

Supplementary Materials

Design, Synthesis and Evaluation of Novel 2-Methoxyestradiol Derivatives as Apoptotic Inducers Through Intrinsic Apoptosis Pathway

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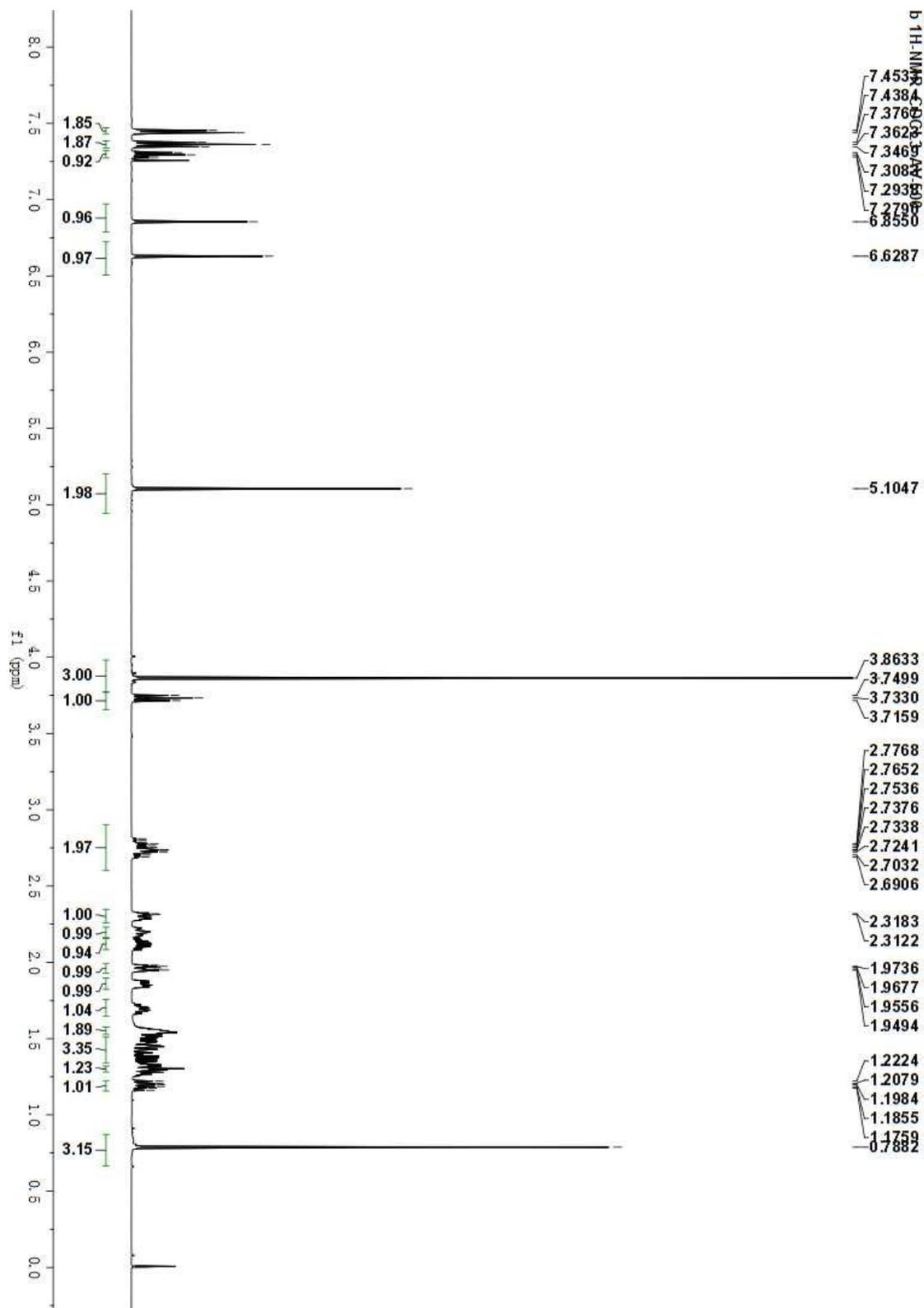
Table of Contents

| | |
|---|----|
| ¹ H NMR spectrum of 5 | 4 |
| HRMS spectrum of 5 | 5 |
| ¹ H NMR spectrum of 6 | 6 |
| HRMS spectrum of 6 | 7 |
| ¹ H NMR spectrum of 7 | 8 |
| ¹³ C NMR spectrum of 7 | 9 |
| HRMS spectrum of 7 | 10 |
| ¹ H NMR spectrum of 8 | 11 |
| ¹³ C NMR spectrum of 8 | 12 |
| HRMS spectrum of 8 | 13 |
| ¹ H NMR spectrum of 9 | 14 |
| ¹³ C NMR spectrum of 9 | 15 |
| HRMS spectrum of 9 | 16 |
| ¹ H NMR spectrum of 10 | 17 |
| ¹³ C NMR spectrum of 10 | 18 |

| | |
|--|----|
| HRMS spectrum of 10 | 19 |
| ¹ H NMR spectrum of 11 | 20 |
| ¹³ C NMR spectrum of 11 | 21 |
| HRMS spectrum of 11 | 22 |
| ¹ H NMR spectrum of 12a | 23 |
| ¹³ C NMR spectrum of 12a | 24 |
| HRMS spectrum of 12a | 25 |
| ¹ H NMR spectrum of 12b | 26 |
| ¹³ C NMR spectrum of 12b | 27 |
| HRMS spectrum of 12b | 28 |
| ¹ H NMR spectrum of 13a | 29 |
| ¹³ C NMR spectrum of 13a | 30 |
| HRMS spectrum of 13a | 31 |
| ¹ H NMR spectrum of 13b | 32 |
| ¹³ C NMR spectrum of 13b | 33 |
| HRMS spectrum of 13b | 34 |
| ¹ H NMR spectrum of 14a | 35 |
| ¹³ C NMR spectrum of 14a | 36 |
| HRMS spectrum of 14a | 37 |
| ¹ H NMR spectrum of 14b | 38 |
| ¹³ C NMR spectrum of 14b | 39 |
| HRMS spectrum of 14b | 40 |
| ¹ H NMR spectrum of 15a | 41 |
| ¹³ C NMR spectrum of 15a | 42 |
| HRMS spectrum of 15a | 43 |
| ¹ H NMR spectrum of 15b | 44 |
| ¹³ C NMR spectrum of 15b | 45 |
| HRMS spectrum of 15b | 46 |
| ¹ H NMR spectrum of 16 | 47 |
| HRMS spectrum of 16 | 48 |

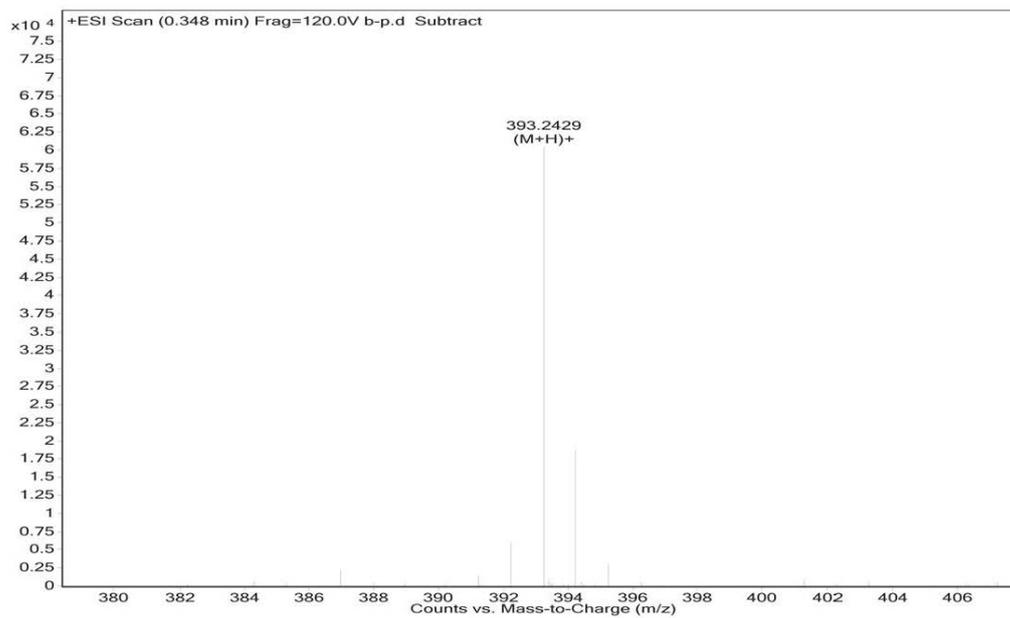
| | |
|--|----|
| ¹ H NMR spectrum of 17 | 49 |
| HRMS spectrum of 17 | 50 |
| ¹ H NMR spectrum of 18 | 51 |
| ¹³ C NMR spectrum of 18 | 52 |
| HRMS spectrum of 18 | 53 |
| ¹ H NMR spectrum of 19 | 54 |
| ¹³ C NMR spectrum of 19 | 55 |
| HRMS spectrum of 19 | 56 |
| ¹ H NMR spectrum of 20a | 57 |
| ¹³ C NMR spectrum of 20a | 58 |
| HRMS spectrum of 20a | 59 |
| ¹ H NMR spectrum of 20b | 60 |
| ¹³ C NMR spectrum of 20b | 61 |
| HRMS spectrum of 20b | 62 |
| ¹ H NMR spectrum of 21a | 63 |
| ¹³ C NMR spectrum of 21a | 64 |
| HRMS spectrum of 21a | 65 |
| ¹ H NMR spectrum of 21b | 66 |
| ¹³ C NMR spectrum of 21b | 67 |
| HRMS spectrum of 21b | 68 |
| ¹ H NMR spectrum of 22a | 69 |
| ¹³ C NMR spectrum of 22a | 70 |
| HRMS spectrum of 22a | 71 |
| ¹ H NMR spectrum of 22b | 72 |
| ¹³ C NMR spectrum of 22b | 73 |
| HRMS spectrum of 22b | 74 |
| ¹ H NMR spectrum of 23a | 75 |
| ¹³ C NMR spectrum of 23a | 76 |
| HRMS spectrum of 23a | 77 |
| ¹ H NMR spectrum of 23b | 78 |

¹H NMR spectrum of **5**

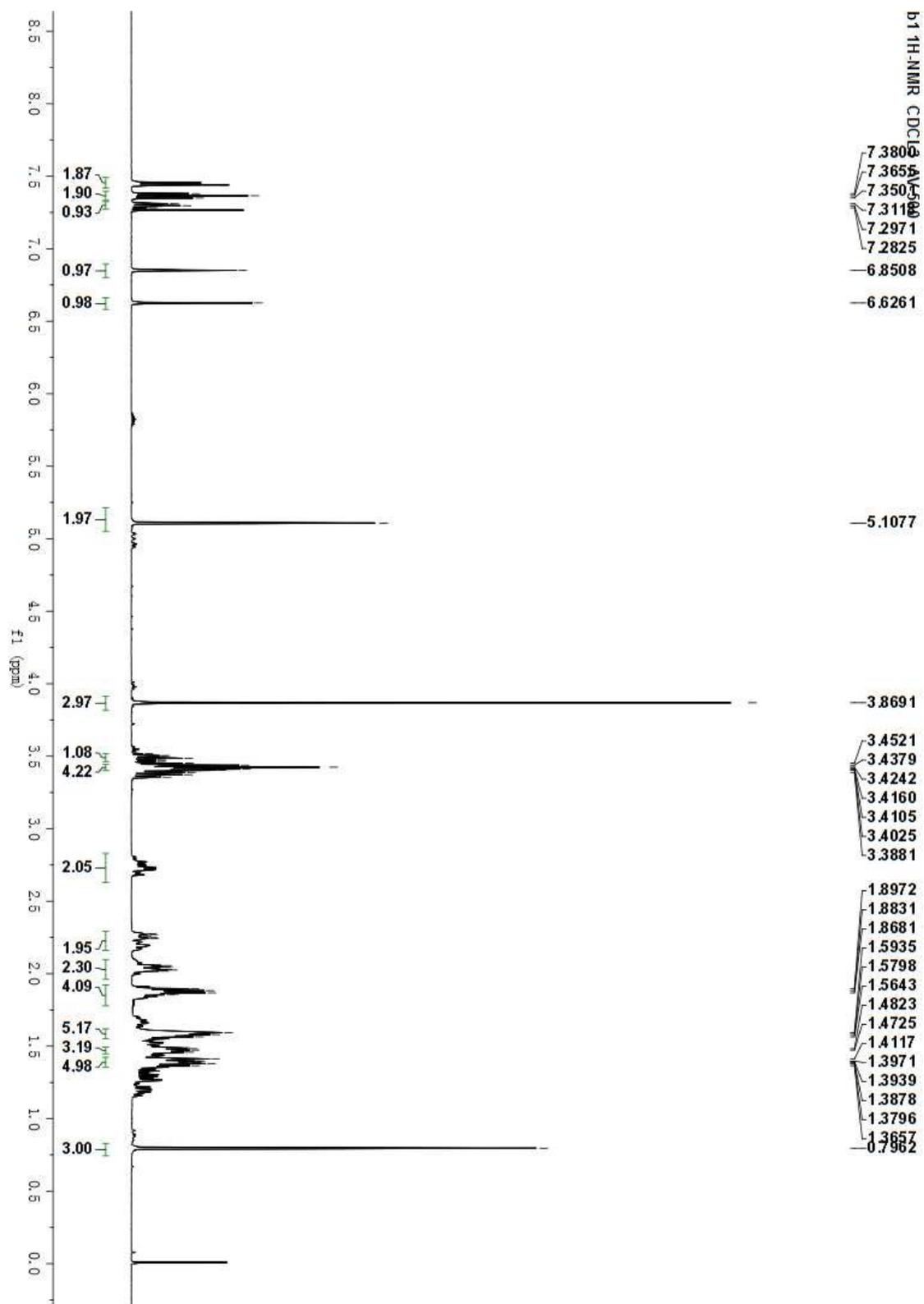


HRMS spectrum of 5

| | | | | | | | |
|----------------------|-------|--------------------|-------|------------------------|--------------|-------------------------------|---------|
| Sample Name | | Position | P2-A6 | Instrument Name | Instrument 1 | User Name | |
| Inj Vol | 0.1 | InjPosition | | SampleType | Sample | IRM Calibration Status | Success |
| Data Filename | b-p.d | ACQ Method | | Comment | | Acquired Time | |

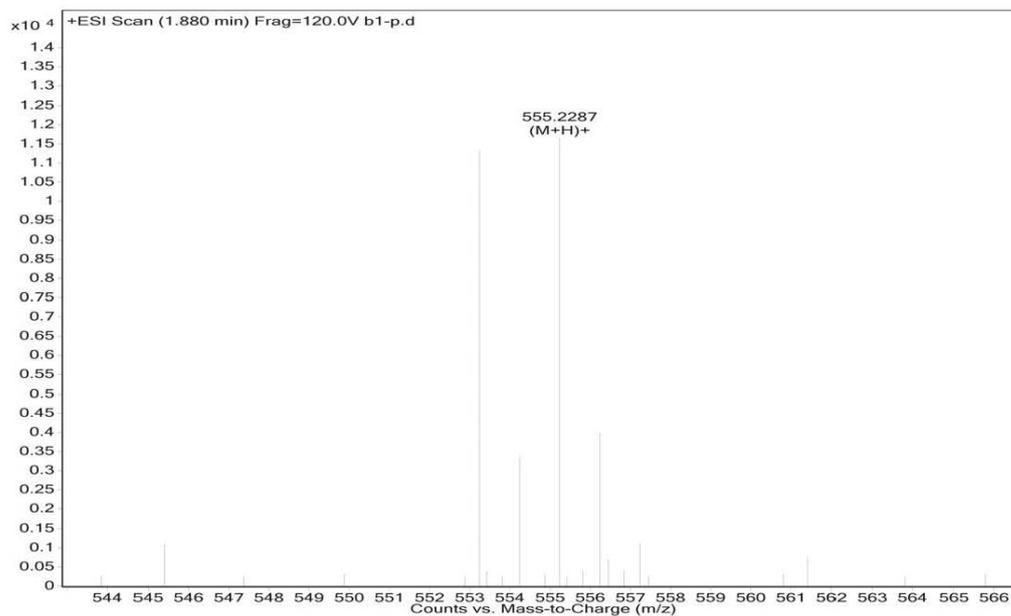


¹H NMR spectrum of 6

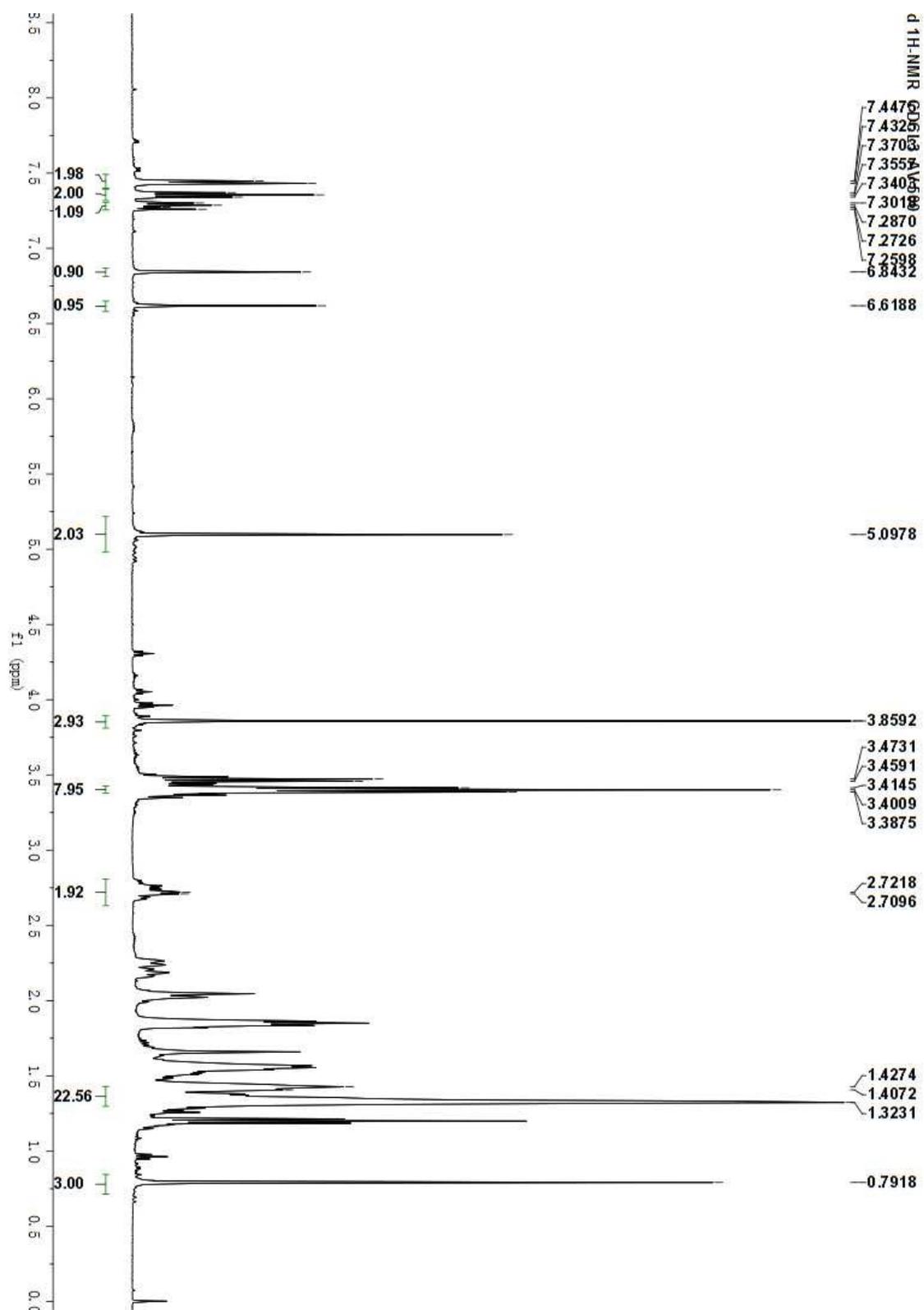


HRMS spectrum of 6

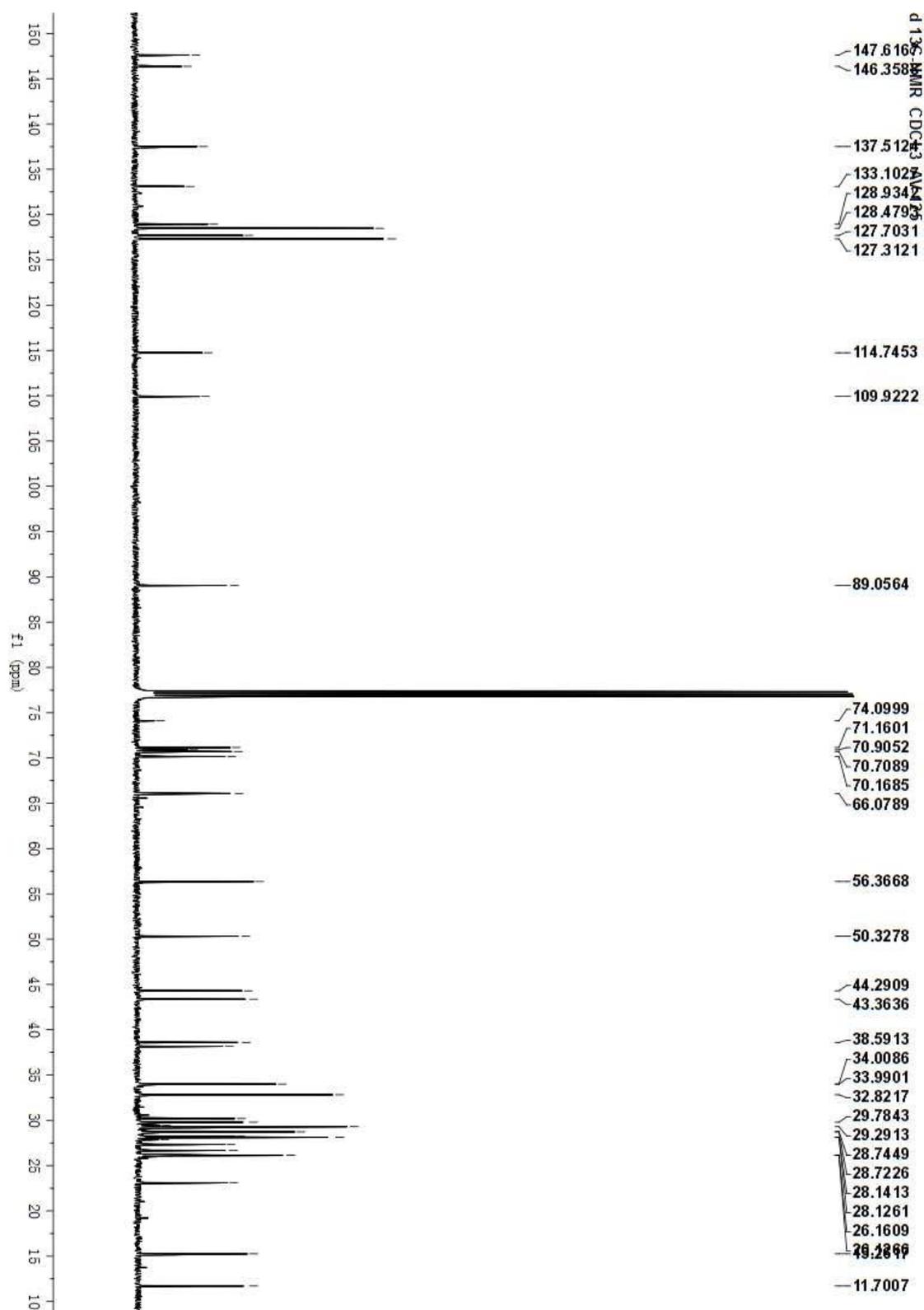
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|----------------------|--------|--------------------|-------|------------------------|--------------|-------------------------------|---------|
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| Inj Vol | 0.1 | InjPosition | | SampleType | Sample | IRM Calibration Status | Success |
| Data Filename | b1-p.d | ACQ Method | | Comment | | Acquired Time | |



¹H NMR spectrum of 7



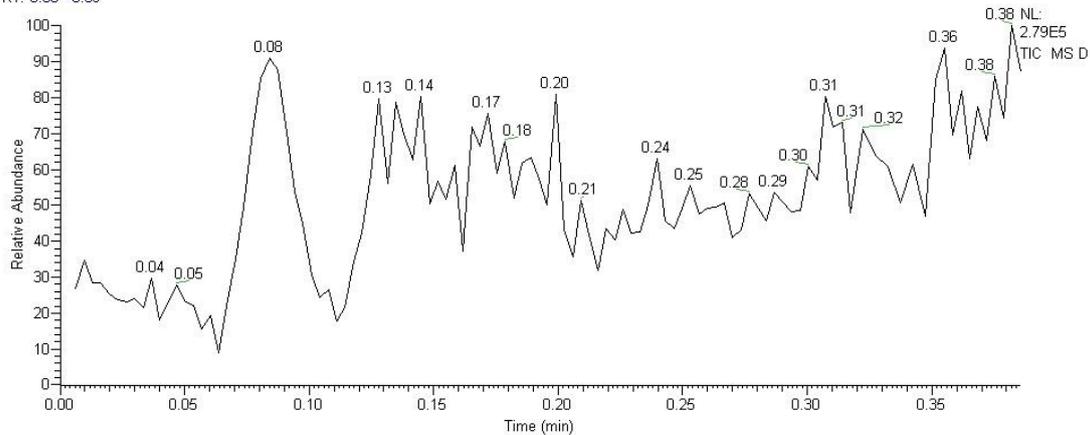
^{13}C NMR spectrum of 7



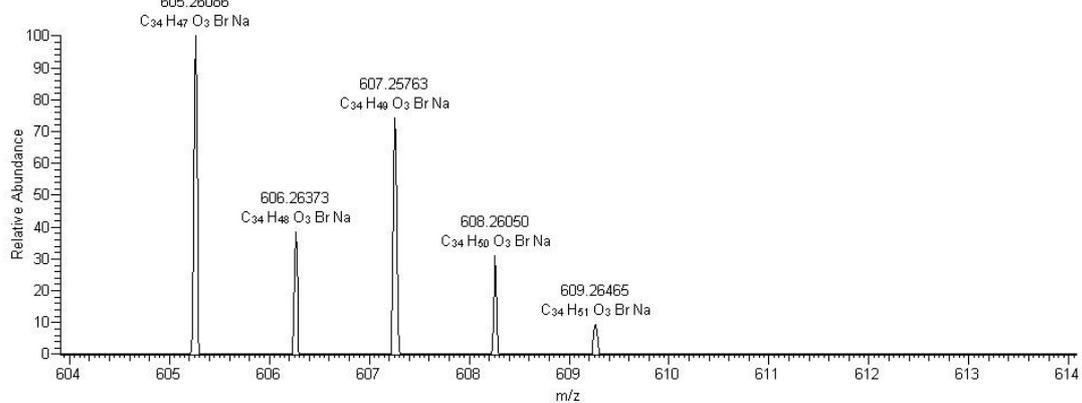
HRMS spectrum of 7

D:\data\

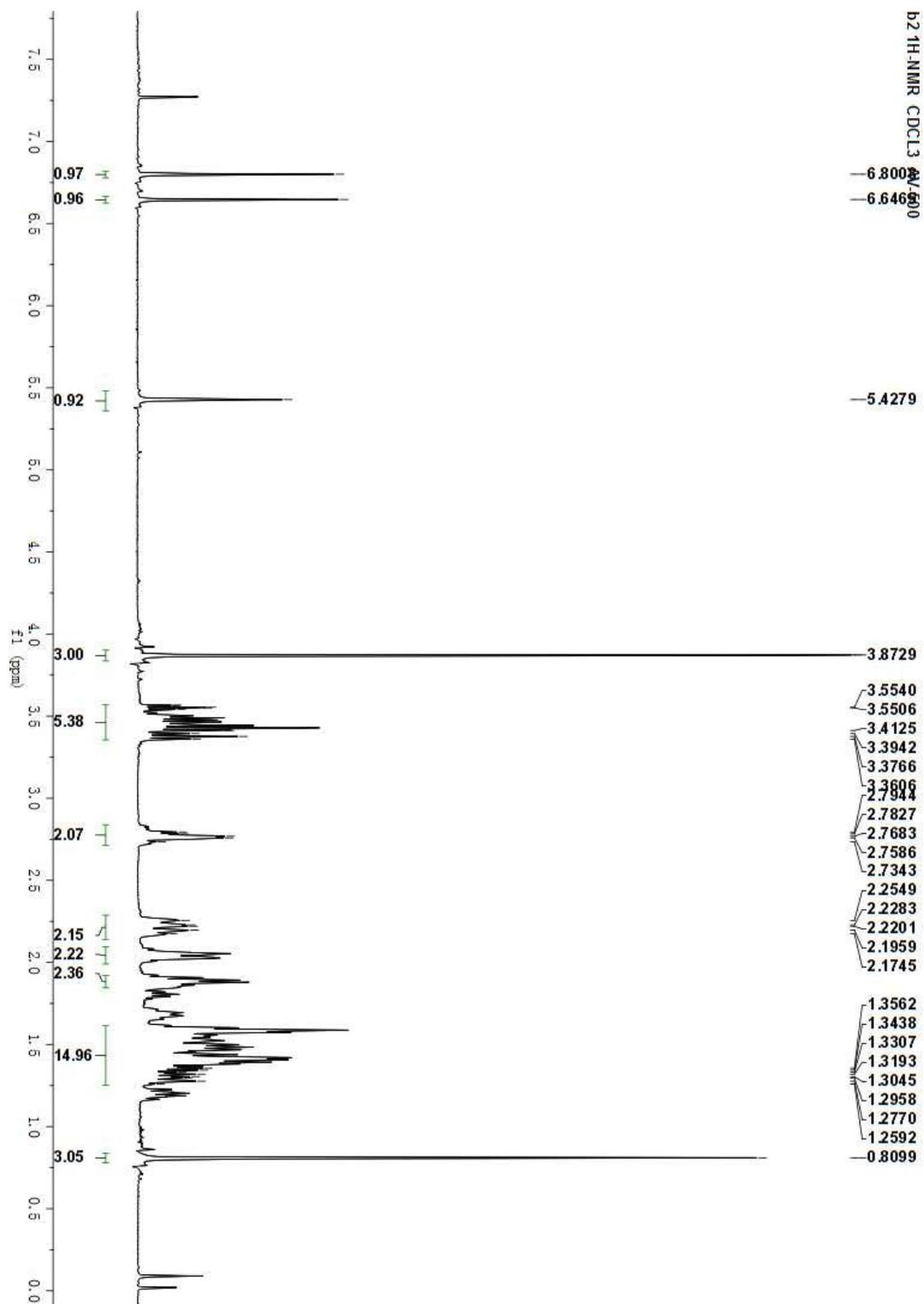
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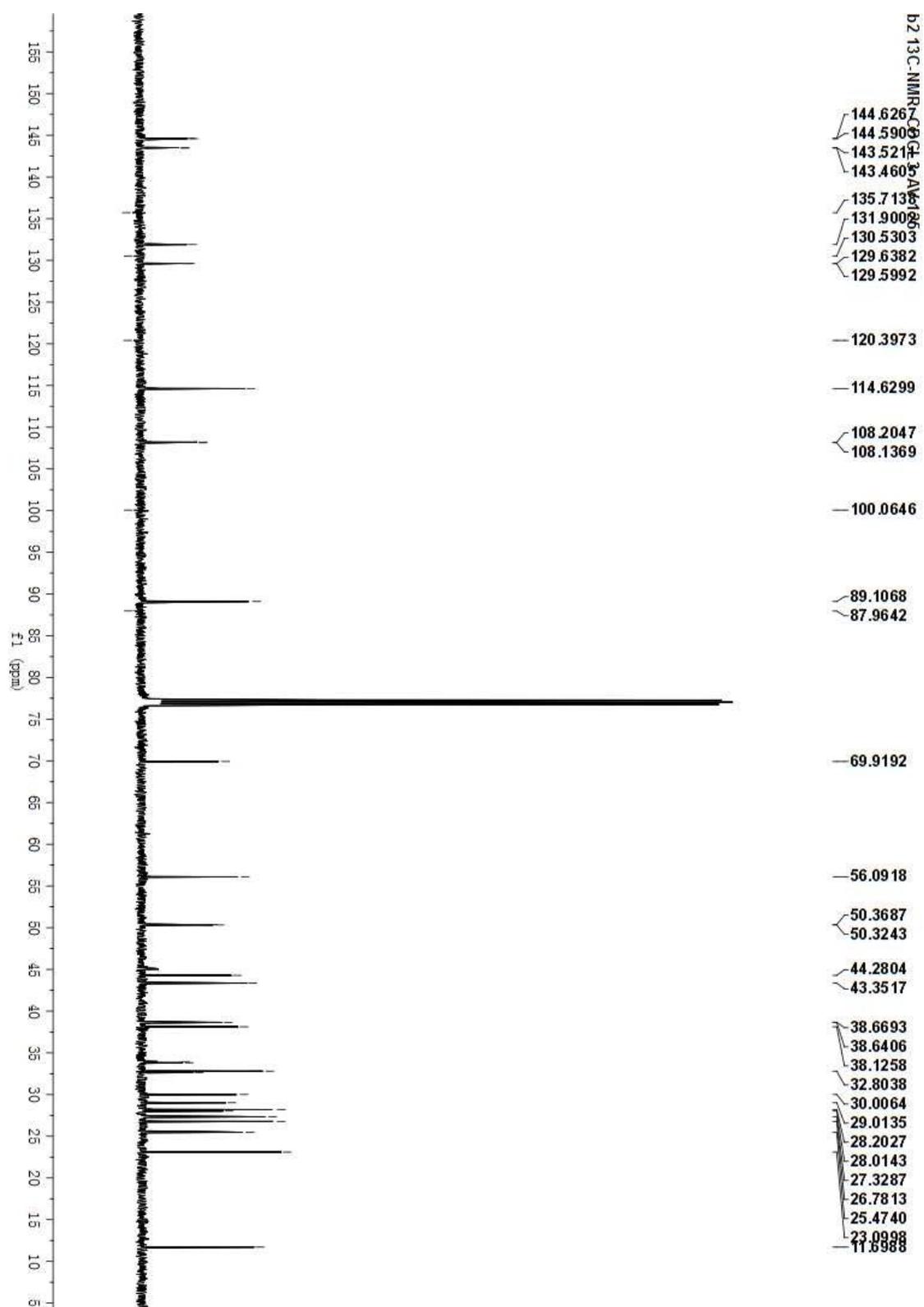
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T: FTMS + p ESI Full ms [500.00-650.00]
605.26086



