

Supporting Information for

Acylphloroglucinols with acetylcholinesterase inhibitory effects from the fruits of *Eucalyptus robusta*

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TABLE OF CONTENTS

| Content | Pages |
|--|---------|
| Figure S1 Key ROESY correlations of 1–4 | S1 |
| Figure S2 Chiral analysis of 6, 8 , and a mixture of 10 and 11 | S1 |
| Figures S3–S8 NMR spectra of 1 in CDCl ₃ | S2–S2 |
| Figure S9 HRESIMS spectrum of 1 | S2 |
| Figures S10–S15 NMR spectra of 2 in CDCl ₃ | S2–S9 |
| Figure S16 HRESIMS spectrum of 2 | S9 |
| Figures S17–S22 NMR spectra of 3 in CDCl ₃ | S10–S13 |
| Figure S23 HRESIMS spectrum of 3 | S13 |
| Figures S24–S29 NMR spectra of 4 in CDCl ₃ | S14–S17 |
| Figure S30 HRESIMS spectrum of 4 | S17 |
| Figures S31–S36 NMR spectra of 5 in CDCl ₃ | S18–S21 |
| Figure S37 HRESIMS spectrum of 5 | S21 |
| Figures S38–S42 NMR spectra of 6 in methanol- <i>d</i> ₄ | S22–S24 |
| Figure S43 HRESIMS spectrum of 6 | S24 |
| Figures S44–S48 NMR spectra of 7 in CDCl ₃ | S25–S27 |
| Figure S49 HRESIMS spectrum of 7 | S27 |
| Figures S50–S54 NMR spectra of 8 in acetone- <i>d</i> ₆ | S28–S30 |
| Figure S55 HRESIMS spectrum of 8 | S30 |
| Figures S56–S60 NMR spectra of 9 in CDCl ₃ | S31–S33 |
| Figure S61 HRESIMS spectrum of 9 | S34 |
| Figures S62–S66 NMR spectra of 10 and 11 in pyridine- <i>d</i> ₅ | S34–S36 |
| Figure S67 HRESIMS spectrum of 10 and 11 | S37 |
| ECD computational data of 2–6 and 8 | S38–S42 |

Figure S1 Key ROESY correlations of **1–4**.

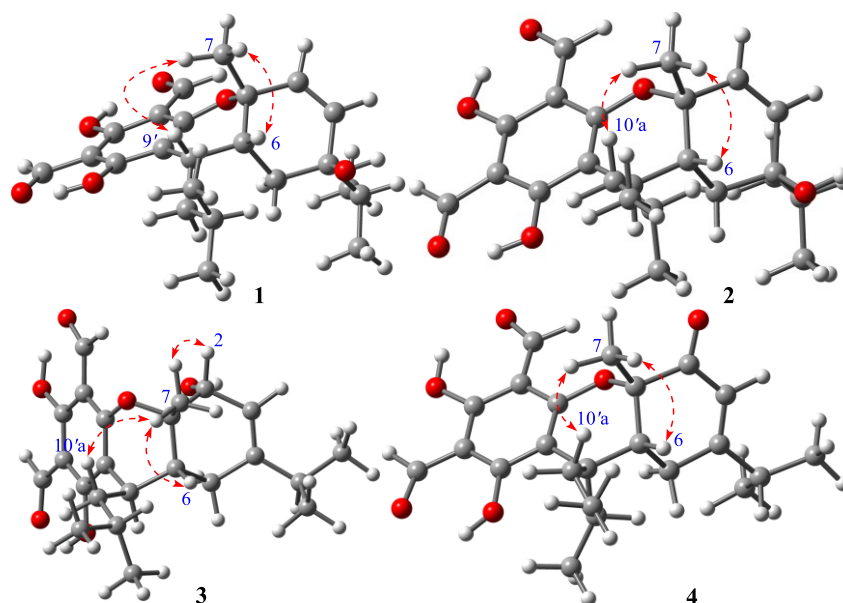


Figure S2 Chiral analysis of **6**, **8**, and a mixture of **10** and **11** by a CHIRALPAK IC column

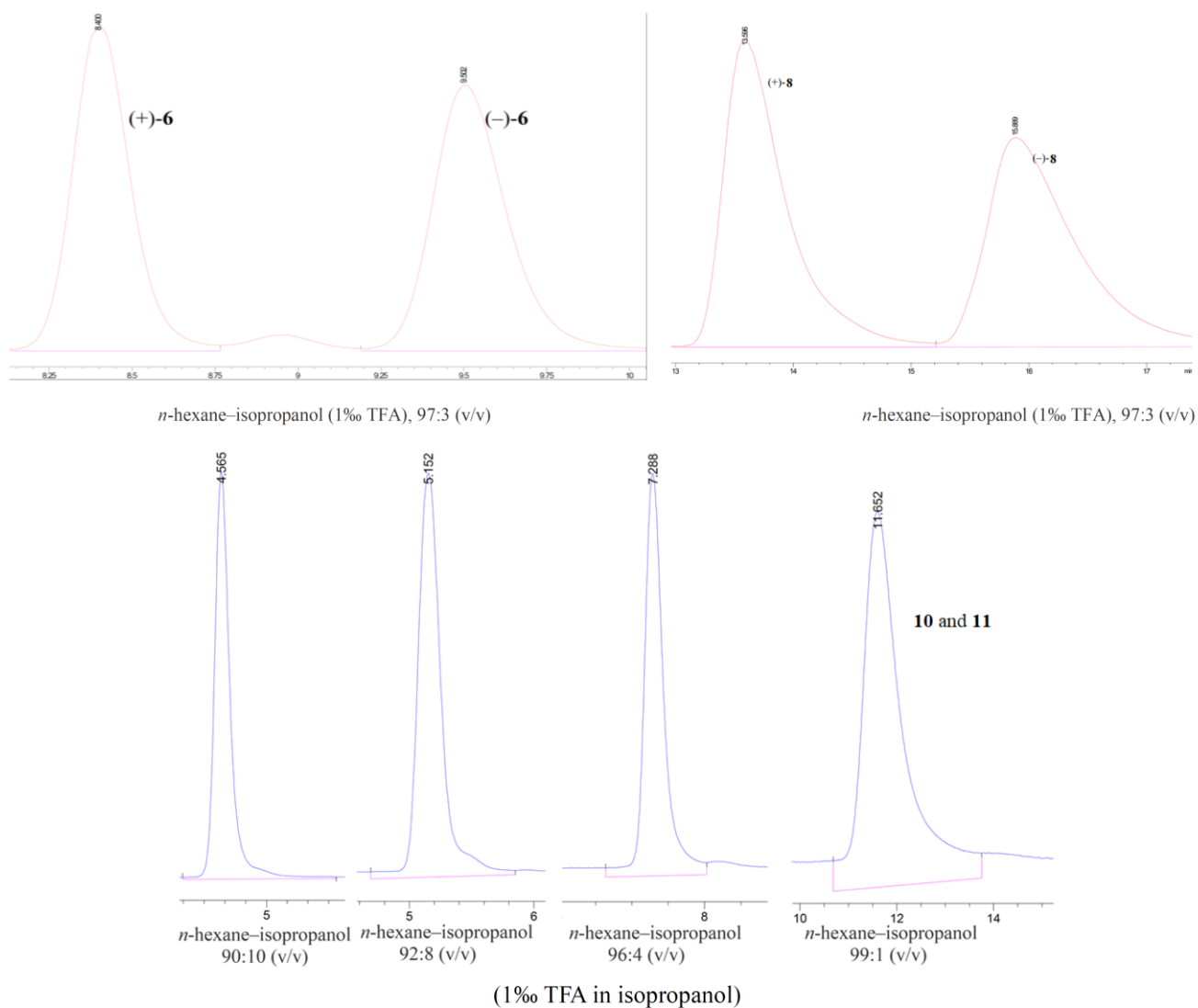


Figure S3 ^1H NMR spectrum of **1** (500 MHz, CDCl_3)

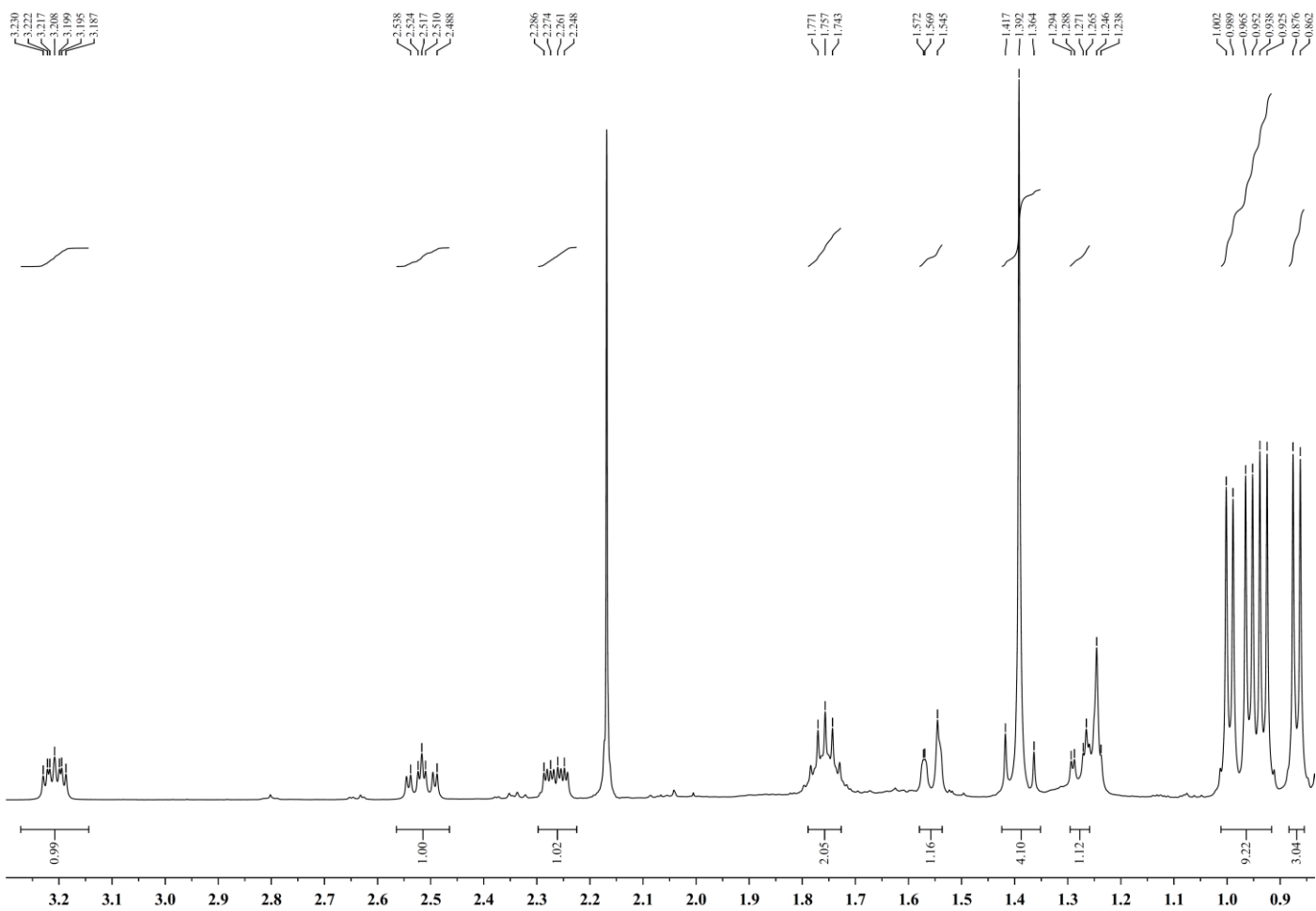
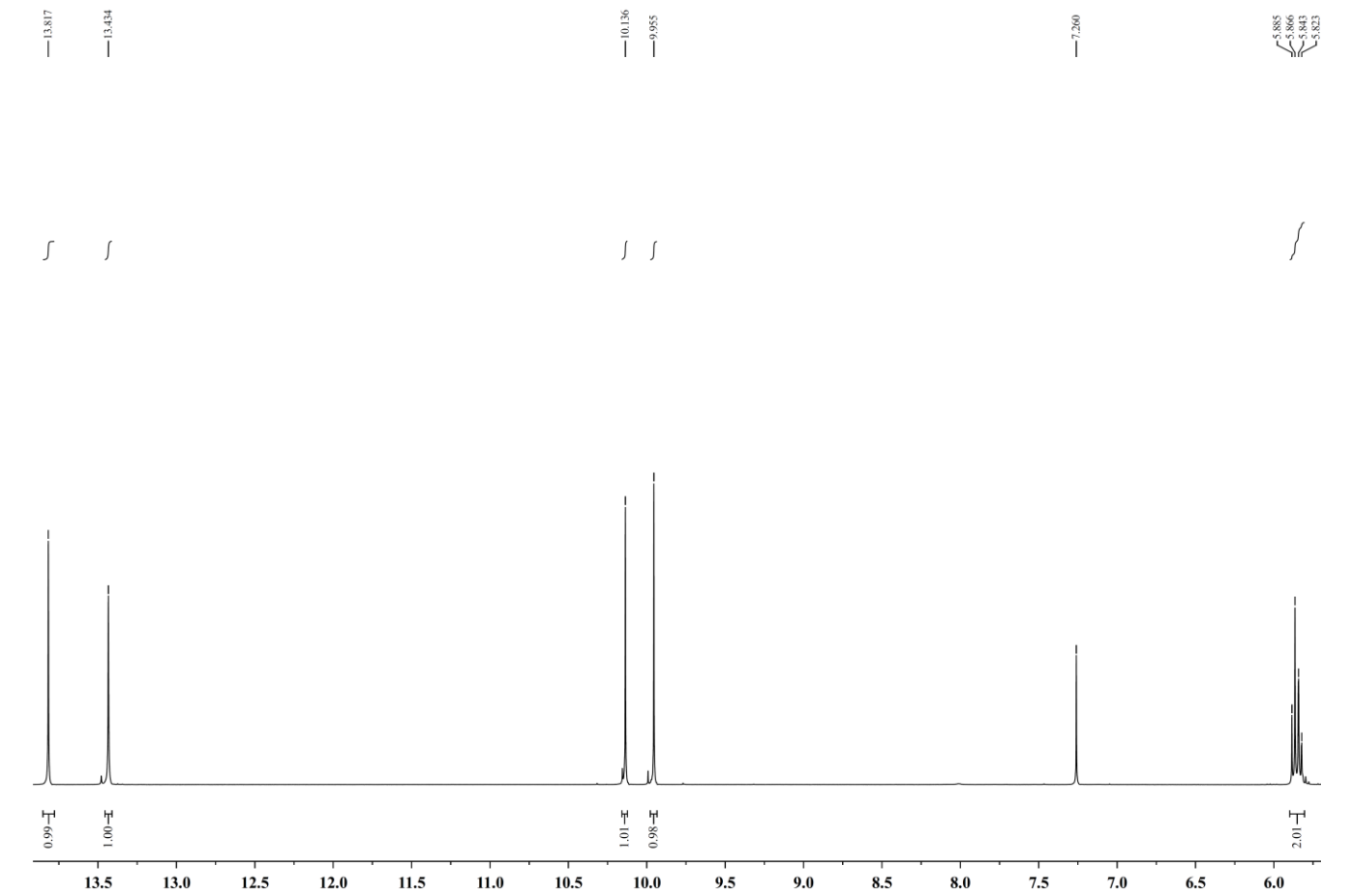


Figure S4 ^{13}C NMR spectrum of **1** (125 MHz, CDCl_3)

