

Supplementary Information

Cysteine Thioesters as Myelin Proteolipid Protein Analogues to Examine the Role of Butyrylcholinesterase in Myelin Decompaction

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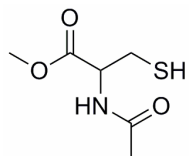
| | |
|---|--------|
| A. Yields and purity of synthesized analogues | S2 |
| B. ¹ H NMR, ¹³ C NMR, HRMS & HPLC spectra | S3-S34 |

A. **Table S1.** Yields and purity of the synthesized compounds.

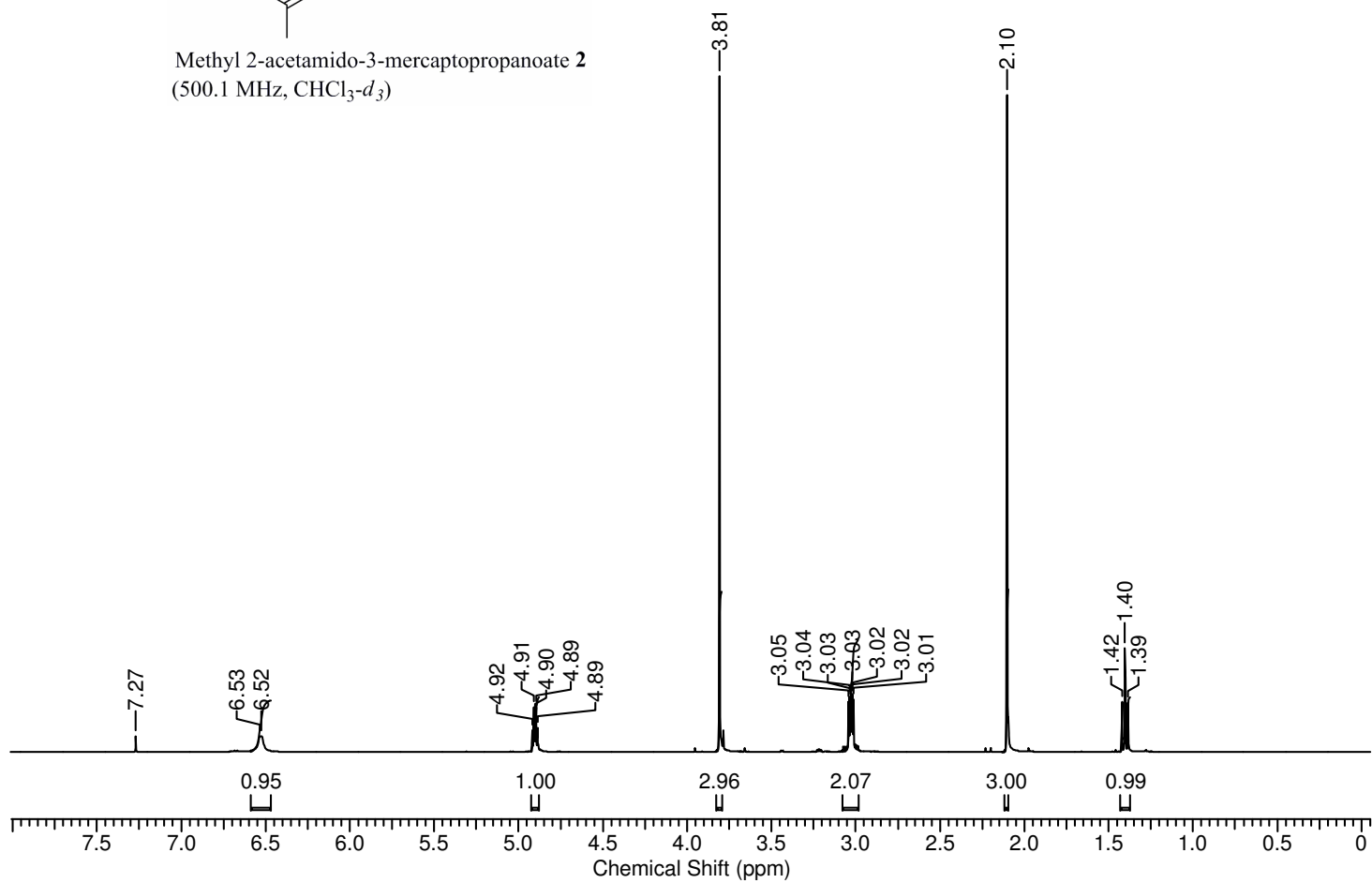
| Comp. # | Name | % Yield | % Purity^a |
|----------------|--|----------------|-----------------------------|
| 2 | Methyl 2-acetamido-3-mercaptopropanoate | 74 | 98.04 |
| 3 | Methyl 2-acetamido-3-(acetylthio)propanoate | 45 | 99.10 |
| 4 | Methyl 2-acetamido-3-(butyrylthio)propanoate | 46 | 98.89 |
| 5 | Methyl 2-acetamido-3-(octanoylthio)propanoate | 70 | 98.34 |
| 6 | Methyl 2-acetamido-3-(decanoylthio)propanoate | 43 | 98.78 |
| 7 | Methyl 2-acetamido-3-(dodecanoylthio)propanoate | 81 | 98.82 |
| 8 | Methyl 2-acetamido-3-(tetradecanoylthio)propanoate | 43 | 99.43 |
| 9 | Methyl 2-acetamido-3-(palmitoylthio)propanoate | 61 | 98.88 |

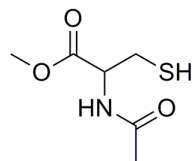
^a The experimental procedure to determine purity of each compound is stated in the legend for the spectrum for each compound.

B. ^1H NMR, ^{13}C NMR, HRMS & HPLC for each compound

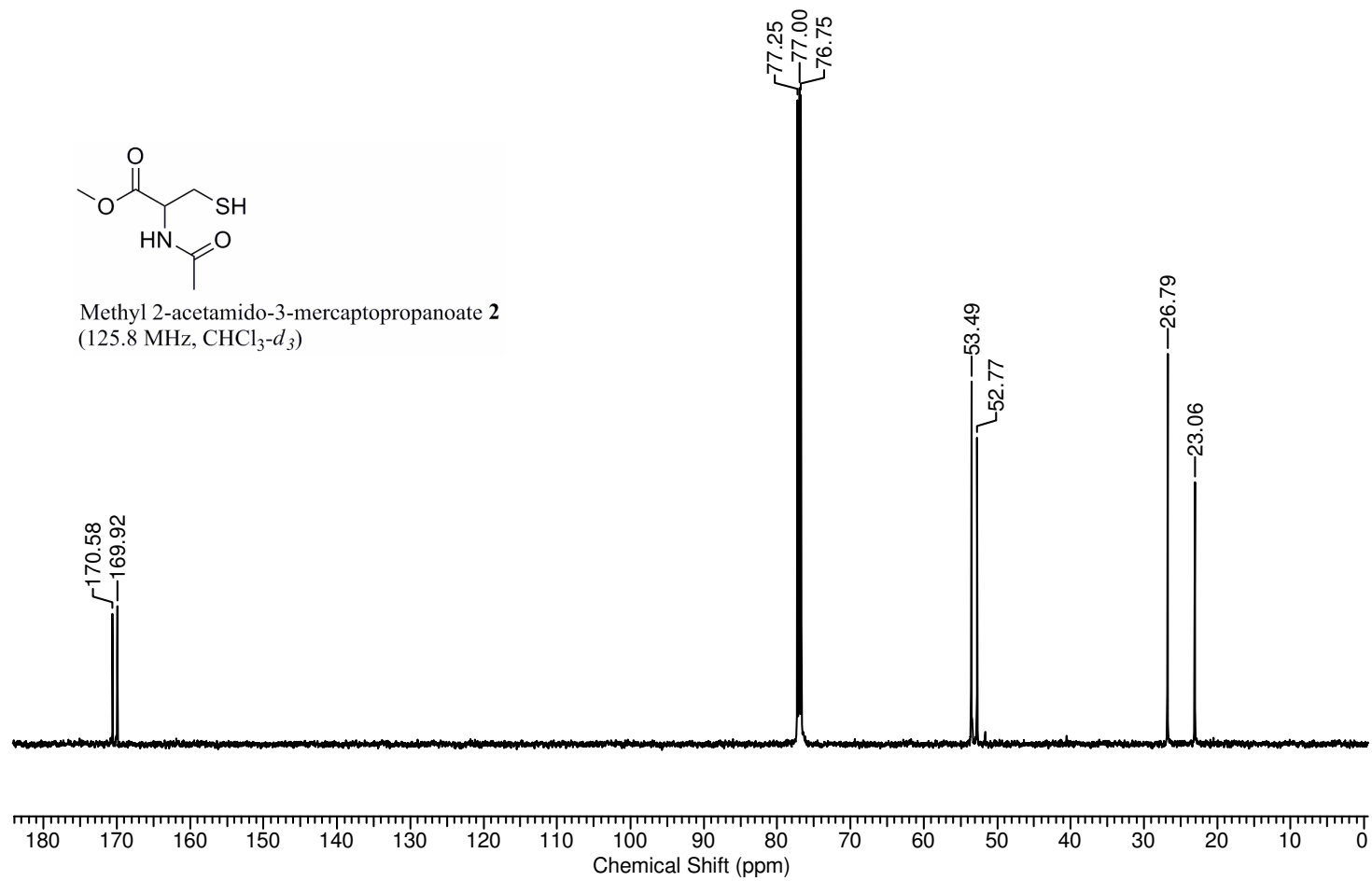


Methyl 2-acetamido-3-mercaptopropanoate **2**
(500.1 MHz, CHCl_3-d_3)





Methyl 2-acetamido-3-mercaptopropanoate **2**
(125.8 MHz, CHCl_3-d_3)



Mass Spectrum Molecular Formula Report

Analysis Info

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Method xiaofengpos.m
Sample Name rab-2
Comment

Acquisition Date 10/3/2008 2:14:36 PM

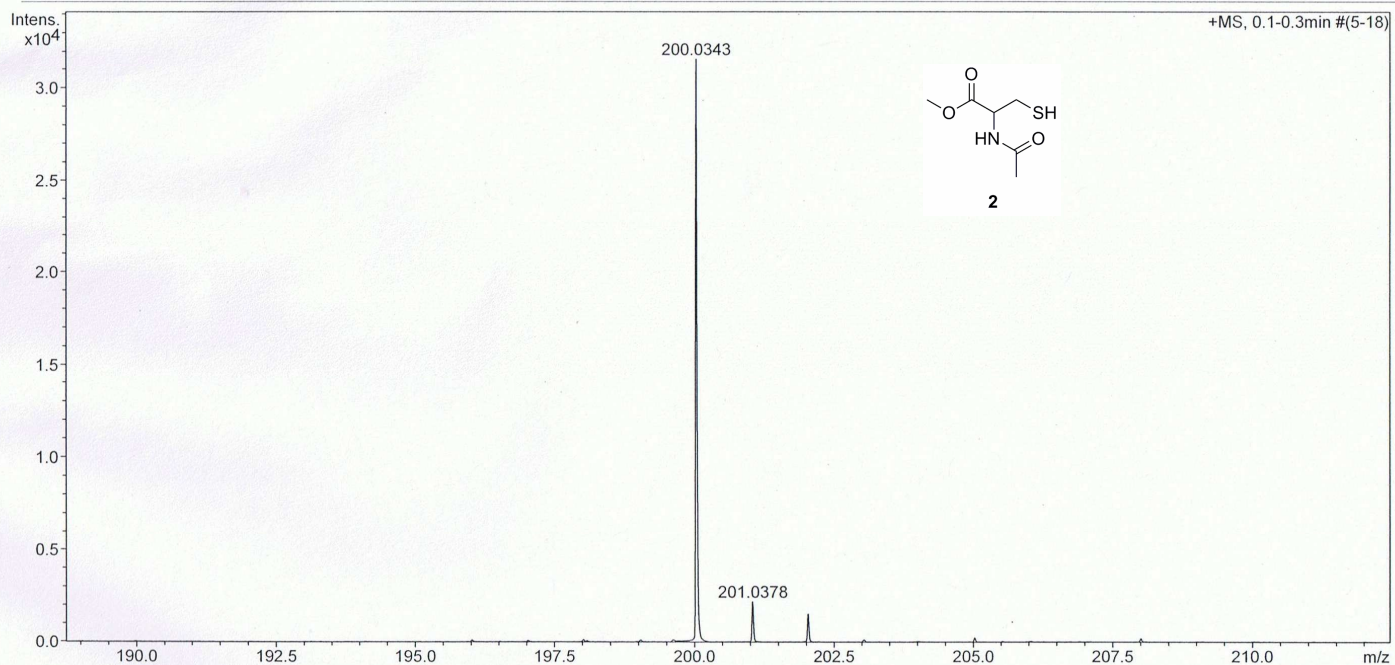
Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
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Scan End 1500 m/z

Ion Polarity Positive
Capillary Exit 150.0 V
Hexapole RF 130.0 V
Skimmer 1 55.0 V
Hexapole 1 26.0 V

Set Corrector Fill 52 V
Set Pulsar Pull 398 V
Set Pulsar Push 398 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 1960 V

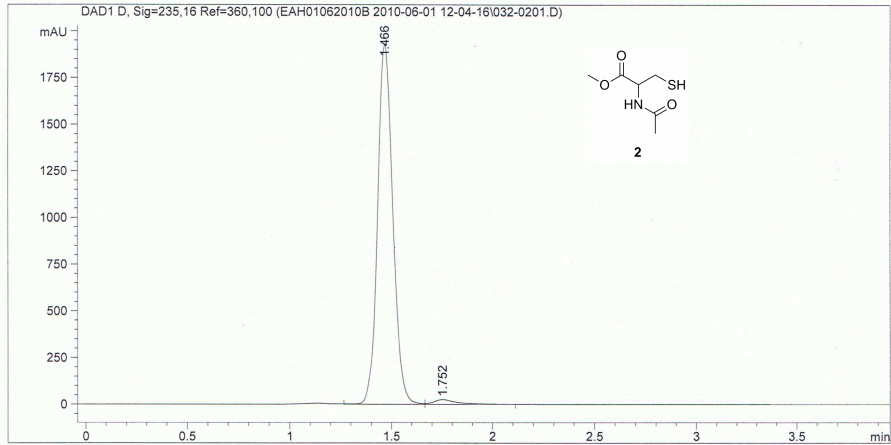


HPLC analysis of methyl 2-acetamido-3-mercaptopropanoate (2)

Purity was determined using an Agilent Technologies 1200 series HPLC system with a photodiode UV-visible detector; column: Eclipse XDB-C₁₈ 4.6 x 150mm 5 µm C₁₈; mobile phase: methanol; injection volume: 60 µL; UV detection: 235 nm; flow rate: 1 mL/min.