¹H NMR spectrum of **8**

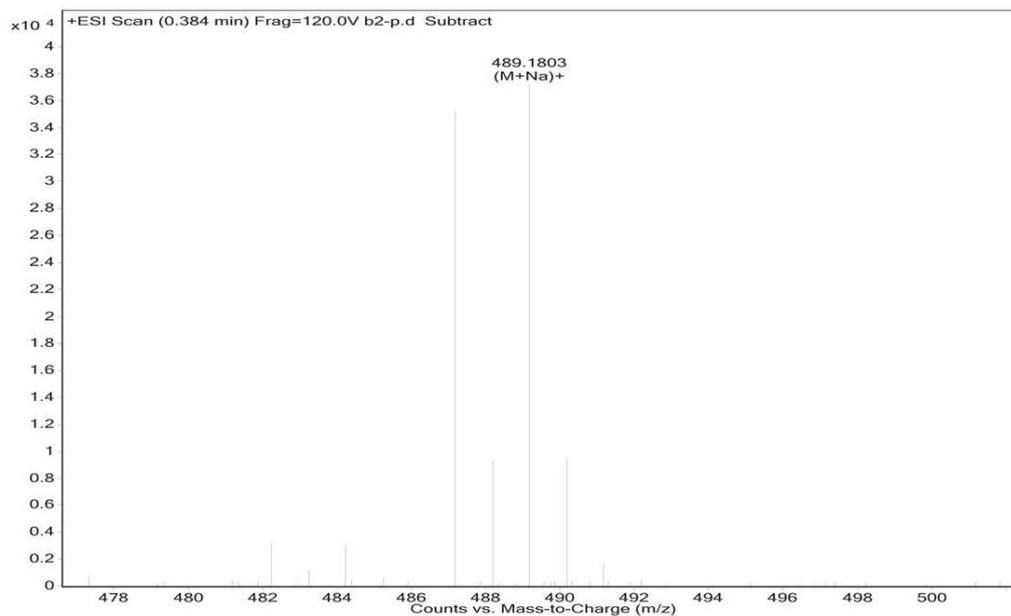


^{13}C NMR spectrum of **8**

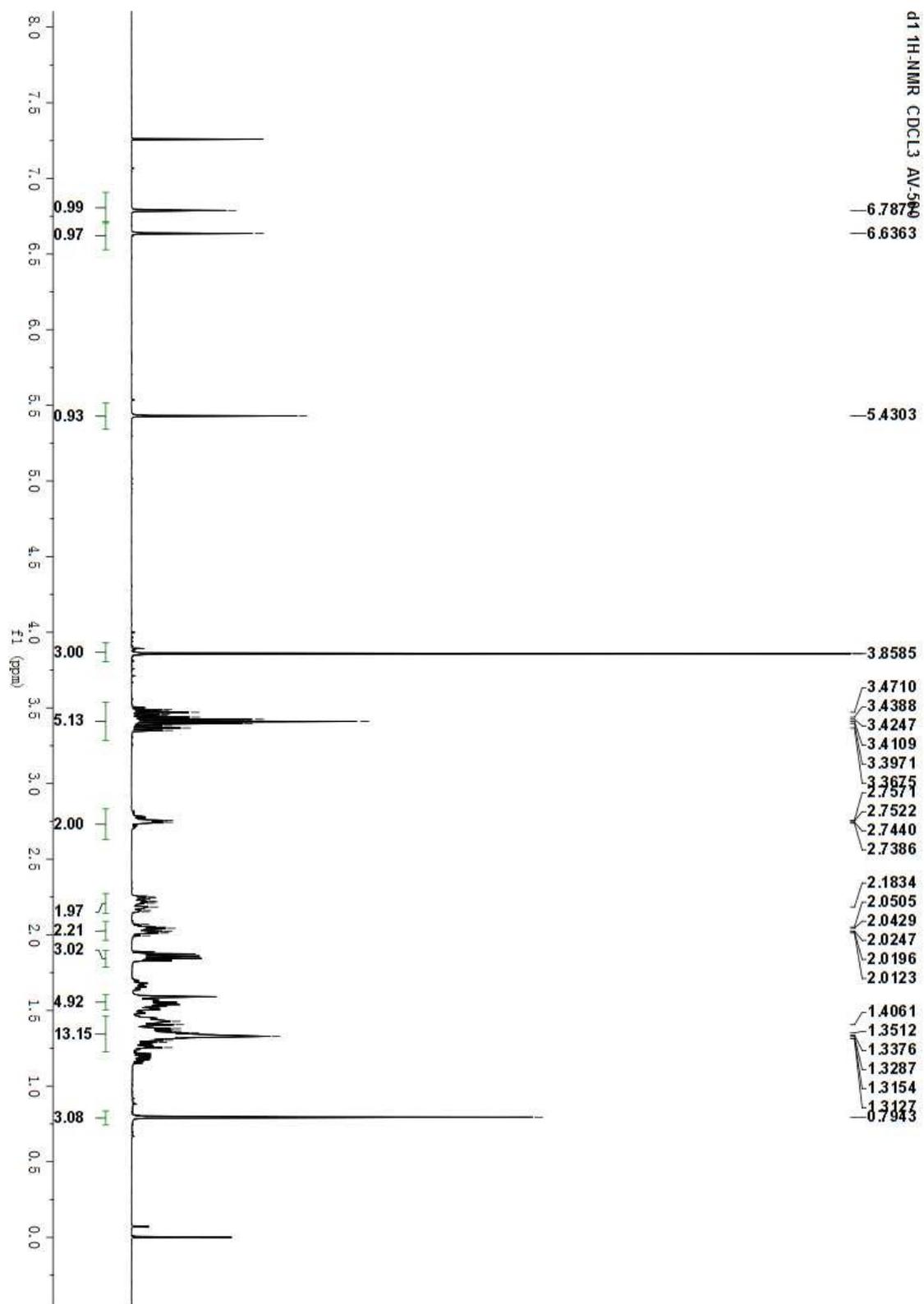


HRMS spectrum of 8

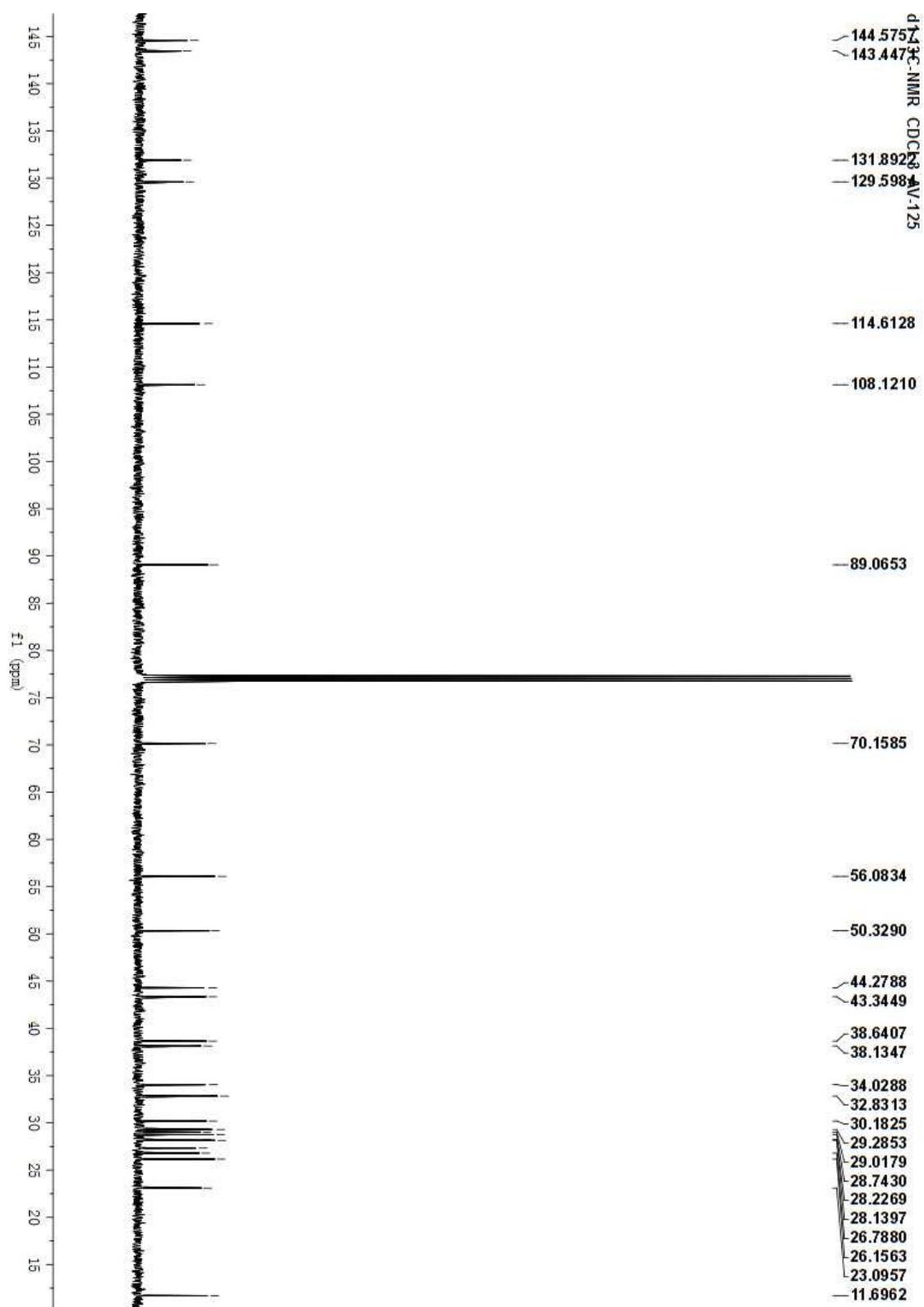
| | | | | | | | |
|----------------------|--------|--------------------|-------|------------------------|--------------|-------------------------------|---------|
| Sample Name | | Position | P2-A8 | Instrument Name | Instrument 1 | User Name | |
| Inj Vol | 0.1 | InjPosition | | SampleType | Sample | IRM Calibration Status | Success |
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¹H NMR spectrum of 9

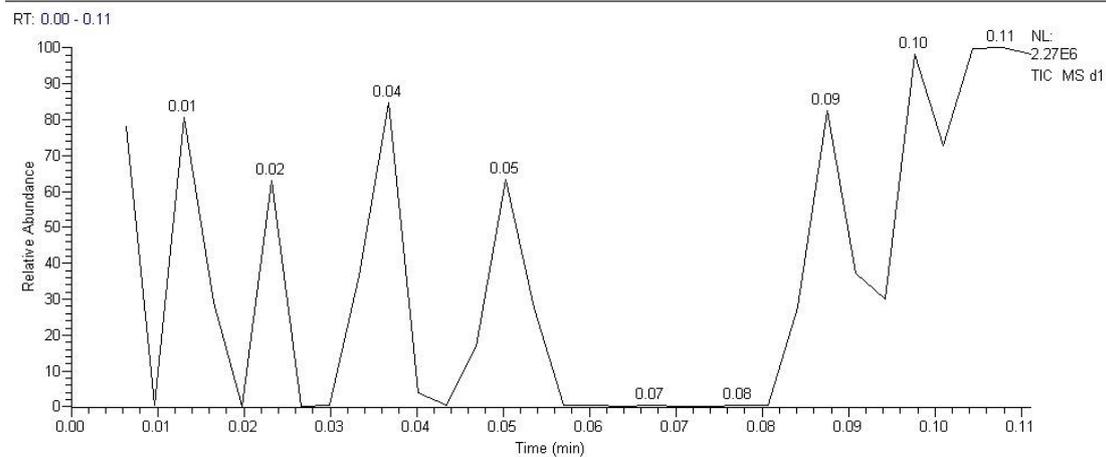


^{13}C NMR spectrum of **9**

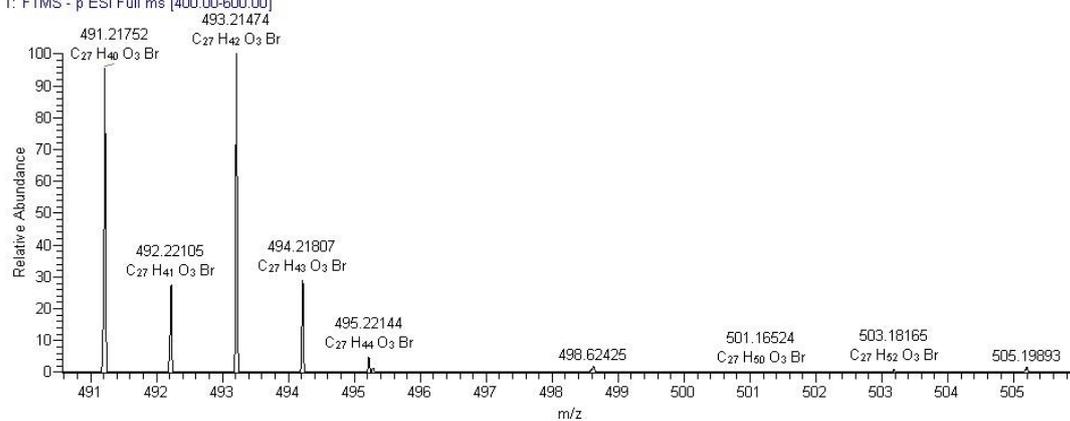


HRMS spectrum of 9

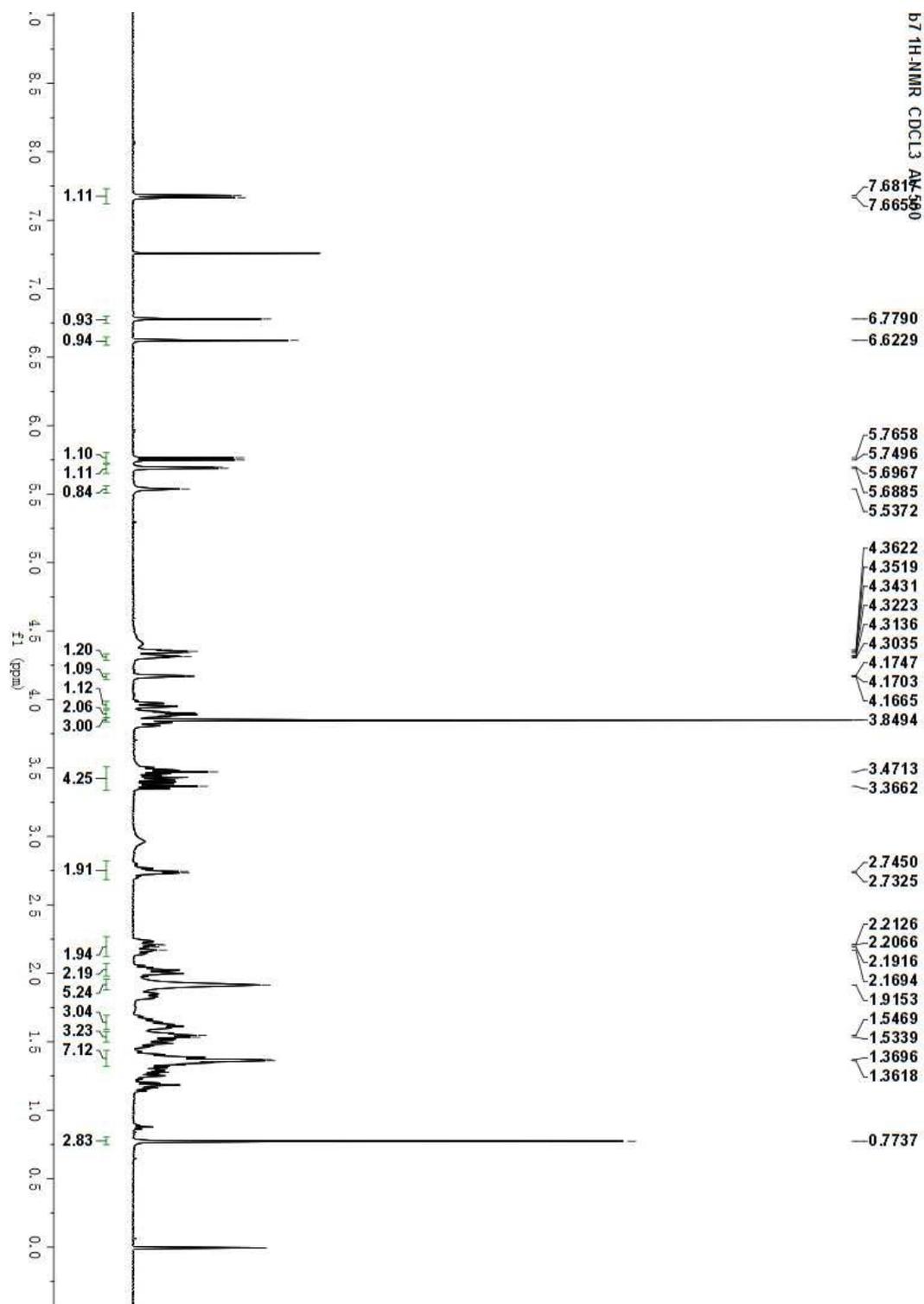
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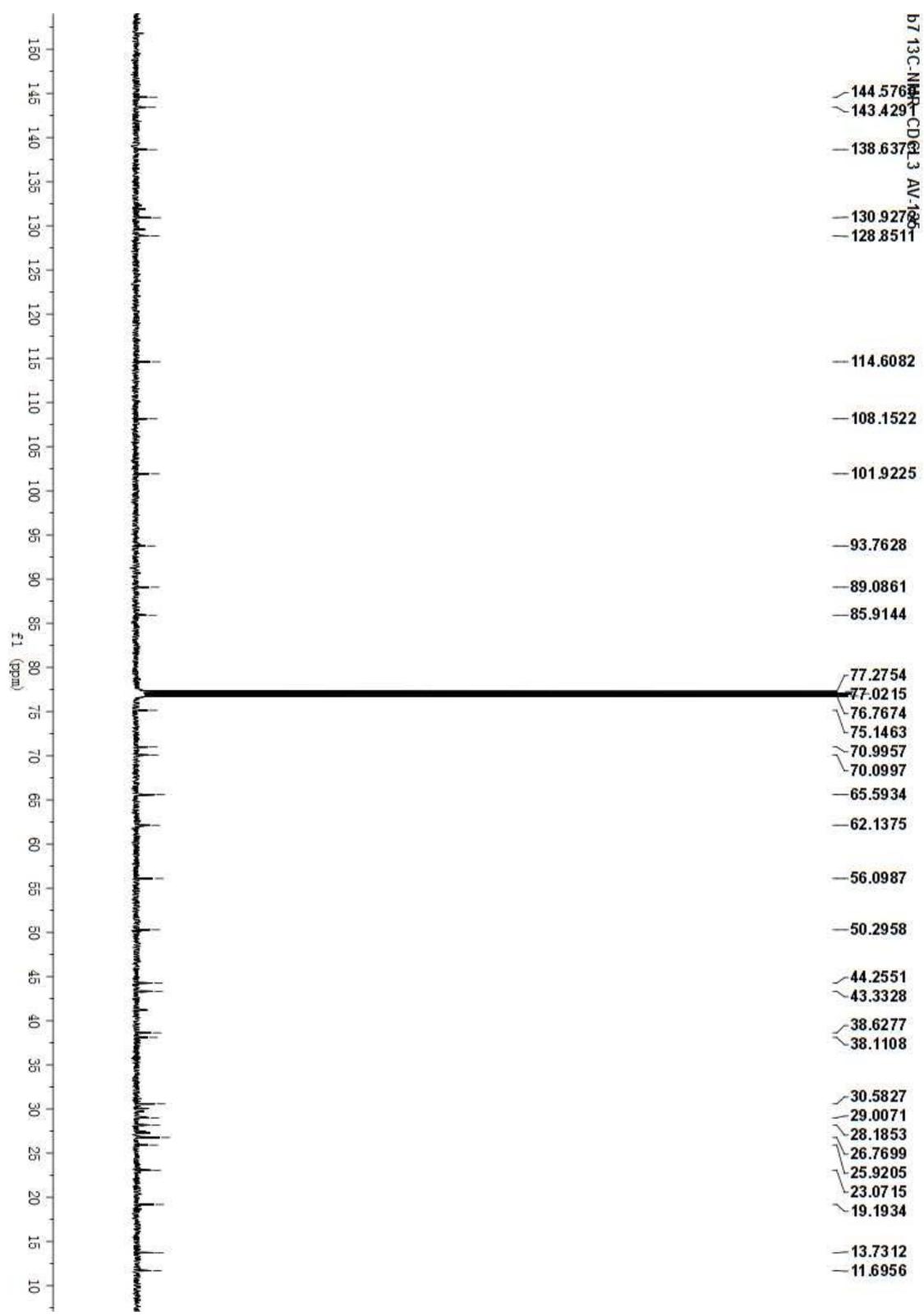
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¹H NMR spectrum of **10**



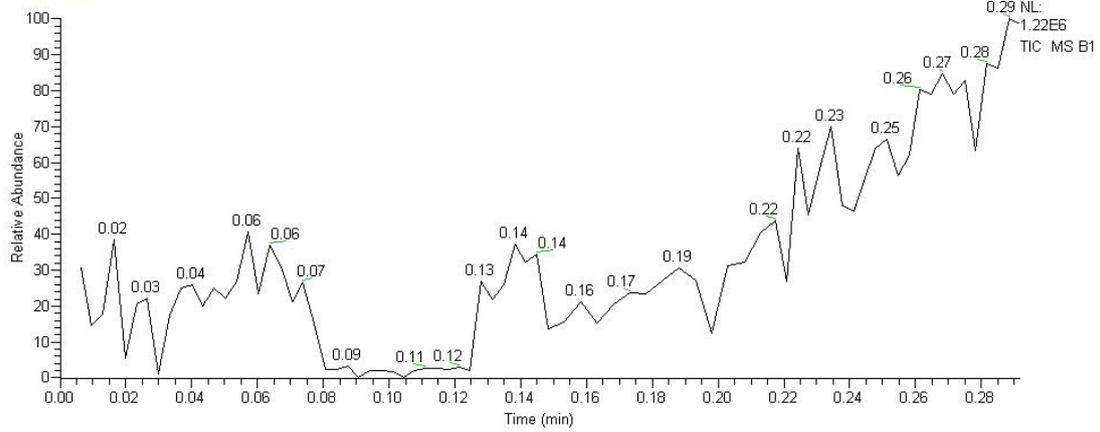
^{13}C NMR spectrum of **10**



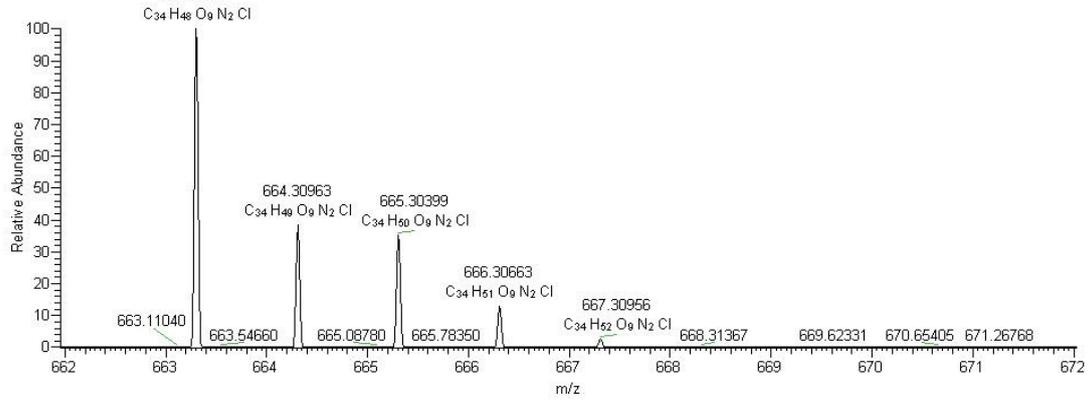
HRMS spectrum of 10

D:\data\

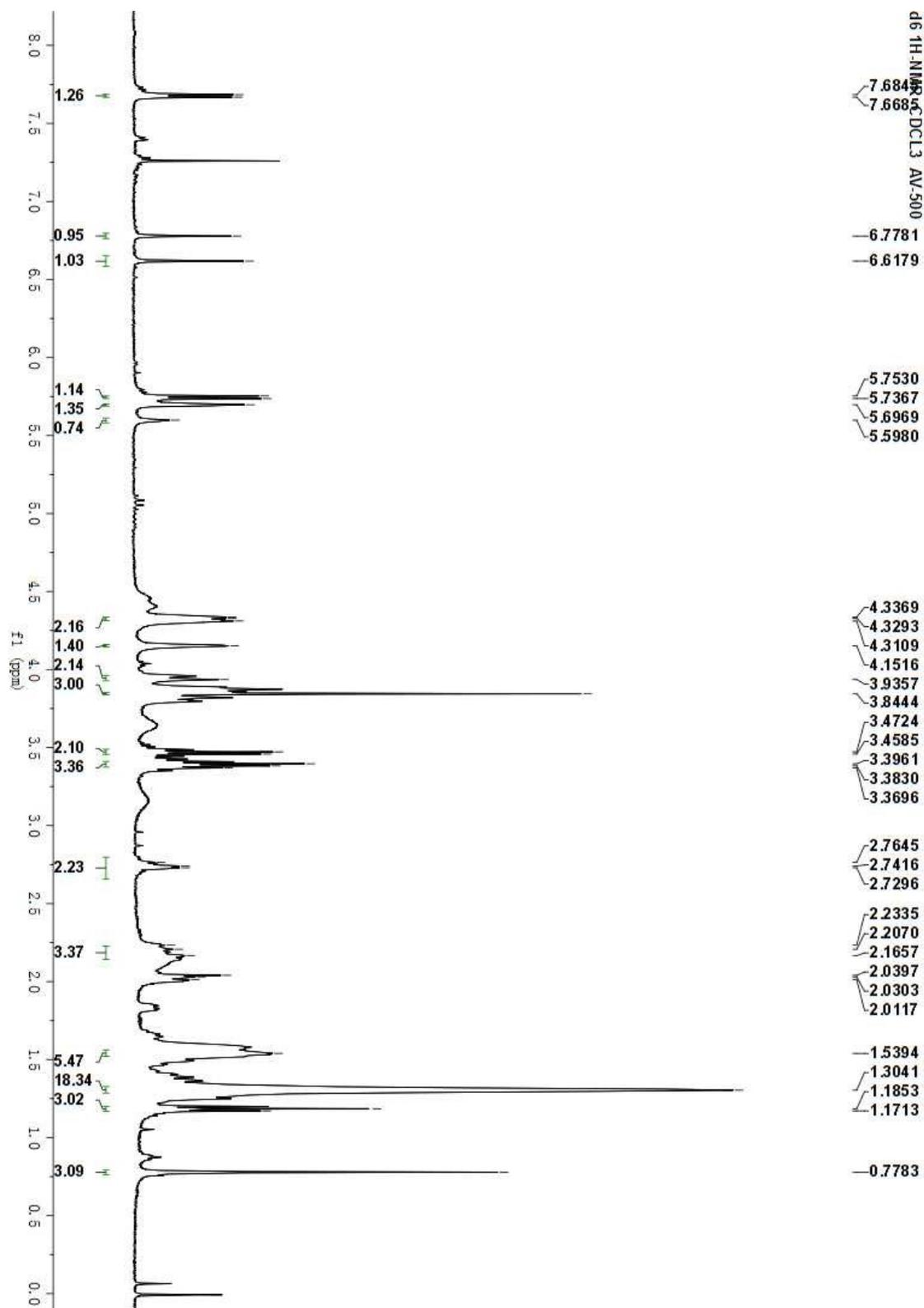
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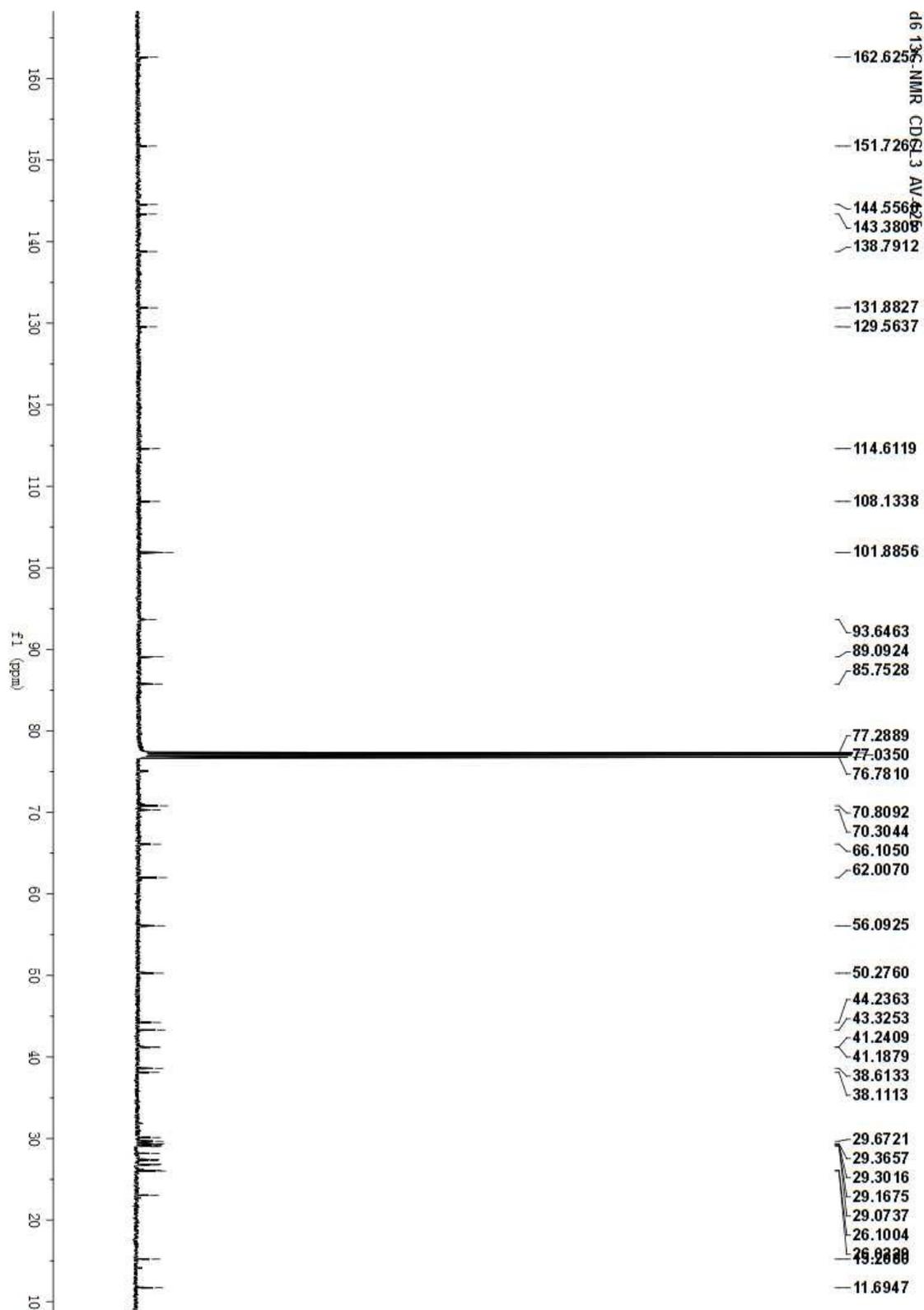
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663.30597



