

Supplementary Materials for:
Panchromatic Absorbers Tethered for Bioconjugation or Surface Attachment

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David F. Bocian,^{2,*} Dewey Holten,^{3,*} and Jonathan S. Lindsey^{1,*}

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North Carolina State University
Raleigh, North Carolina 27695-8204

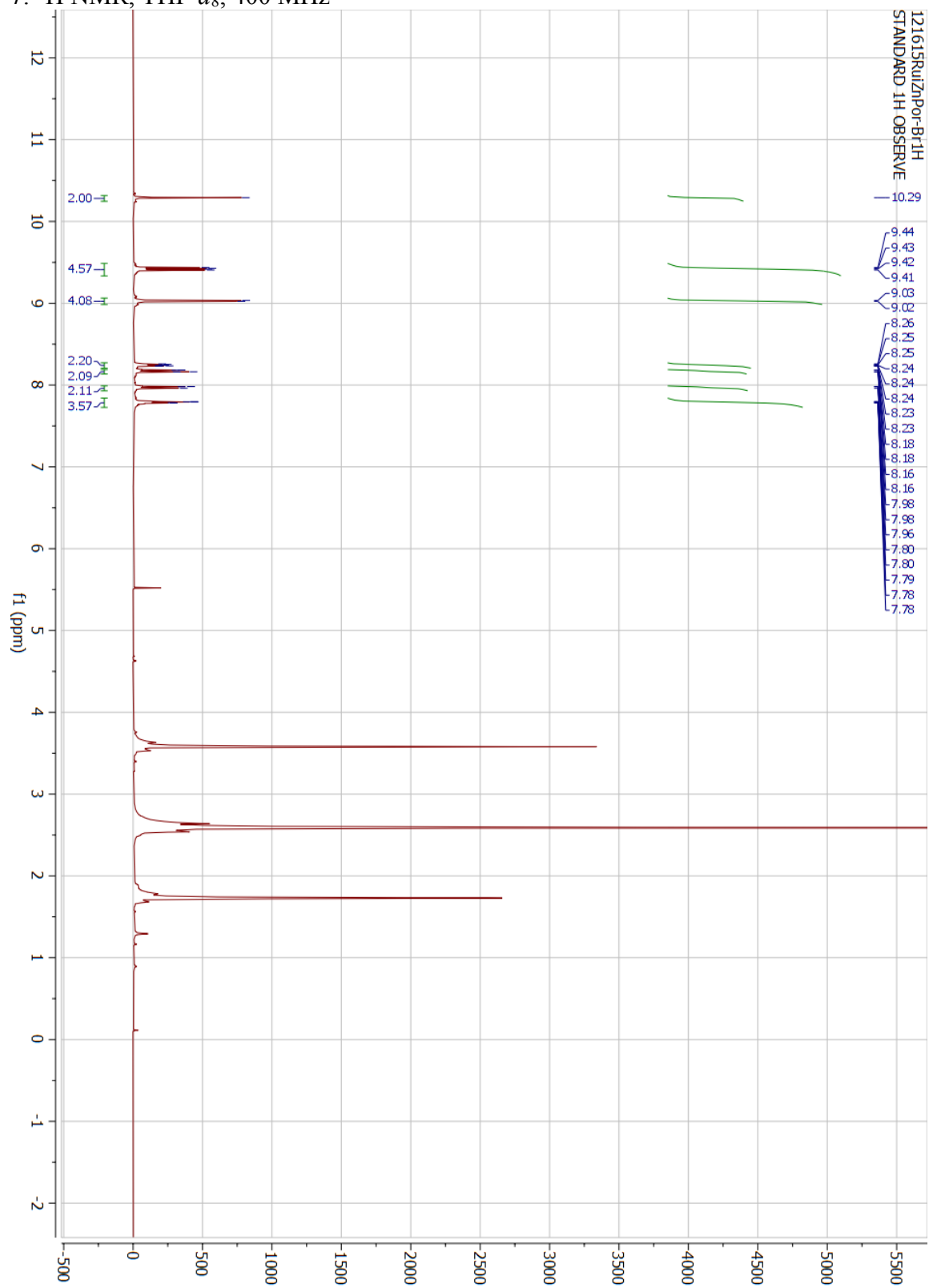
² Department of Chemistry
University of California
Riverside, California 92521-0403

³ Department of Chemistry
Washington University
St. Louis, Missouri 63130-4889

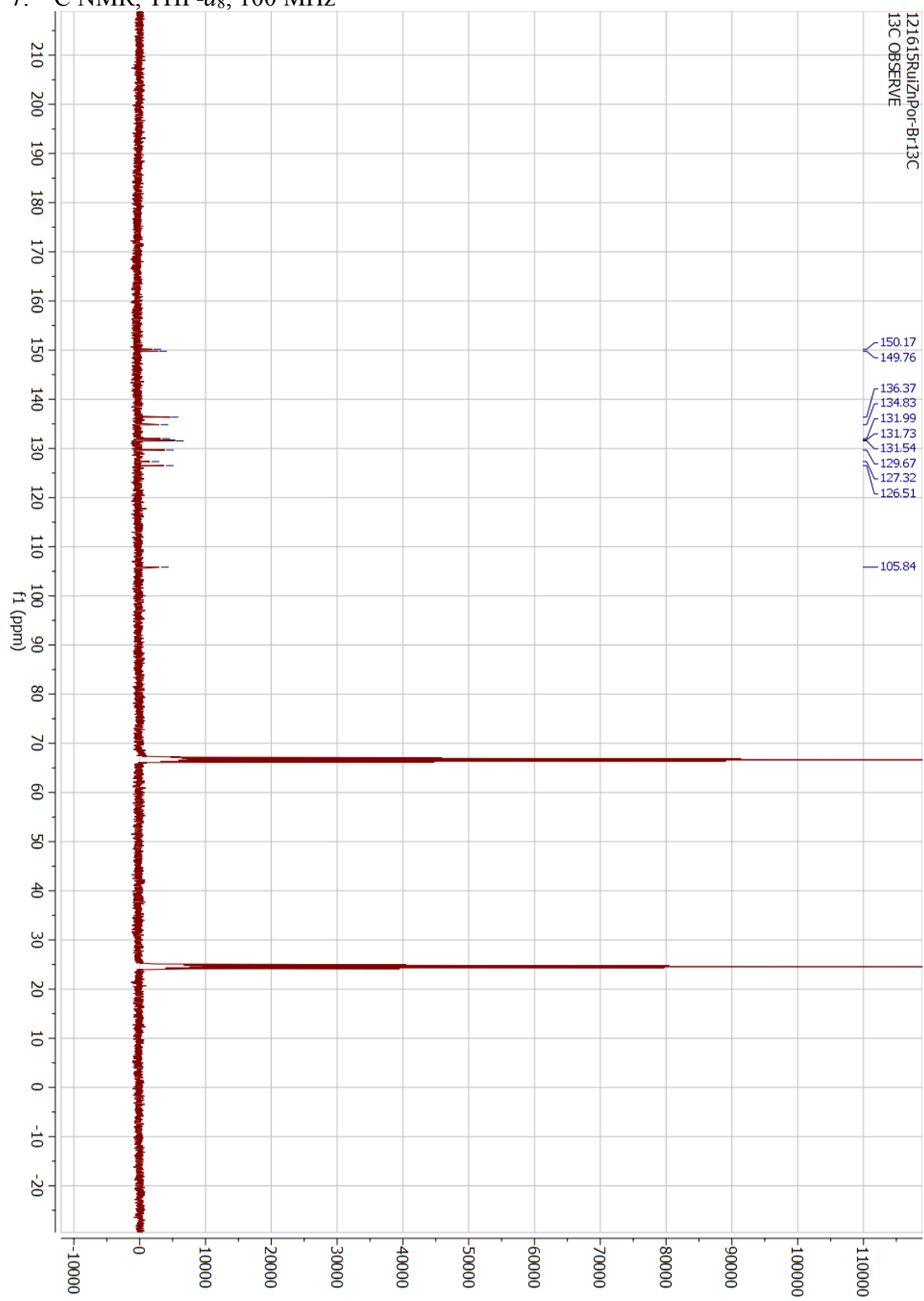
^a Equal contributions

¹H NMR spectra, ¹³C{¹H} spectra, MALDI-MS spectra, ESI-MS spectra, and absorption spectra (where available) for new compounds are provided in the following pages.

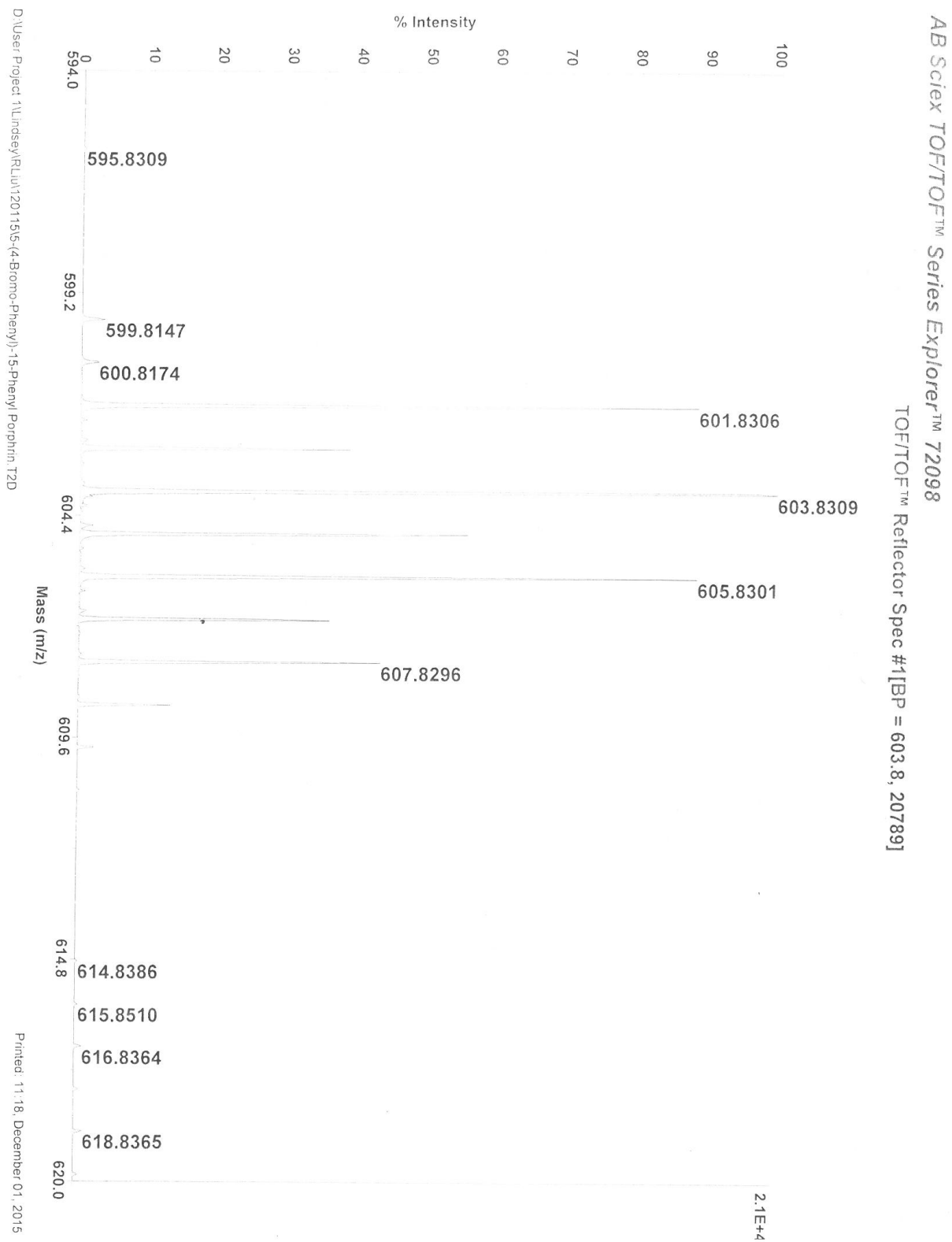
7: ^1H NMR, THF- d_8 , 400 MHz



7: ^{13}C NMR, THF- d_8 , 100 MHz



7: MALDI-MS



7: ESI-MS

NC STATE UNIVERSITY

Mass Spectrometry Facility

Department of Chemistry

P.O. Box 8204

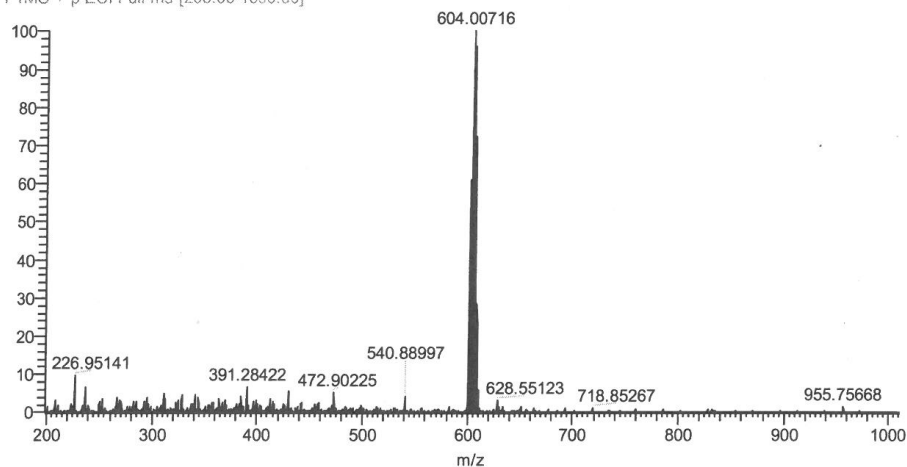
Raleigh, NC 27695-8204

<http://www.ncsu.edu/chemistry/msf>

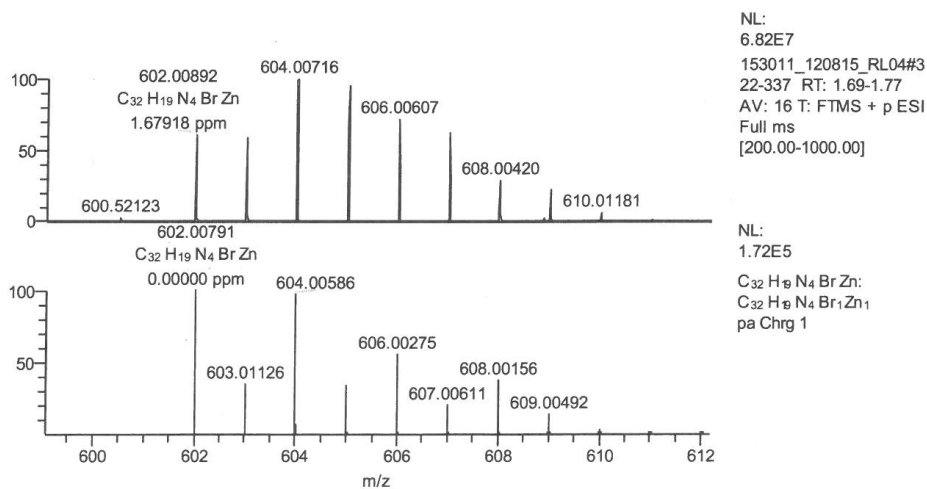
120815 RL04 Full Scan

153011_120815_RL04 #322-337 RT: 1.69-1.77 AV: 16 NL: 6.82E7

T: FTMS + p ESI Full ms [200.00-1000.00]



120815 RL04 Experimental and Theoretical Isotopic Distribution for $C_{32}H_{19}BrN_4Zn [M]^+$



NL:
6.82E7
153011_120815_RL04#3
22-337 RT: 1.69-1.77
AV: 16 T: FTMS + p ESI
Full ms
[200.00-1000.00]

NL:
1.72E5
 $C_{32}H_{19}N_4BrZn$:
 $C_{32}H_{19}N_4Br_1Zn_1$
pa Chrg 1



7: Absorption spectrum (toluene)

Spectrum/Peak Report

Date 6/9/2016 Time 13:04:52 Page 1 of 1

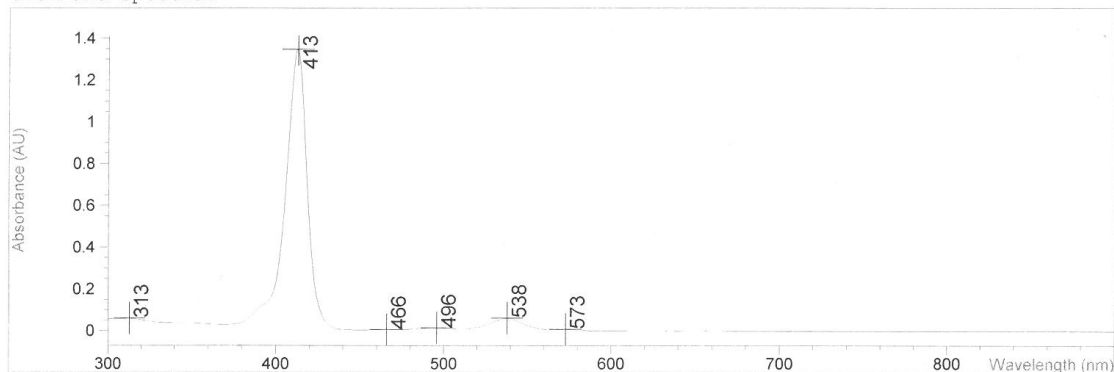
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Information : Default Method

Data File : C:\Chem32\1\DATA\Rui\060916ZNPORBR.SD

Created : 6/9/16 12:46:53

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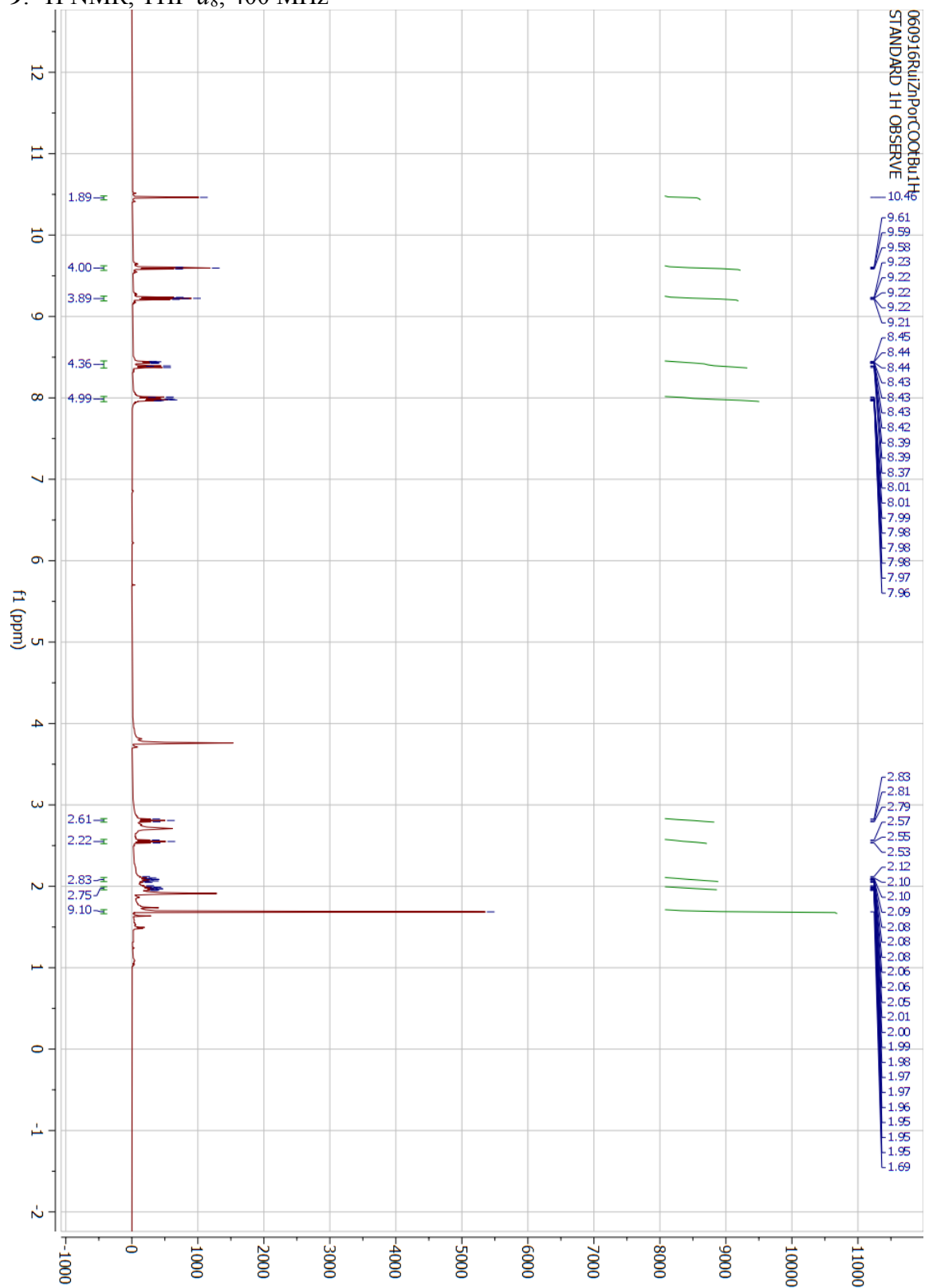
| # | Name | Peaks (nm) | Abs (AU) |
|---|------|------------|-----------|
| 1 | | 413.0 | 1.34620 |
| 1 | | 538.0 | 6.1114E-2 |
| 1 | | 313.0 | 5.9897E-2 |
| 1 | | 496.0 | 1.4721E-2 |
| 1 | | 573.0 | 7.0415E-3 |
| 1 | | 466.0 | 6.7382E-3 |

Report generated by : Lindsey Lab

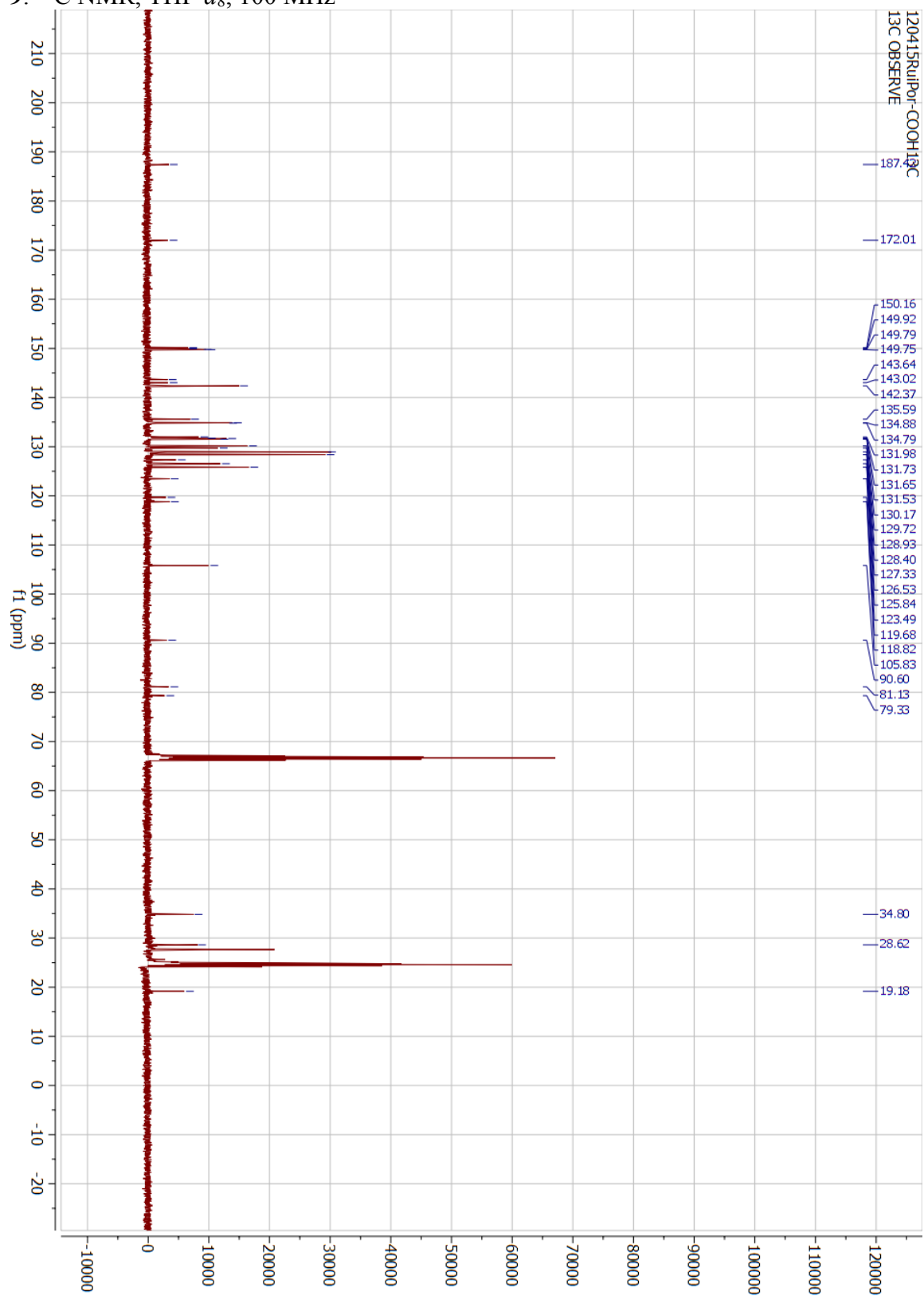
Signature:

