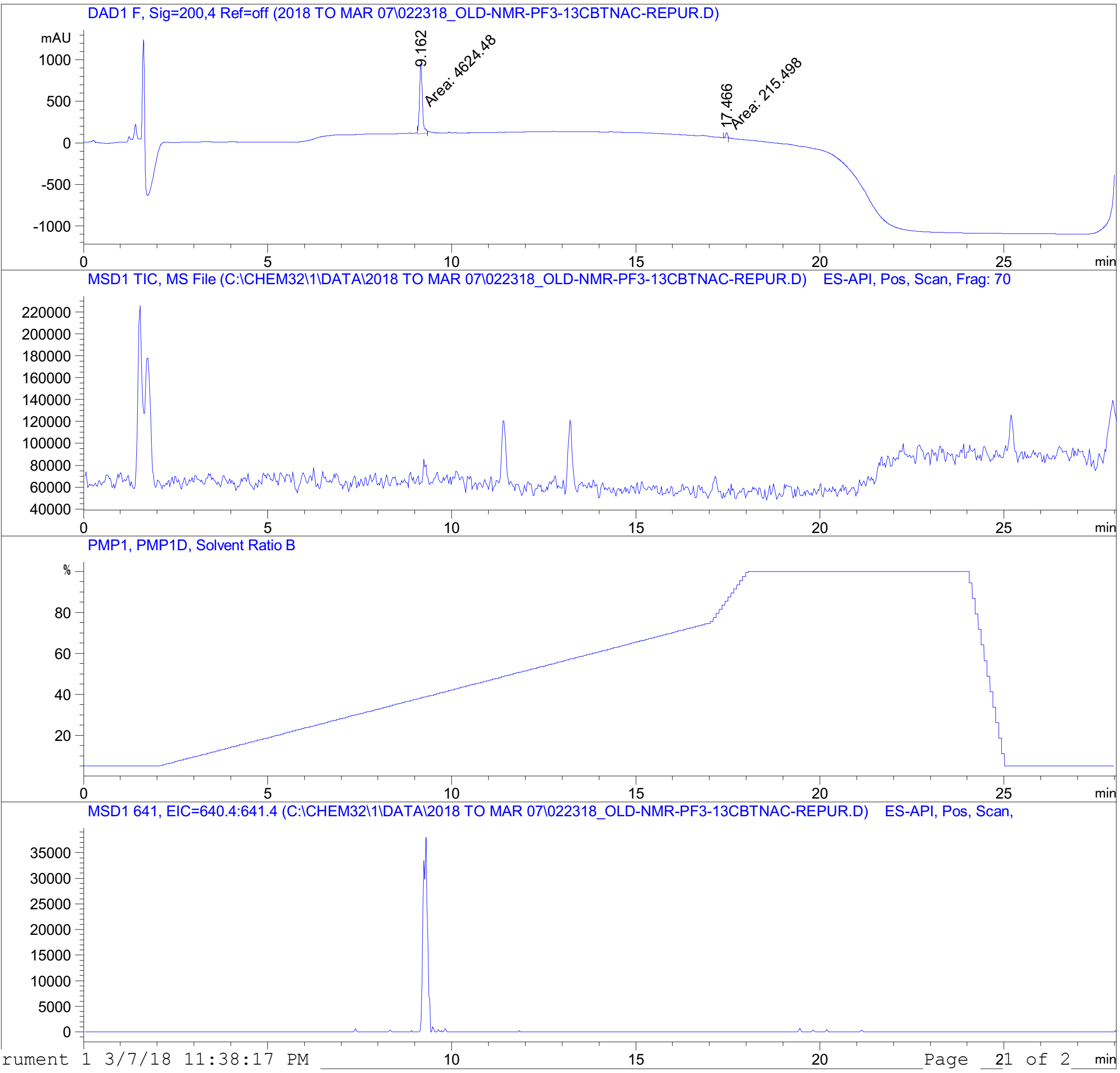
MSD1 523, EIC=522.7:523.7 (C:\CHEM32\1\DATA\2018 TO MAR 07\010518\010518_1MMPEPFOLD-3S_1.D)   ES-API, Pos, Scan, Frag

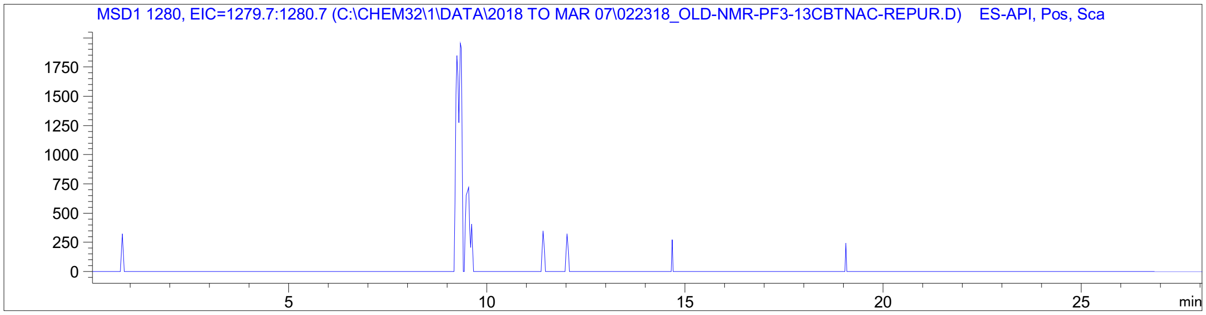


```
=====================================================================
                         Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 B, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]        %
----|-------|----|-------|----------|----------|--------|
   1   7.201 MF    0.1101 1.22979e4  1862.15747  94.9863
   2   7.419 FM    0.1554  649.12140   69.64057   5.0137

Totals :                  1.29470e4  1931.79804



Signal 2: MSD1 TIC, MS File

=====================================================================
                          *** End of Report ***
```

CBTag 1.0-13CBTNAc (amidine) (24). Synthesized and purified following Method 2.

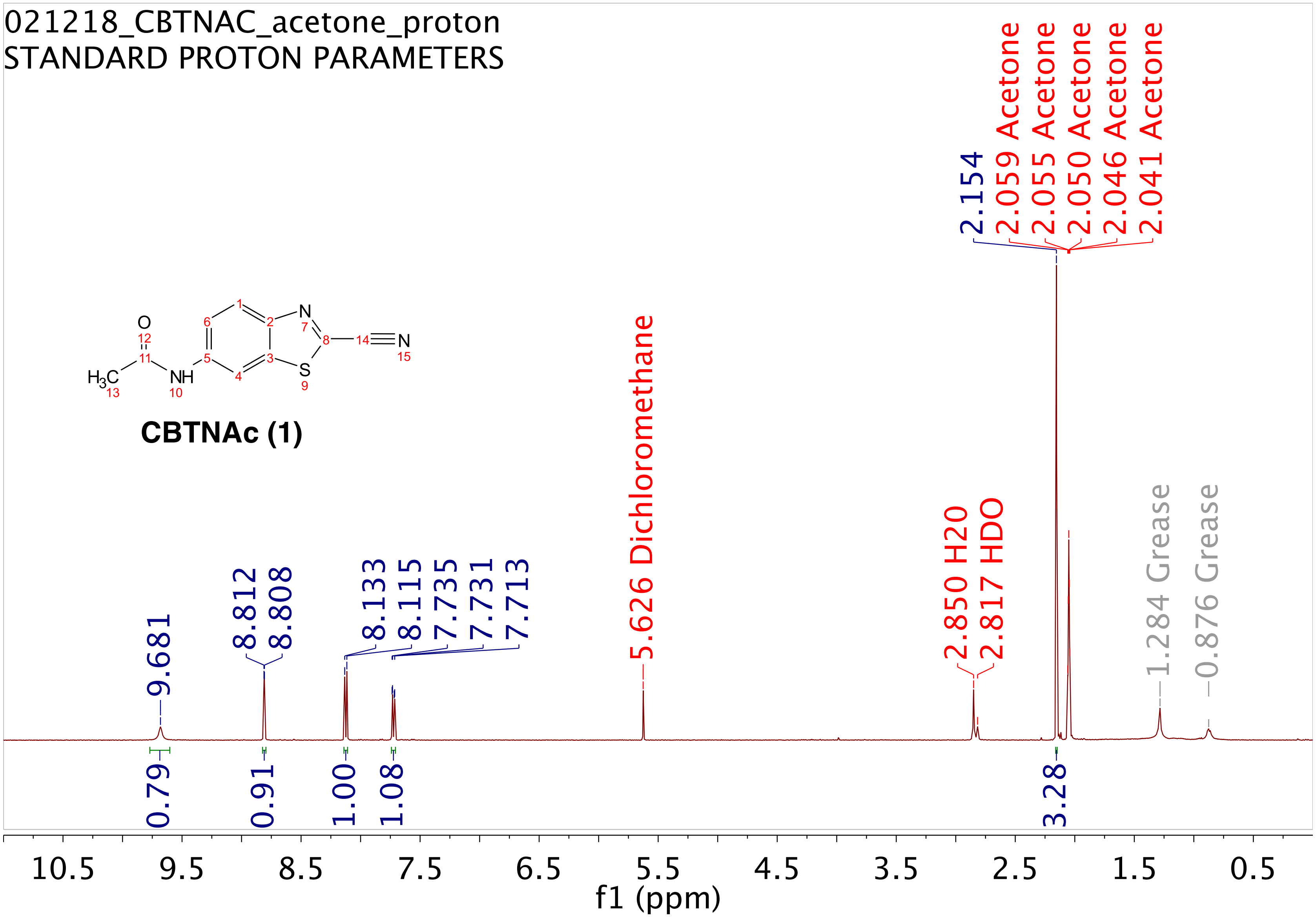
```
Data File C:\CHEM32\1\DATA\2018 TO MAR 07\022318_OLD-NMR-PF3-13CBTNAC-REPUR.D
Sample Name: 022318_old-nmr-pf3-13cbtnac-repur

    =====================================================================
    Acq. Operator   : SGLK                            Seq. Line :   1
    Acq. Instrument : Instrument 1                     Location : Vial 52
    Injection Date  : 2/23/18 5:33:18 PM                    Inj :   1
                                                     Inj Volume : 1.000 µl
    Different Inj Volume from Sequence !      Actual Inj Volume : 75.000 µl
    Acq. Method     : D:\CHEM32\1\METHODS\AP_C18_INSERT.M
    Last changed    : 2/23/18 4:30:31 PM by SGLK
    Analysis Method : Z:\DESKTOP\BERTOZZI LAB\LCMS INFO\LCMS METHODS TO 112917\SGLK_BERTOZZIBP_