¹H NMR spectrum of **11**

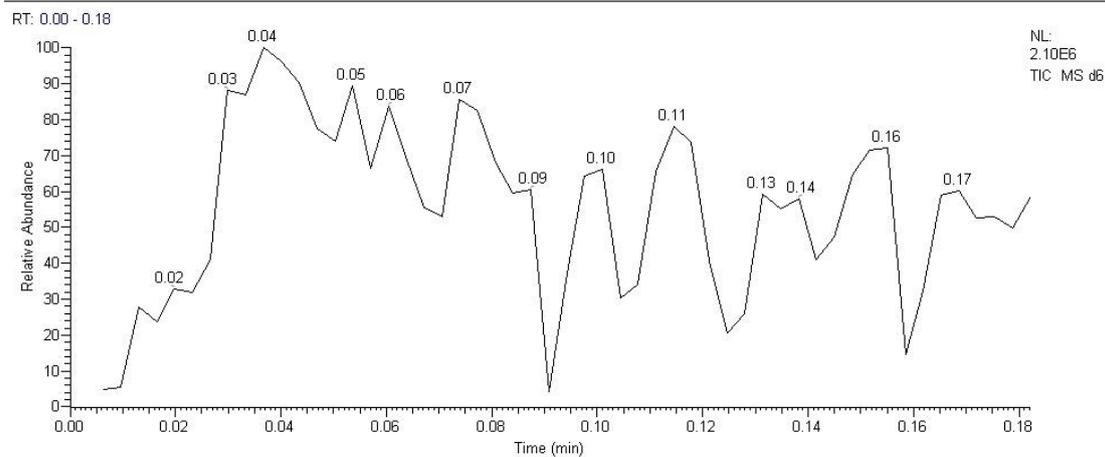


¹³C NMR spectrum of **11**

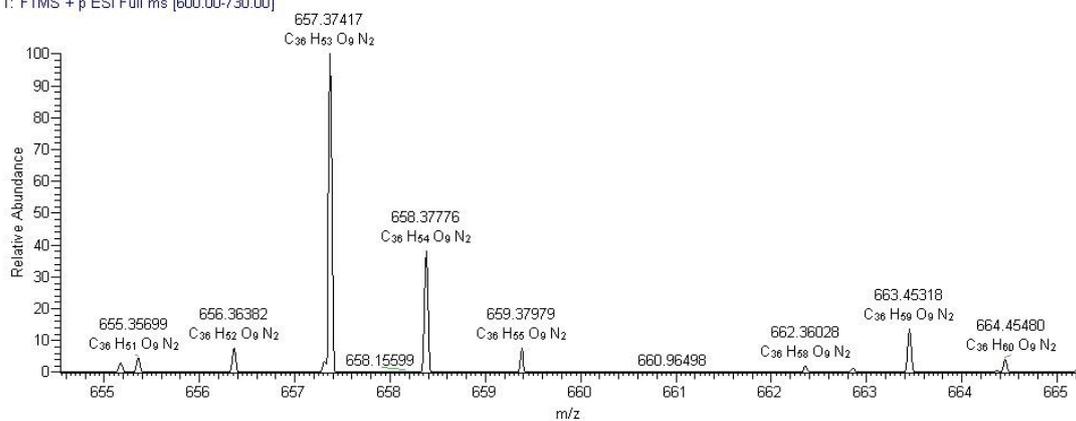


HRMS spectrum of 11

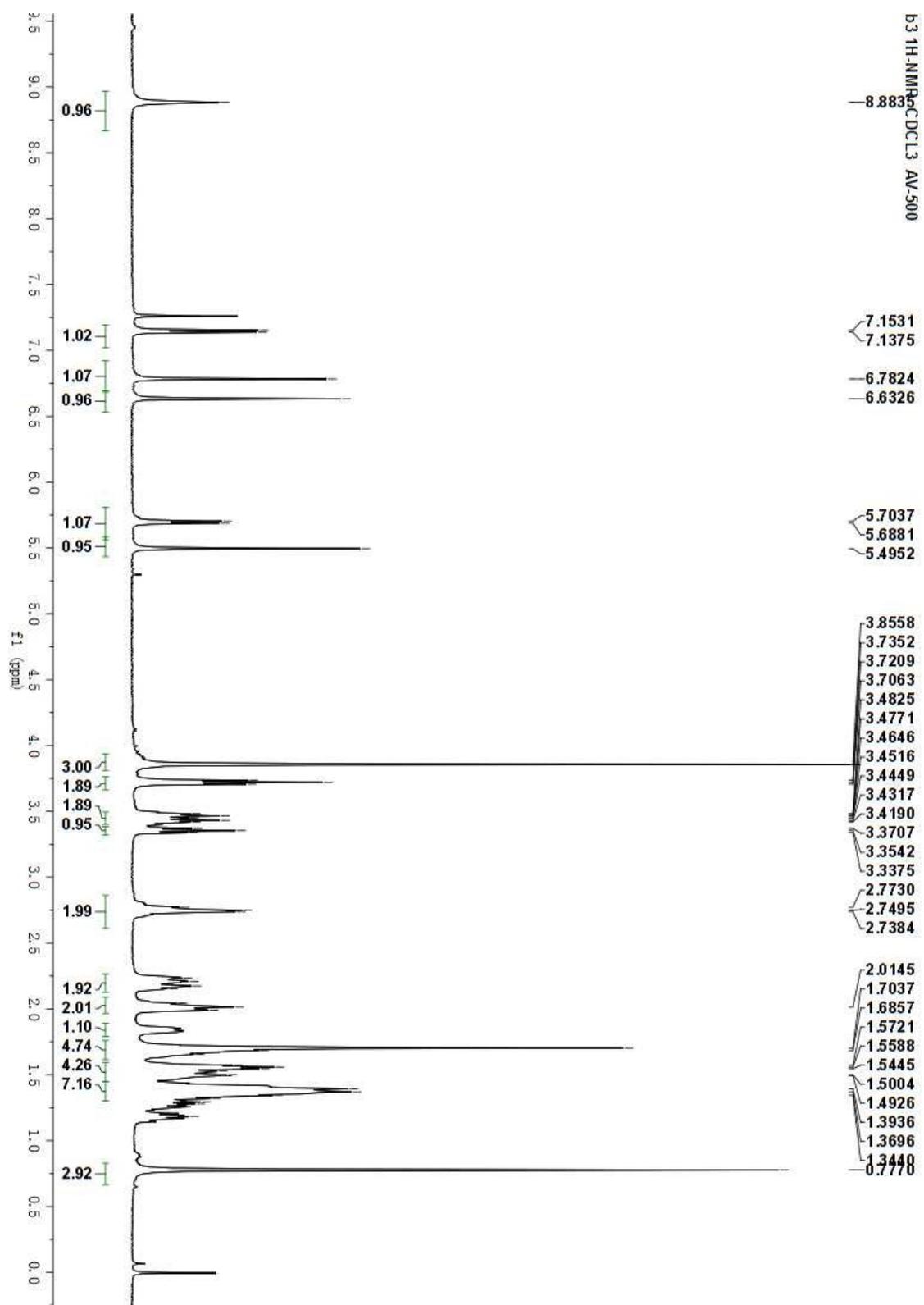
D:\data\



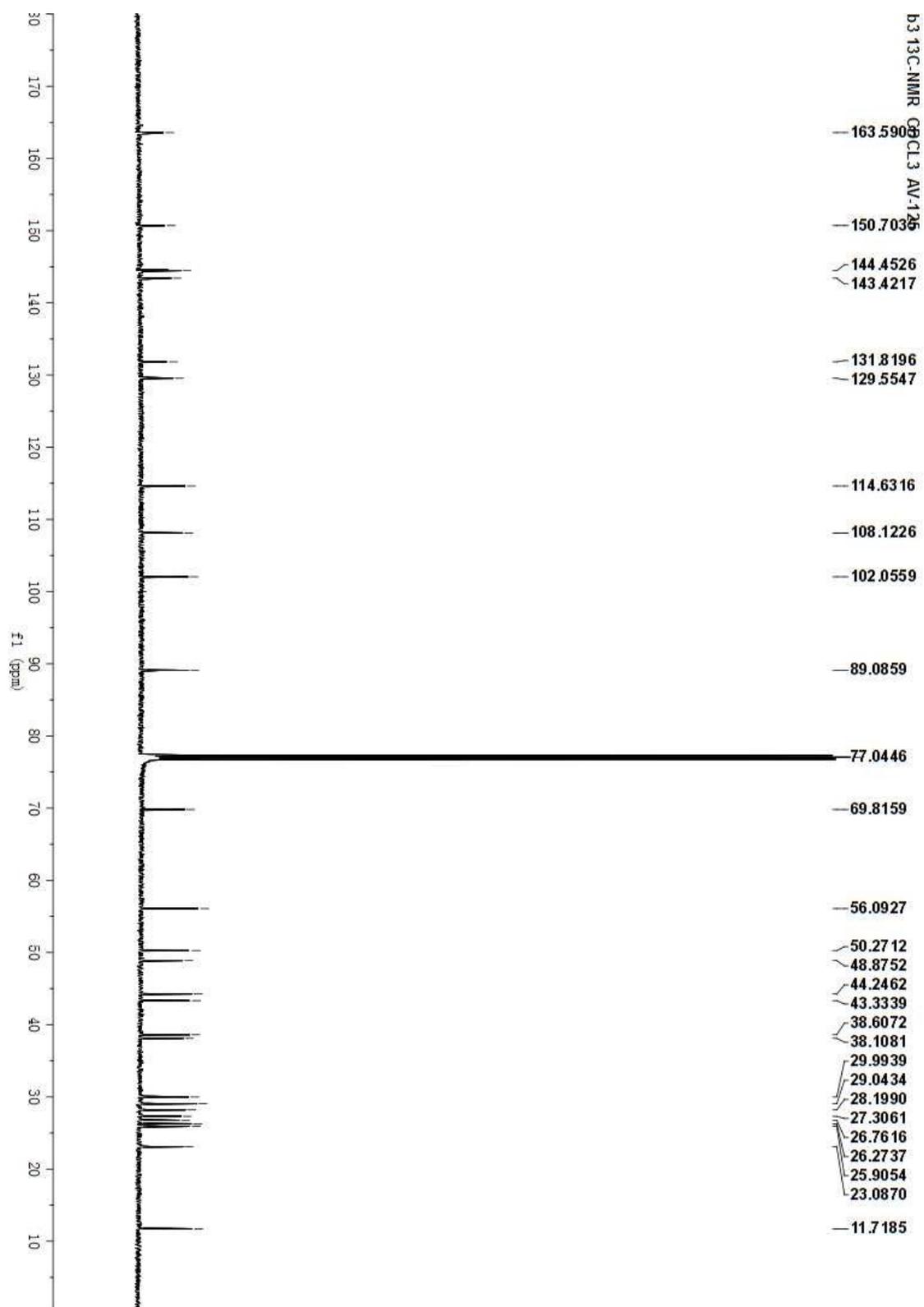
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¹H NMR spectrum of 12a

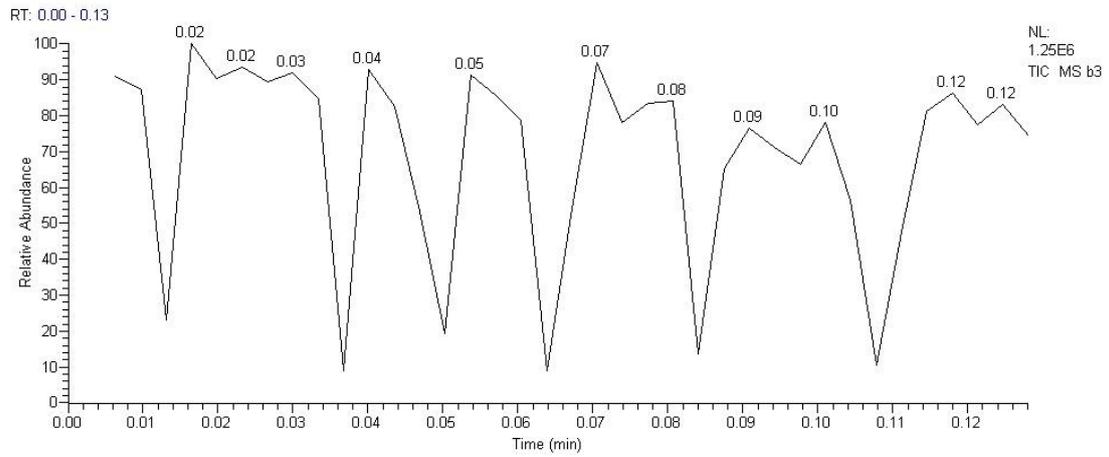


^{13}C NMR spectrum of **12a**

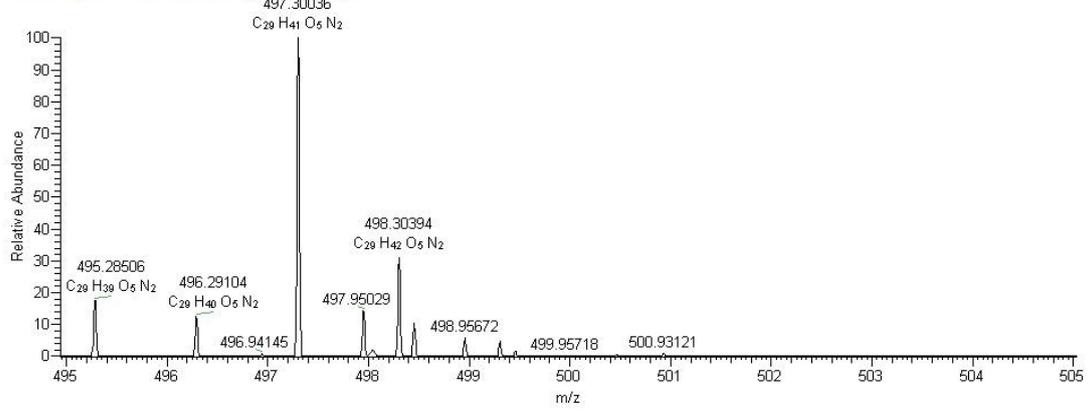


HRMS spectrum of 12a

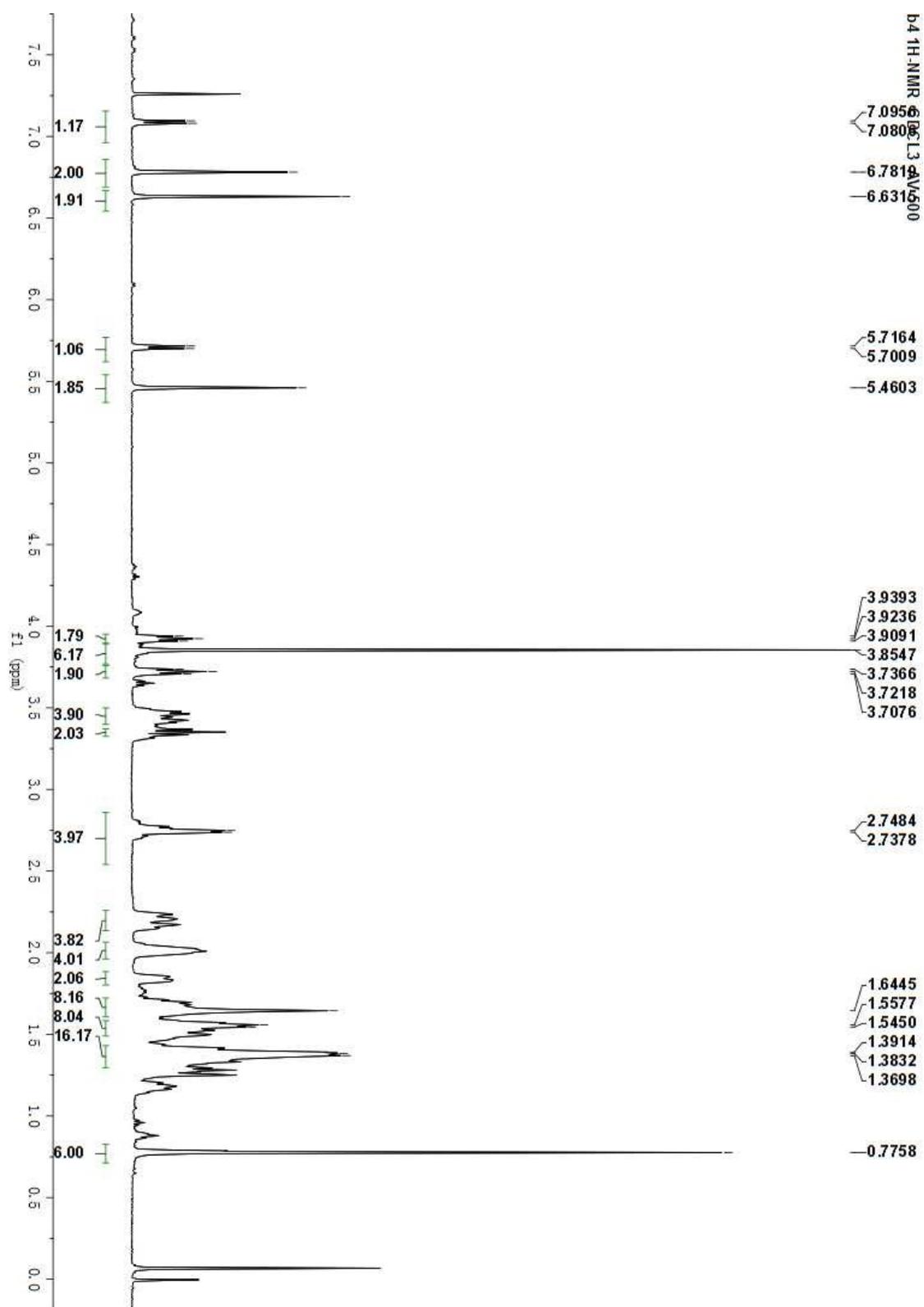
D:\data\



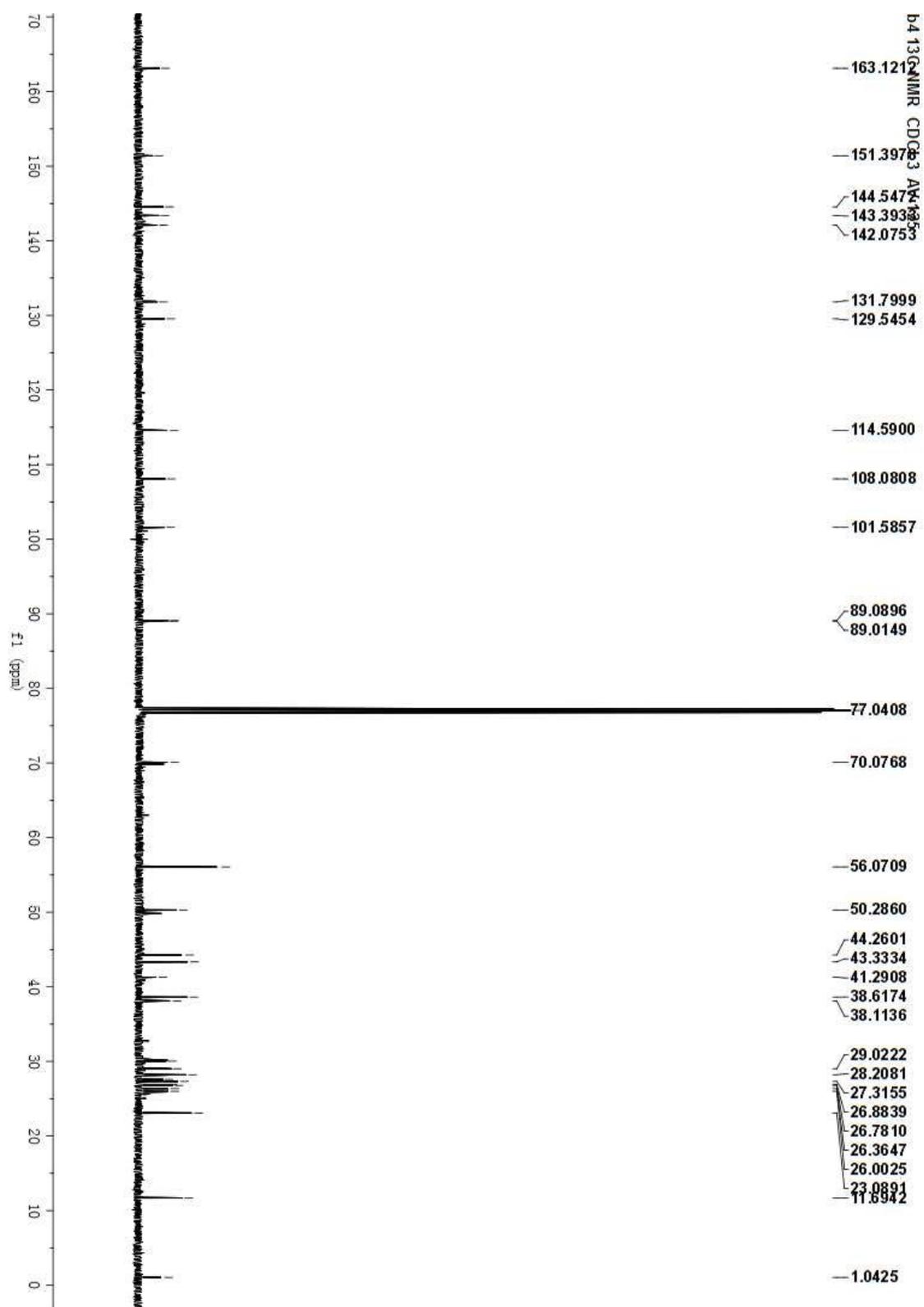
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¹H NMR spectrum of 12b

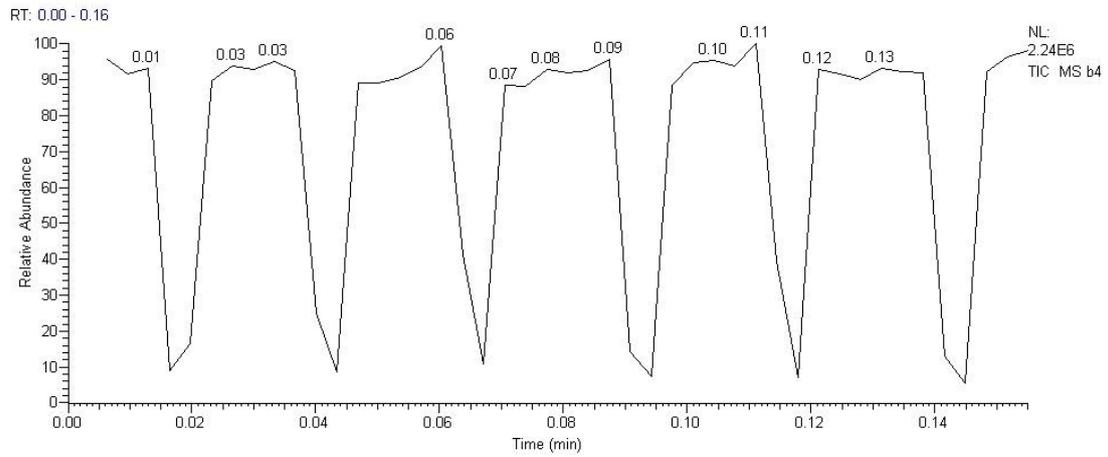


^{13}C NMR spectrum of **12b**

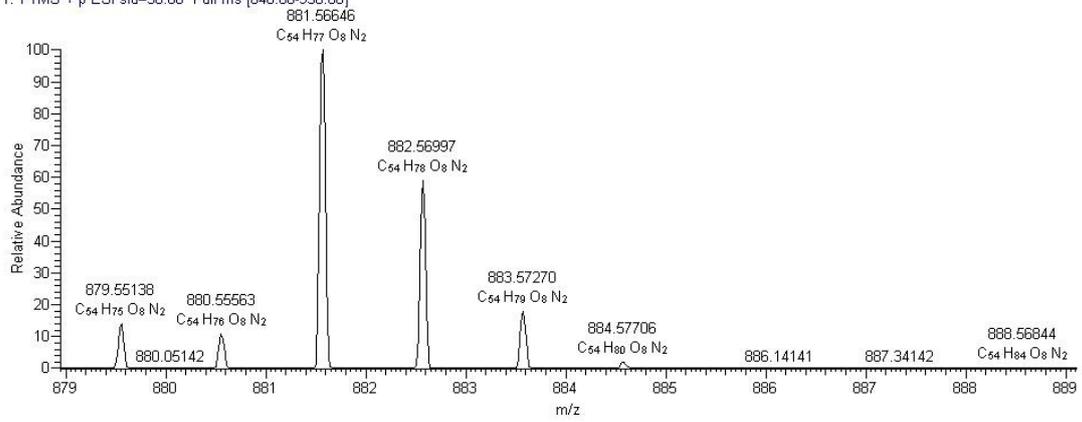


HRMS spectrum of 12b

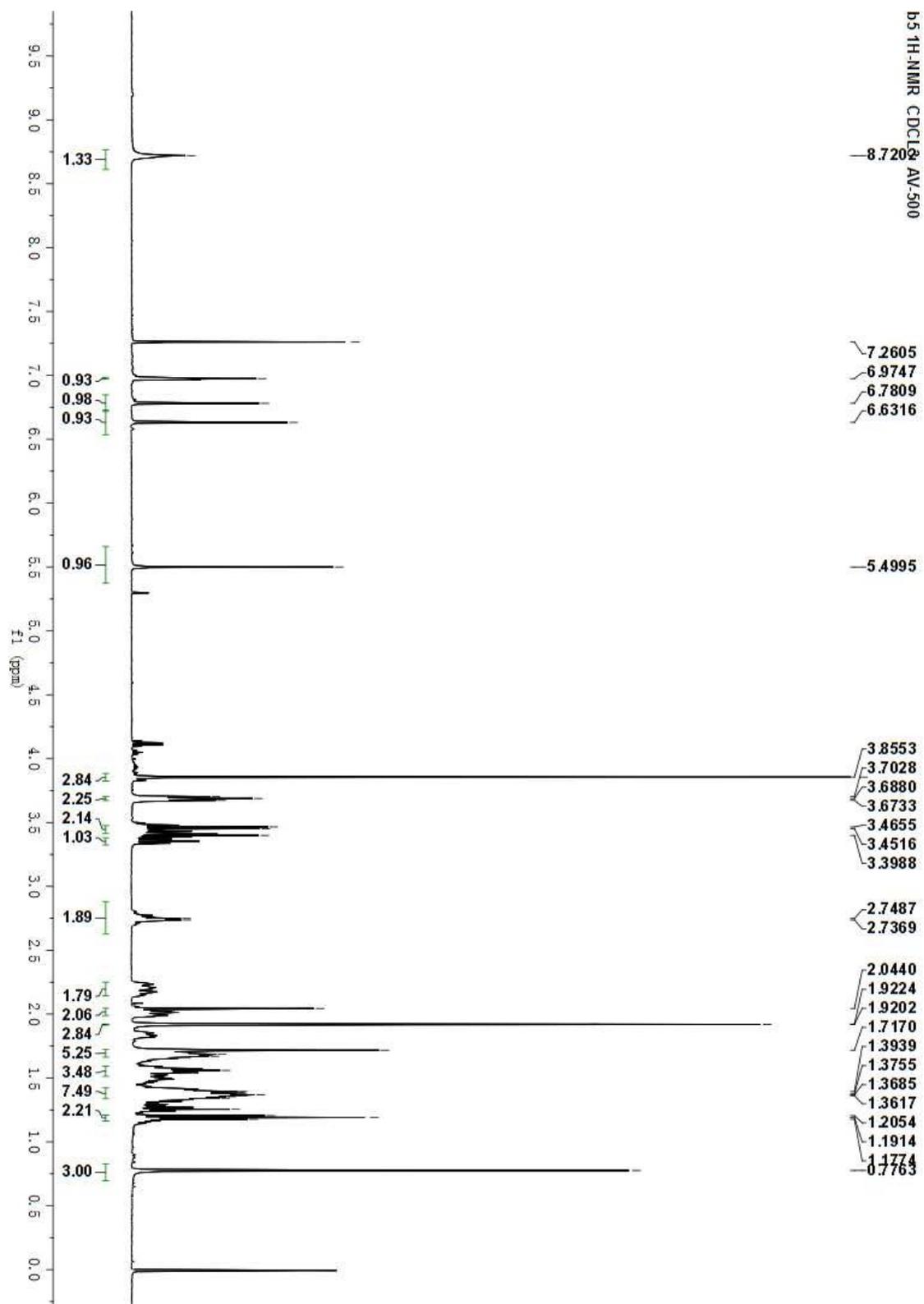
D:\data\



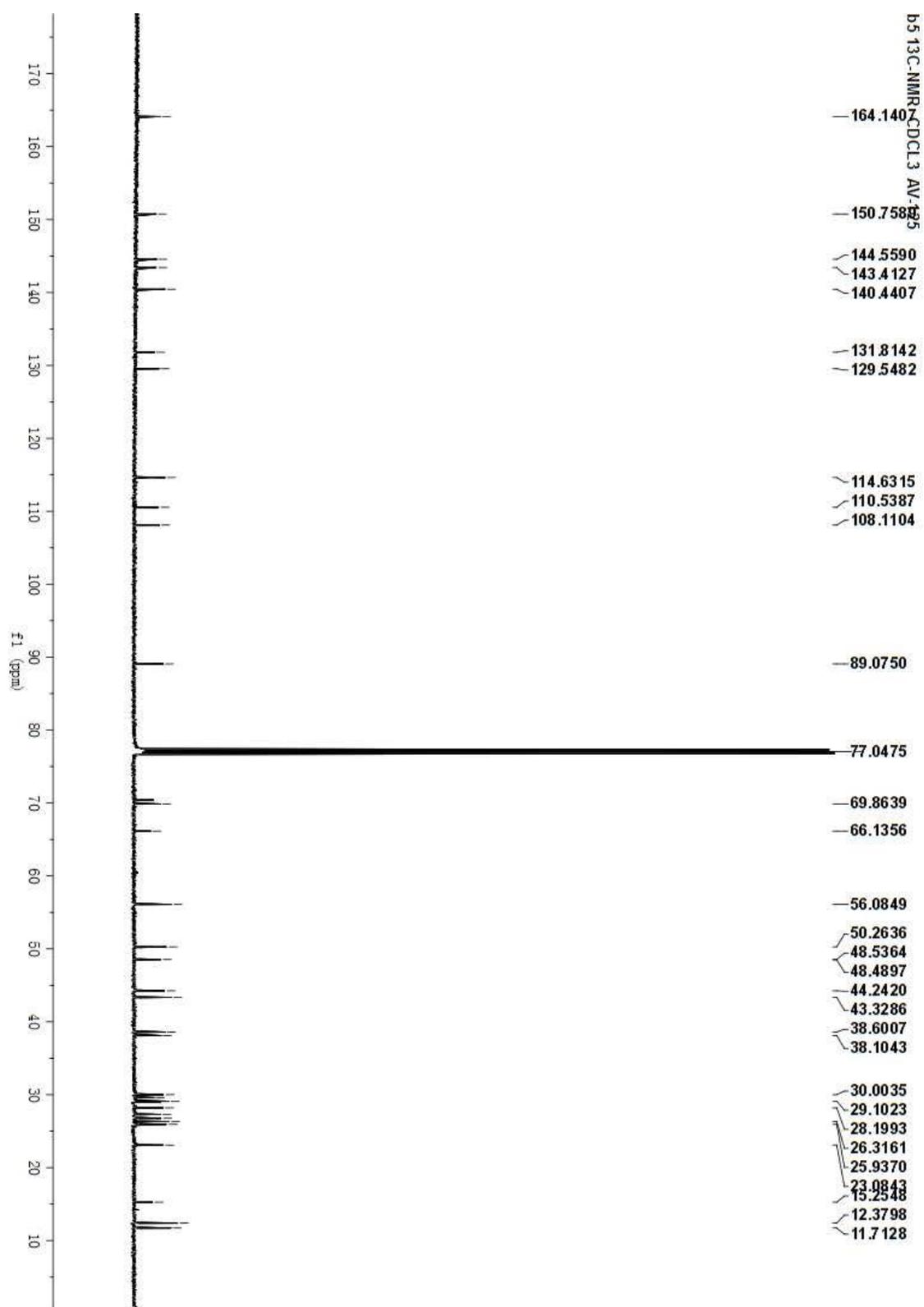
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¹H NMR spectrum of 13a