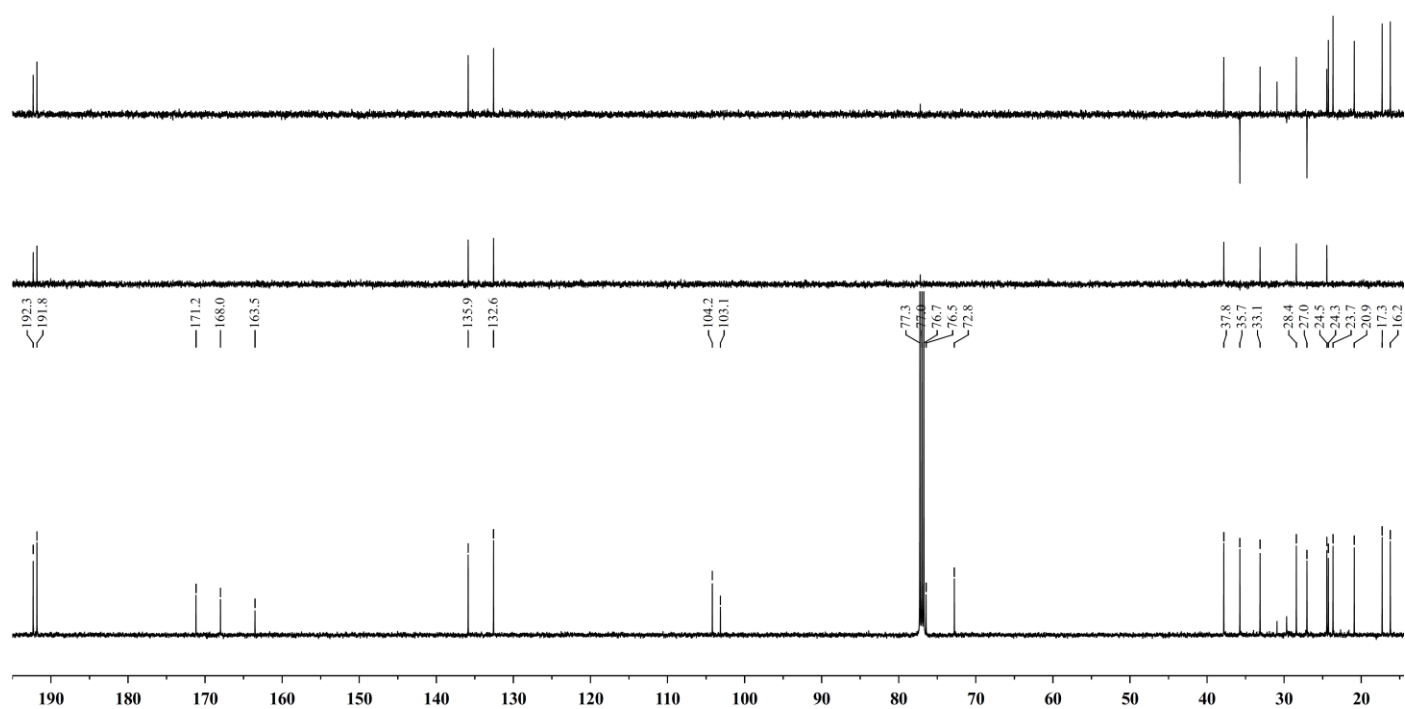


Figure S5 HSQC spectrum of **1**

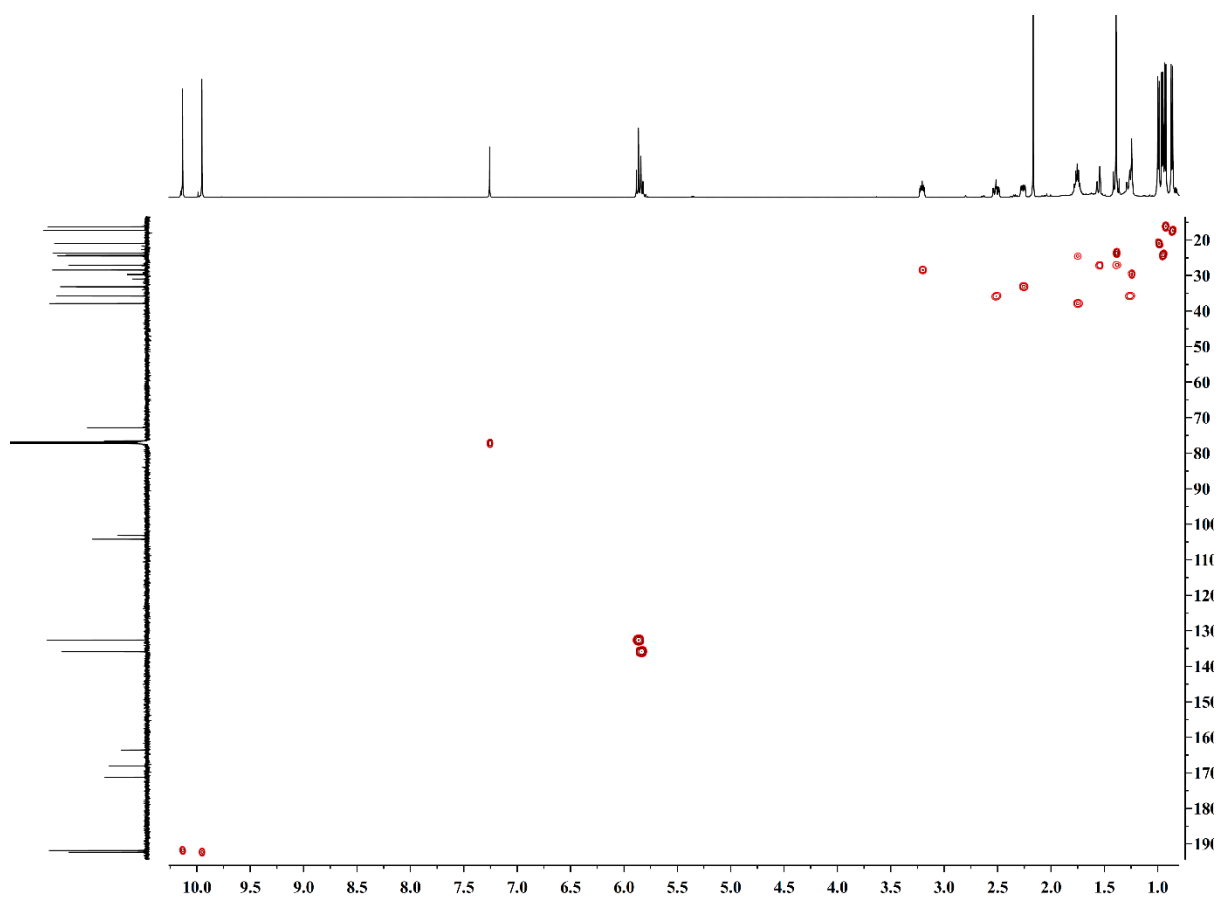


Figure S6 HMBC spectrum of **1**

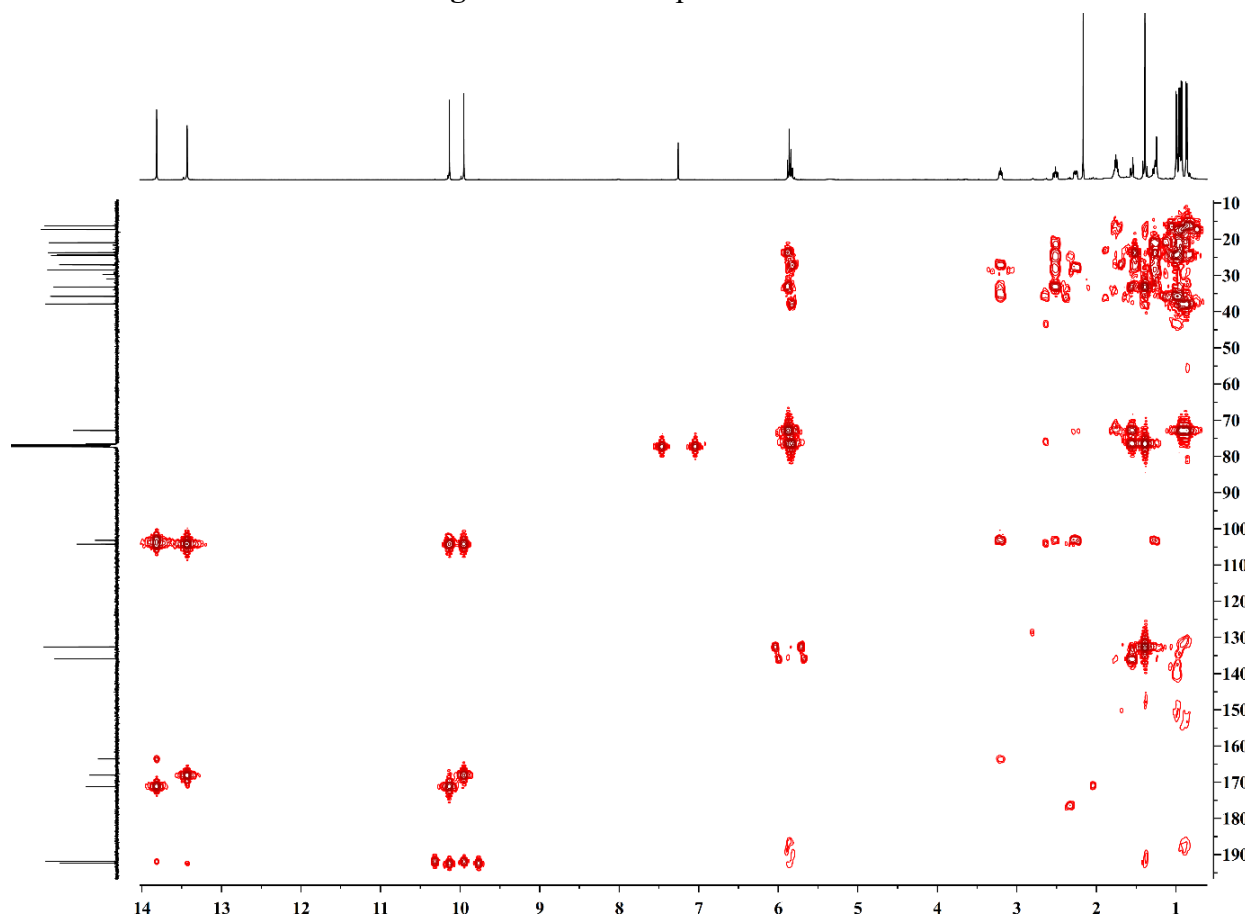


Figure S7 ^1H - ^1H COSY spectrum of **1**

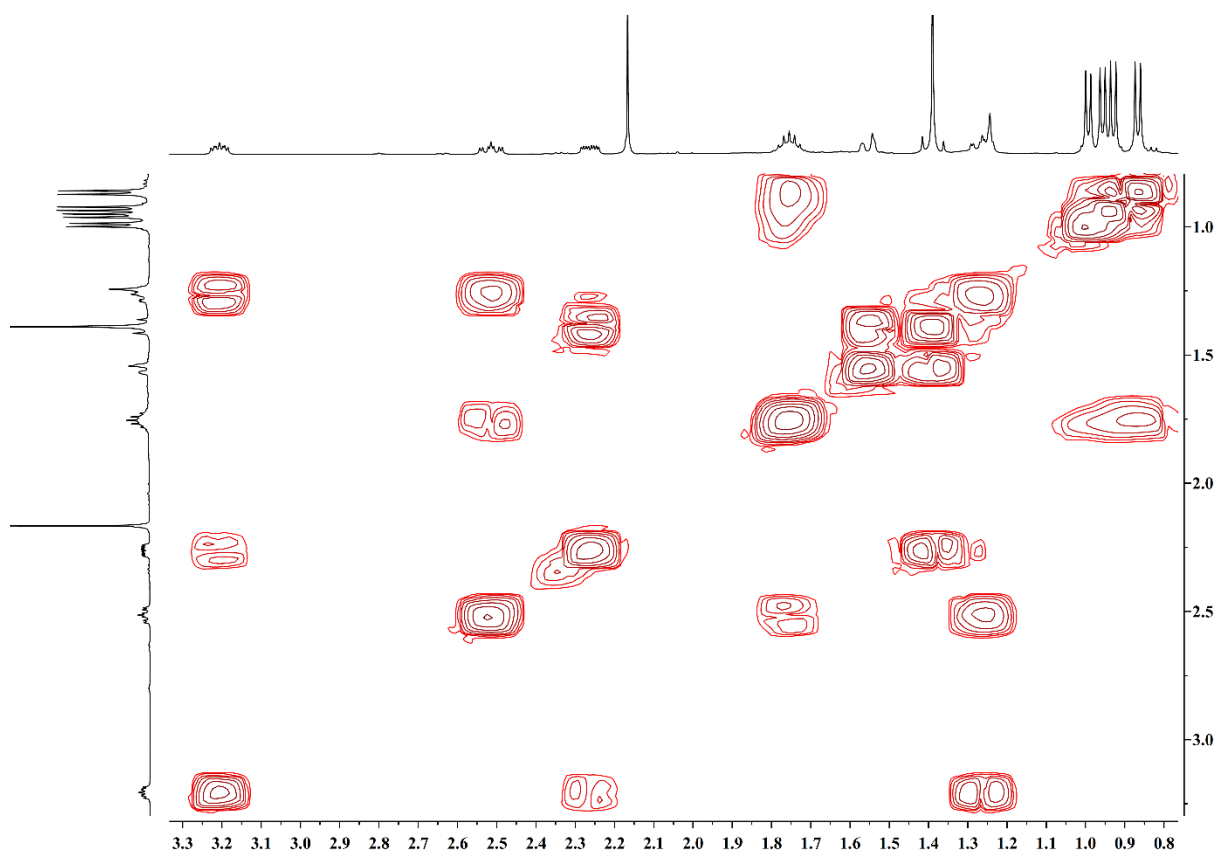


Figure S8 ROESY spectrum of 1

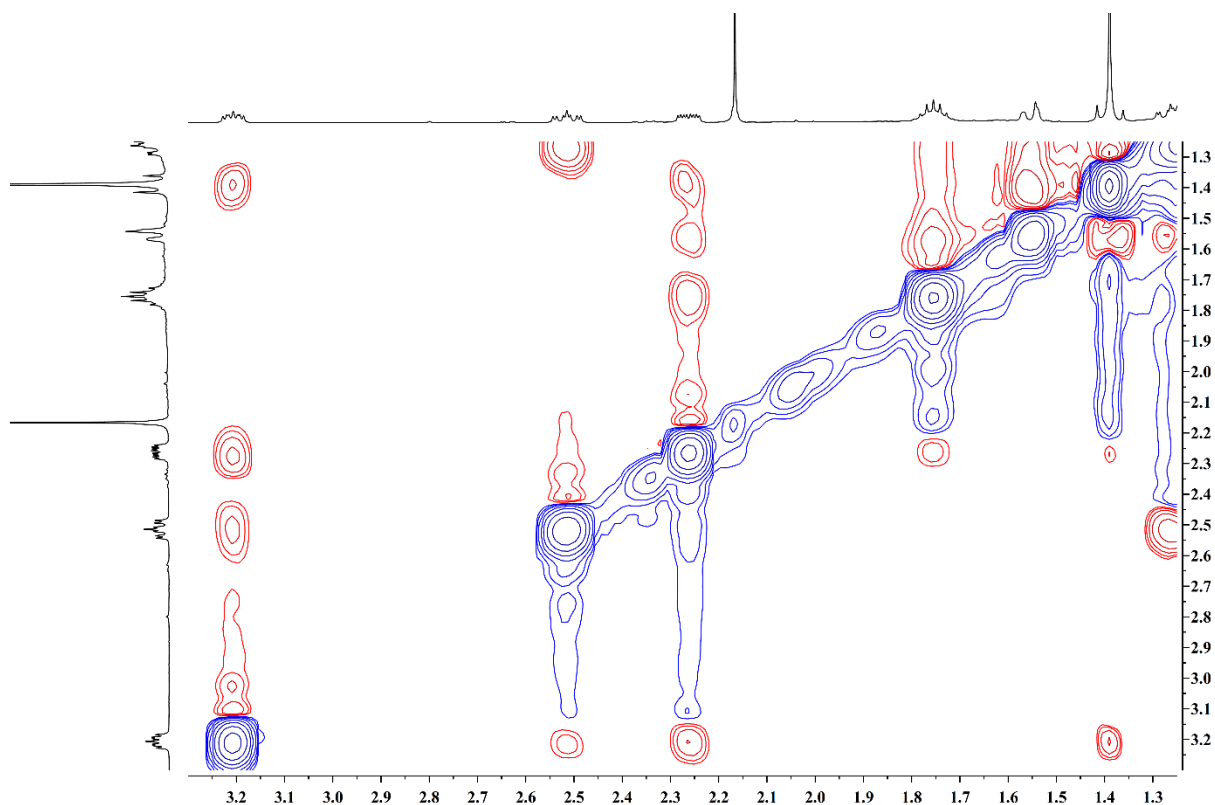
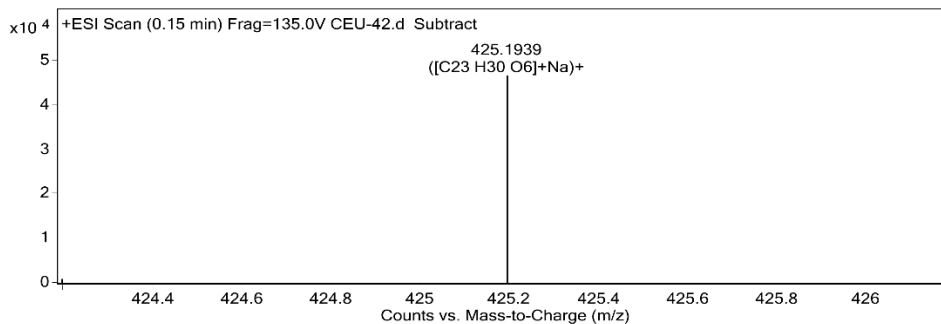


Figure S9 HRESIMS spectrum of 1

User Spectra

Fragmentor Voltage 135 Collision Energy 0 Ionization Mode ESI



Peak List

| m/z | z | Abund | Formula | Ion |
|----------|---|----------|------------|---------|
| 274.2735 | 1 | 18487.52 | | |
| 318.3002 | 1 | 26547.79 | | |
| 425.1939 | 1 | 46856.73 | C23 H30 O6 | (M+Na)+ |
| 426.1973 | 1 | 12582.23 | C23 H30 O6 | (M+Na)+ |
| 441.1679 | 1 | 13739.56 | | |
| 453.1691 | 1 | 40827.04 | | |
| 623.2886 | 2 | 20494.45 | | |
| 623.7908 | 2 | 16000.04 | | |

Formula Calculator Element Limits

| Element | Min | Max |
|---------|-----|-----|
| C | 3 | 60 |
| H | 0 | 120 |
| O | 0 | 30 |

Formula Calculator Results

| Formula | CalculatedMass | CalculatedMz | Mz | Diff. (mDa) | Diff. (ppm) | DBE |
|------------|----------------|--------------|----------|-------------|-------------|--------|
| C23 H30 O6 | 402.2042 | 425.1935 | 425.1939 | -0.40 | -0.94 | 9.0000 |

Figure S10 ^1H NMR spectrum of **2** (500 MHz, CDCl_3)