*** End Spectrum/Peak Report ***

9: ^1H NMR, THF- d_8 , 400 MHz



9: ^{13}C NMR, THF- d_8 , 100 MHz



9: ESI-MS

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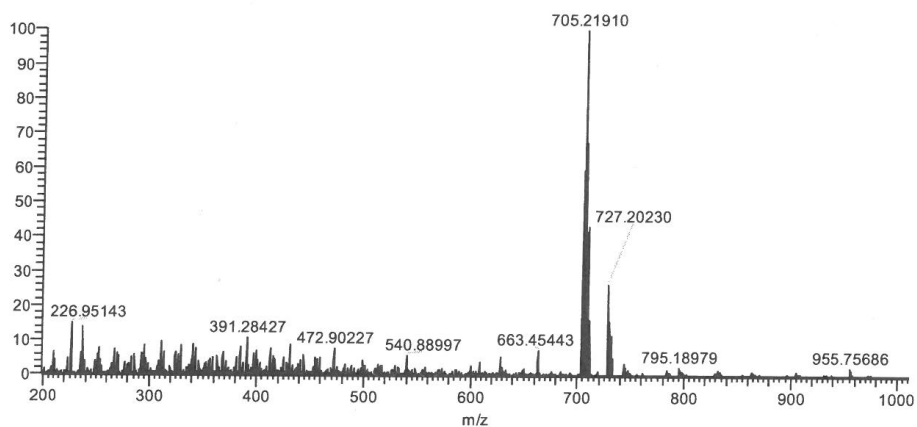
Raleigh, NC 27695-8204

<http://www.ncsu.edu/chemistry/msf>

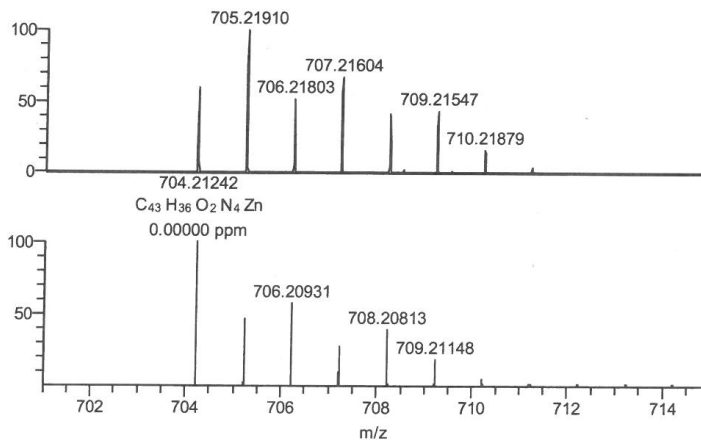
120815 RL03 Full Scan

153010_120815_RL03 #558-573 RT: 2.93-3.01 16 NL: 3.71E7

T: FTMS + p ESI Full ms [200.00-1000.00]



120815 RL03 Experimental and Theoretical Isotopic Distribution for $C_{43}H_{36}N_4O_2Zn [M]^+$



NL:
3.71E7
153010_120815_RL03#5
58-573 RT: 2.93-3.01
AV: 16 T: FTMS + p ESI
Full ms
[200.00-1000.00]

NL:
2.99E5
 $C_{43}H_{36}O_2N_4Zn$:
 $C_{43}H_{36}O_2N_4Zn_1$
pa Chrg 1



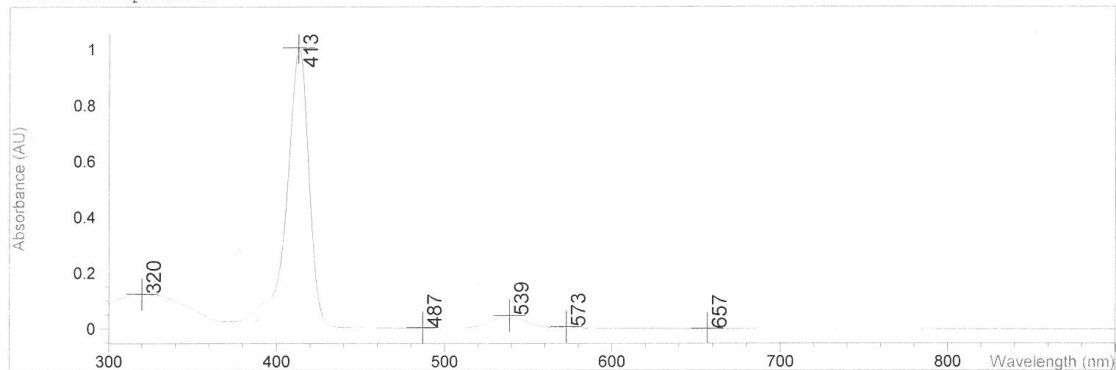
9: Absorption spectrum (toluene)

Spectrum/Peak Report

Date 6/9/2016 Time 13:05:15 Page 1 of 1

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12:50:34

Overlaid Spectra:



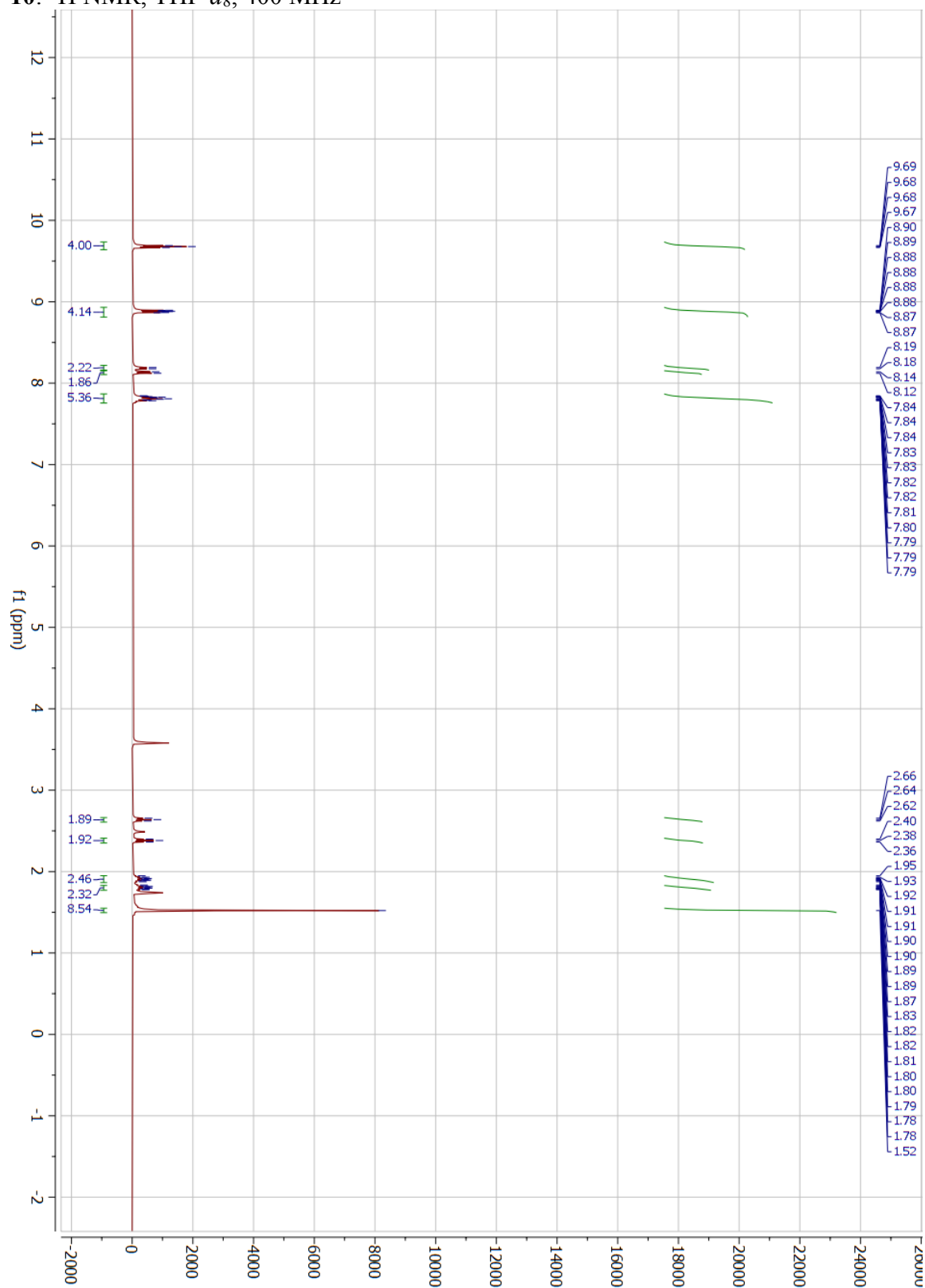
| # | Name | Peaks (nm) | Abs (AU) |
|---|------|------------|-----------|
| 1 | | 413.0 | 1.00640 |
| 1 | | 320.0 | 0.12468 |
| 1 | | 539.0 | 4.7800E-2 |
| 1 | | 573.0 | 7.1979E-3 |
| 1 | | 487.0 | 4.3850E-3 |
| 1 | | 657.0 | 1.4977E-3 |

Report generated by : Lindsey Lab

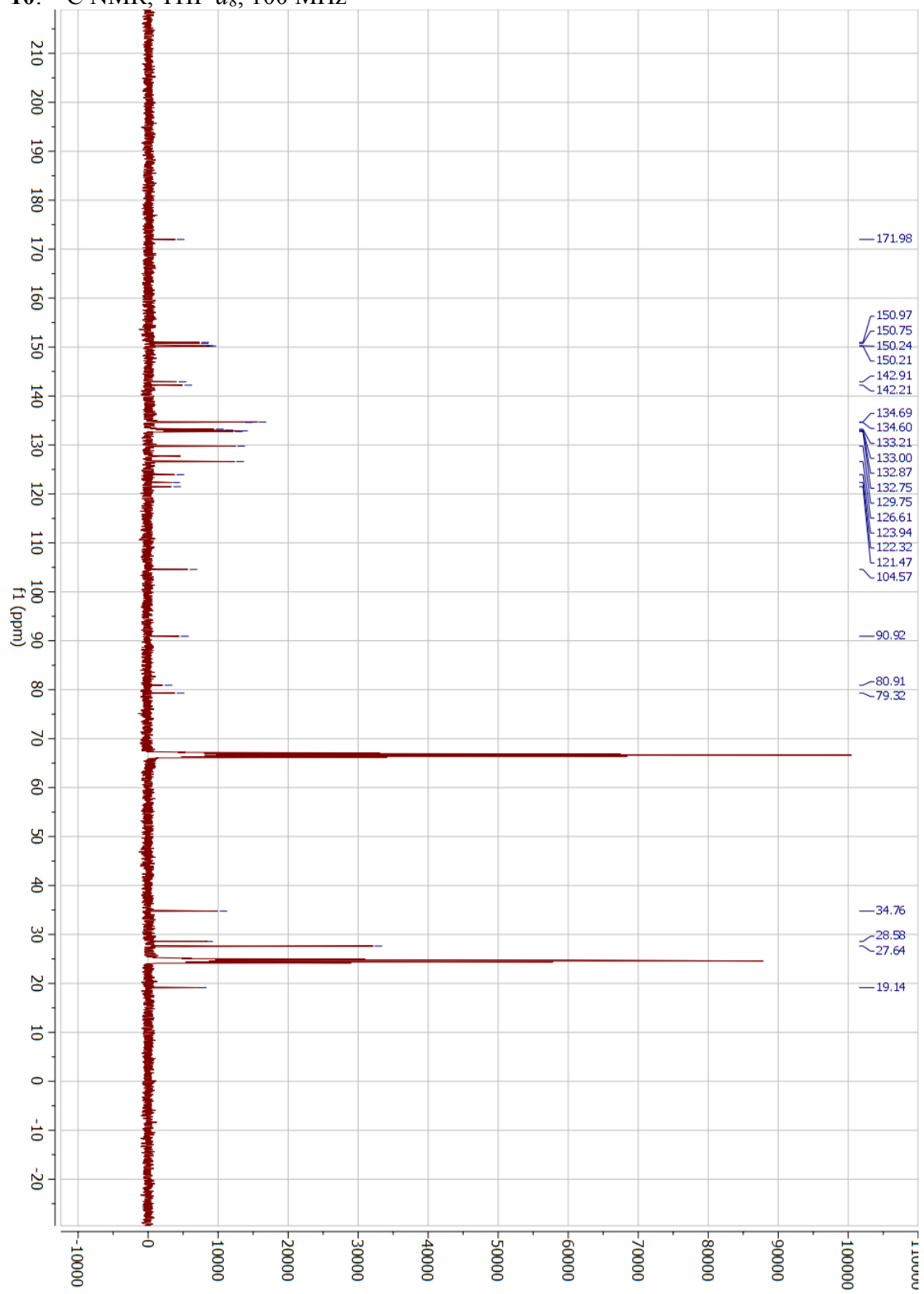
Signature:

*** End Spectrum/Peak Report ***

10: ^1H NMR, THF- d_8 , 400 MHz



10: ^{13}C NMR, THF- d_8 , 100 MHz

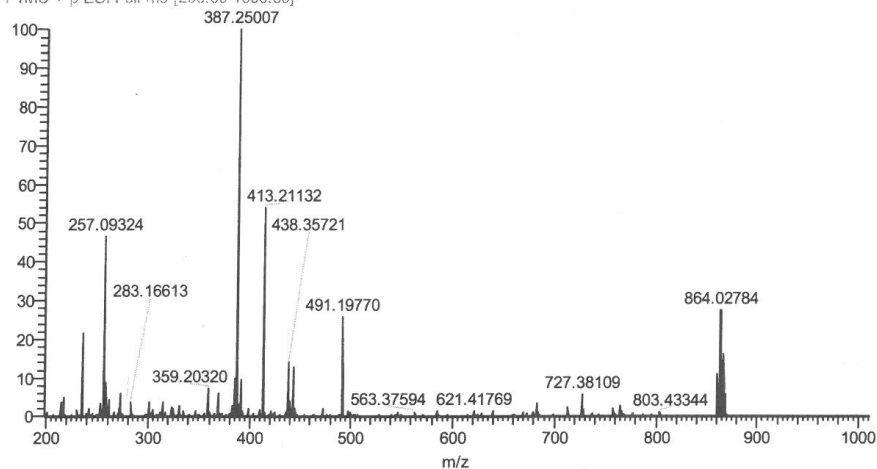


10: ESI-MS

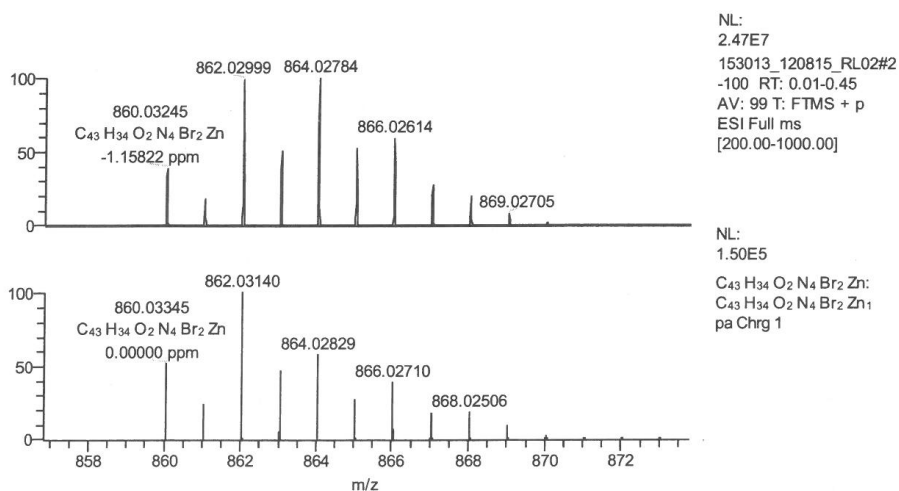
NC STATE UNIVERSITY
 Mass Spectrometry Facility
 Department of Chemistry
 P.O. Box 8204
 Raleigh, NC 27695-8204
<http://www.ncsu.edu/chemistry/msf>

120815 RL02 Full Scan

153013_120815_RL02 #2-100 RT: 0.01-0.45 AV: 99 NL: 9.01E7
 T: FTMS + p ESI Full ms [200.00-1000.00]



120815 RL02 Experimental and Theoretical Isotopic Distribution for $C_{43}H_{34}Br_2N_4O_2Zn [M]^+$



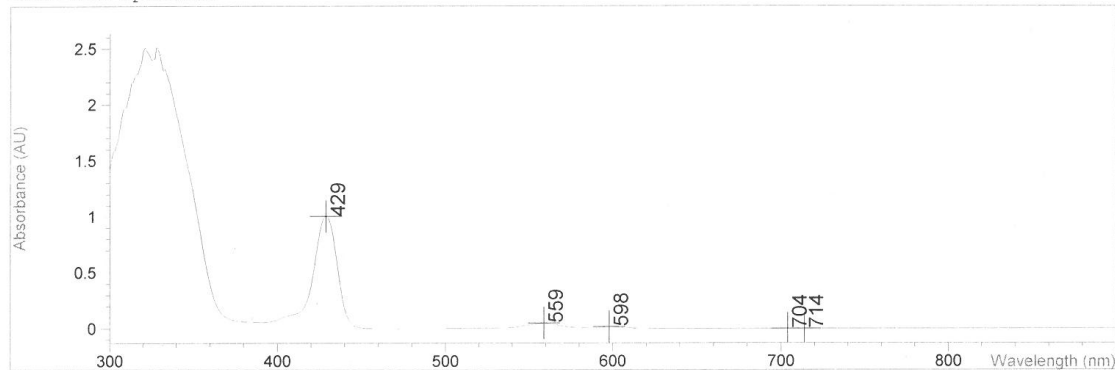
10: Absorption spectrum (toluene)

Spectrum/Peak Report

Date 6/9/2016 Time 13:04:32 Page 1 of 1

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Information : Default Method
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13:03:26

Overlaid Spectra:



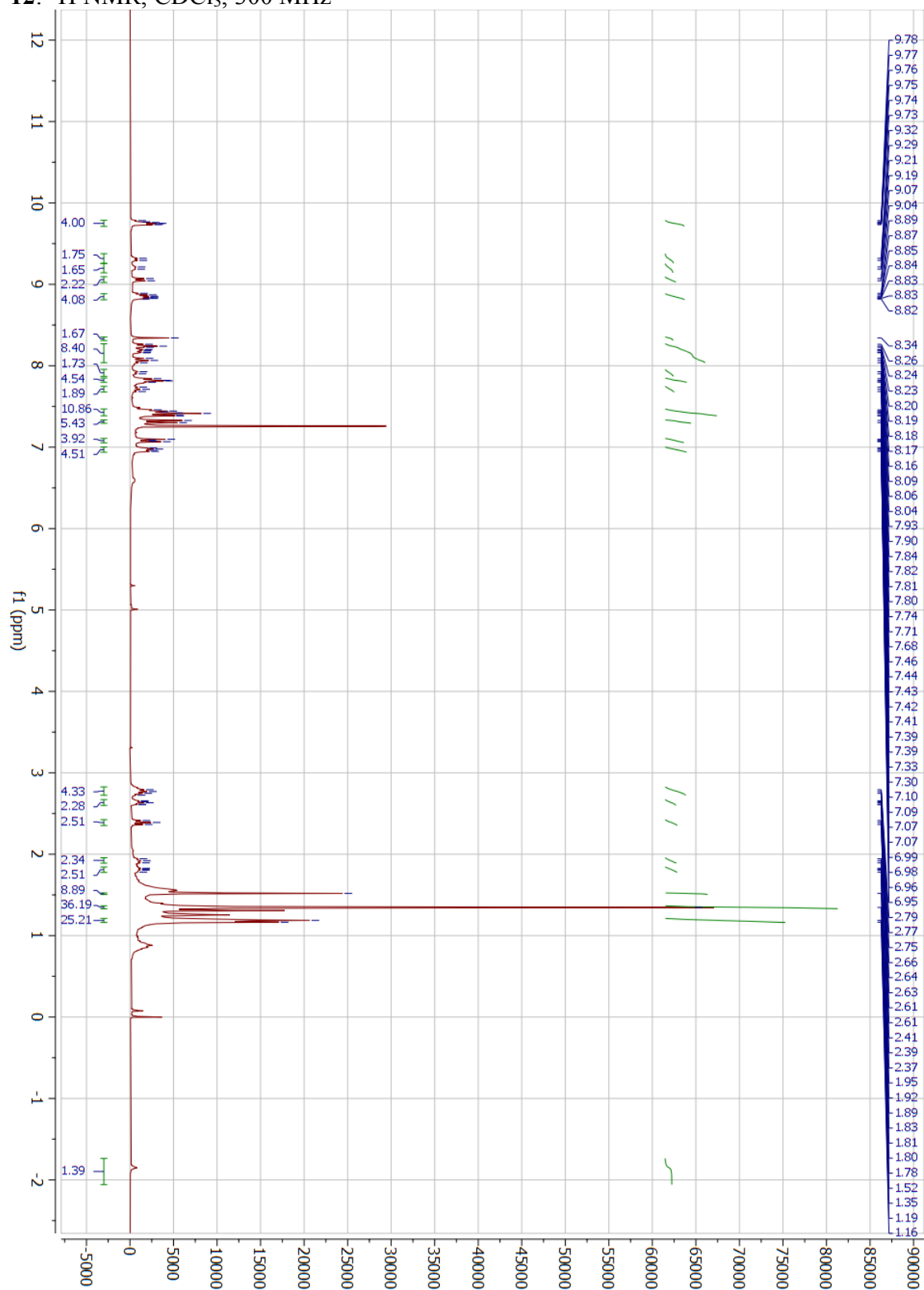
| # | Name | Peaks (nm) | Abs (AU) |
|---|------|-------------|-------------|
| 1 | | 429.0 | 1.00520 |
| 1 | | 559.0 | 4.8405E-2 |
| 1 | | 598.0 | 1.7118E-2 |
| 1 | | 714.0 | -9.1267E-4 |
| 1 | | 704.0 | -9.2983E-4 |
| 1 | | 000000000.0 | -1.7977E308 |