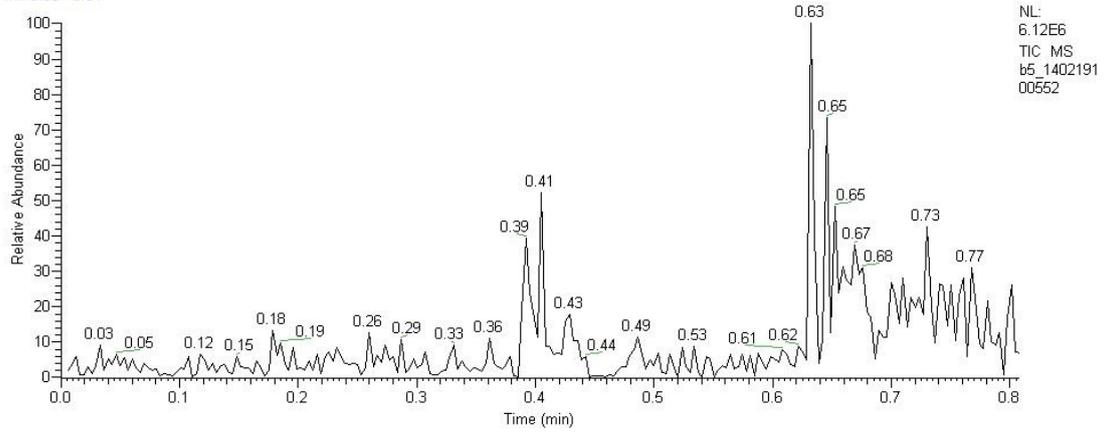
^{13}C NMR spectrum of **13a**



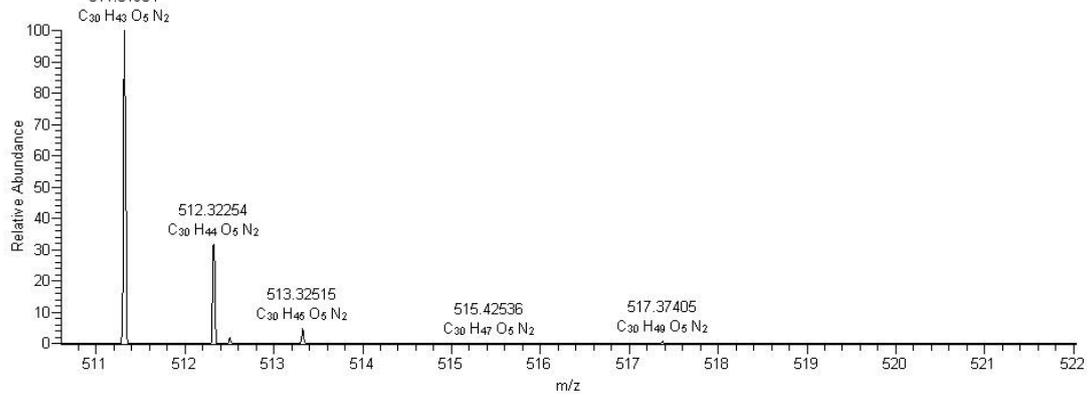
HRMS spectrum of 13a

D:\data\

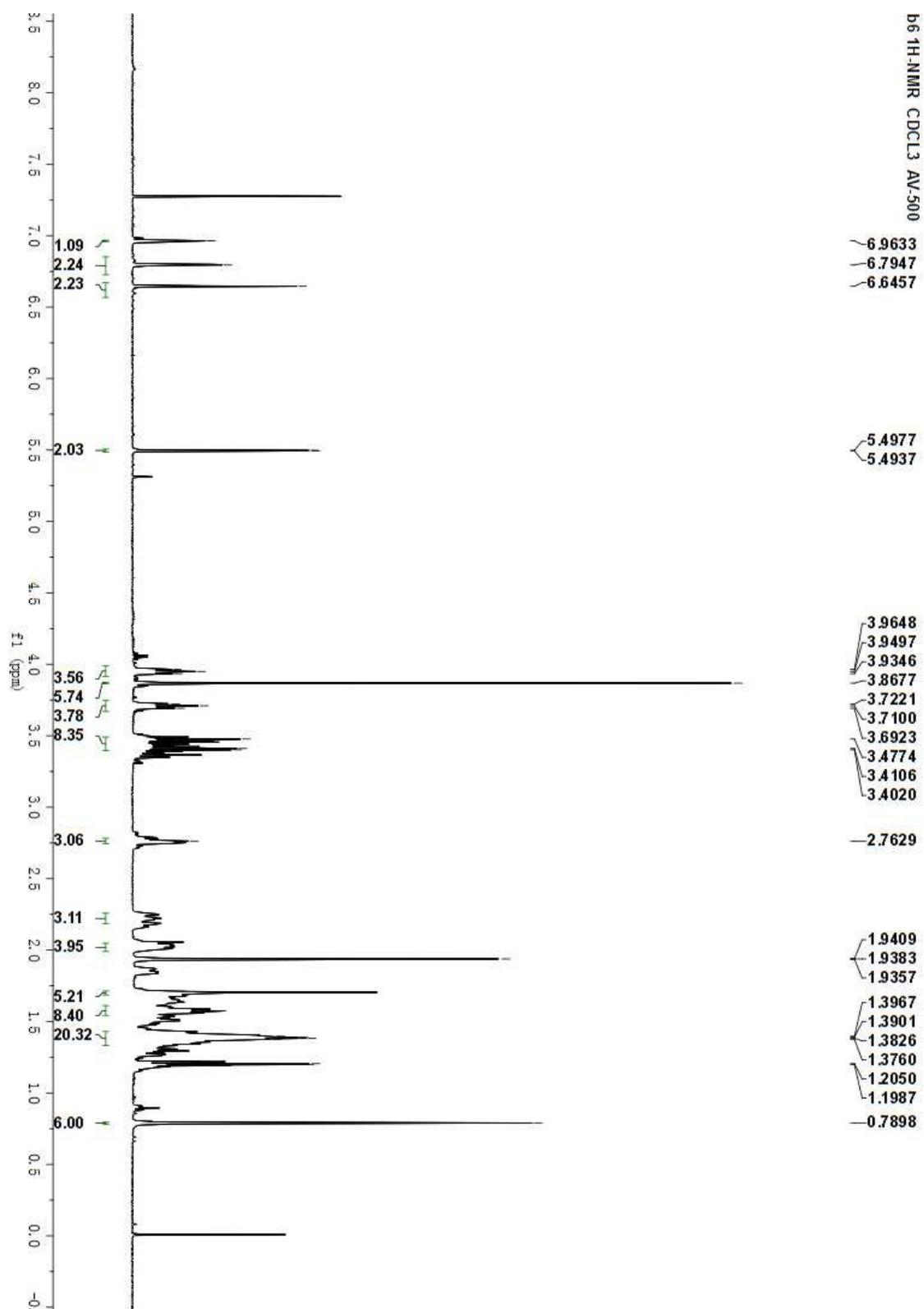
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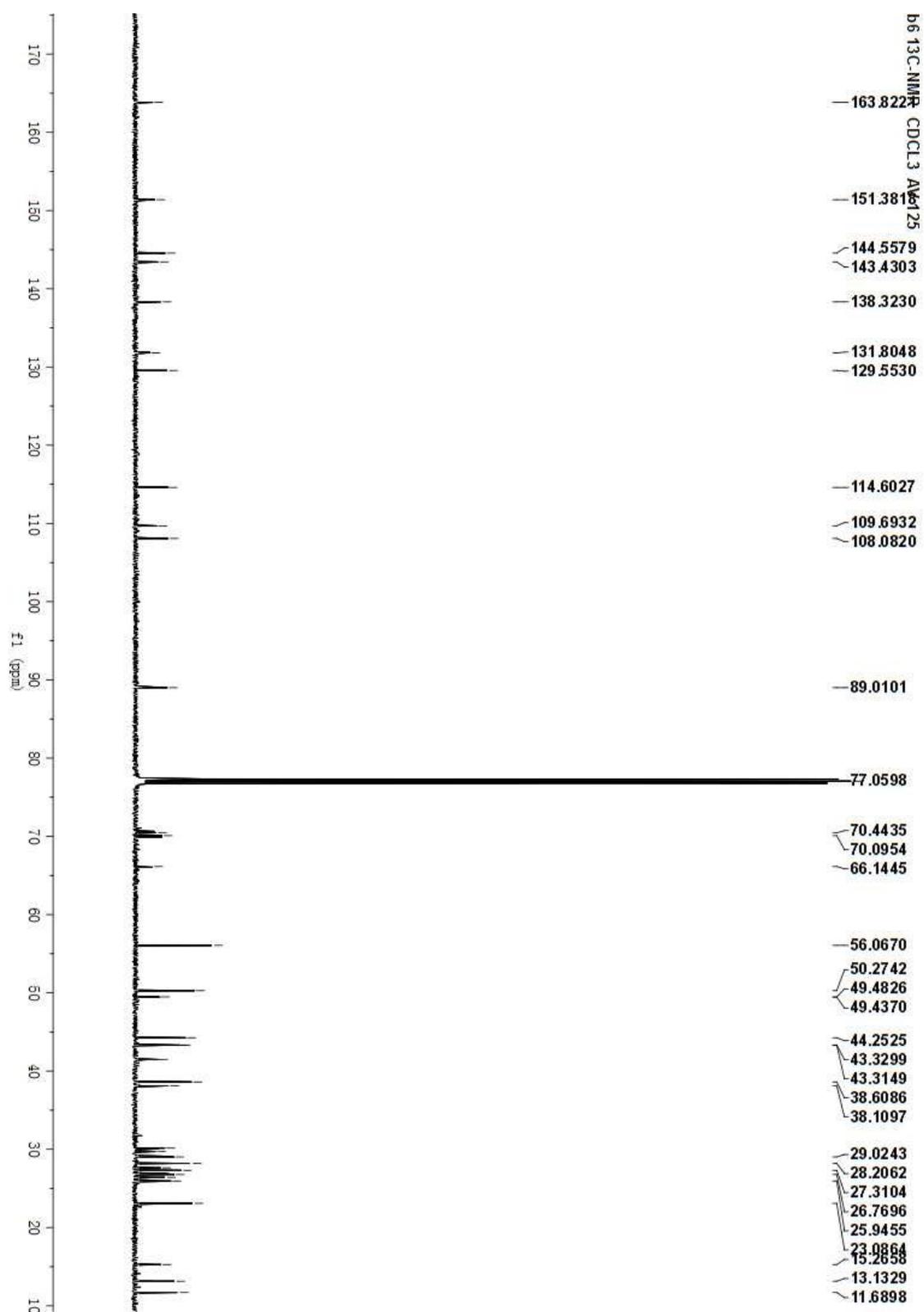
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511.31904



¹H NMR spectrum of 13b

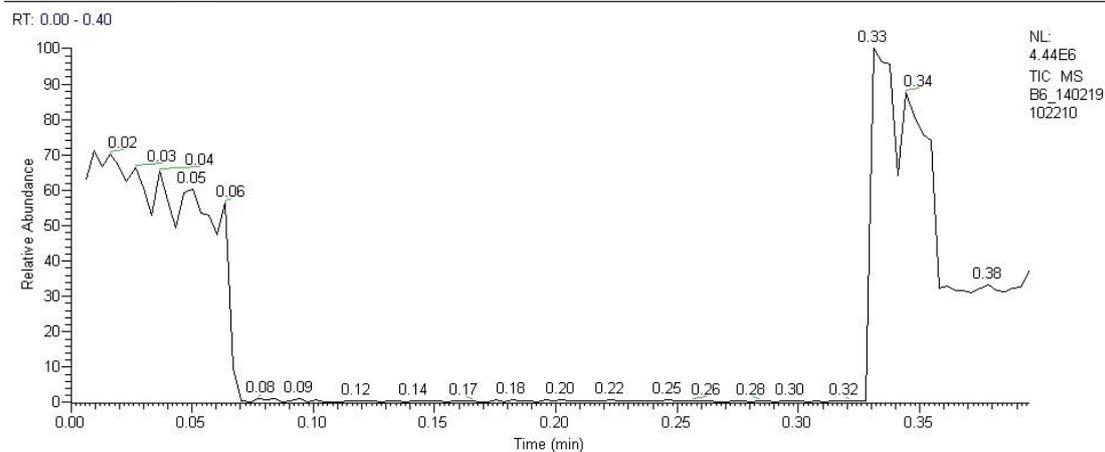


^{13}C NMR spectrum of **13b**

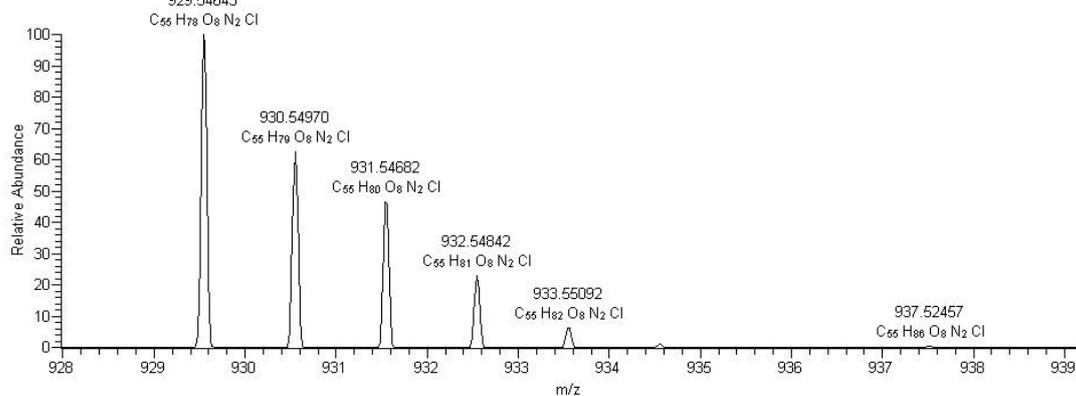


HRMS spectrum of 13b

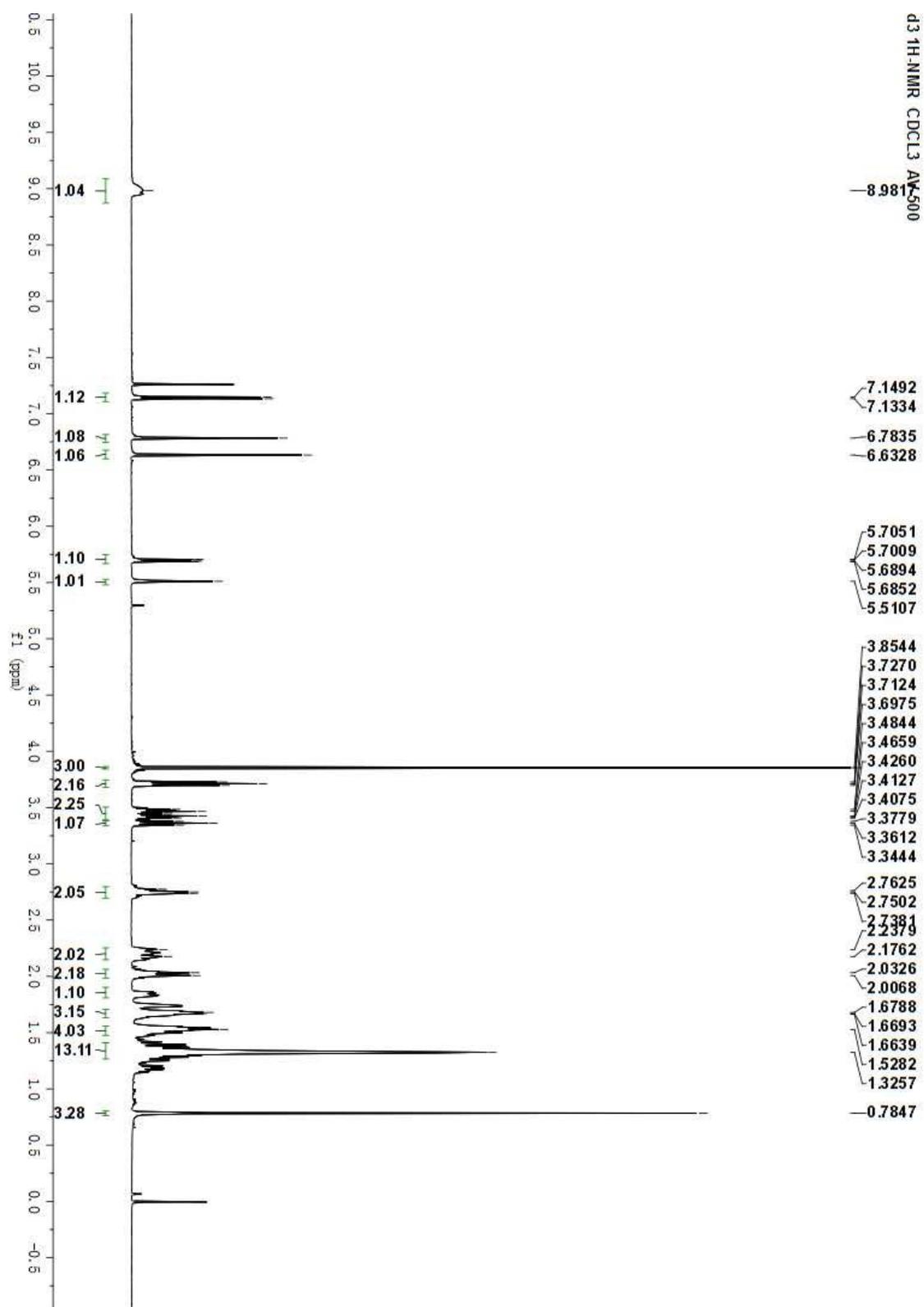
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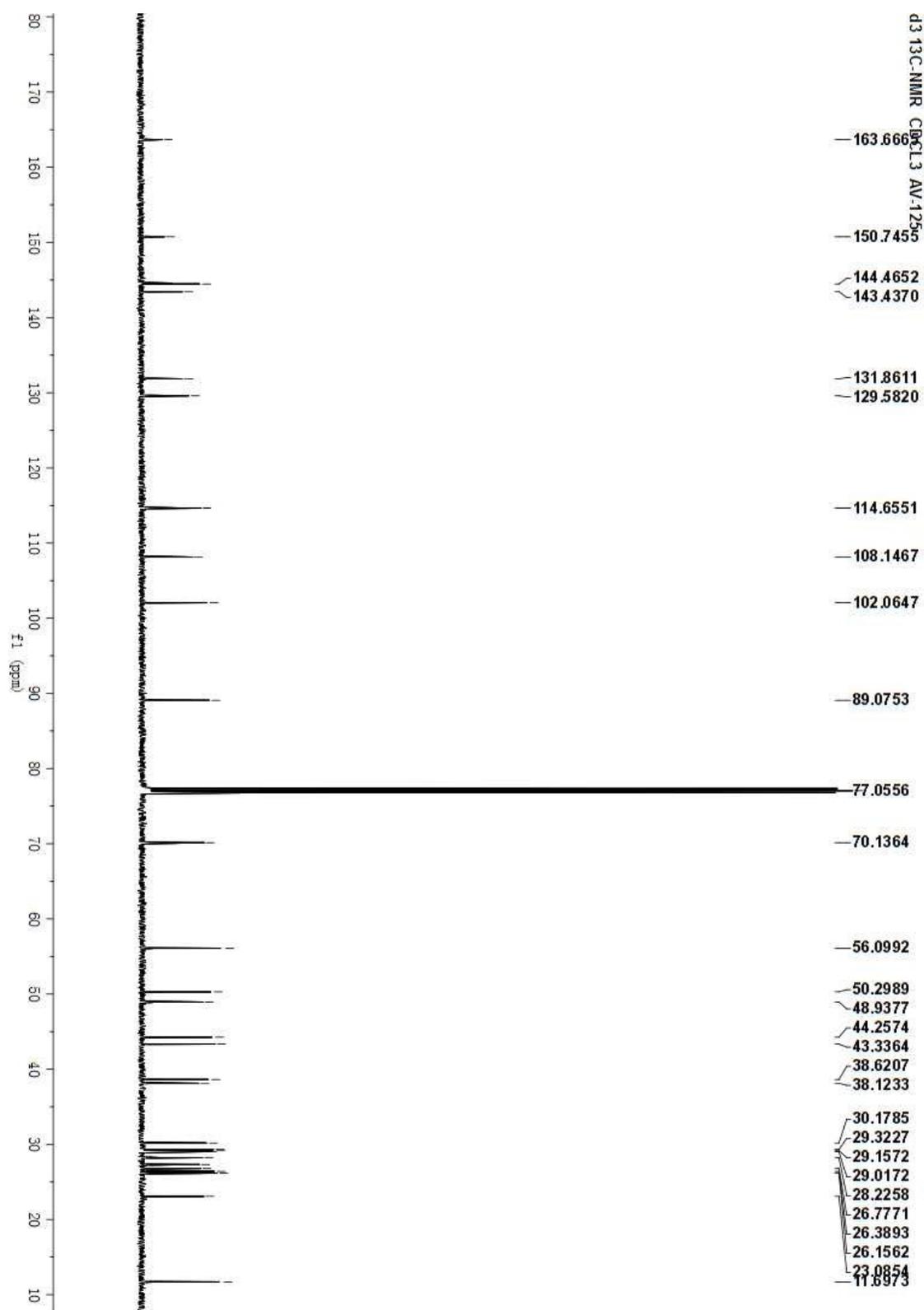
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¹H NMR spectrum of 14a

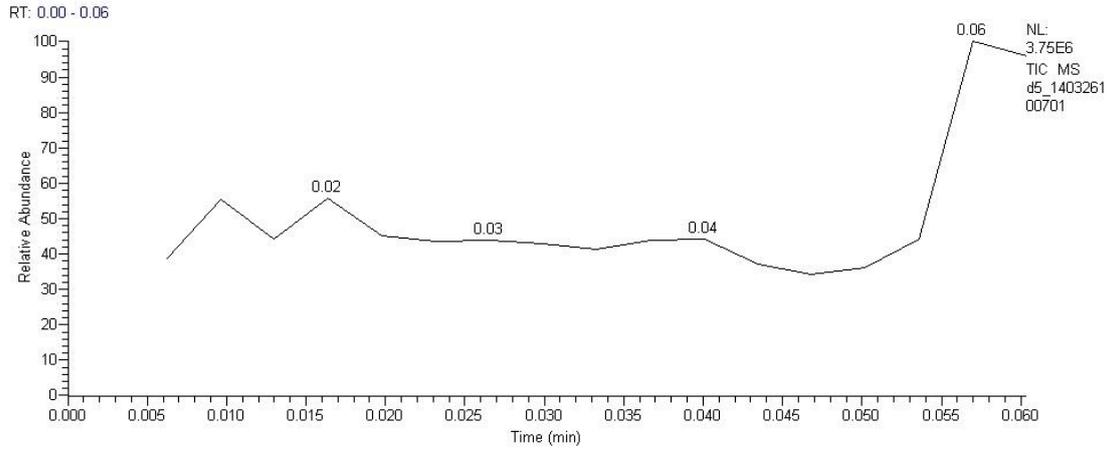


^{13}C NMR spectrum of **14a**

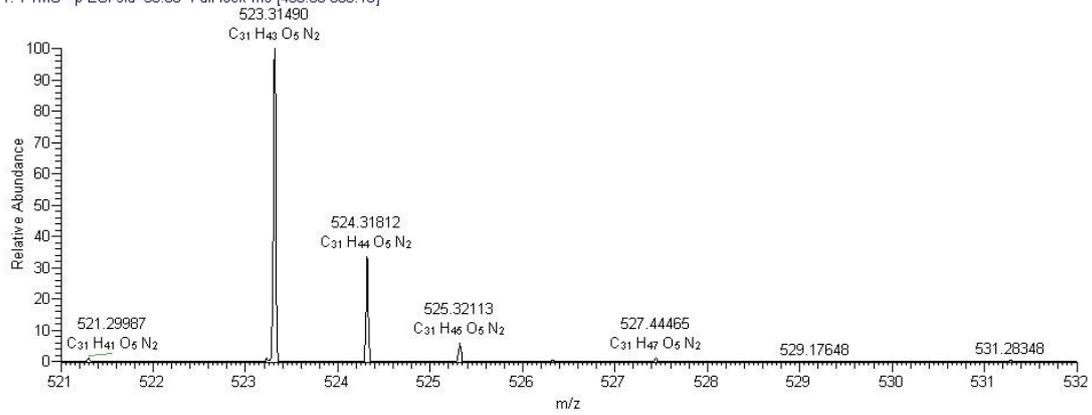


HRMS spectrum of 14a

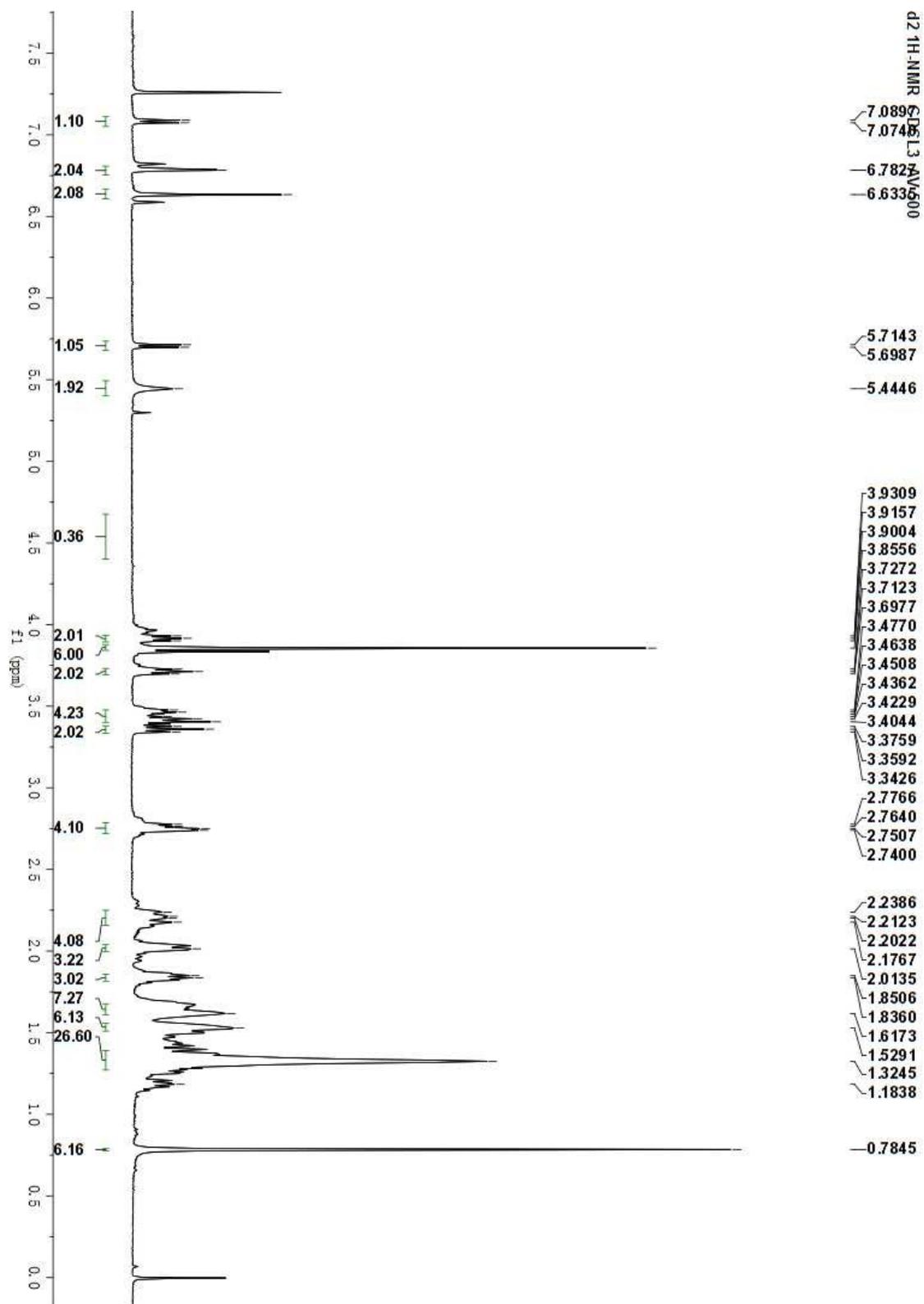
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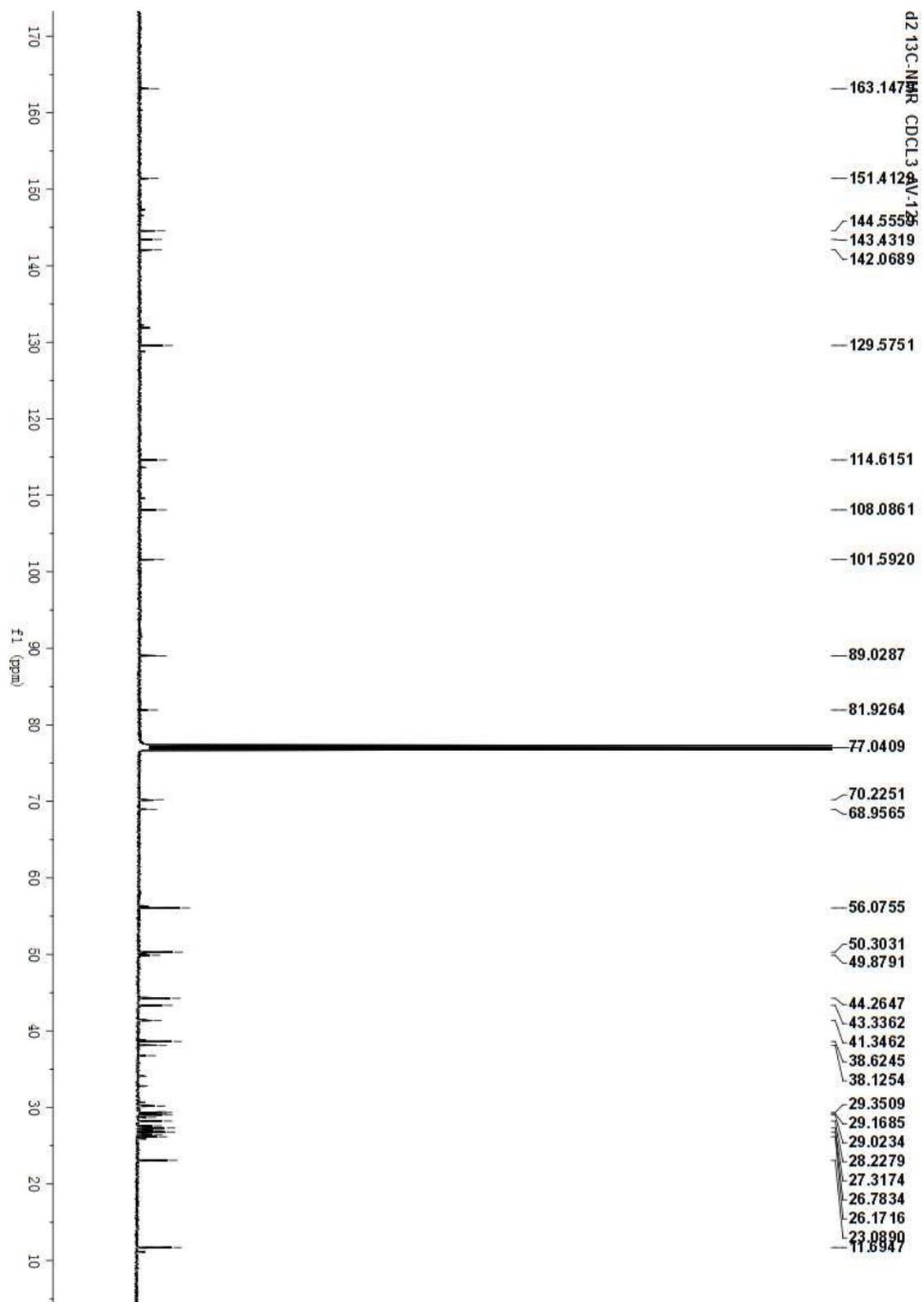
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¹H NMR spectrum of 14b