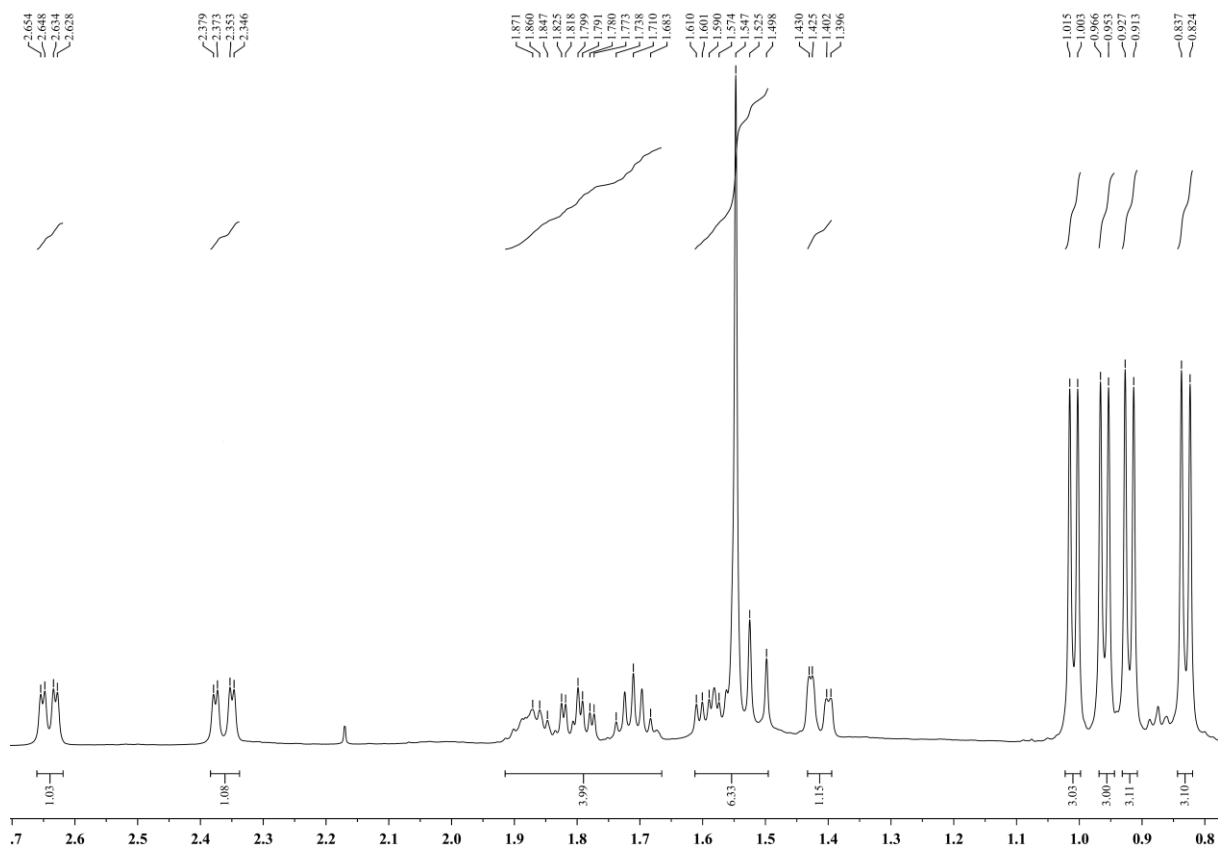
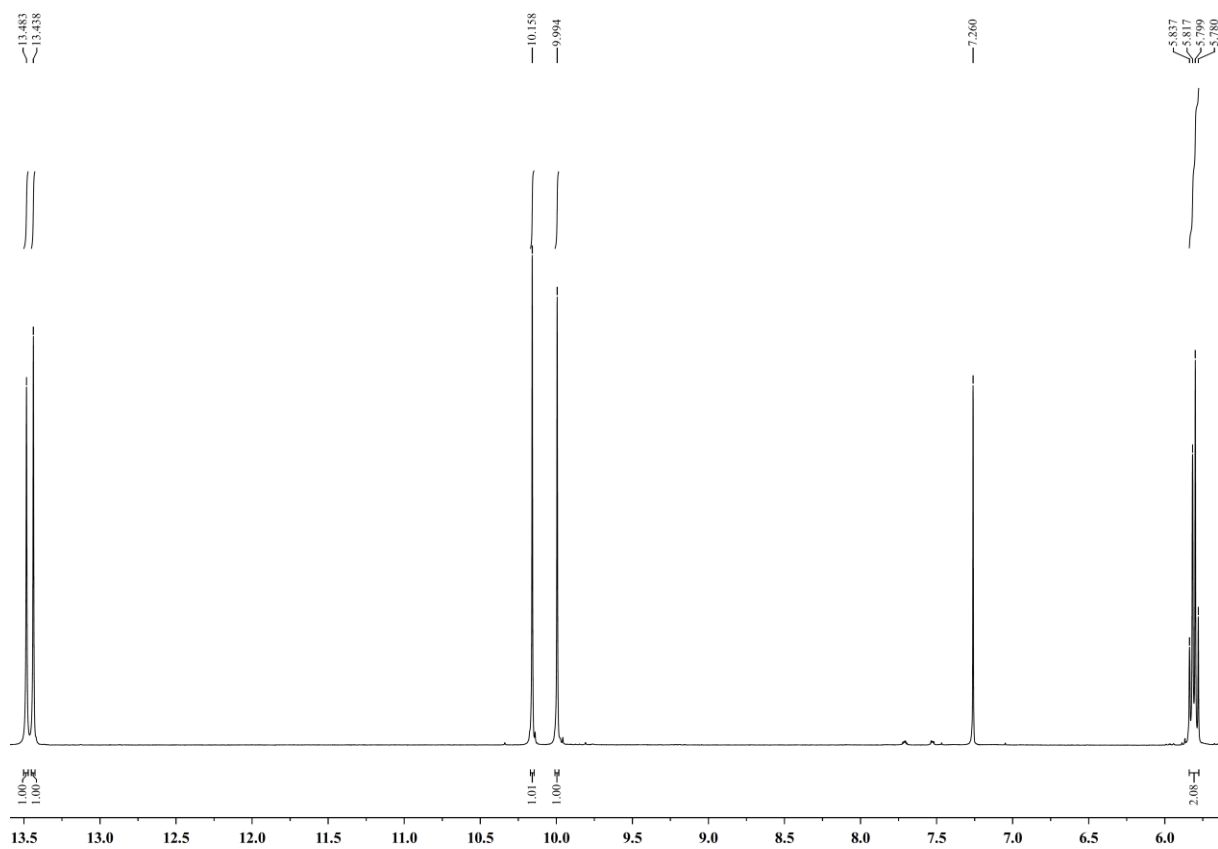


Figure S11 ^{13}C NMR spectrum of **2** (125 MHz, CDCl_3)