Data File C:\CHEM32\1\DATA\JEREMY\JER091008CFRACS 2008-10-09 15-09-59\EAH01062010B 2010-06-01 12-0
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                                                    Inj Volume: 60 µl
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                : (modified after loading)
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Use Multiplier & Dilution Factor with ISTDs
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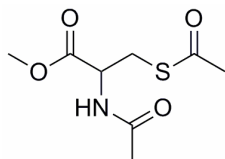
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| 1 | 1.466 | VV | 0.0807 | 1.00686e4 | 1934.15417 | 98.0426 |
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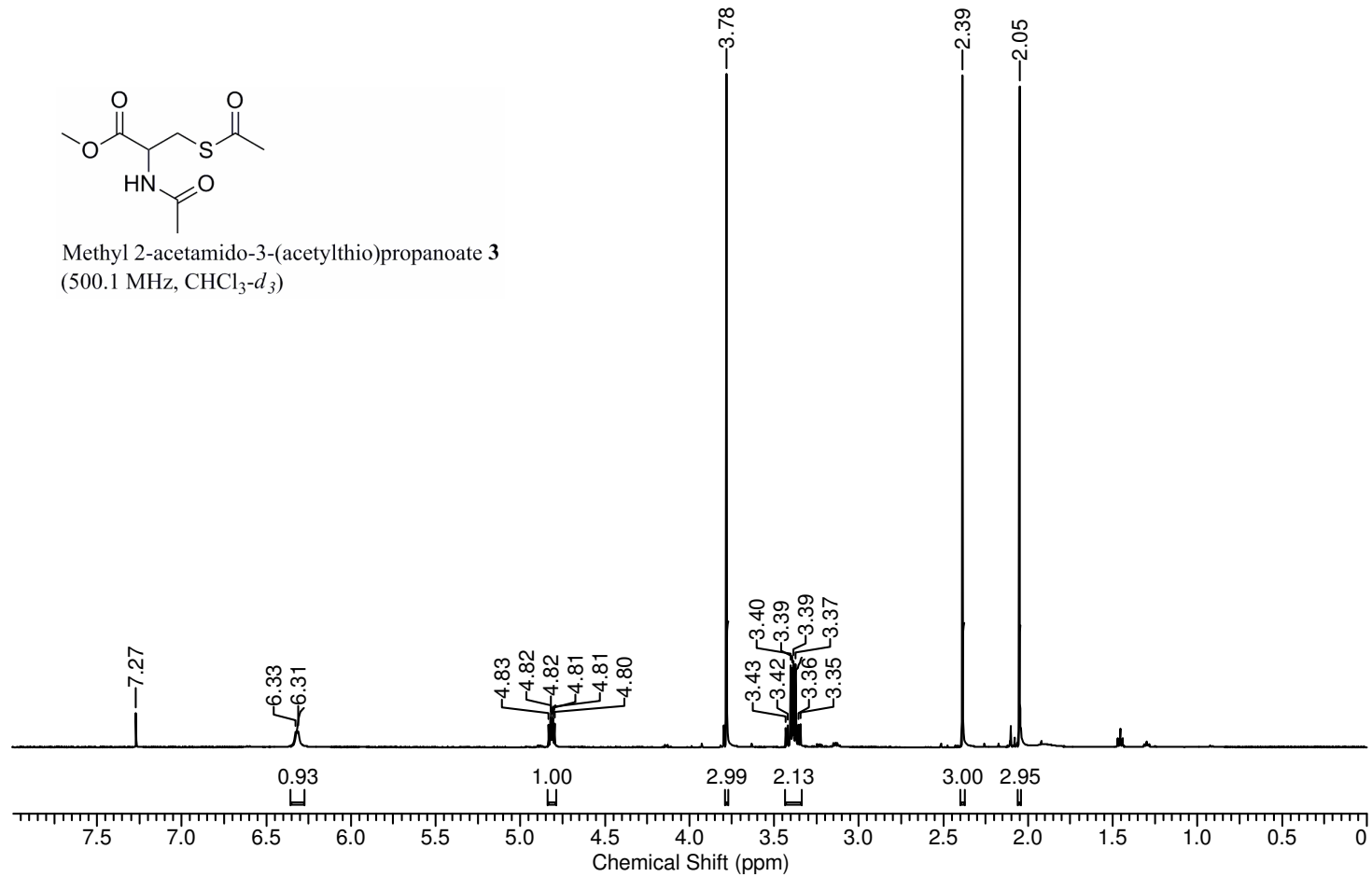
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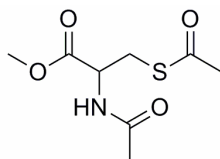
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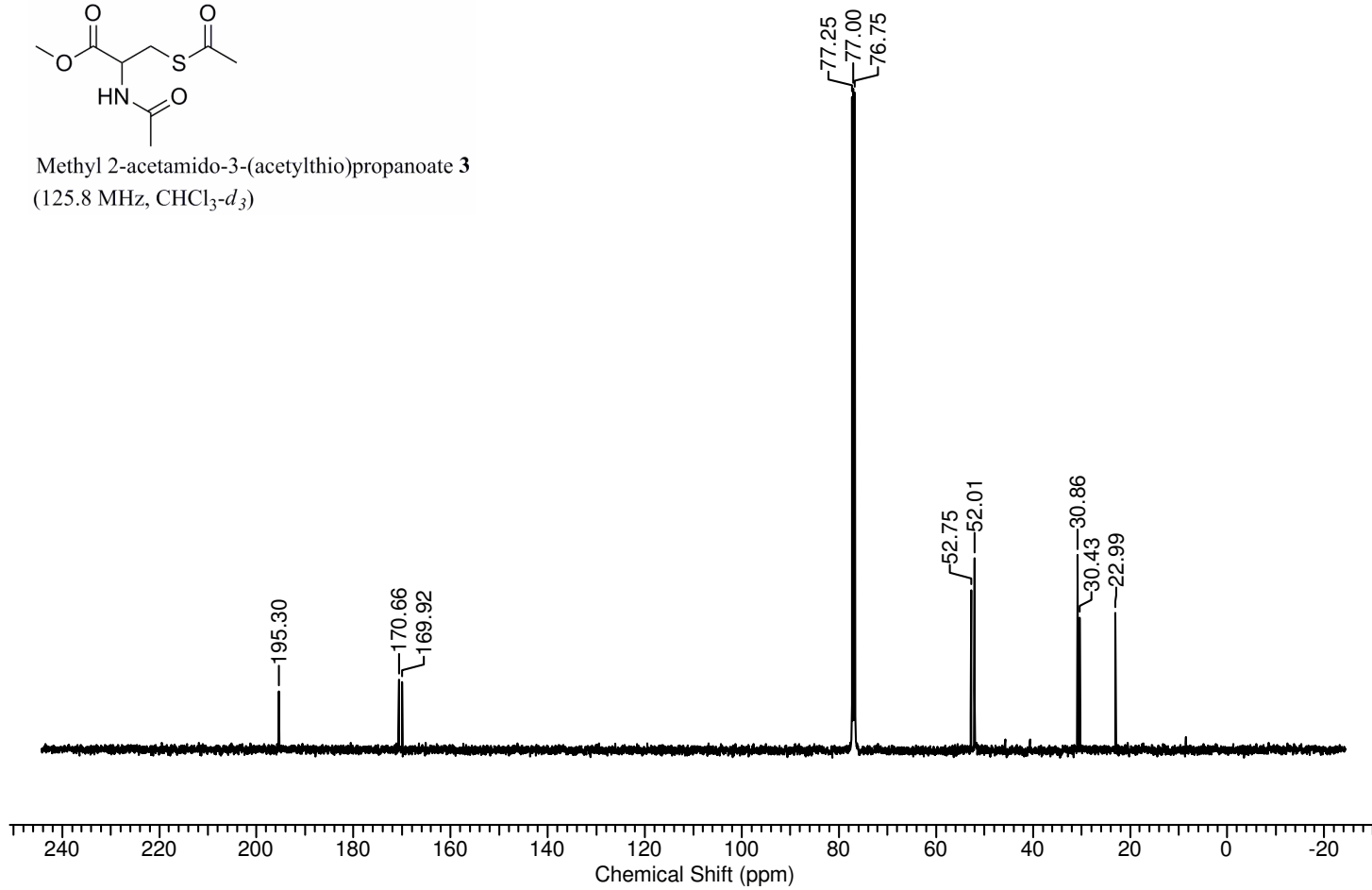


Methyl 2-acetamido-3-(acetylthio)propanoate **3**
(500.1 MHz, CHCl_3-d_3)





Methyl 2-acetamido-3-(acetylthio)propanoate **3**
(125.8 MHz, CHCl_3-d_3)



Mass Spectrum Molecular Formula Report

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Method xiaofengpos.m
Sample Name rab-4
Comment

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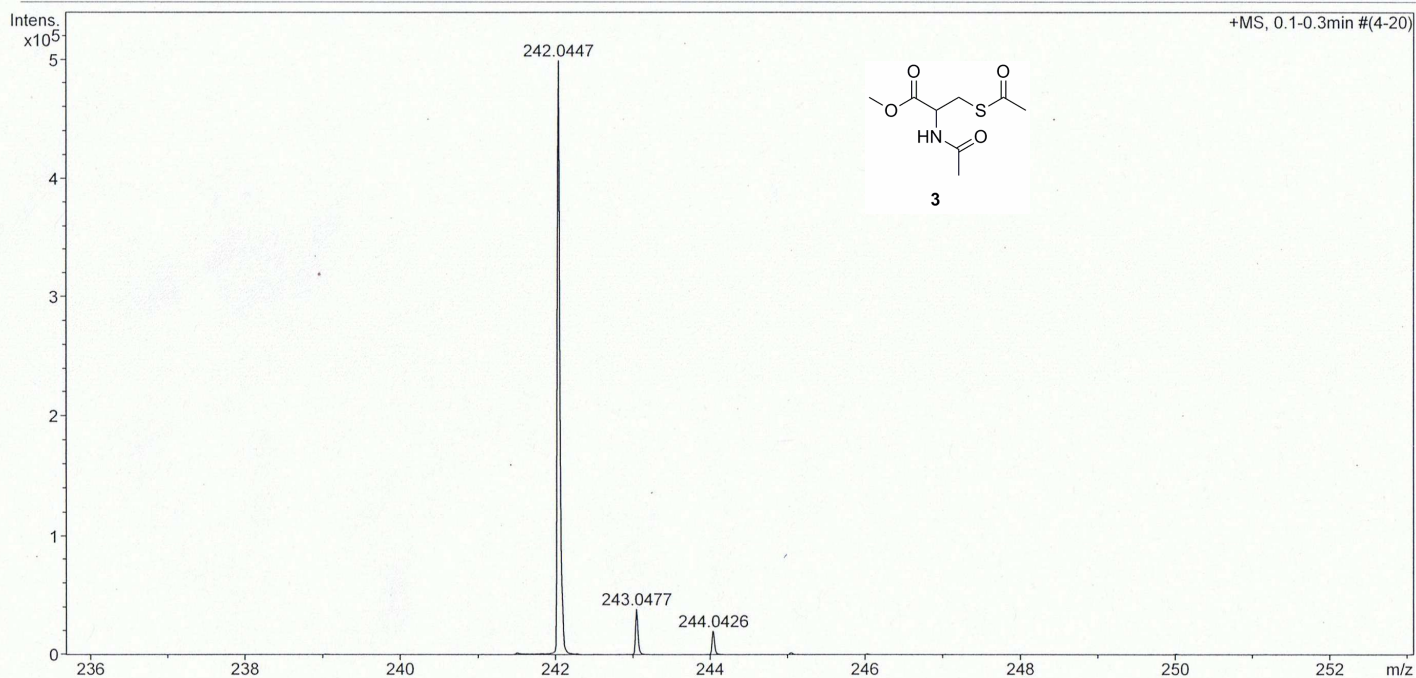
Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
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Scan End 1500 m/z

Ion Polarity Positive
Capillary Exit 150.0 V
Hexapole RF 130.0 V
Skimmer 1 55.0 V
Hexapole 1 26.0 V

Set Corrector Fill 52 V
Set Pulsar Pull 398 V
Set Pulsar Push 398 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 1960 V

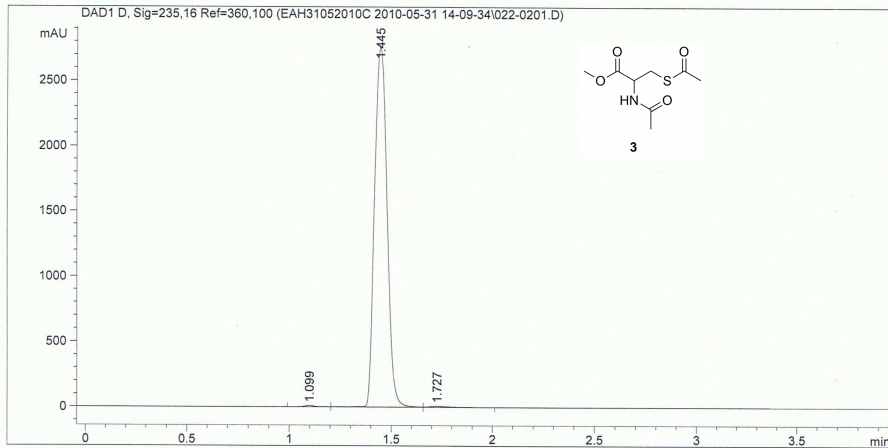


HPLC analysis of methyl 2-acetamido-3-(acetylthio)propanoate (2)

Purity was determined using an Agilent Technologies 1200 series HPLC system with a photodiode UV-visible detector; column: Eclipse XDB-C₁₈ 4.6 x 150mm 5 µm C₁₈; mobile phase: methanol; injection volume: 20 µL; UV detection: 235 nm; flow rate: 1 mL/min.