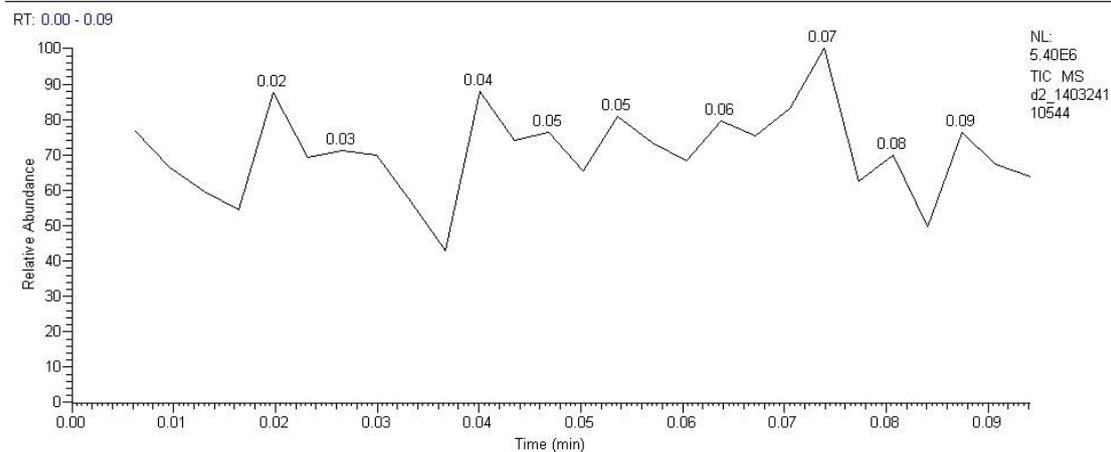


¹³C NMR spectrum of **14b**

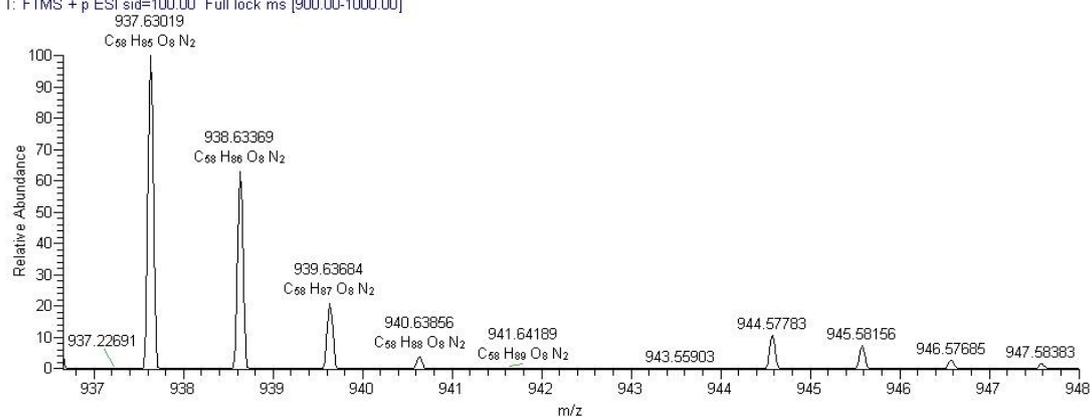


HRMS spectrum of 14b

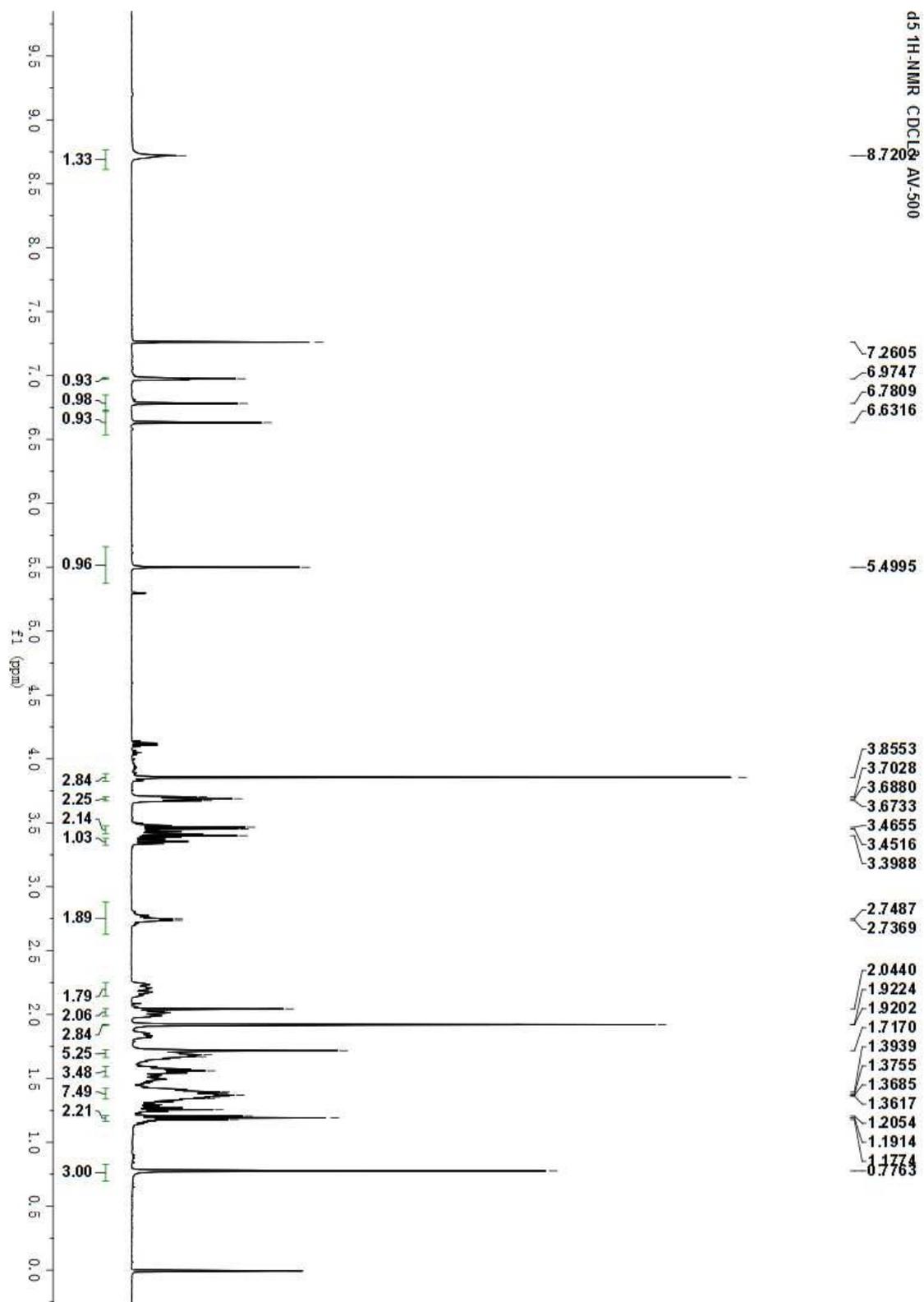
D:\data\



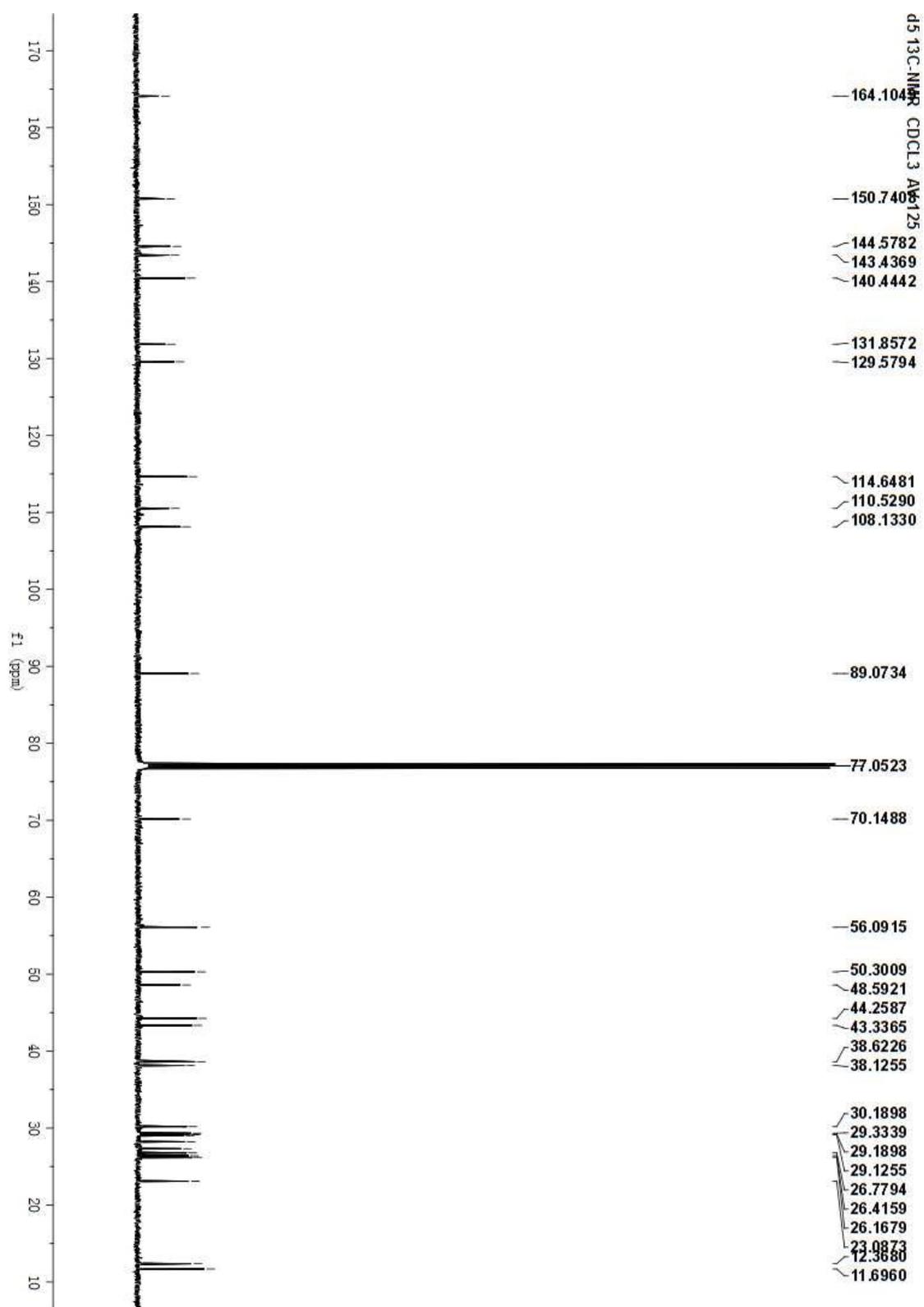
d2_140324110544 #2-26 RT: 0.01-0.09 AV: 25 NL: 2.63E5
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¹H NMR spectrum of 15a

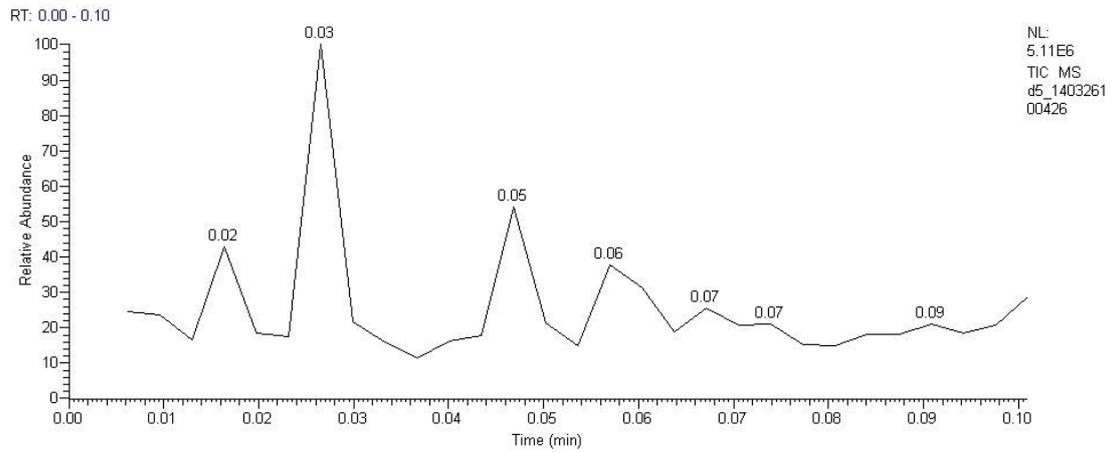


^{13}C NMR spectrum of **15a**

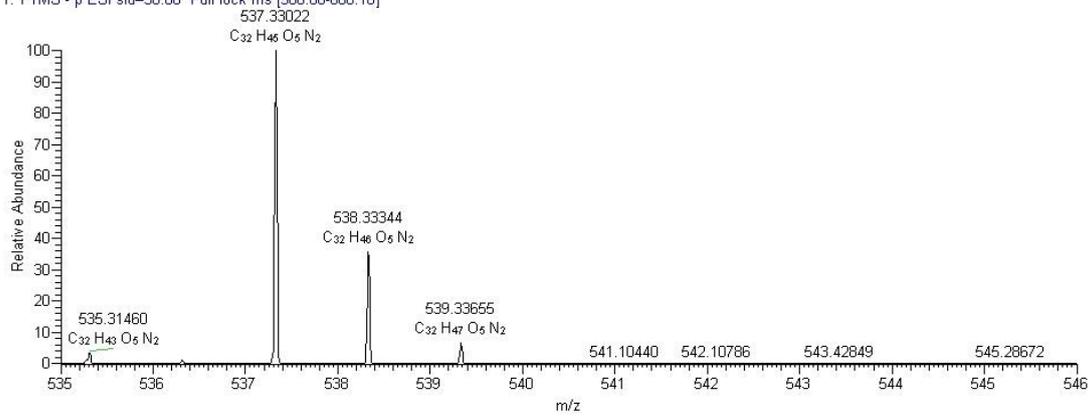


HRMS spectrum of 15a

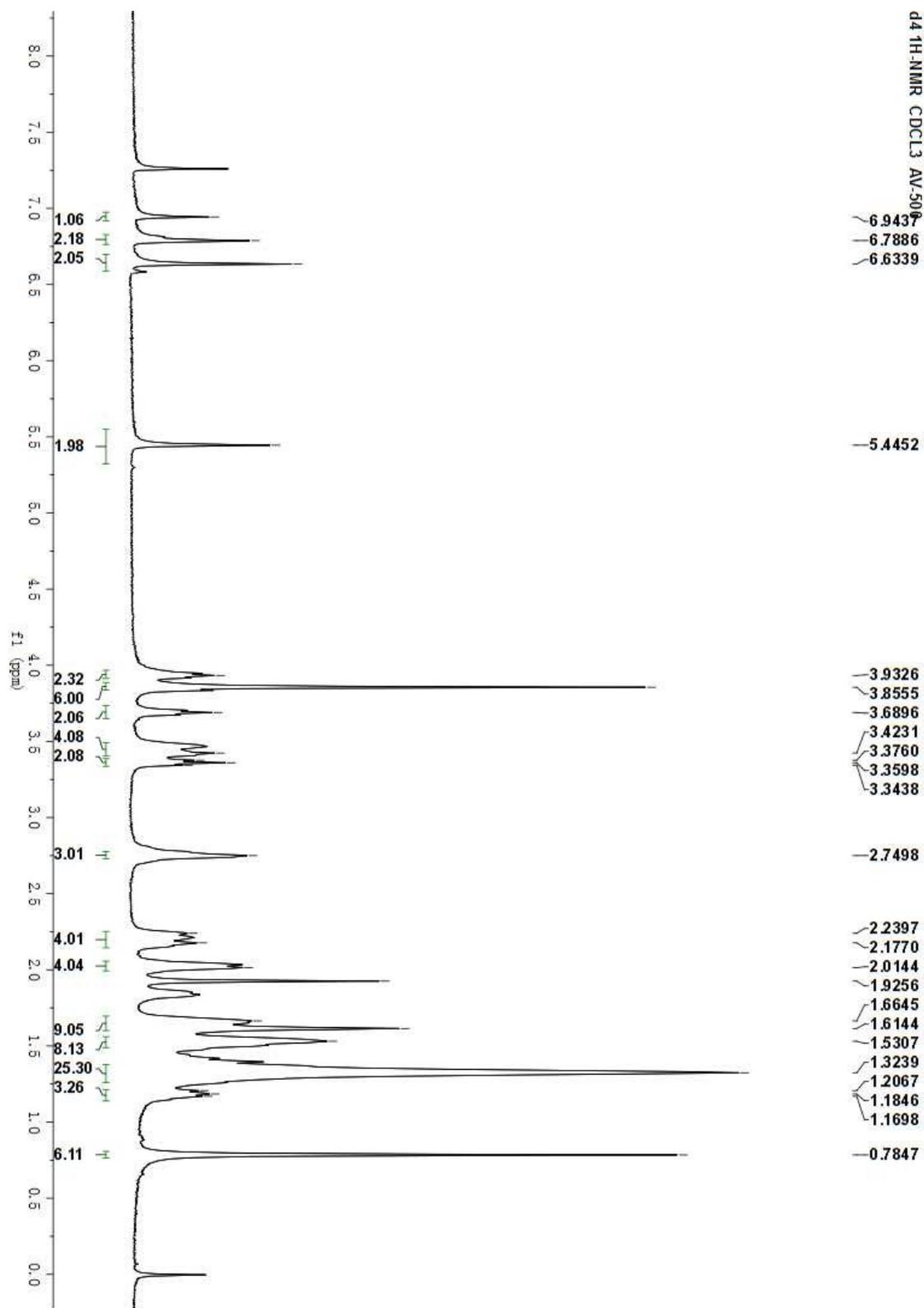
D:\data\



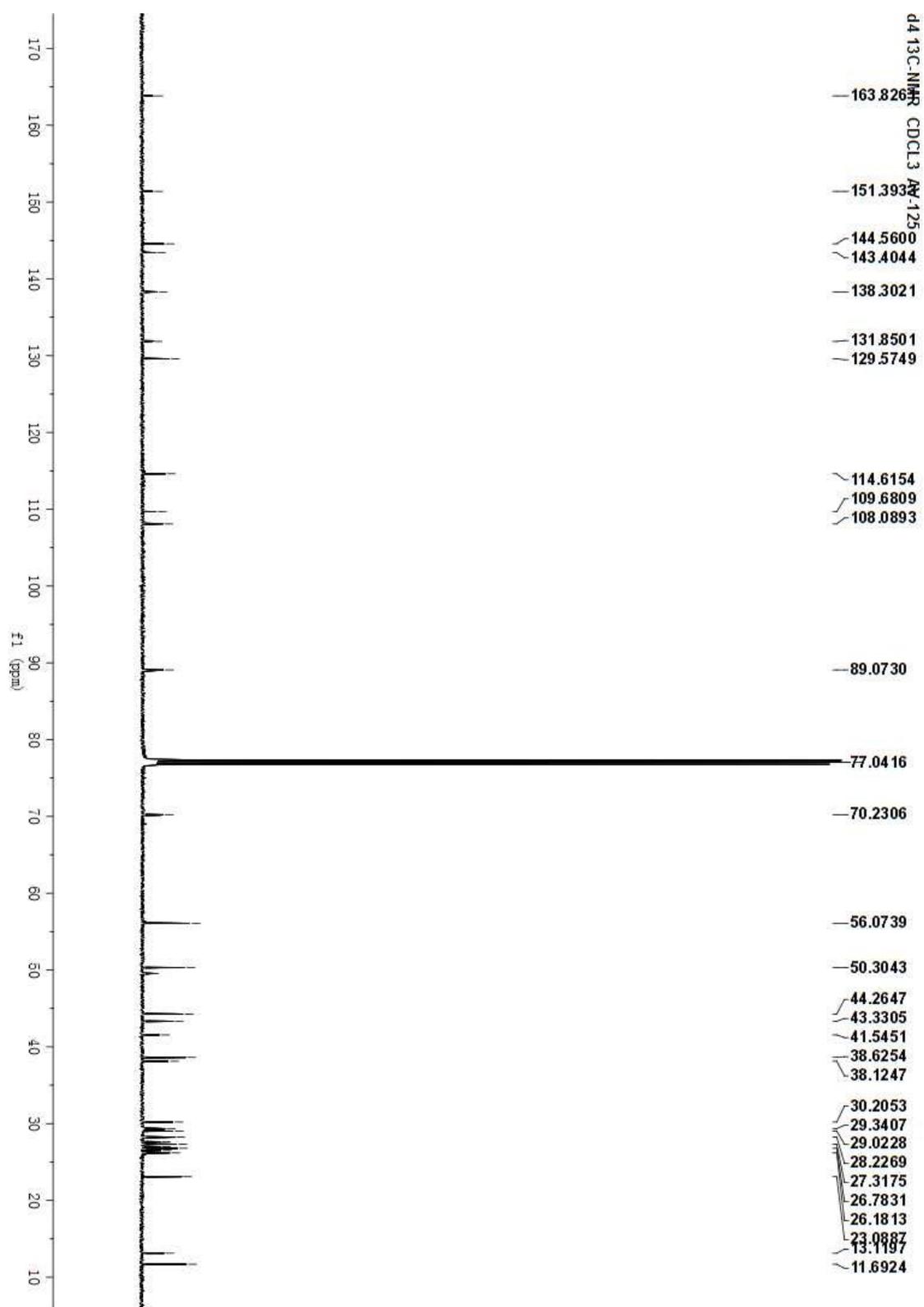
d5_140326100426 #2-29 RT: 0.01-0.10 AV: 28 NL: 2.86E5
T: FTMS - p ESI sid=50.00 Full lock ms [500.00-600.10]



¹H NMR spectrum of **15b**

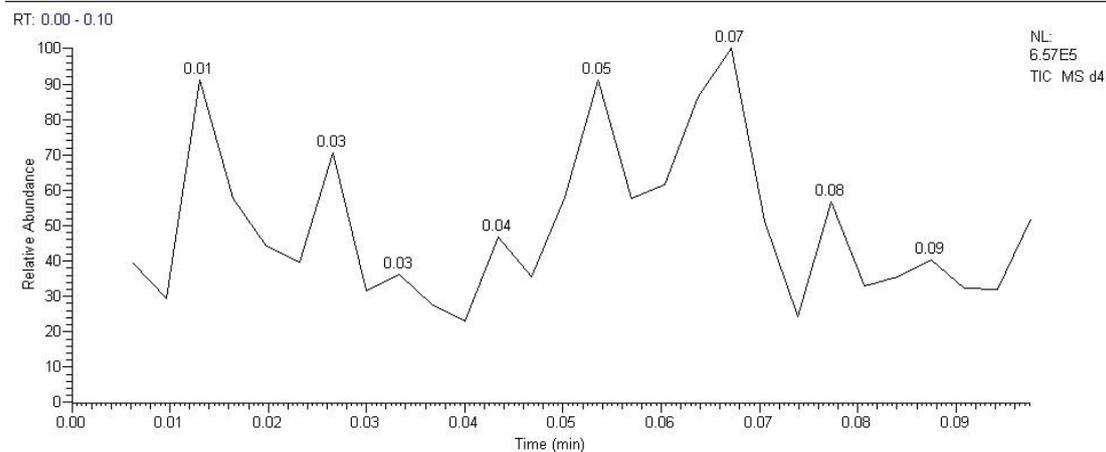


^{13}C NMR spectrum of **15b**

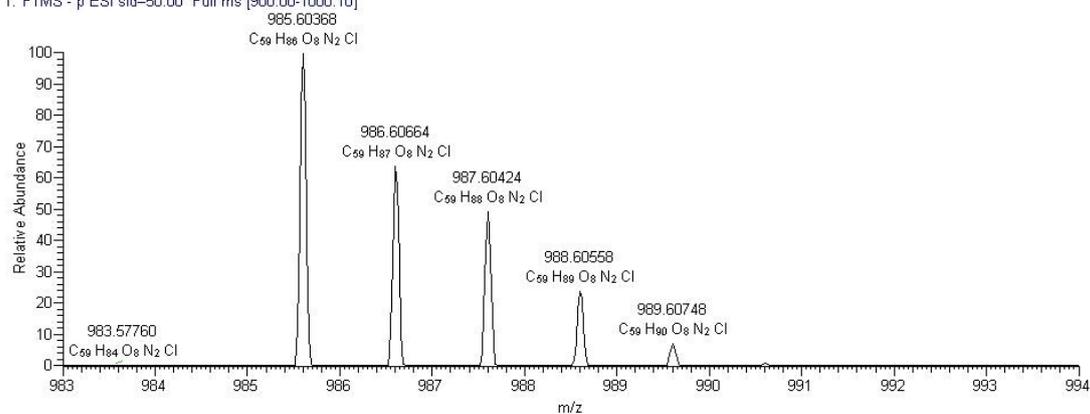


HRMS spectrum of **15b**

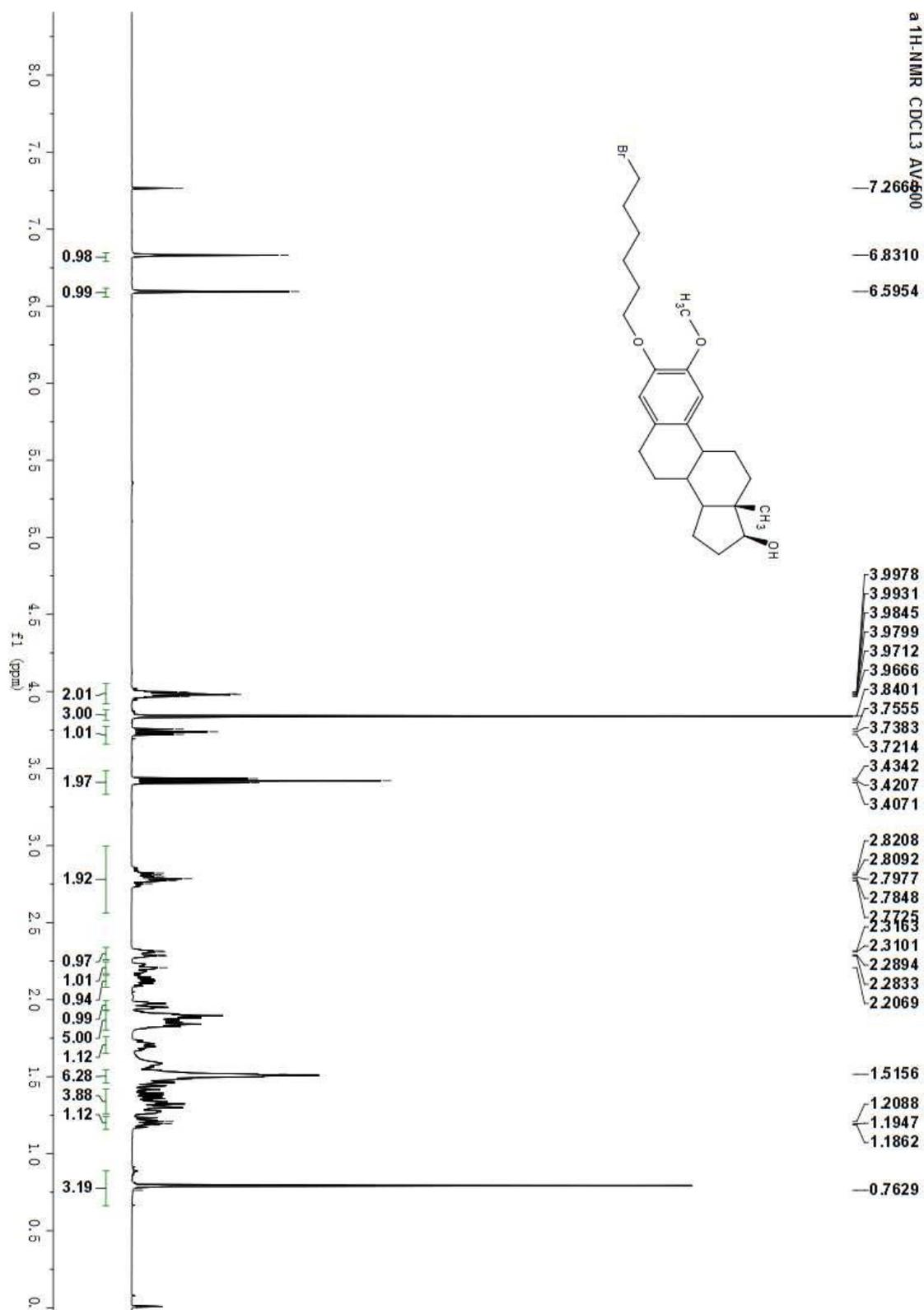
D:\data\



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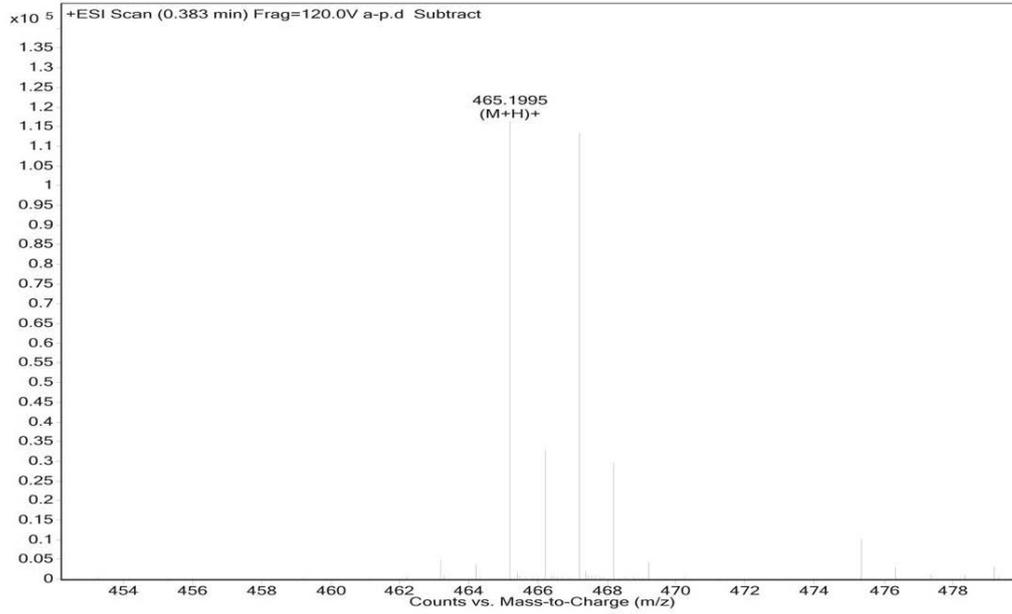


¹H NMR spectrum of **16**

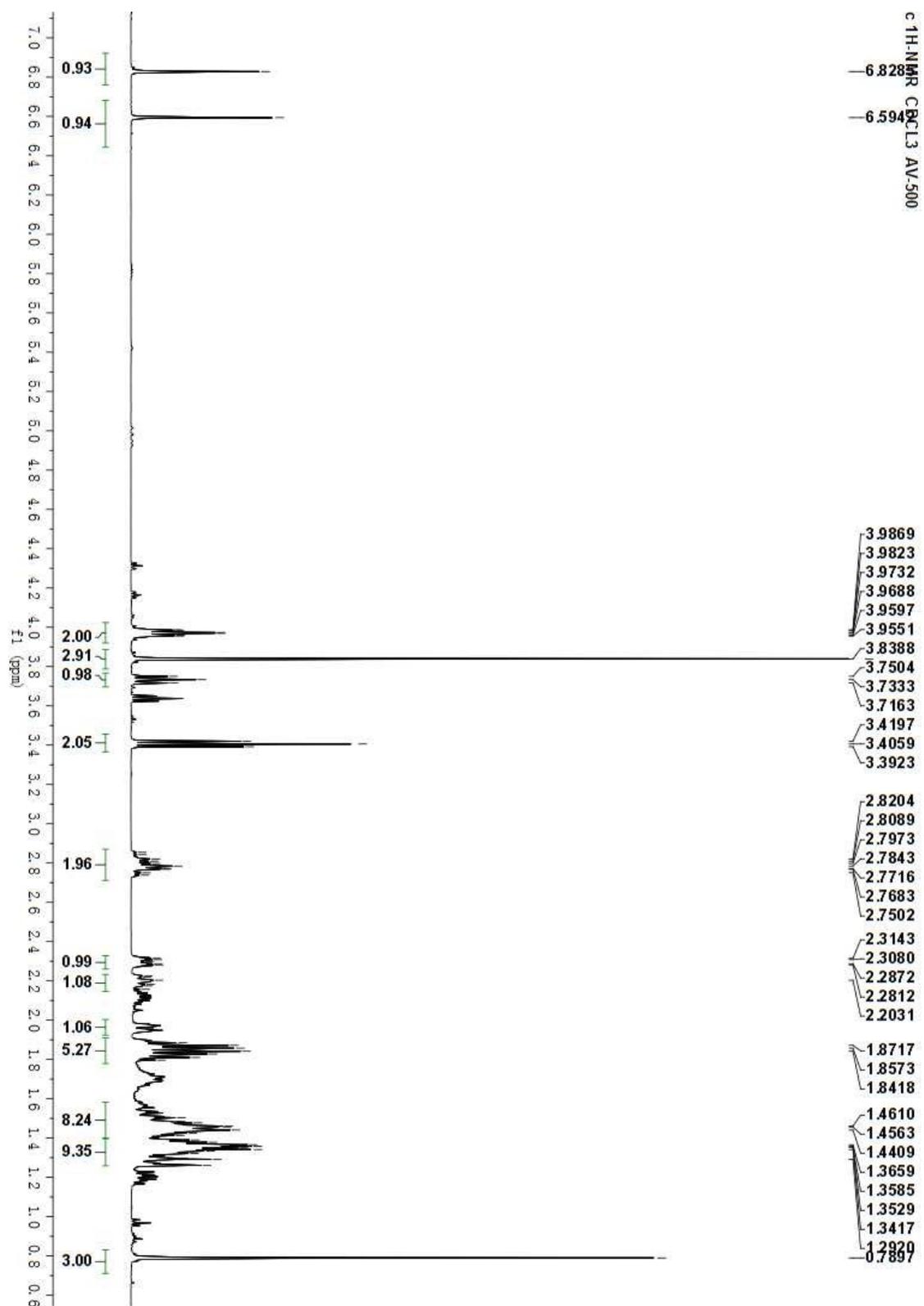


HRMS spectrum of 16

| | | | | | | | |
|----------------------|-------|--------------------|-------|------------------------|--------------|-------------------------------|---------|
| Sample Name | | Position | P2-A1 | Instrument Name | Instrument 1 | User Name | |
| Inj Vol | 0.1 | InjPosition | | SampleType | Sample | IRM Calibration Status | Success |
| Data Filename | a-p.d | ACQ Method | | Comment | | Acquired Time | |