                      WITHINSERT.M
    Last changed    : 3/6/18 6:13:20 PM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

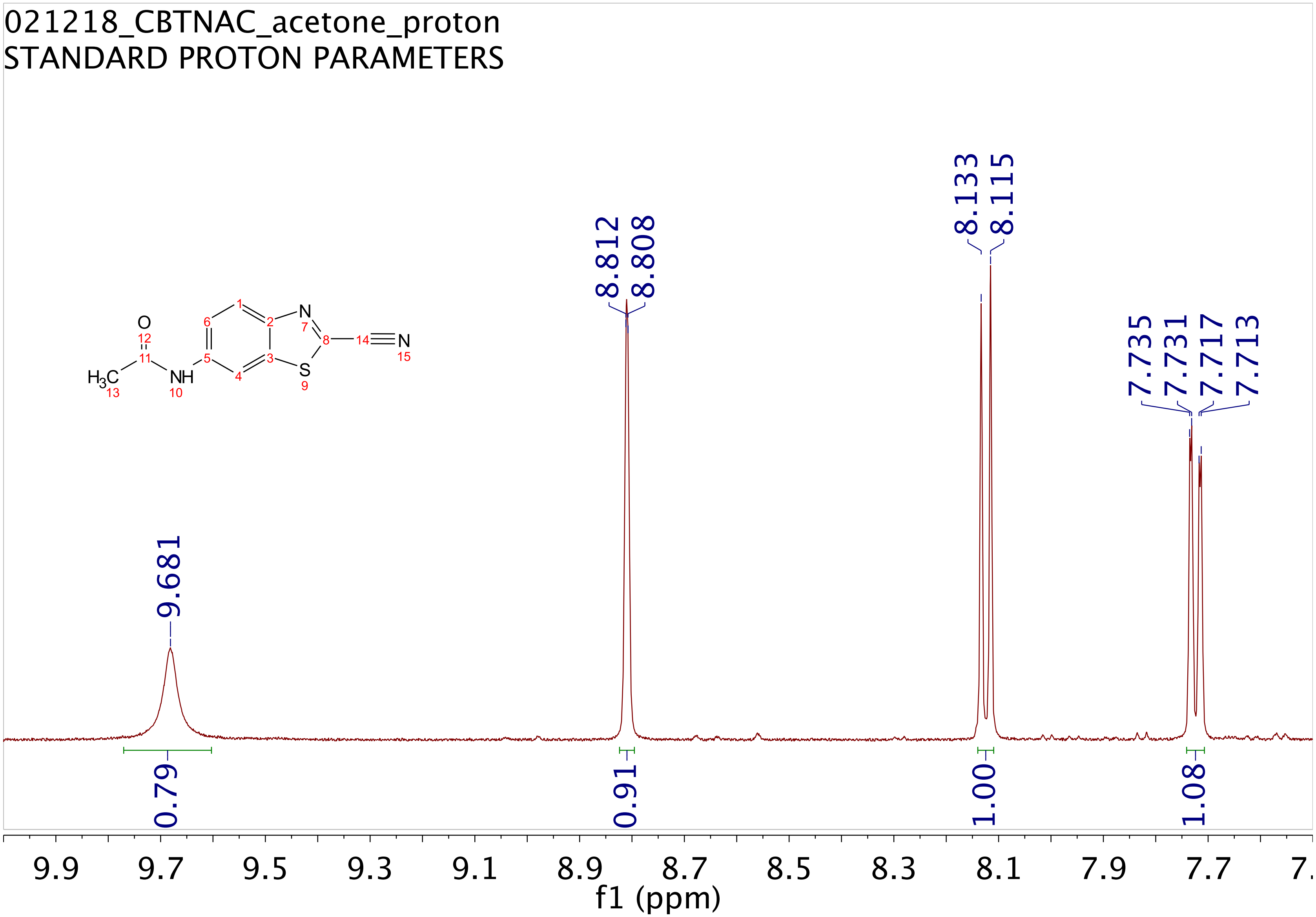


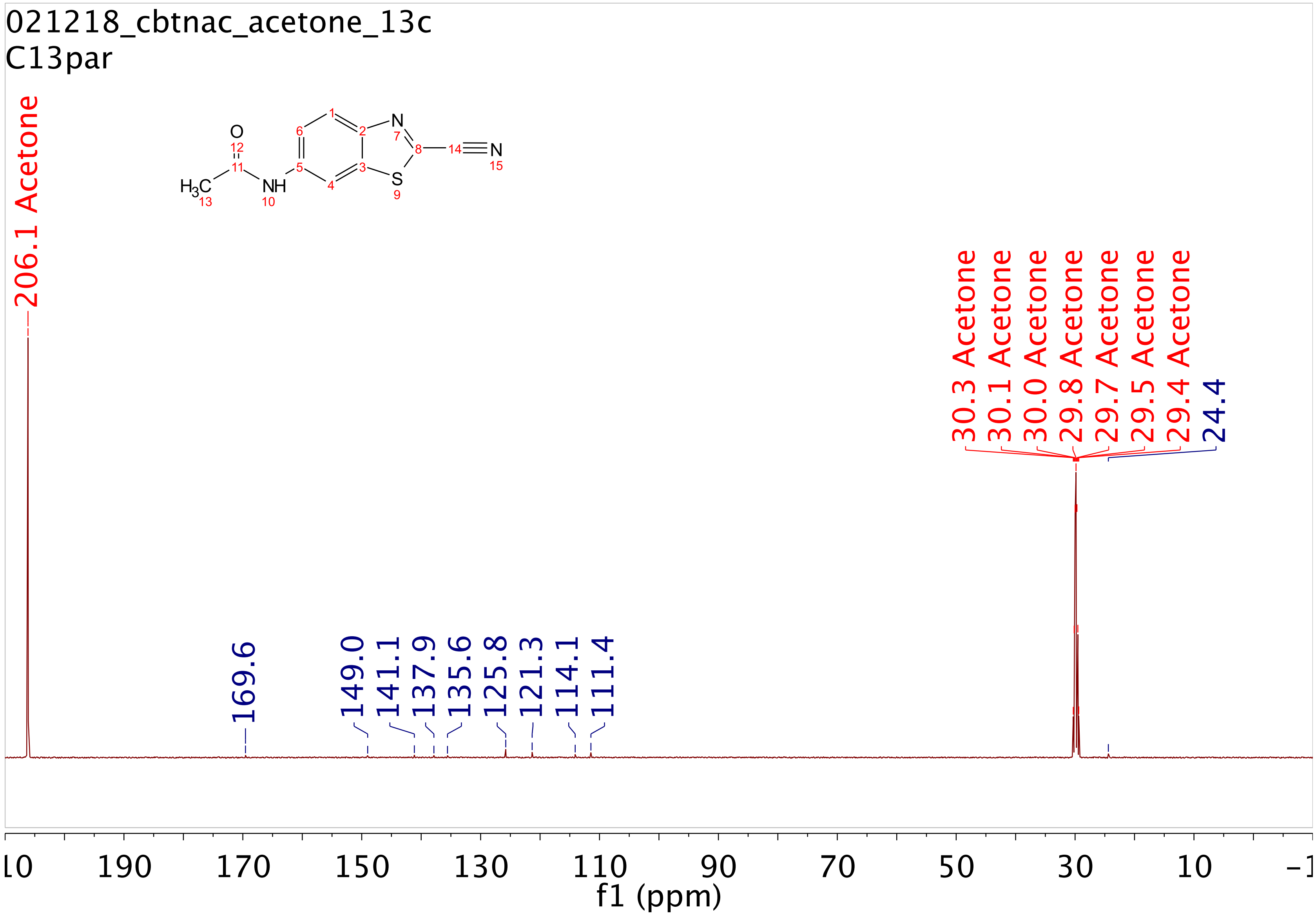


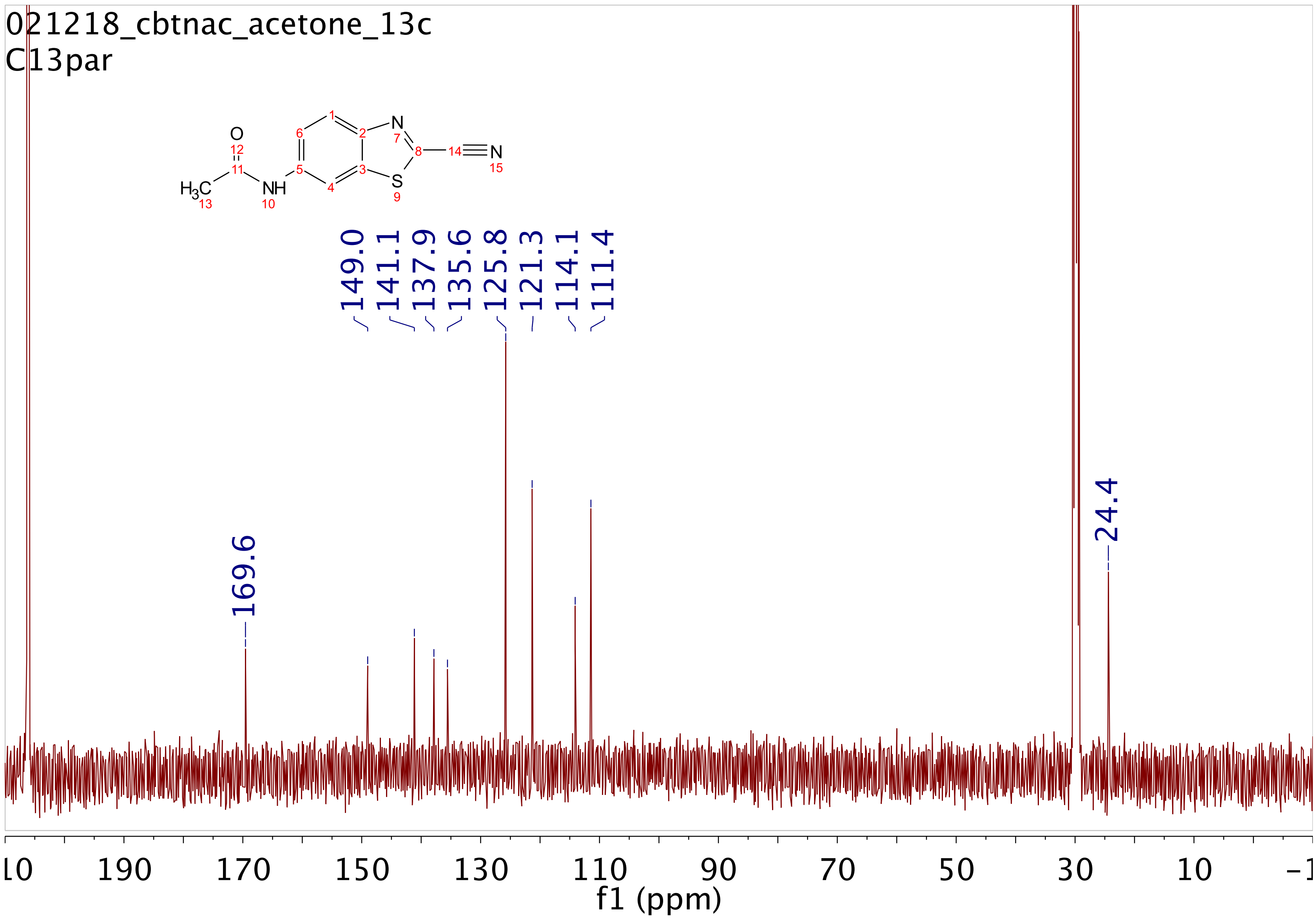
```
=====================================================================
                         Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 F, Sig=200,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]        %
----|-------|----|-------|----------|----------|--------|
   1   9.162 MM    0.0911 4624.47559  846.48572  95.5475
   2  17.466 MM    0.0596  215.49754   60.21696   4.4525

Totals :                  4839.97313  906.70268



Signal 2: MSD1 TIC, MS File

=====================================================================
                          *** End of Report ***
```

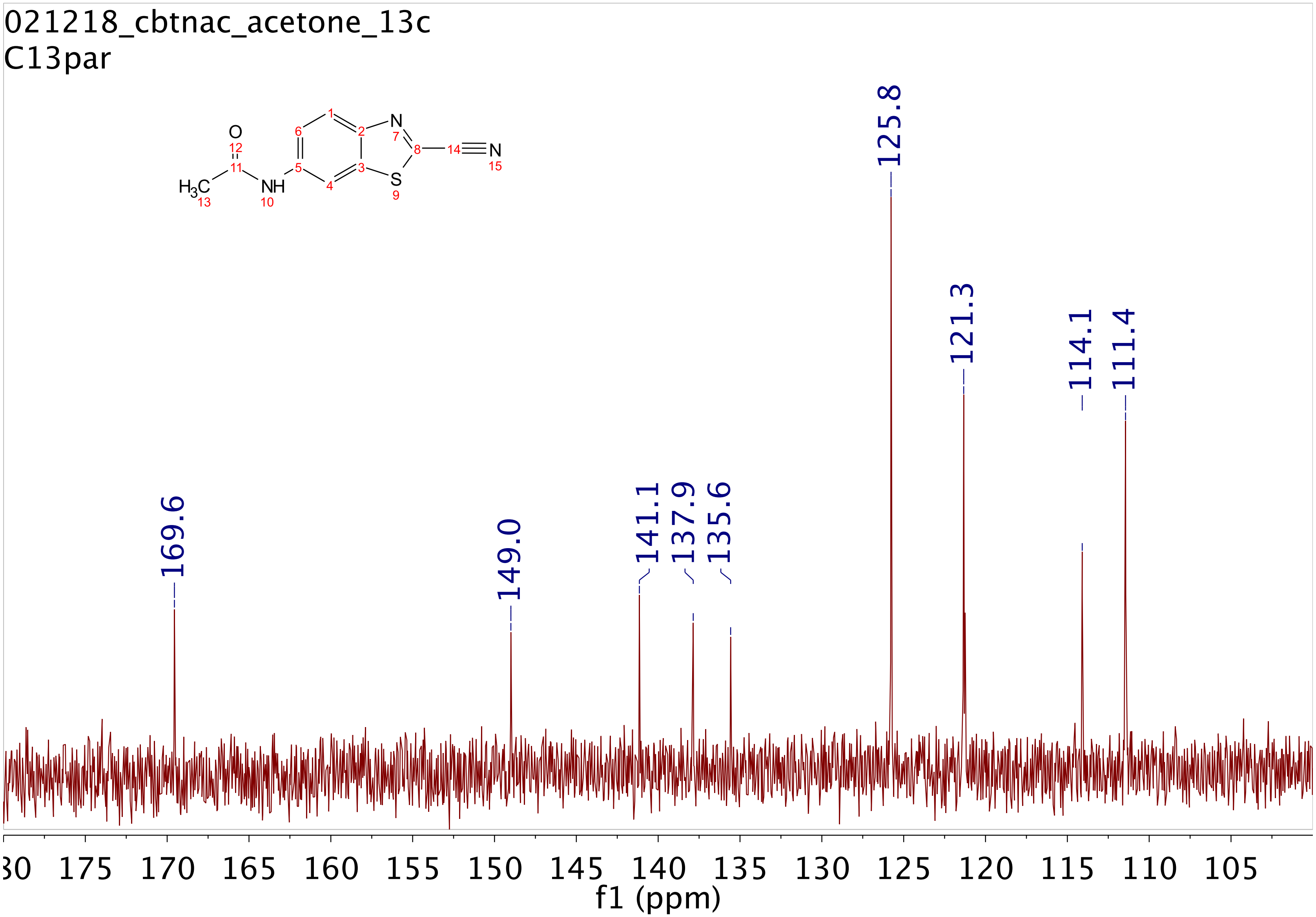
NMR Spectra

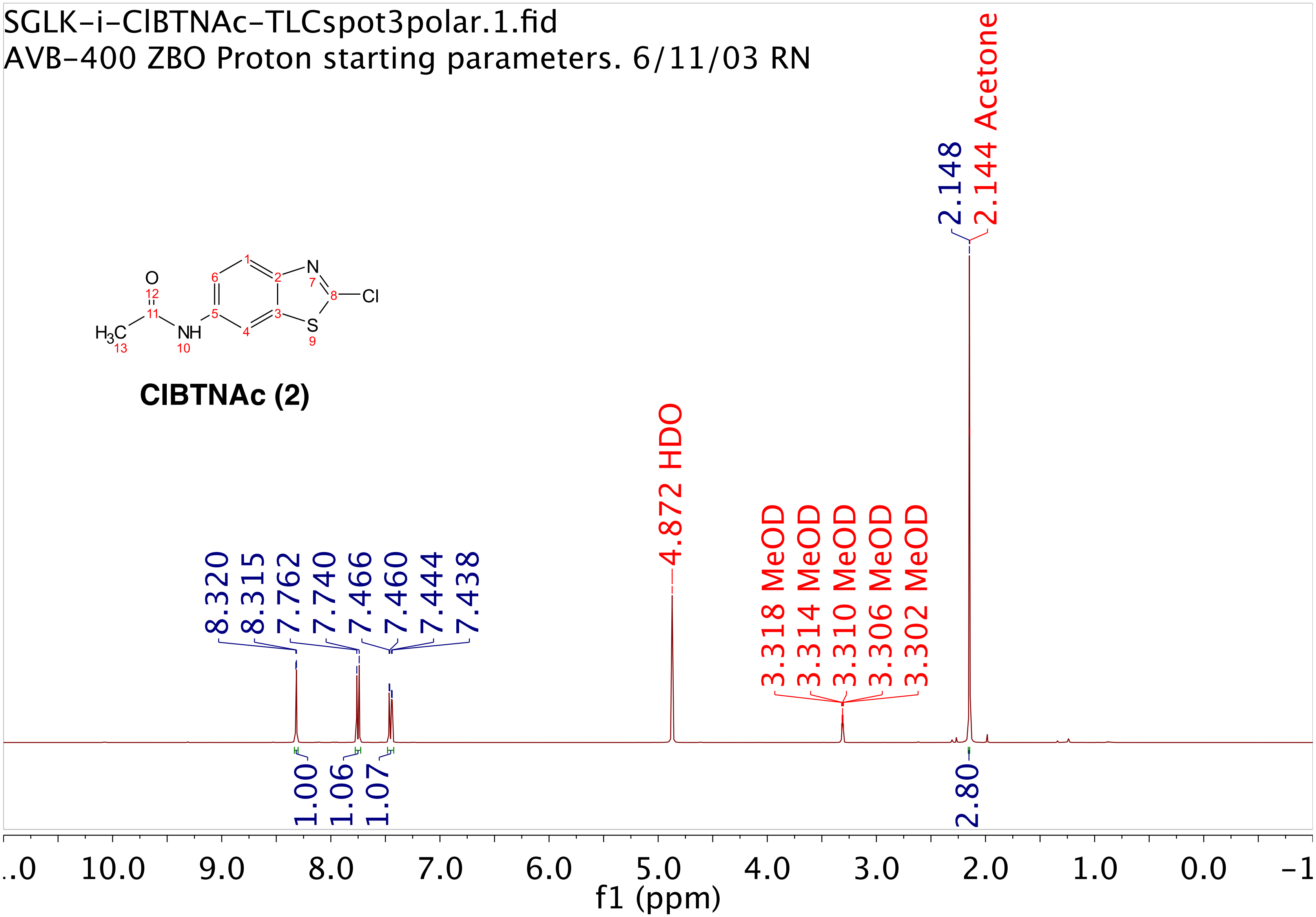

021218_CBTNAC_acetone_proton
STANDARD PROTON PARAMETERS
CBTNAc (1)
O
H3C
NH
N
S
N
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
9.681
8.812
8.808
8.133
8.115
7.735
7.731
7.713
5.626 Dichloromethane
2.850 H20
2.817 HDO
2.154
2.059 Acetone
2.055 Acetone
2.050 Acetone
2.046 Acetone
2.041 Acetone
1.284 Grease
0.876 Grease
0.79
0.91
1.00
1.08
3.28
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

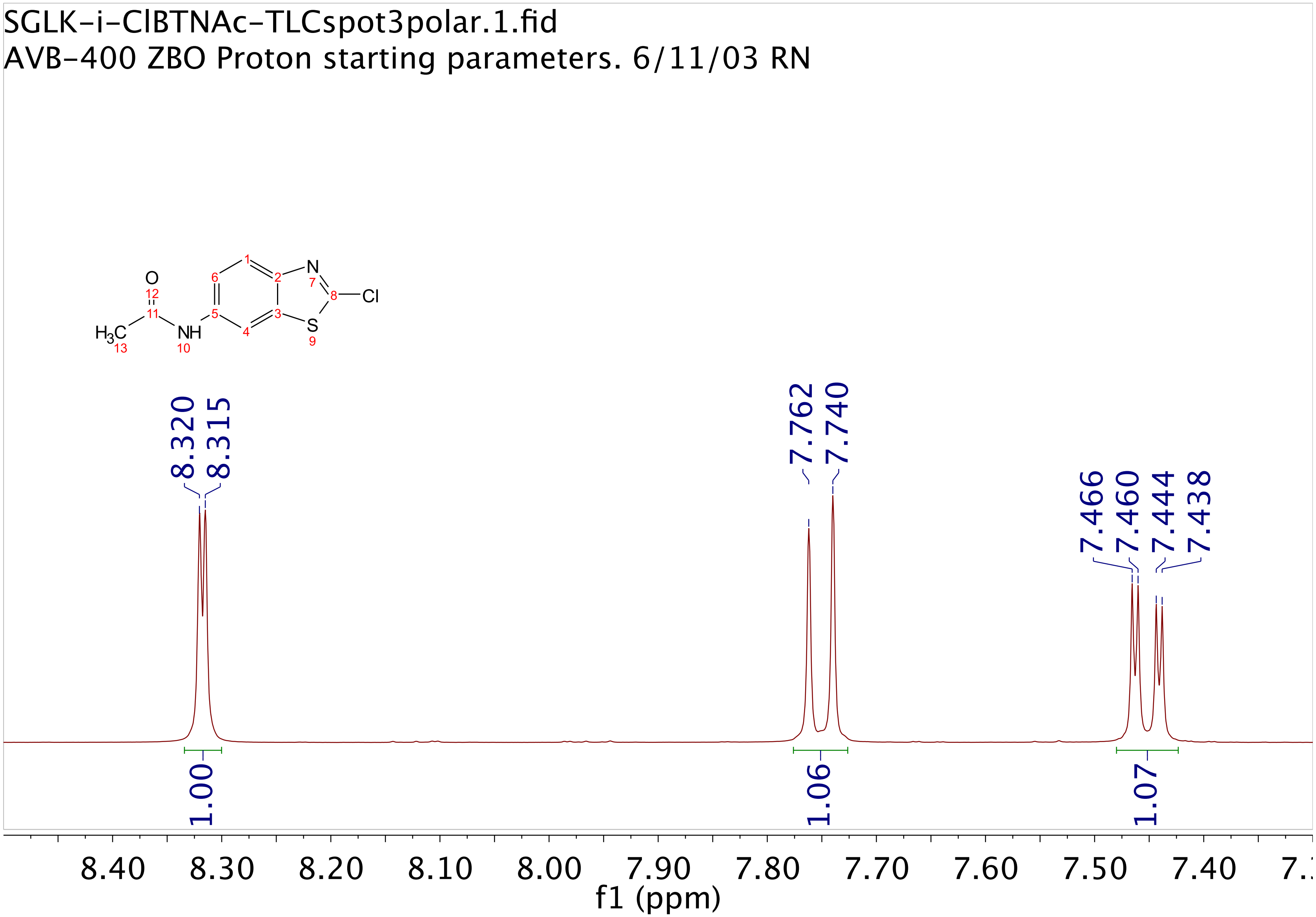

021218_CBTNAC_acetone_proton
STANDARD PROTON PARAMETERS
O
12
11
H3C
13
NH
10
1
2
3
4
5
6
N
7
8
S
9
14
N
15
9.681
8.812
8.808
8.133
8.115
7.735
7.731
7.717
7.713
0.79
0.91
1.00
1.08
9.9
9.7
9.5
9.3
9.1
8.9
8.7
8.5
8.3
8.1
7.9
7.7
7.