Report generated by : Lindsey Lab

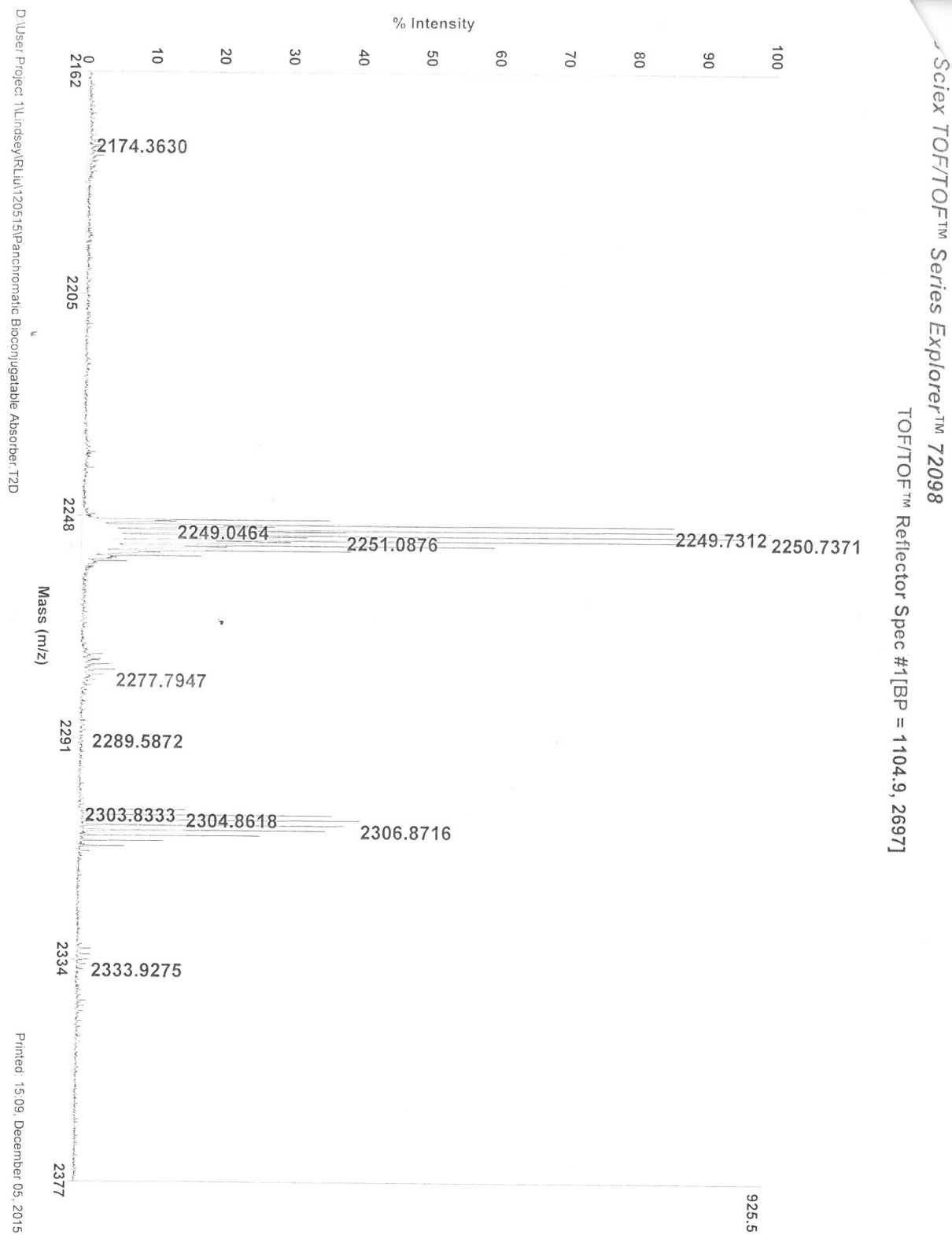
Signature:

*** End Spectrum/Peak Report ***

12: ^1H NMR, CDCl_3 , 300 MHz



12: MALDI-MS



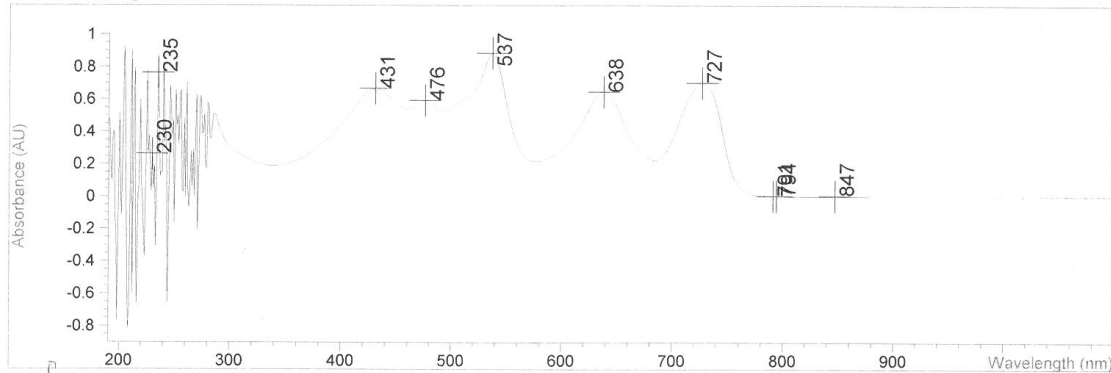
12: Absorption spectrum (toluene)

Spectrum/Peak Report

Date 6/7/2016 Time 14:13:07 Page 1 of 1

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Information : Default Method
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3/25/16 13:30:44

Overlaid Spectra:



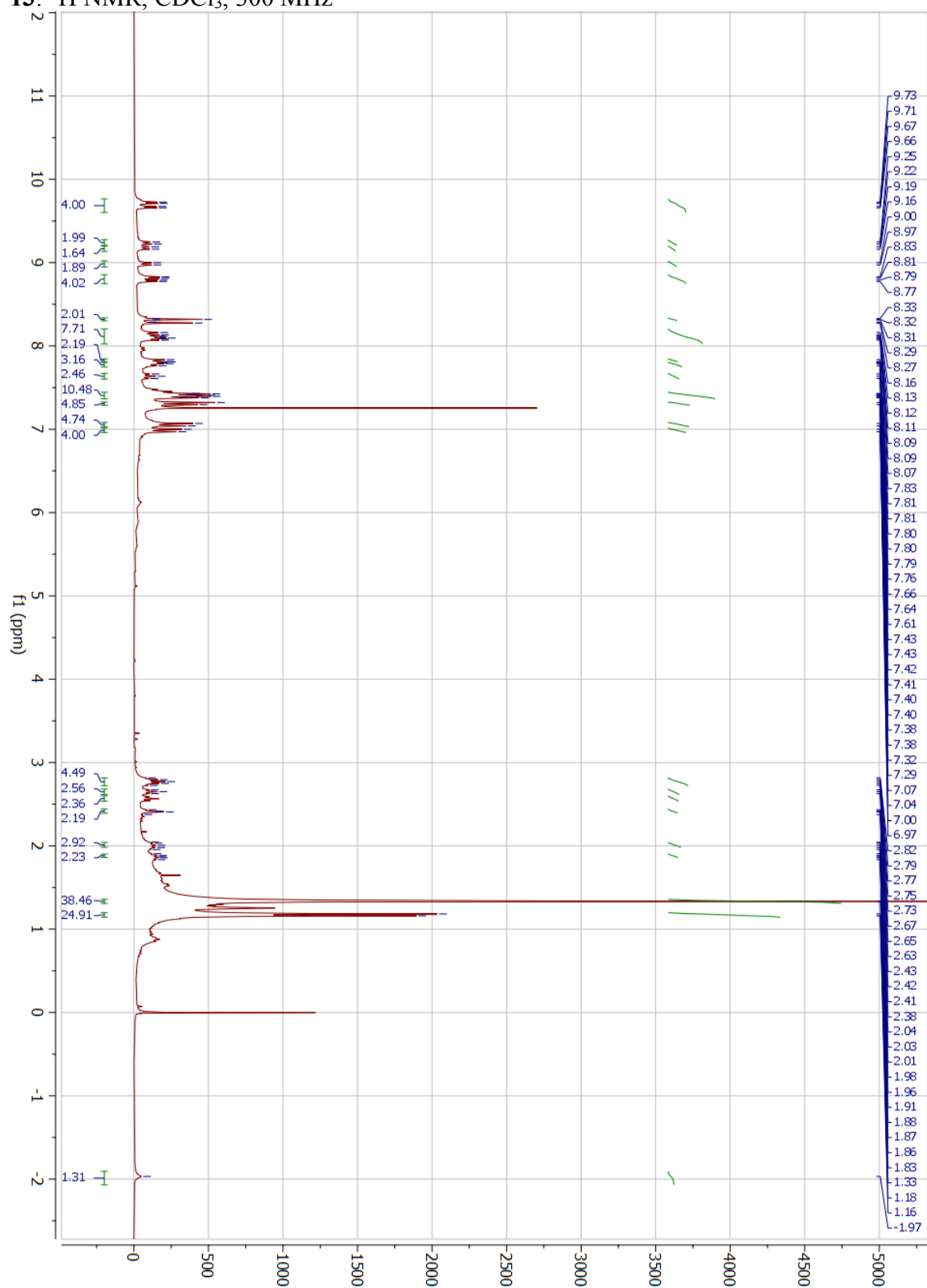
| # | Name | Peaks (nm) | Abs (AU) |
|---|------|------------|-----------|
| 1 | | 537.0 | 0.88411 |
| 1 | | 235.0 | 0.76264 |
| 1 | | 727.0 | 0.70325 |
| 1 | | 431.0 | 0.66651 |
| 1 | | 638.0 | 0.64723 |
| 1 | | 476.0 | 0.59303 |
| 1 | | 230.0 | 0.26232 |
| 1 | | 794.0 | 5.4092E-3 |
| 1 | | 791.0 | 5.2538E-3 |
| 1 | | 847.0 | 4.7388E-3 |

Report generated by : Lindsey Lab

Signature:

*** End Spectrum/Peak Report ***

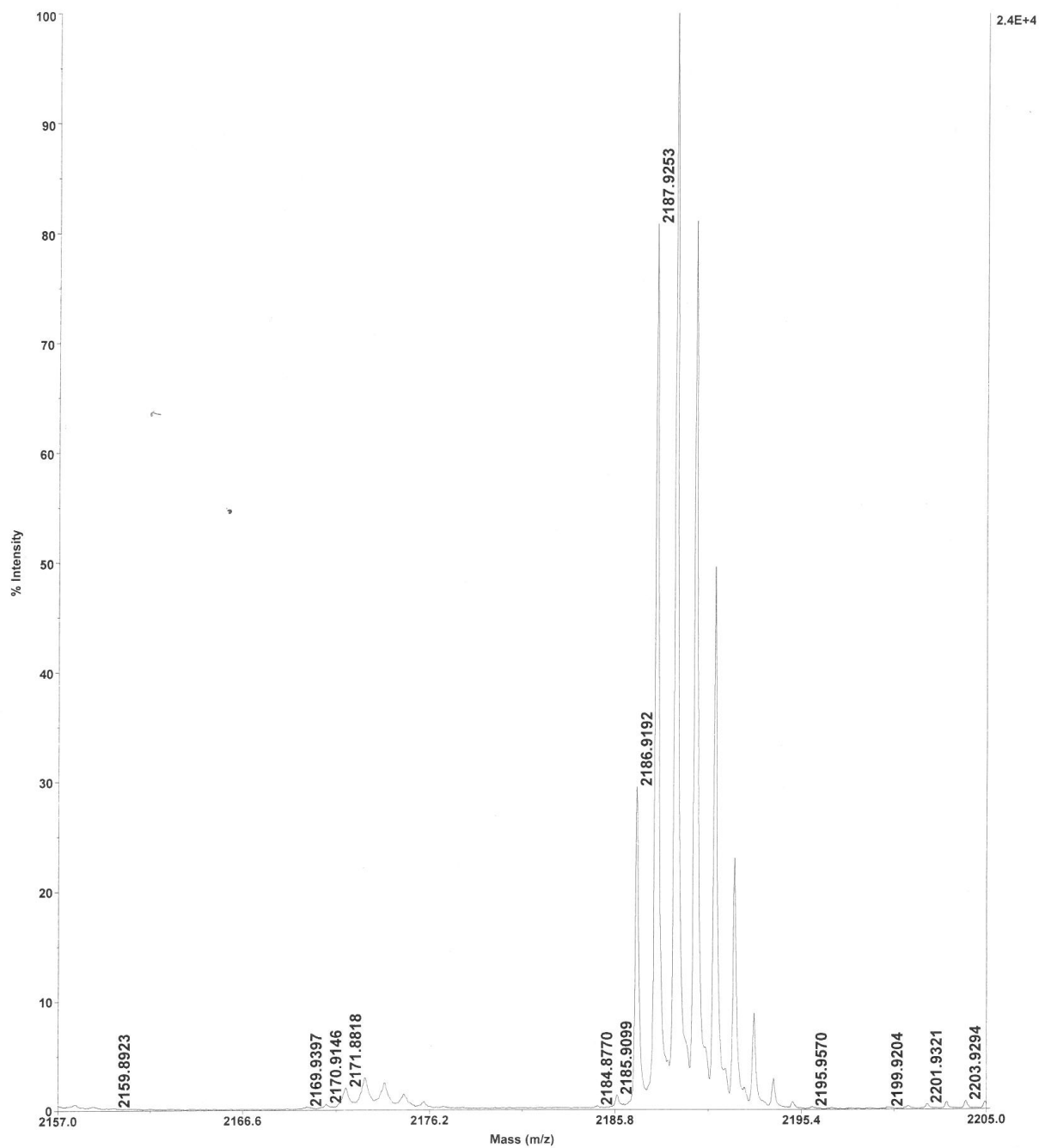
13: ^1H NMR, CDCl_3 , 300 MHz



13: MALDI-MS

AB Sciex TOF/TOF™ Series Explorer™ 72098

TOF/TOF™ Reflector Spec #1[BP = 729.3, 27070]



D:\User Project 1\Lindsey\RLiu\Before2016\120915\Deprotection of t-butyl from P2tPor 2.T2D

Printed: 14:00, June 07, 2016

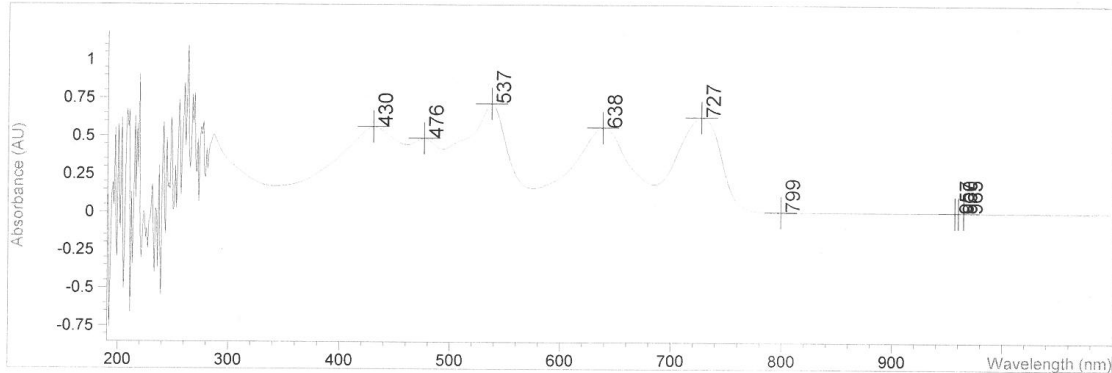
13: Absorption spectrum (toluene)

Spectrum/Peak Report

Date 6/11/2016 Time 13:41:39 Page 1 of 1

Method file : <untitled>
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12/9/15 14:22:40

Overlaid Spectra:



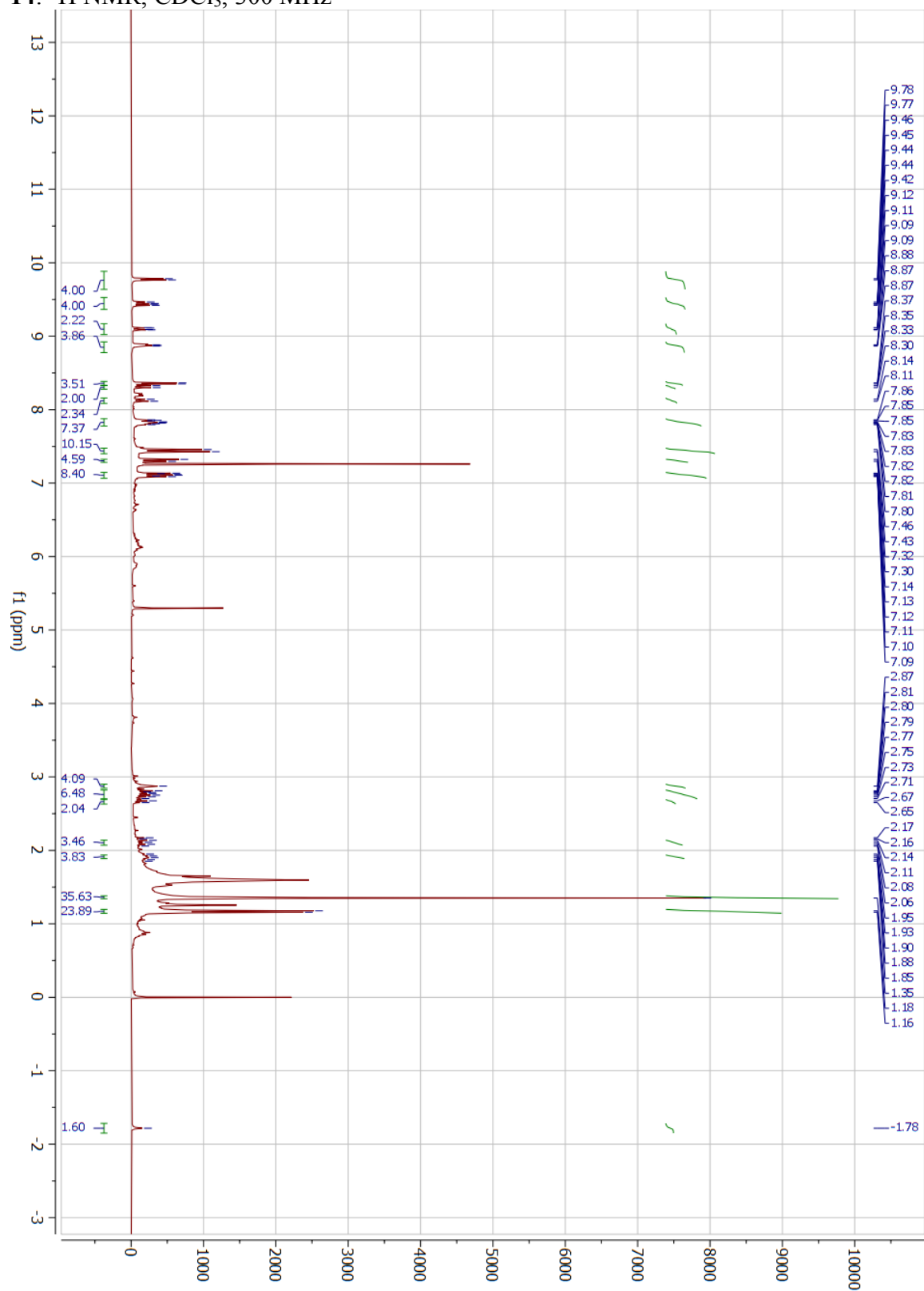
| # | Name | Peaks (nm) | Abs (AU) |
|---|------|-------------|-------------|
| 1 | | 537.0 | 0.71428 |
| 1 | | 727.0 | 0.62812 |
| 1 | | 430.0 | 0.56336 |
| 1 | | 638.0 | 0.55953 |
| 1 | | 476.0 | 0.48743 |
| 1 | | 799.0 | 6.5522E-3 |
| 1 | | 960.0 | 5.3821E-3 |
| 1 | | 957.0 | 5.3663E-3 |
| 1 | | 965.0 | 5.2128E-3 |
| 1 | | 000000000.0 | -1.7977E308 |

Report generated by : Lindsey Lab

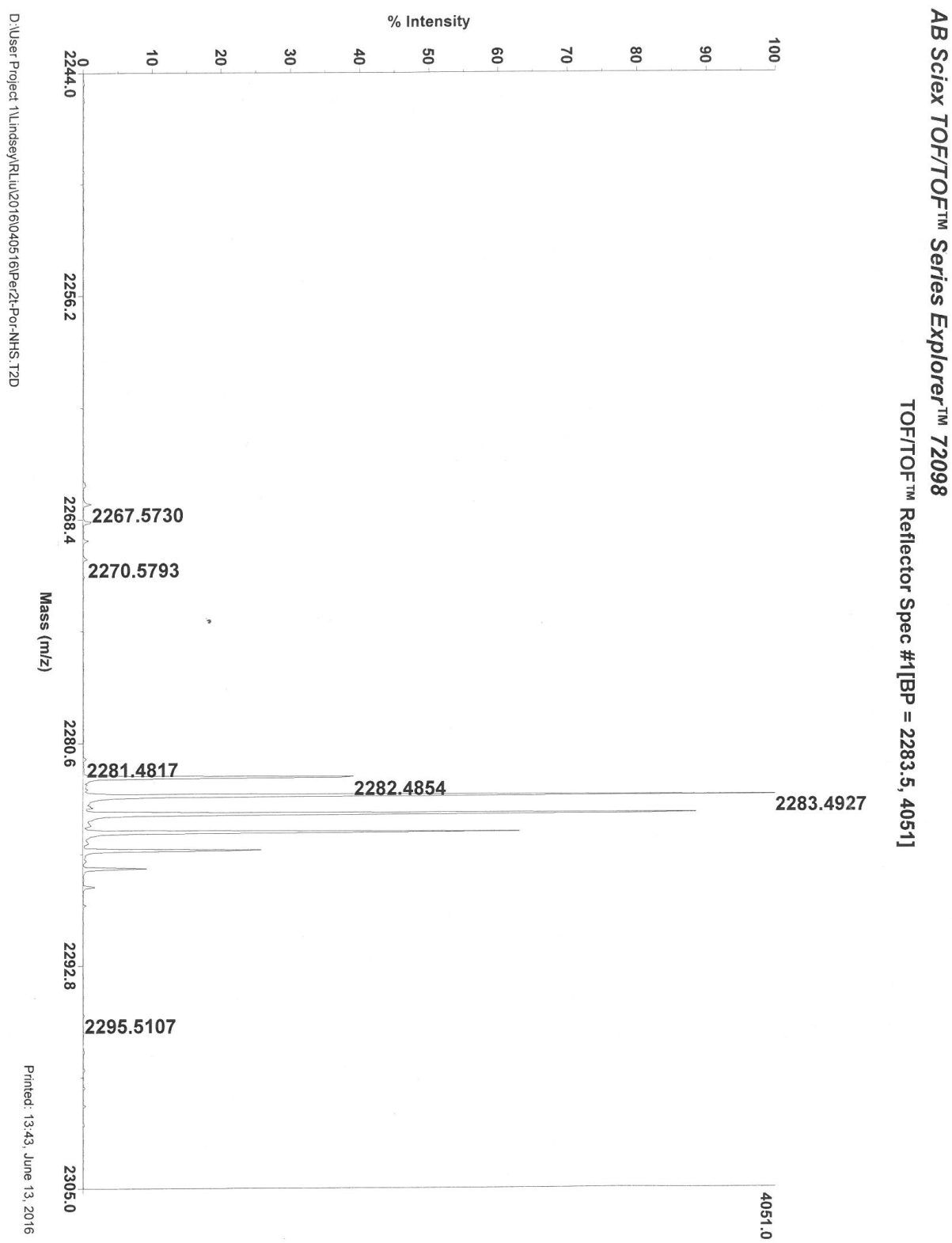
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*** End Spectrum/Peak Report ***