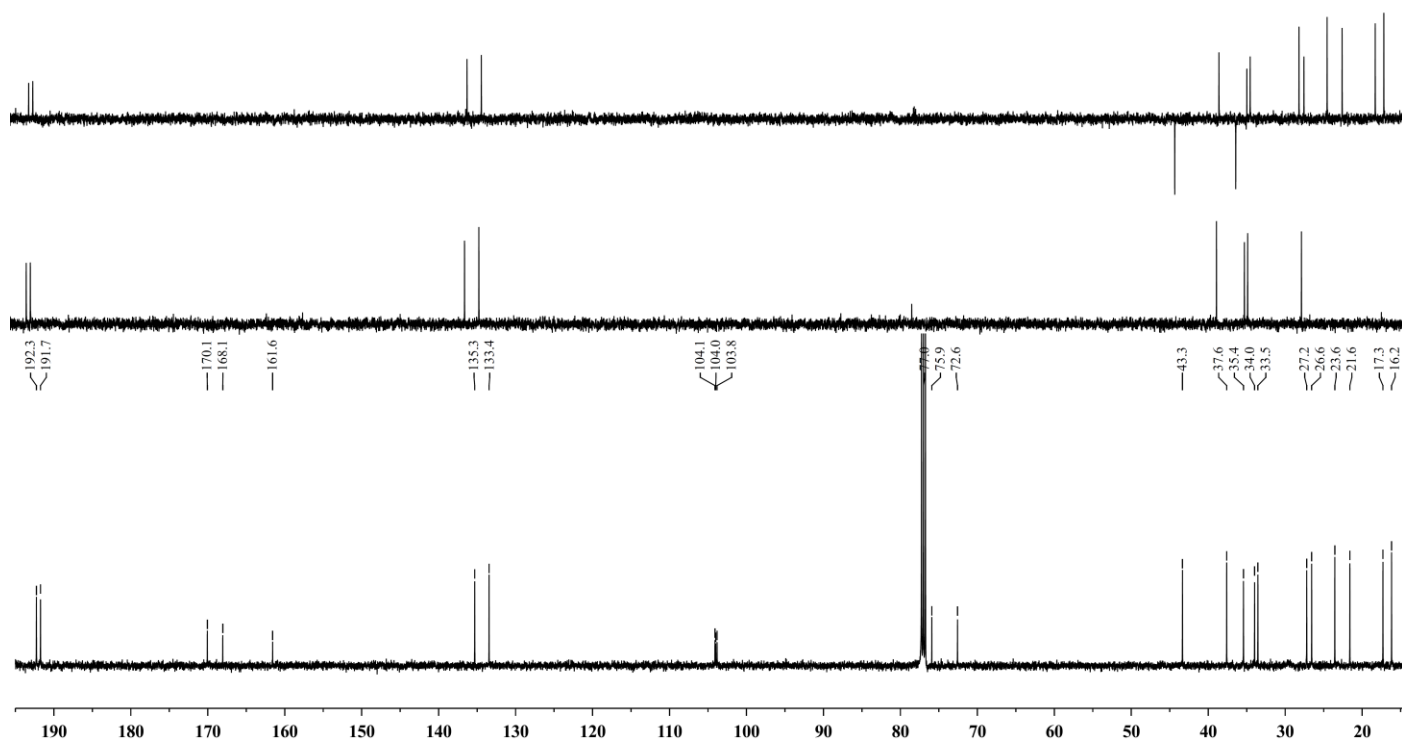


Figure S12 HSQC spectrum of **2**

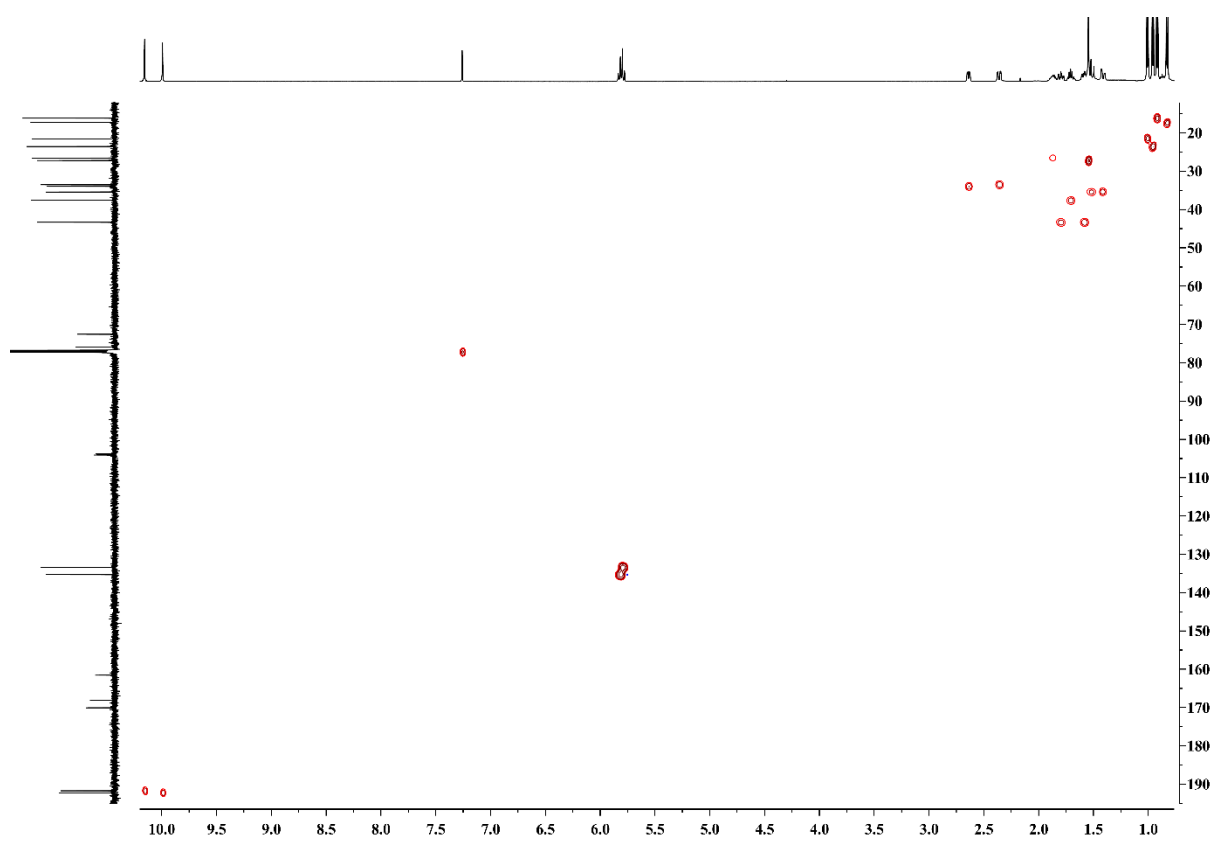


Figure S13 HMBC spectrum of **2**

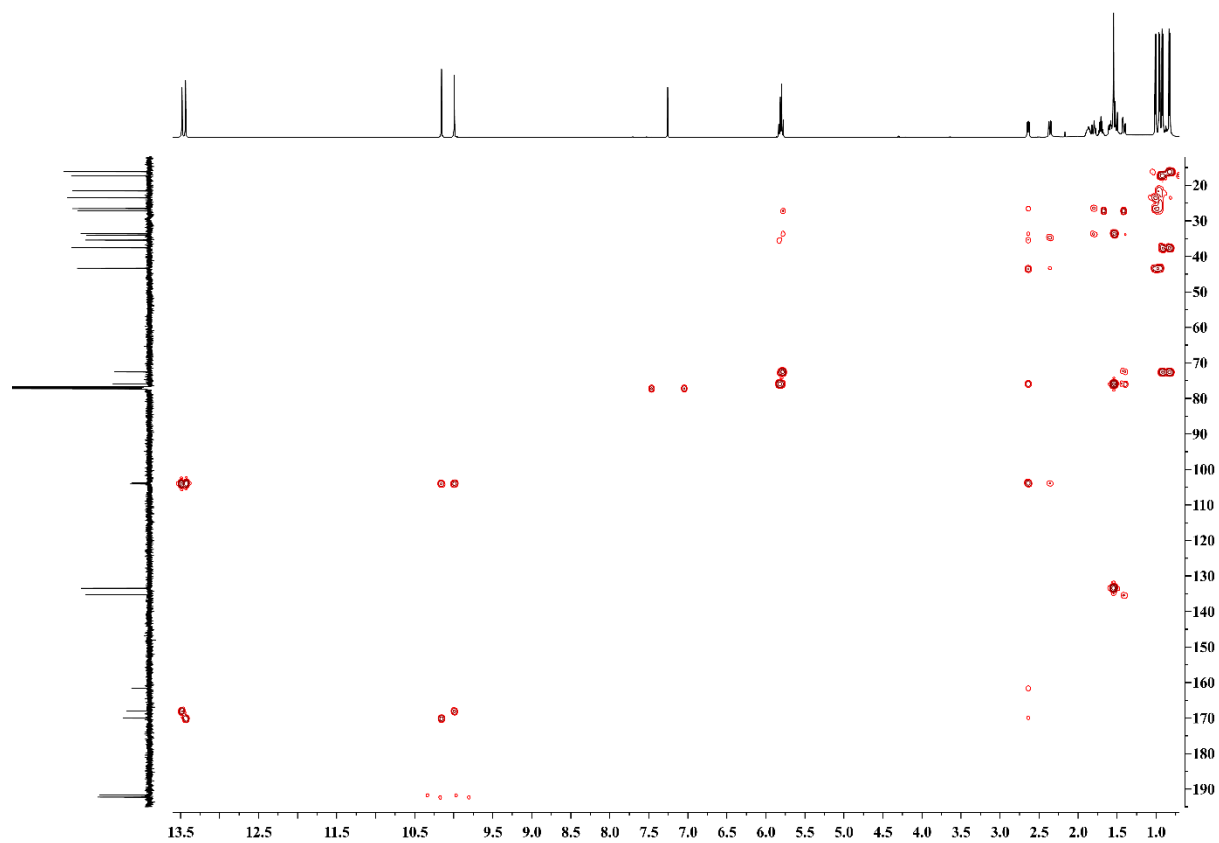


Figure S14 ^1H - ^1H COSY spectrum of **2**

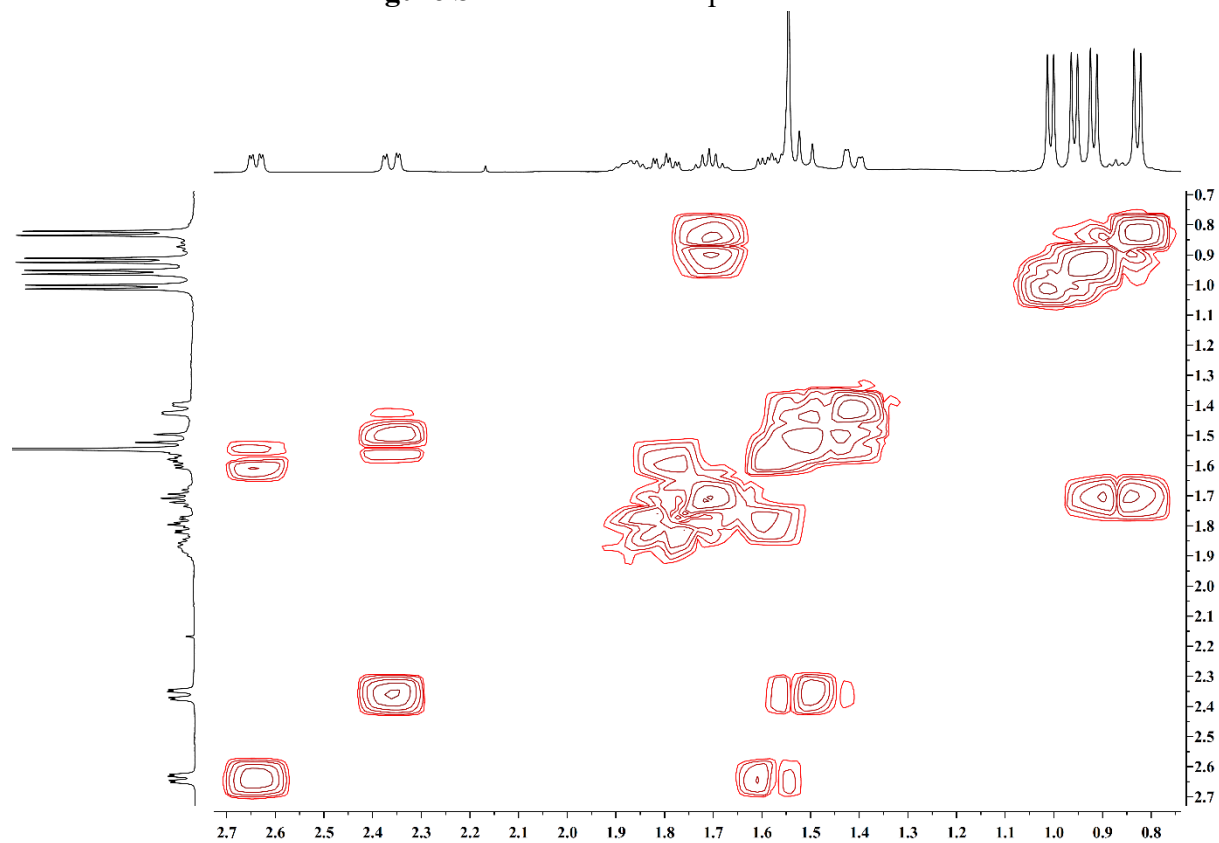


Figure S15 ROESY spectrum of 2

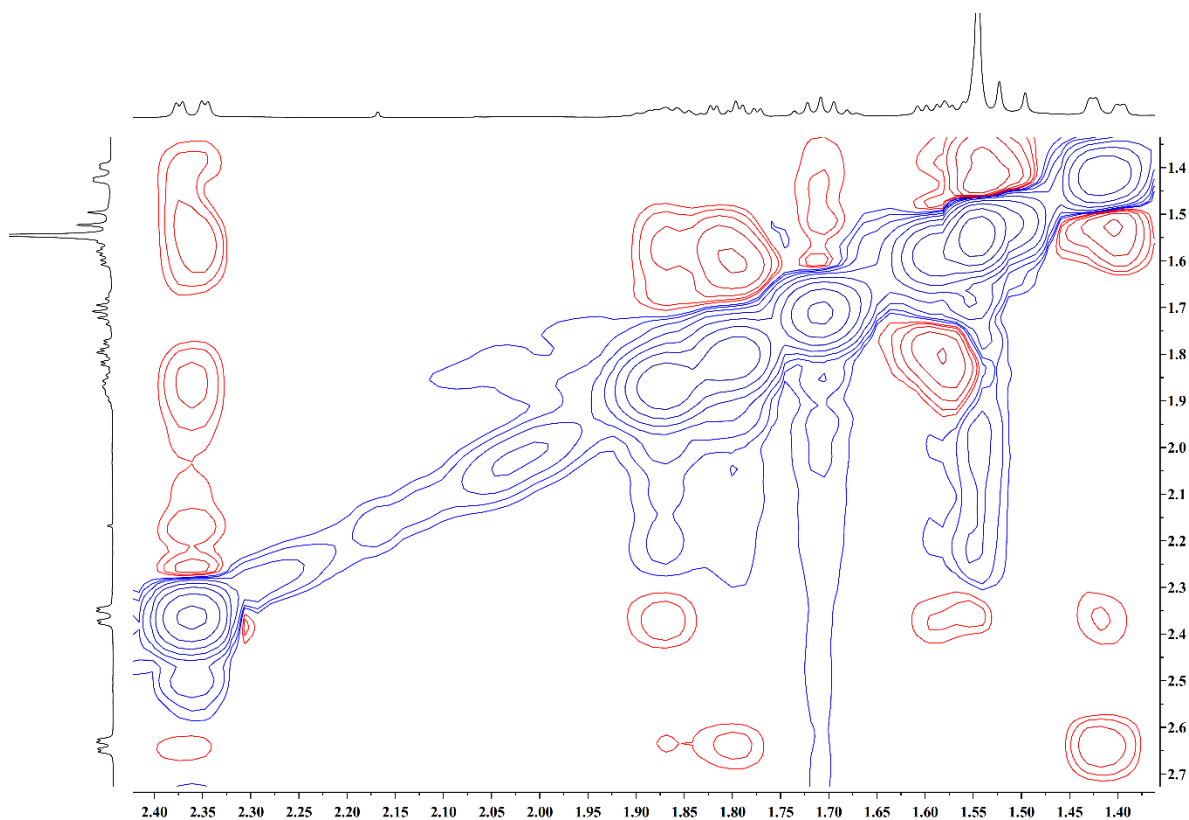
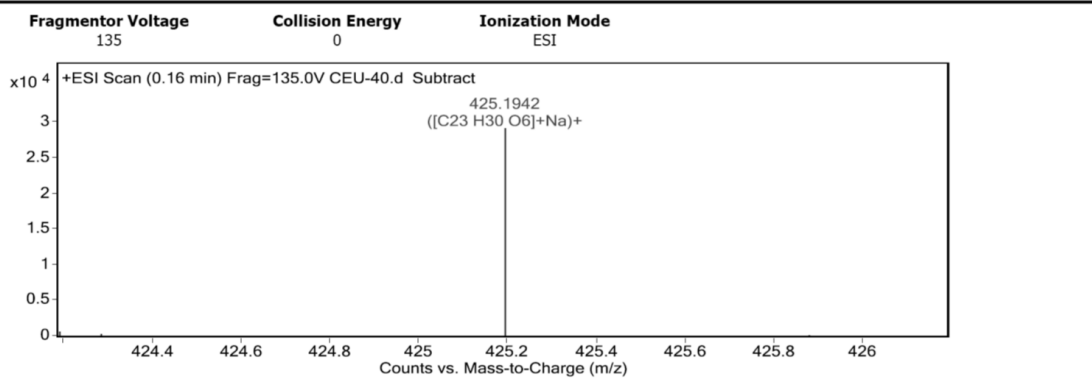


Figure S16 HRESIMS spectrum of 2

User Spectra



Peak List

| m/z | z | Abund | Formula | Ion |
|----------|---|----------|------------|---------|
| 212.1167 | 1 | 34253.24 | | |
| 262.1097 | 2 | 16016.45 | | |
| 301.1415 | 1 | 25177.3 | | |
| 317.1149 | 1 | 16980.58 | | |
| 425.1942 | 1 | 29122.36 | C23 H30 O6 | (M+Na)+ |
| 453.1698 | 1 | 20429.21 | | |
| 471.237 | 1 | 8633.81 | | |
| 623.2906 | 2 | 10431.4 | | |

Formula Calculator Element Limits

| Element | Min | Max |
|---------|-----|-----|
| C | 3 | 60 |
| H | 0 | 120 |
| O | 0 | 30 |

Formula Calculator Results

| Formula | CalculatedMass | CalculatedMz | Mz | Diff. (mDa) | Diff. (ppm) | DBE |
|------------|----------------|--------------|----------|-------------|-------------|--------|
| C23 H30 O6 | 402.2042 | 425.1935 | 425.1942 | -0.70 | -1.65 | 9.0000 |

Figure S17 ^1H NMR spectrum of **3** (800 MHz, CDCl_3)

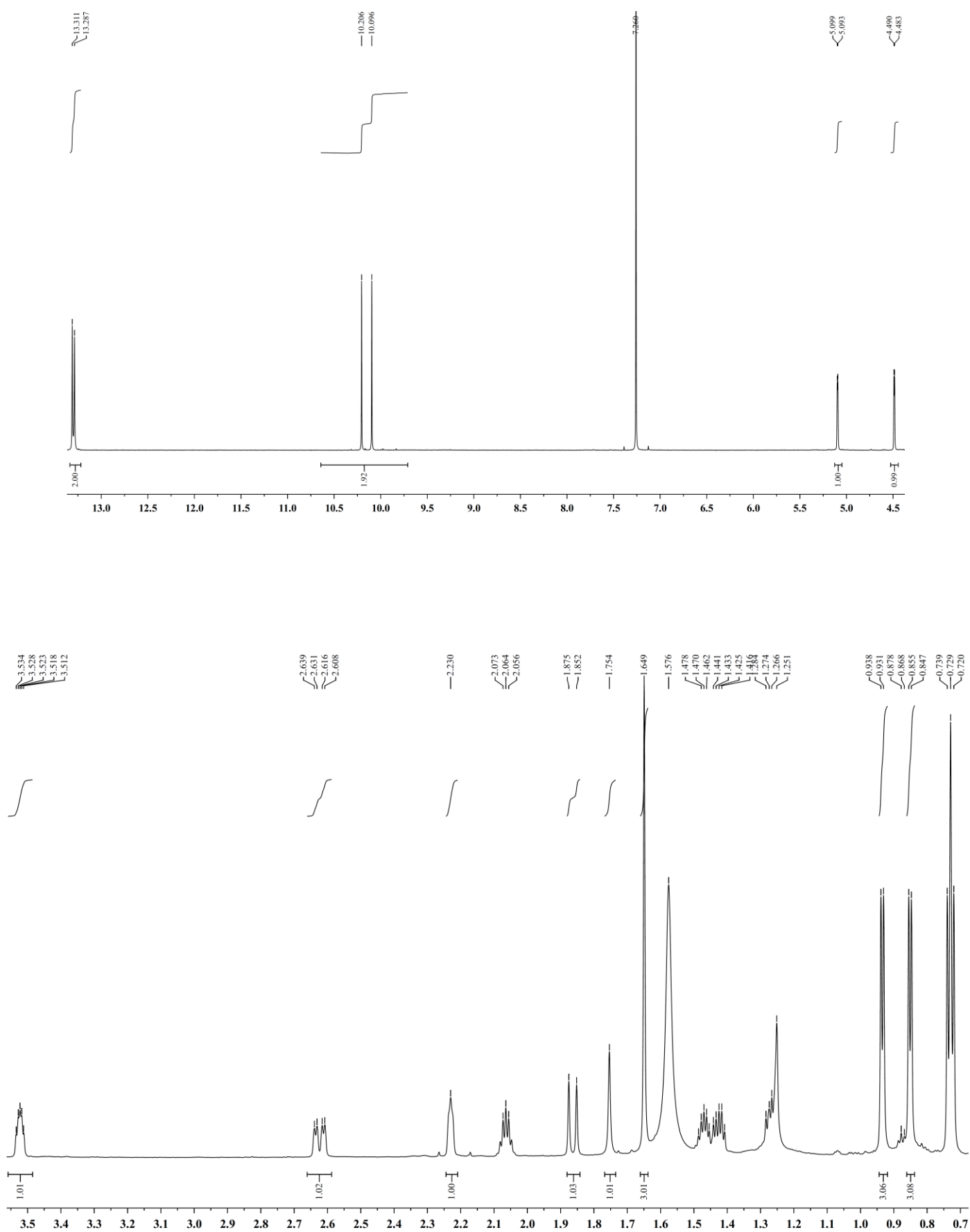


Figure S18 ^{13}C NMR spectrum of **3** (200 MHz, CDCl_3)