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                                                    Inj Volume: 20 µl
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Last changed   : 5/31/2010 2:26:19 PM by Ian
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Area Percent Report

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Dilution       : 1.0000
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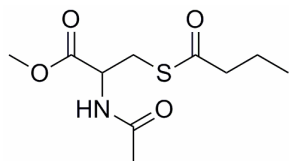
Signal 1: DAD1 D, Sig=235,16 Ref=360,100

| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
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| 1 | 1.099 | BV | 0.0630 | 43.74969 | 10.42287 | 0.3671 |
| 2 | 1.445 | VV | 0.0697 | 1.18105e4 | 2771.47900 | 99.1010 |
| 3 | 1.727 | VB | 0.1022 | 63.39398 | 8.78621 | 0.5319 |

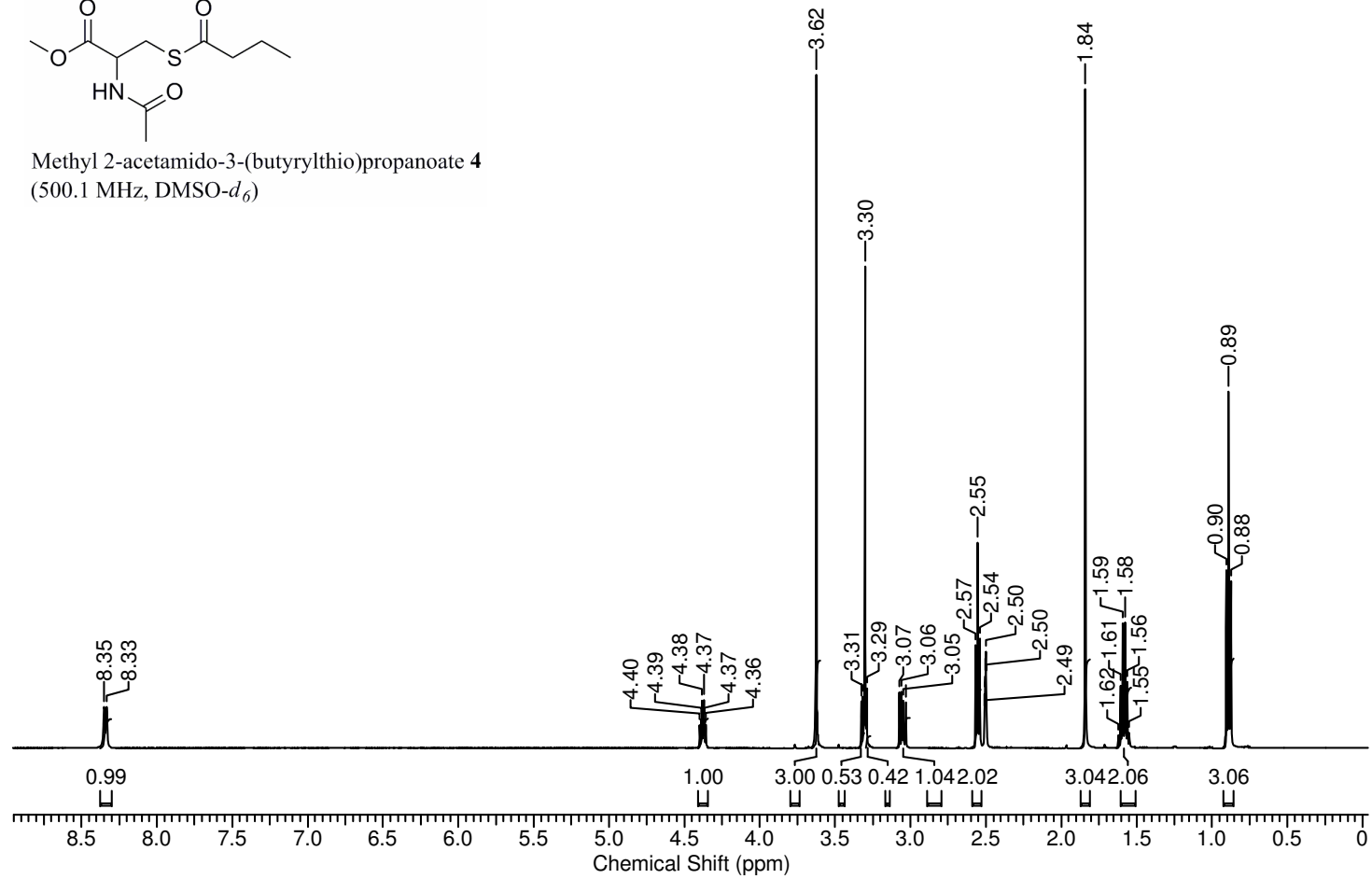
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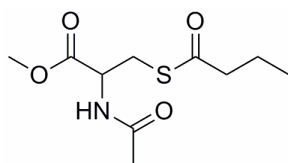
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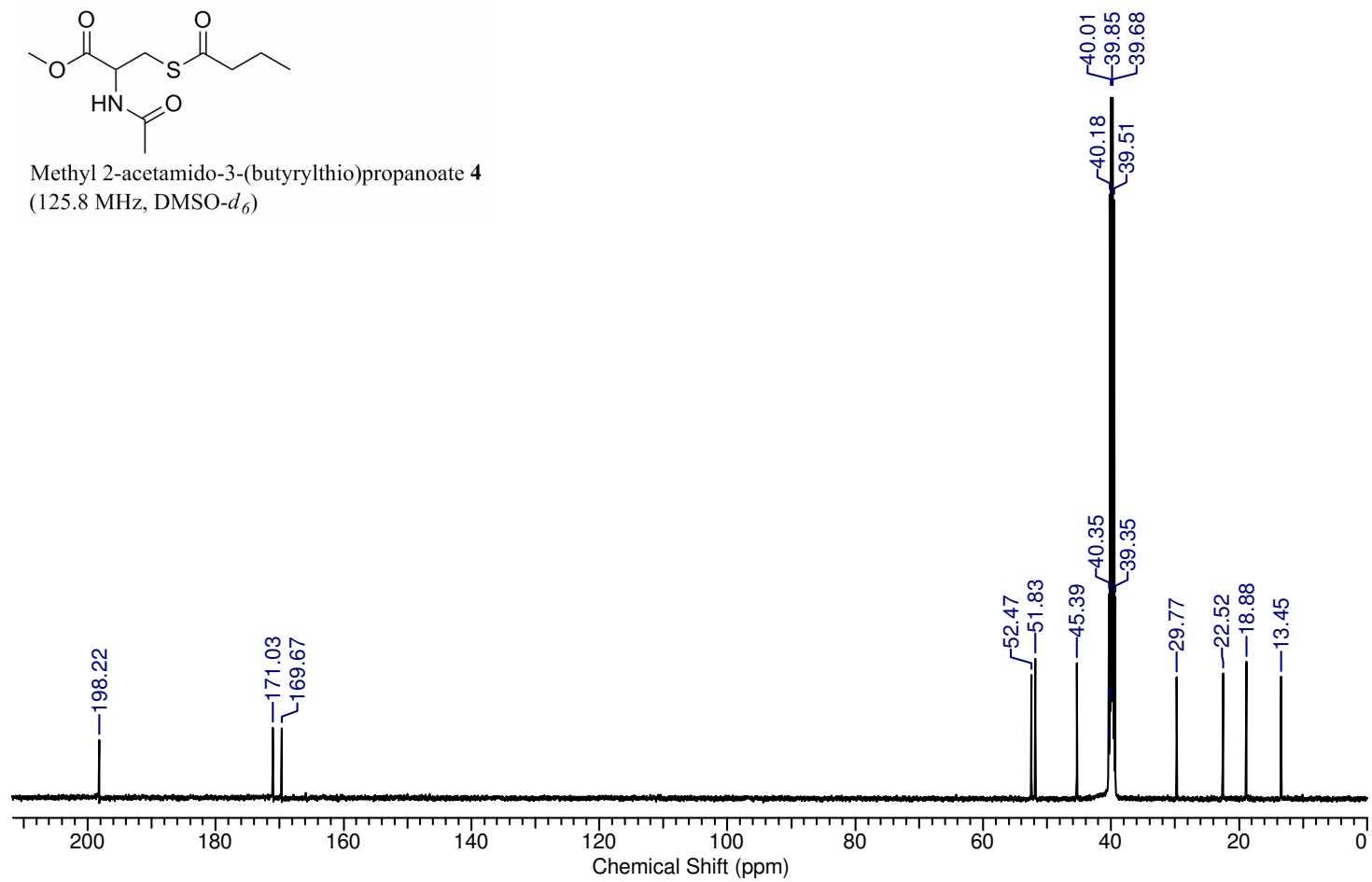


Methyl 2-acetamido-3-(butyrylthio)propanoate **4**
(500.1 MHz, DMSO-*d*₆)





Methyl 2-acetamido-3-(butyrylthio)propanoate **4**
(125.8 MHz, DMSO-*d*₆)



Mass Spectrum Molecular Formula Report

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Method xiaofengpos.m
Sample Name rab-5
Comment

Acquisition Date 10/3/2008 1:32:09 PM

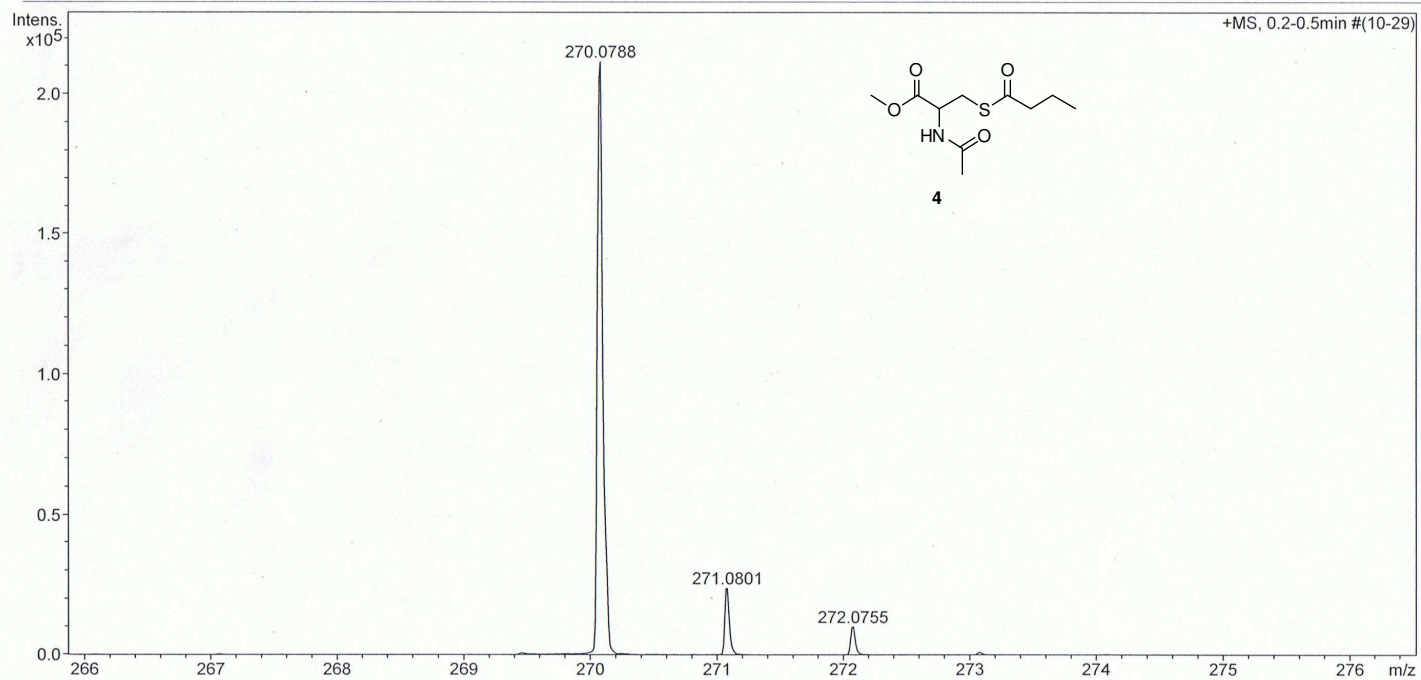
Operator
Instrument Administrator
microTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 1500 m/z

Ion Polarity Positive
Capillary Exit 150.0 V
Hexapole RF 130.0 V
Skimmer 1 55.0 V
Hexapole 1 26.0 V

Set Corrector Fill 52 V
Set Pulsar Pull 398 V
Set Pulsar Push 398 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 1960 V

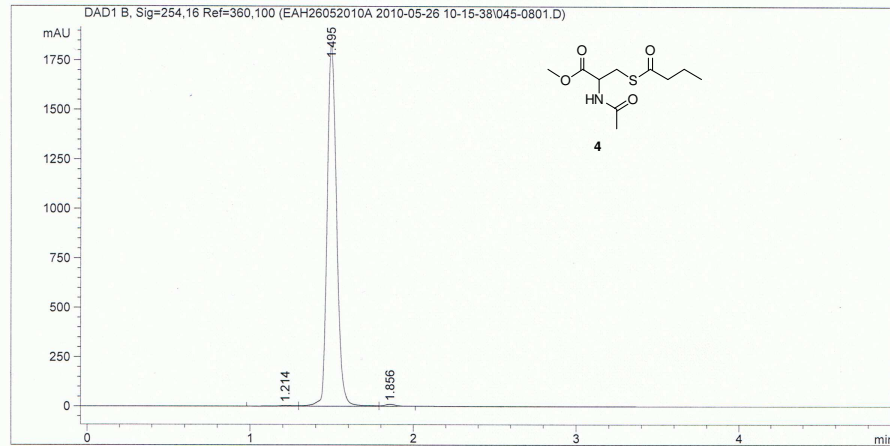


HPLC analysis of methyl 2-acetamido-3-(butyrylthio)propanoate (4)

Purity was determined using an Agilent Technologies 1200 series HPLC system with a photodiode UV-visible detector; column: Eclipse XDB-C₁₈ 4.6 x 150mm 5 µm C₁₈; mobile phase: methanol; injection volume: 20 µL; UV detection: 254 nm; flow rate: 1 mL/min.