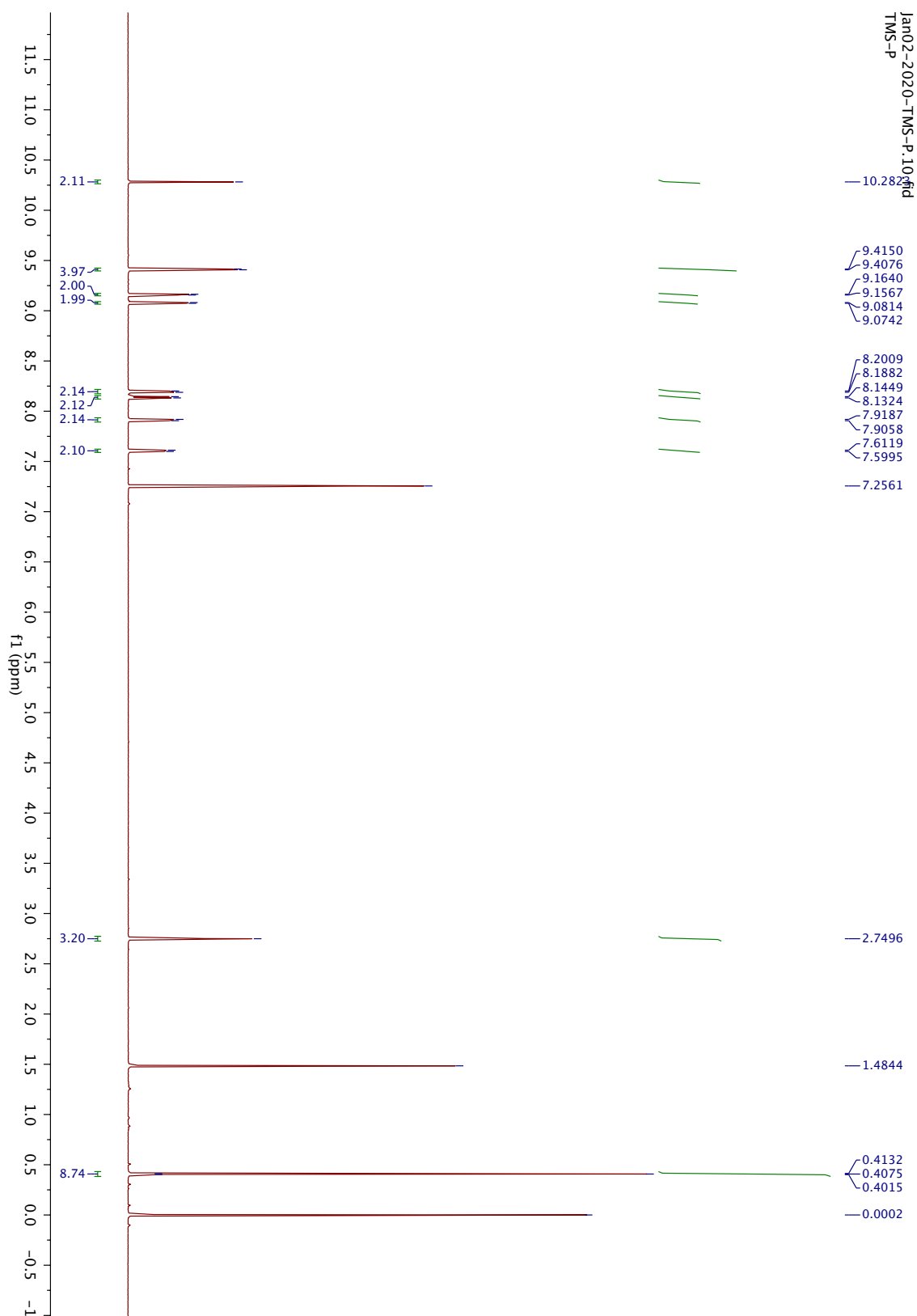
14: ^1H NMR, CDCl_3 , 300 MHz



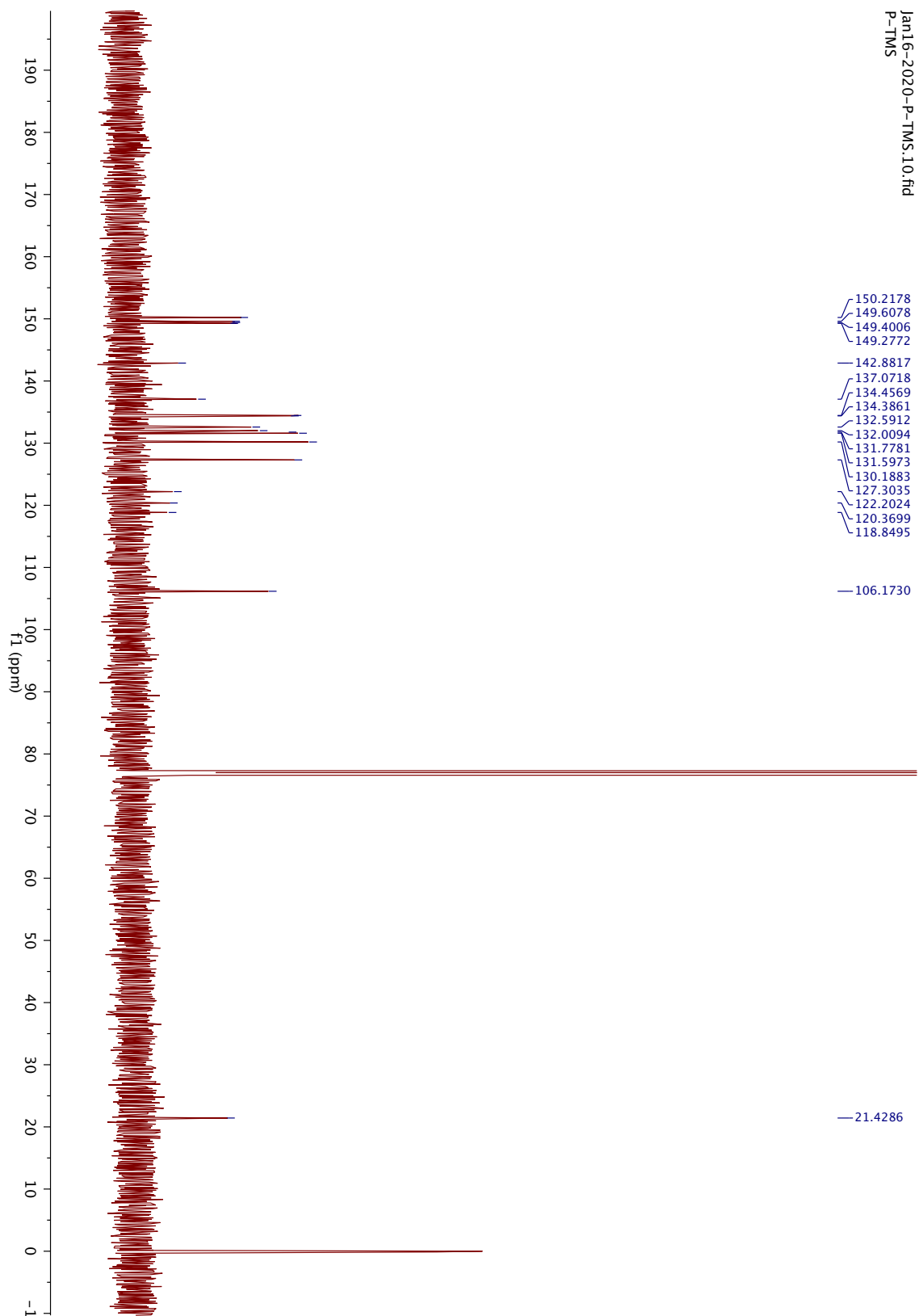
14: MALDI-MS

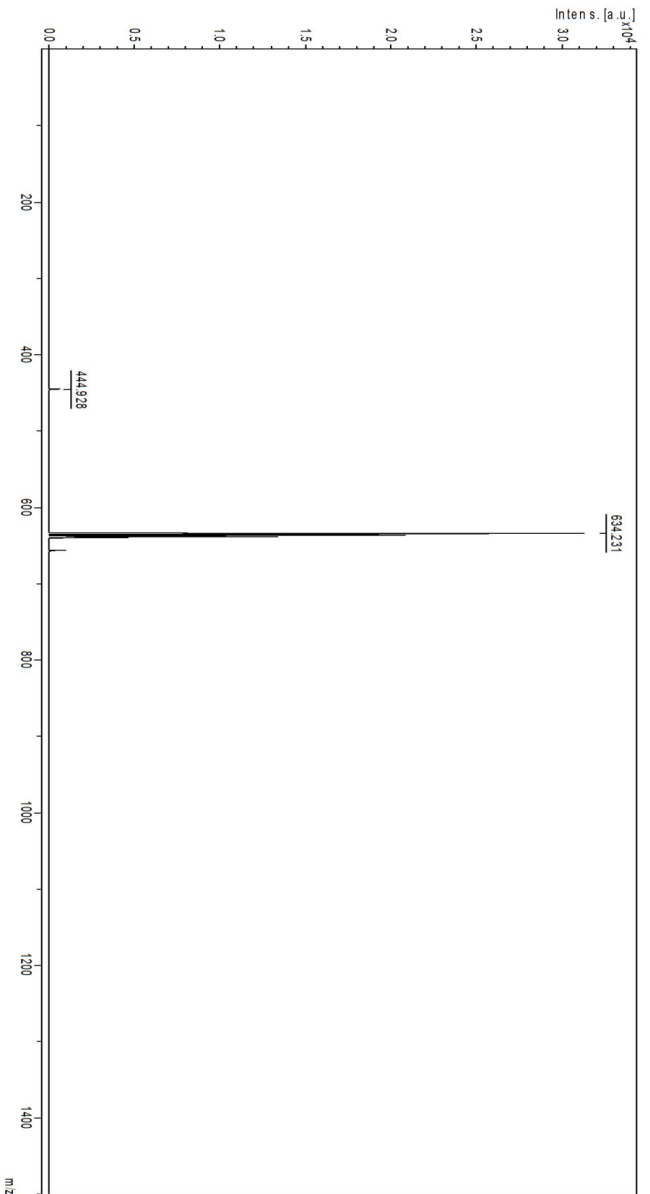


20: ^1H NMR, CDCl_3 , 600 MHz



20: ^{13}C NMR, CDCl_3 , 151 MHz





Target
Target type 0280784
Target serial number 1004015
Position 120

Laser
Laser beam attenuation 75
Laser beam focus 36
Laser repetition rate 2000 Hz
Number of shots 500

Spectrometer
positive voltage polarity POS
PIE delay 130 ns
ion source voltage 1 19 kV
ion source voltage 2 16.85 kV
Lens voltage 8.3 kV
Linear detector voltage 2.783 kV
Deflection on
Deflection mass

MSMS parent mass
LIFT voltage 1
LIFT voltage 2
LIFT 1 Pulser time depending on the parent mass
LIFT 2 Pulser time

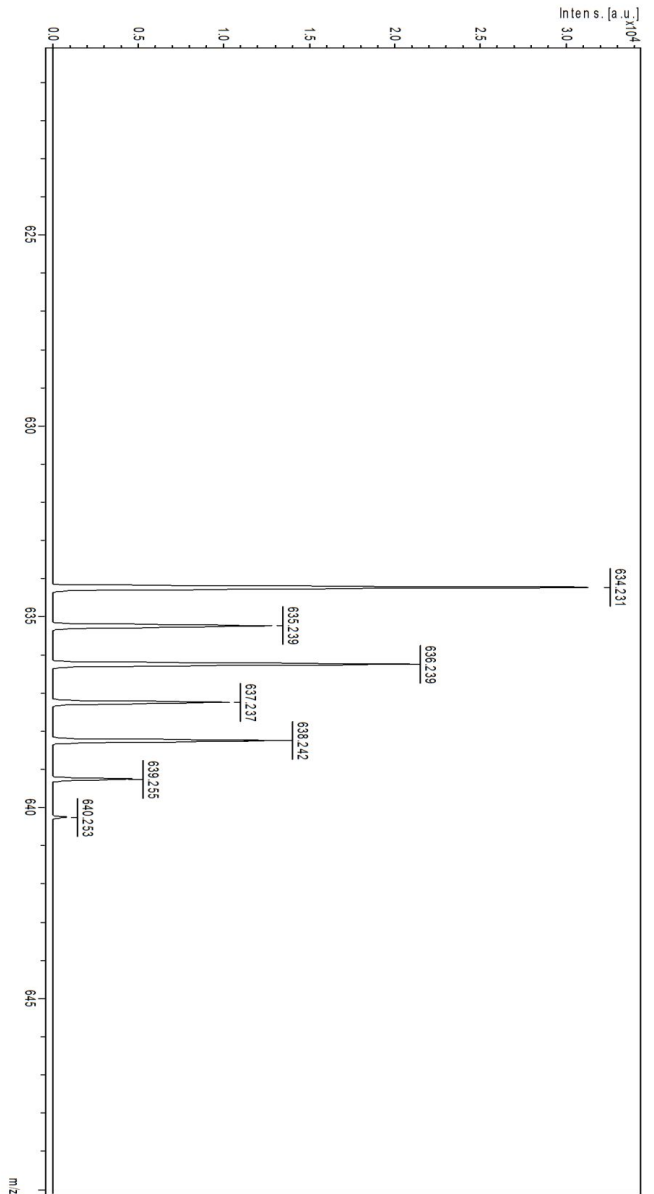
Reflector voltage 1 21 kV
Reflector voltage 2 9.6 kV
Reflector detector volt. 1.662 kV

Instrument
Instrument type autolex
Instrument serial 1857351.00828
Name of computer FLEX-PC
Operator ID or name admin
flexControl version flexControl 3.4.168.0
flexAnalysis version 3.4.79.0

Date of Acquisition 2020-01-27T15:06:18.040-05:00 printed: 1/27/2020 3:43:20 PM
Acquisition method D:\Methods\flexControl\Methods\Lindsey_Zhiyuan\RP_0-1500_Da.par
Processing method
File Name D:\Data\Lindsey\Jay\20200127P-TMS\0_1201

| | |
|--------------|-------------|
| Performed by | Viewed by |
| Date / Sign | Date / Sign |

Bruker Daltonics



Target
Target type 0280784
Target serial number 1004015
Position 120

Laser
Laser beam attenuation 75
Laser beam focus 36
Laser repetition rate 2000 Hz
Number of shots 500

Spectrometer
positive voltage polarity POS
PIE delay 130 ns
Ion source voltage 1 19 kV
Ion source voltage 2 16.85 kV
Lens voltage 8.3 kV
Linear detector voltage 2.783 kV
Deflection on
Deflection mass

MSMS parent mass
LIFT voltage 1
LIFT voltage 2
LIFT 1 Pulser time
depending on the parent
mass
LIFT 2 Pulser time

Reflector voltage 1 21 kV
Reflector voltage 2 9.6 kV
Reflector detector volt. 1.662 kV

Instrument
Instrument type autoflex
Instrument serial 1857351.00828
Name of computer FLEX-PC
Operator ID or name admin
flexControl version flexControl 3.4.168.0
flexAnalysis version 3.4.79.0

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printed: 1/27/2020 3:42:57 PM

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| Performed by | Viewed by |
| Date / Sign | Date / Sign |

Bruker Daltonics

20: Absorption spectrum (toluene)

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Spectrum/Peak Report

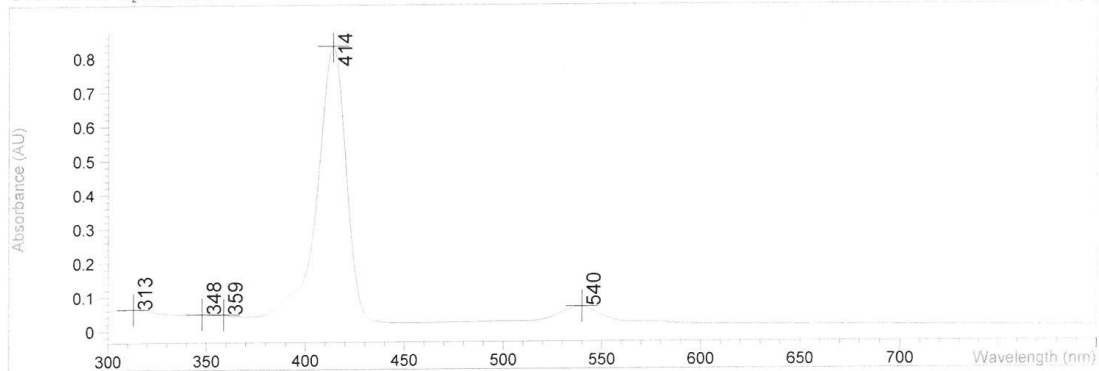
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Date 9/23/2022 Time 12:01:14 Page 1 of 1

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Created : 1/17/20 15:33:49

Compound 20

Overlaid Spectra:



| # | Name | Peaks (nm) | Abs (AU) |
|---|------|------------|-----------|
| 1 | | 414.0 | 0.83416 |
| 1 | | 540.0 | 6.8727E-2 |
| 1 | | 313.0 | 6.4114E-2 |
| 1 | | 348.0 | 4.8937E-2 |
| 1 | | 359.0 | 4.7909E-2 |

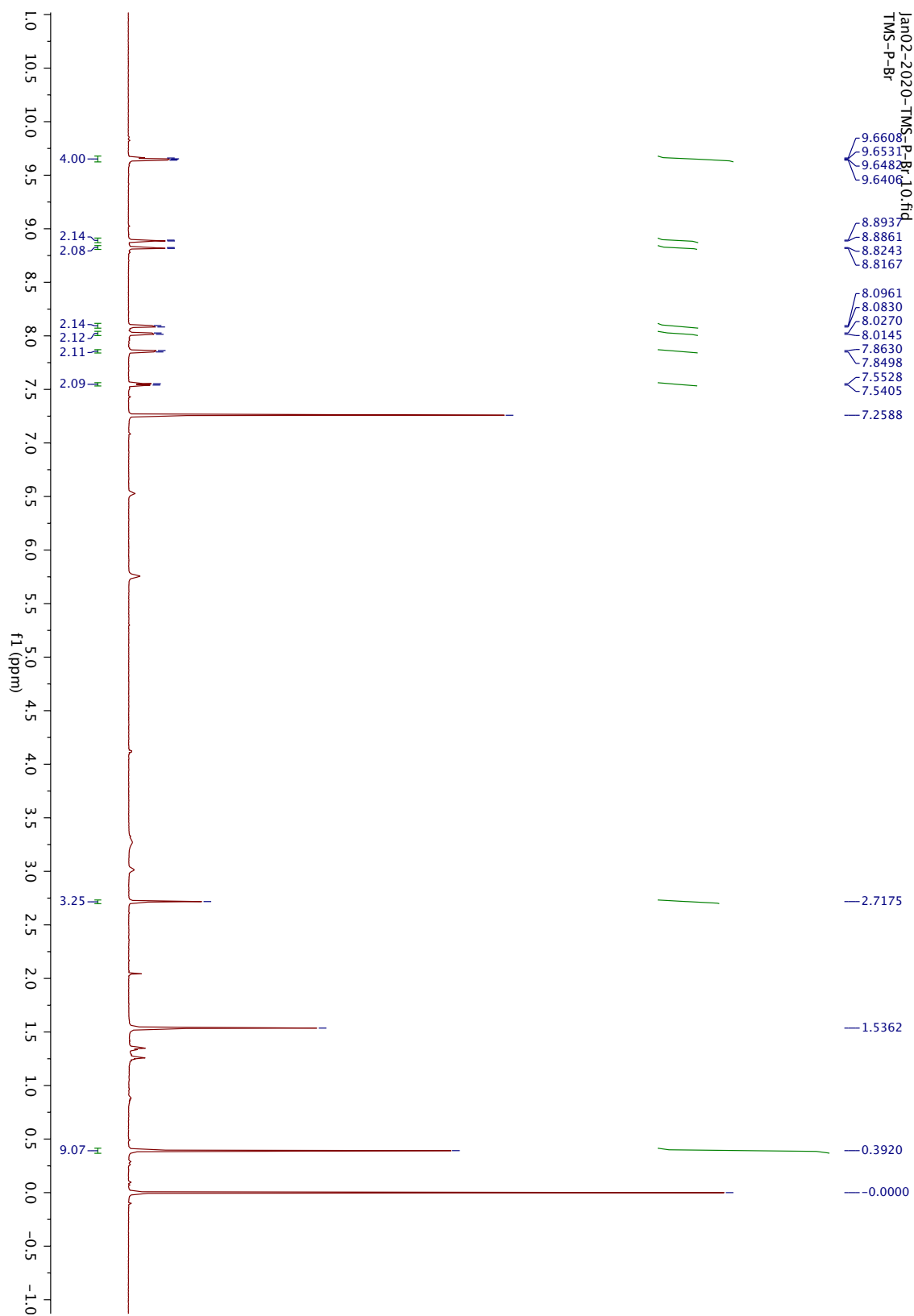
Report generated by : jon

Signature:

*** End Spectrum/Peak Report ***

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21: ^1H NMR, CDCl_3 , 600 MHz





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Target serial number 1004015
Position 123

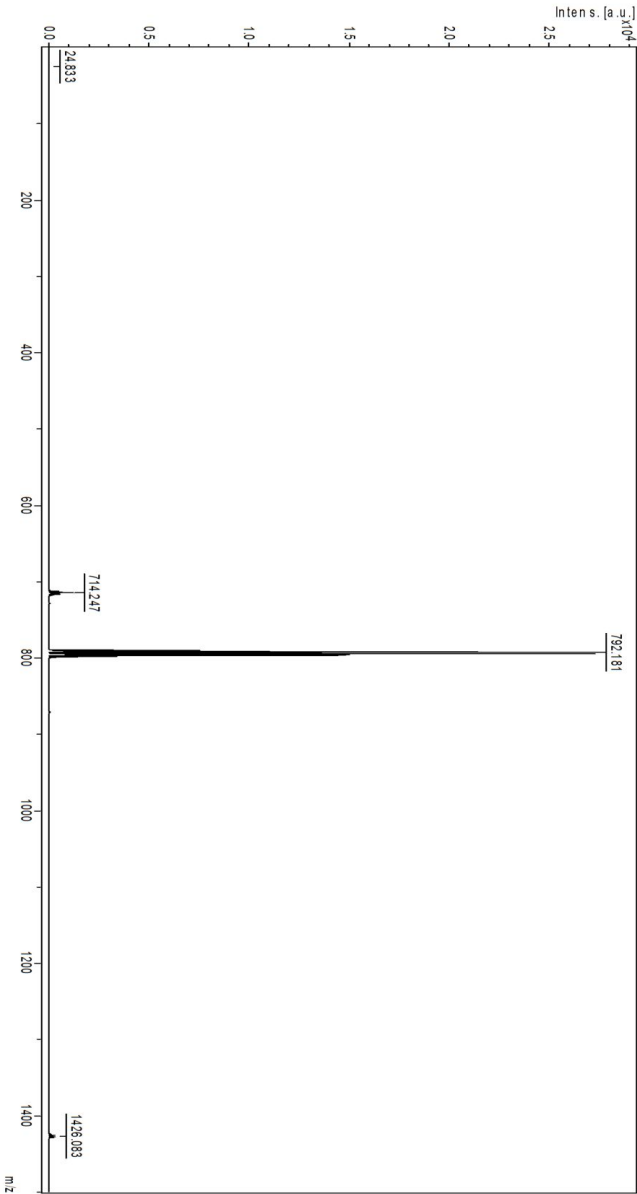
Laser
Laser beam attenuation 60
Laser beam focus 36
Laser repetition rate 2000 Hz
Number of shots 500

Spectrometer
positive voltage polarity POS
PIE delay 130 ns
ion source voltage 1 19 kV
ion source voltage 2 16.85 kV
Lens voltage 8.3 kV
Linear detector voltage 2.783 kV
Detection on

MSMS parent mass
LIFT voltage 1
LIFT voltage 2
LIFT 1 Pulser time
depending on the parent
mass
LIFT 2 Pulser time

Reflector voltage 1 21 kV
Reflector voltage 2 9.6 kV
Reflector detector volt. 1.662 kV

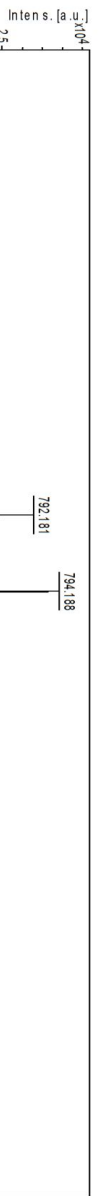
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Instrument type autoflex
Instrument serial 1857351.00828
Name of computer FLEX-PC
Operator ID or name admin
flexControl version flexControl 3.4.168.0
flexAnalysis version 3.4.79.0