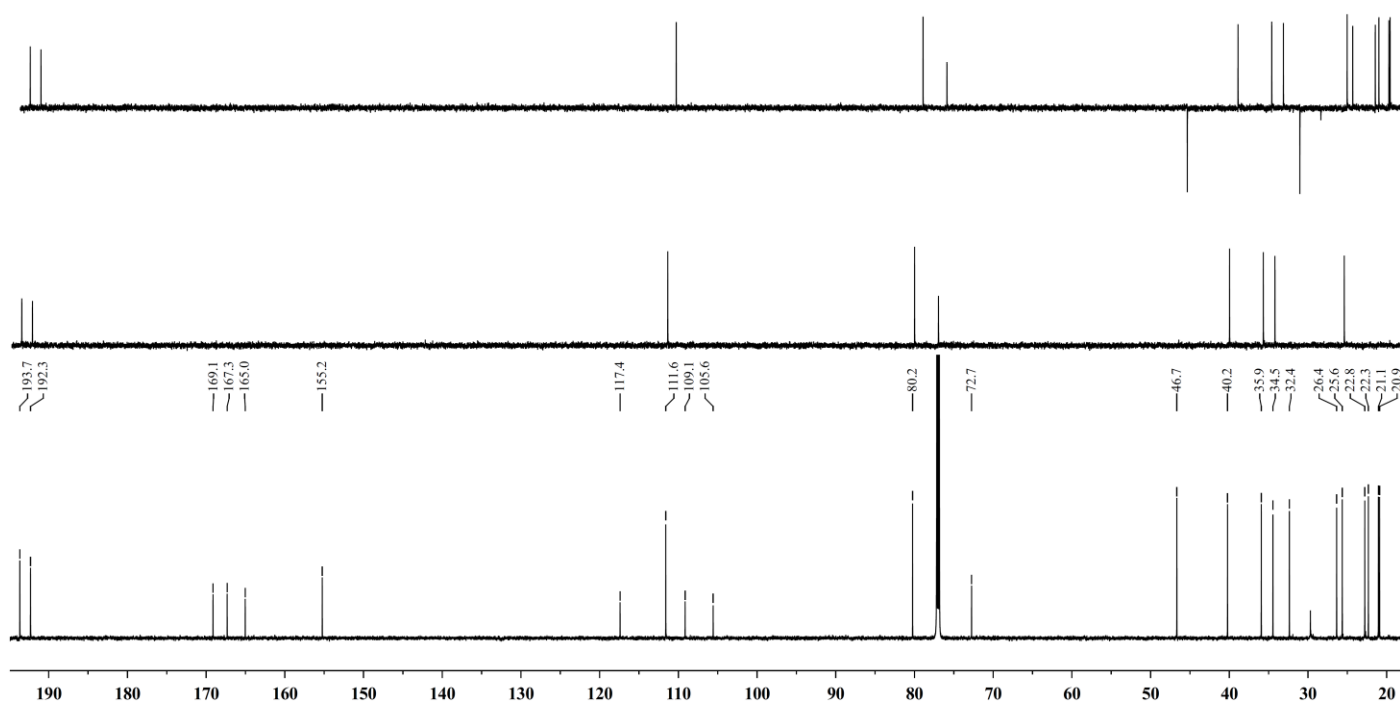


Figure S19 HSQC spectrum of **3**

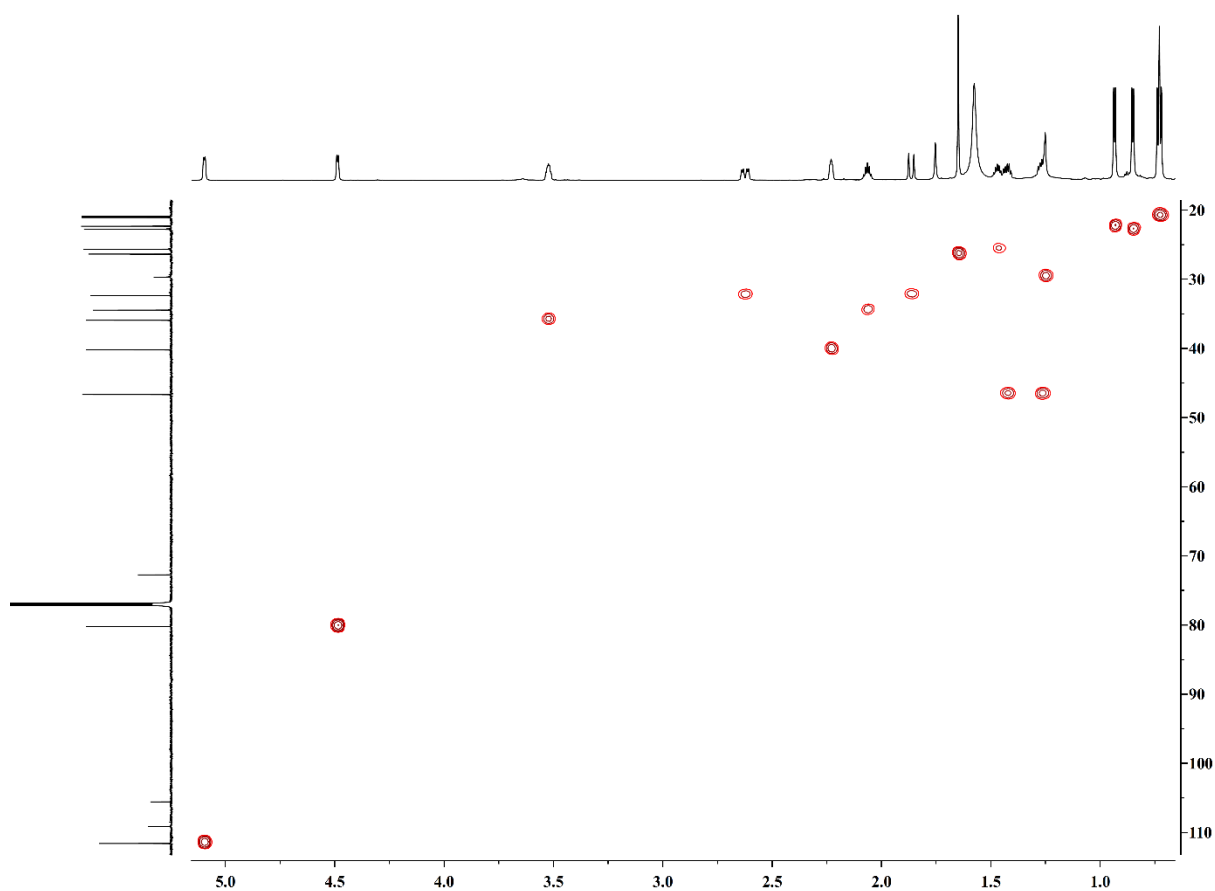


Figure S20 HMBC spectrum of **3**

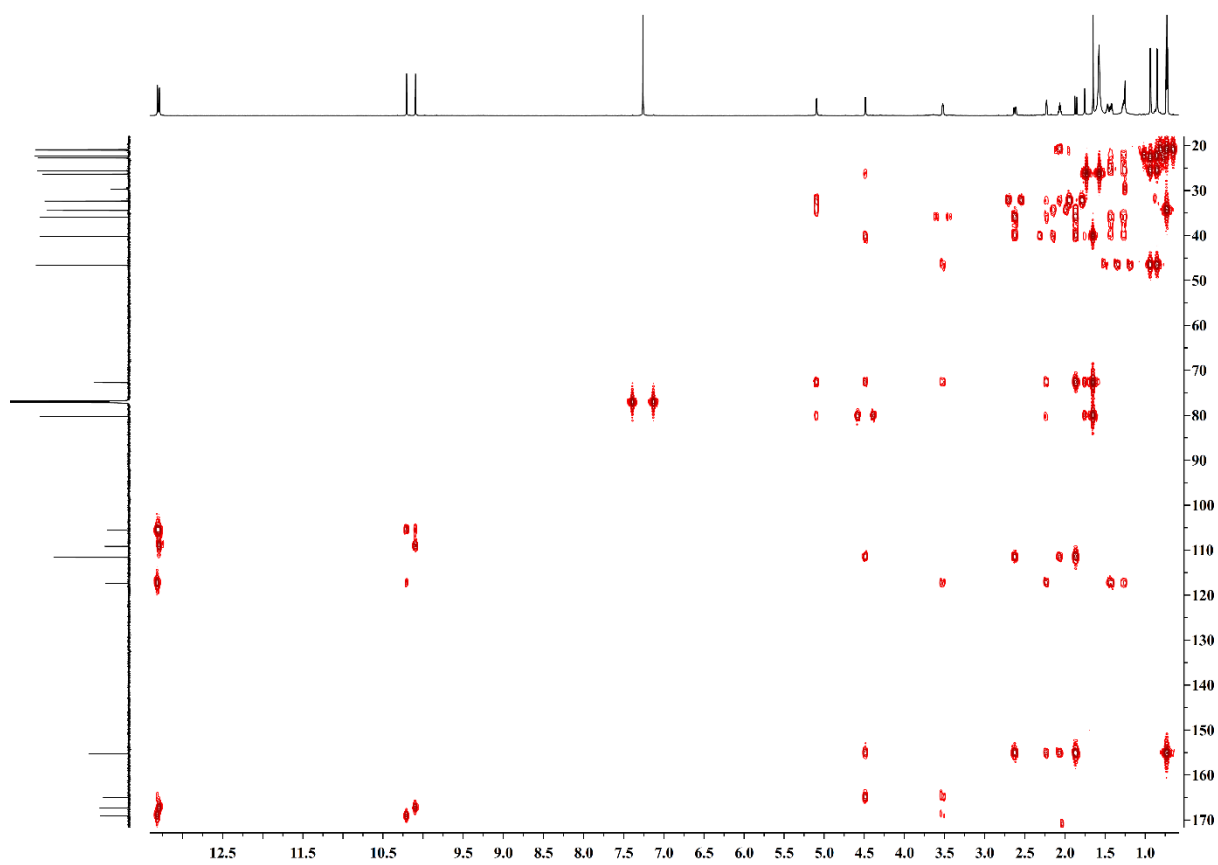


Figure S21 ^1H - ^1H COSY spectrum of **3**

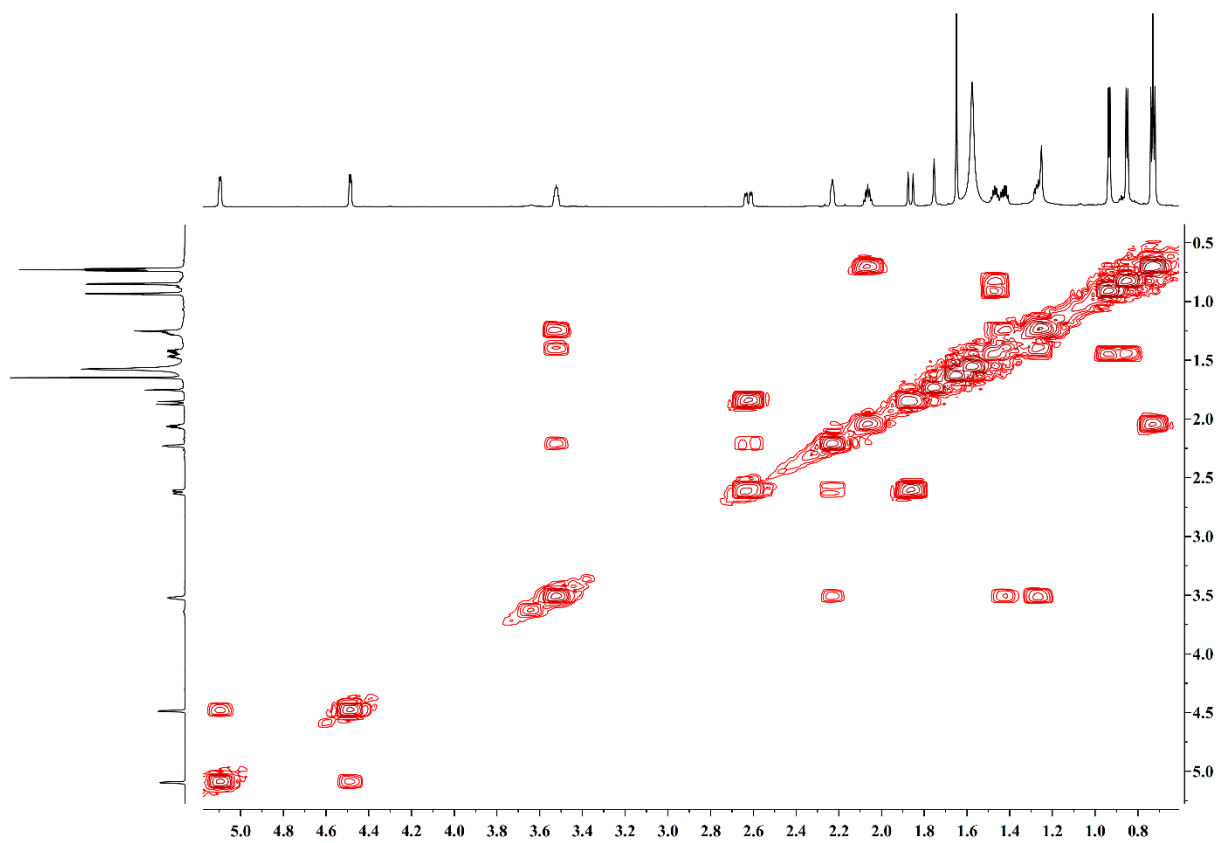


Figure S22 ROESY spectrum of 3

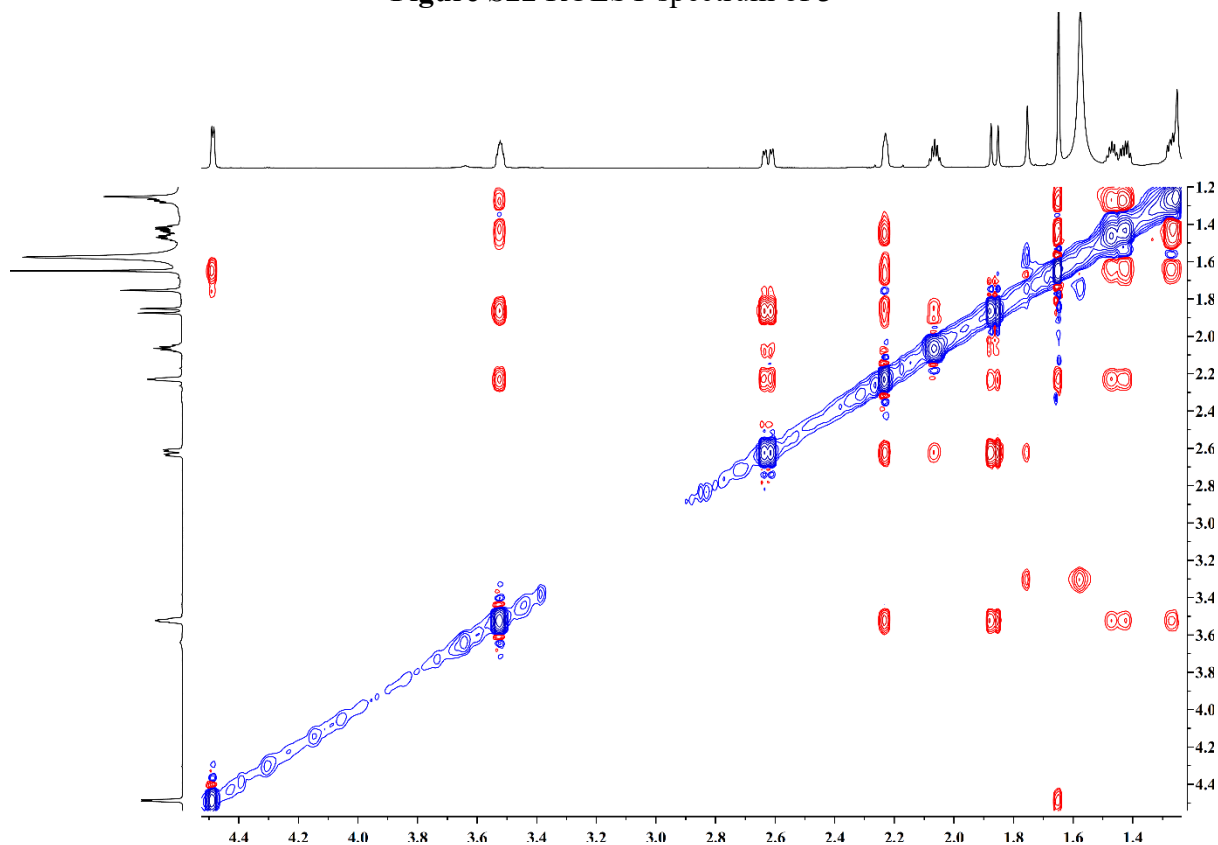
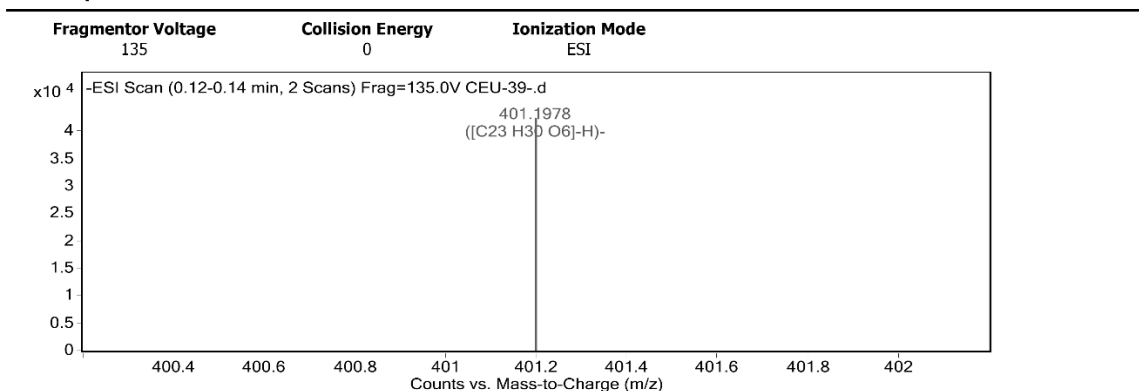


Figure S23 HRESIMS spectrum of 3

User Spectra



Peak List

| m/z | z | Abund | Formula | Ion |
|-----------|---|-----------|------------|--------|
| 96.9696 | | 80985.78 | | |
| 112.9853 | 1 | 64266.77 | | |
| 401.1978 | 1 | 42660.04 | C23 H30 O6 | (M-H)- |
| 955.9718 | 1 | 23164.42 | | |
| 982.995 | 1 | 200408.41 | | |
| 983.9939 | 1 | 32954.03 | | |
| 996.0123 | 1 | 22085.45 | | |
| 1033.9889 | 1 | 38626.57 | | |

Formula Calculator Element Limits

| Element | Min | Max |
|---------|-----|-----|
| C | 3 | 60 |
| H | 0 | 120 |
| O | 0 | 30 |

Formula Calculator Results

| Formula | CalculatedMass | CalculatedMz | Mz | Diff. (mDa) | Diff. (ppm) | DBE |
|------------|----------------|--------------|----------|-------------|-------------|--------|
| C23 H30 O6 | 402.2042 | 401.1970 | 401.1978 | -0.80 | -1.99 | 9.0000 |

Figure S24 ^1H NMR spectrum of **4** (500 MHz, CDCl_3)

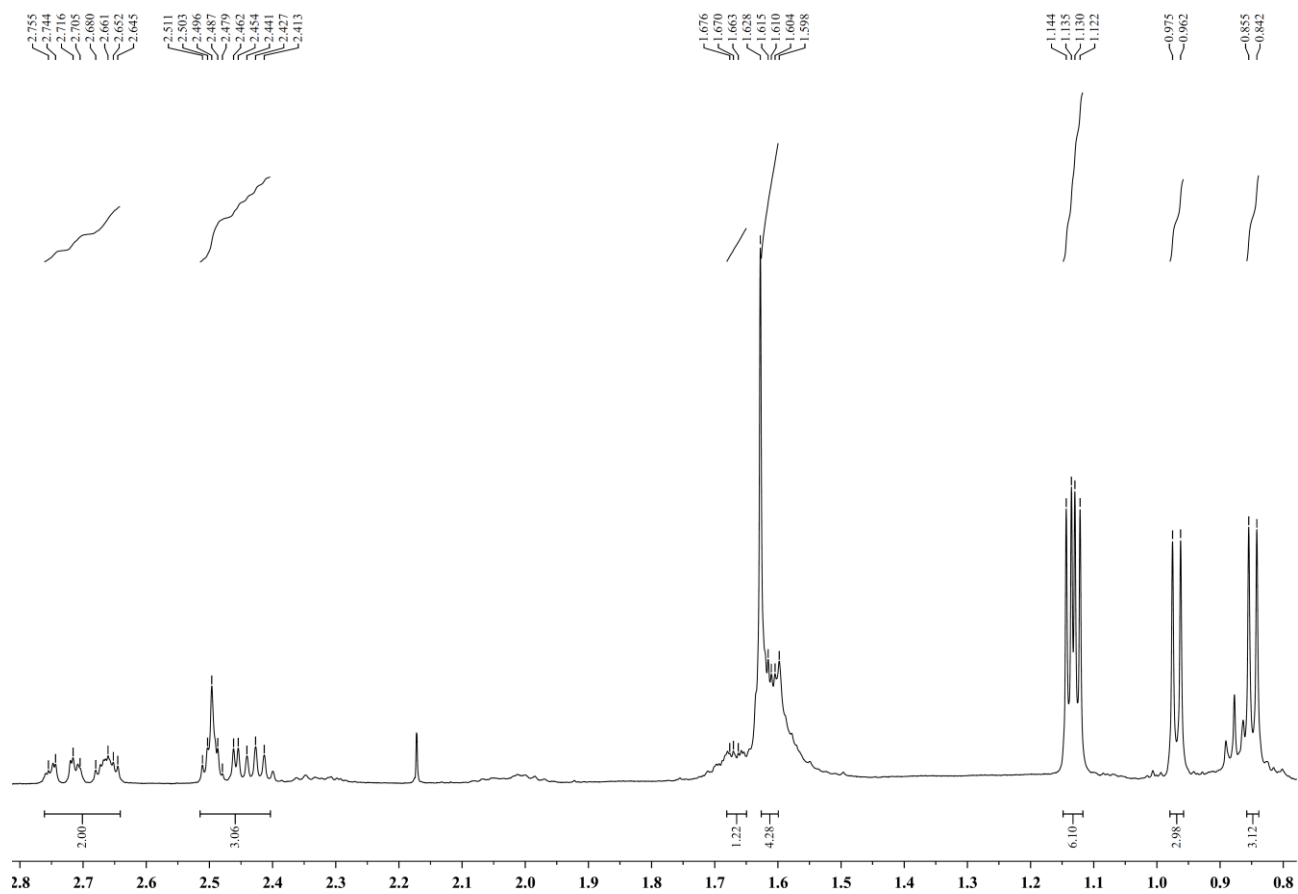
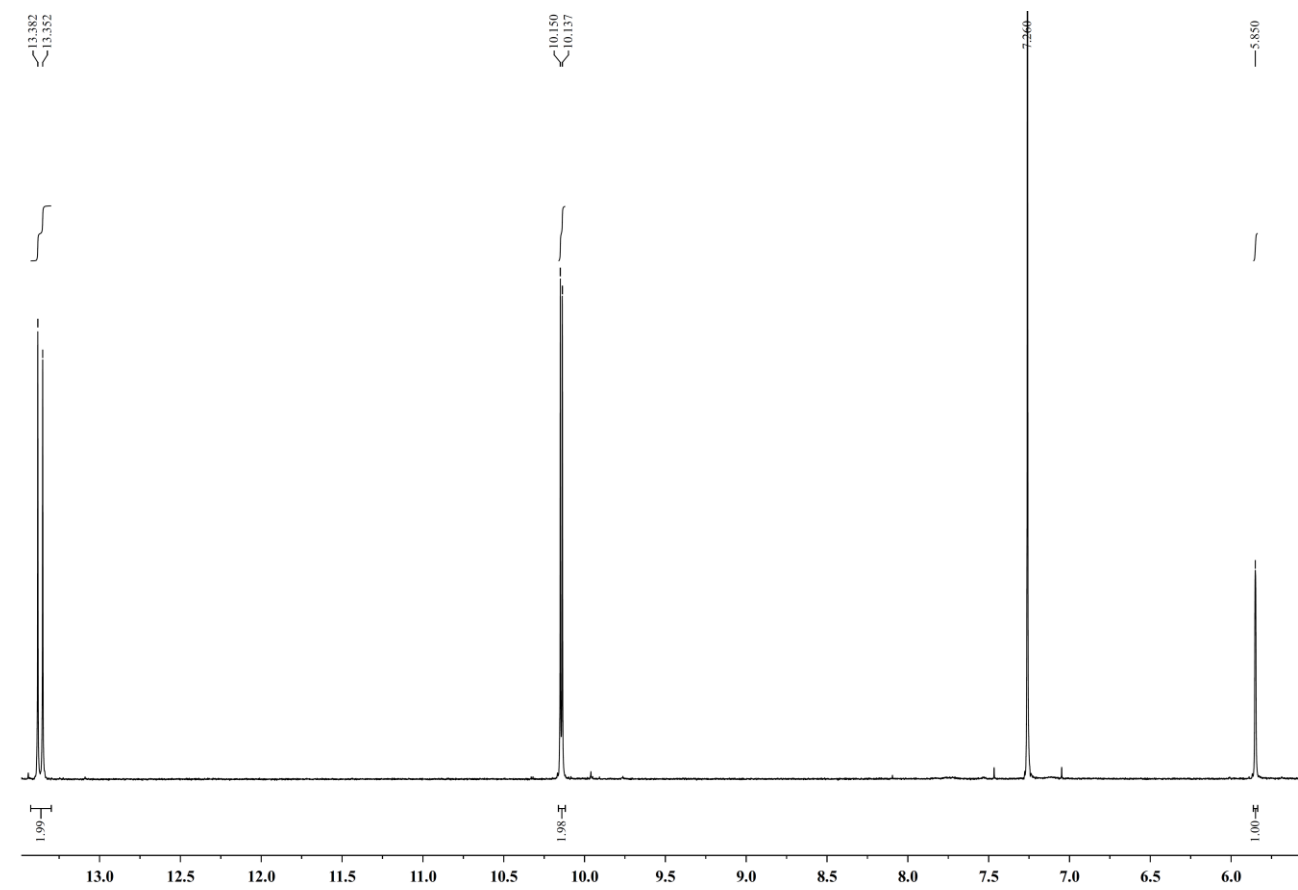