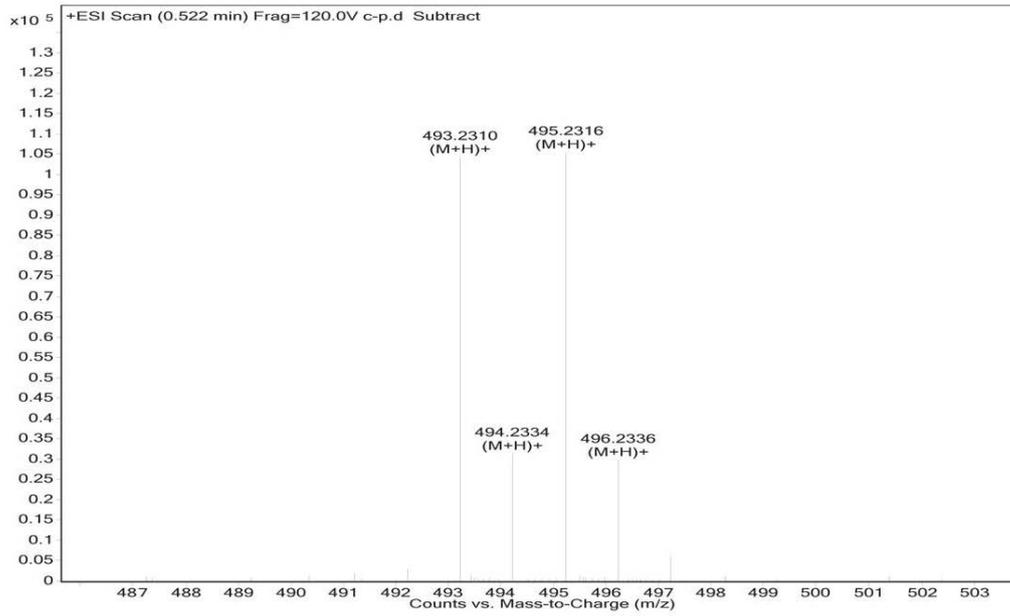


¹H NMR spectrum of 17

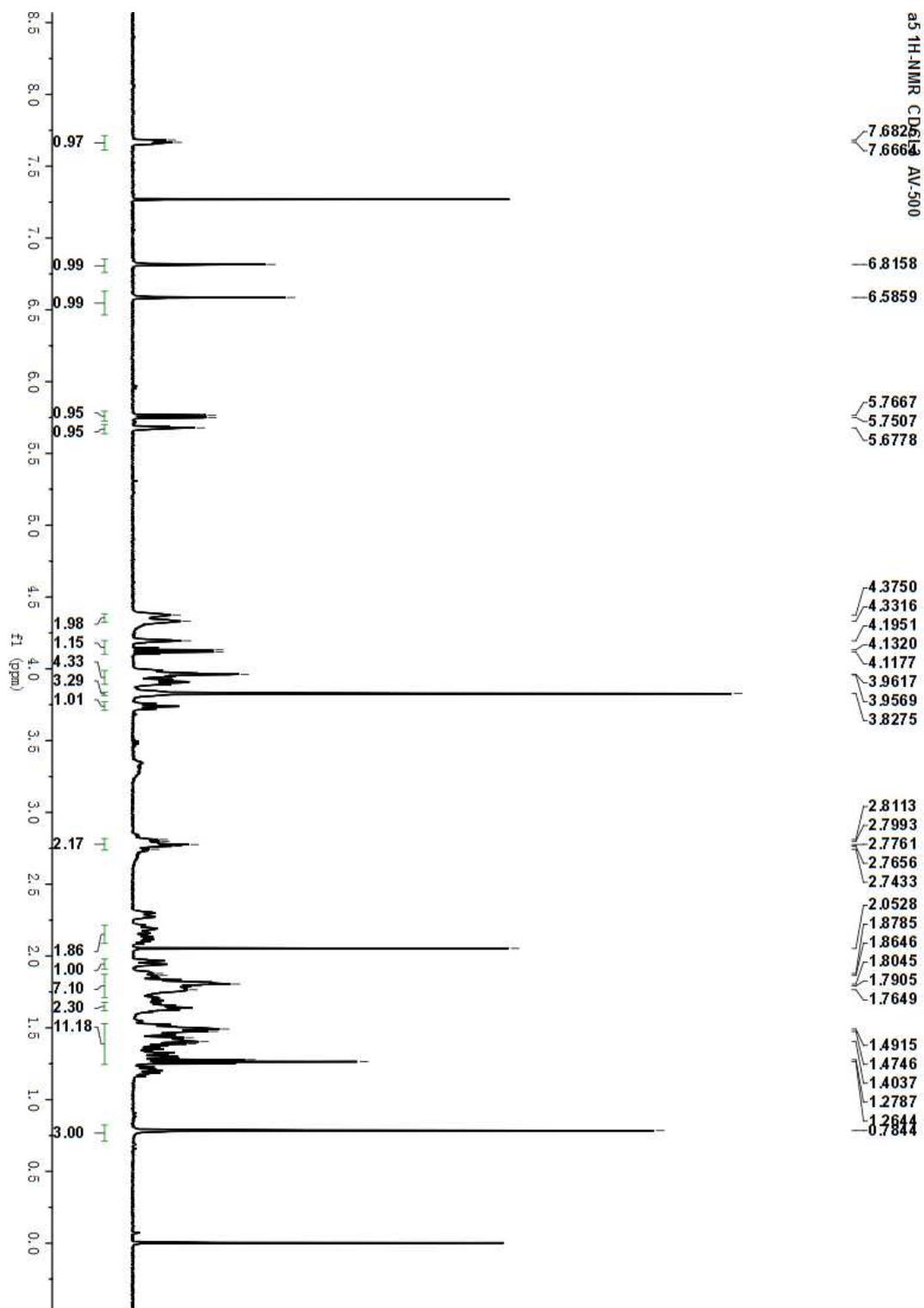


HRMS spectrum of 17

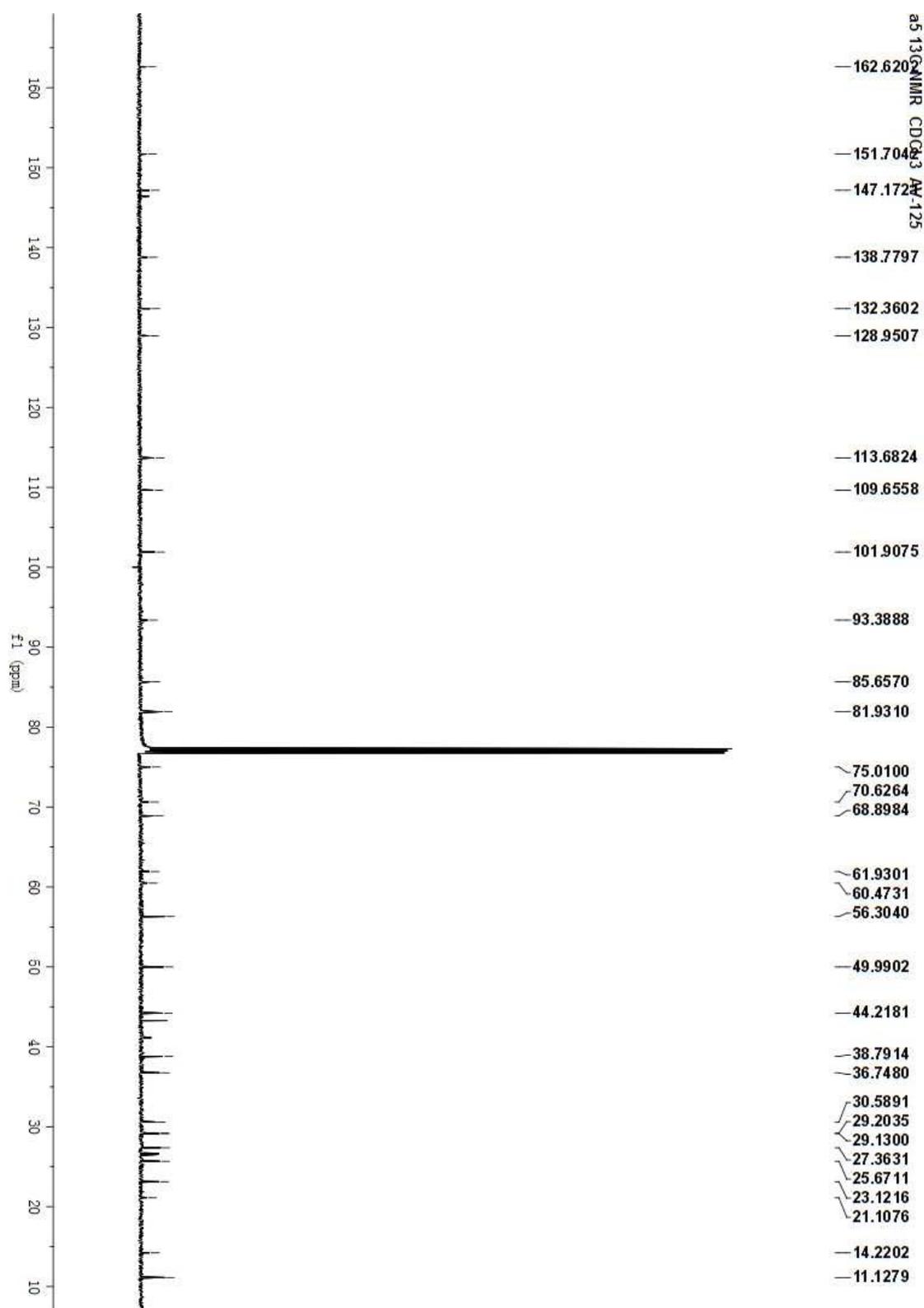
| | | | | | | | |
|---------------|-------|-------------|-------|-----------------|--------------|------------------------|---------|
| Sample Name | | Position | P2-A9 | Instrument Name | Instrument 1 | User Name | |
| Inj Vol | 0.1 | InjPosition | | SampleType | Sample | IRM Calibration Status | Success |
| Data Filename | c-p.d | ACQ Method | | Comment | | Acquired Time | |



¹H NMR spectrum of **18**

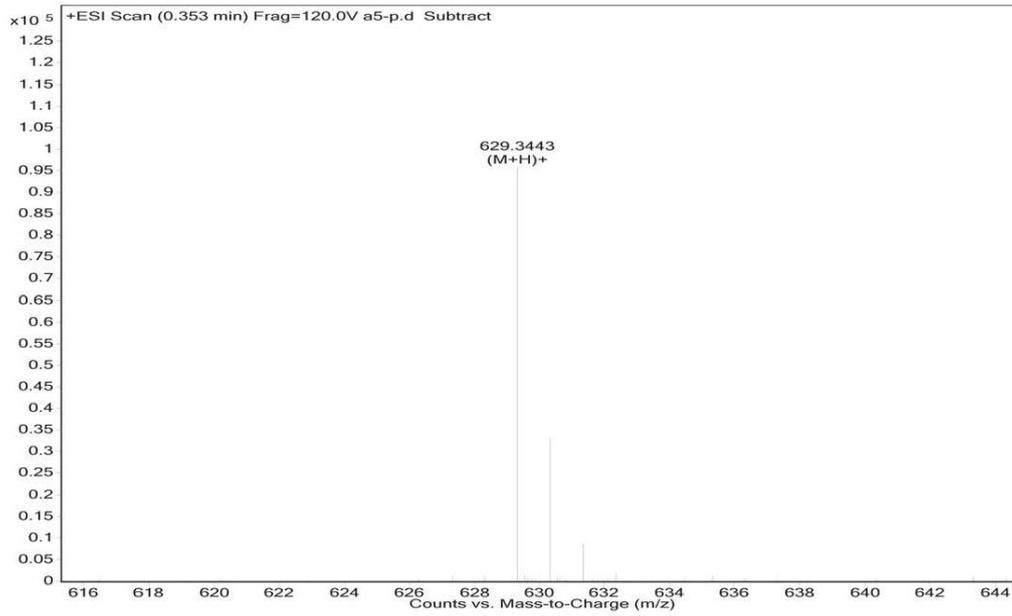


^{13}C NMR spectrum of **18**

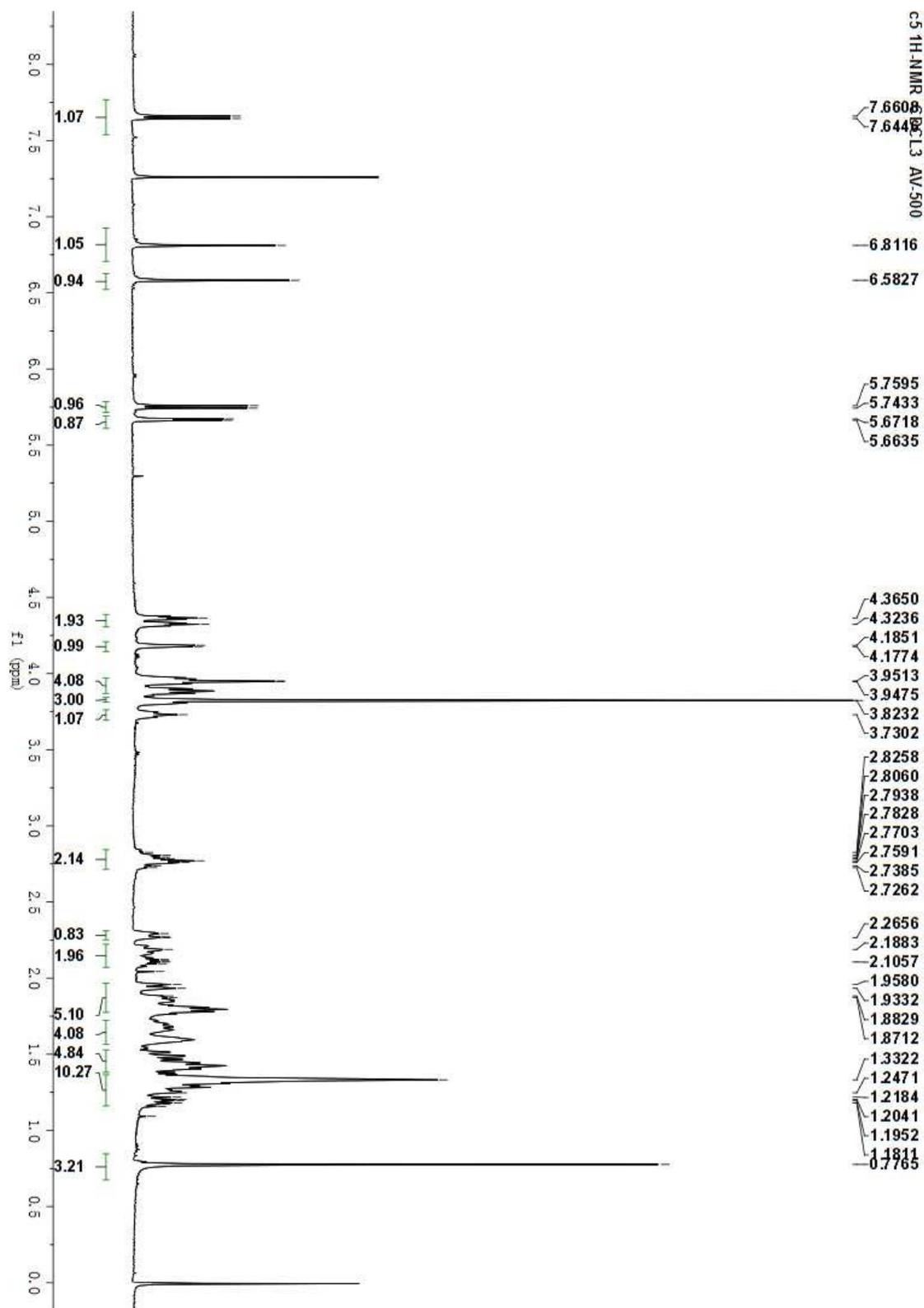


HRMS spectrum of 18

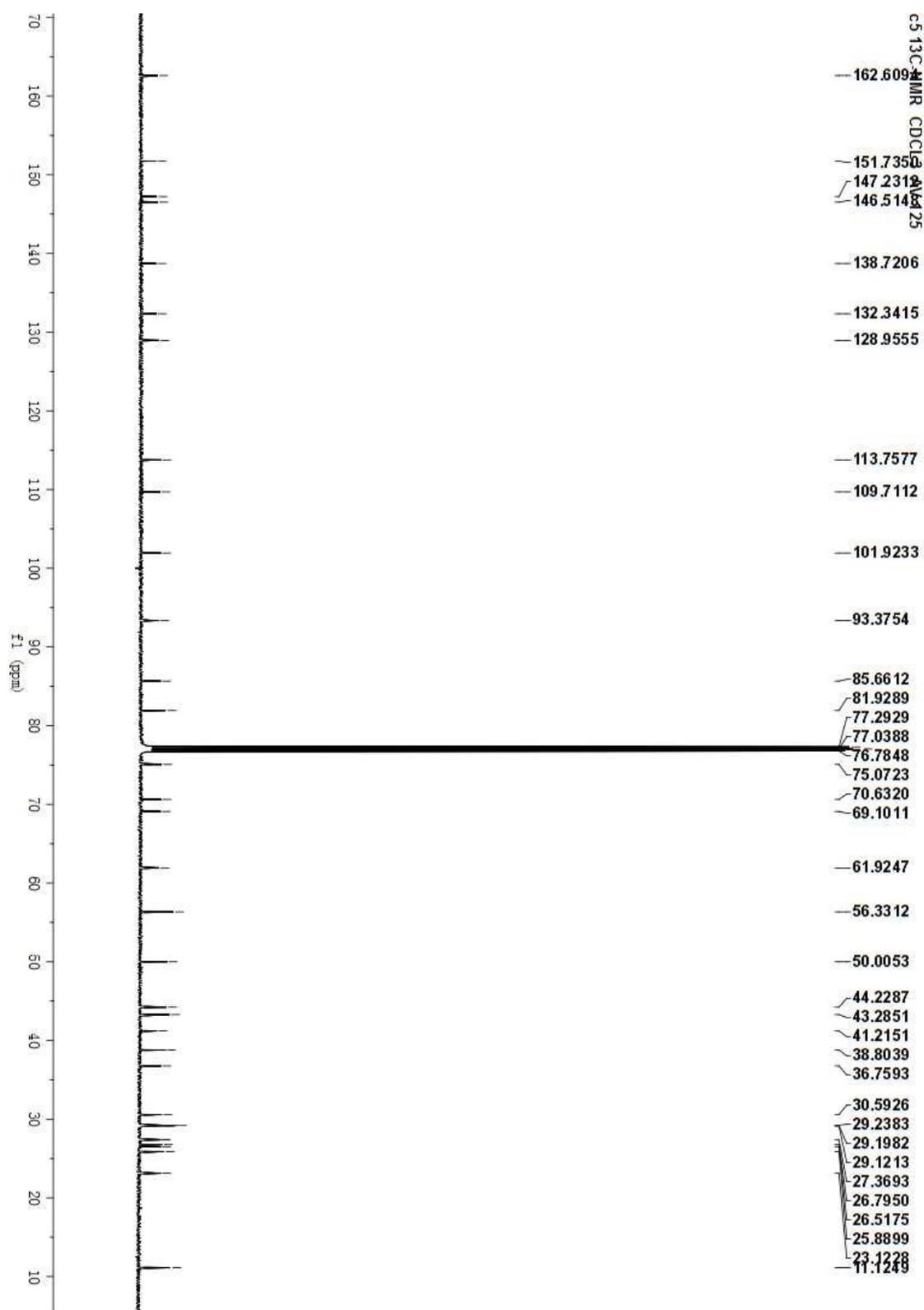
| | | | | | | | |
|---------------|--------|-------------|-------|-----------------|--------------|------------------------|---------|
| Sample Name | | Position | P2-A5 | Instrument Name | Instrument 1 | User Name | |
| Inj Vol | 0.1 | InjPosition | | SampleType | Sample | IRM Calibration Status | Success |
| Data Filename | a5-p.d | ACQ Method | | Comment | | Acquired Time | |



¹H NMR spectrum of **19**

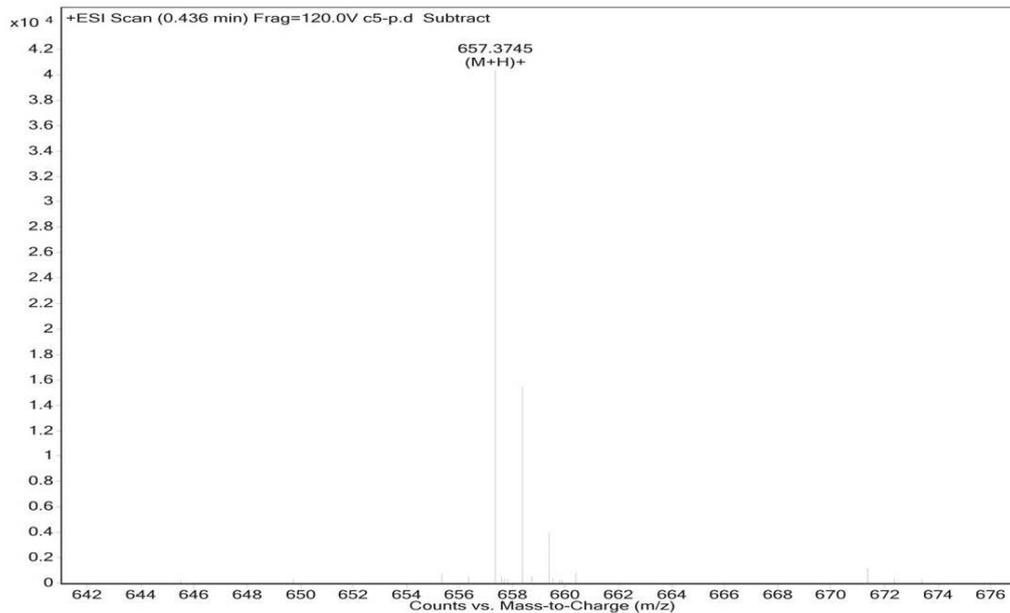


¹³C NMR spectrum of 19

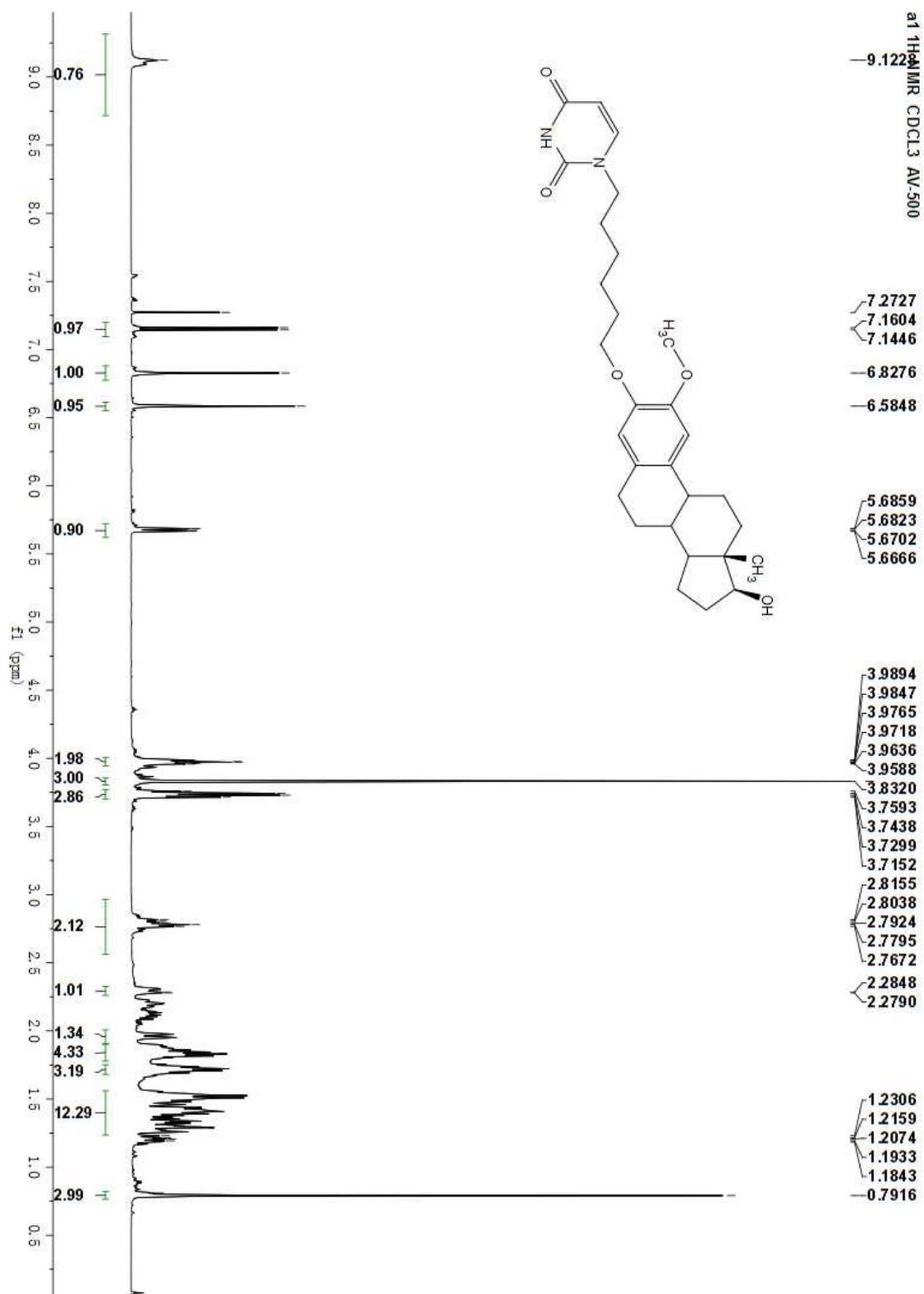


HRMS spectrum of 19

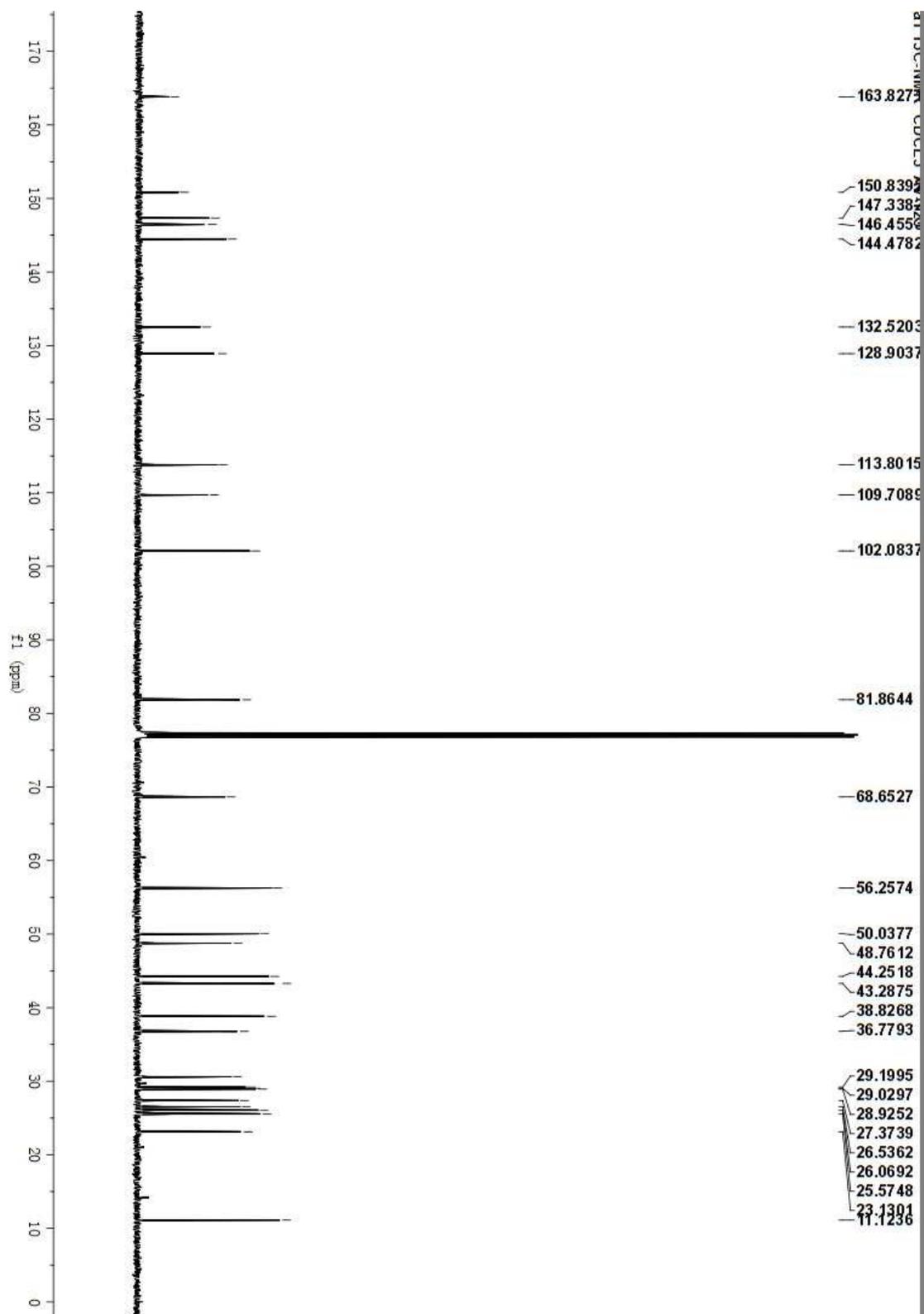
| | | | | | | | |
|---------------|--------|-------------|-------|-----------------|--------------|------------------------|---------|
| Sample Name | | Position | P2-B5 | Instrument Name | Instrument 1 | User Name | |
| Inj Vol | 0.1 | InjPosition | | SampleType | Sample | IRM Calibration Status | Success |
| Data Filename | c5-p.d | ACQ Method | | Comment | | Acquired Time | |