f1 (ppm)

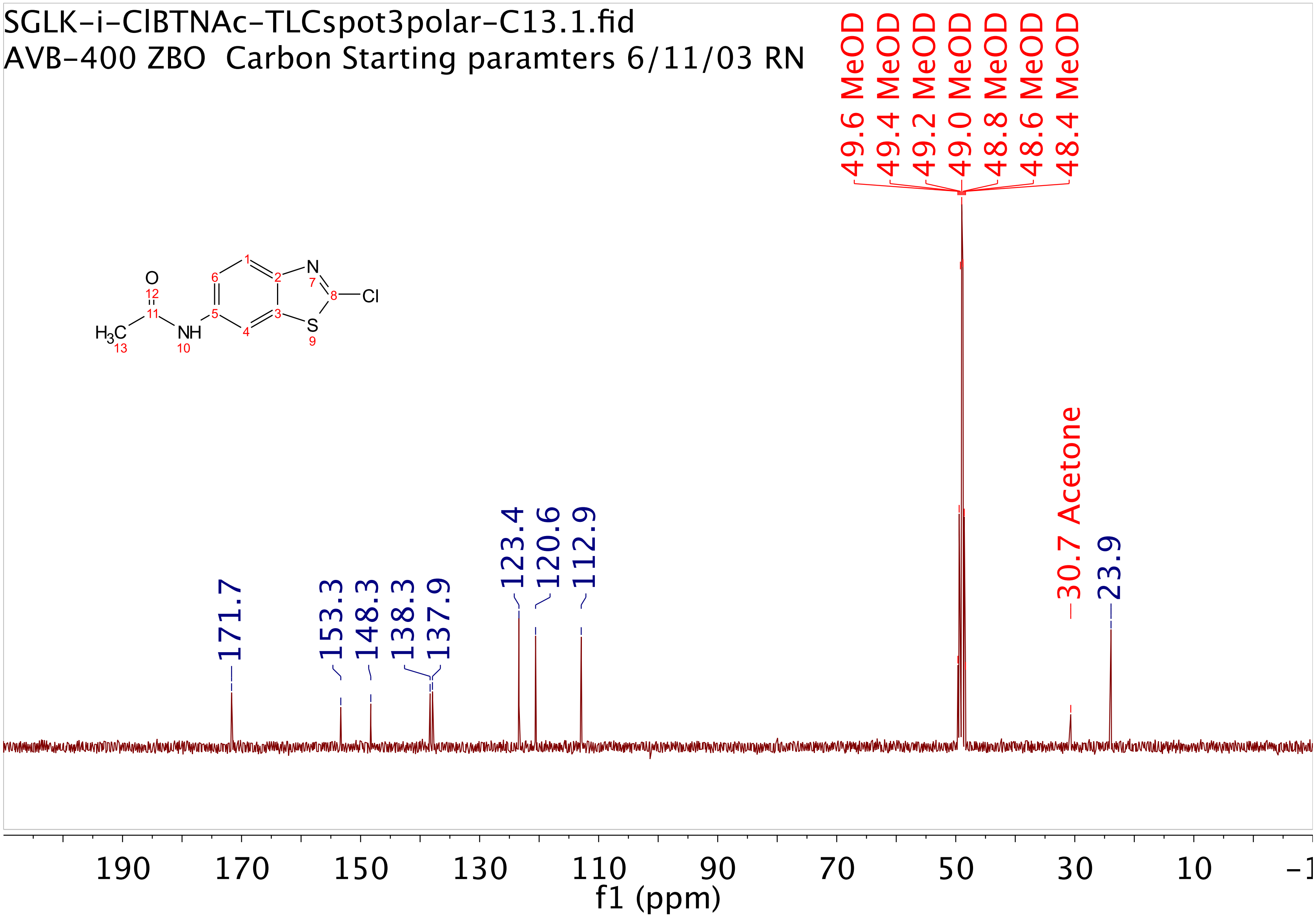

021218_cbtnac_acetone_13c
C13par
206.1 Acetone
169.6
149.0
141.1
137.9
135.6
125.8
121.3
114.1
111.4
30.3 Acetone
30.1 Acetone
30.0 Acetone
29.8 Acetone
29.7 Acetone
29.5 Acetone
29.4 Acetone
24.4
O
12
11
H_3C
13
NH
10
6
5
4
1
2
3
N
7
8
S
9
14
N
15
10
190
170
150
130
110
90
70
50
30
10
-1
f1 (ppm)

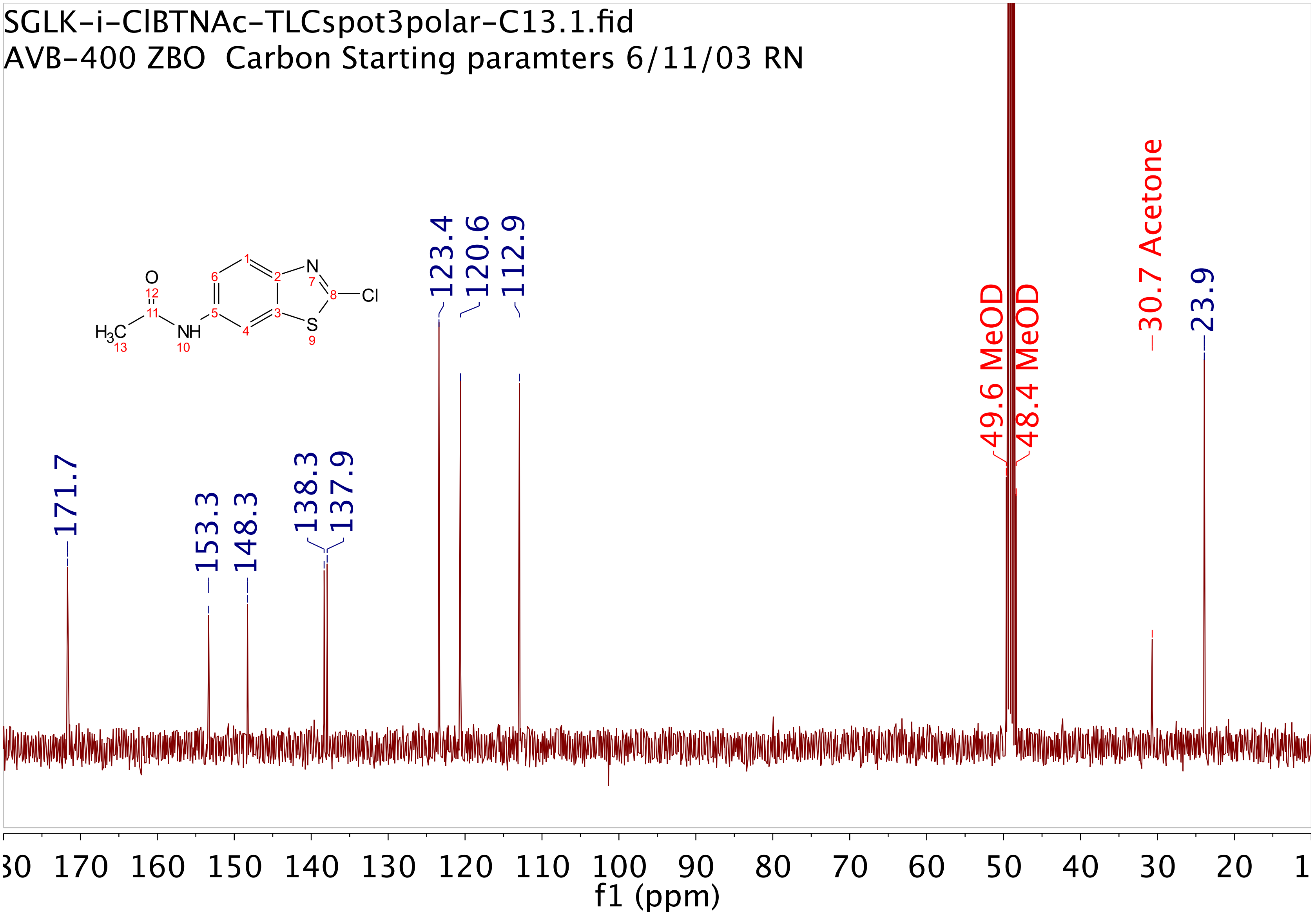

021218_cbtnac_acetone_13c
C13par
O
12
11
H3C
13
NH
10
5
6
1
2
N
7
8
14
N
15
3
4
S
9
149.0
141.1
137.9
135.6
125.8
121.3
114.1
111.4
169.6
24.4
10
190
170
150
130
110
90
70
50
30
10
-1
f1 (ppm)

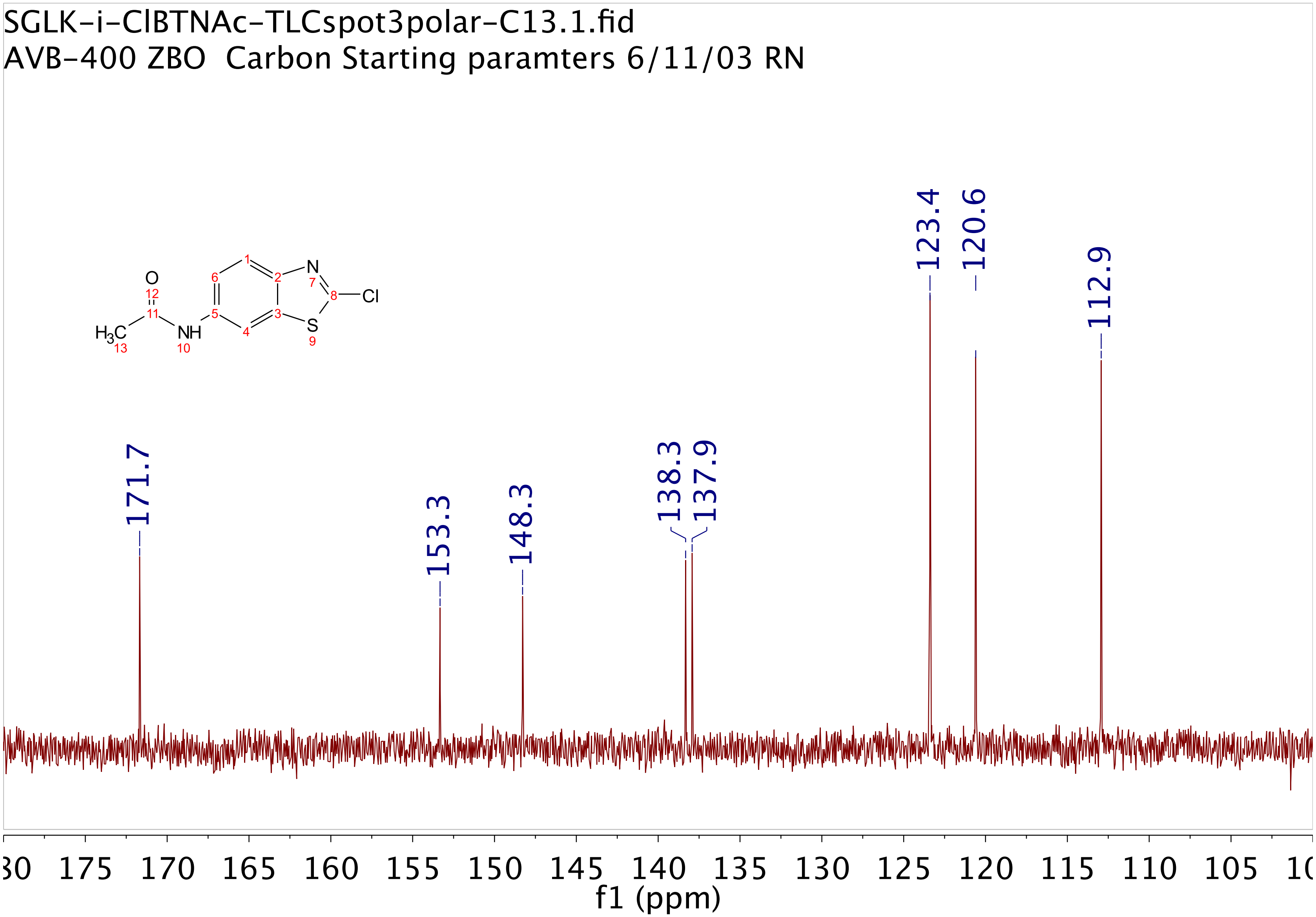

021218_cbtnac_acetone_13c
C13par
O
12
11
H3C
13
NH
10
1
2
3
4
5
6
N
7
8
S
9
14
N
15
169.6
149.0
141.1
137.9
135.6
125.8
121.3
114.1
111.4
30
175
170
165
160
155
150
145
140
135
130
125
120
115
110
105
f1 (ppm)

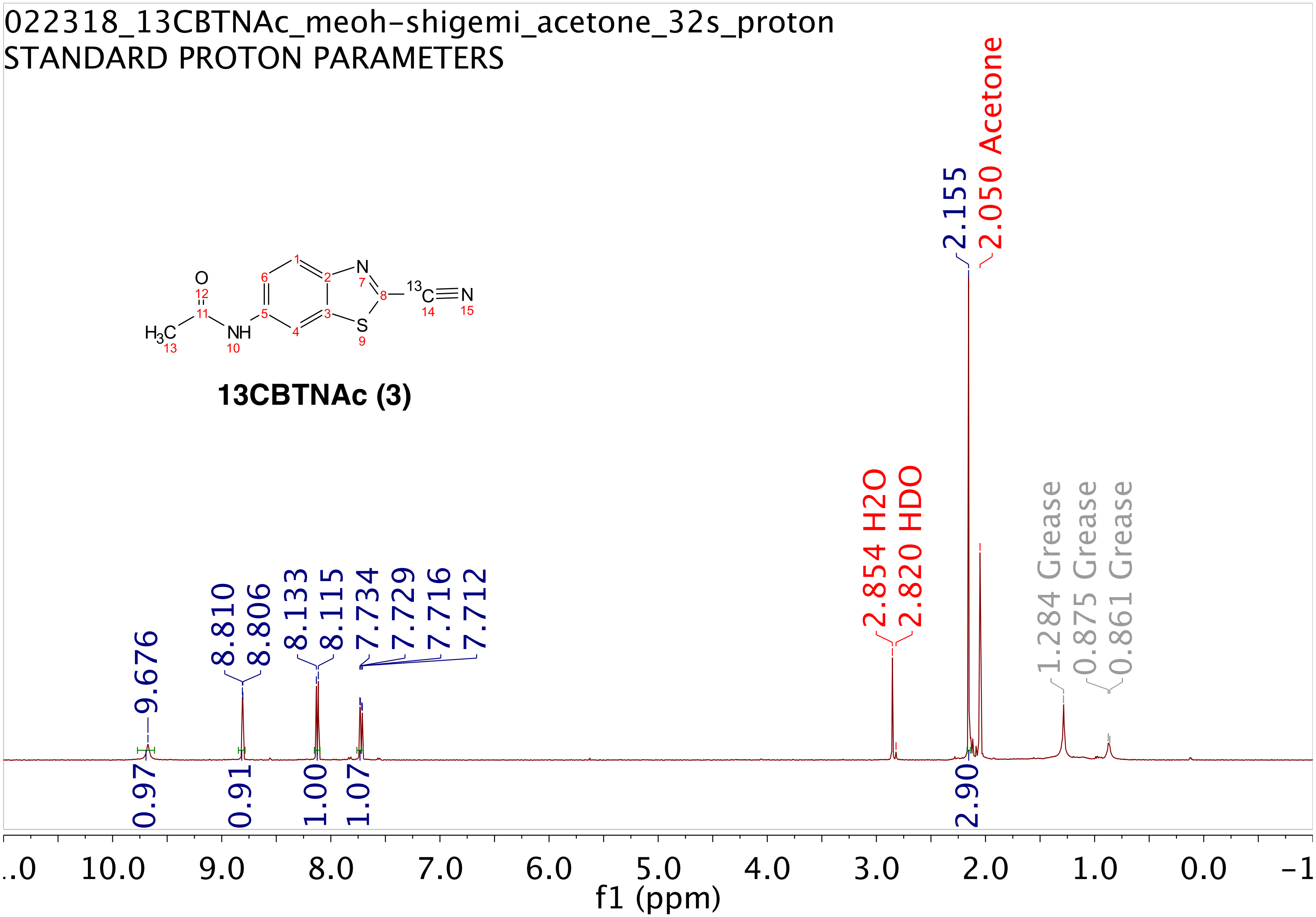

SGLK-i-ClBTNAc-TLCspot3polar.1.fid
AVB-400 ZBO Proton starting parameters. 6/11/03 RN
O
12
11
H3C
13
NH
10
6
5
1
4
2
3
N
7
8
Cl
S
9
ClBTNAc (2)
8.320
8.315
7.762
7.740
7.466
7.460
7.444
7.438
4.872 HDO
3.318 MeOD
3.314 MeOD
3.310 MeOD
3.306 MeOD
3.302 MeOD
2.148
2.144 Acetone
1.00
1.06
1.07
2.80
..0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1
f1 (ppm)

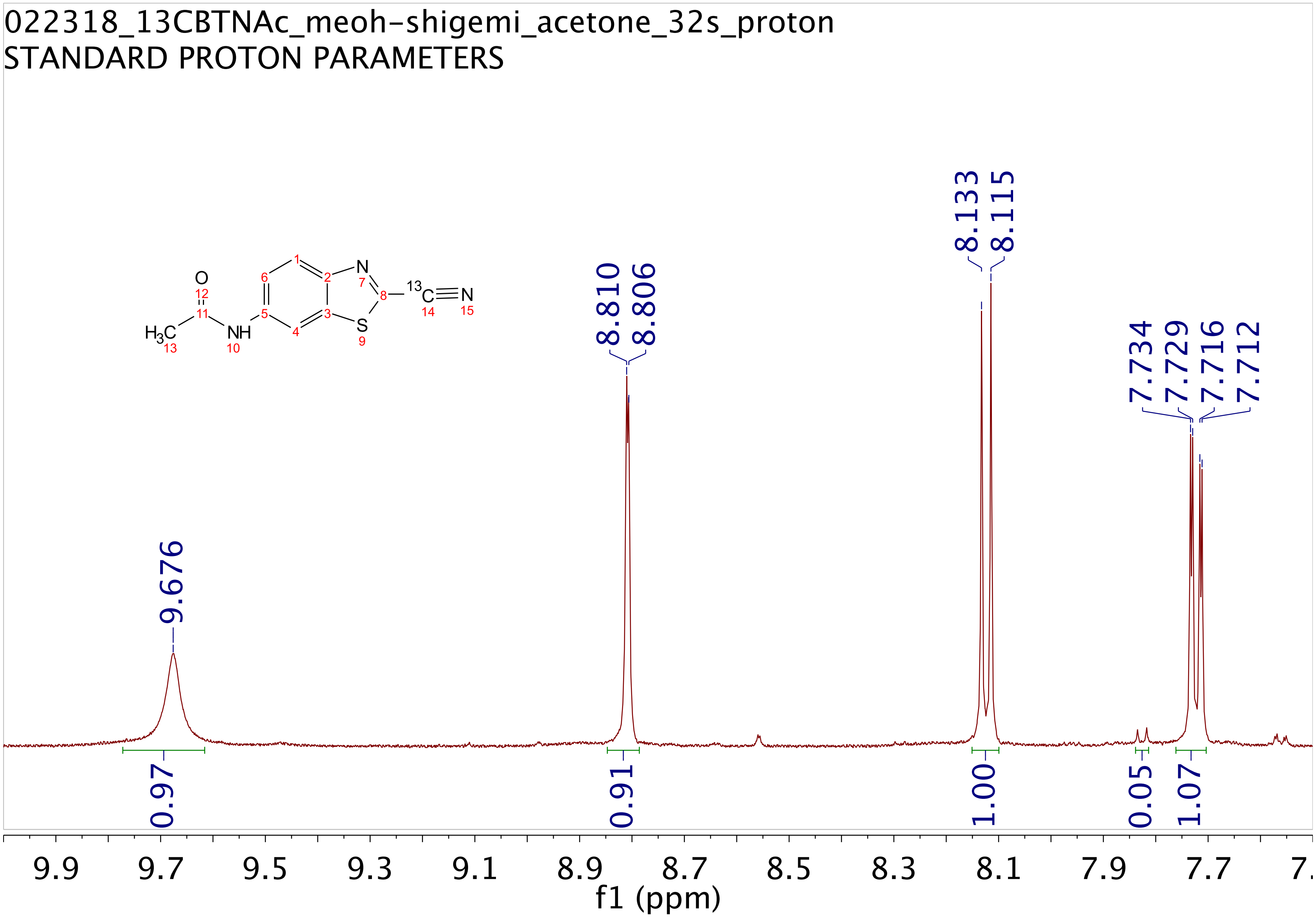

SGLK-i-ClBTNAc-TLCspot3polar.1.fid
AVB-400 ZBO Proton starting parameters. 6/11/03 RN
O
12
11
H_3C
13
NH
10
5
6
1