Data File C:\CHEM32\1\DATA\JEREMY\JER091008CFRACS 2008-10-09 15-09-59\EAH26052010A 2010-05-26 10-1
Sample Name: RAB-5

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                                                    Inj Volume: 20 µl
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                : 2010-05-26 10-15-38\REV PHASE METHANOL 20UL.M
Last changed    : 5/5/2010 2:09:53 PM by Ian
Analysis Method : C:\CHEM32\1\DATA\JEREMY\JER091008CFRACS 2008-10-09 15-09-59\EAH26052010A
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Last changed    : 5/26/2010 1:49:28 PM by Ian
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Method Info     : Reverse Phase Methanol
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Area Percent Report

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Dilution       : 1.0000
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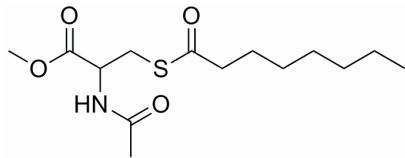
Signal 1: DAD1 B, Sig=254,16 Ref=360,100

| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
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| 1 | 1.214 | BV | 0.1054 | 34.47628 | 4.30508 | 0.4628 |
| 2 | 1.495 | VV | 0.0627 | 7367.03809 | 1841.66760 | 98.8906 |
| 3 | 1.856 | VB | 0.0720 | 48.17263 | 10.03880 | 0.6466 |

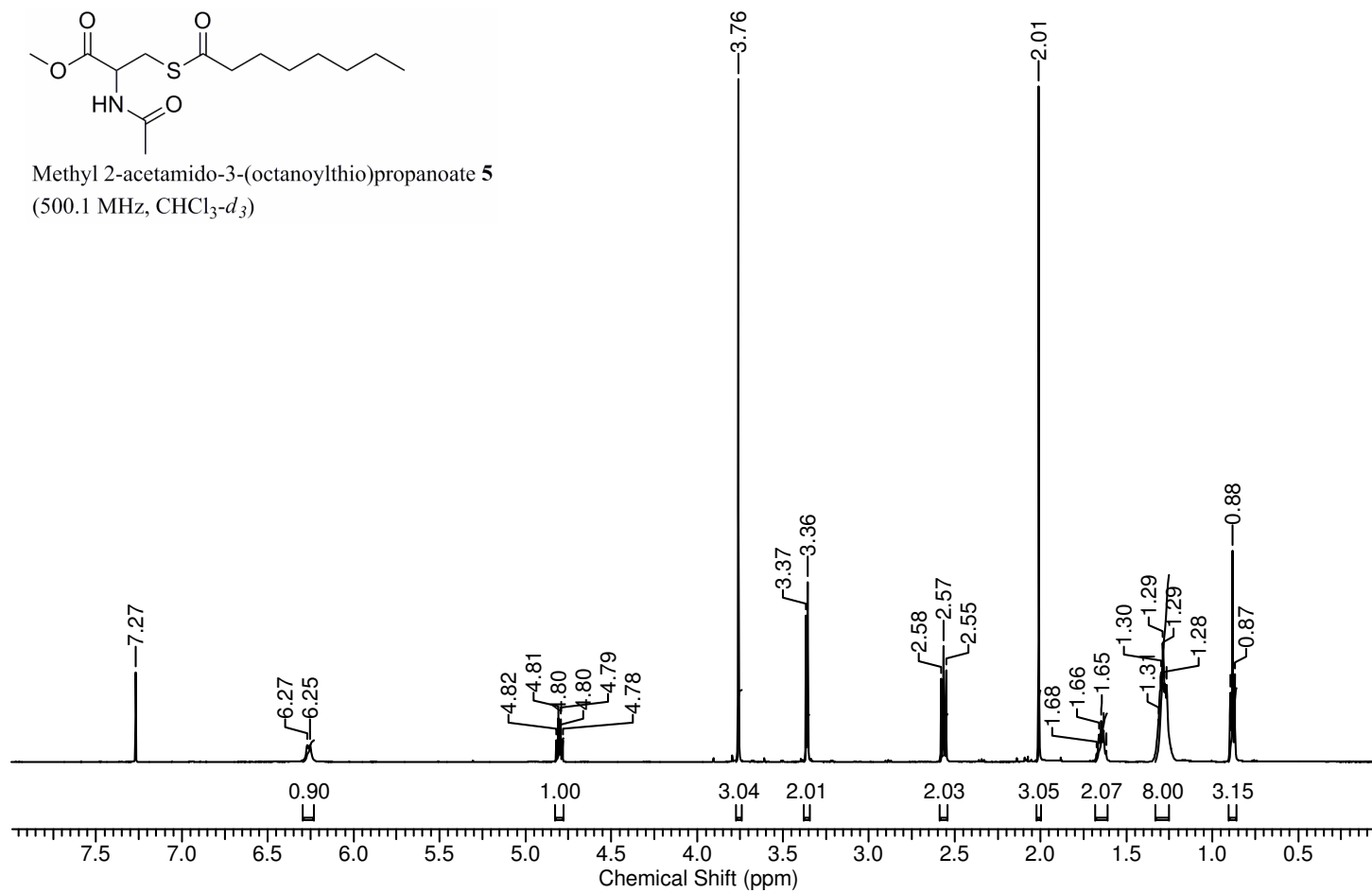
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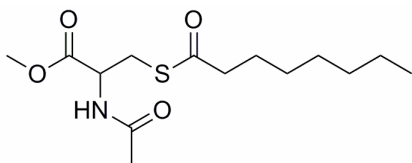
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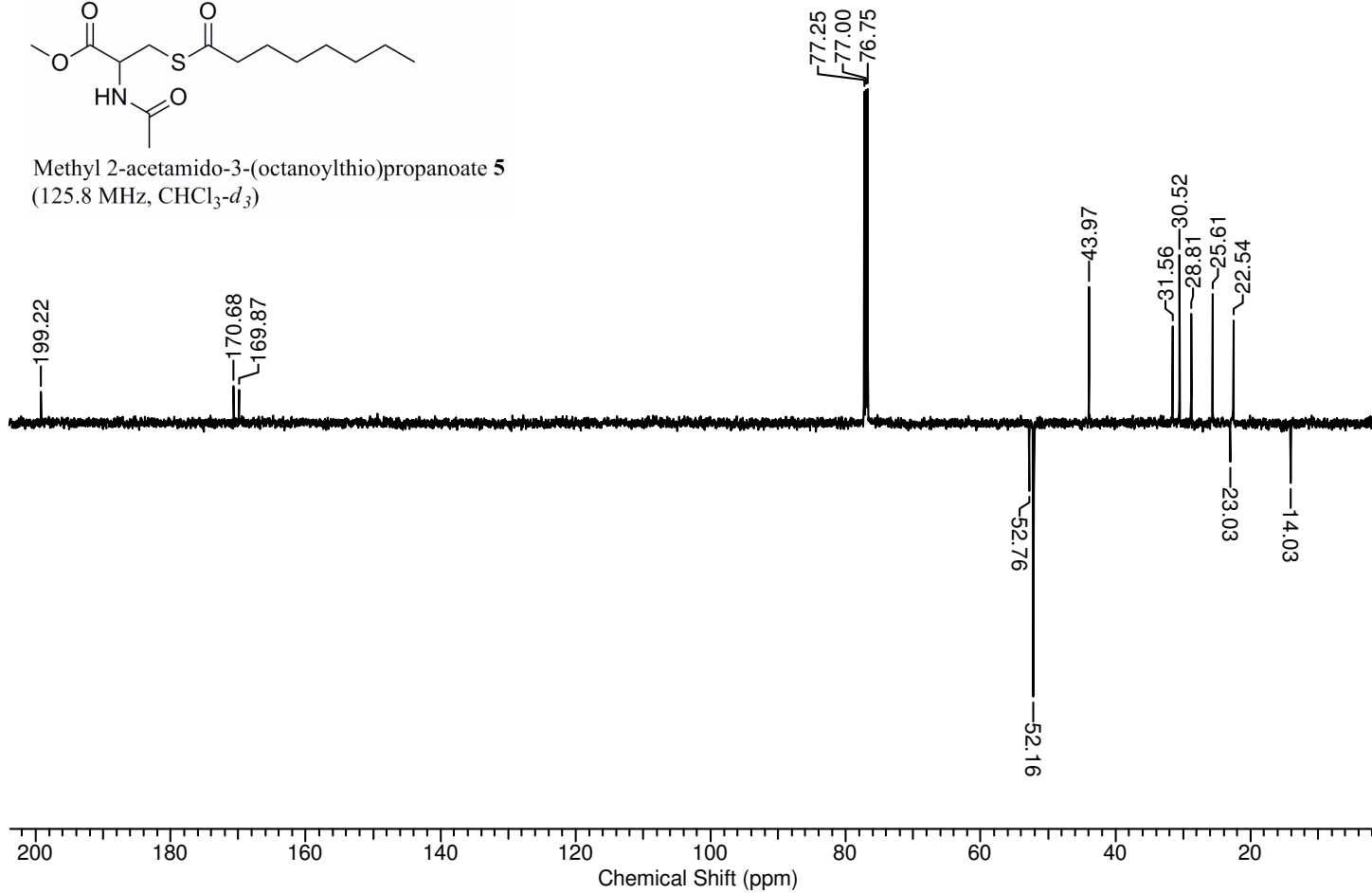


Methyl 2-acetamido-3-(octanoylthio)propanoate **5**
(500.1 MHz, CHCl_3-d_3)





Methyl 2-acetamido-3-(octanoylthio)propanoate **5**
(125.8 MHz, CHCl_3-d_3)



Mass Spectrum Molecular Formula Report

Analysis Info

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Method xiaofengpos.m
Sample Name EAH-17
Comment

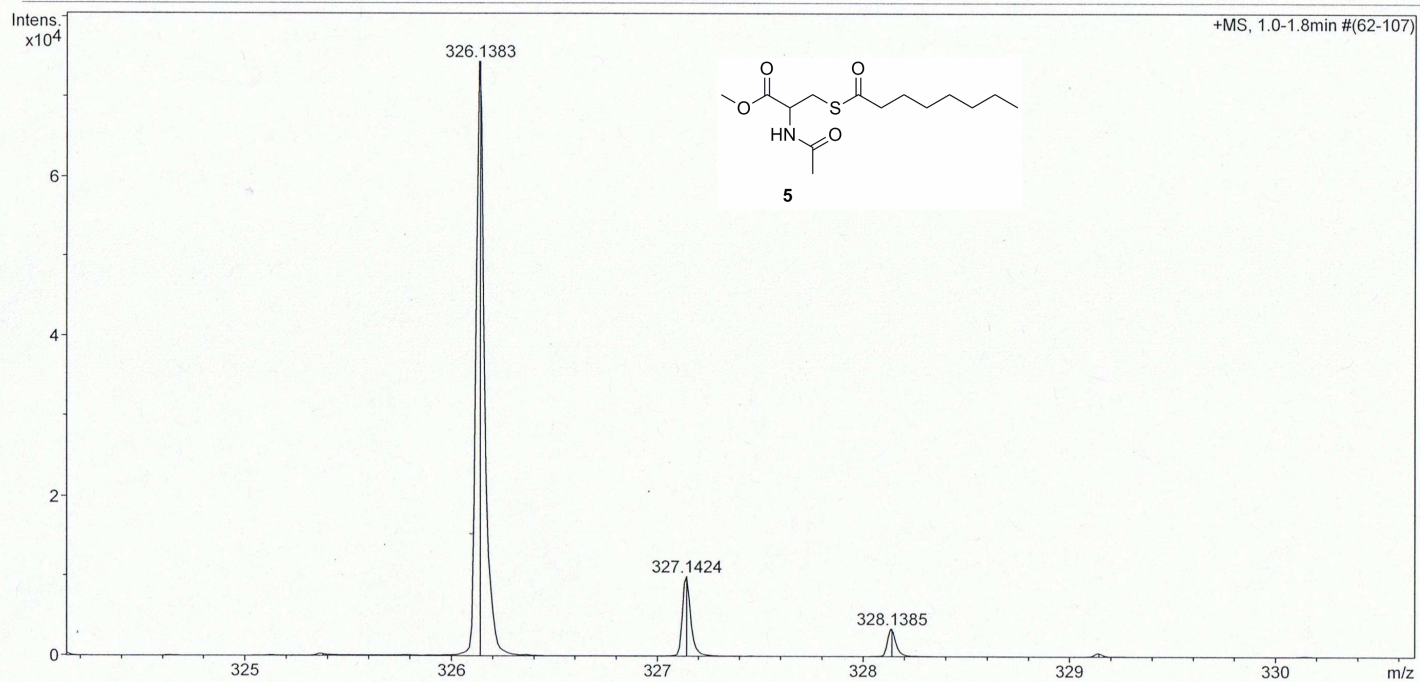
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Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

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Scan End 1500 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 55.0 V
Hexapole 1 26.0 V

Set Corrector Fill 52 V
Set Pulsar Pull 398 V
Set Pulsar Push 398 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 1960 V



HPLC analysis of methyl 2-acetamido-3-(octanoylthio)propanoate (5)

Purity was determined using an Agilent Technologies 1200 series HPLC system with a photodiode UV-visible detector; column: Eclipse XDB-C₁₈ 4.6 x 150mm 5 µm C₁₈; mobile phase: methanol; injection volume: 50 µL; UV detection: 220 nm; flow rate: 1 mL/min.

Data File C:\CHEM32\1\DATA\EMMA HIGGINS\EAH12022010E 2010-02-12 15-48-16\056-1001.D
Sample Name: EAH-17

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                                                    Inj Volume: 50 µl
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HEN METHANOL 50UL FRACON.M
Last changed    : 1/28/2010 2:13:55 PM by Ian
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DA.M (REV PHASE HEN METHANOL 50UL FRACON.M)
Last changed    : 5/25/2010 3:57:52 PM by Ian
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Area Percent Report

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Use Multiplier & Dilution Factor with ISTDs
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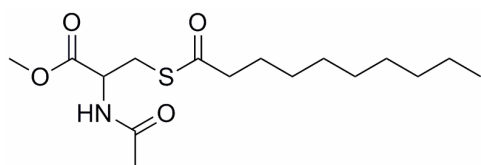
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| 1 | 1.435 | VV | 0.0998 | 128.47316 | 18.31710 | 1.6633 |
| 2 | 1.691 | VB | 0.0716 | 7595.43359 | 1594.50146 | 98.3367 |