¹H NMR spectrum of 20a

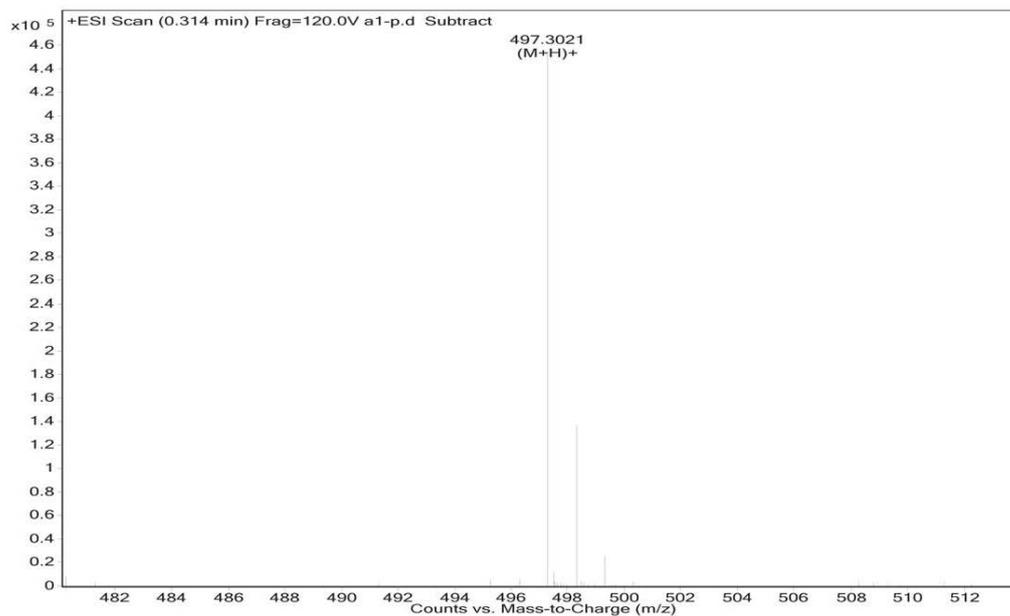


^{13}C NMR spectrum of **20a**

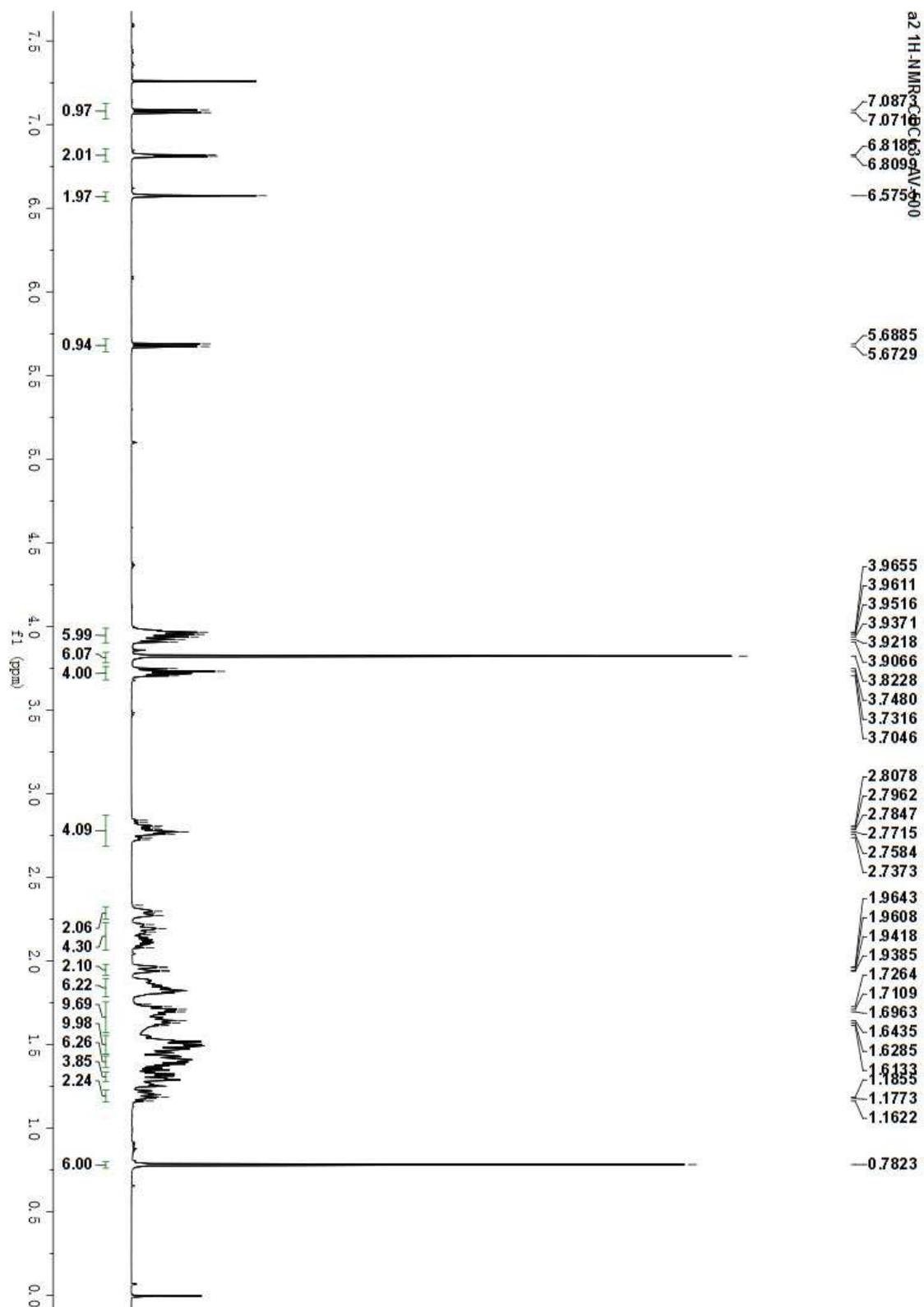


HRMS spectrum of 20a

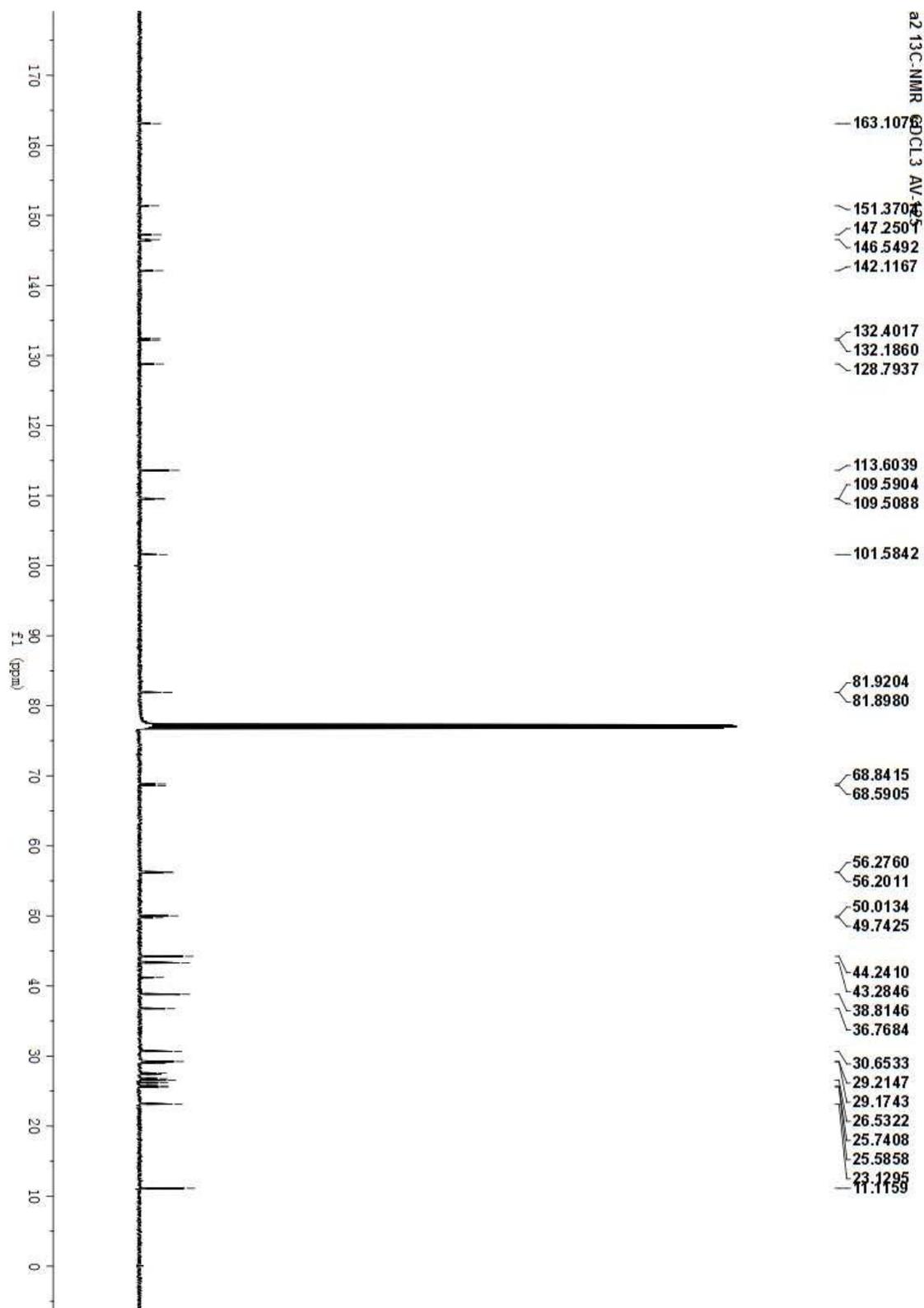
| | | | | | | | |
|---------------|--------|-------------|-------|-----------------|--------------|------------------------|---------|
| Sample Name | | Position | P2-A2 | Instrument Name | Instrument 1 | User Name | |
| Inj Vol | 0.1 | InjPosition | | SampleType | Sample | IRM Calibration Status | Success |
| Data Filename | a1-p.d | ACQ Method | | Comment | | Acquired Time | |



¹H NMR spectrum of 20b

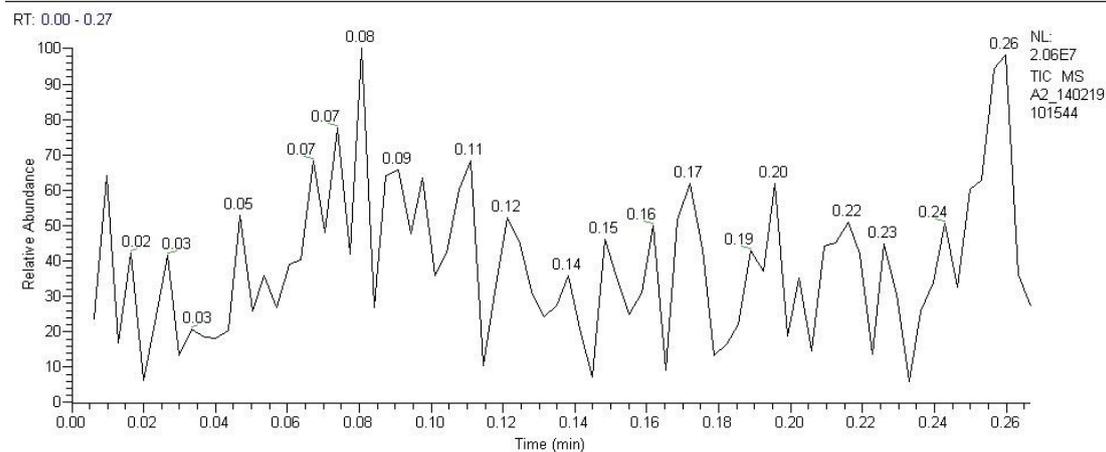


¹³C NMR spectrum of **20b**

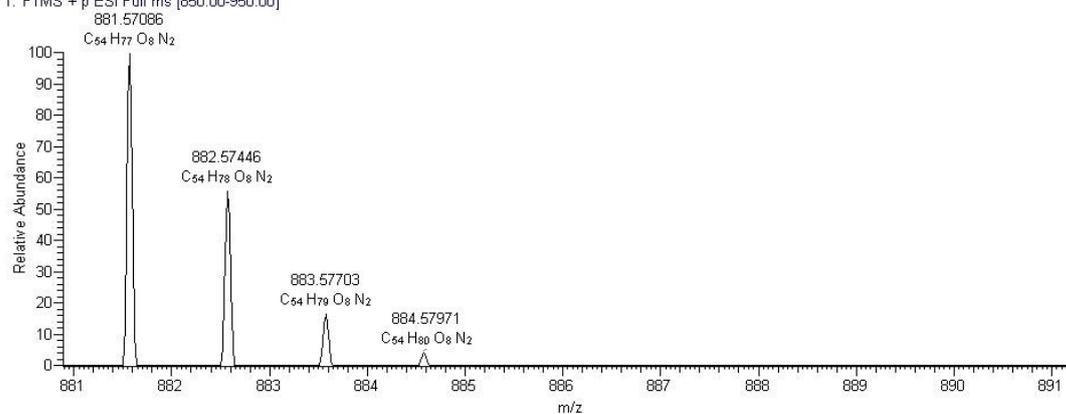


HRMS spectrum of 20b

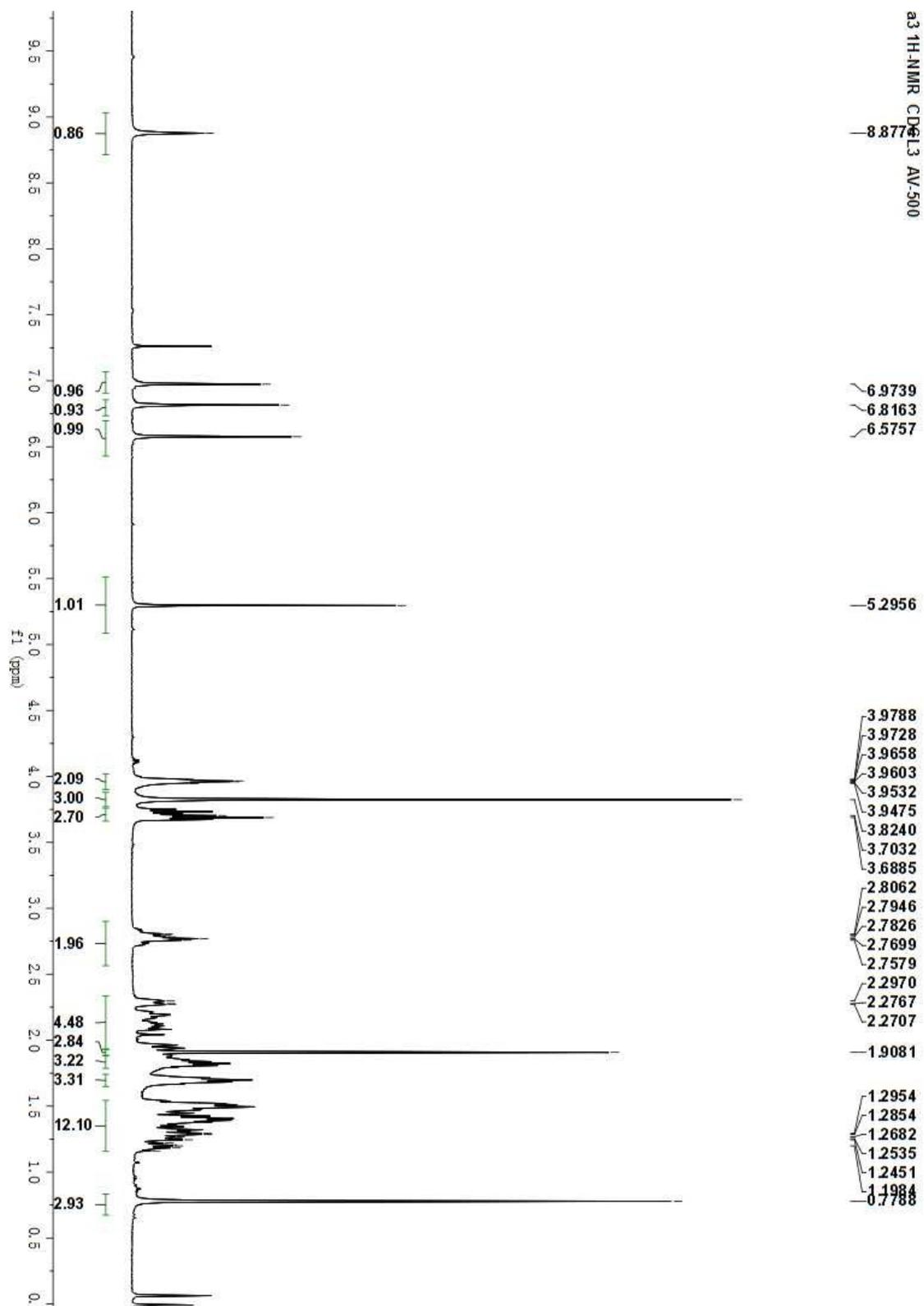
D:\data\



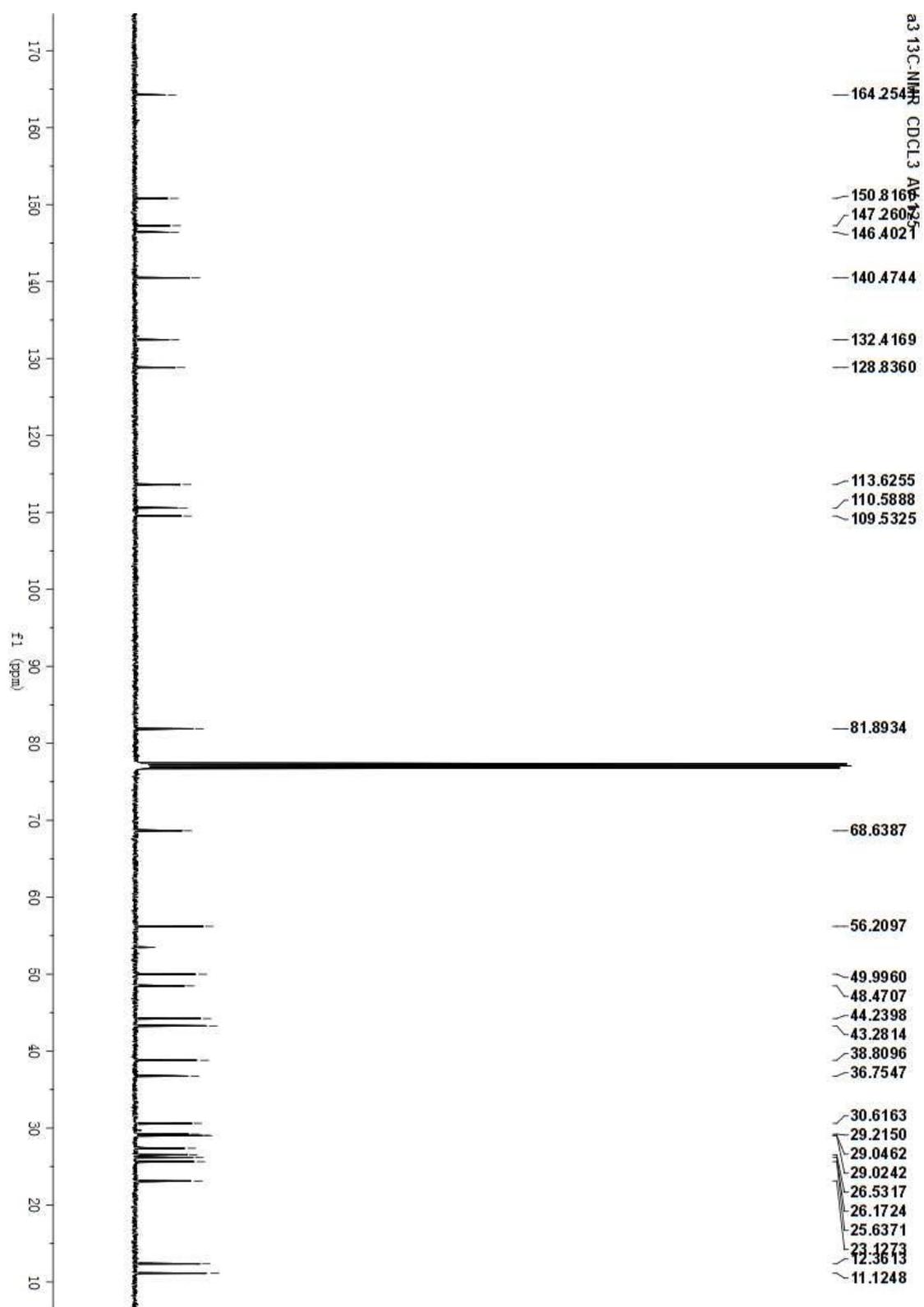
A2_140219101544 #1 RT: 0.01 AV: 1 NL: 8.99E5
T: FTMS + p ESI Full ms [950.00-950.00]



¹H NMR spectrum of 21a

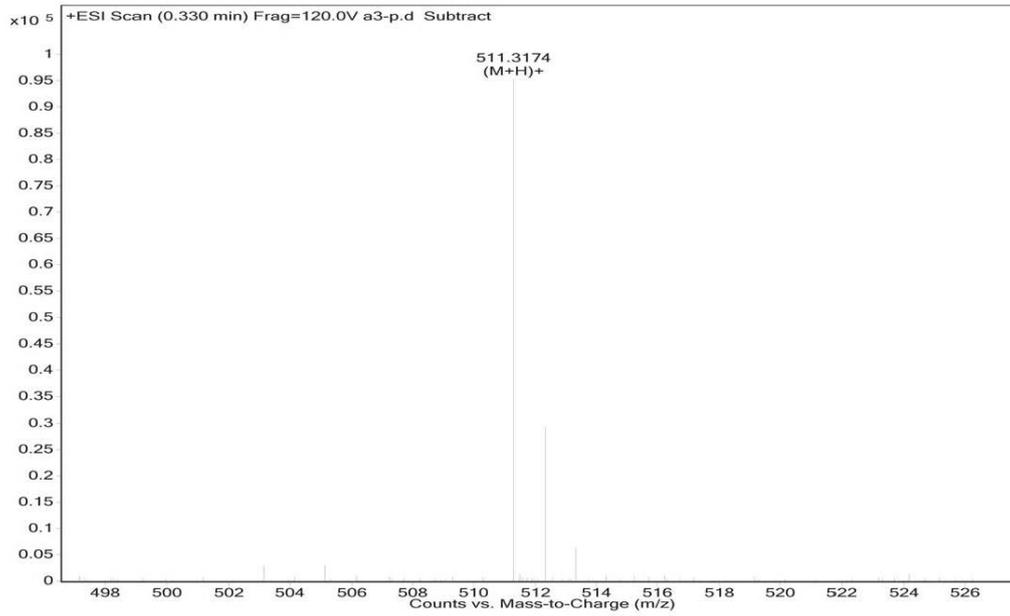


^{13}C NMR spectrum of **21a**

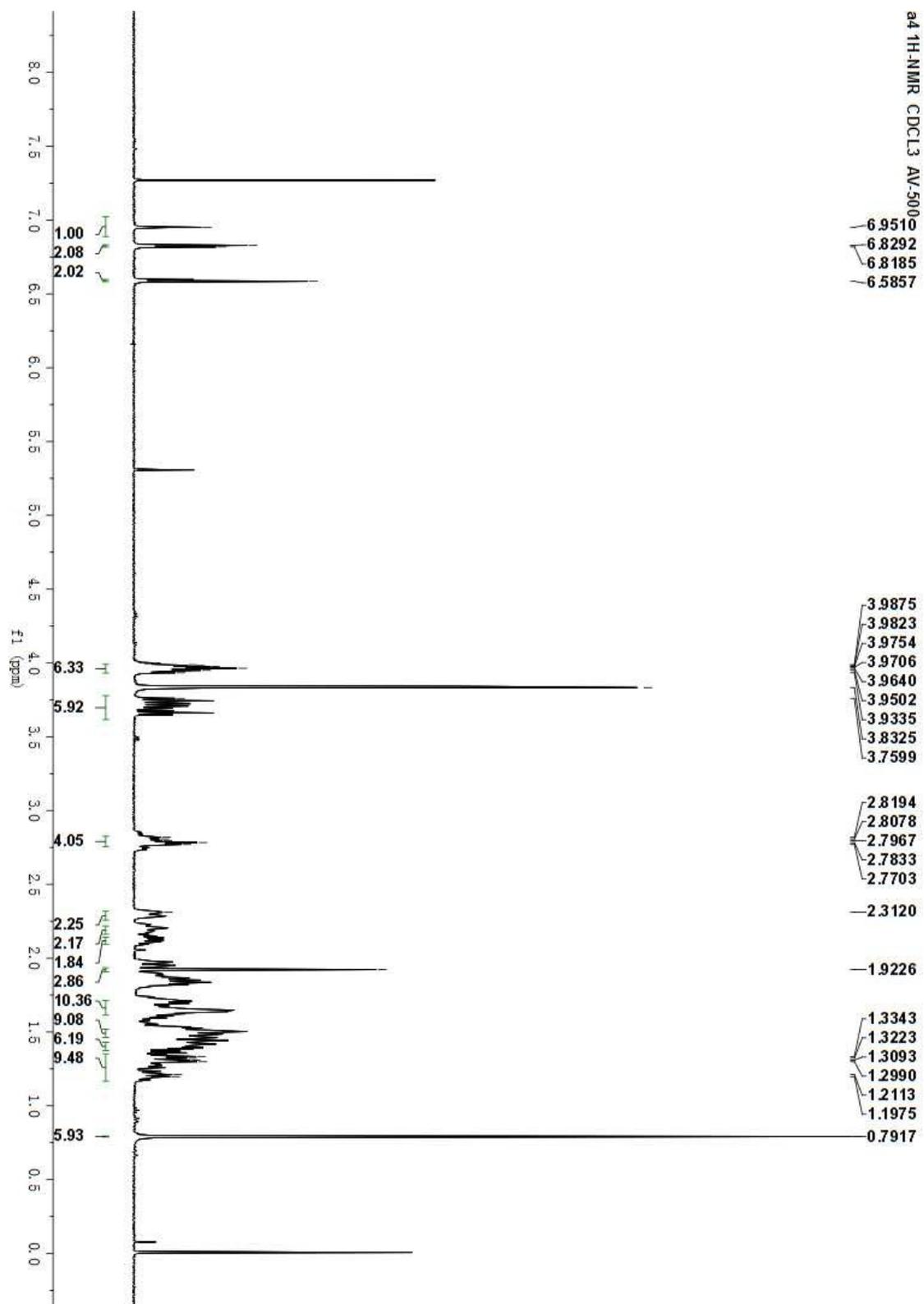


HRMS spectrum of 21a

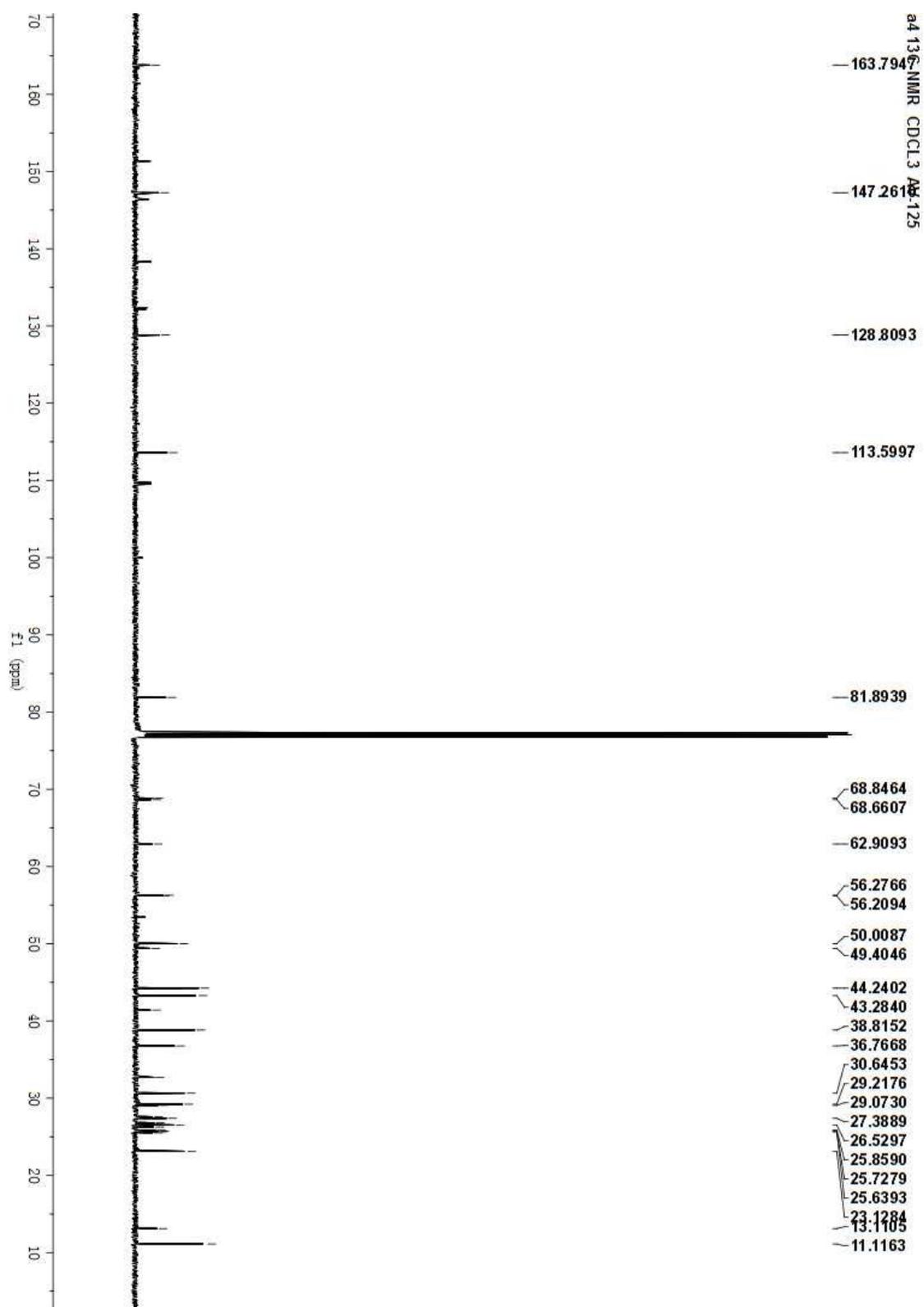
| | | | | | | | |
|---------------|--------|-------------|-------|-----------------|--------------|------------------------|---------|
| Sample Name | | Position | P2-A3 | Instrument Name | Instrument 1 | User Name | |
| Inj Vol | 0.1 | InjPosition | | SampleType | Sample | IRM Calibration Status | Success |
| Data Filename | a3-p.d | ACQ Method | | Comment | | Acquired Time | |