2
3
4
N
7
8
Cl
S
9
8.320
8.315
7.762
7.740
7.466
7.460
7.444
7.438
1.00
1.06
1.07
8.40
8.30
8.20
8.10
8.00
7.90
7.80
7.70
7.60
7.50
7.40
f1 (ppm)

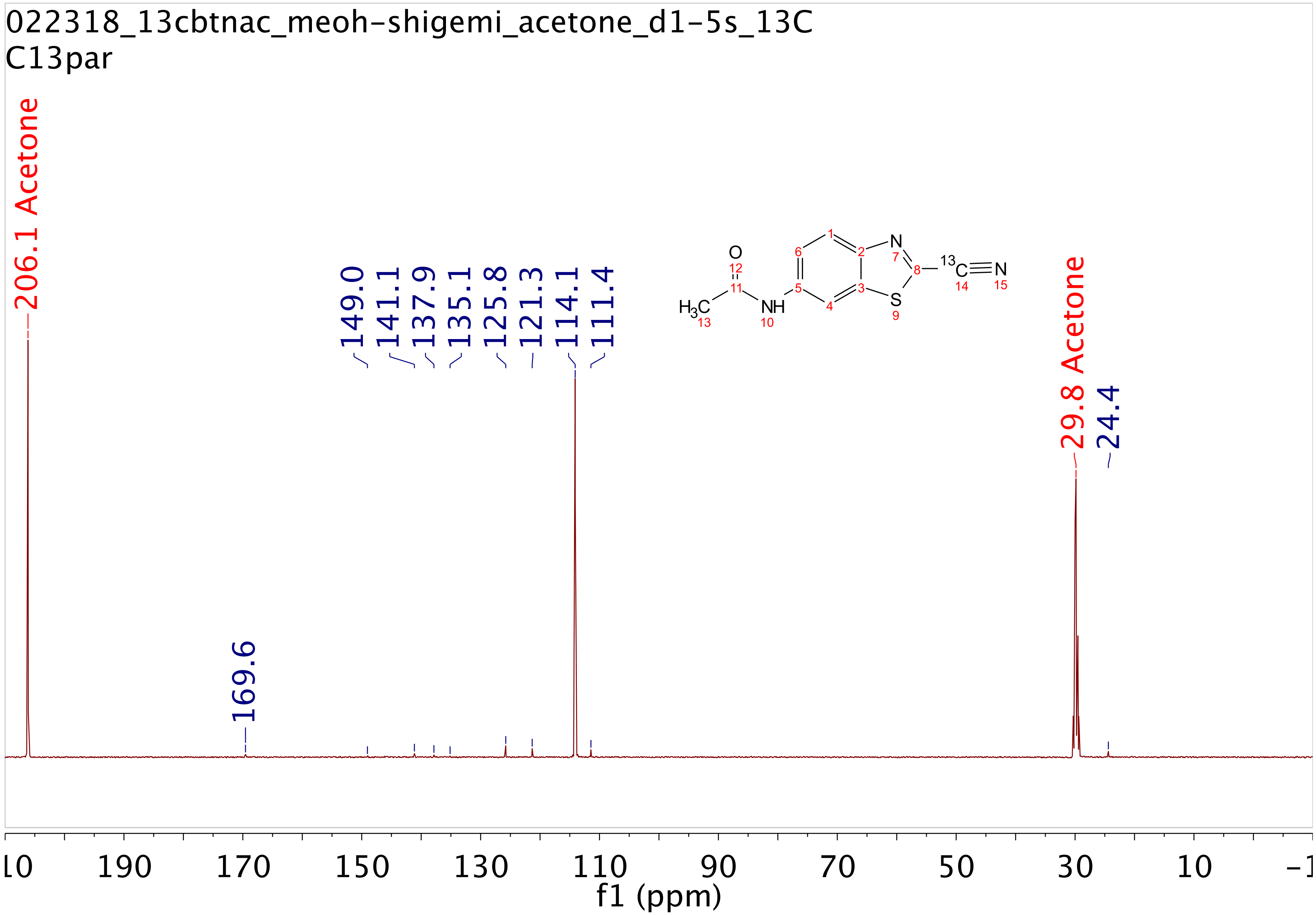

SGLK-i-ClBTNAc-TLCspot3polar-C13.1.fid
AVB-400 ZBO Carbon Starting paramters 6/11/03 RN
49.6 MeOD
49.4 MeOD
49.2 MeOD
49.0 MeOD
48.8 MeOD
48.6 MeOD
48.4 MeOD
O
12
11
H3C
13
NH
10
6
1
5
4
2
3
N
7
8
Cl
S
9
30.7 Acetone
171.7
153.3
148.3
138.3
137.9
123.4
120.6
112.9
23.9
190
170
150
130
110
90
70
50
30
10
-1
f1 (ppm)

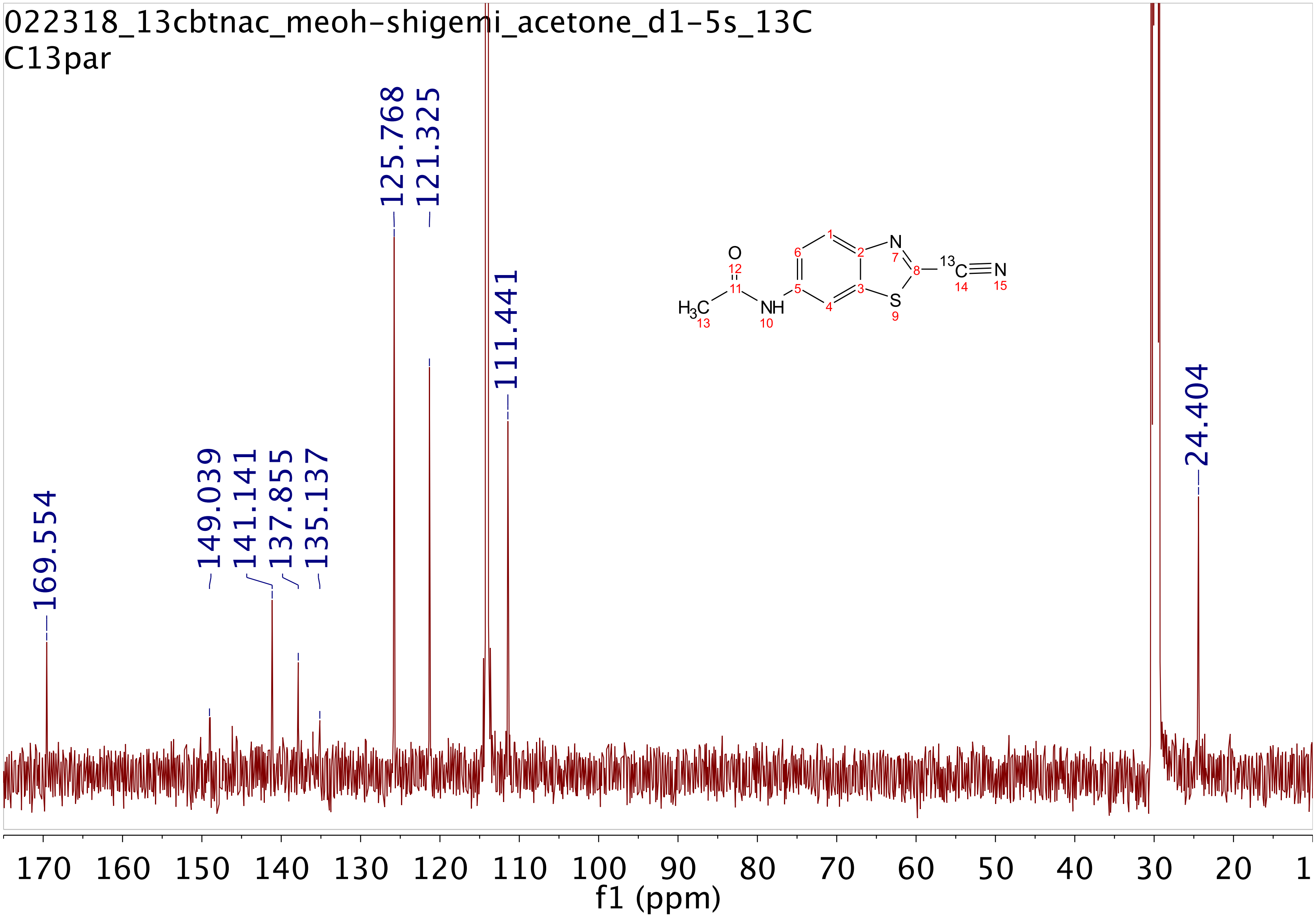

SGLK-i-ClBTNAc-TLCspot3polar-C13.1.fid
AVB-400 ZBO Carbon Starting paramters 6/11/03 RN
O
12
11
H_3C
13
NH
10
6
5
1
4
2
3
N
7
8
Cl
S
9
171.7
153.3
148.3
138.3
137.9
123.4
120.6
112.9
49.6 MeOD
48.4 MeOD
30.7 Acetone
23.9
30
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
1
f1 (ppm)

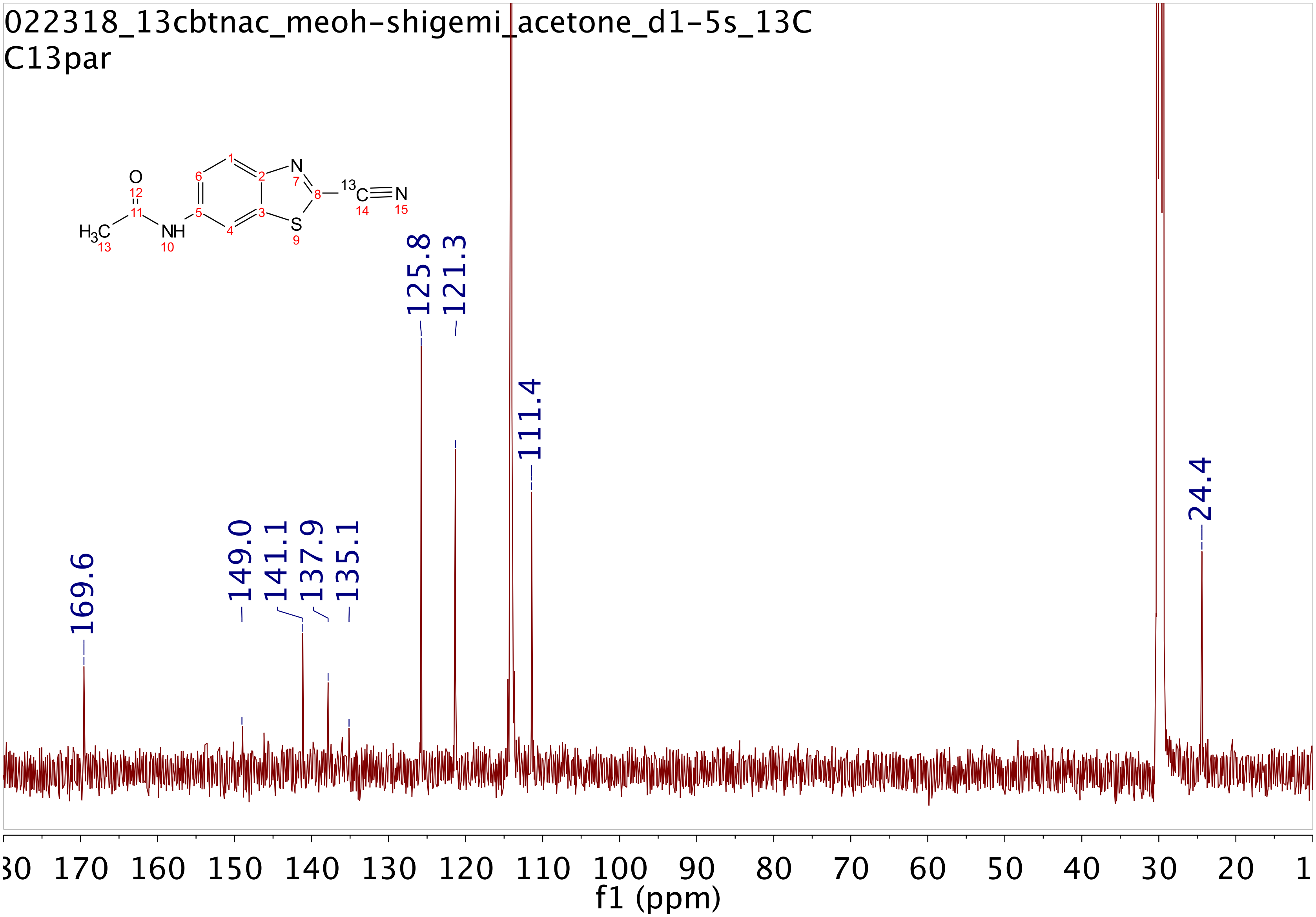

SGLK-i-ClBTNAc-TLCspot3polar-C13.1.fid
AVB-400 ZBO Carbon Starting paramters 6/11/03 RN
O
12
11
H_3C
13
NH
10
6
5
4
1
2
3
N
7
8
Cl
S
9
171.7
153.3
148.3
138.3
137.9
123.4
120.6
112.9
30
175
170
165
160
155
150
145
140
135
130
125
120
115
110
105
1(
f1 (ppm)

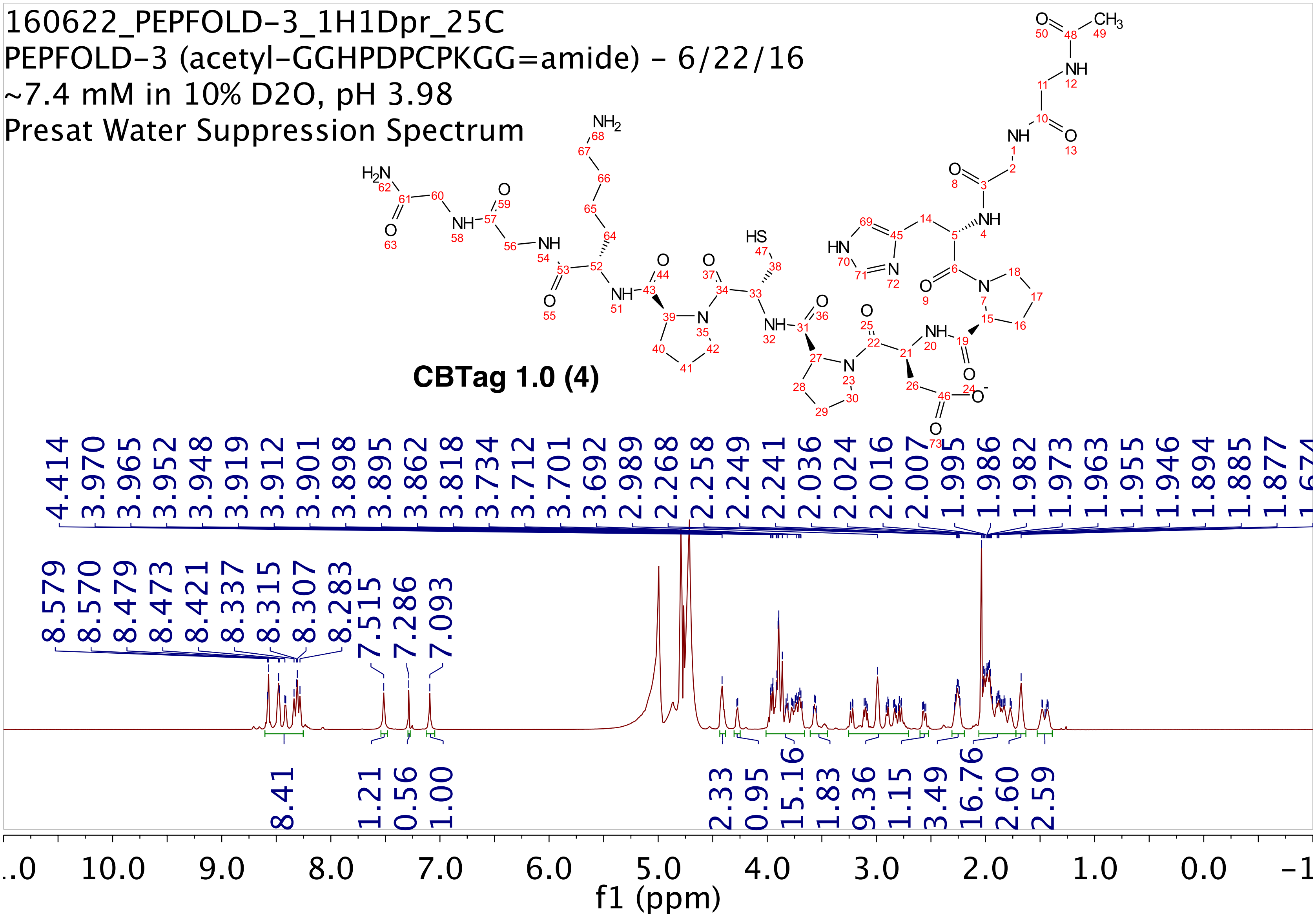

022318_13CBTNAc_meoh-shigemi_acetone_32s_proton
STANDARD PROTON PARAMETERS
13CBTNAc (3)
O
12
11
H3C
13
NH
10
5
6
1
2
4
3
N
7
8
S
9
13C
14
N
15
9.676
8.810
8.806
8.133
8.115
7.734
7.729
7.716
7.712
2.854 H2O
2.820 HDO
2.155