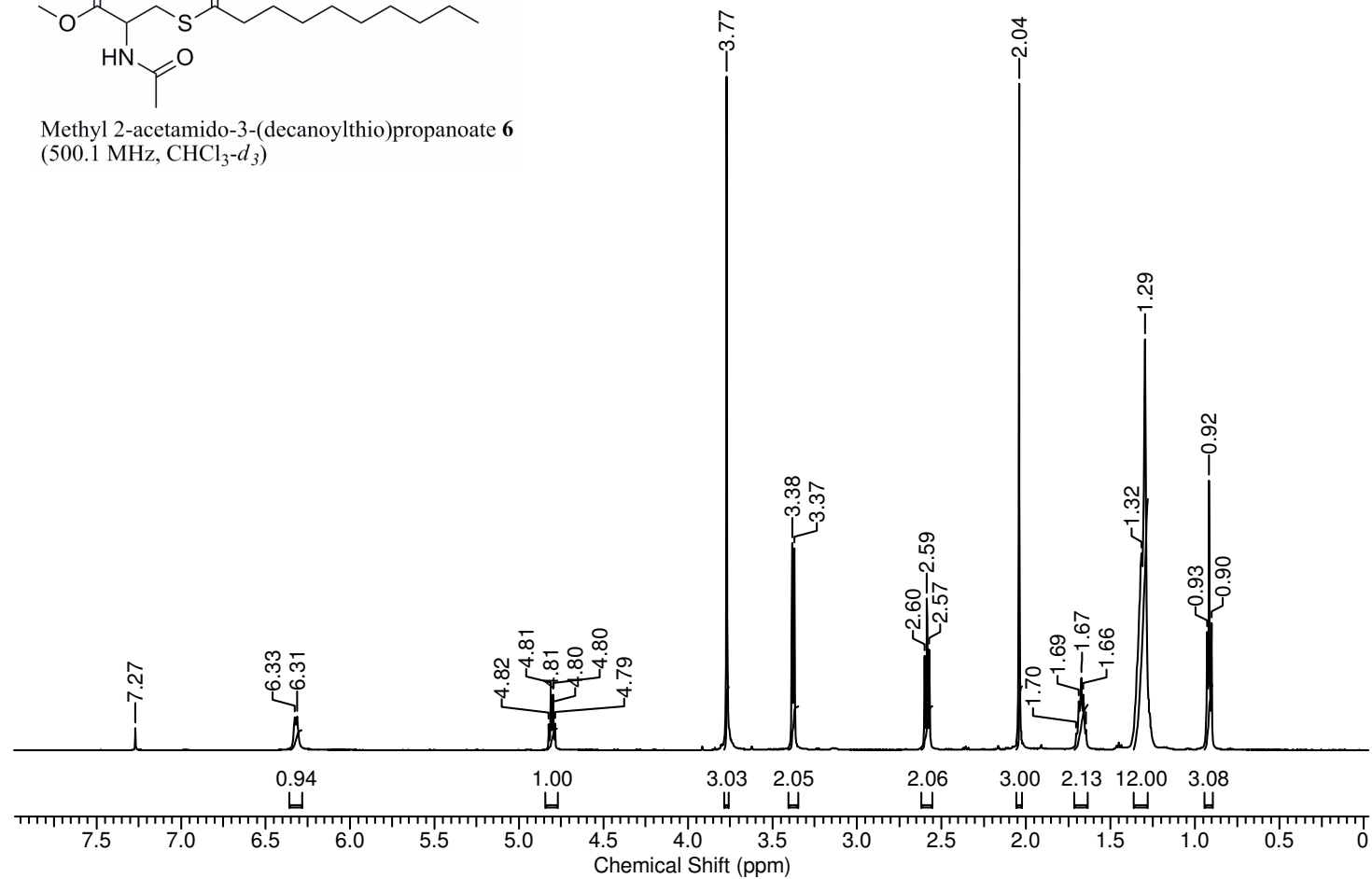
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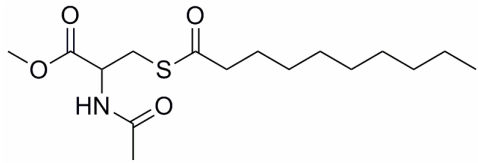
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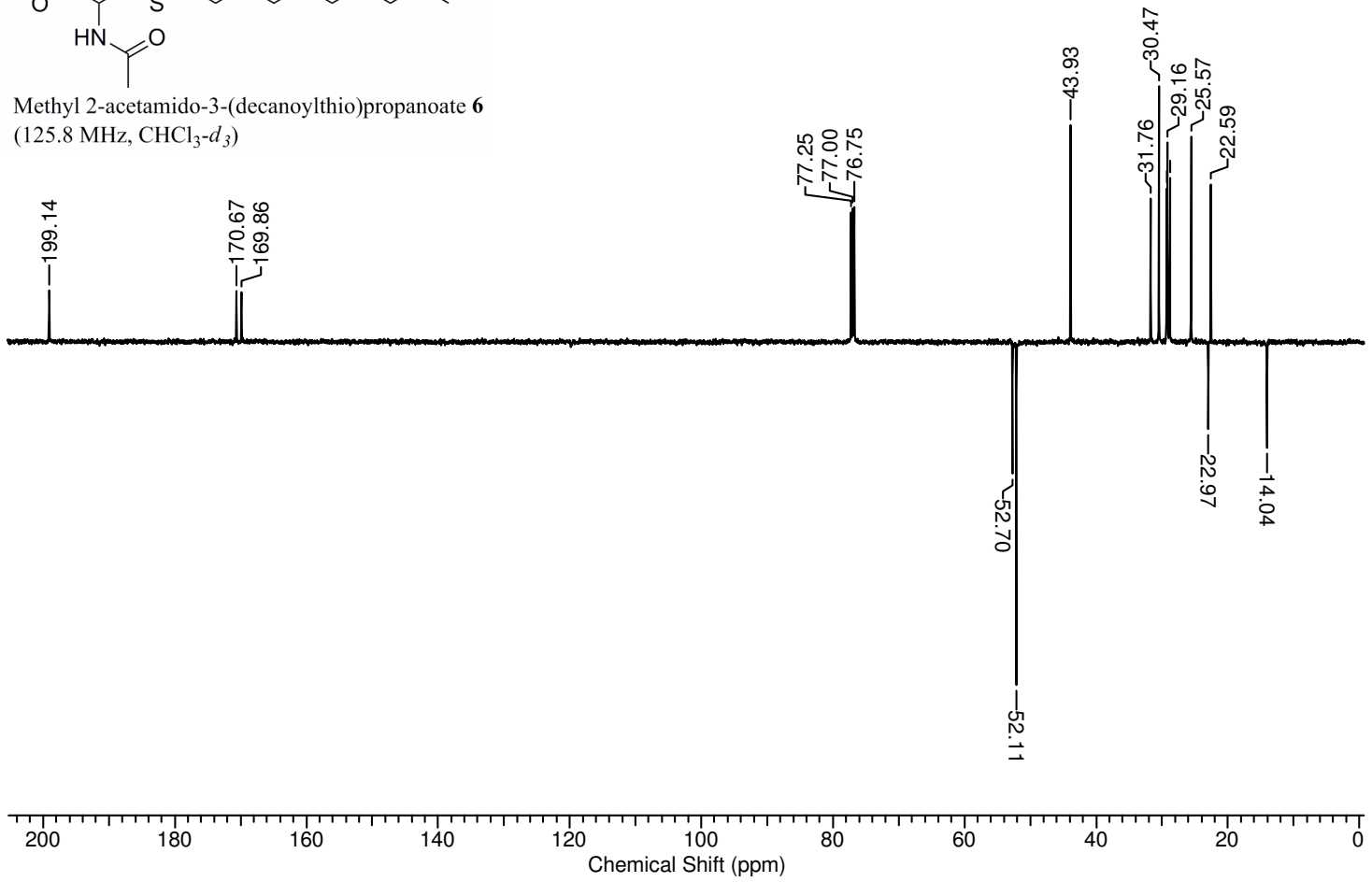


Methyl 2-acetamido-3-(decanoylthio)propanoate **6**
(500.1 MHz, CHCl₃-d₃)





Methyl 2-acetamido-3-(decanoylthio)propanoate **6**
(125.8 MHz, CHCl_3-d_3)



Mass Spectrum Molecular Formula Report

Analysis Info

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Method xiaofengpos.m
Sample Name EAH-16
Comment

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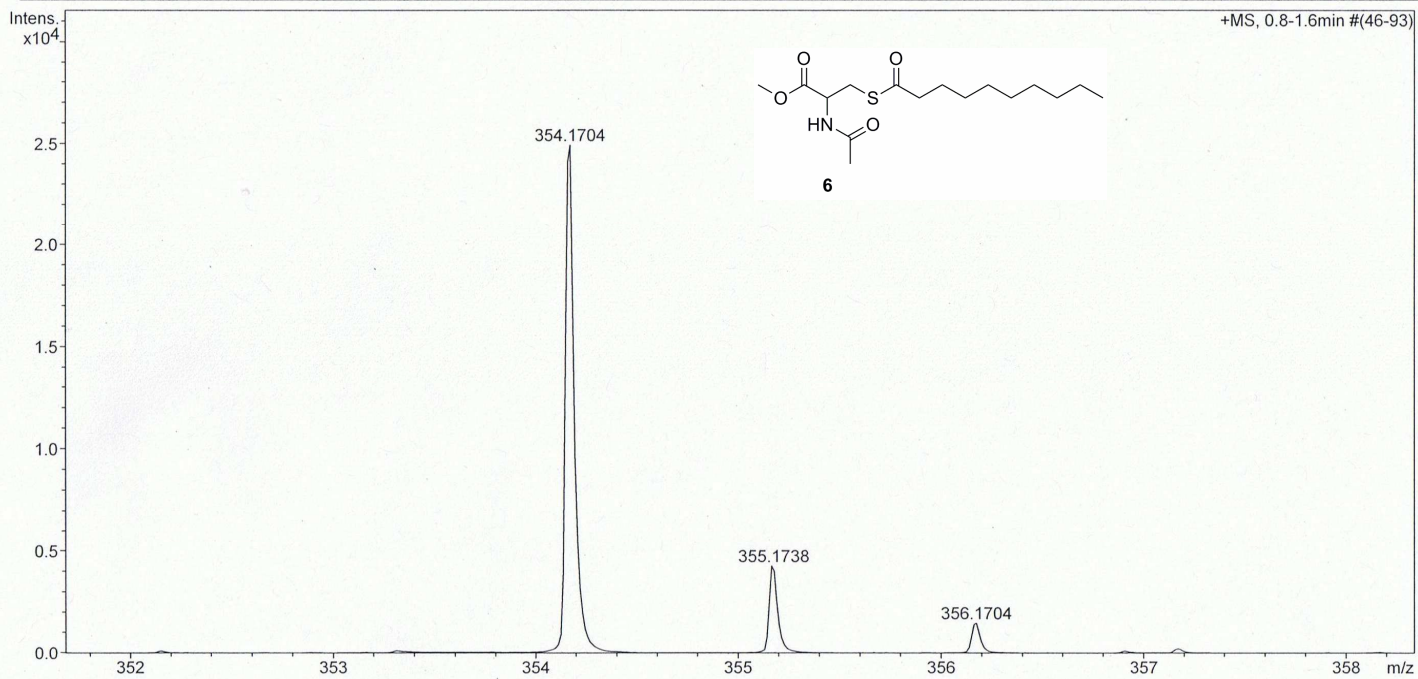
Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
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Scan Begin 50 m/z
Scan End 1500 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 55.0 V
Hexapole 1 26.0 V

Set Corrector Fill 52 V
Set Pulsar Pull 398 V
Set Pulsar Push 398 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 1960 V

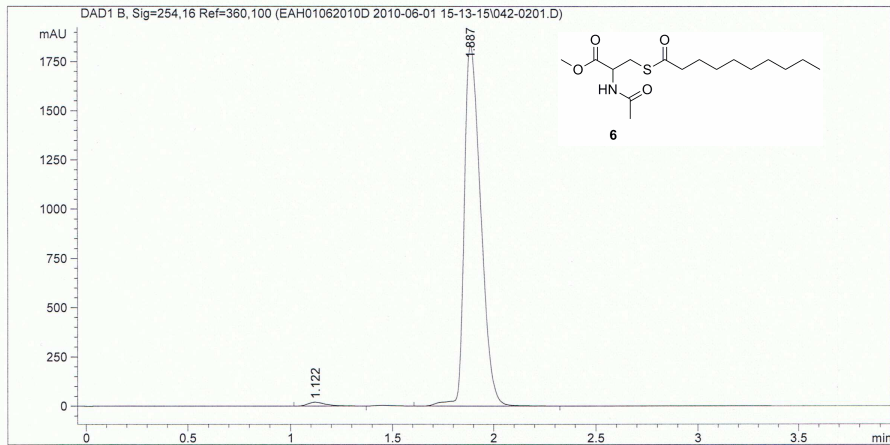


HPLC analysis of methyl 2-acetamido-3-(decanoylthio)propanoate (6)

Purity was determined using an Agilent Technologies 1200 series HPLC system with a photodiode UV-visible detector; column: Eclipse XDB-C₁₈ 4.6 x 150mm 5 µm C₁₈; mobile phase: methanol; injection volume: 70 µL; UV detection: 254 nm; flow rate: 1 mL/min.

Data File C:\CHEM32\1\DATA\JEREMY\JER091008CFRACS 2008-10-09 15-09-59\EAH01062010D 2010-06-01 15-1
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                                                    Inj Volume: 70 µl
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Last changed    : 6/1/2010 3:13:02 PM by Ian
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Area Percent Report

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Dilution       : 1.0000
Use Multiplier & Dilution Factor with ISTDs
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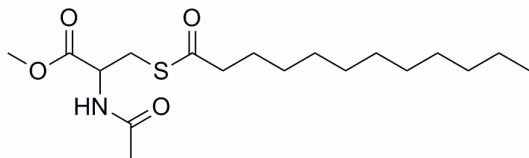
Signal 1: DAD1 B, Sig=254,16 Ref=360,100

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| 1 | 1.122 | BB | 0.0938 | 128.19121 | 20.27837 | 1.2187 |
| 2 | 1.887 | VB | 0.0898 | 1.03904e4 | 1841.08044 | 98.7813 |