Figure S25 ^{13}C NMR spectrum of 4 (125 MHz, CDCl_3)

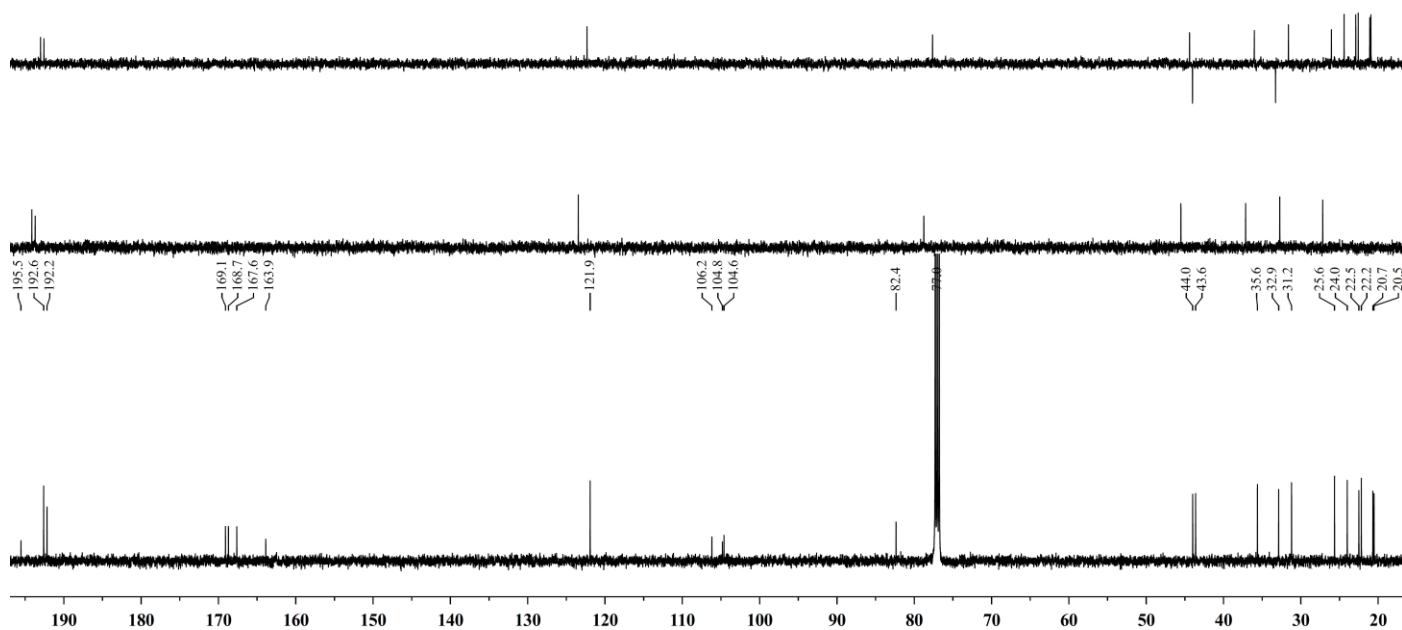


Figure S26 HSQC spectrum of 4

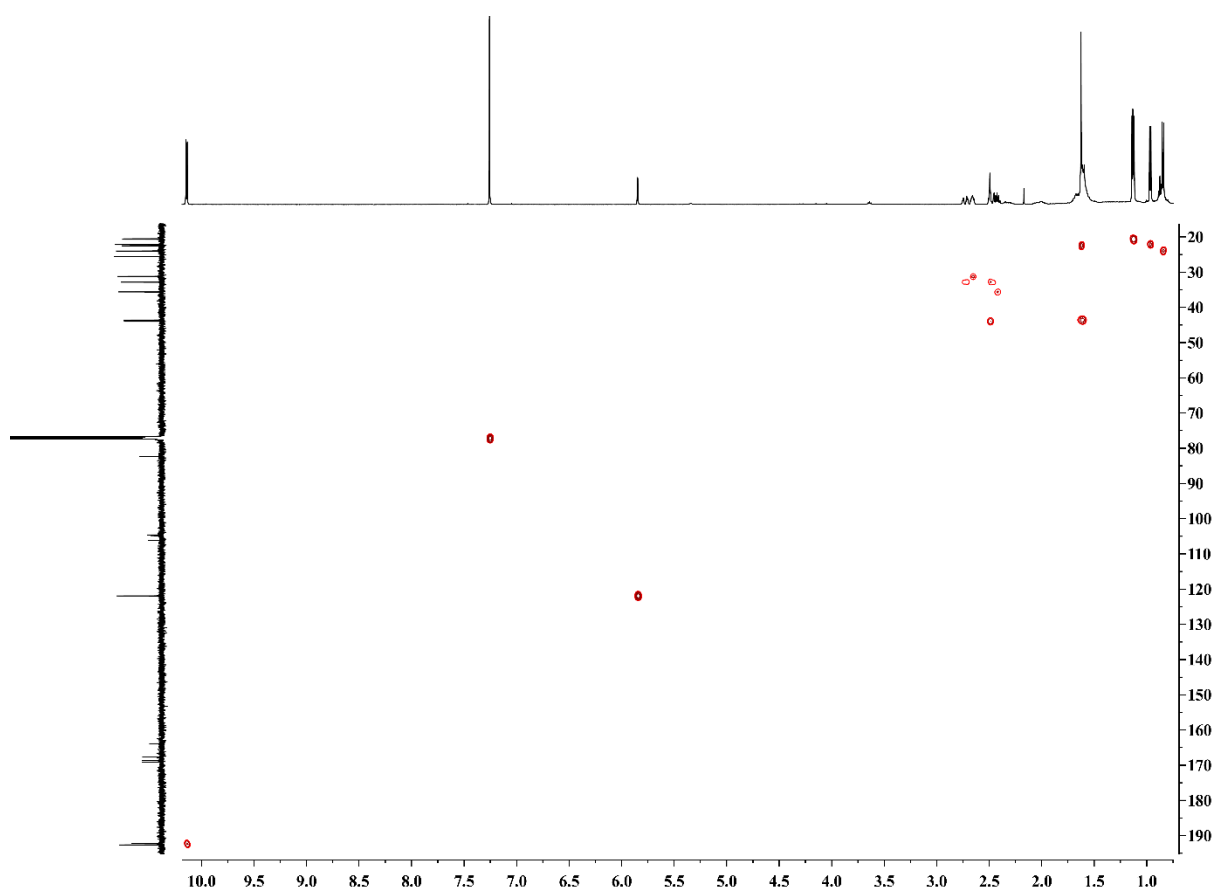


Figure S27 HMBC spectrum of 4

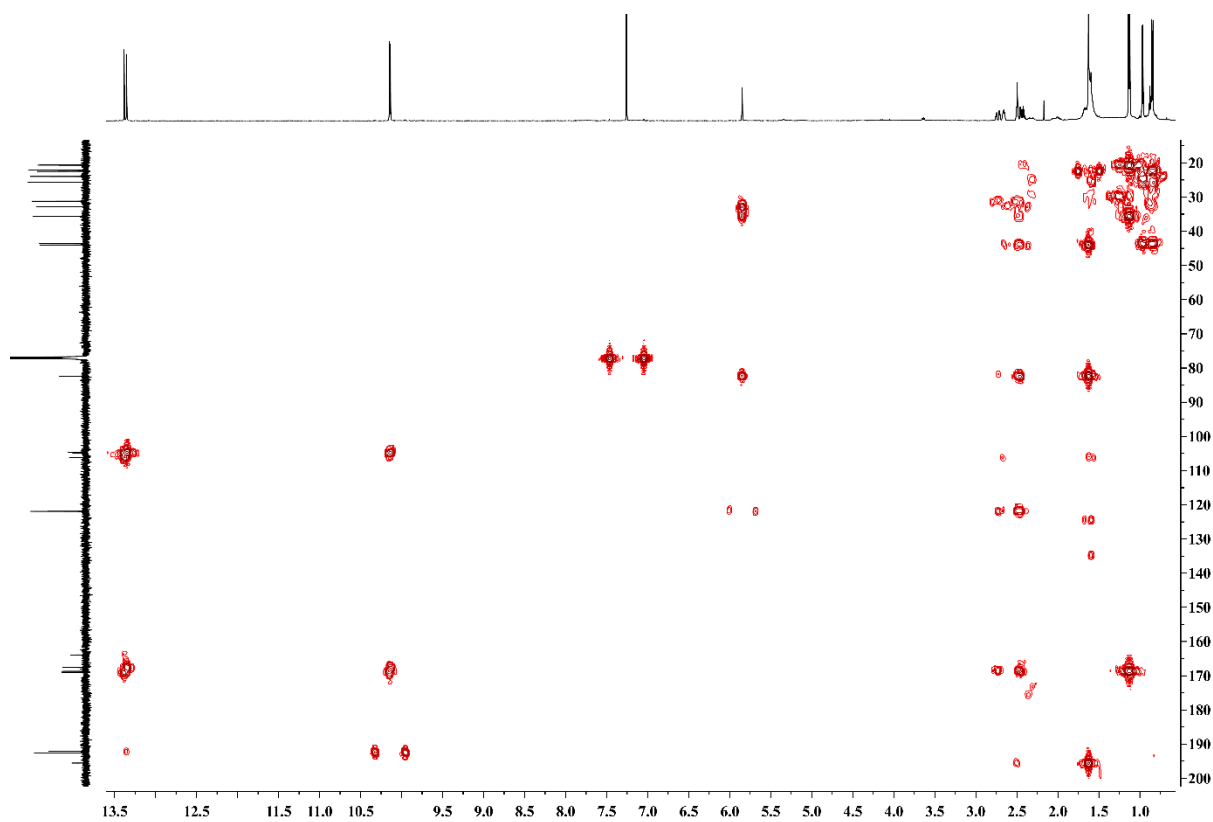


Figure S28 ^1H - ^1H COSY spectrum of 4

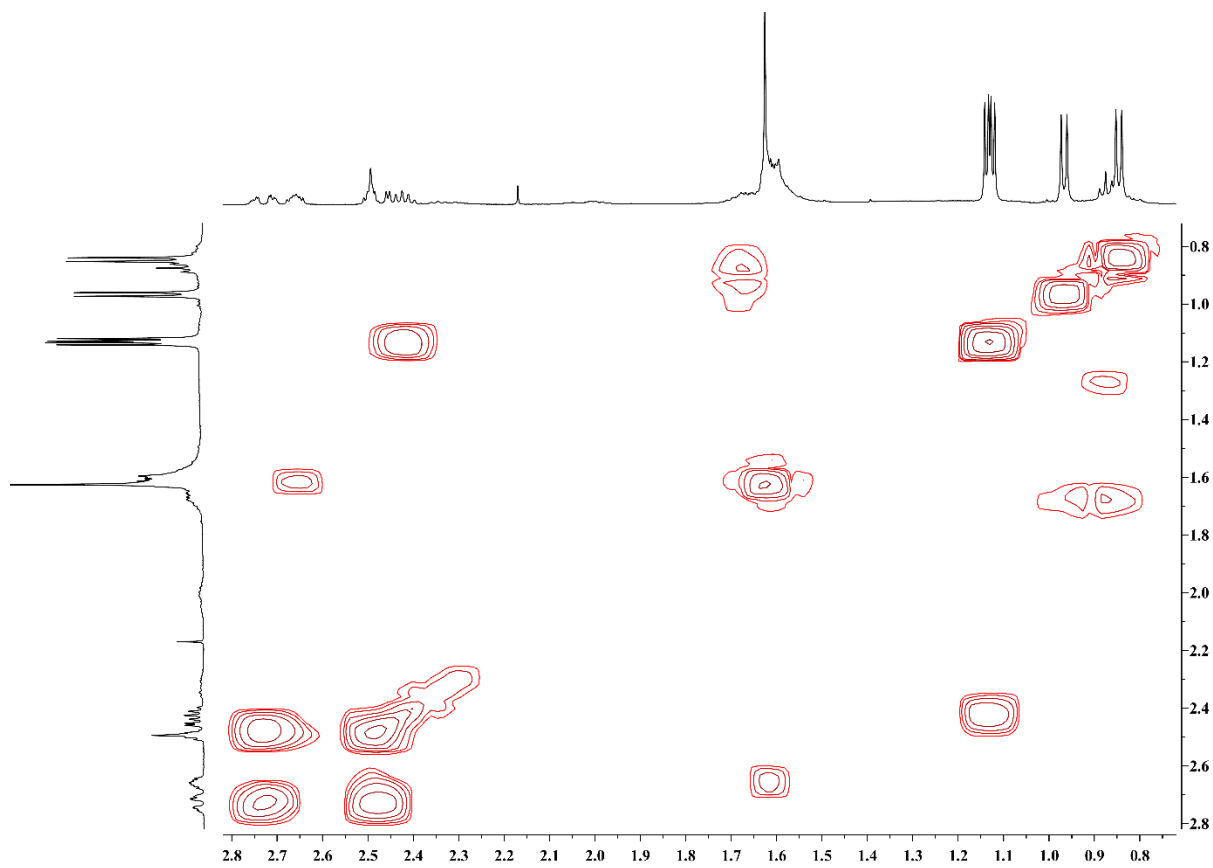


Figure S29 ROESY spectrum of 4

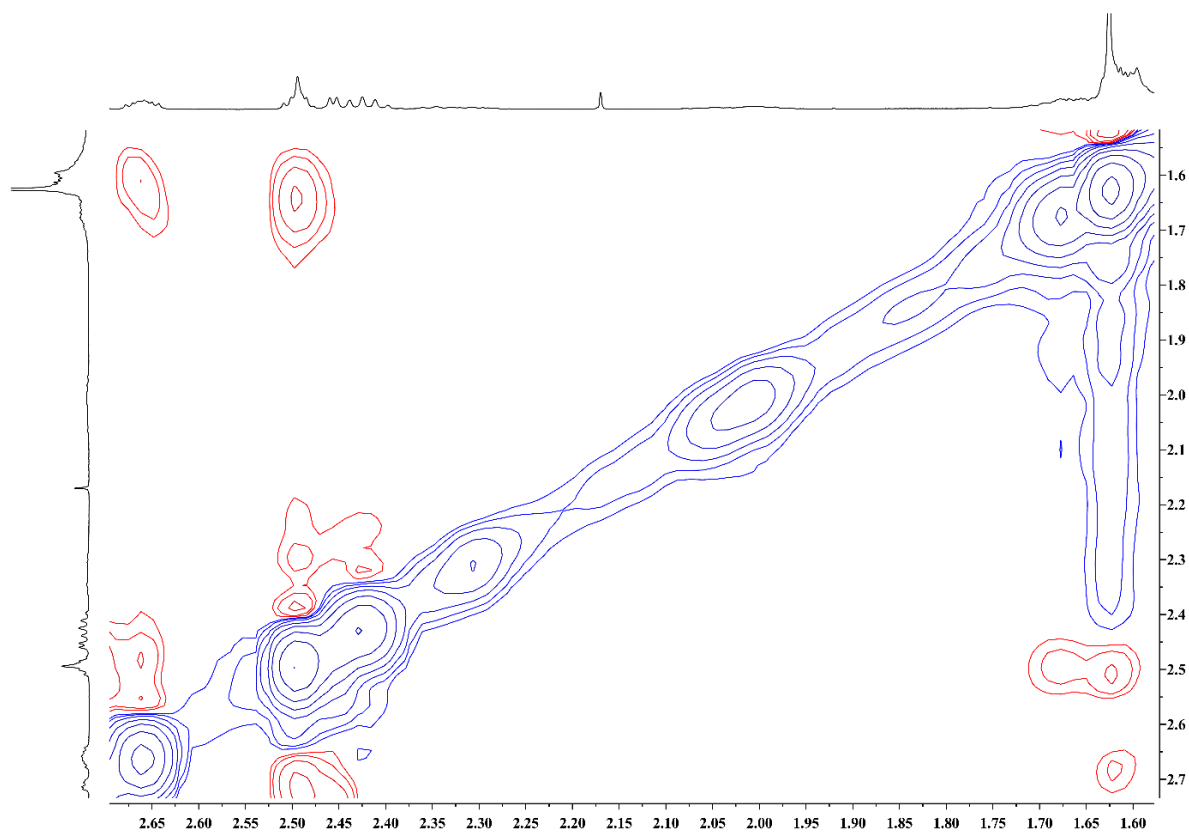
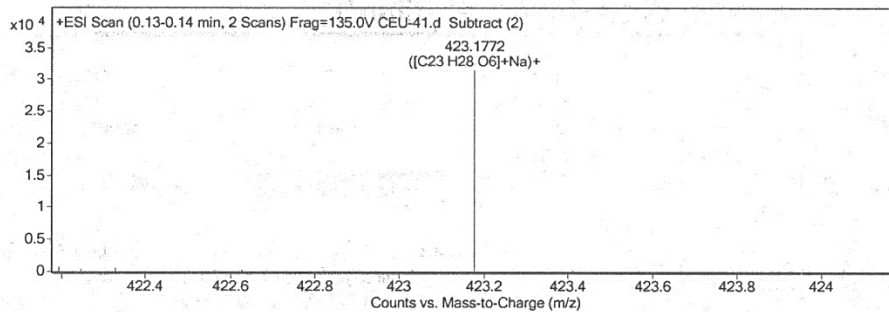