2.050 Acetone
1.284 Grease
0.875 Grease
0.861 Grease
0.97
0.91
1.00
1.07
2.90
..0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1
f1 (ppm)


022318_13CBTNAc_meoh-shigemi_acetone_32s_proton
STANDARD PROTON PARAMETERS
O
12
11
H3C
13
NH
10
6
5
1
2
4
3
N
7
8
S
9
13C
14
N
15
9.676
8.810
8.806
8.133
8.115
7.734
7.729
7.716
7.712
0.97
0.91
1.00
0.05
1.07
9.9
9.7
9.5
9.3
9.1
8.9
8.7
8.5
8.3
8.1
7.9
7.7
7.
f1 (ppm)

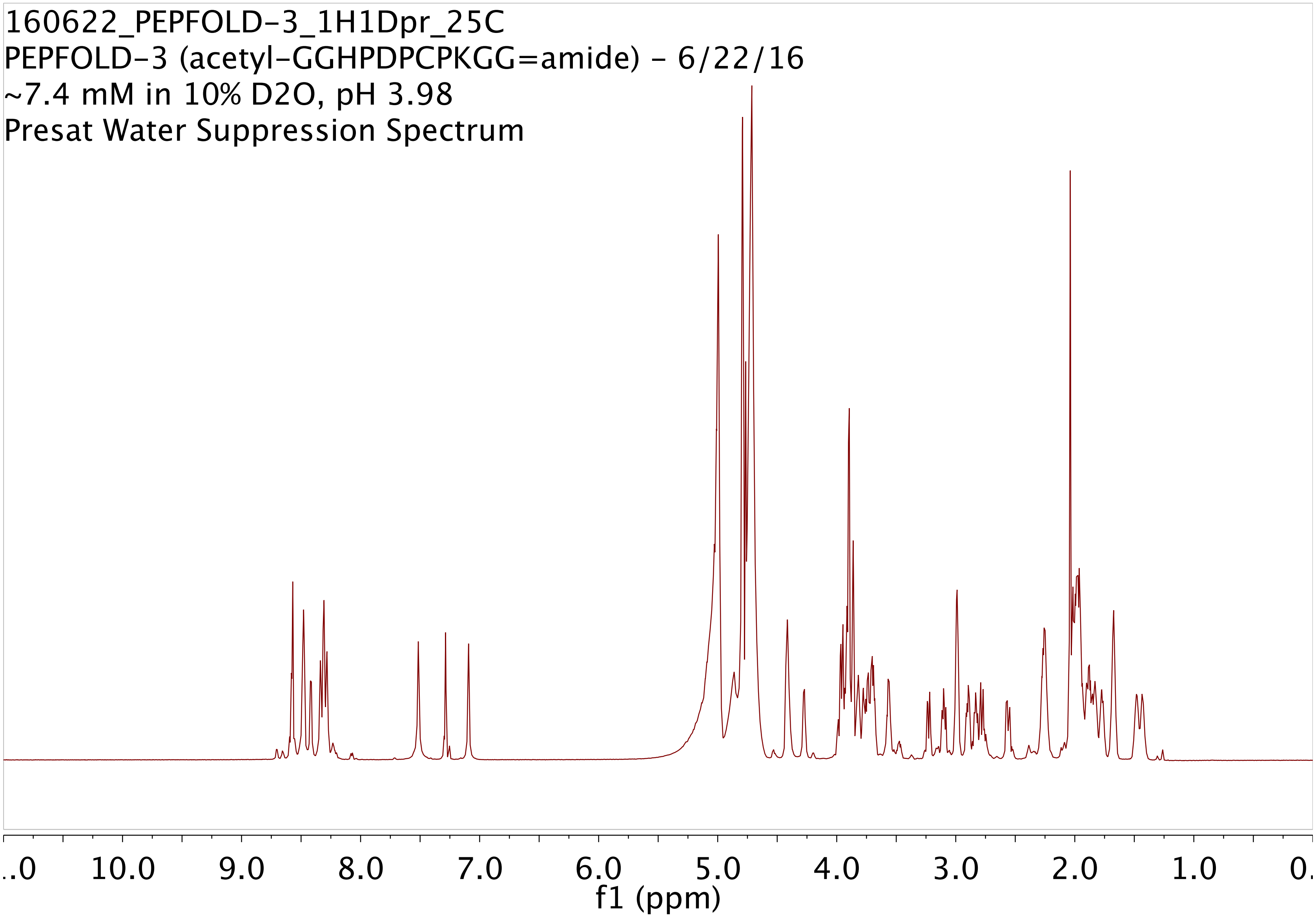

022318_13cbtnac_meoh-shigemi_acetone_d1-5s_13C
C13par
206.1 Acetone
169.6
149.0
141.1
137.9
135.1
125.8
121.3
114.1
111.4
29.8 Acetone
24.4
O
12
11
H_3C
13
NH
10
5
6
1
2
3
4
N
7
8
S
9
^{13}C
14
N
15
10
190
170
150
130
110
90
70
50
30
10
-1
f1 (ppm)

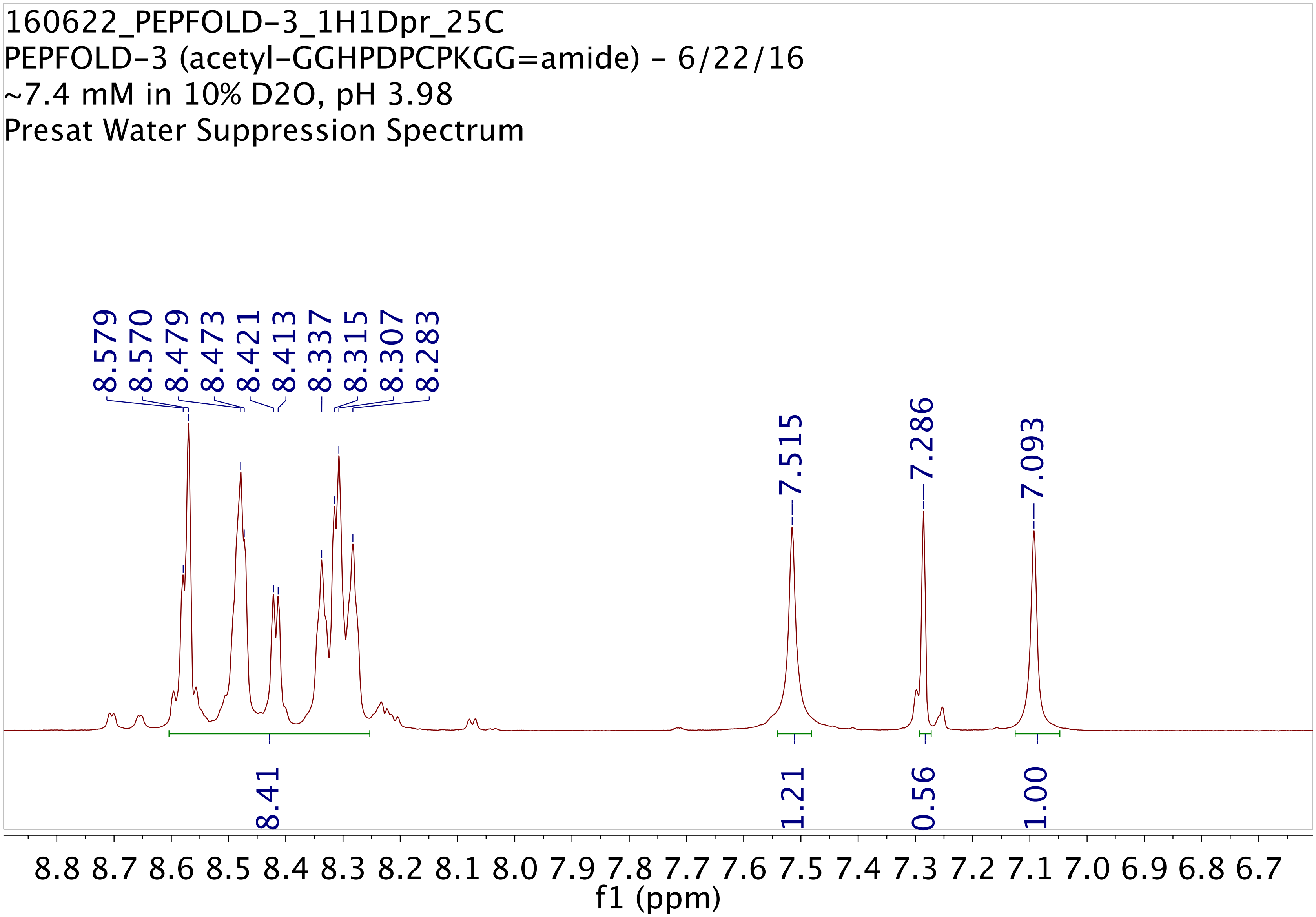

022318_13cbtnac_meoh-shigemi_acetone_d1-5s_13C
C13par
169.554
149.039
141.141
137.855
135.137
125.768
121.325
111.441
24.404
O
12
11
H3C
13
NH
10
5
6
1
2
3
4
N
7
8
S
9
13C
14
N
15
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
1
f1 (ppm)


022318_13cbtnac_meoh-shigemi_acetone_d1-5s_13C
C13par
O
12
11
H_3C
13
NH
10
5
6
1
2
3
4
N
7
8
S
9
^{13}C
14
N
15
169.6
149.0
141.1
137.9
135.1
125.8
121.3
111.4
24.4
30
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
1
f1 (ppm)

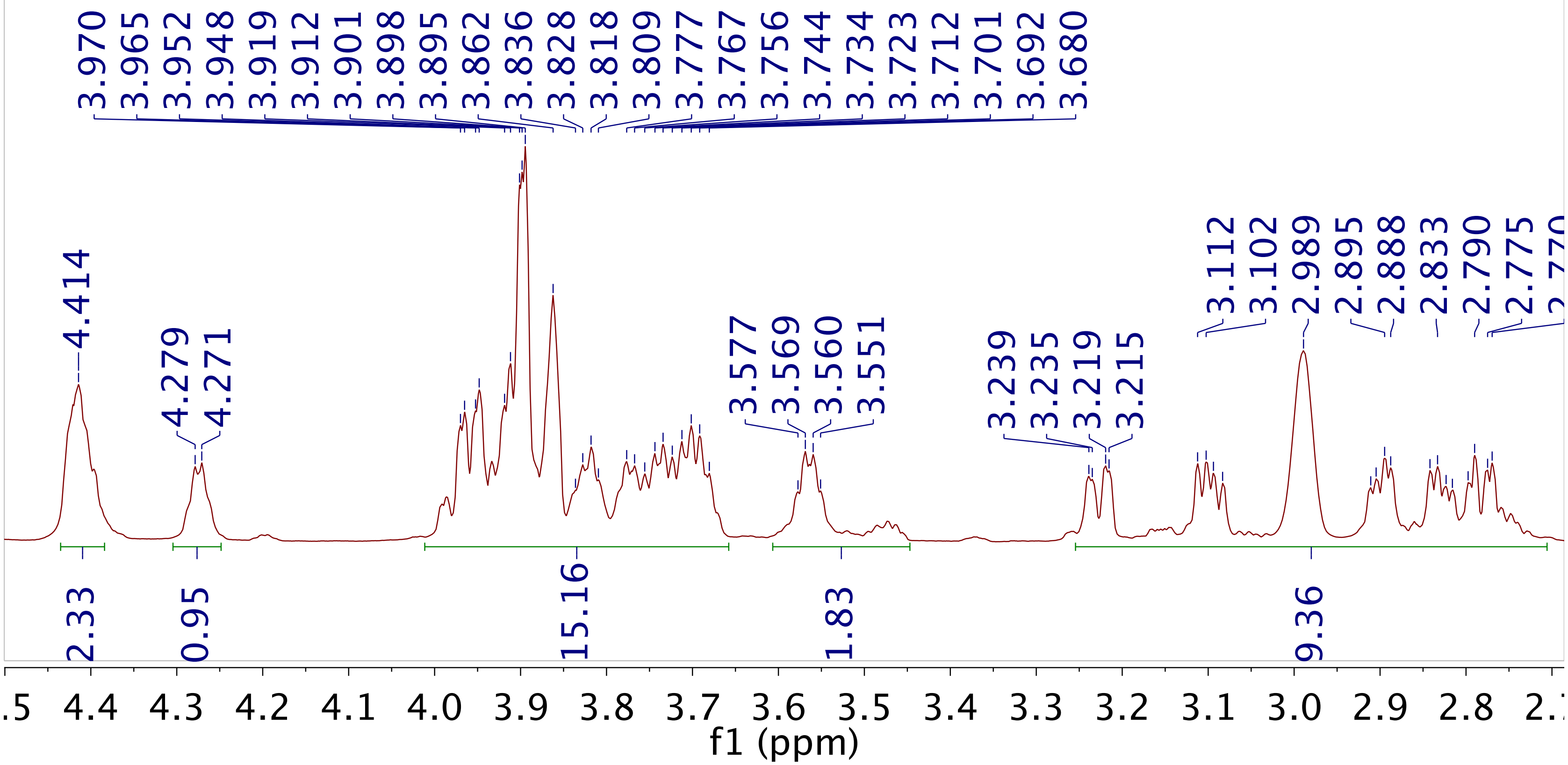

160622_PEPFOLD-3_1H1Dpr_25C
PEPFOLD-3 (acetyl-GGHPDPCPKGG=amide) - 6/22/16
~7.4 mM in 10% D2O, pH 3.98
Presat Water Suppression Spectrum