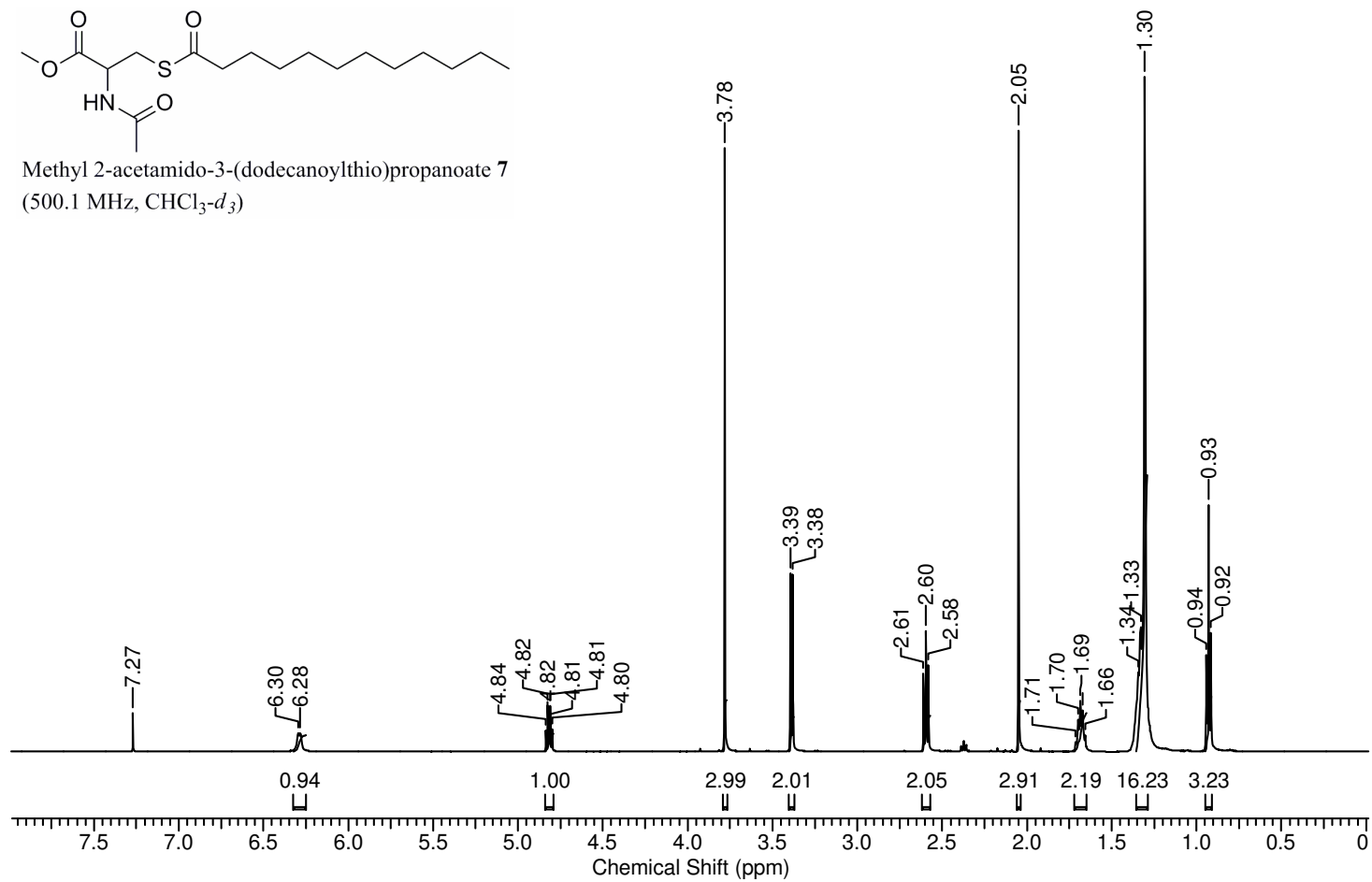
Totals : 1.05186e4 1861.35882

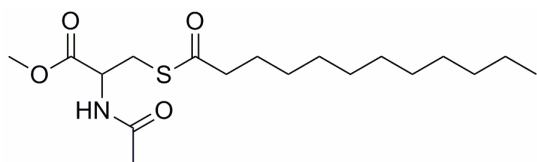
Instrument 1 6/1/2010 3:35:24 PM Ian

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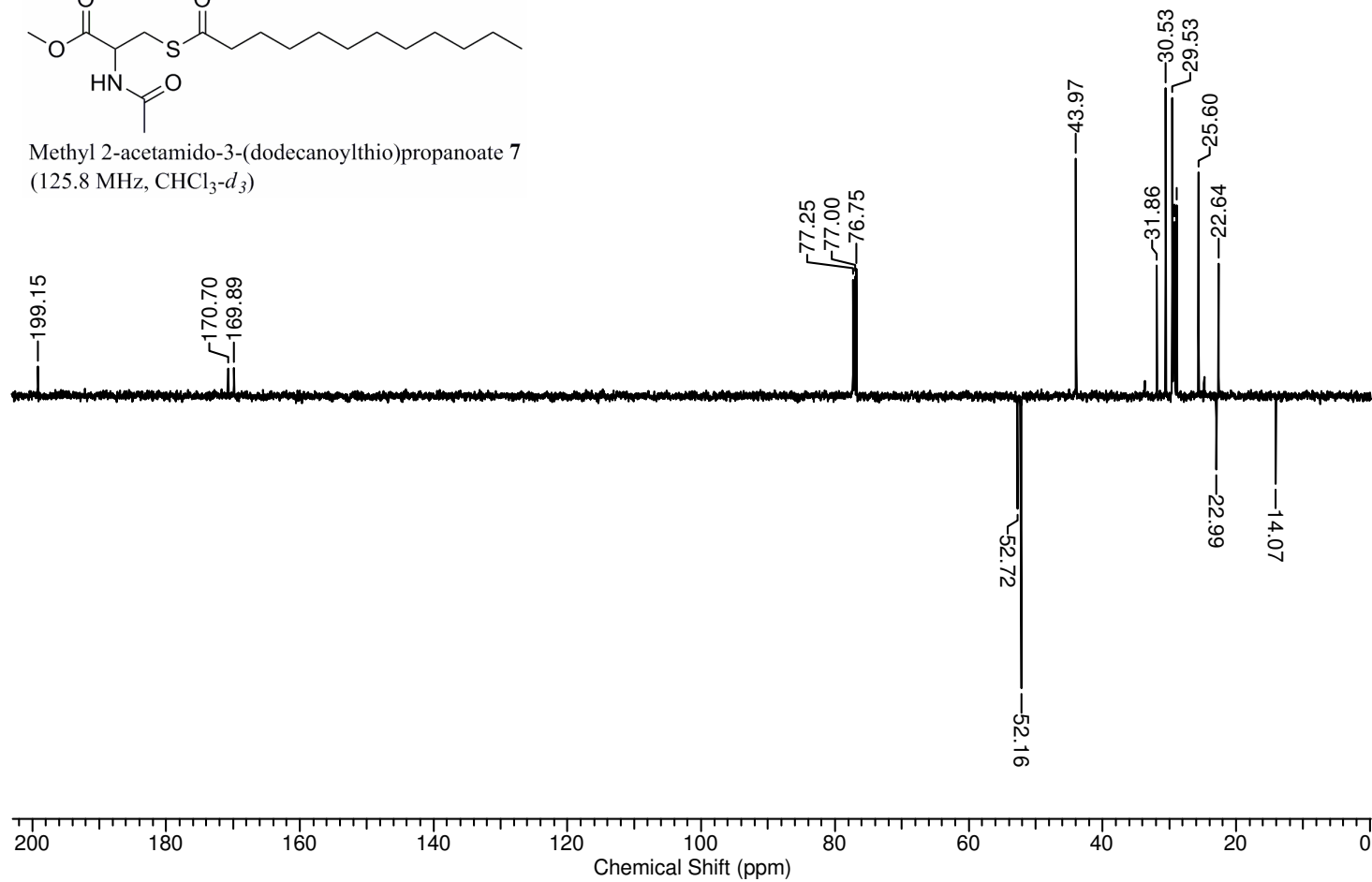


Methyl 2-acetamido-3-(dodecanoylthio)propanoate **7**
(500.1 MHz, CHCl_3-d_3)





Methyl 2-acetamido-3-(dodecanoylthio)propanoate **7**
(125.8 MHz, CHCl_3-d_3)



Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 3 08000004.d
Method xiaofengpos.m
Sample Name rab-6
Comment

Acquisition Date 10/3/2008 1:57:36 PM

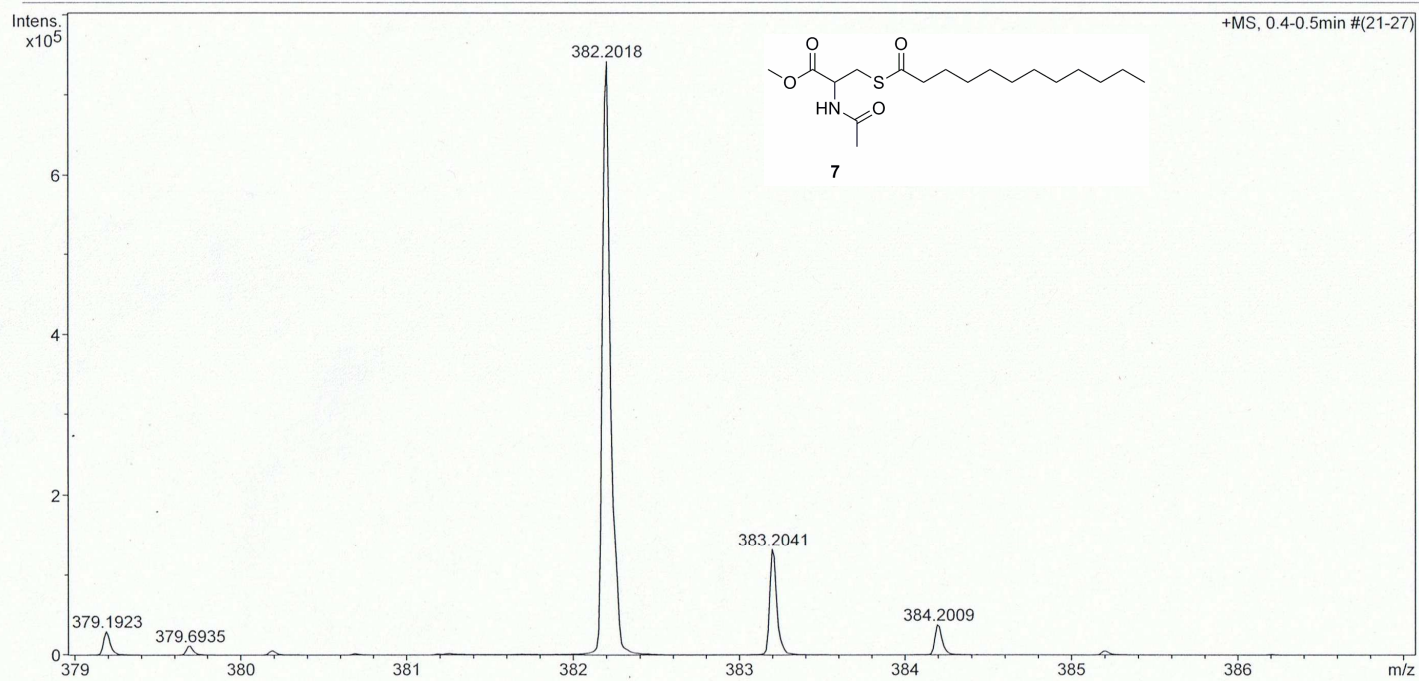
Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 1500 m/z

Ion Polarity Positive
Capillary Exit 150.0 V
Hexapole RF 130.0 V
Skimmer 1 55.0 V
Hexapole 1 26.0 V

Set Corrector Fill 52 V
Set Pulsar Pull 398 V
Set Pulsar Push 398 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 1960 V

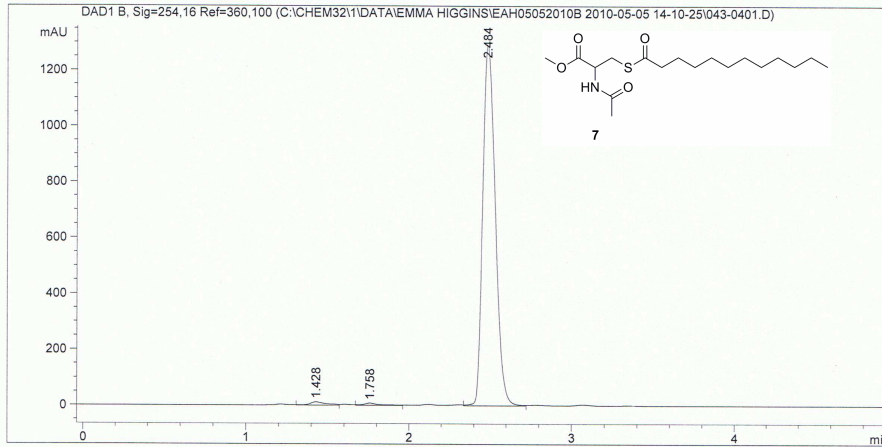


HPLC analysis of methyl 2-acetamido-3-(dodecanoylthio)propanoate (7)

Purity was determined using an Agilent Technologies 1200 series HPLC system with a photodiode UV-visible detector; column: Eclipse XDB-C₁₈ 4.6 x 150mm 5 µm C₁₈; mobile phase: methanol; injection volume: 20 µL; UV detection: 254 nm; flow rate: 1 mL/min.

Data File C:\CHEM32\1\DATA\EMMA HIGGINS\EAH05052010B 2010-05-05 14-10-25\043-0401.D
Sample Name: EAH-12

```
=====
Acq. Operator   : Ian                               Seq. Line :    4
Acq. Instrument : Instrument 1                       Location  : Vial 43
Injection Date  : 5/5/2010 2:35:03 PM              Inj       :    1
                                                    Inj Volume: 20 µl
Acq. Method     : C:\Chem32\1\DATA\EMMA HIGGINS\EAH05052010B 2010-05-05 14-10-25\REV PHASE
                  METHANOL 20UL.M
Last changed    : 5/5/2010 2:09:53 PM by Ian
Analysis Method : C:\CHEM32\1\DATA\EMMA HIGGINS\EAH05052010B 2010-05-05 14-10-25\043-0401.D\
                  DA.M (REV PHASE METHANOL 20UL.M)
Last changed    : 5/5/2010 2:09:53 PM by Ian
                  (Current integration events modified)
Method Info     : Reverse Phase Methanol
=====
```



Area Percent Report

```
Sorted By      : Signal
Multiplier     : 1.0000
Dilution       : 1.0000
Use Multiplier & Dilution Factor with ISTDs
```

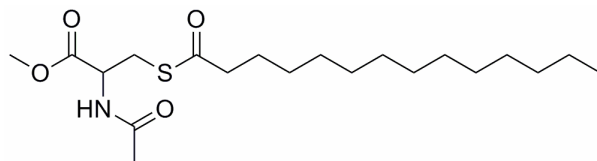
Signal 1: DAD1 B, Sig=254,16 Ref=360,100

| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 1.428 | VV | 0.0970 | 83.15818 | 11.97593 | 1.1704 |
| 2 | 1.758 | VB | 0.0954 | 55.89657 | 8.01217 | 0.7867 |
| 3 | 2.484 | VV | 0.0847 | 6965.81787 | 1295.59766 | 98.0428 |