¹H NMR spectrum of 21b

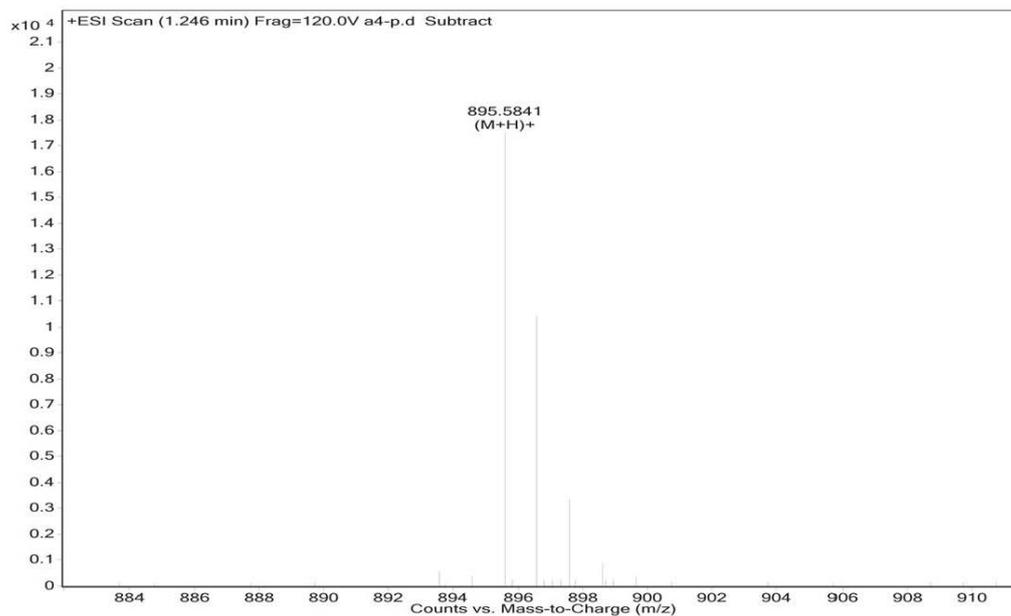


^{13}C NMR spectrum of **21b**

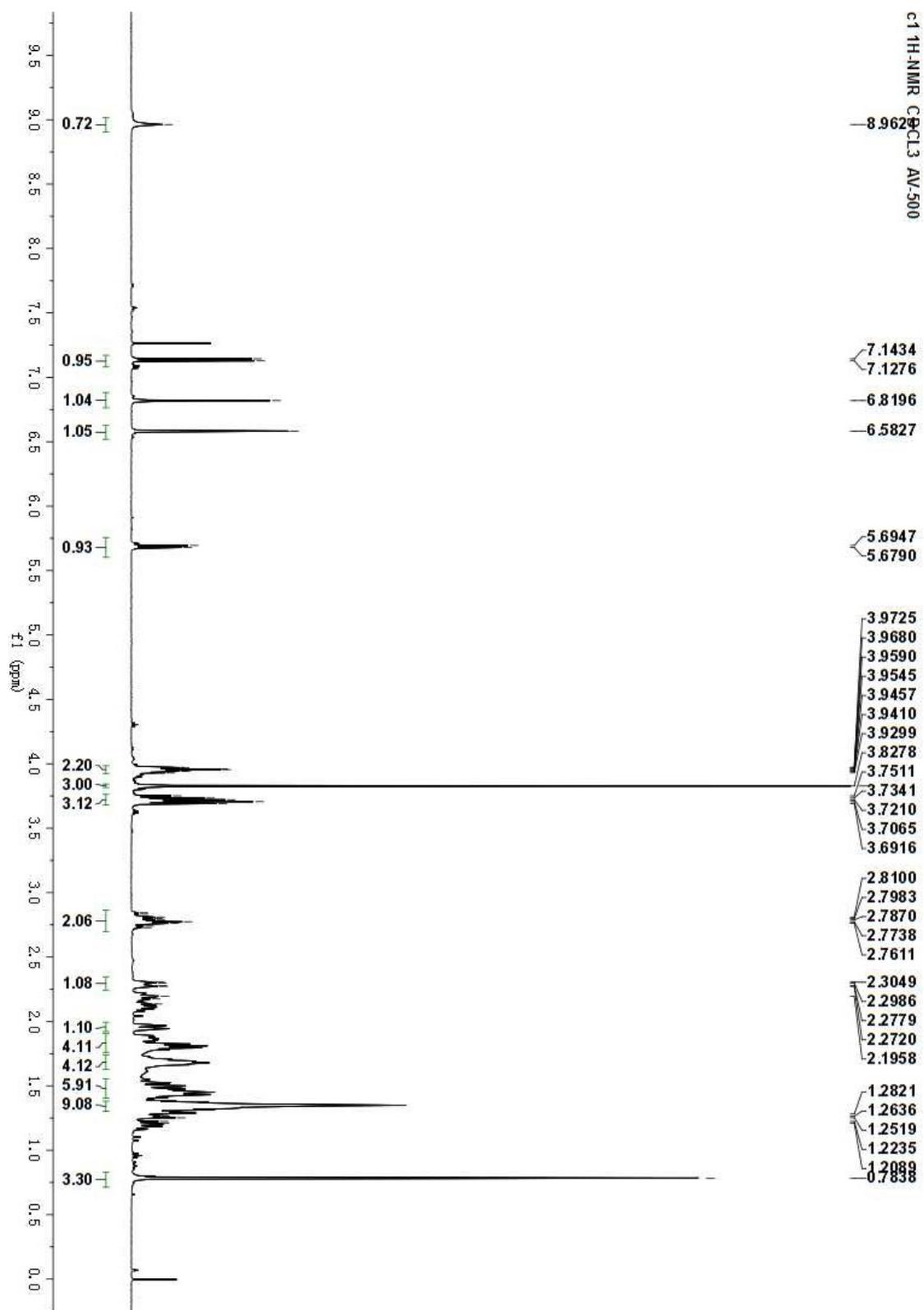


HRMS spectrum of **21b**

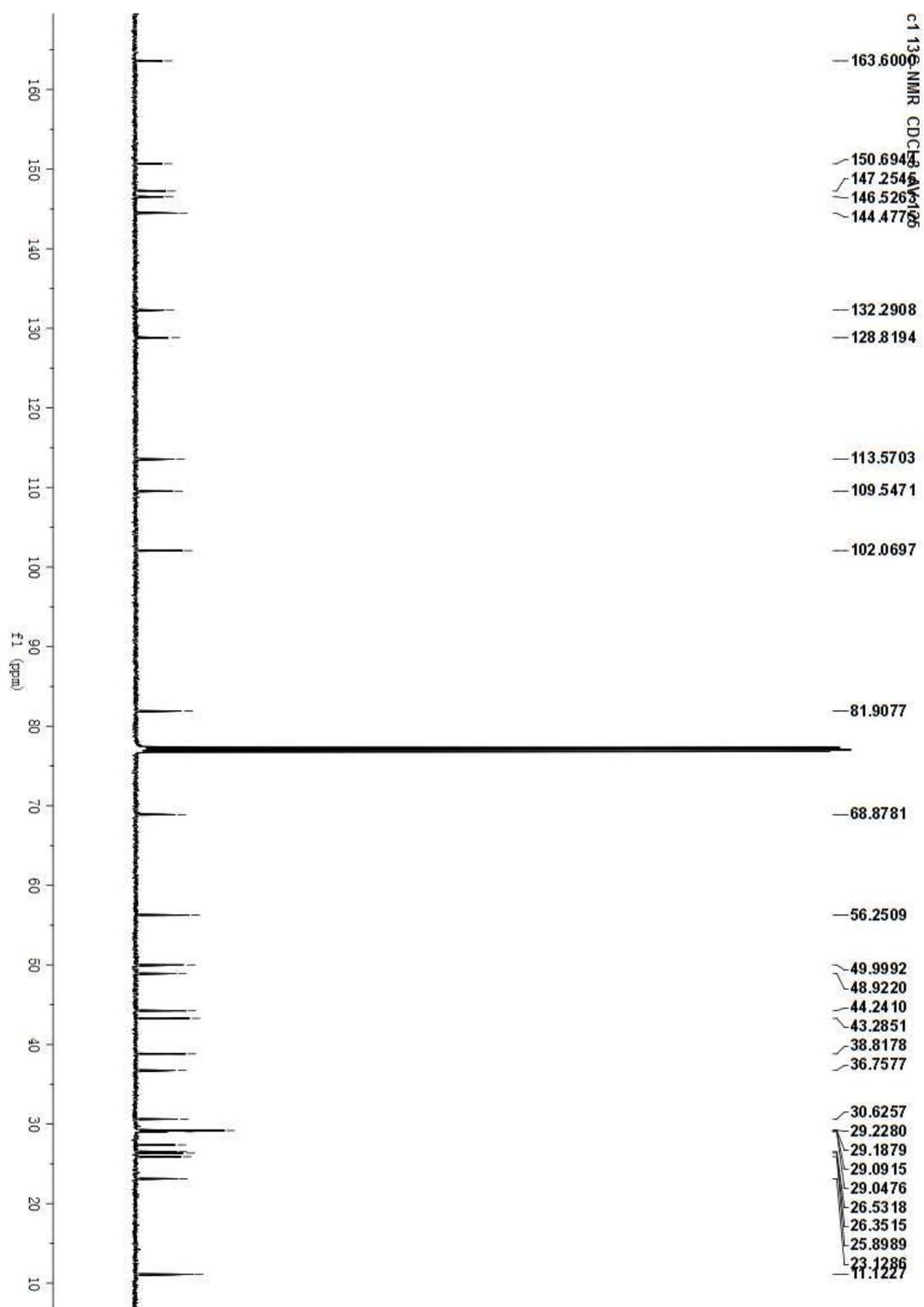
| | | | | | | | |
|---------------|--------|-------------|-------|-----------------|--------------|------------------------|---------|
| Sample Name | 0.1 | Position | P2-A4 | Instrument Name | Instrument 1 | User Name | |
| Inj Vol | 0.1 | InjPosition | | SampleType | Sample | IRM Calibration Status | Success |
| Data Filename | a4-p.d | ACQ Method | | Comment | | Acquired Time | |



¹H NMR spectrum of 22a

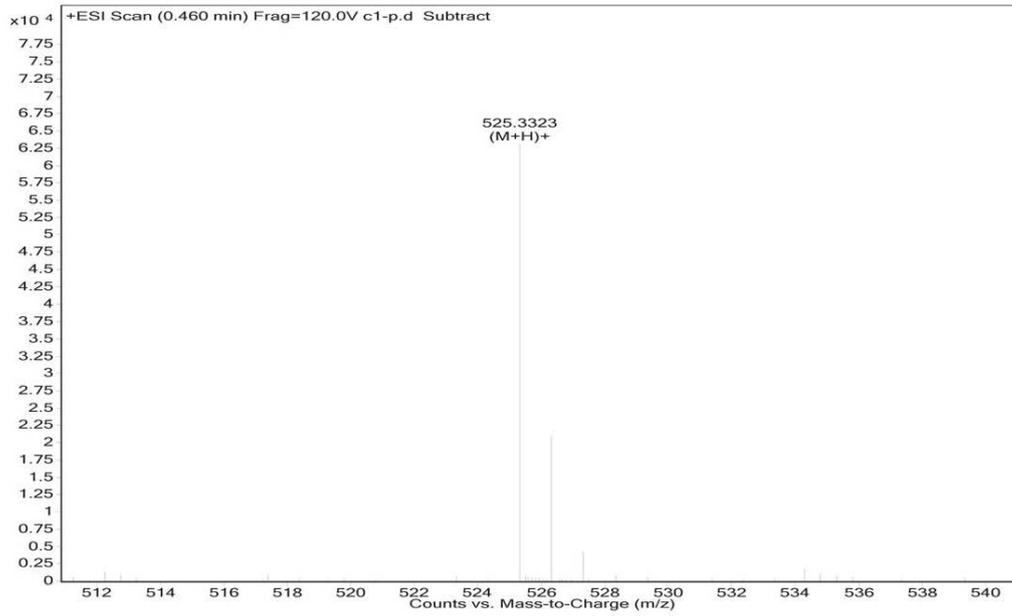


^{13}C NMR spectrum of **22a**

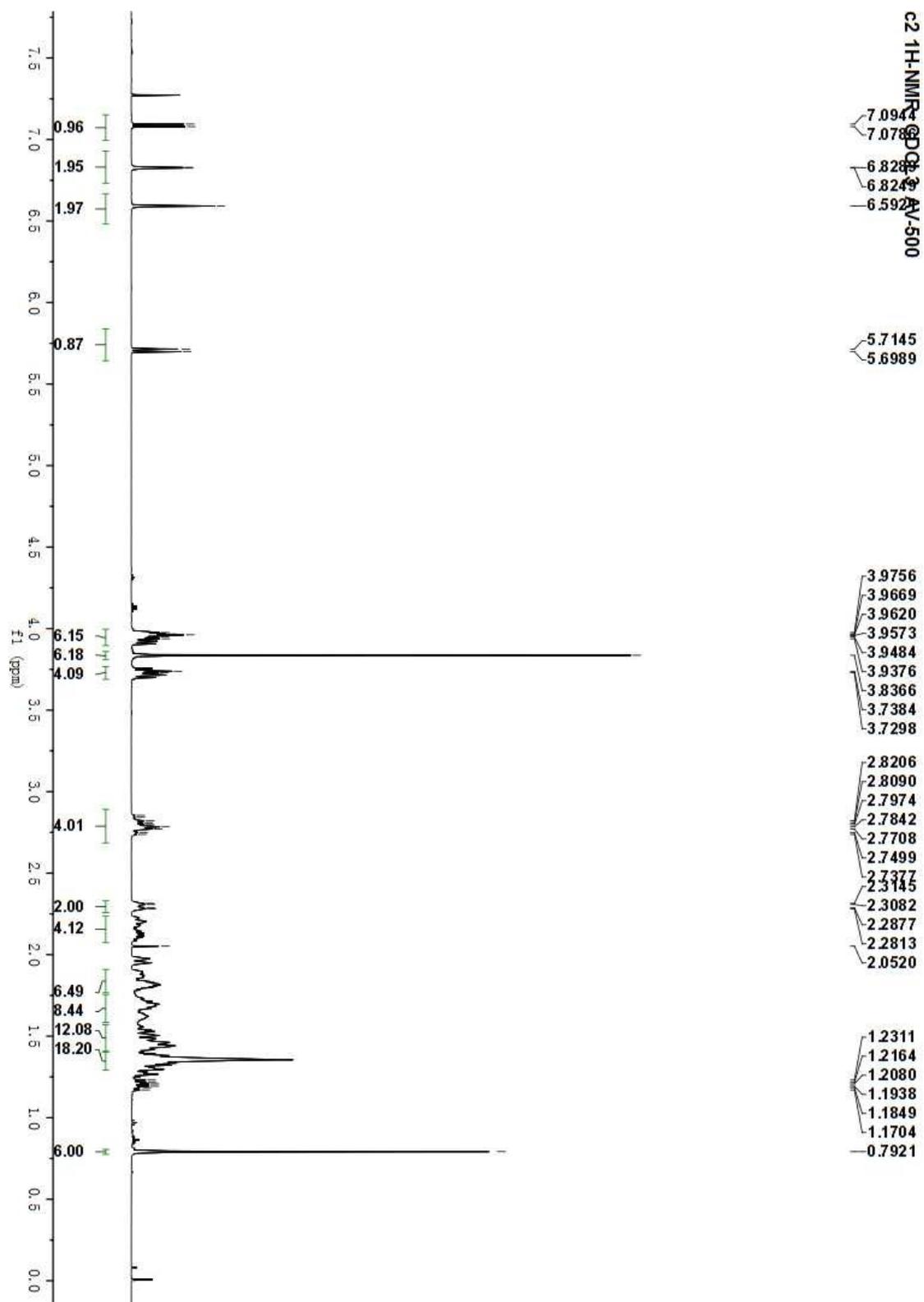


HRMS spectrum of 22a

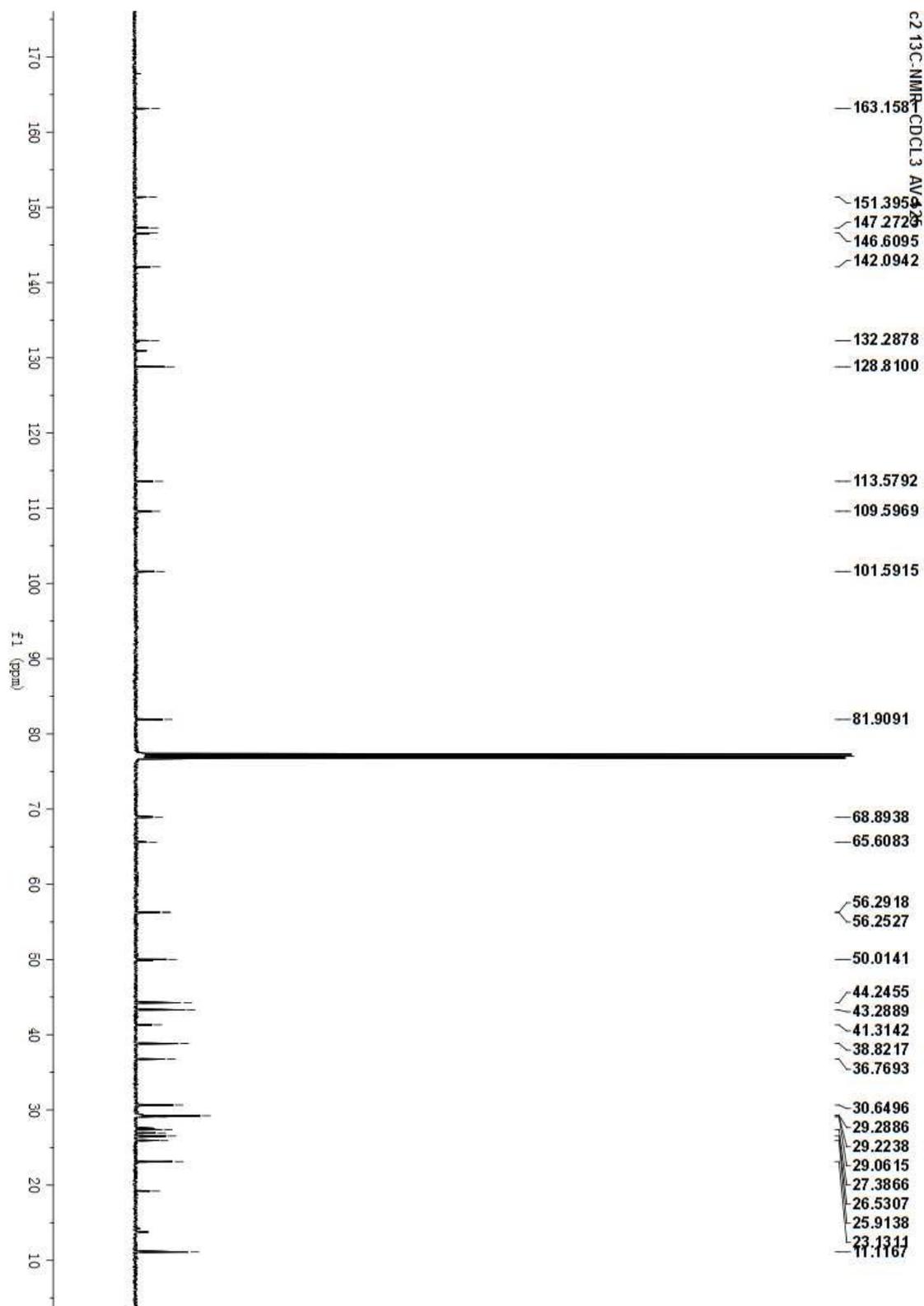
| | | | | | | | |
|---------------|--------|-------------|-------|-----------------|--------------|------------------------|---------|
| Sample Name | | Position | P2-B1 | Instrument Name | Instrument 1 | User Name | |
| Inj Vol | 0.1 | InjPosition | | SampleType | Sample | IRM Calibration Status | Success |
| Data Filename | c1-p.d | ACQ Method | | Comment | | Acquired Time | |



¹H NMR spectrum of 22b

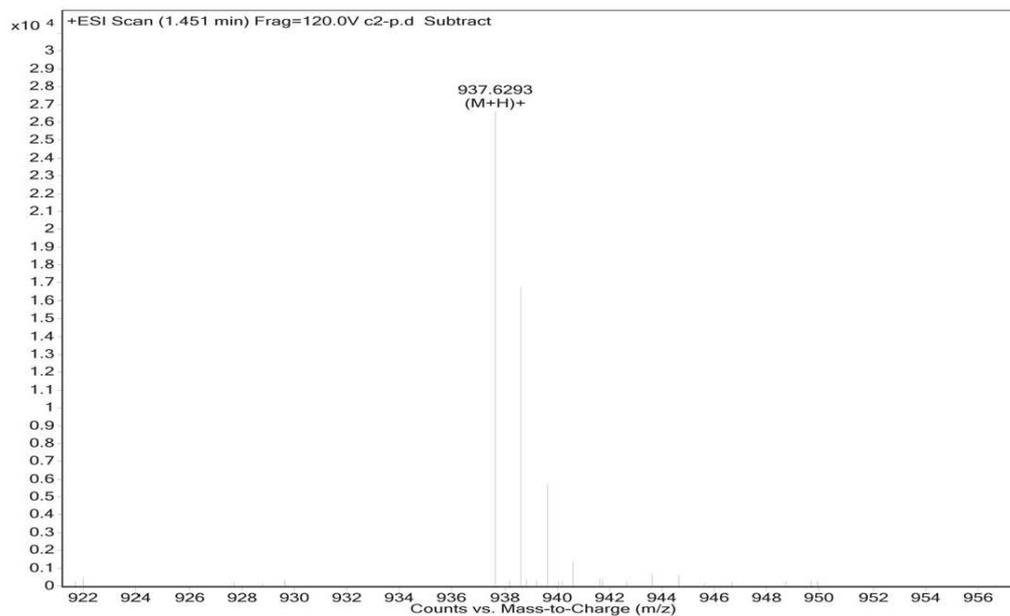


¹³C NMR spectrum of **22b**

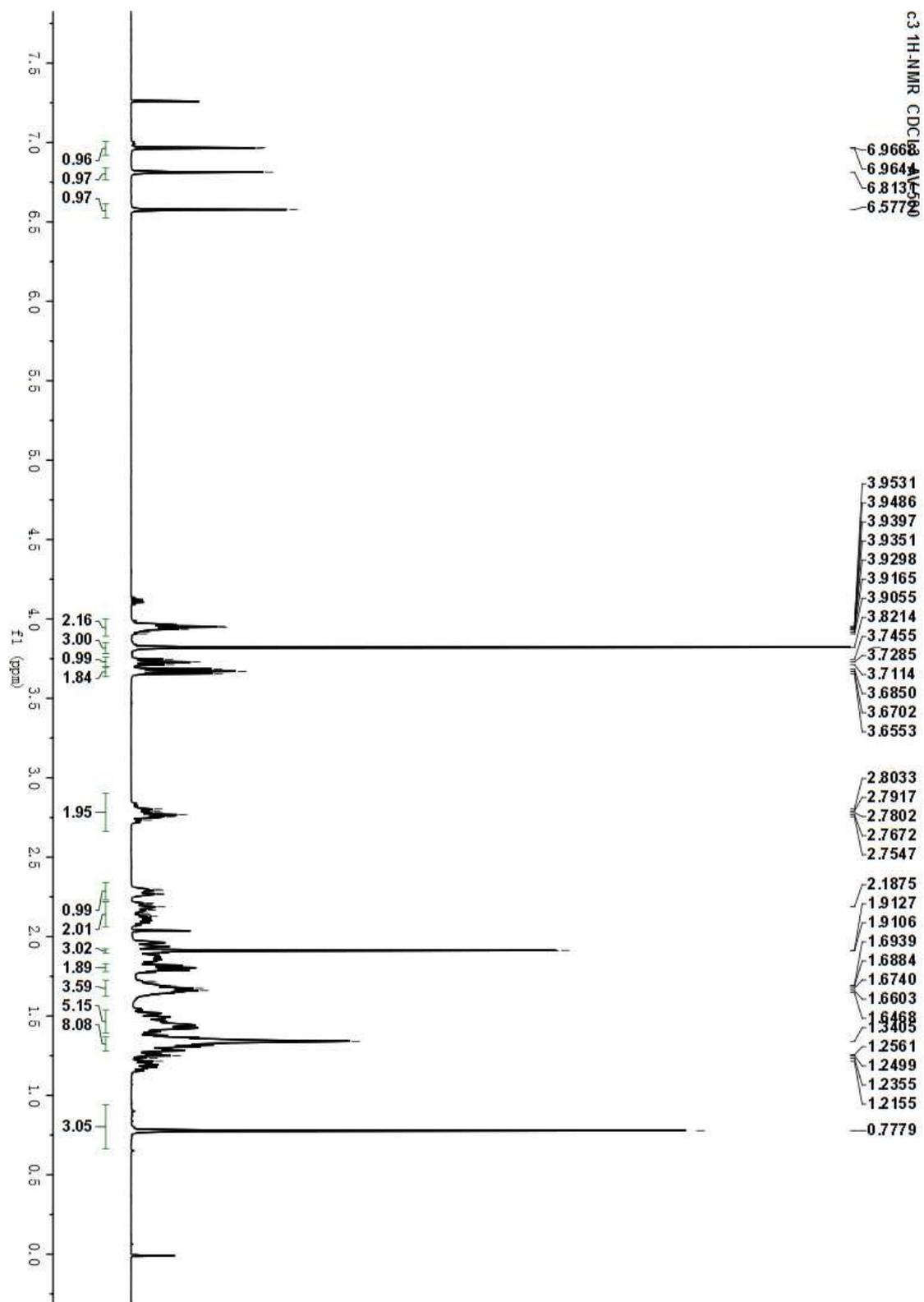


HRMS spectrum of 22b

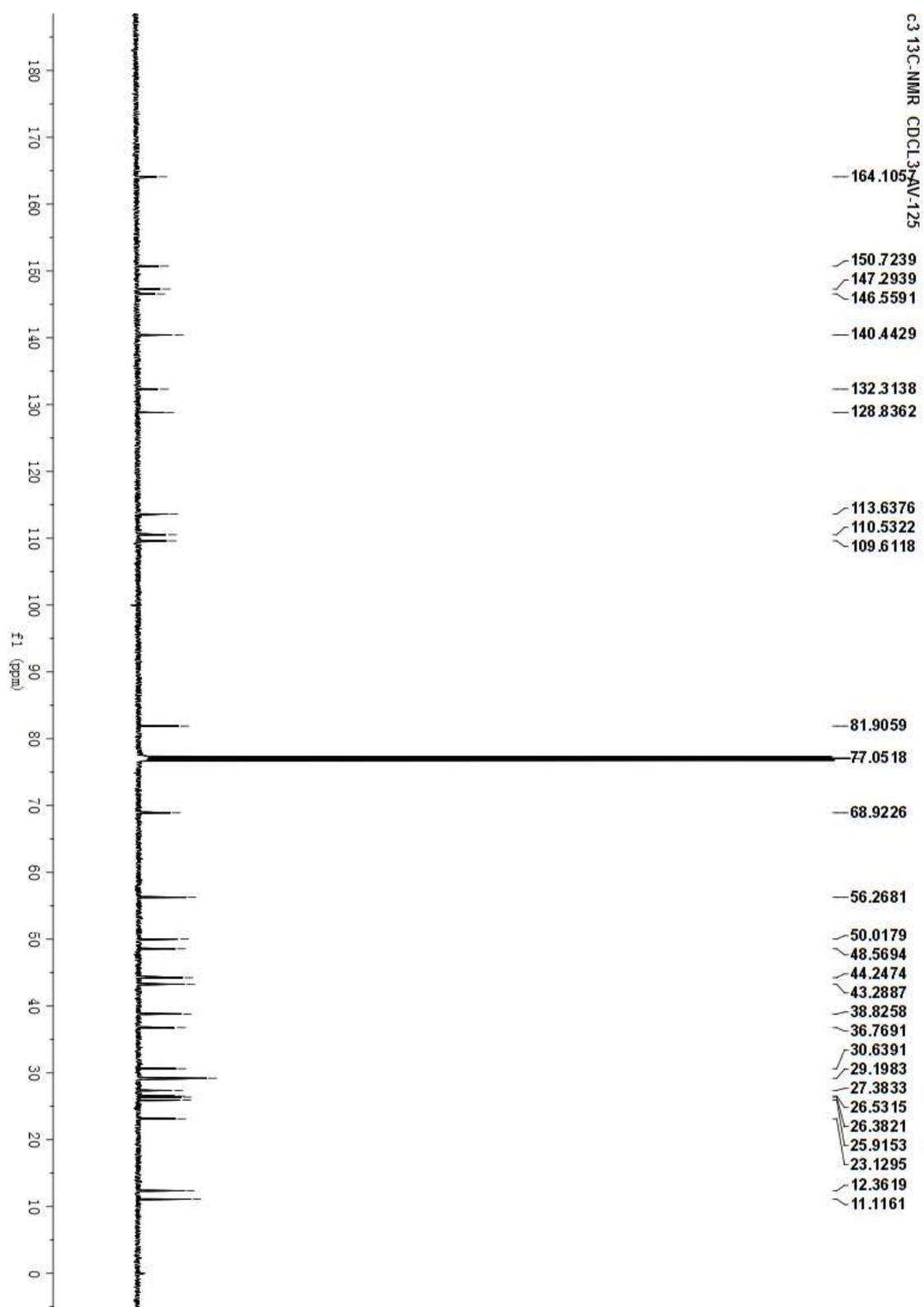
| | | | | | | | |
|---------------|--------|-------------|-------|-----------------|--------------|------------------------|---------|
| Sample Name | | Position | P2-B2 | Instrument Name | Instrument 1 | User Name | |
| Inj Vol | 0.1 | InjPosition | | SampleType | Sample | IRM Calibration Status | Success |
| Data Filename | c2-p.d | ACQ Method | | Comment | | Acquired Time | |



¹H NMR spectrum of 23a

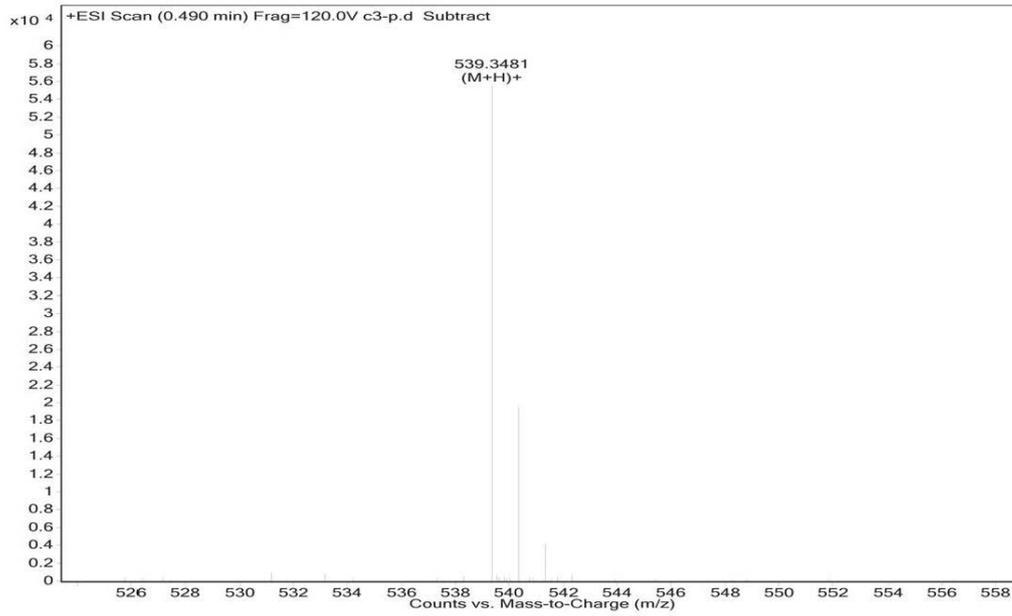


^{13}C NMR spectrum of **23a**

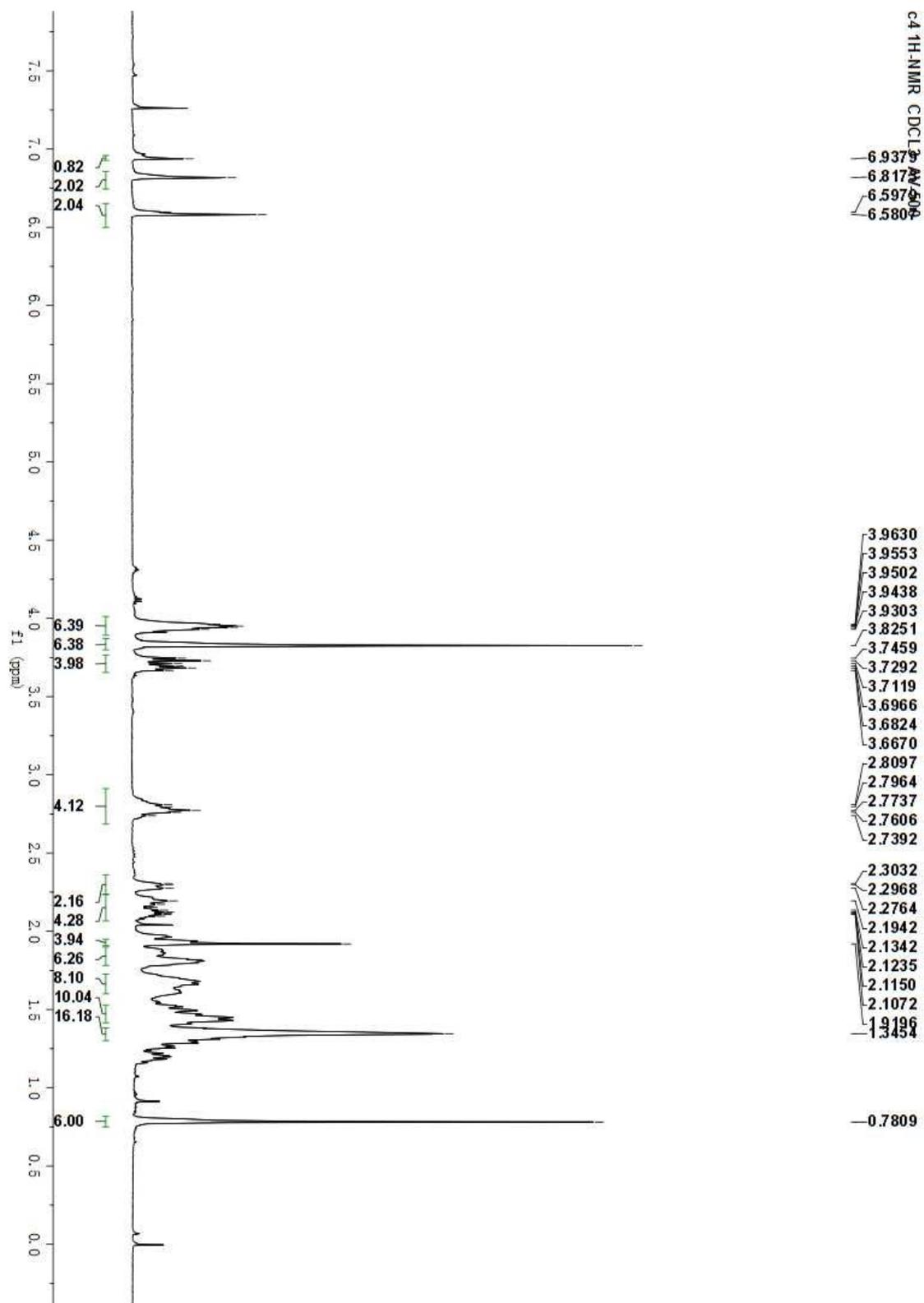


HRMS spectrum of 23a

| | | | | | | | |
|---------------|--------|-------------|-------|-----------------|--------------|------------------------|---------|
| Sample Name | | Position | P2-B3 | Instrument Name | Instrument 1 | User Name | |
| Inj Vol | 0.1 | InjPosition | | SampleType | Sample | IRM Calibration Status | Success |
| Data Filename | c3-p.d | ACQ Method | | Comment | | Acquired Time | |



¹H NMR spectrum of 23b



HRMS spectrum of 23b

| | | | | | | | |
|---------------|--------|-------------|-------|-----------------|--------------|------------------------|---------|
| Sample Name | | Position | P2-B4 | Instrument Name | Instrument 1 | User Name | |
| Inj Vol | 0.1 | InjPosition | | SampleType | Sample | IRM Calibration Status | Success |
| Data Filename | c4-p.d | ACQ Method | | Comment | | Acquired Time | |