NH2
H2N
O
NH
HS
HN
N
O-
CH3
4.414
3.970
3.965
3.952
3.948
3.919
3.912
3.901
3.898
3.895
3.862
3.818
3.734
3.712
3.701
3.692
2.989
2.268
2.258
2.249
2.241
2.036
2.024
2.016
2.007
1.995
1.986
1.982
1.973
1.963
1.955
1.946
1.894
1.885
1.877
1.67
8.579
8.570
8.479
8.473
8.421
8.337
8.315
8.307
8.283
7.515
7.286
7.093
8.41
1.21
0.56
1.00
2.33
0.95
15.16
1.83
9.36
1.15
3.49
16.76
2.60
2.59
.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1
f1 (ppm)

CBTag 1.0 (4)

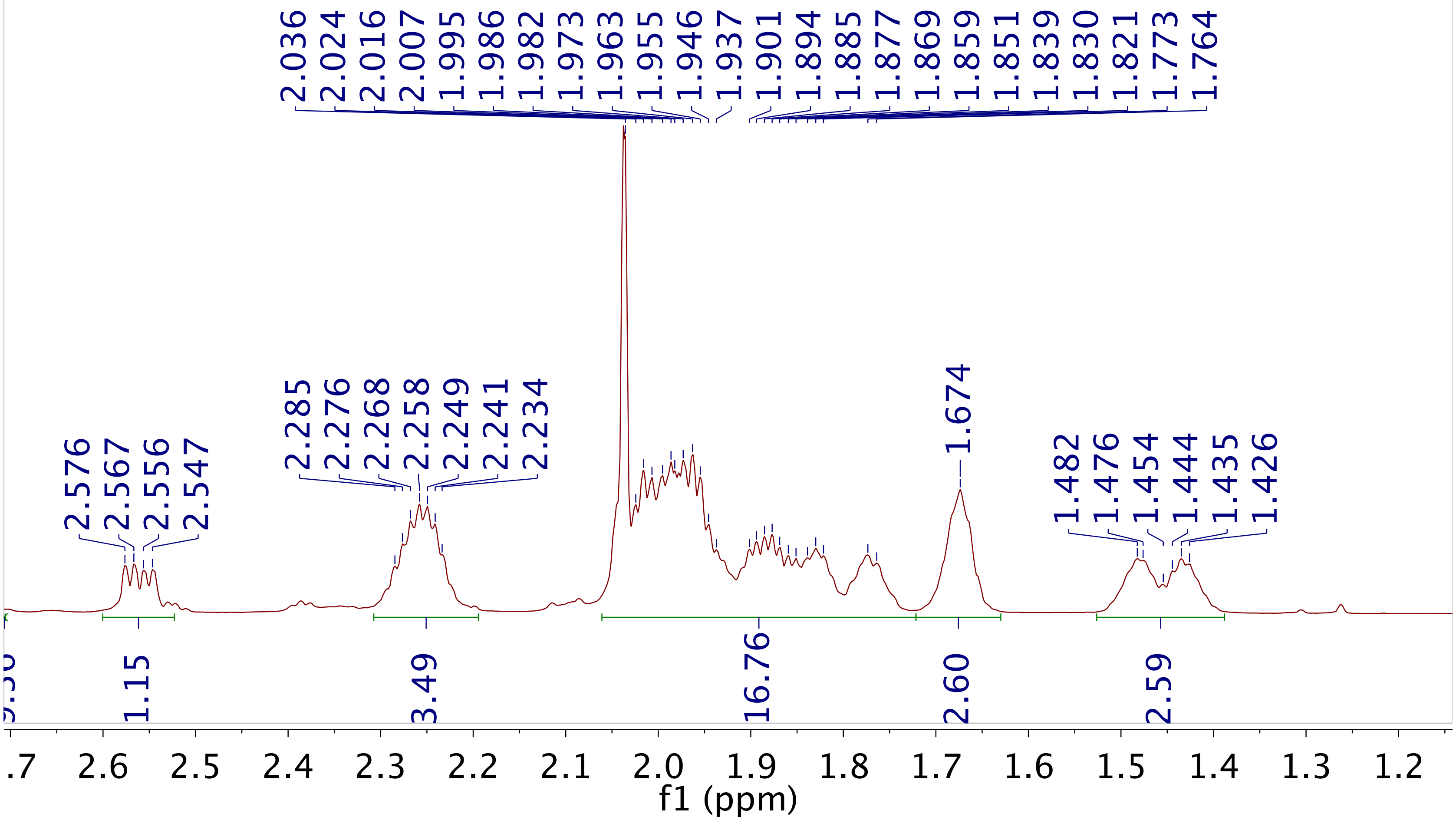

160622_PEPFOLD-3_1H1Dpr_25C
PEPFOLD-3 (acetyl-GGHPDPCPKGG=amide) - 6/22/16
~7.4 mM in 10% D2O, pH 3.98
Presat Water Suppression Spectrum
.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.
f1 (ppm)

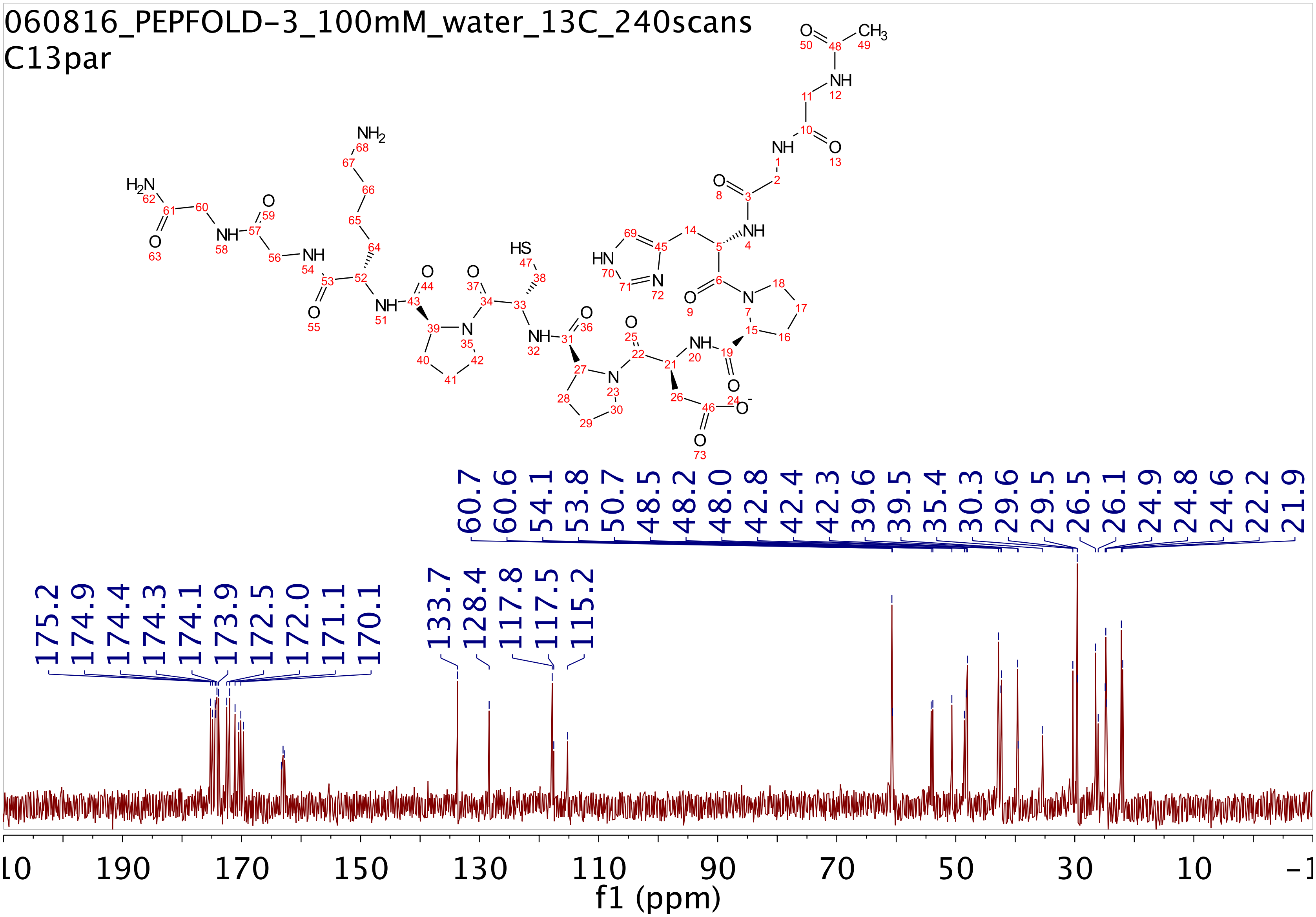

160622_PEPFOLD-3_1H1Dpr_25C
PEPFOLD-3 (acetyl-GGHPDPCPKGG=amide) - 6/22/16
~7.4 mM in 10% D2O, pH 3.98
Presat Water Suppression Spectrum
8.579
8.570
8.479
8.473
8.421
8.413
8.337
8.315
8.307
8.283
7.515
7.286
7.093
8.41
1.21
0.56
1.00
8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7
f1 (ppm)

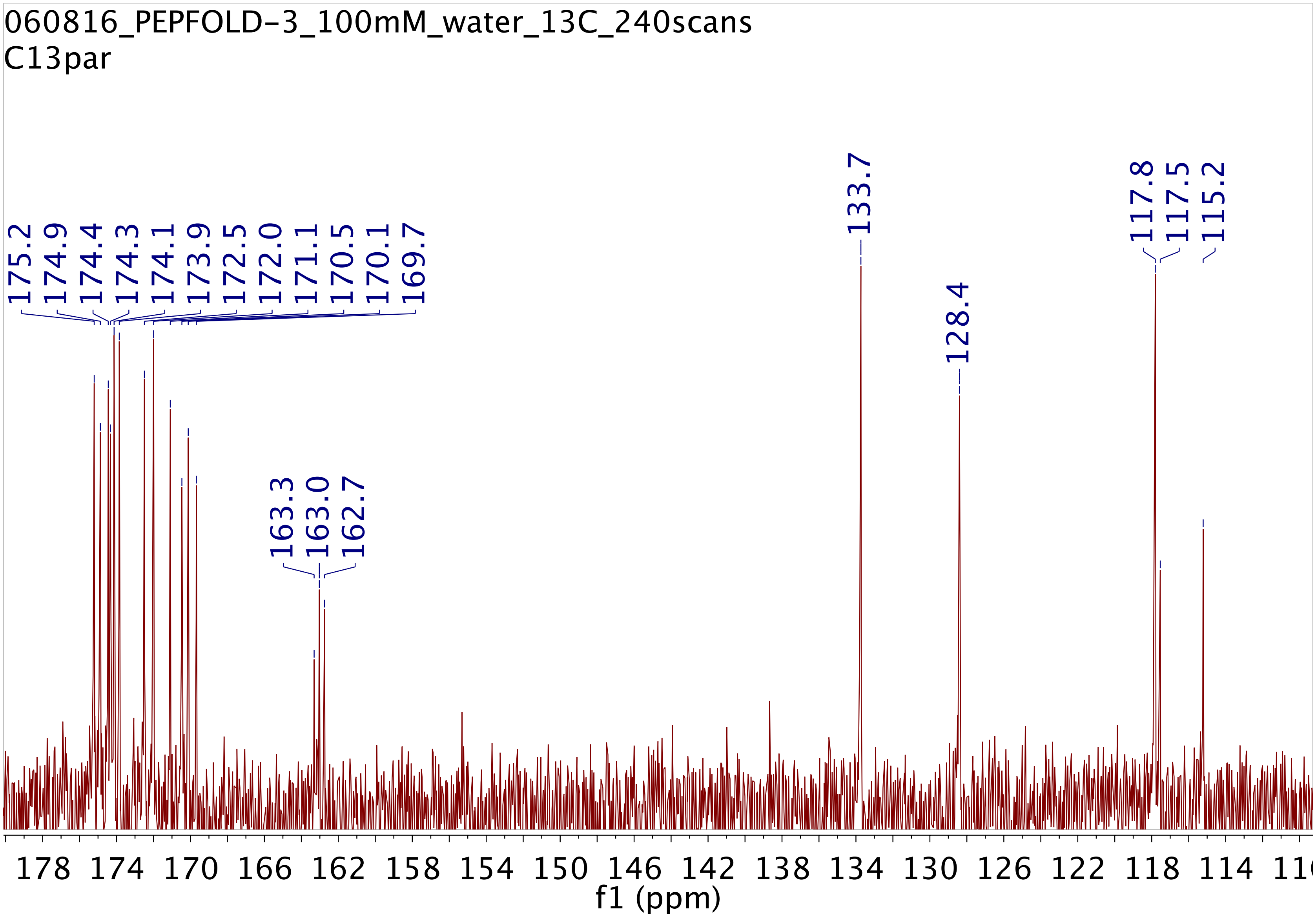
160622_PEPFOLD-3_1H1Dpr_25C
PEPFOLD-3 (acetyl-GGHPDPCPKGG=amide) - 6/22/16
~7.4 mM in 10% D2O, pH 3.98
Presat Water Suppression Spectrum

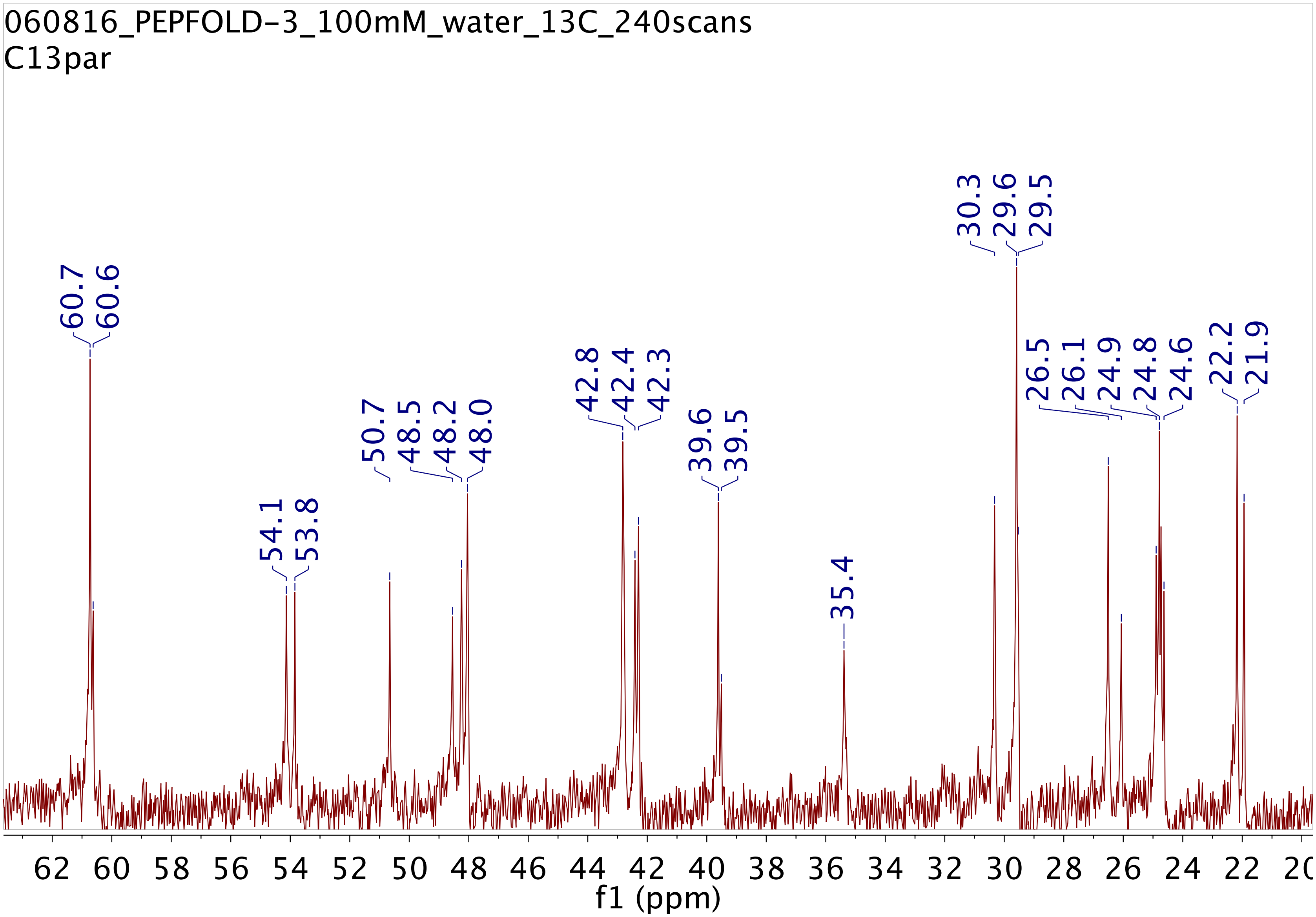


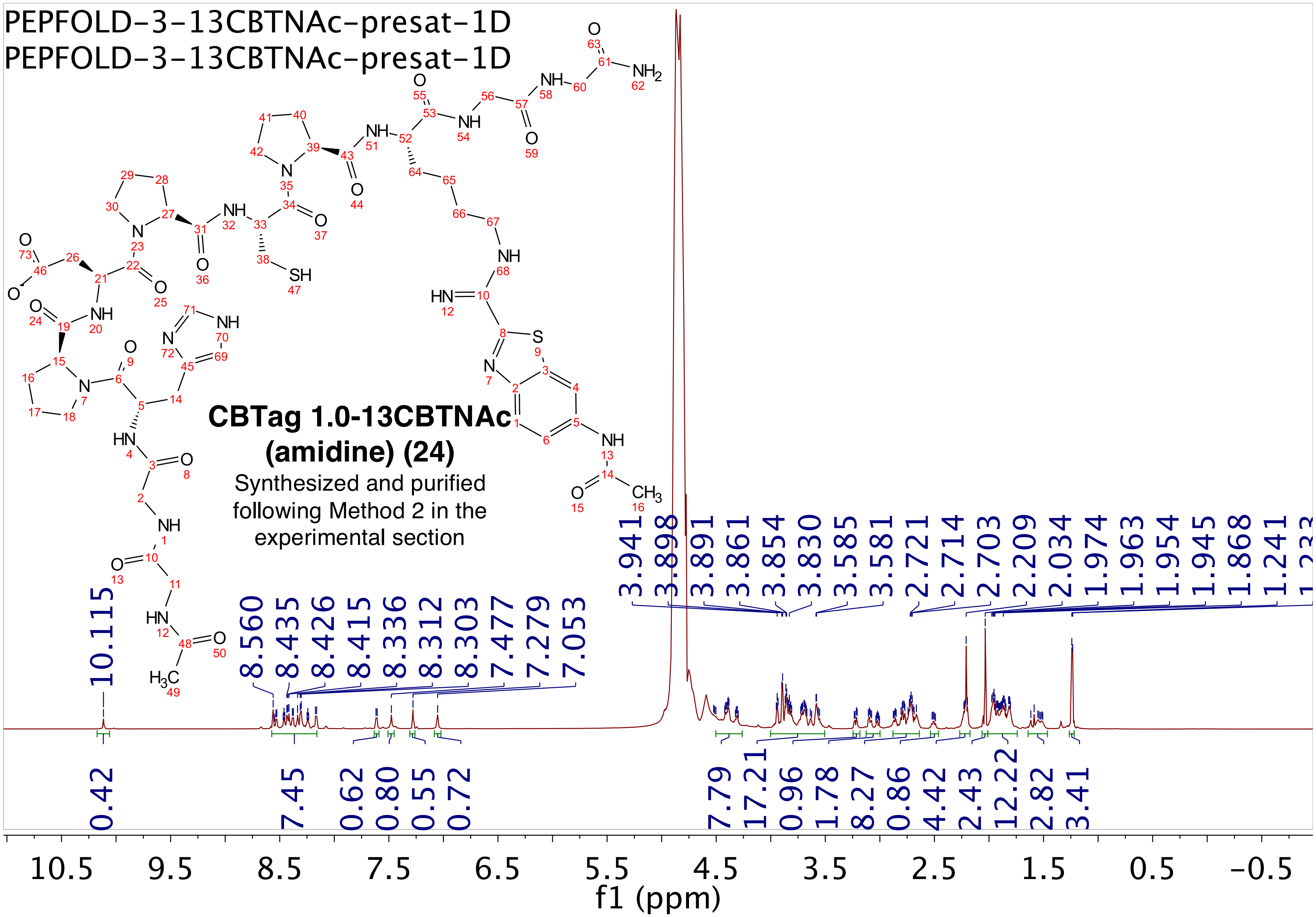
160622_PEPFOLD-3_1H1Dpr_25C
PEPFOLD-3 (acetyl-GGHPDPCPKGG=amide) - 6/22/16