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Processing method
File Name D:\Data\Lindsey\Jay\20200127Br-P-TMS\0_1231

| | |
|--------------|-------------|
| Performed by | Viewed by |
| Date / Sign | Date / Sign |

Bruker Daltonics



Target
Target type 0280784
Target serial number 1004015
Position 123

Laser
Laser beam attenuation 60
Laser beam focus 36
Laser repetition rate 2000 Hz
Number of shots 500

Spectrometer
positive voltage polarity POS
P/E delay 130 ns
Ion source voltage 1 19 kV
Ion source voltage 2 16.85 kV
Lens voltage 8.3 kV
Linear detector voltage 2.783 kV
Deflection on

MSMS parent mass
LIFT voltage 1
LIFT voltage 2
LIFT 1 Pulser time
depending on the parent
mass
LIFT 2 Pulser time

Reflector voltage 1 21 kV
Reflector voltage 2 9.6 kV
Reflector detector volt. 1.662 kV

Instrument
Instrument type autoflex
Instrument serial 1857351.00828
Name of computer FLEX-PC
Operator ID or name admin
flexControl version flexControl 3.4.168.0
flexAnalysis version 3.4.79.0

Date of Acquisition 2020-01-27T15:08:35.912-05:00
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Processing method
File Name D:\Data\Lindsey\Jay\20200127\Br-P-TMS\0_1231

printed: 1/27/2020 3:44:46 PM

| | |
|--------------|-------------|
| Performed by | Viewed by |
| Date / Sign | Date / Sign |

Bruker Daltonics

21: Absorption spectrum (toluene)

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Spectrum/Peak Report

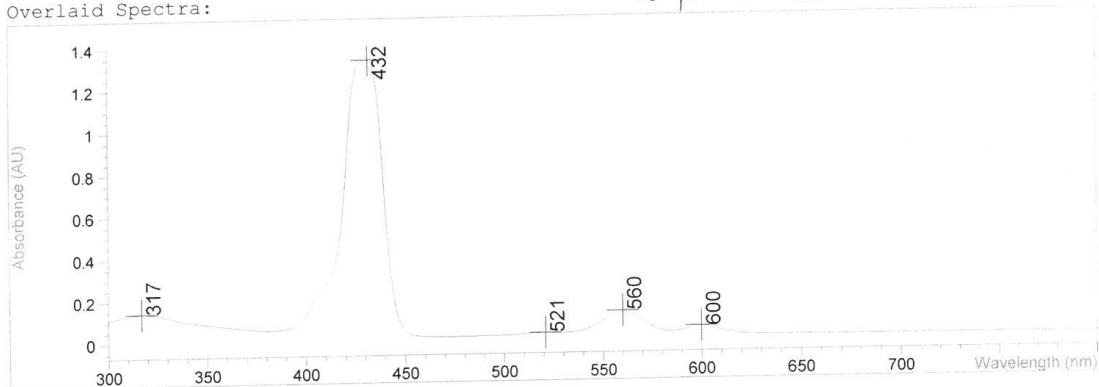
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Date 9/23/2022 Time 12:00:48 Page 1 of 1

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Overlaid Spectra:

Compound 21



| # | Name | Peaks (nm) | Abs (AU) |
|---|------|------------|-----------|
| 1 | | 432.0 | 1.33510 |
| 1 | | 317.0 | 0.14086 |
| 1 | | 560.0 | 0.12602 |
| 1 | | 600.0 | 4.9747E-2 |
| 1 | | 521.0 | 2.6982E-2 |

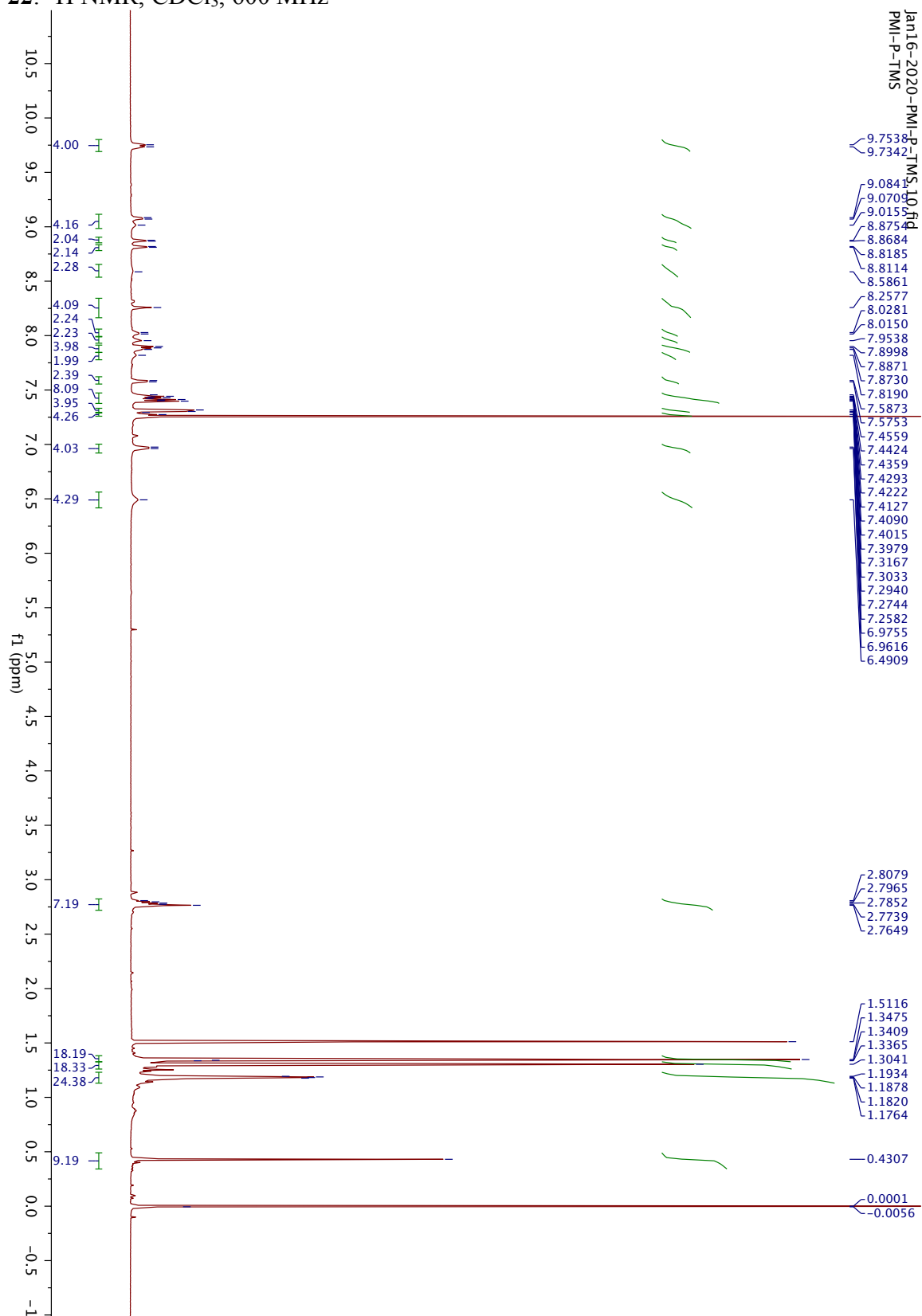
Report generated by : jon

Signature:

*** End Spectrum/Peak Report ***

=====

22: ^1H NMR, CDCl_3 , 600 MHz





Target

Target type 0280784
Target serial number 1004015
Position K20

Laser

Laser beam attenuation 50
Laser beam focus 36
Laser repetition rate 2000 Hz
Number of shots 500

Spectrometer

positive voltage polarity POS
PIE delay 130 ns
ion source voltage 1 19 kV
ion source voltage 2 16.85 kV
Lens voltage 8.3 kV
Linear detector voltage 2.783 kV
Detection on

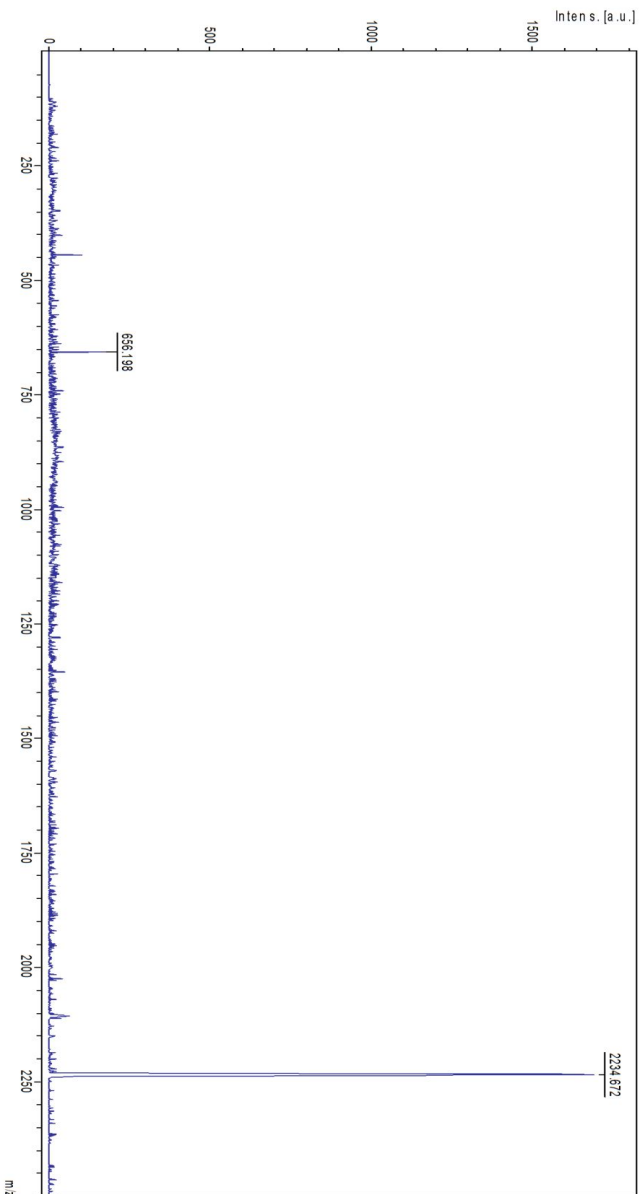
MSMS parent mass

LIFT voltage 1
LIFT voltage 2
LIFT 1 Pulser time depending on the parent mass
LIFT 2 Pulser time

Reflector voltage 1 21 kV
Reflector voltage 2 9.6 kV
Reflector detector volt. 1.662 kV

Instrument

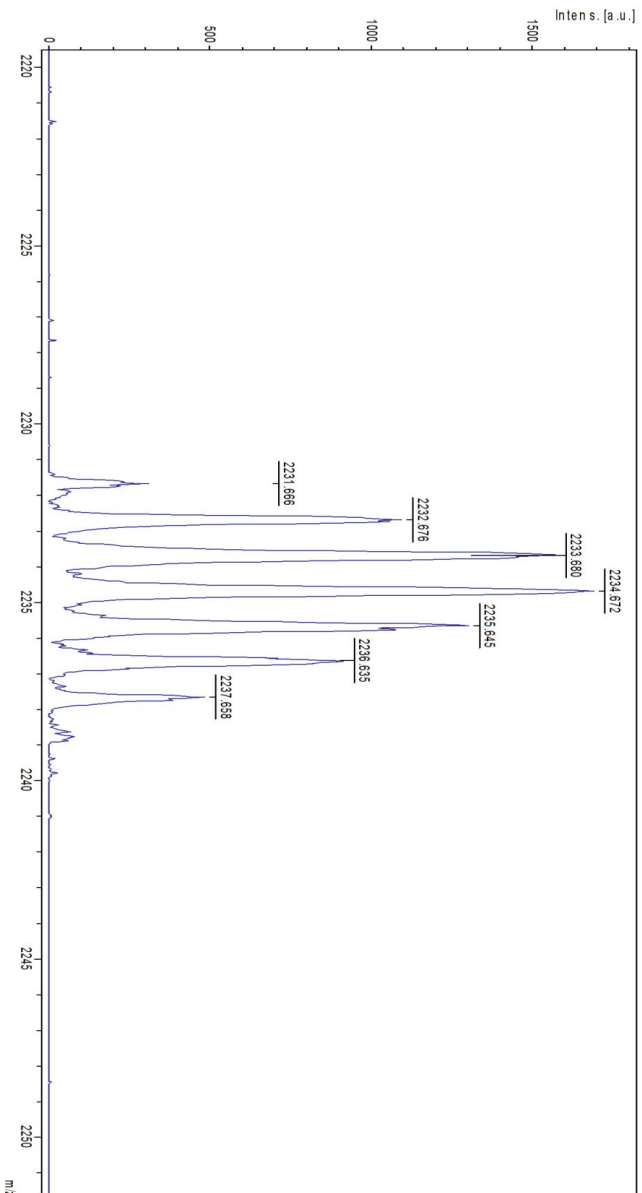
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Operator ID or name admin
flexControl version flexControl 3.4.168.0
flexAnalysis version 3.4.79.0



Date of Acquisition 2020-01-27T15:11:10.766-05:00 printed: 1/27/2020 3:46:07 PM
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| | |
|--------------|-------------|
| Performed by | Viewed by |
| Date / Sign | Date / Sign |

Bruker Daltonics



Target
Target type 0280784
Target serial number 1004015
Position K20

Laser
Laser beam attenuation 50
Laser beam focus 36
Laser repetition rate 2000 Hz
Number of shots 500

Spectrometer
positive voltage polarity POS
PIE delay 130 ns
Ion source voltage 1 19 kV
Ion source voltage 2 16.85 kV
Lens voltage 8.3 kV
Linear detector voltage 2.763 kV
Deflection on

MSMS parent mass
LIFT voltage 1
LIFT voltage 2
LIFT 1 Pulser time
depending on the parent
mass
LIFT 2 Pulser time

Instrument
Instrument type autoflex
Instrument serial 1857351.00828
Name of computer FLEX-PC
Operator ID or name admin
flexControl version flexControl 3.4.168.0
flexAnalysis version 3.4.79.0

Reflector voltage 1 21 kV
Reflector voltage 2 9.6 kV
Reflector detector volt. 1.662 kV

Date of Acquisition 2020-01-27T15:11:10.768-05:00
Acquisition method D:\Methods\flexControl\Methods\Lindsey_Zhiyuan\RP_0-1500_Da.par
Processing method
File Name D:\Data\Lindsey\Jay\20200127\PMI-P-TMSIO_K201

printed: 1/27/2020 3:45:59 PM

| Performed by | Viewed by |
|--------------|-------------|
| Date / Sign | Date / Sign |

Bruker Daltonics

22: Absorption spectrum (toluene)

=====

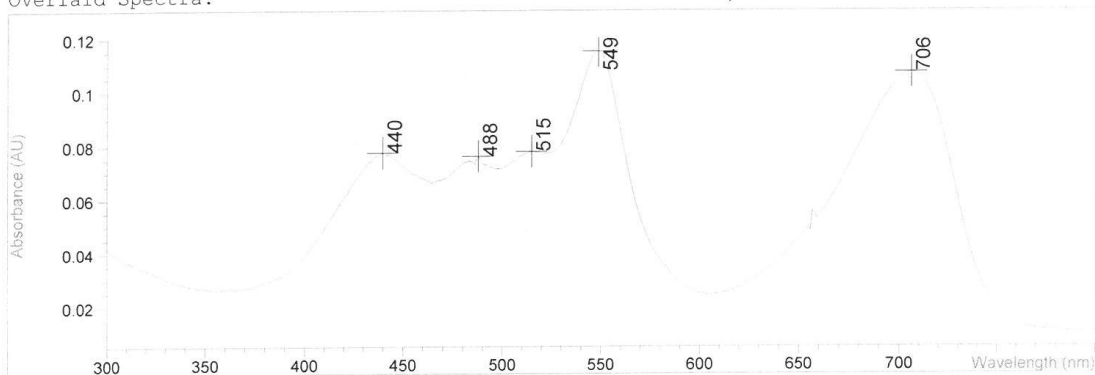
Spectrum/Peak Report

=====

Date 9/23/2022 Time 12:01:49 Page 1 of 1

Method file : <method not saved>
Information : Default Method
Data File : C:\Chem32\1\DATA\JayRong\Solar_Cell\ABS for paper\PMI-P-TMS_1.SD
Created : 1/17/20 15:21:06

Overlaid Spectra:



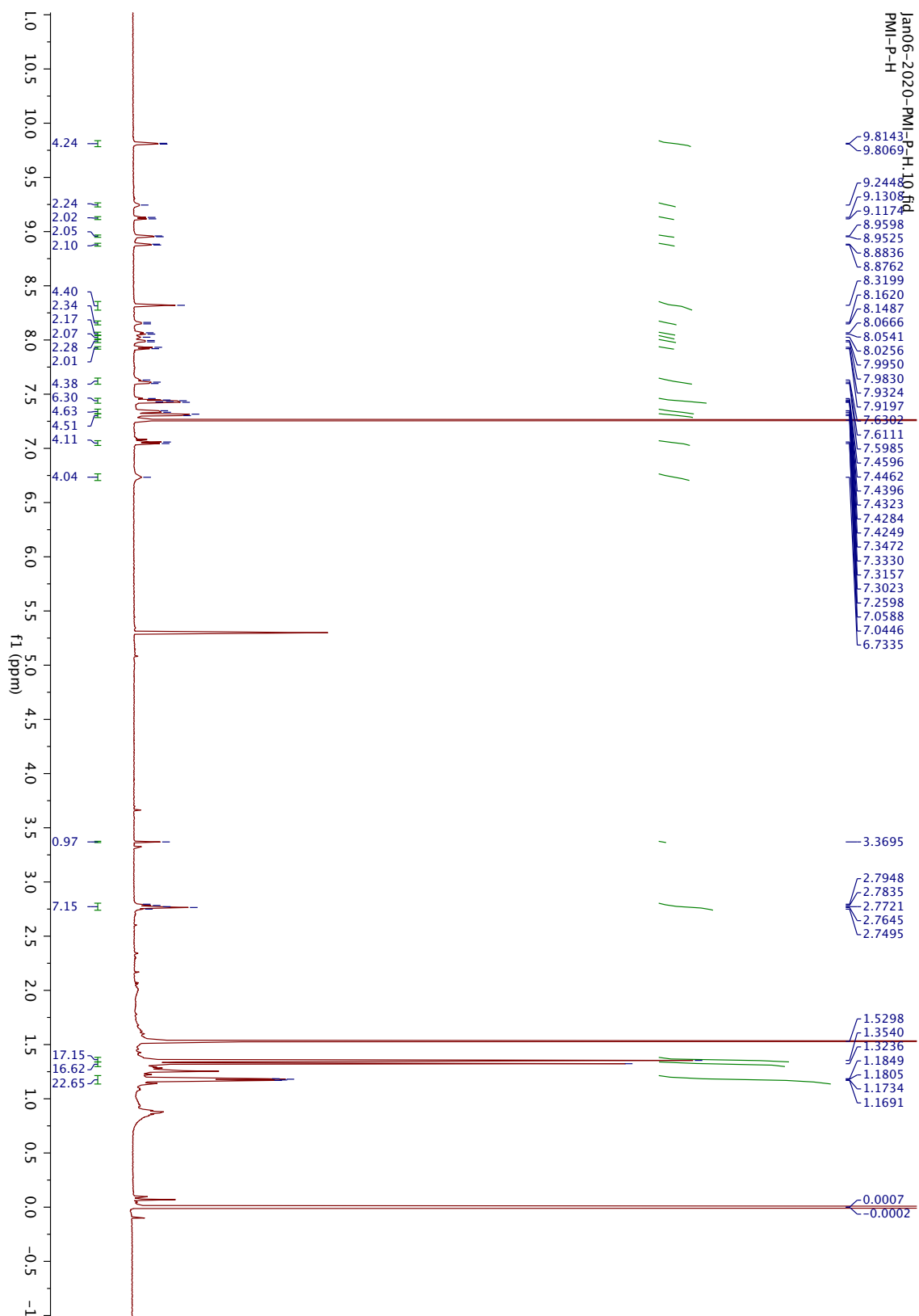
| # | Name | Peaks (nm) | Abs (AU) |
|---|------|------------|-----------|
| 1 | | 549.0 | 0.11524 |
| 1 | | 706.0 | 0.10732 |
| 1 | | 515.0 | 7.7922E-2 |
| 1 | | 440.0 | 7.7526E-2 |
| 1 | | 488.0 | 7.6225E-2 |

Report generated by : jon

Signature:

*** End Spectrum/Peak Report ***

23: ^1H NMR, CDCl_3 , 600 MHz





Target

Target type 0280784
Target serial number 1004015
Position K23

Laser

Laser beam attenuation 38
Laser beam focus 36
Laser repetition rate 2000 Hz
Number of shots 500

Spectrometer

positive voltage polarity POS
PIE delay 130 ns
ion source voltage 1 19 kV
ion source voltage 2 16.85 kV
Lens voltage 8.3 kV
Linear detector voltage 2.783 kV
Deflection on

Deflection mass

MSMS parent mass

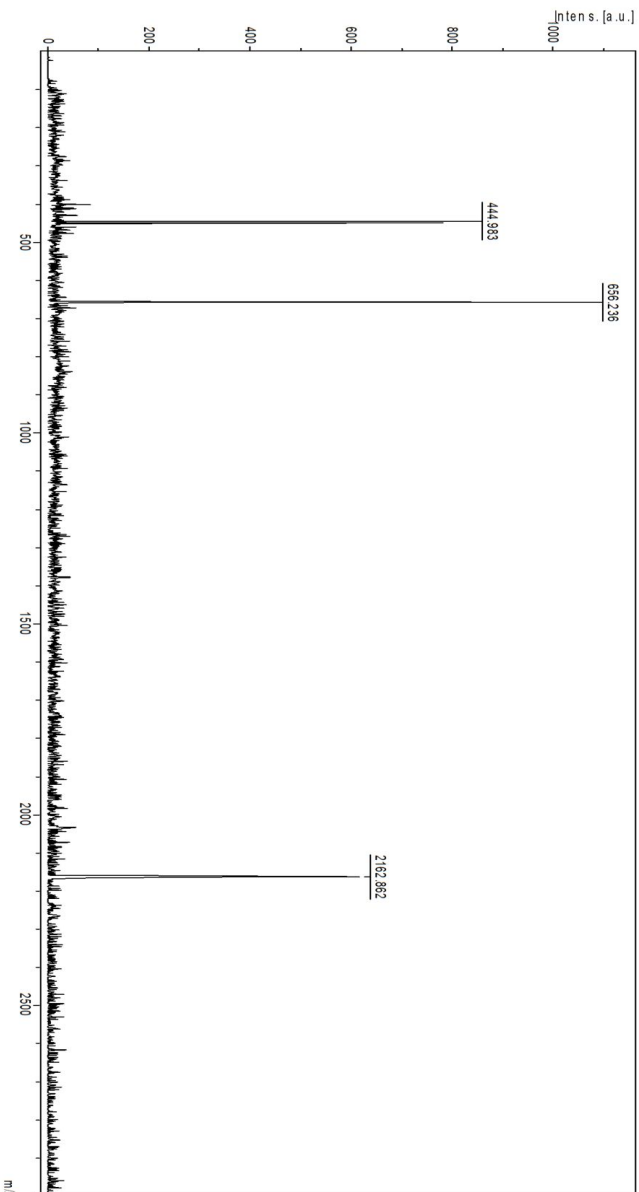
LIFT voltage 1
LIFT voltage 2
LIFT 1 Pulser time
depending on the parent
mass

LIFT 2 Pulser time

Reflector voltage 1 21 kV
Reflector voltage 2 9.6 kV
Reflector detector volt. 1.662 kV

Instrument

Instrument type autoflex
Instrument serial 1857351.00828
Name of computer FLEX-PC
Operator ID or name admin
flexControl version flexControl 3.4.168.0
flexAnalysis version