Figure S30 HRESIMS spectrum of 4

User Spectra

Fragmentor Voltage: 135
Collision Energy: 0
Ionization Mode: ESI



Peak List

| m/z | z | Abund | Formula | Ion |
|----------|---|-----------|------------|---------|
| 102.1279 | 1 | 547299.38 | | |
| 103.1311 | 1 | 37837.59 | | |
| 299.1093 | 1 | 31369.39 | | |
| 301.1407 | 1 | 217539.23 | | |
| 302.144 | 1 | 36303.66 | | |
| 305.1566 | 1 | 76515.82 | | |
| 317.1147 | 1 | 93489.31 | | |
| 321.1304 | 1 | 30060.03 | | |
| 423.1772 | 1 | 31510.83 | C23 H28 O6 | (M+Na)+ |
| 579.2923 | 1 | 52332.01 | | |

Formula Calculator Element Limits

| Element | Min | Max |
|---------|-----|-----|
| C | 3 | 60 |
| H | 0 | 120 |
| O | 0 | 30 |

Formula Calculator Results

| Formula | CalculatedMass | CalculatedMz | Mz | Diff. (mDa) | Diff. (ppm) | DBE |
|------------|----------------|--------------|----------|-------------|-------------|---------|
| C23 H28 O6 | 400.1886 | 423.1778 | 423.1772 | 0.60 | 1.42 | 10.0000 |

Figure S31 ^1H NMR spectrum of **5** (500 MHz, CDCl_3)

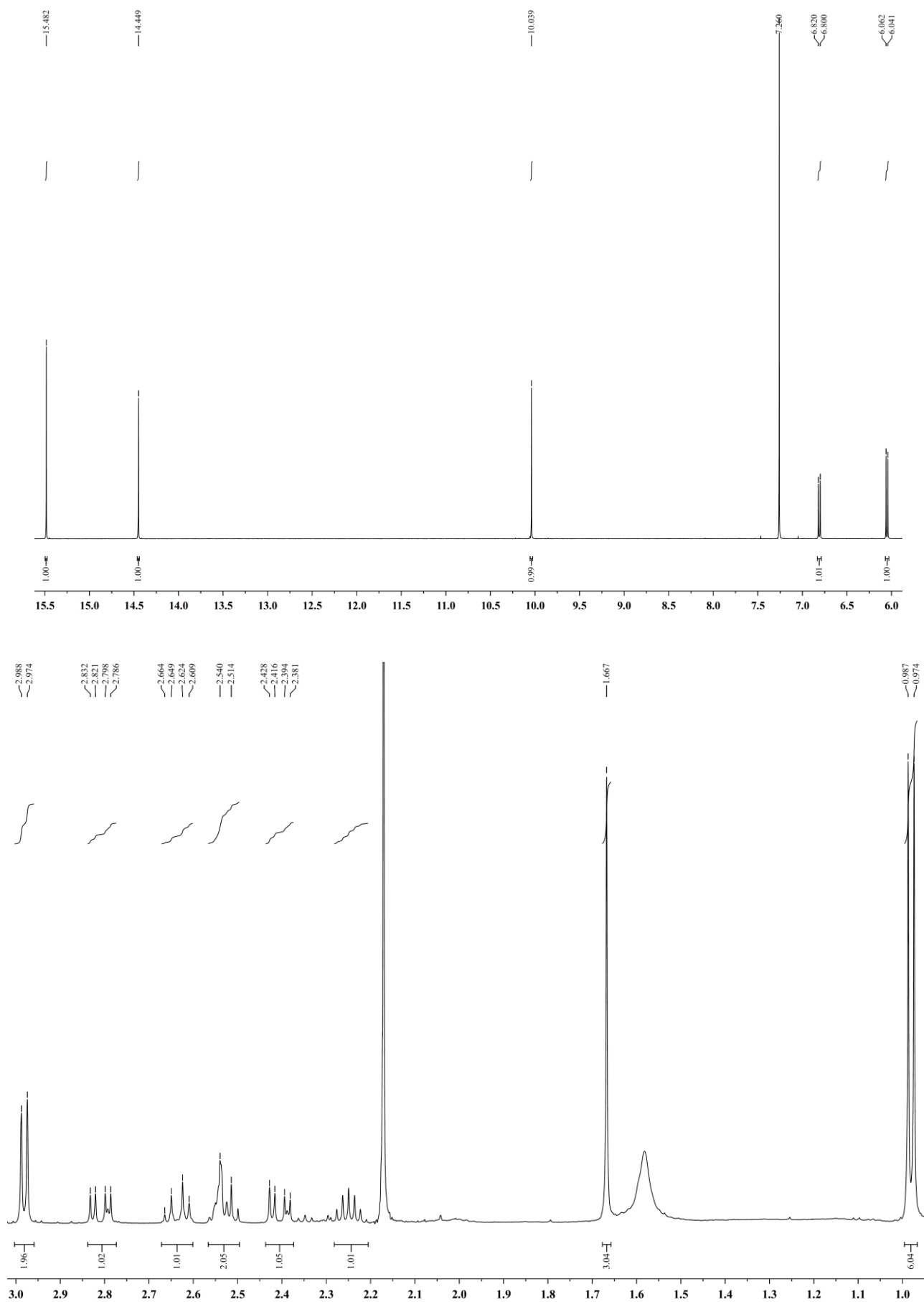


Figure S32 ^{13}C NMR spectrum of **5** (125 MHz, CDCl_3)