~7.4 mM in 10% D2O, pH 3.98
Presat Water Suppression Spectrum




060816_PEPFOLD-3_100mM_water_13C_240scans
C13par
175.2
174.9
174.4
174.3
174.1
173.9
172.5
172.0
171.1
170.1
133.7
128.4
117.8
117.5
115.2
60.7
60.6
54.1
53.8
50.7
48.5
48.2
48.0
42.8
42.4
42.3
39.6
39.5
35.4
30.3
29.6
29.5
26.5
26.1
24.9
24.8
24.6
22.2
21.9
10
190
170
150
130
110
90
70
50
30
10
-1
f1 (ppm)
CH_3
NH
HS
HN
N
NH_2
H_2N
O
O^-

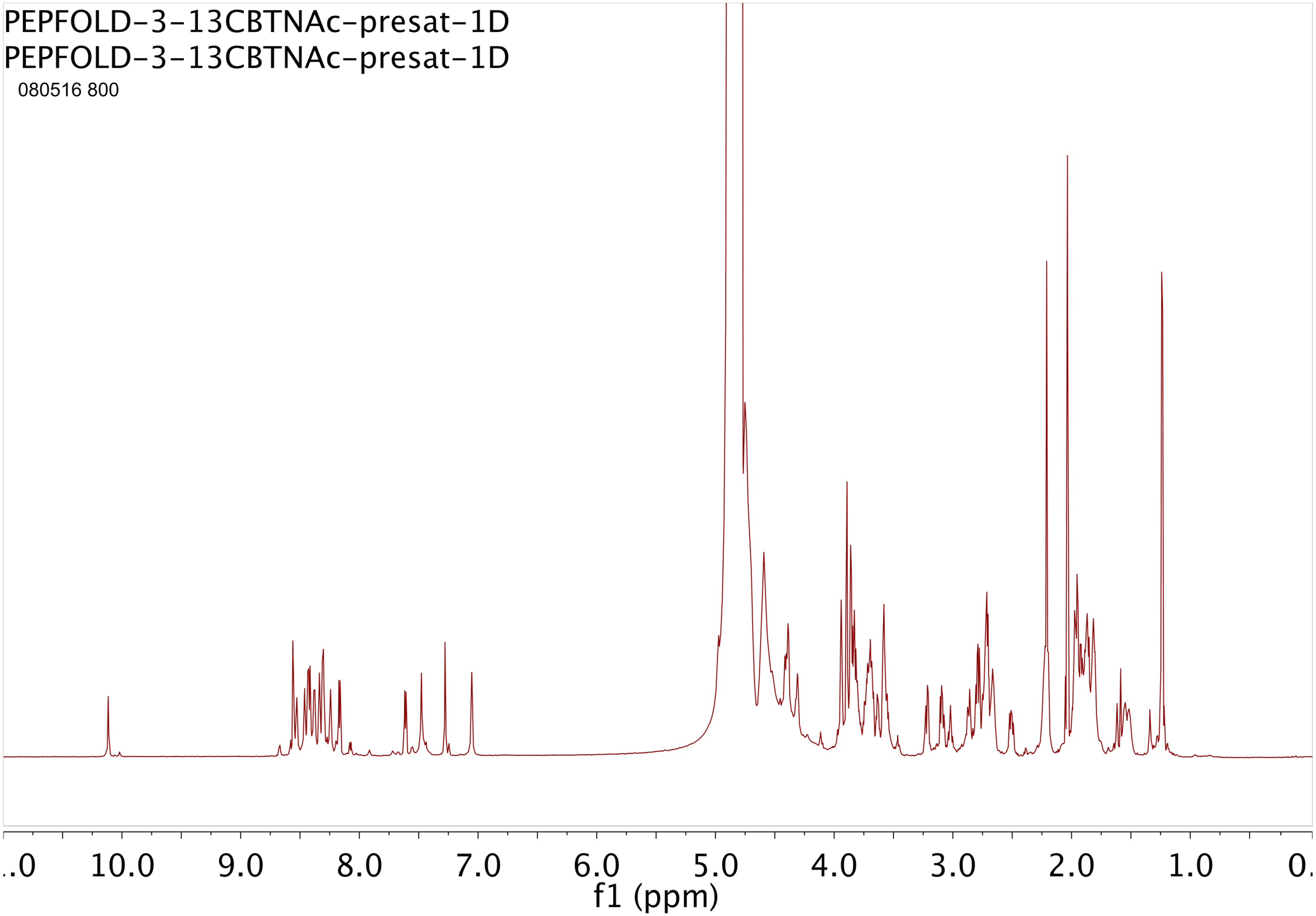

060816_PEPFOLD-3_100mM_water_13C_240scans
C13par
175.2
174.9
174.4
174.3
174.1
173.9
172.5
172.0
171.1
170.5
170.1
169.7
163.3
163.0
162.7
133.7
128.4
117.8
117.5
115.2
178
174
170
166
162
158
154
150
146
142
138
134
130
126
122
118
114
f1 (ppm)

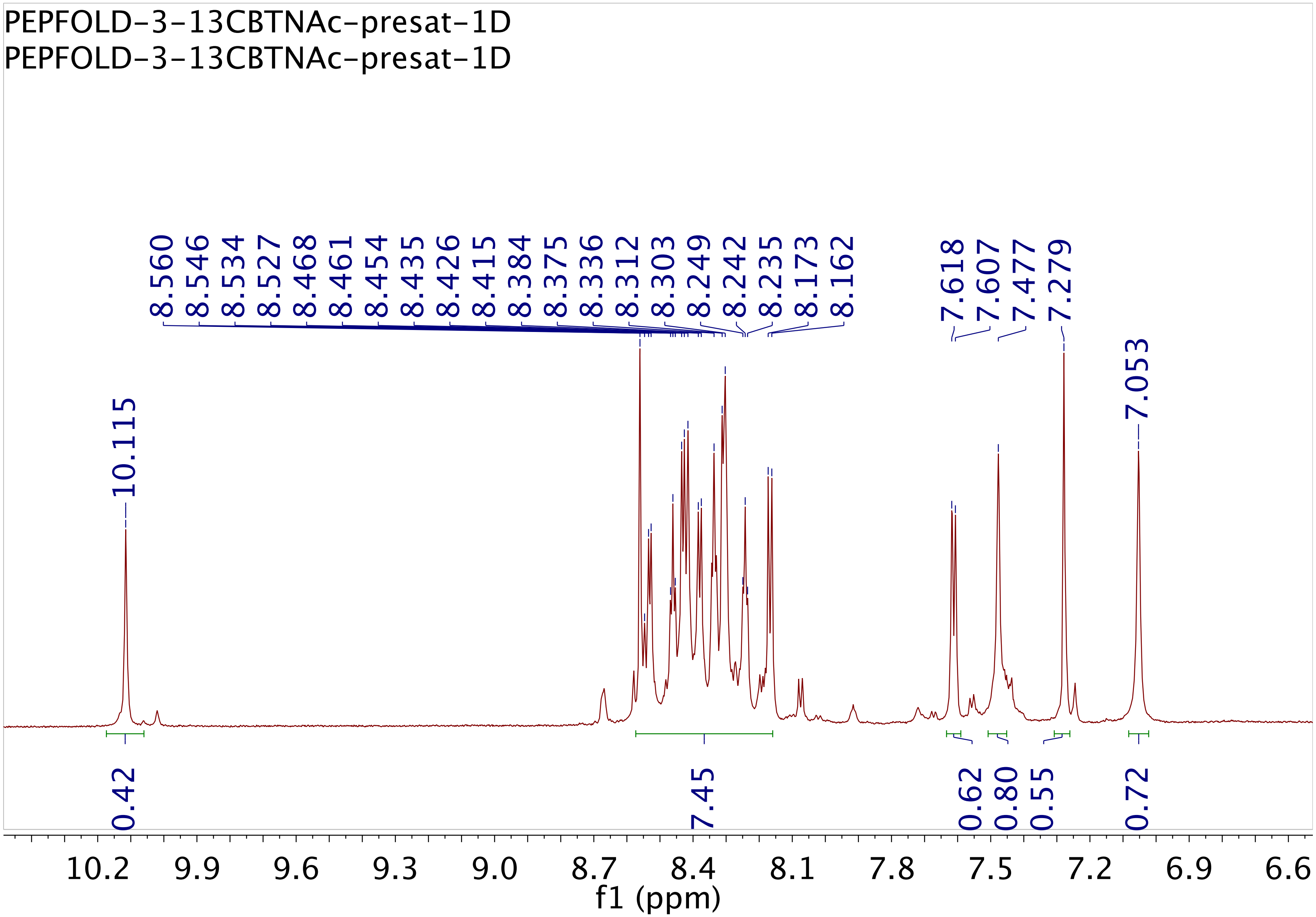

060816_PEPFOLD-3_100mM_water_13C_240scans
C13par
60.7
60.6
54.1
53.8
50.7
48.5
48.2
48.0
42.8
42.4
42.3
39.6
39.5
35.4
30.3
29.6
29.5
26.5
26.1
24.9
24.8
24.6
22.2
21.9
62
60
58
56
54
52
50
48
46
44
42
40
38
36
34
32
30
28
26
24
22
2
f1 (ppm)

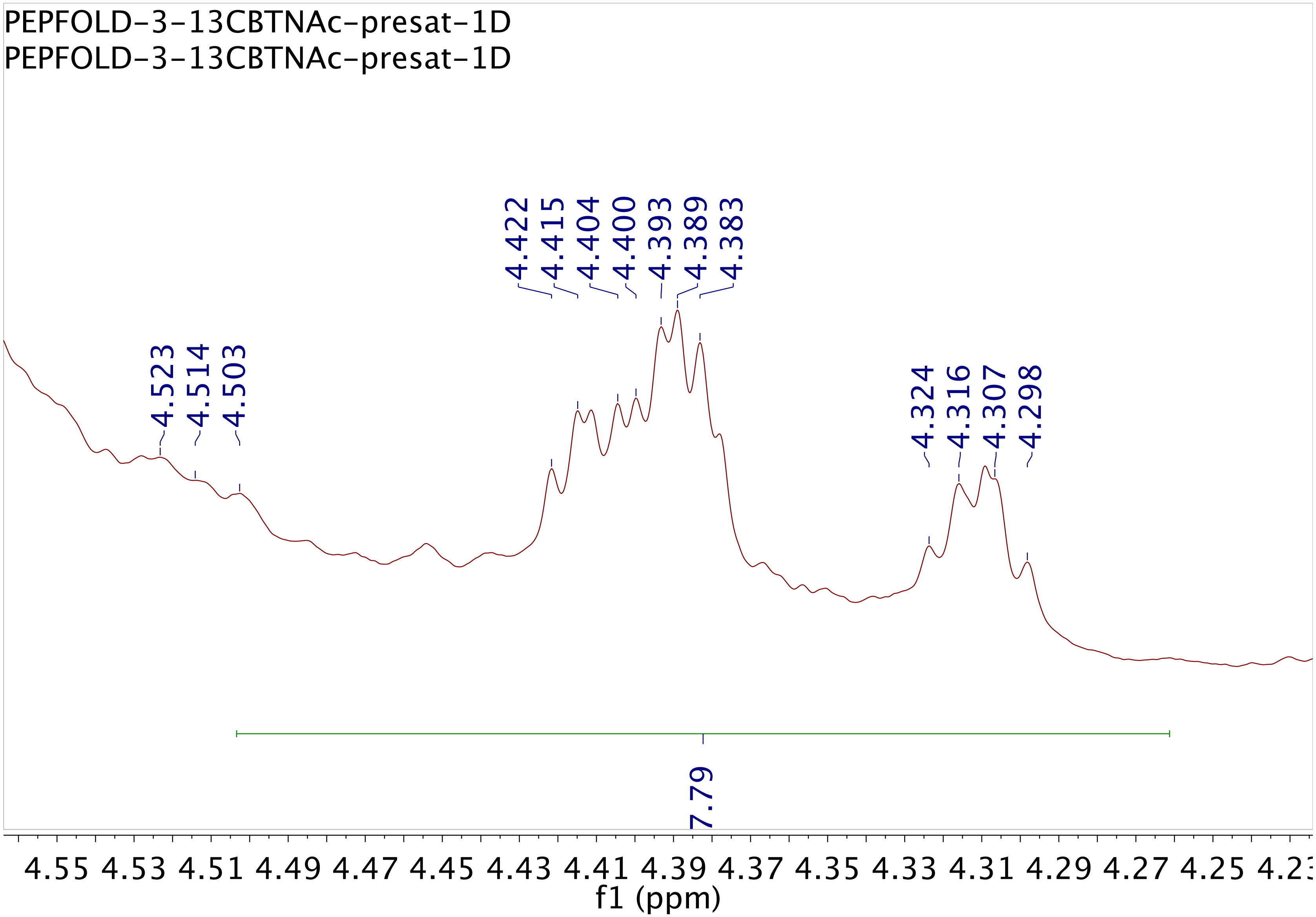


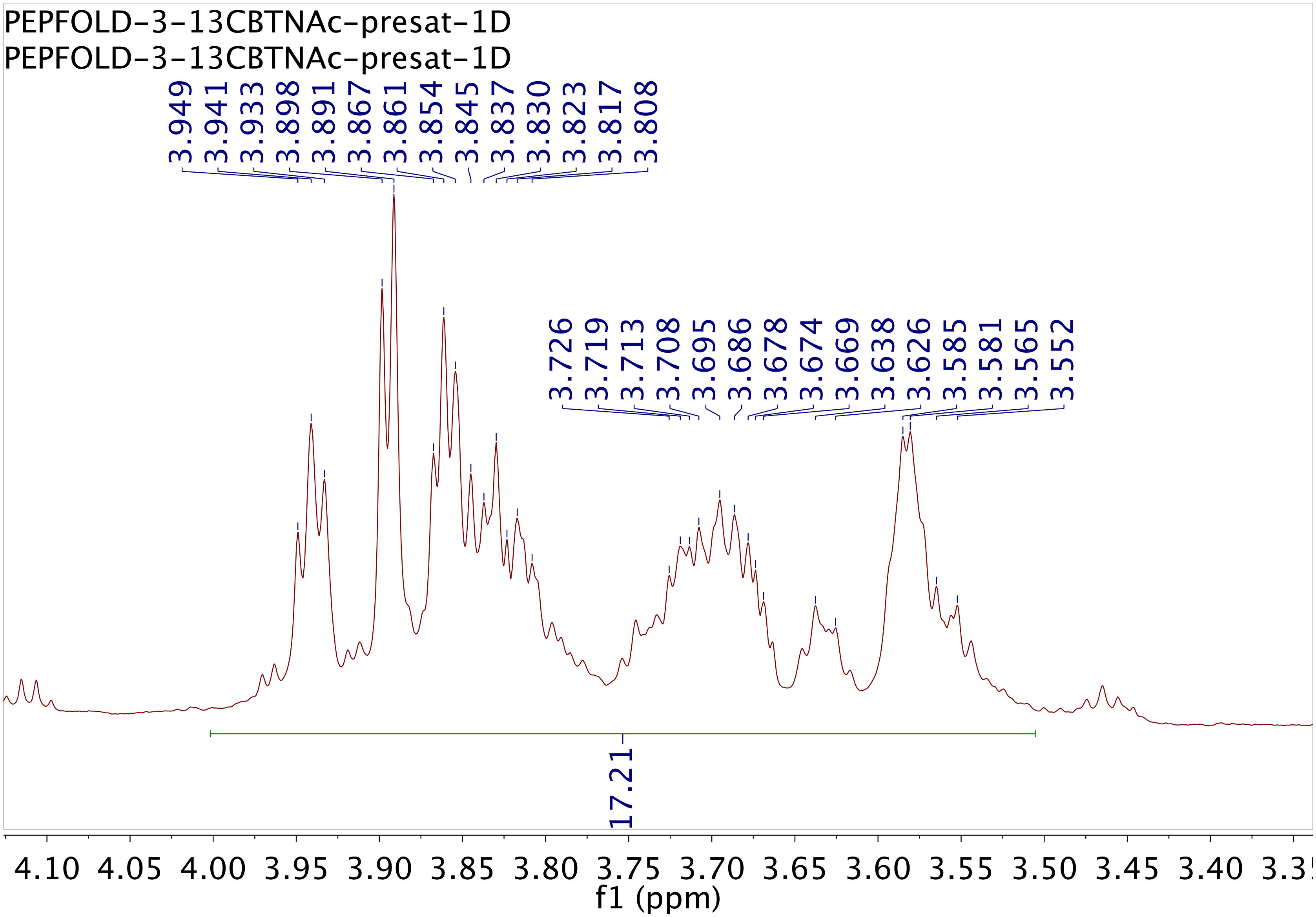
CBTag 1.0-13CBTNAc (amidine) (24)

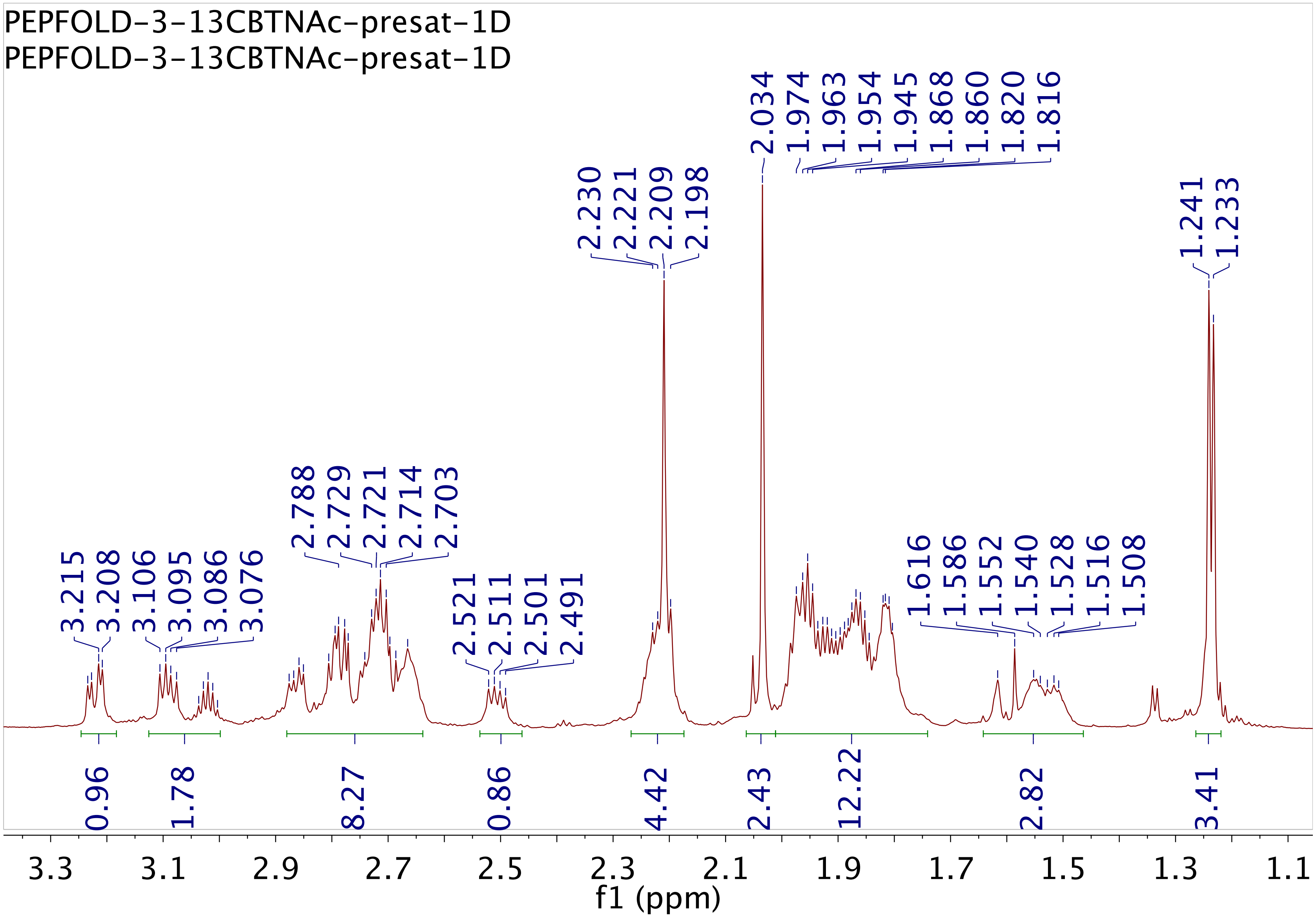
Synthesized and purified following Method 2 in the experimental section

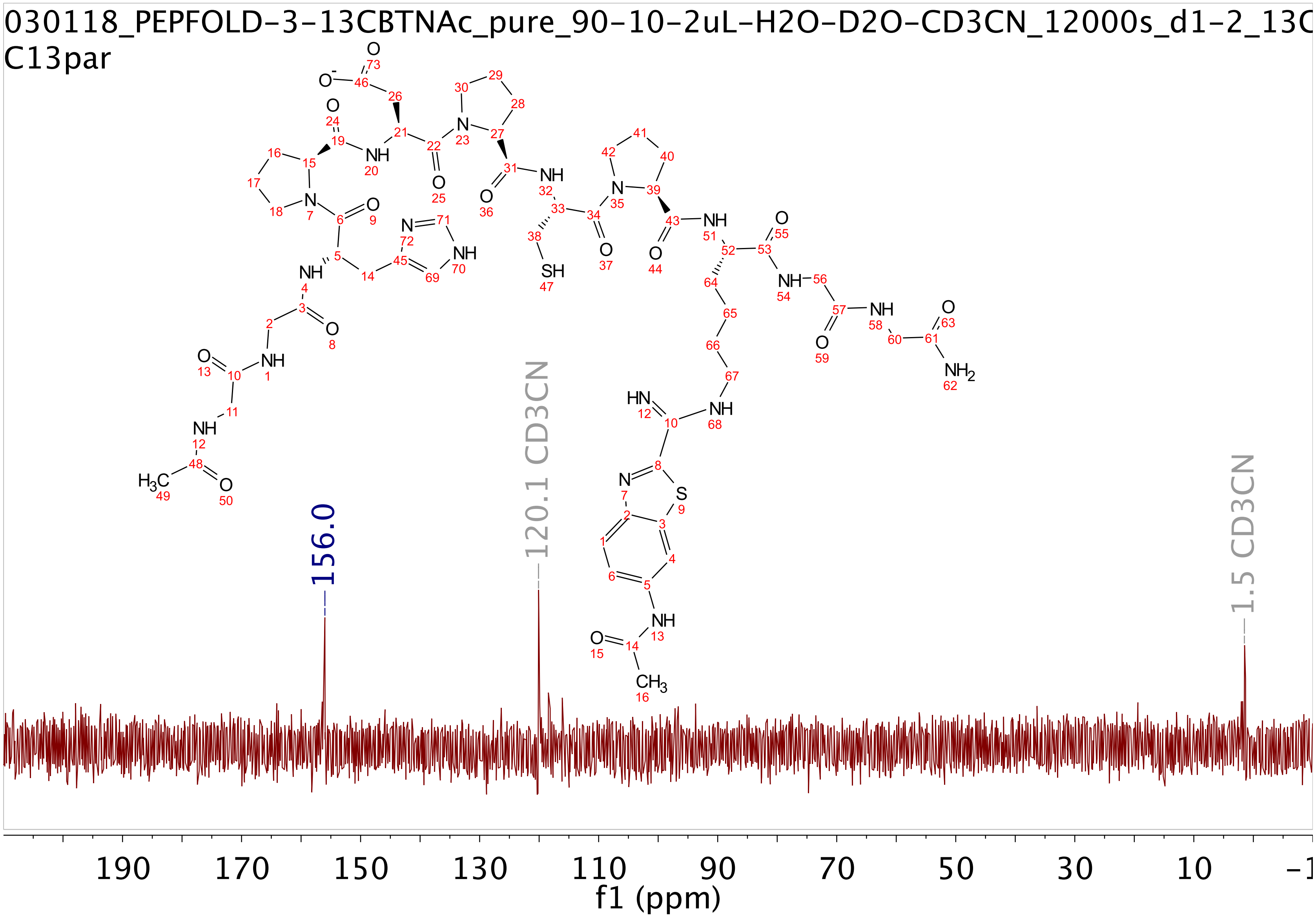

PEPFOLD-3-13CBTNAc-presat-1D
PEPFOLD-3-13CBTNAc-presat-1D
080516 800
.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.
f1 (ppm)