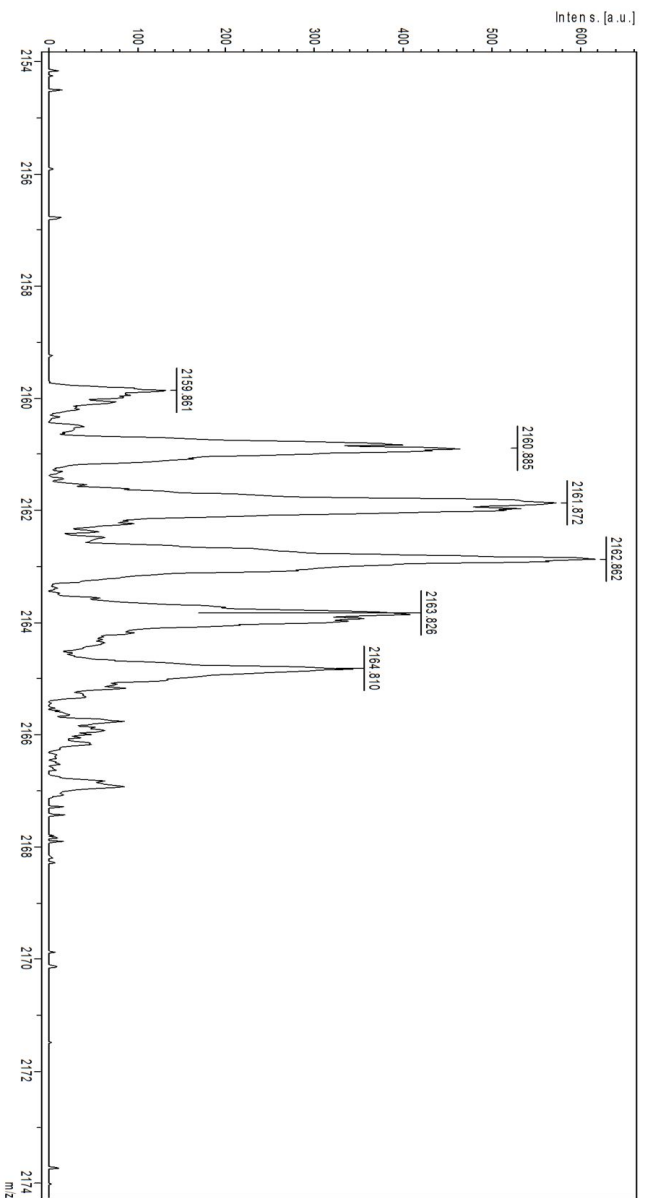


Date of Acquisition 2020-01-27T15:41:07.820-05:00 printed: 1/27/2020 3:47:20 PM
Acquisition method D:\Methods\flexControl\Methods\Lindsey_Zhiyuan\RP_0-1500_Da.par
Processing method
File Name D:\Data\Lindsey\Jay\20200127PM-LP-H10_K231

Performed by
Date / Sign

Viewed by
Date / Sign

Bruker Daltonics



Target
Target type 0280784
Target serial number 1004015
Position K23

Laser
Laser beam attenuation 38
Laser beam focus 36
Laser repetition rate 2000 Hz
Number of shots 500

Spectrometer
positive voltage polarity POS
PIE delay 130 ns
Ion source voltage 1 19 kV
Ion source voltage 2 16.85 kV
Lens voltage 8.3 kV
Linear detector voltage 2.763 kV
Deflection on

MSMS parent mass
LIFT voltage 1
LIFT voltage 2
LIFT 1 Pulser time
depending on the parent
mass
LIFT 2 Pulser time

Reflector voltage 1 21 kV
Reflector voltage 2 9.6 kV
Reflector detector volt. 1.662 kV

Instrument
Instrument type autoflex
Instrument serial 1857351.00828
Name of computer FLEX-PC
Operator ID or name admin
flexControl version flexControl 3.4.168.0
flexAnalysis version

Date of Acquisition 2020-01-27T15:41:07.820-05:00
Acquisition method D:\Methods\flexControl\Methods\Lindsey_Zhiyuan\RP_0-1500_Da.par
Processing method
File Name D:\Data\Lindsey\Jay\20200127\PM1-P-H10_K231

printed: 1/27/2020 3:47:10 PM

| Performed by | | Viewed by | |
|--------------|--|-------------|--|
| Date / Sign | | Date / Sign | |

Bruker Daltonics

23: Absorption spectrum (toluene)

=====

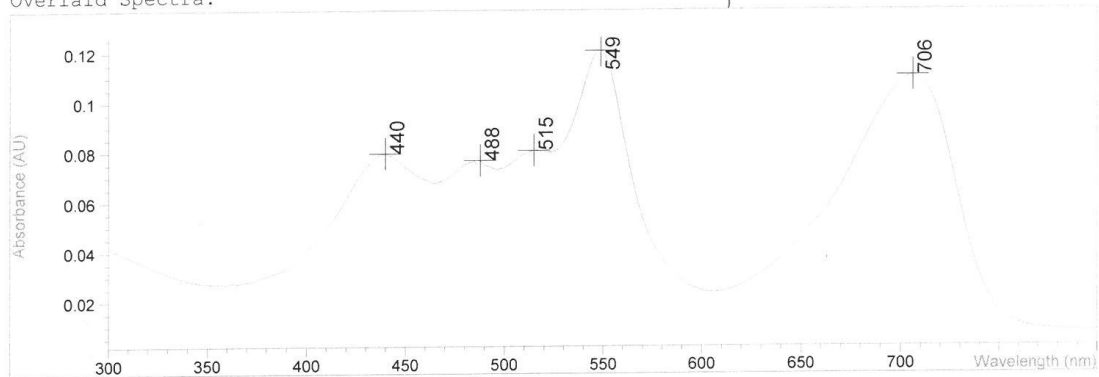
Spectrum/Peak Report

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Date 9/23/2022 Time 12:01:55 Page 1 of 1

Method file : <method not saved>
Information : Default Method
Data File : C:\Chem32\1\DATA\JayRong\Solar_Cell\ABS for paper\PMI-P-H_1.SD
Created : 1/17/20 15:27:08

Overlaid Spectra:



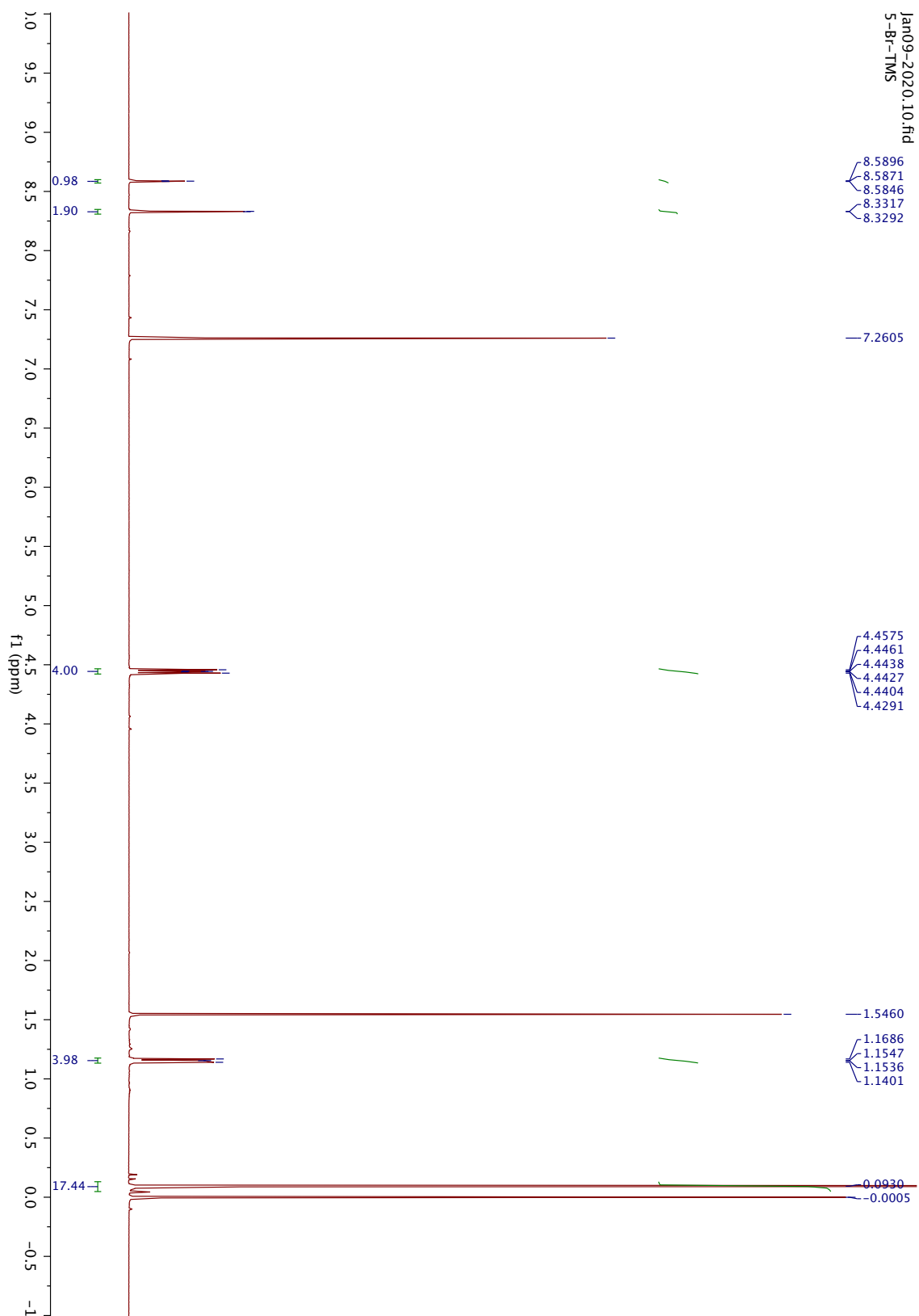
| # | Name | Peaks (nm) | Abs (AU) |
|---|------|------------|-----------|
| 1 | | 549.0 | 0.12052 |
| 1 | | 706.0 | 0.11034 |
| 1 | | 515.0 | 8.0578E-2 |
| 1 | | 440.0 | 7.9451E-2 |
| 1 | | 488.0 | 7.6578E-2 |

Report generated by : jon

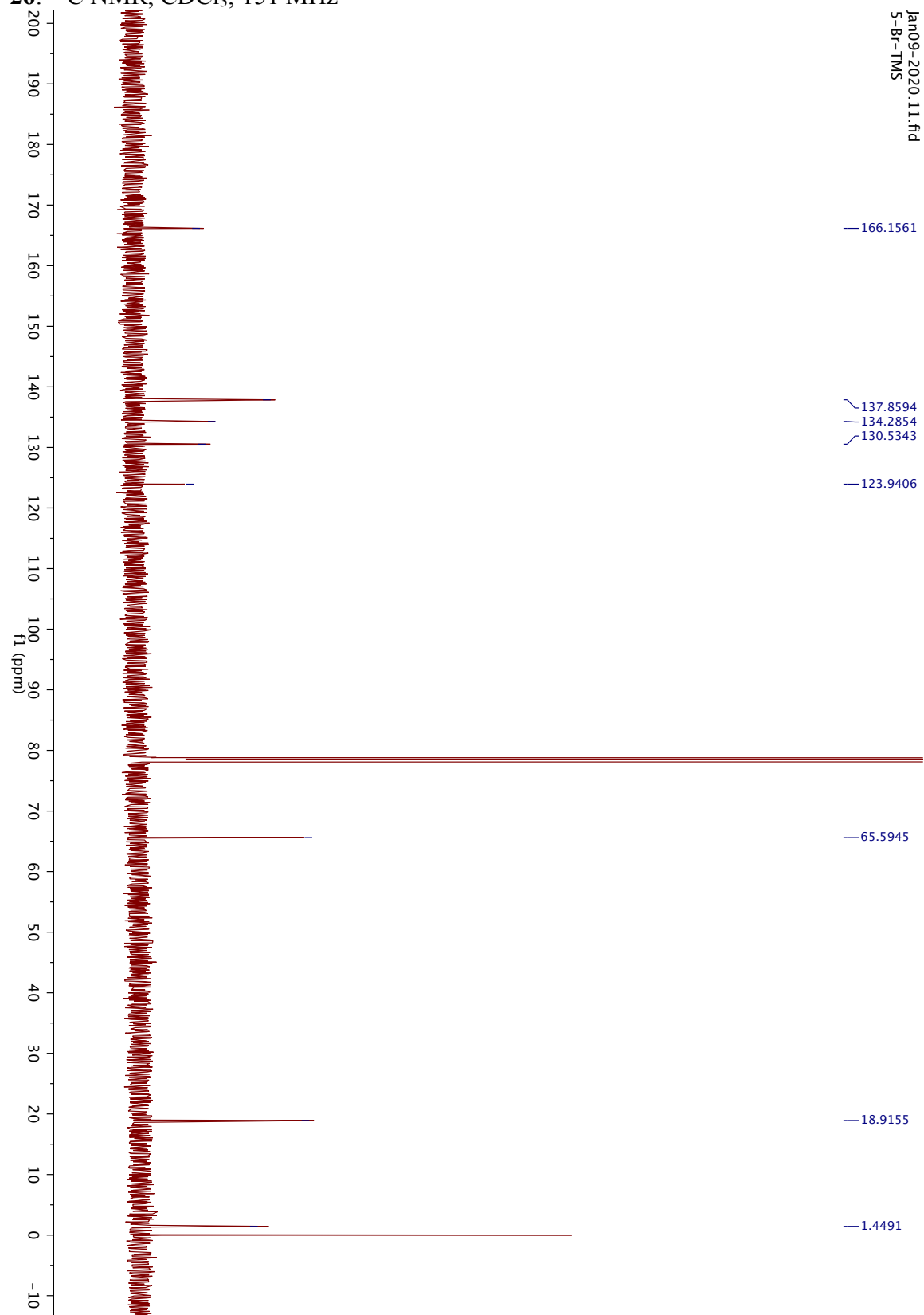
Signature:

*** End Spectrum/Peak Report ***

26: ^1H NMR, CDCl_3 , 600 MHz



26: ^{13}C NMR, CDCl_3 , 151 MHz



26: ESI-MS

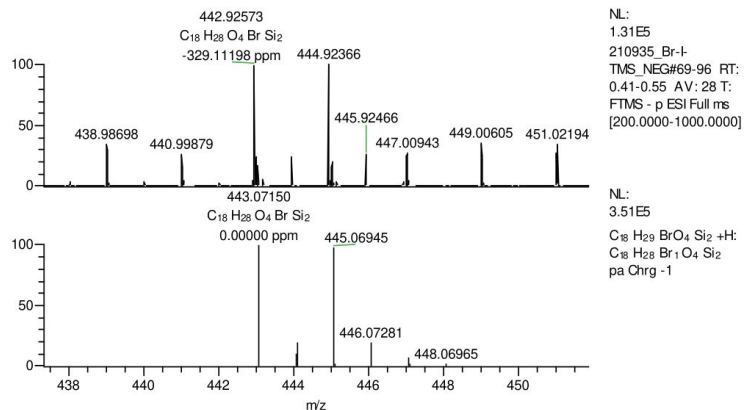
NC STATE UNIVERSITY

Molecular Education, Technology and
Research Innovation Center

Raleigh, NC 27695

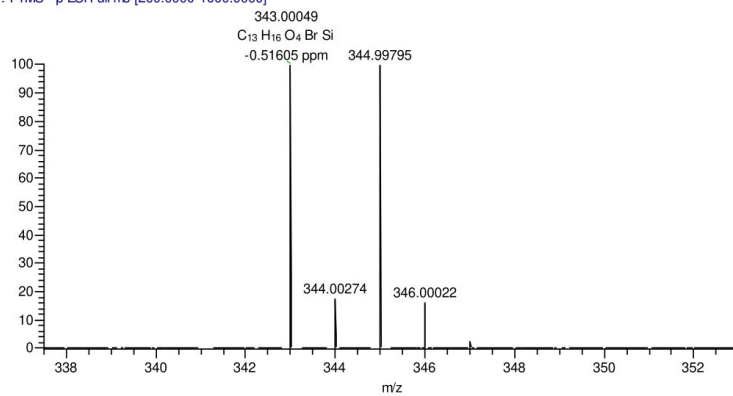
<https://research.ncsu.edu/metric/>

Br-I-TMS Experimental and Theoretical Isotopic Distribution for $C_{18}H_{29}BrO_4Si_2 [M-H]^+$

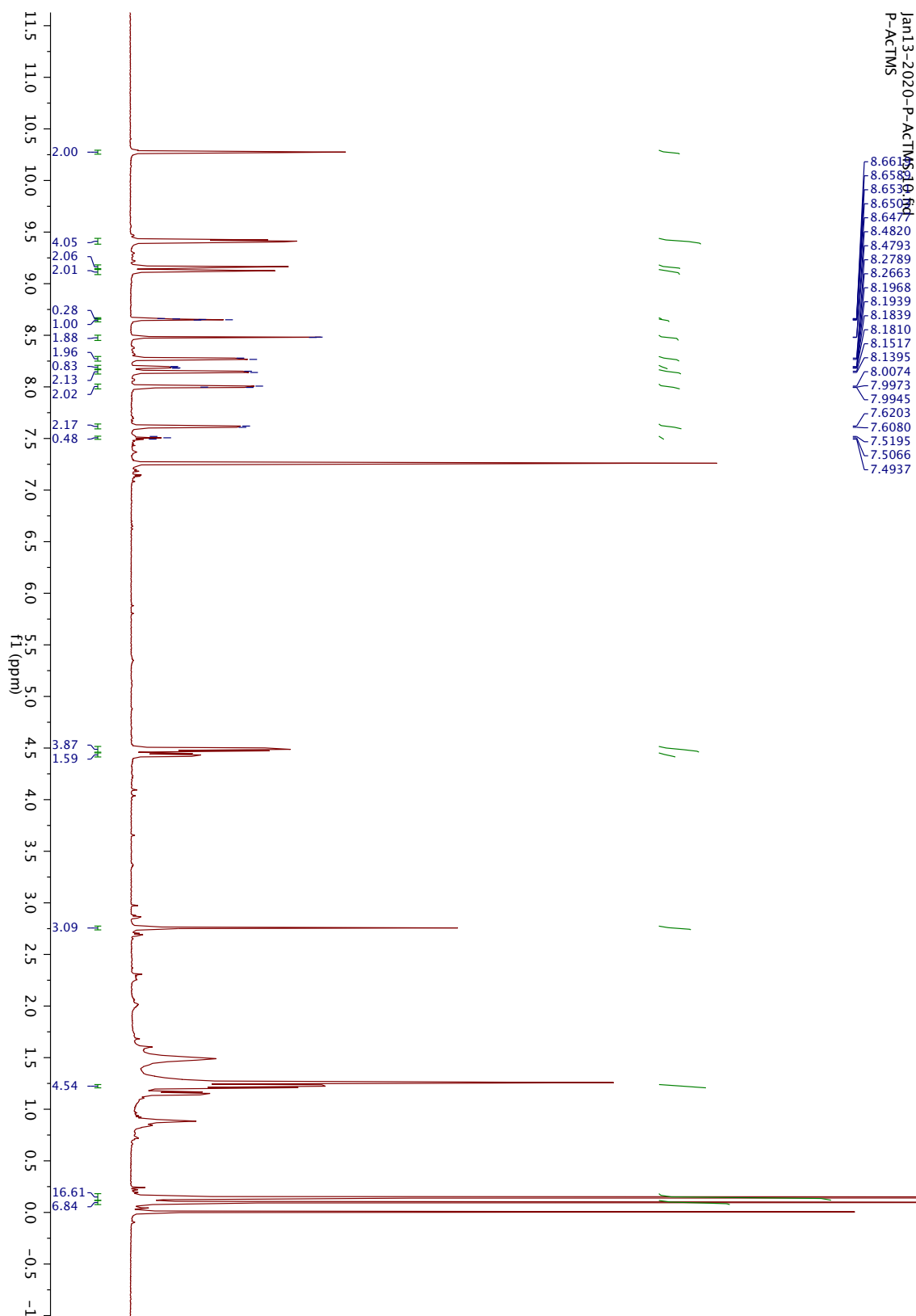


Br-I-TMS Scan 338-352 m/z

210935_Br-I-TMS_NEG #69-96 RT: 0.41-0.55 AV: 28 NL: 2.66E7
T: FTMS - p ESI Full ms [200.0000-1000.0000]



27: ^1H NMR, CDCl_3 , 600 MHz





Target
Target type 0280784
Target serial number 1004015
Position O21

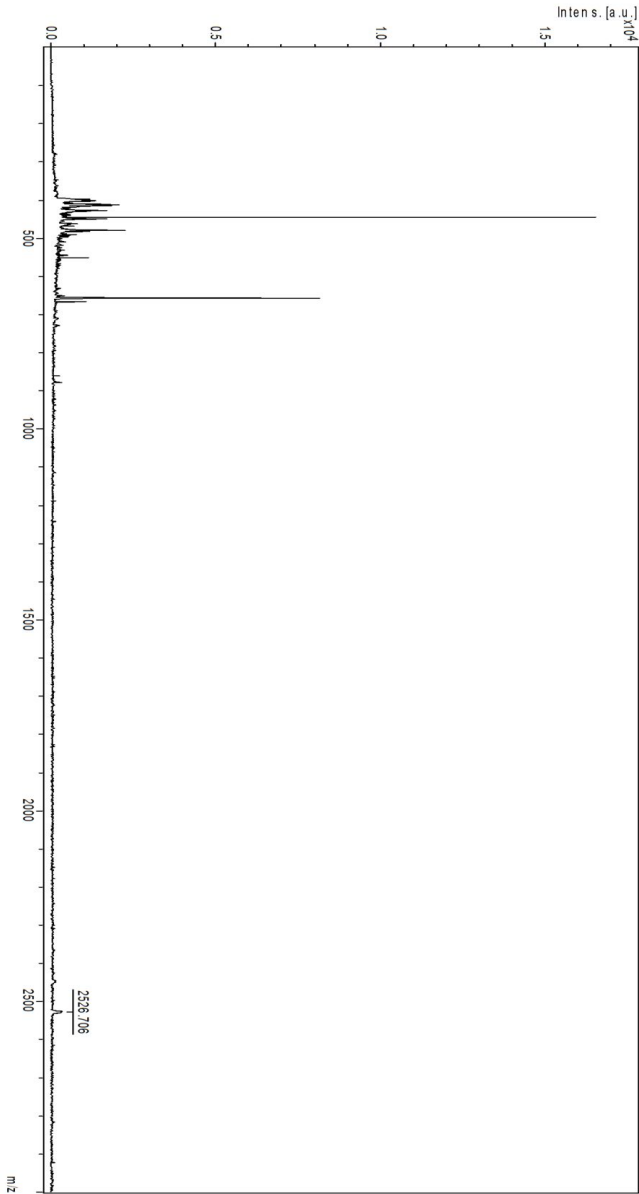
Laser
Laser beam attenuation 12
Laser beam focus 36
Laser repetition rate 2000 Hz
Number of shots 500

Spectrometer
positive voltage polarity POS
PIE delay 130 ns
ion source voltage 1 19 kV
ion source voltage 2 16.85 kV
Lens voltage 8.3 kV
Linear detector voltage 2.783 kV
Detection on

MSMS parent mass
LIFT voltage 1
LIFT voltage 2
LIFT 1 Pulser time depending on the parent mass
LIFT 2 Pulser time

Reflector voltage 1 21 kV
Reflector voltage 2 9.6 kV
Reflector detector volt. 1.662 kV