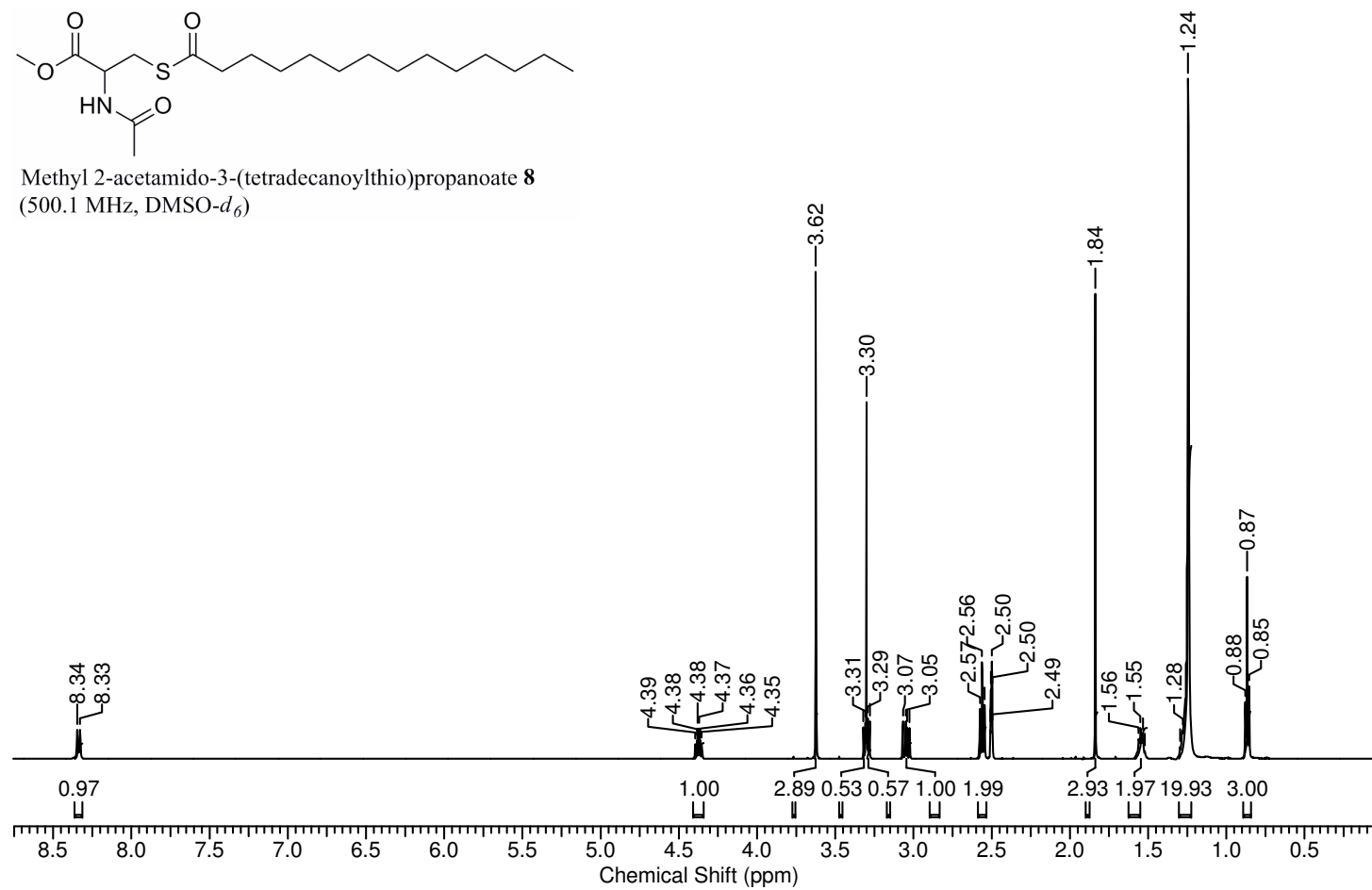
Totals : 7104.87262 1315.58575

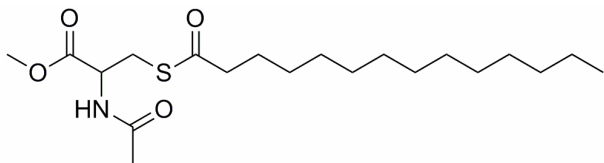
Instrument 1 5/25/2010 3:43:56 PM Ian

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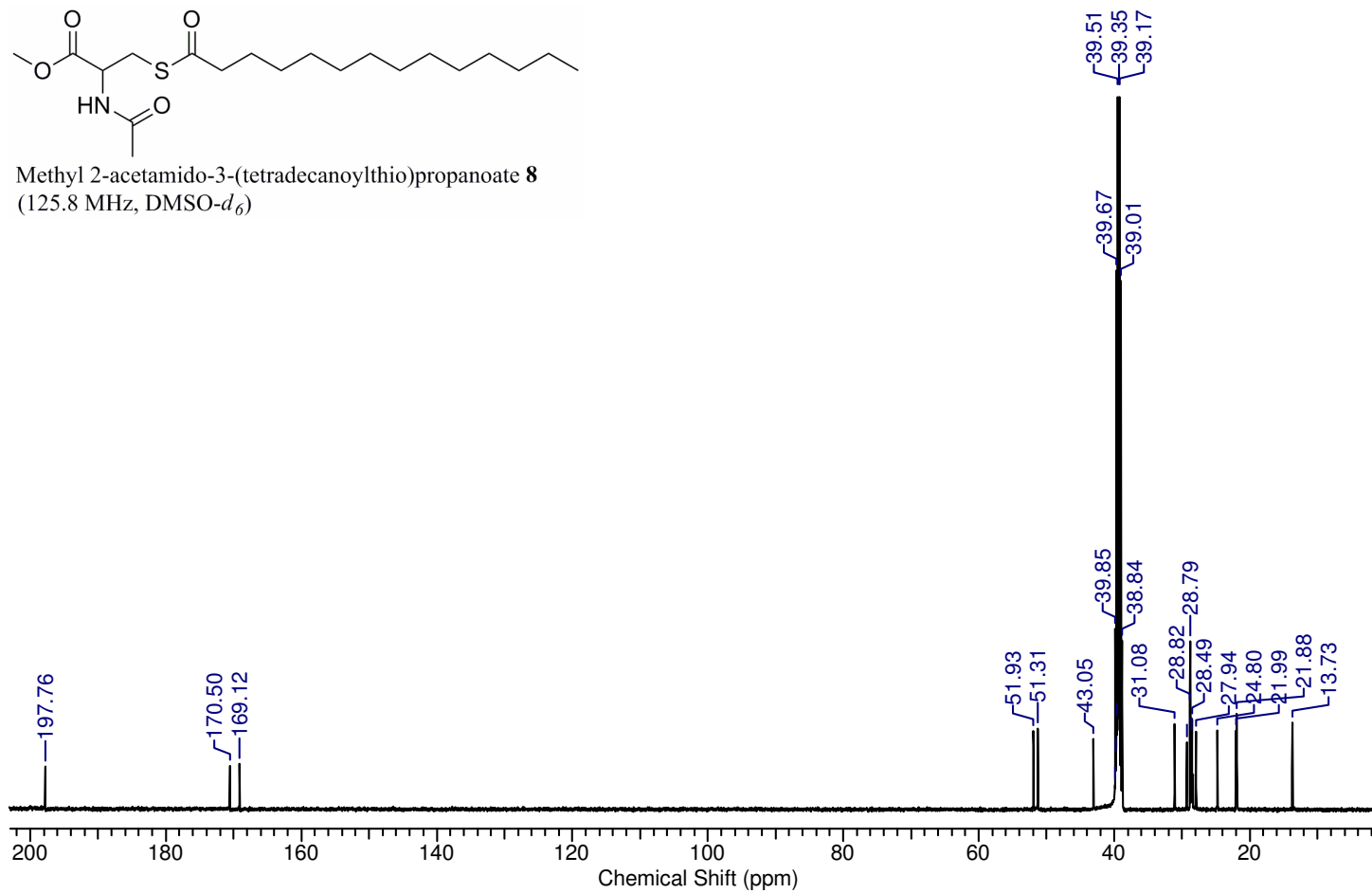


Methyl 2-acetamido-3-(tetradecanoylthio)propanoate **8**
(500.1 MHz, DMSO-*d*₆)





Methyl 2-acetamido-3-(tetradecanoylthio)propanoate **8**
(125.8 MHz, DMSO- d_6)



Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 3 08000002.d
Method xiaofengpos.m
Sample Name rab-7
Comment

Acquisition Date 10/3/2008 1:41:51 PM

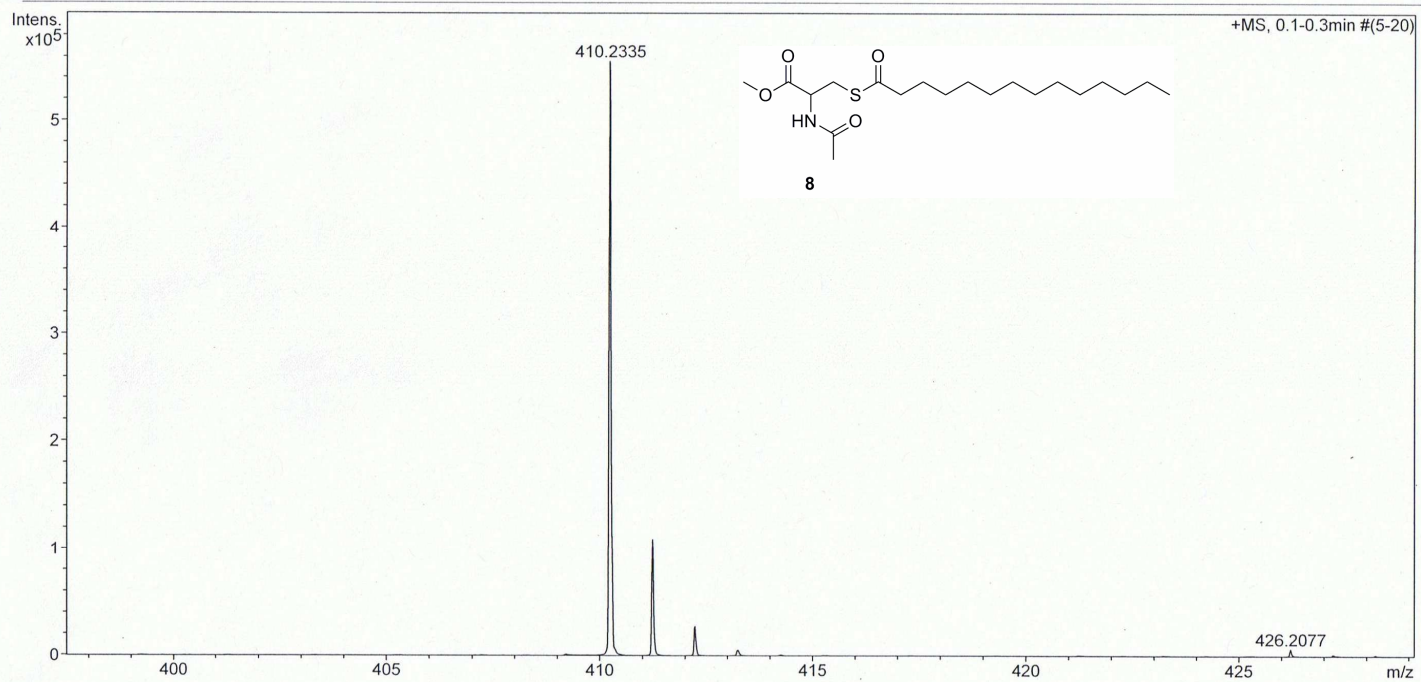
Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 1500 m/z

Ion Polarity Positive
Capillary Exit 150.0 V
Hexapole RF 130.0 V
Skimmer 1 55.0 V
Hexapole 1 26.0 V

Set Corrector Fill 52 V
Set Pulsar Pull 398 V
Set Pulsar Push 398 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 1960 V

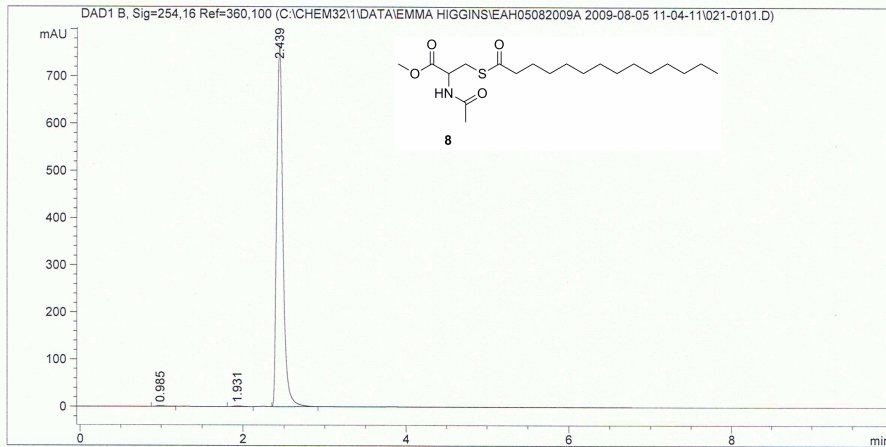


HPLC analysis of methyl 2-acetamido-3-(tetradecanoylthio)propanoate (8)

Purity was determined using an Agilent Technologies 1200 series HPLC system with a photodiode UV-visible detector; column: Eclipse XDB-C18 4.6 x 150mm 5 µm C18; mobile phase: methanol; injection volume: 10 µL; UV detection: 254 nm; flow rate: 1 mL/min.

Data File C:\CHEM32\1\DATA\EMMA HIGGINS\EAH05082009A 2009-08-05 11-04-11\021-0101.D
Sample Name: RAB-7

```
=====
Acq. Operator   : Ian                               Seq. Line :    1
Acq. Instrument : Instrument 1                       Location  : Vial 21
Injection Date  : 8/5/2009 11:05:37 AM              Inj       :    1
                                                    Inj Volume: 10 µl
Acq. Method     : C:\Chem32\1\DATA\EMMA HIGGINS\EAH05082009A 2009-08-05 11-04-11\REV PHASE
CH3CN 10UL.M
Last changed    : 8/5/2009 10:44:41 AM by Ian
Analysis Method : C:\CHEM32\1\DATA\EMMA HIGGINS\EAH05082009A 2009-08-05 11-04-11\021-0101.D\
DA.M (REV PHASE CH3CN 10UL.M)
Last changed    : 8/5/2009 10:44:41 AM by Ian
Method Info     : Reverse Phase Methanol
=====
```



Area Percent Report

```
Sorted By      : Signal
Multiplier     : 1.0000
Dilution       : 1.0000
Use Multiplier & Dilution Factor with ISTDs
```

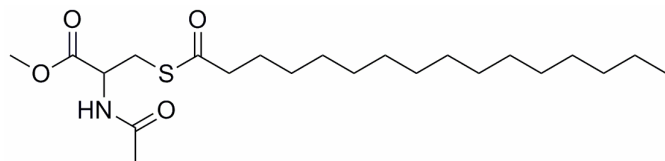
Signal 1: DAD1 B, Sig=254,16 Ref=360,100

| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 0.985 | BB | 0.1075 | 14.30312 | 1.82387 | 0.3507 |
| 2 | 1.931 | BB | 0.1092 | 8.83584 | 1.26975 | 0.2166 |
| 3 | 2.439 | BB | 0.0818 | 4055.52686 | 766.10217 | 99.4327 |