PEPFOLD-3-13CBTNAc-presat-1D
PEPFOLD-3-13CBTNAc-presat-1D
10.115
8.560
8.546
8.534
8.527
8.468
8.461
8.454
8.435
8.426
8.415
8.384
8.375
8.336
8.312
8.303
8.249
8.242
8.235
8.173
8.162
7.618
7.607
7.477
7.279
7.053
0.42
7.45
0.62
0.80
0.55
0.72
10.2
9.9
9.6
9.3
9.0
8.7
8.4
8.1
7.8
7.5
7.2
6.9
6.6
f1 (ppm)


PEPFOLD-3-13CBTNAc-presat-1D
PEPFOLD-3-13CBTNAc-presat-1D
4.523
4.514
4.503
4.422
4.415
4.404
4.400
4.393
4.389
4.383
4.324
4.316
4.307
4.298
7.79
4.55 4.53 4.51 4.49 4.47 4.45 4.43 4.41 4.39 4.37 4.35 4.33 4.31 4.29 4.27 4.25 4.2
f1 (ppm)


PEPFOLD-3-13CBTNAc-presat-1D
PEPFOLD-3-13CBTNAc-presat-1D
3.949
3.941
3.933
3.898
3.891
3.867
3.861
3.854
3.845
3.837
3.830
3.823
3.817
3.808
3.726
3.719
3.713
3.708
3.695
3.686
3.678
3.674
3.669
3.638
3.626
3.585
3.581
3.565
3.552
17.21
4.10
4.05
4.00
3.95
3.90
3.85
3.80
3.75
3.70
3.65
3.60
3.55
3.50
3.45
3.40
3.3
f1 (ppm)


PEPFOLD-3-13CBTNAc-presat-1D
PEPFOLD-3-13CBTNAc-presat-1D
3.215
3.208
3.106
3.095
3.086
3.076
2.788
2.729
2.721
2.714
2.703
2.521
2.511
2.501
2.491
2.230
2.221
2.209
2.198
2.034
1.974
1.963
1.954
1.945
1.868
1.860
1.820
1.816
1.616
1.586
1.552
1.540
1.528
1.516
1.508
1.241
1.233
0.96
1.78
8.27
0.86
4.42
2.43
12.22
2.82
3.41
3.3
3.1
2.9
2.7
2.5
2.3
2.1
1.9
1.7
1.5
1.3
1.1
f1 (ppm)


030118_PEPFOLD-3-13CBTNAc_pure_90-10-2uL-H2O-D2O-CD3CN_12000s_d1-2_13C
C13par
156.0
120.1 CD3CN
1.5 CD3CN
190
170
150
130
110
90
70
50
30
10
-1
f1 (ppm)