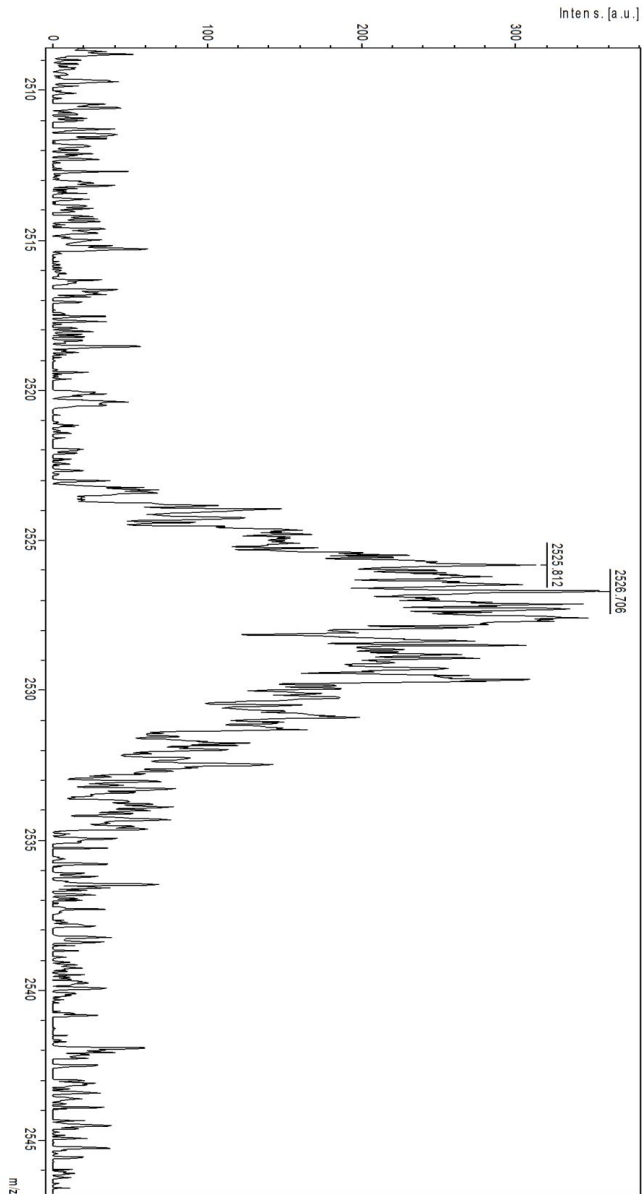
Instrument
Instrument type autoflex
Instrument serial 1857351.00828
Name of computer FLEX-PC
Operator ID or name admin
flexControl version flexControl 3.4.168.0
flexAnalysis version



Date of Acquisition 2020-01-27T15:39:26.971-05:00 printed: 1/27/2020 4:02:06 PM
Acquisition method D:\Methods\flexControl\Methods\Lindsey_Zhiyuan\RP_0-1500_Da.par
Processing method
File Name D:\Data\Lindsey\Jay\20200127PM-LP-ACTMS10_O21\1

| | |
|--------------|-------------|
| Performed by | Viewed by |
| Date / Sign | Date / Sign |

Bruker Daltonics



Target
Target type 0280784
Target serial number 1004015
Position O21

Laser
Laser beam attenuation 12
Laser beam focus 36
Laser repetition rate 2000 Hz
Number of shots 500

Spectrometer
positive voltage polarity POS
PIE delay 130 ns
Ion source voltage 1 19 kV
Ion source voltage 2 16.85 kV
Lens voltage 8.3 kV
Linear detector voltage 2.783 kV
Deflection on
Deflection mass

MSMS parent mass
LIFT voltage 1
LIFT voltage 2
LIFT 1 Pulser time
depending on the parent
mass
LIFT 2 Pulser time

Reflector voltage 1 21 kV
Reflector voltage 2 9.6 kV
Reflector detector volt. 1.662 kV

Instrument
Instrument type autoflex
Instrument serial 1857351.00828
Name of computer FLEX-PC
Operator ID or name admin
flexControl version flexControl 3.4.168.0
flexAnalysis version

Date of Acquisition 2020-01-27T15:39:26.971-05:00 printed: 1/27/2020 4:02:51 PM
Acquisition method D:\Methods\flexControl\Methods\Lindsey_Zhiyuan\RP_0-1500_Da.par
Processing method
File Name D:\Data\Lindsey\day20200127PM-LP-ActMS0_02111

| | |
|--------------|-------------|
| Performed by | Viewed by |
| Date / Sign | Date / Sign |

Bruker Daltonics

27: Absorption spectrum (toluene)

=====

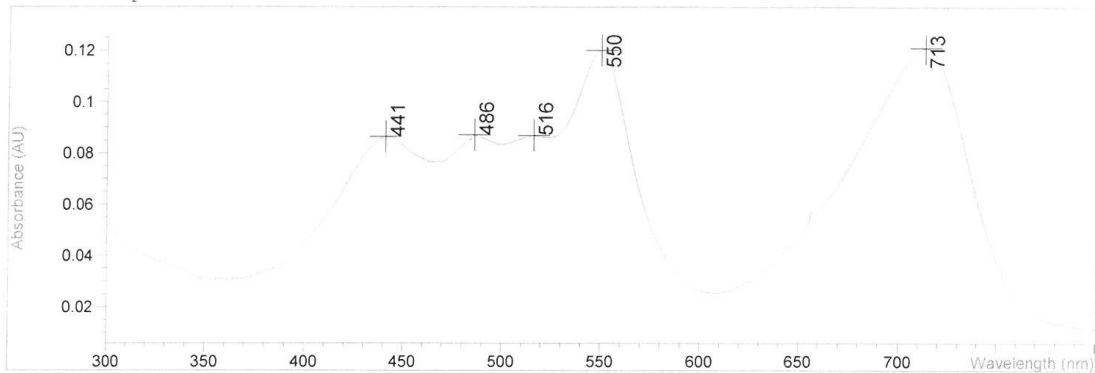
Spectrum/Peak Report

=====

Date 9/23/2022 Time 12:02:02 Page 1 of 1

Method file : <method not saved>
Information : Default Method
Data File : C:\Chem32\1\DATA\JayRong\Solar_Cell\ABS for paper\PMI-P-ACTMS_1.SD
Created : 1/17/20 15:16:12

Overlaid Spectra:



| # | Name | Peaks (nm) | Abs (AU) |
|---|------|------------|-----------|
| 1 | | 713.0 | 0.12108 |
| 1 | | 550.0 | 0.12002 |
| 1 | | 486.0 | 8.7032E-2 |
| 1 | | 516.0 | 8.6899E-2 |
| 1 | | 441.0 | 8.6447E-2 |

Report generated by : jon

Signature:

*** End Spectrum/Peak Report ***

=====

28: Absorption spectrum (toluene)

=====

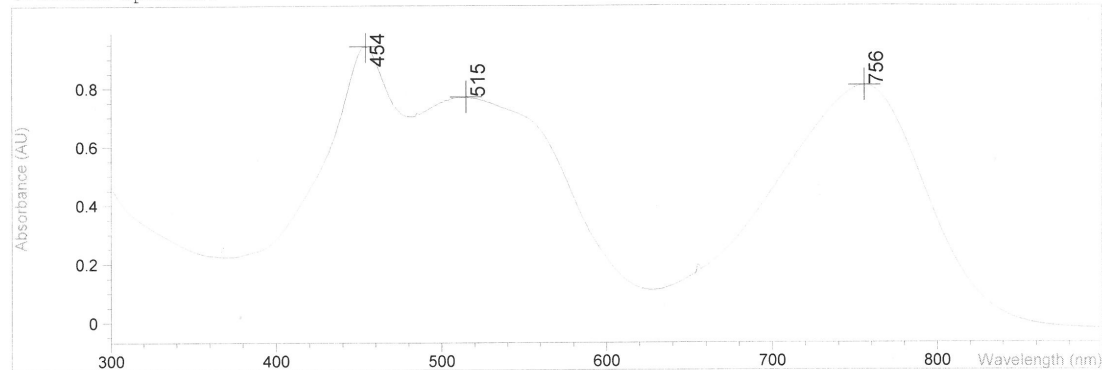
Spectrum/Peak Report

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Date 9/24/2022 Time 15:26:47 Page 1 of 1

Method file : <method not saved>
Information : Default Method
Data File : C:\Chem32\1\DATA\Masa\PERYLENE TRIAD 28 J8 (75).SD Created :
9/24/22 13:10:57

Overlaid Spectra:



| # | Name | Peaks (nm) | Abs (AU) |
|---|------|------------|----------|
| 1 | | 454.0 | 0.94268 |
| 1 | | 756.0 | 0.80966 |
| 1 | | 515.0 | 0.77060 |

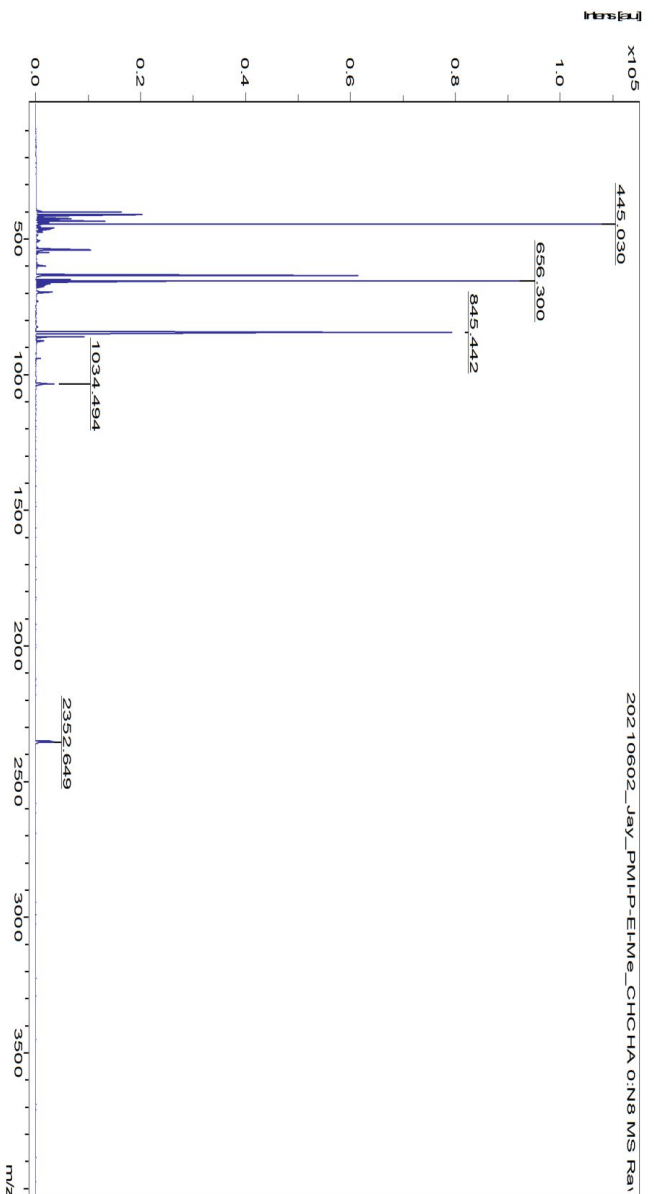
Report generated by : jon

Signature:

*** End Spectrum/Peak Report ***



20210602_Jay_PMI-P-EI-Me_CHCA
20210602_Jay_PMI-P-EI-Me_CHCA



Target

Target type 0280784
Target serial number 1004015
Position N8

Laser

Laser beam attenuation 42
Laser beam focus 36
Laser repetition rate 2000 Hz
Number of shots 500

Spectrometer

positive voltage polarity POS
PIE delay 130 ns
ion source voltage 1 19 kV
ion source voltage 2 16.85 kV
Lens voltage 8.3 kV
Linear detector voltage 2.728 kV
Deflection on

Deflection mass

MS/MS parent mass

LIFT voltage 1
LIFT voltage 2
LIFT 1 Pulser time
depending on the parent
mass

LIFT 2 Pulser time

Reflector voltage 1 21 kV
Reflector voltage 2 9.6 kV
Reflector detector volt. 1.662 kV

Instrument

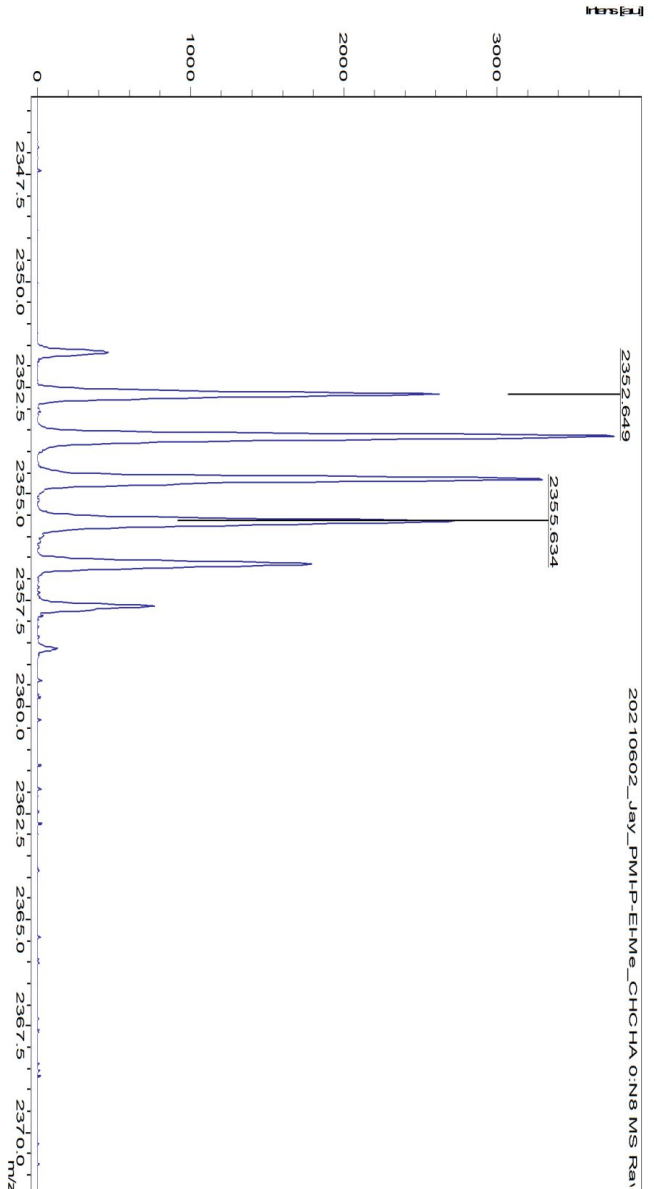
Instrument type autotex
Instrument serial 1857351.00828
Name of computer FLEX-PC
Operator ID or name admin
flexControl version flexControl 3.4.168.0
flexAnalysis version 3.4.79.0

Date of Acquisition 2021-06-02T15:07:25.722-04:00 printed: 9/23/2022 3:02:21 PM
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Processing method
File Name D:\Data\Lindsey\Jay\20210602_Jay_PMI-P-EI-Me_CHCA\10_N8\1

Performed by
Date / Sign

Viewed by
Date / Sign

Bruker Daltonics



Target
Target type 0280784
Target serial number 1004015
Position N8

Laser
Laser beam attenuation 42
Laser beam focus 36
Laser repetition rate 2000 Hz
Number of shots 500

Spectrometer
positive voltage polarity POS
PIE delay 130 ns
Ion source voltage 1 19 kV
Ion source voltage 2 16.85 kV
Lens voltage 8.3 kV
Linear detector voltage 2.728 kV
Deflection on

MSMS parent mass
LIFT voltage 1
LIFT voltage 2
LIFT 1 Pulser time
depending on the parent
mass
LIFT 2 Pulser time

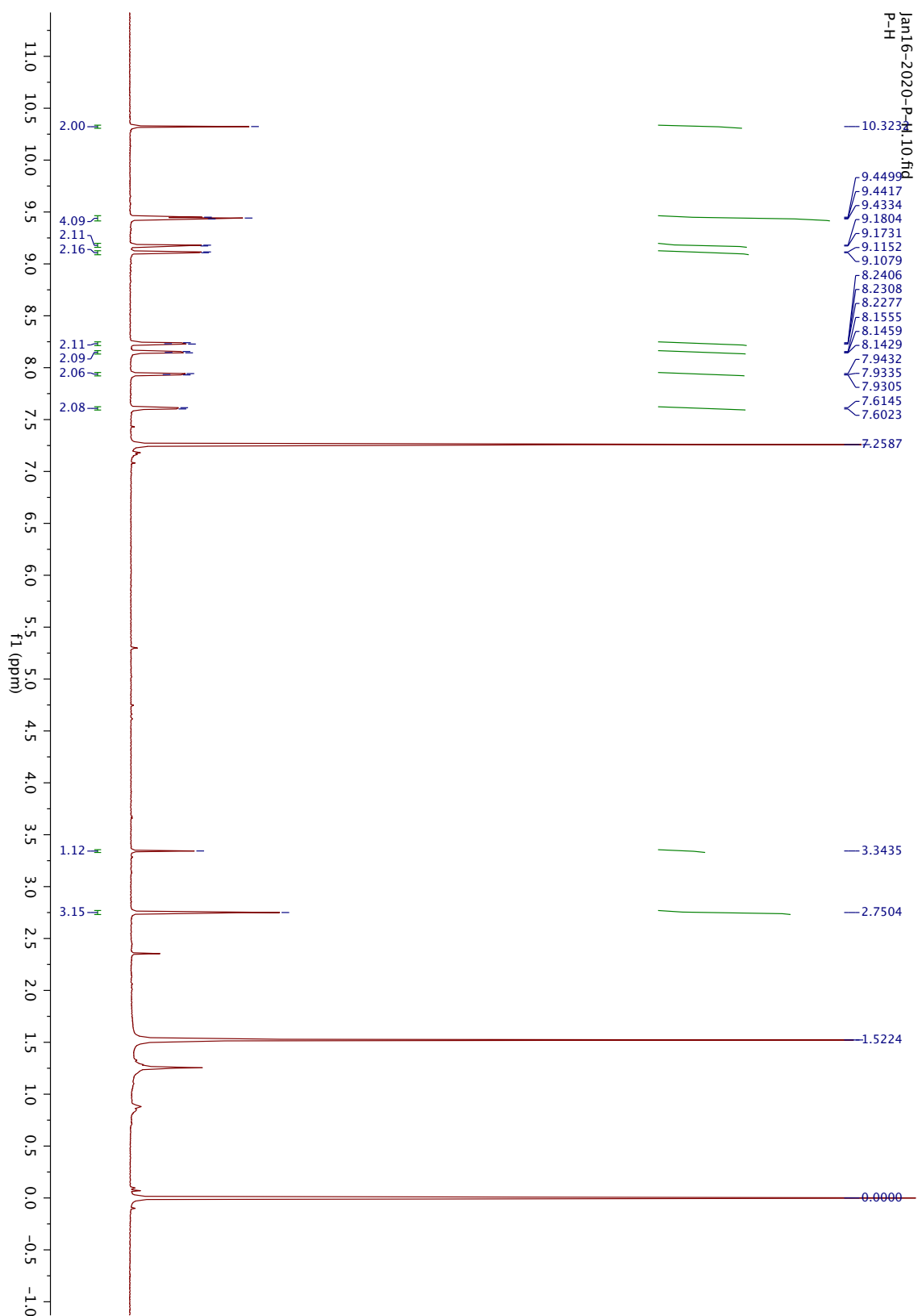
Reflector voltage 1 21 kV
Reflector voltage 2 9.6 kV
Reflector detector volt. 1.662 kV

Instrument
Instrument type autoflex
Instrument serial 1857351.00828
Name of computer FLEX-PC
Operator ID or name admin
FlexControl version flexControl 3.4.168.0
flexAnalysis version 3.4.79.0

Date of Acquisition 2021-06-02T15:07:25.722-04:00 printed: 9/23/2022 3:02:55 PM
Acquisition method D:\Methods\flexControl\Methods\Lindsey_Zhiyuan\RP_0-1500_Da.par
Processing method
File Name D:\Data\Lindsey\Jay\20210602_Jay_PMI-P-El-Me_CHCHA0_N811

| | |
|--------------|-------------|
| Performed by | Viewed by |
| Date / Sign | Date / Sign |

30: ^1H NMR, CDCl_3 , 600 MHz





Target

Target type 0280784
Target serial number 1004015
Position M20

Laser

Laser beam attenuation 60
Laser beam focus 36
Laser repetition rate 2000 Hz
Number of shots 500

Spectrometer

positive voltage polarity POS
PIE delay 130 ns
ion source voltage 1 19 kV
ion source voltage 2 16.85 kV
Lens voltage 8.3 kV
Linear detector voltage 2.783 kV
Detection on

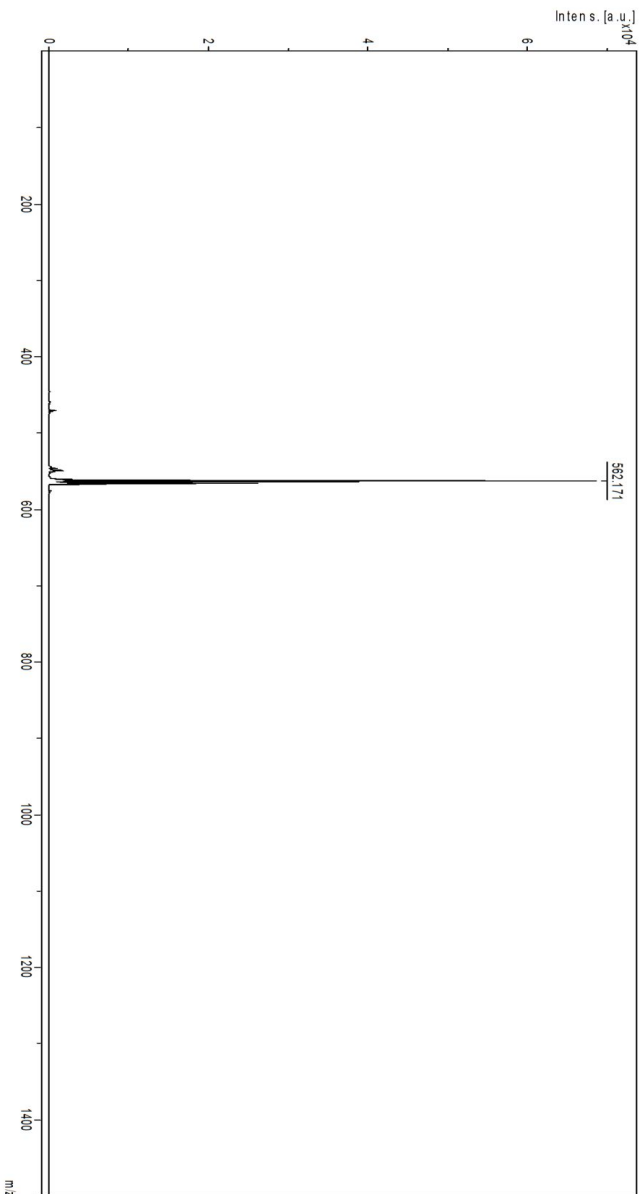
MSMS parent mass

LIFT voltage 1
LIFT voltage 2
LIFT 1 Pulser time depending on the parent mass
LIFT 2 Pulser time

Reflector voltage 1 21 kV
Reflector voltage 2 9.6 kV
Reflector detector volt. 1.662 kV

Instrument

Instrument type autoflex
Instrument serial 1857351.00828
Name of computer FLEX-PC
Operator ID or name admin
flexControl version flexControl 3.4.168.0
flexAnalysis version 3.4.79.0



Date of Acquisition 2020-01-27T15:09:18.224-05:00 printed: 1/27/2020 3:48:34 PM
Acquisition method D:\Methods\flexControl\Methods\Lindsey_Zhiyuan\RP_0-1500_Da.par
Processing method
File Name D:\Data\Lindsey\Jay\20200127P-H10_M201

Performed by
Date / Sign

Viewed by
Date / Sign

Bruker Daltonics



Target

Target type 0280784
Target serial number 1004015
Position M20

Laser

Laser beam attenuation 60
Laser beam focus 36
Laser repetition rate 2000 Hz
Number of shots 500

Spectrometer

positive voltage polarity POS
PIE delay 130 ns
Ion source voltage 1 19 kV
Ion source voltage 2 16.85 kV
Lens voltage 8.3 kV
Linear detector voltage 2.783 kV
Deflection on