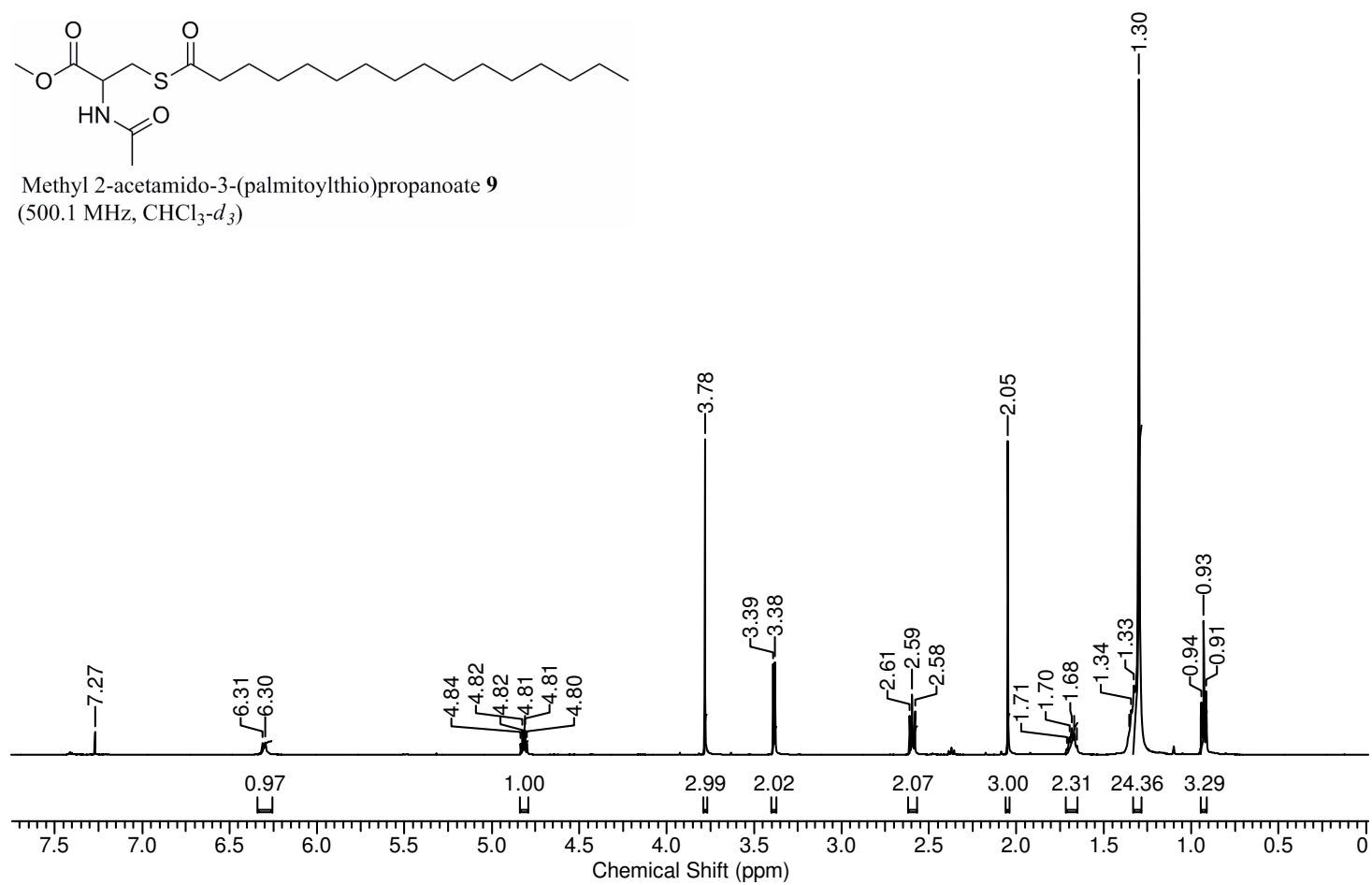
Totals : 4078.66582 769.19580

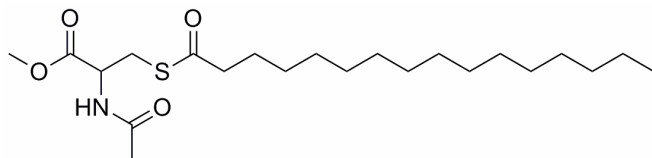
Instrument 1 5/25/2010 3:54:34 PM Ian

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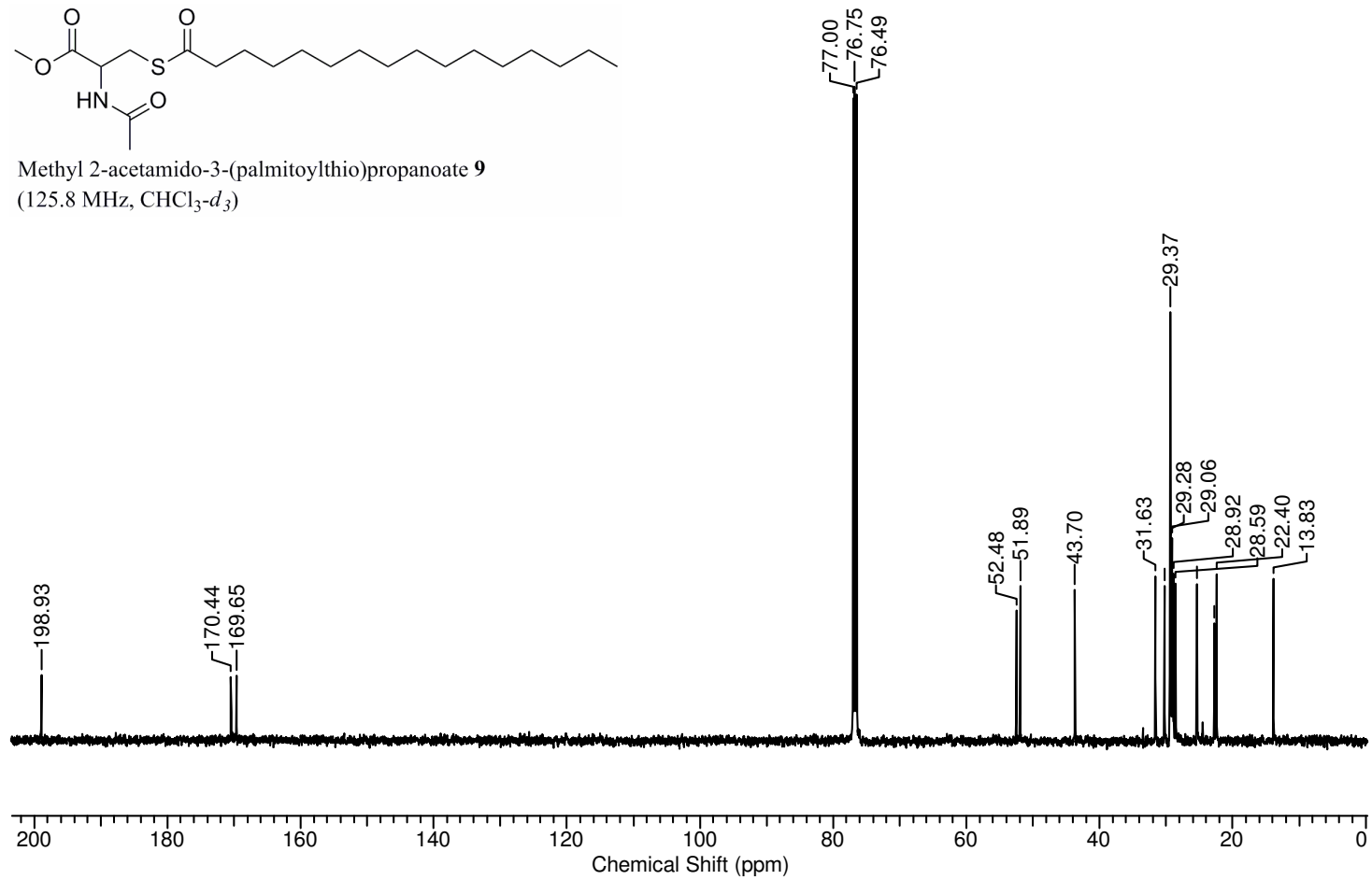


Methyl 2-acetamido-3-(palmitoylthio)propanoate **9**
 (500.1 MHz, CHCl_3-d_3)





Methyl 2-acetamido-3-(palmitoylthio)propanoate **9**
(125.8 MHz, CHCl_3-d_3)



Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Jan 28 10000004.d
Method xiaofengpos.m
Sample Name EAH-3
Comment

Acquisition Date

1/28/2010 1:57:37 PM

Operator

Administrator

Instrument

micrOTOF

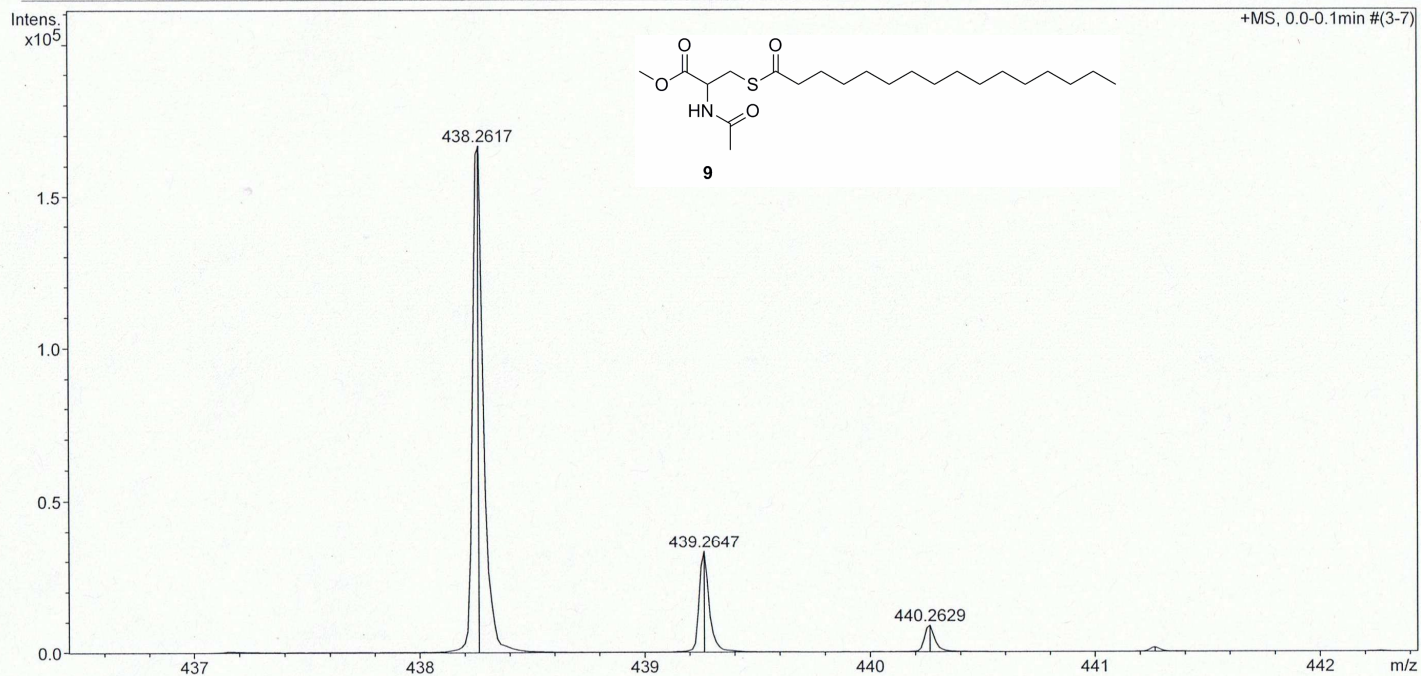
57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 1500 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 55.0 V
Hexapole 1 26.0 V

Set Corrector Fill 52 V
Set Pulsar Pull 398 V
Set Pulsar Push 398 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 1960 V

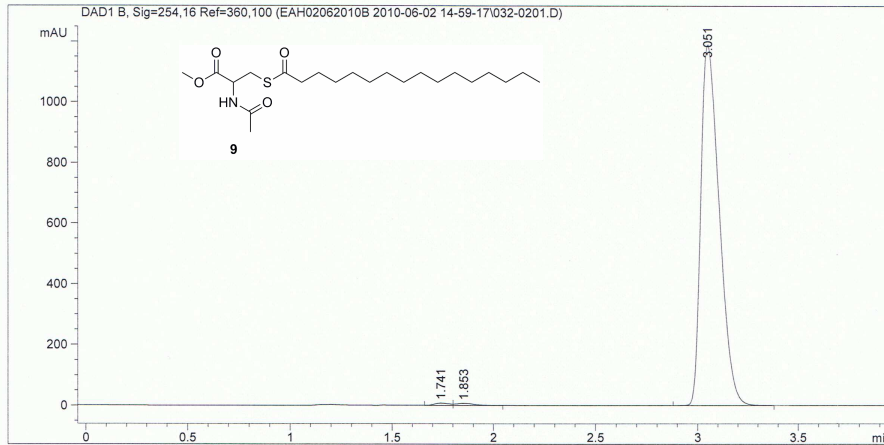


HPLC analysis of methyl 2-acetamido-3-(palmitoylthio)propanoate (9)

Purity was determined using an Agilent Technologies 1200 series HPLC system with a photodiode UV-visible detector; column: Eclipse XDB-C18 4.6 x 150mm 5 µm C18; mobile phase: methanol; injection volume: 50 µL; UV detection: 254 nm; flow rate: 1 mL/min.

Data File C:\CHEM32\1\DATA\JEREMY\JER091008CFRACS 2008-10-09 15-09-59\EAH02062010B 2010-06-02 14-5
Sample Name: EAH-3 frac

```
=====
Acq. Operator   : Ian                      Seq. Line :    2
Acq. Instrument : Instrument 1              Location  : Vial 32
Injection Date  : 6/2/2010 3:08:40 PM      Inj       :    1
                                           Inj Volume: 50 µl
Acq. Method    : C:\Chem32\1\DATA\JEREMY\JER091008CFRACS 2008-10-09 15-09-59\EAH02062010B
                                           2010-06-02 14-59-17\REV PHASE METHANOL 20UL.M
Last changed   : 6/2/2010 2:56:03 PM by Ian
Analysis Method : C:\CHEM32\1\DATA\JEREMY\JER091008CFRACS 2008-10-09 15-09-59\EAH02062010B
                                           2010-06-02 14-59-17\032-0201.D\DA.M (REV PHASE METHANOL 20UL.M)
Last changed   : 6/2/2010 3:16:03 PM by Ian
                                           (modified after loading)
Method Info    : Alzheimer project - ShutDown
=====
```



Area Percent Report

```
=====
Sorted By      : Signal
Multiplier    : 1.0000
Dilution      : 1.0000
Use Multiplier & Dilution Factor with ISTDs
=====
```

Signal 1: DAD1 B, Sig=254,16 Ref=360,100

| Peak # | RetTime [min] | Type | Width [min] | Area [mAU*s] | Height [mAU] | Area % |
|--------|---------------|------|-------------|--------------|--------------|---------|
| 1 | 1.741 | VV | 0.0774 | 39.90322 | 7.83817 | 0.5230 |
| 2 | 1.853 | VB | 0.1011 | 45.76357 | 6.92376 | 0.5998 |
| 3 | 3.051 | BB | 0.0978 | 7544.26270 | 1192.38586 | 98.8772 |

Totals : 7629.92948 1207.14780

Instrument 1 6/2/2010 3:16:07 PM Ian

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