Deflection mass

MSMS parent mass

LIFT voltage 1

LIFT voltage 2

LIFT 1 Pulser time
depending on the parent
mass

LIFT 2 Pulser time

Reflector voltage 1 21 kV
Reflector voltage 2 9.6 kV
Reflector detector volt. 1.662 kV

Instrument

Instrument type autoflex
Instrument serial 1857351.00828
Name of computer FLEX-PC
Operator ID or name admin
flexControl version flexControl 3.4.168.0
flexAnalysis version 3.4.79.0

Date of Acquisition 2020-01-27T15:09:18.224-05:00
Acquisition method D:\Methods\flexControl\Methods\Lindsey_Zhiyuan\RP_0-1500_Da.par
Processing method
File Name D:\Data\Lindsey\Jay\20200127P-H10_M201

printed: 1/27/2020 3:48:27 PM

| | |
|--------------|-------------|
| Performed by | Viewed by |
| Date / Sign | Date / Sign |

Bruker Daltonics

30: Absorption spectrum (toluene)

=====

Spectrum/Peak Report

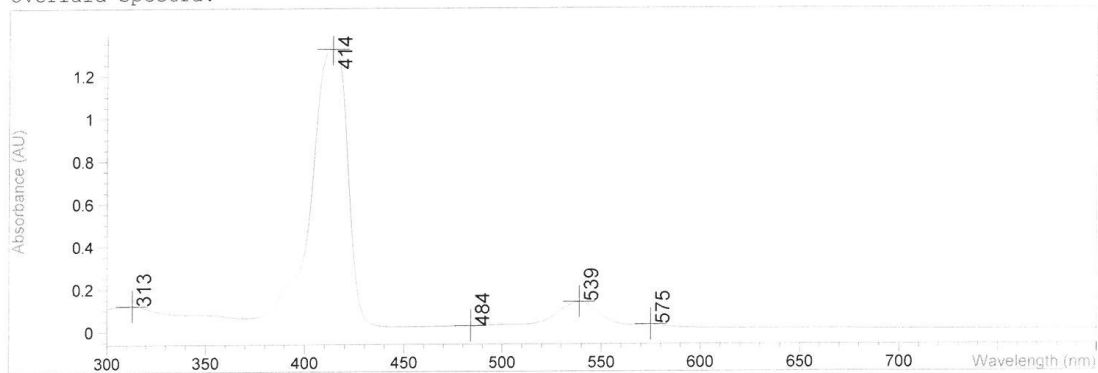
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Date 9/23/2022 Time 12:01:24 Page 1 of 1

Method file : <method not saved>
Information : Default Method
Data File : C:\Chem32\1\DATA\JayRong\Solar_Cell\ABS for paper\P-H_1.SD
Created : 1/17/20 15:36:25

Compound 30

Overlaid Spectra:



| # | Name | Peaks (nm) | Abs (AU) |
|---|------|------------|-----------|
| 1 | | 414.0 | 1.32440 |
| 1 | | 539.0 | 0.13791 |
| 1 | | 313.0 | 0.12170 |
| 1 | | 575.0 | 3.1120E-2 |
| 1 | | 484.0 | 2.5795E-2 |

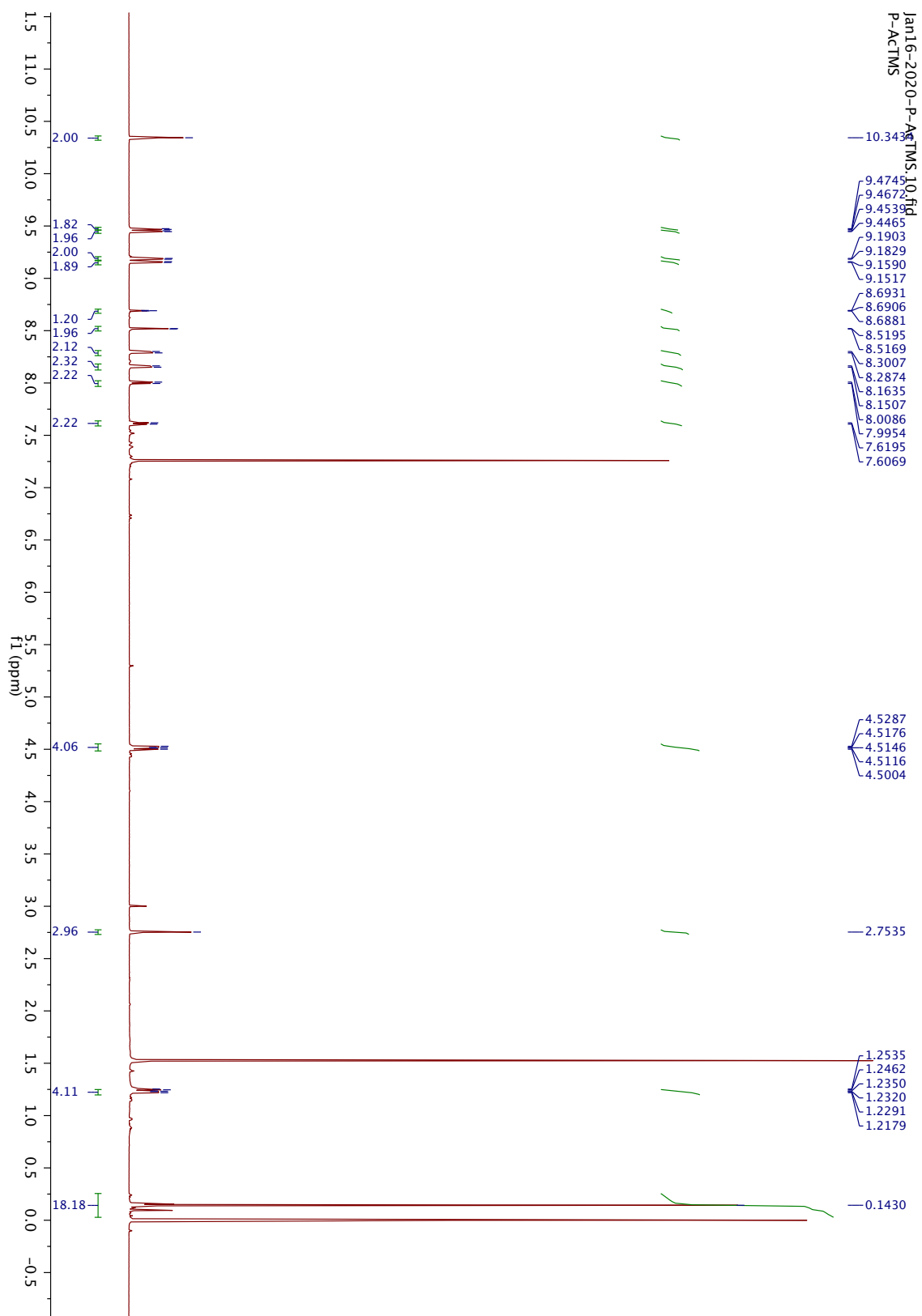
Report generated by : jon

Signature:

*** End Spectrum/Peak Report ***

=====

31: ^1H NMR, CDCl_3 , 600 MHz





Target
Target type 0280784
Target serial number 1004015
Position M23

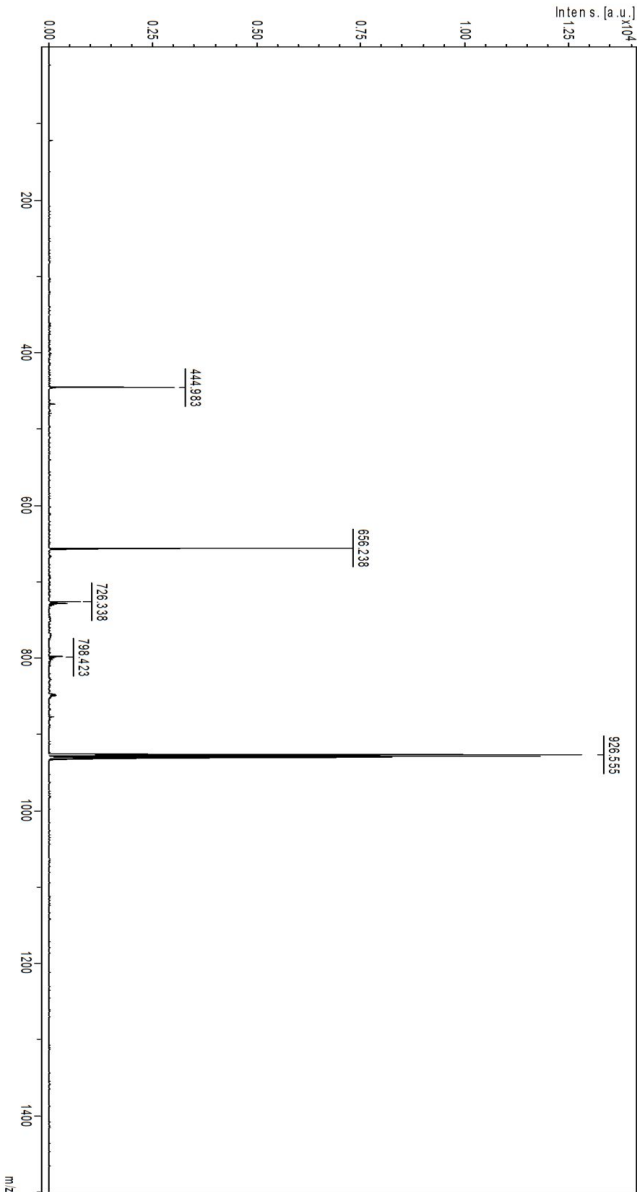
Laser
Laser beam attenuation 60
Laser beam focus 36
Laser repetition rate 2000 Hz
Number of shots 500

Spectrometer
positive voltage polarity POS
PIE delay 130 ns
ion source voltage 1 19 kV
ion source voltage 2 16.85 kV
Lens voltage 8.3 kV
Linear detector voltage 2.783 kV
Detection on

MSMS parent mass
LIFT voltage 1
LIFT voltage 2
LIFT 1 Pulser time
depending on the parent
mass
LIFT 2 Pulser time

Reflector voltage 1 21 kV
Reflector voltage 2 9.6 kV
Reflector detector volt. 1.662 kV

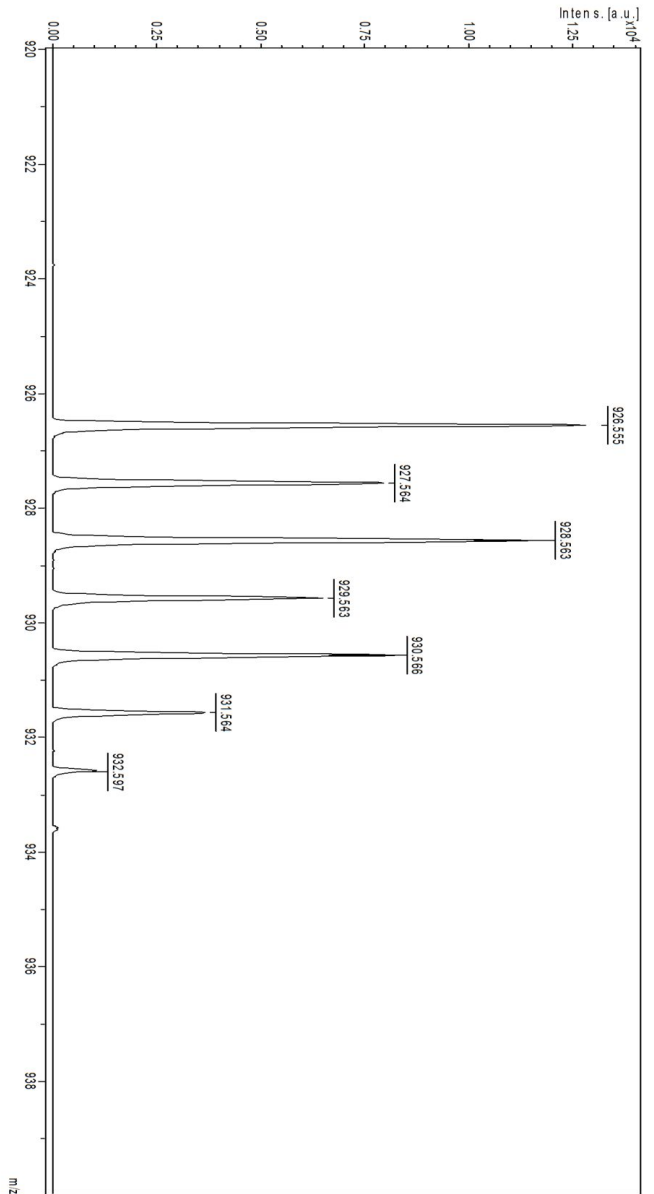
Instrument
Instrument type autoflex
Instrument serial 1857351.00828
Name of computer FLEX-PC
Operator ID or name admin
flexControl version flexControl 3.4.168.0
flexAnalysis version 3.4.79.0



Date of Acquisition 2020-01-27T15:09:50.649-05:00 printed: 1/27/2020 3:49:26 PM
Acquisition method D:\Methods\flexControl\Methods\Lindsey_Zhiyuan\RP_0-1500_Da.par
Processing method
File Name D:\Data\Lindsey\Jday20200127P-ActMS10_M231

| | |
|--------------|-------------|
| Performed by | Viewed by |
| Date / Sign | Date / Sign |

Bruker Daltonics



Target

Target type 0280784
Target serial number 1004015
Position M23

Laser

Laser beam attenuation 60
Laser beam focus 36
Laser repetition rate 2000 Hz
Number of shots 500

Spectrometer

positive voltage polarity POS
PIE delay 130 ns
Ion source voltage 1 19 kV
Ion source voltage 2 16.85 kV
Lens voltage 8.3 kV
Linear detector voltage 2.763 kV
Deflection on

MSMS parent mass
LIFT voltage 1
LIFT voltage 2
LIFT 1 Pulser time
depending on the parent
mass
LIFT 2 Pulser time

Reflector voltage 1 21 kV
Reflector voltage 2 9.6 kV
Reflector detector volt. 1.662 kV

Instrument

Instrument type autoflex
Instrument serial 1857351.00828
Name of computer FLEX-PC
Operator ID or name admin
flexControl version flexControl 3.4.168.0
flexAnalysis version 3.4.79.0

Date of Acquisition 2020-01-27T15:09:50.649-05:00
Acquisition method D:\Methods\flexControl\Methods\Lindsey_Zhiyuan\RP_0-1500_Da.par
Processing method
File Name D:\Data\Lindsey\day20200127P-ActMS\0_M231

printed: 1/27/2020 3:49:19 PM

| Performed by | | Viewed by | |
|--------------|--|-------------|--|
| Date / Sign | | Date / Sign | |

Bruker Daltonics

31: Absorption spectrum (toluene)

=====

Spectrum/Peak Report

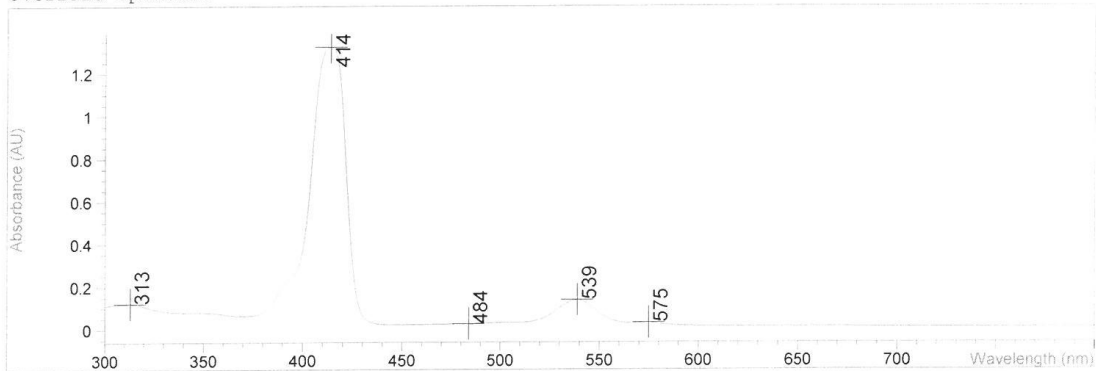
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Date 9/23/2022 Time 12:01:24 Page 1 of 1

Method file : <method not saved>
Information : Default Method
Data File : C:\Chem32\1\DATA\JayRong\Solar_Cell\ABS for paper\P-H_1.SD
Created : 1/17/20 15:36:25

Compound 30

Overlaid Spectra:



| # | Name | Peaks (nm) | Abs (AU) |
|---|------|------------|-----------|
| 1 | | 414.0 | 1.32440 |
| 1 | | 539.0 | 0.13791 |
| 1 | | 313.0 | 0.12170 |
| 1 | | 575.0 | 3.1120E-2 |
| 1 | | 484.0 | 2.5795E-2 |

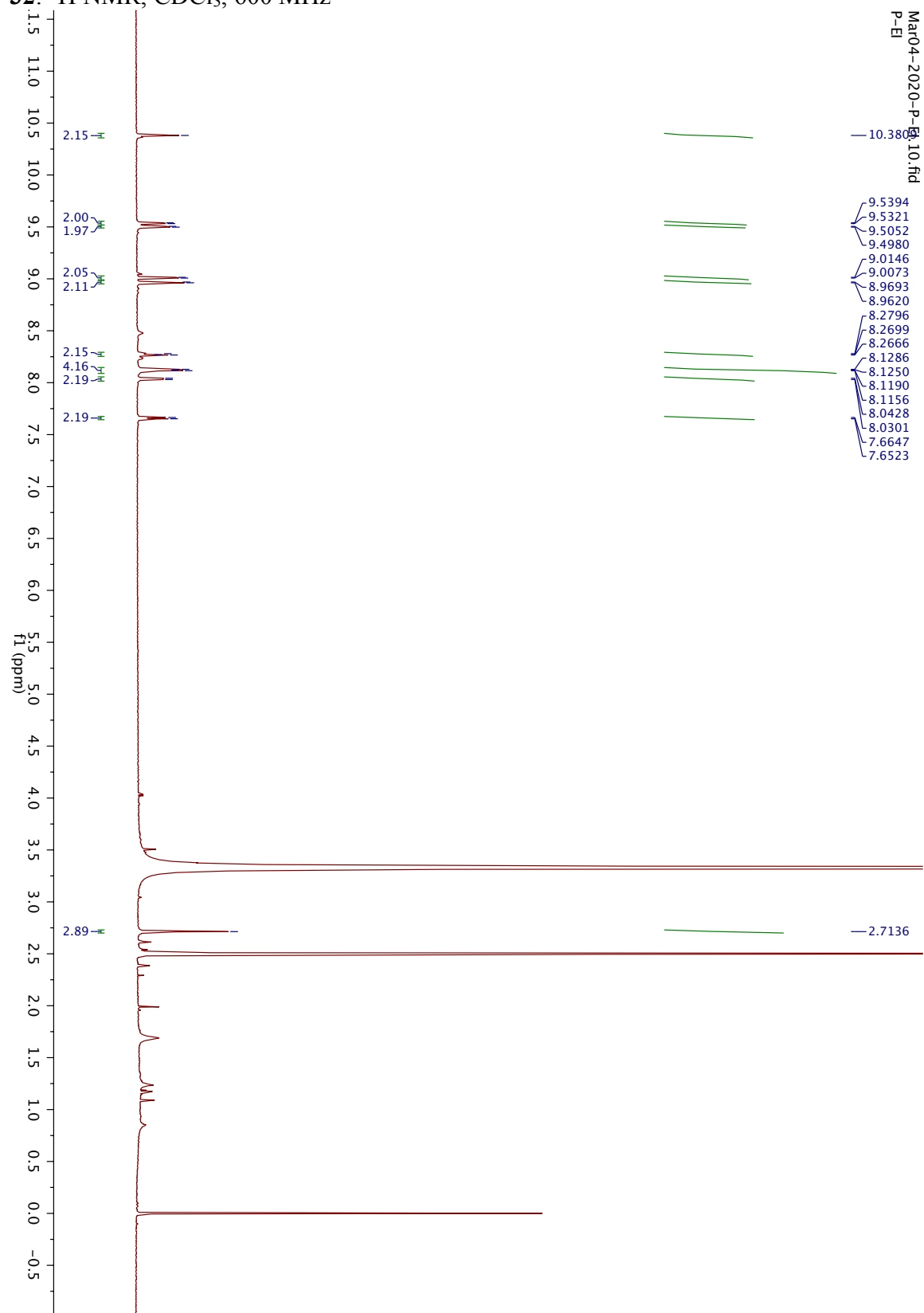
Report generated by : jon

Signature:

*** End Spectrum/Peak Report ***

=====

32: ^1H NMR, CDCl_3 , 600 MHz



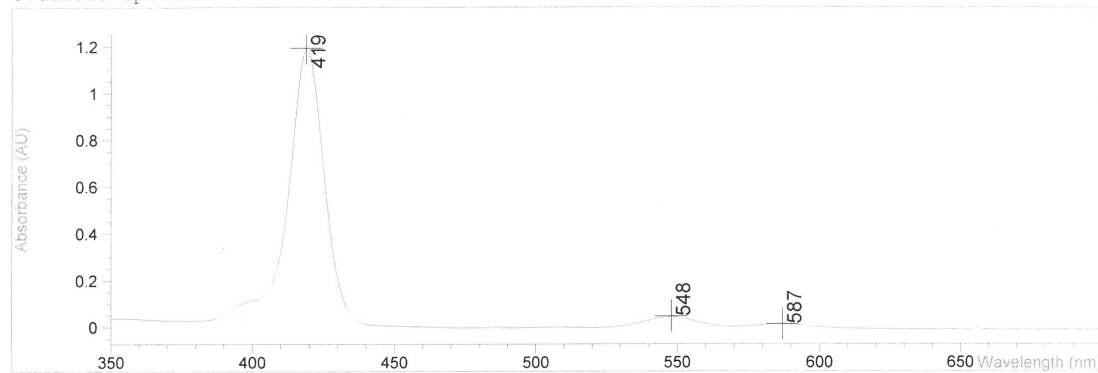
32: Absorption spectrum (DMSO)

Spectrum/Peak Report

Date 9/24/2022 Time 15:27:30 Page 1 of 1

Method file : <method not saved>
Information : Default Method
Data File : C:\Chem32\1\DATA\Masa\J37 PORPHYRIN DMSO.SD Created : 9/23/22
19:47:19

Overlaid Spectra:



| # | Name | Peaks (nm) | Abs (AU) |
|---|------|------------|-----------|
| 1 | * | 419.0 | 1.19270 |
| 1 | | 548.0 | 4.6544E-2 |
| 1 | | 587.0 | 1.3256E-2 |

Report generated by : jon

Signature:

*** End Spectrum/Peak Report ***

32: ESI-MS

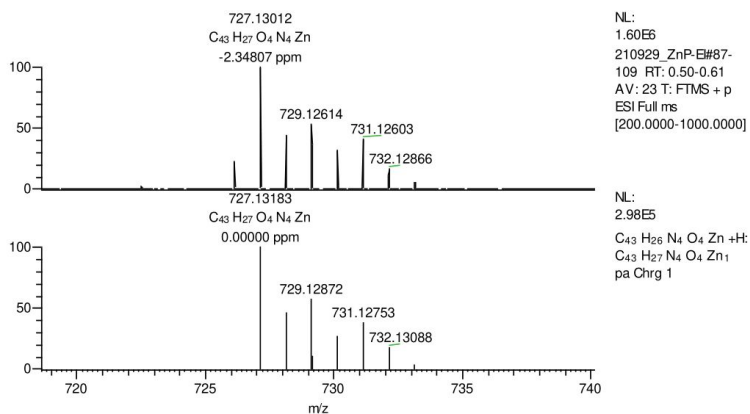
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<https://research.ncsu.edu/metric/>

ZnP-EI Experimental and Theoretical Isotopic Distribution for $C_{43}H_{26}N_4O_4Zn$ [M+H]⁺



ZnP-EI Experimental and Theoretical Isotopic Distribution for $C_{43}H_{26}N_4O_4Zn$ [M-H]⁻