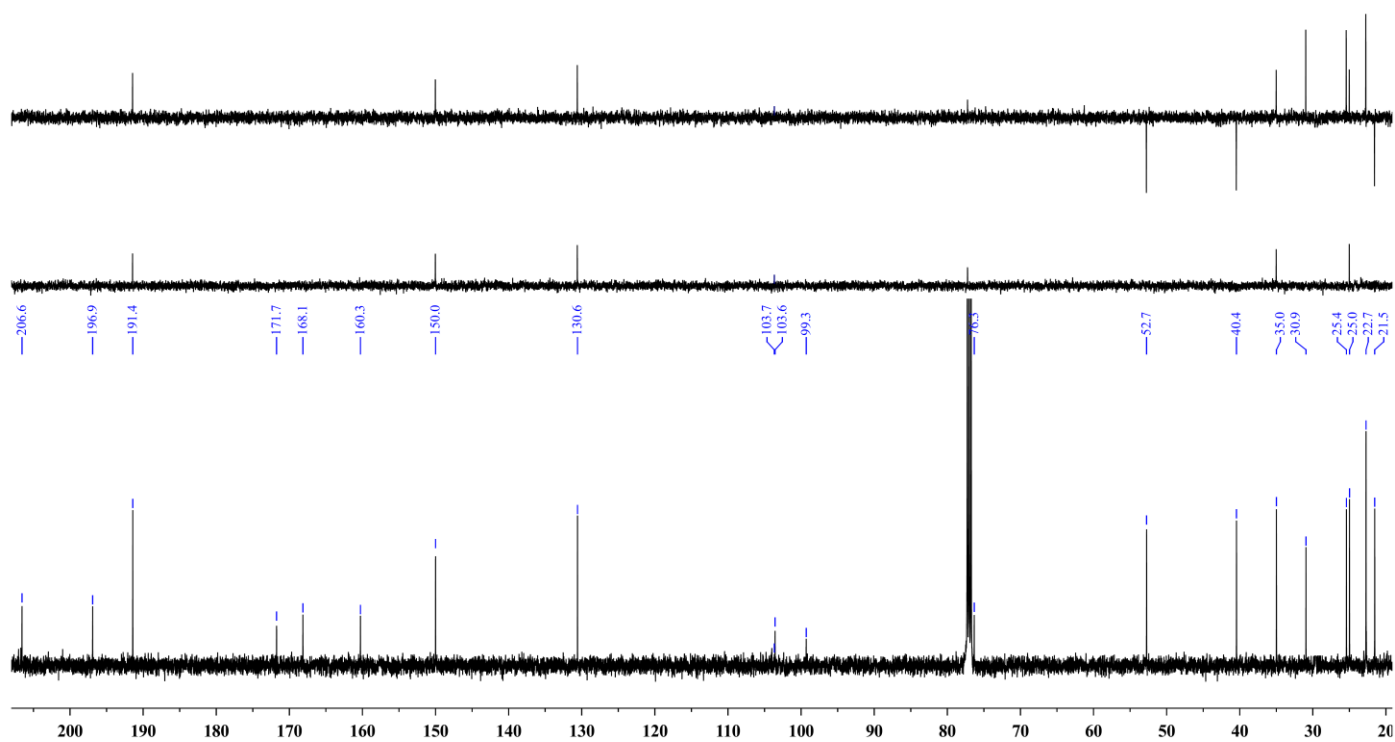


Figure S33 HSQC spectrum of **5**

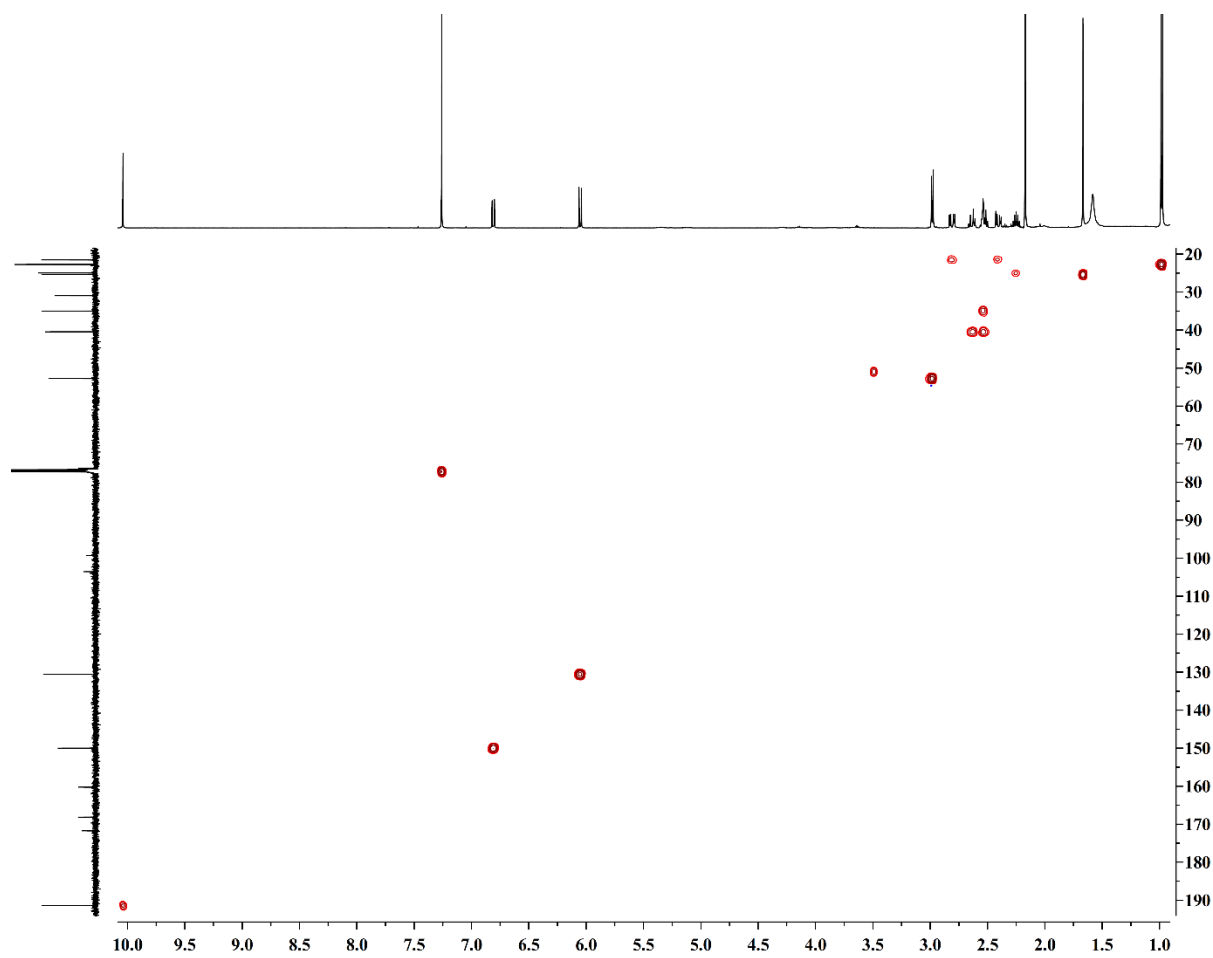


Figure S34 HMBC spectrum of **5**

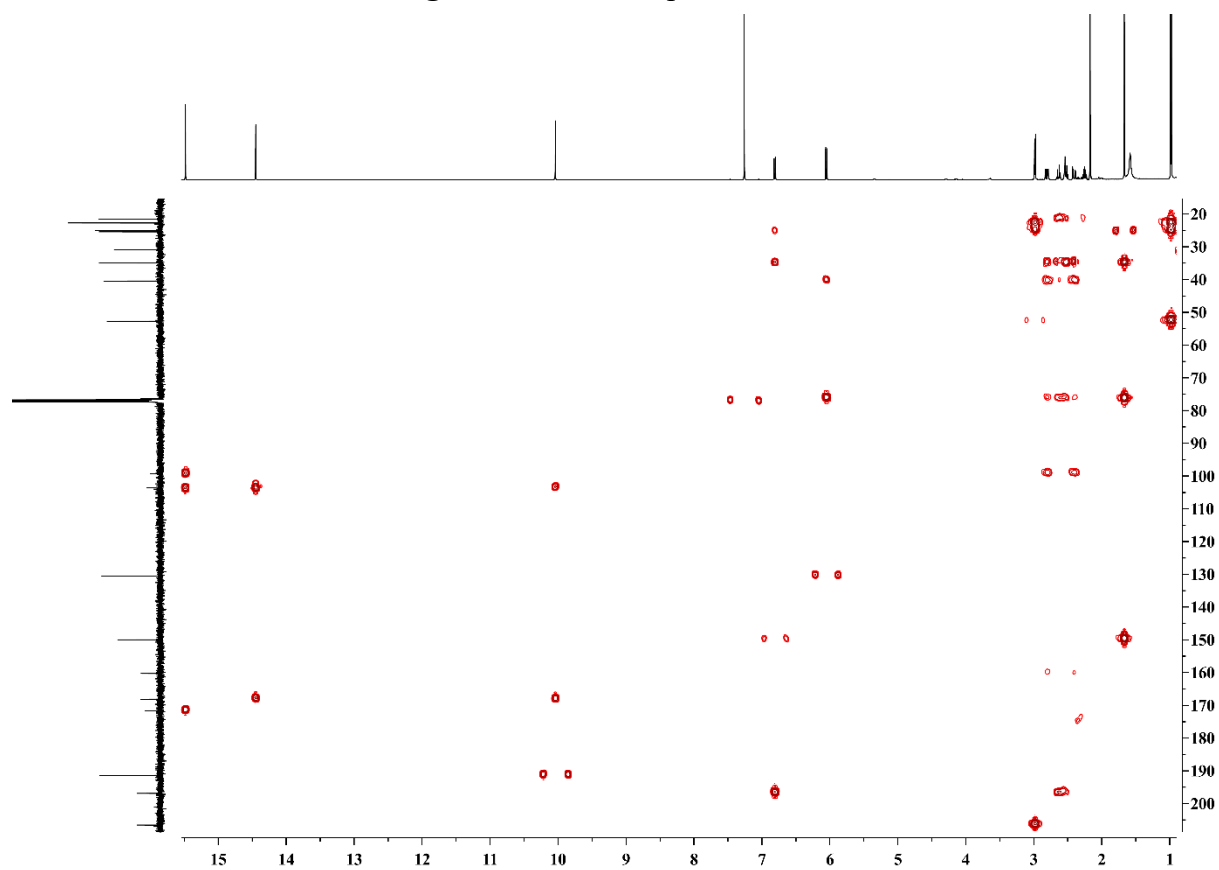


Figure S35 ^1H - ^1H COSY spectrum of **5**

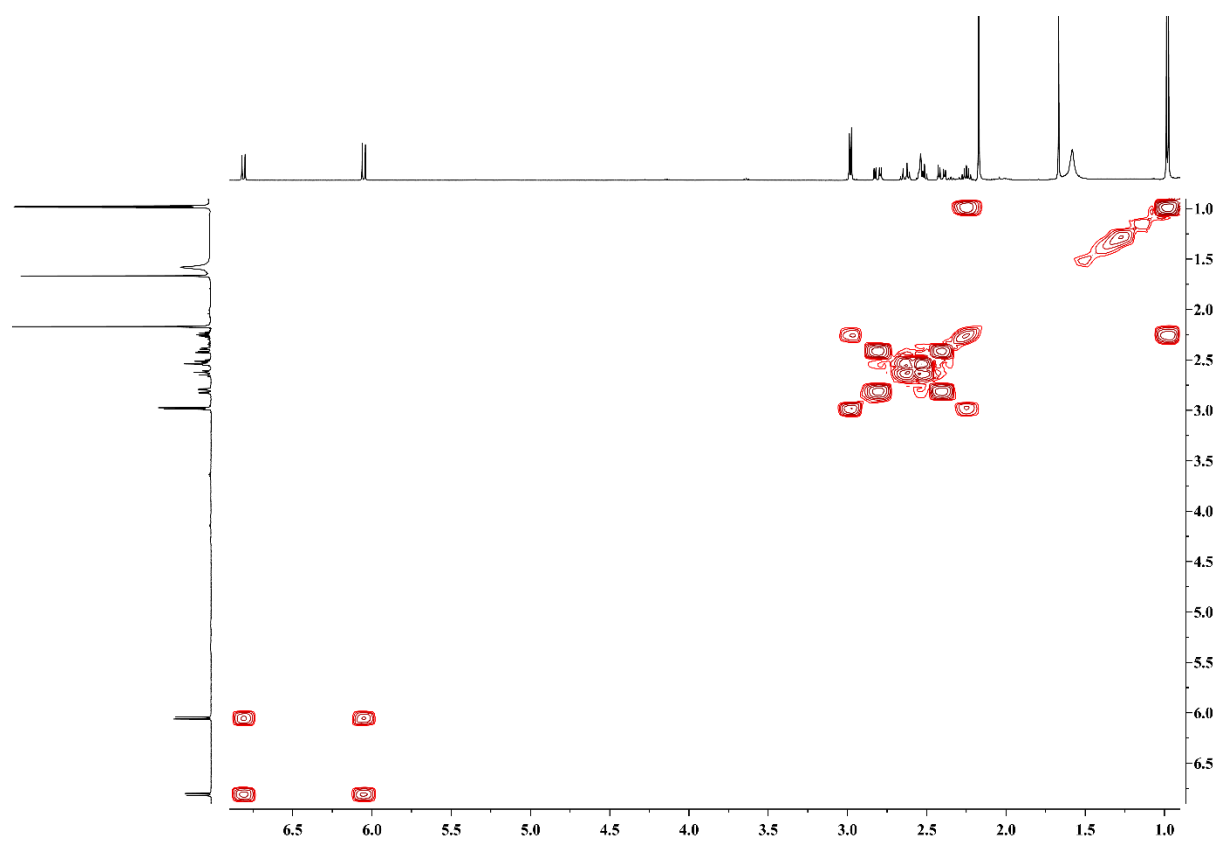


Figure S36 ROESY spectrum of 5

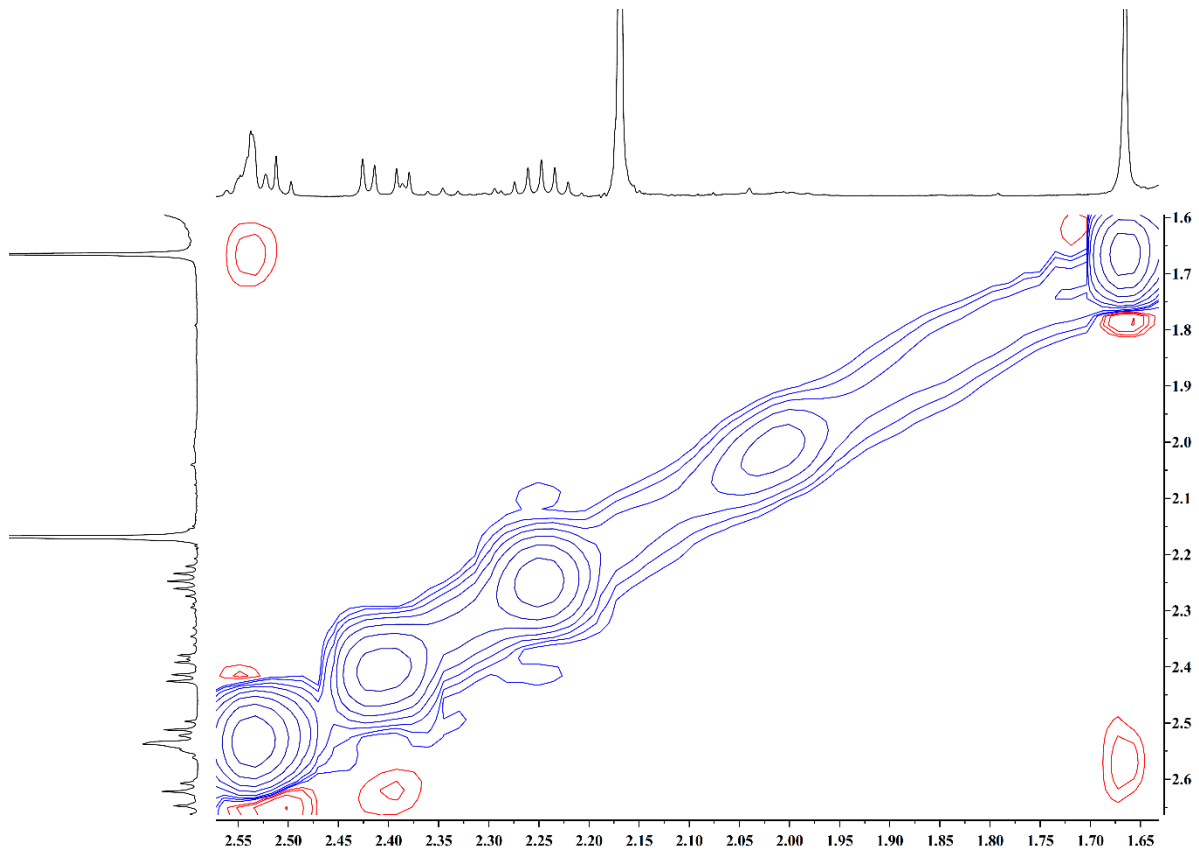
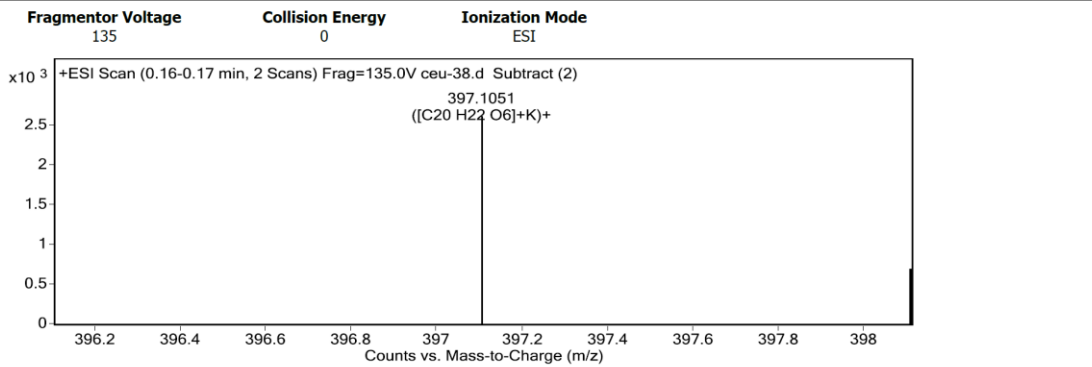


Figure S37 HRESIMS spectrum of 5

User Spectra



Peak List

| m/z | z | Abund | Formula | Ion |
|----------|---|---------|--|--------------------|
| 299.1104 | | 1642.38 | | |
| 397.1051 | 1 | 2617.18 | C ₂₀ H ₂₂ O ₆ | (M+K) ⁺ |
| 486.322 | 1 | 4717.21 | | |
| 487.325 | 1 | 1856.47 | | |
| 529.4404 | 1 | 1980.77 | | |
| 543.4557 | 1 | 1933.51 | | |
| 764.5753 | 1 | 1882.27 | | |
| 765.5764 | 1 | 1455.62 | | |

Formula Calculator Element Limits

| Element | Min | Max |
|---------|-----|-----|
| C | 3 | 60 |
| H | 0 | 120 |
| O | 0 | 10 |

Formula Calculator Results

| Formula | CalculatedMass | CalculatedMz | Mz | Diff. (mDa) | Diff. (ppm) | DBE |
|--|----------------|--------------|----------|-------------|-------------|---------|
| C ₂₀ H ₂₂ O ₆ | 358.1416 | 397.1048 | 397.1051 | -0.30 | -0.76 | 10.0000 |

Figure S38 ^1H NMR spectrum of **6** (500 MHz, CD_3OD)

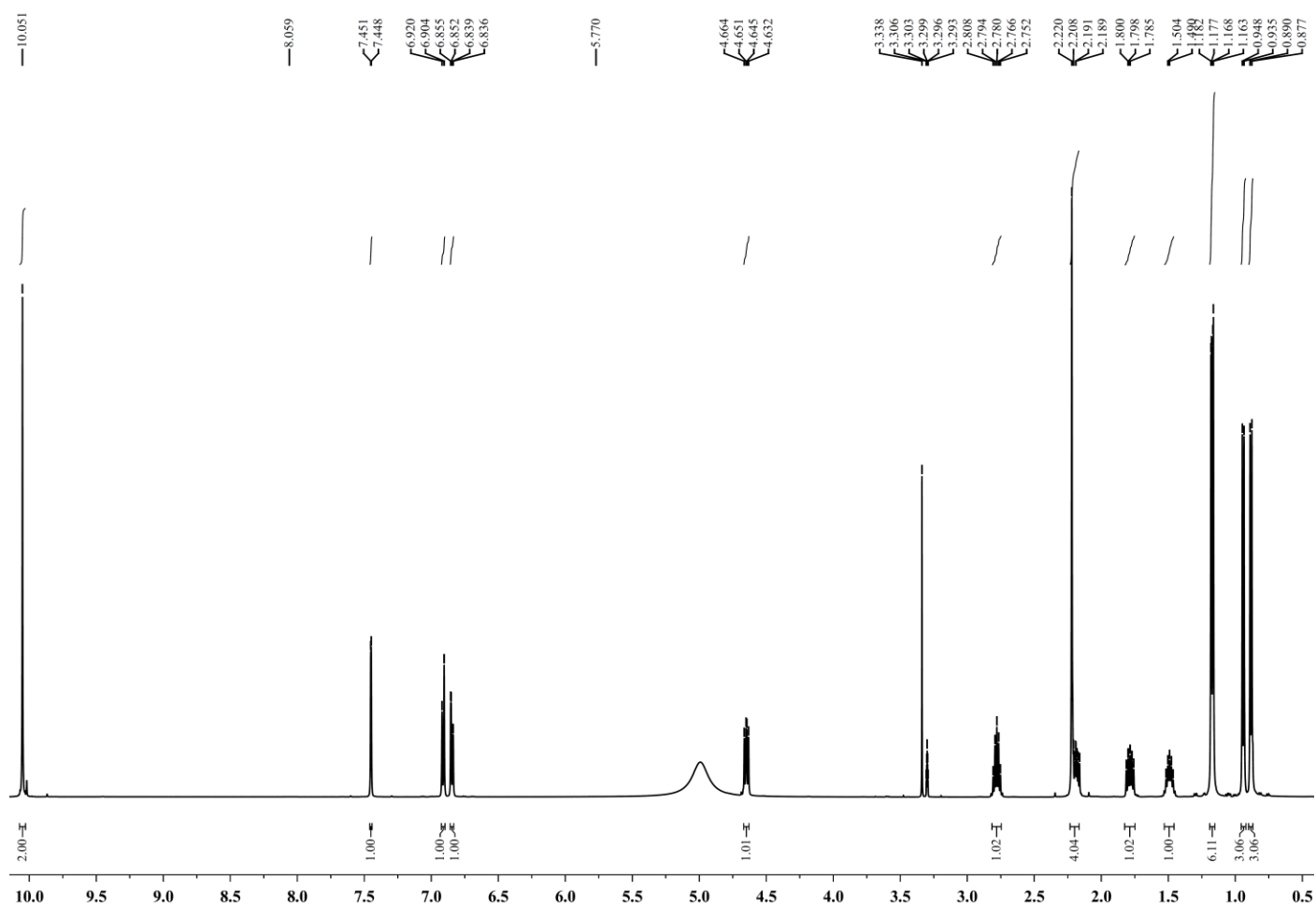


Figure S39 ^{13}C NMR spectrum of **6** (125 MHz, CD_3OD)

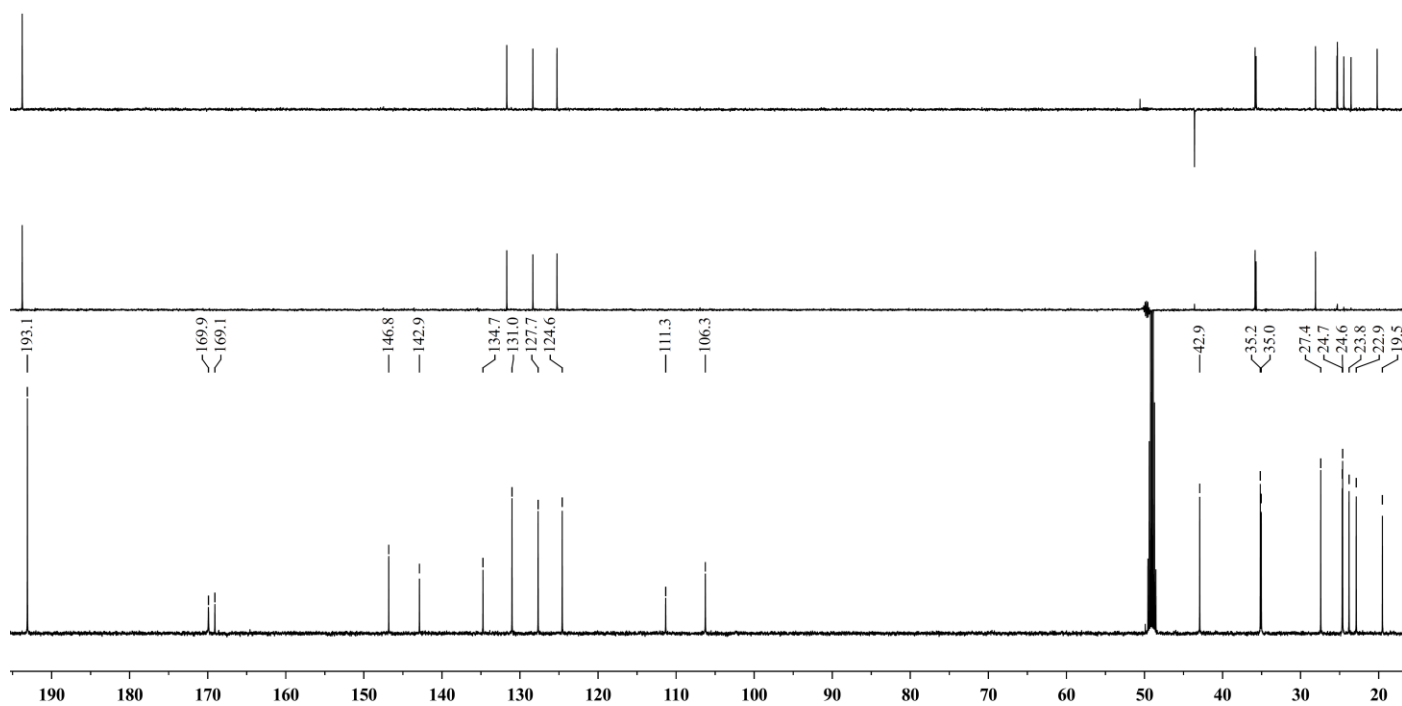


Figure S40 HSQC spectrum of **6**

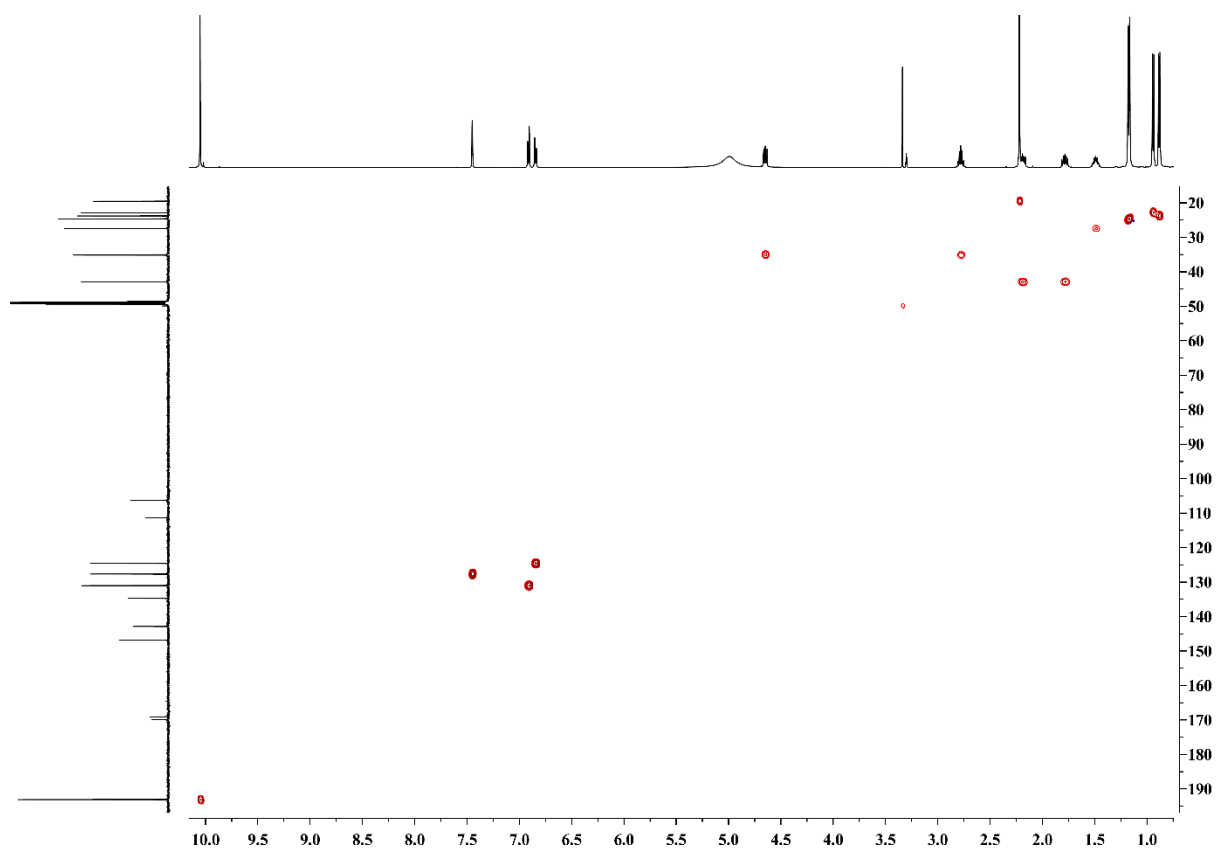


Figure S41 HMBC spectrum of **6**

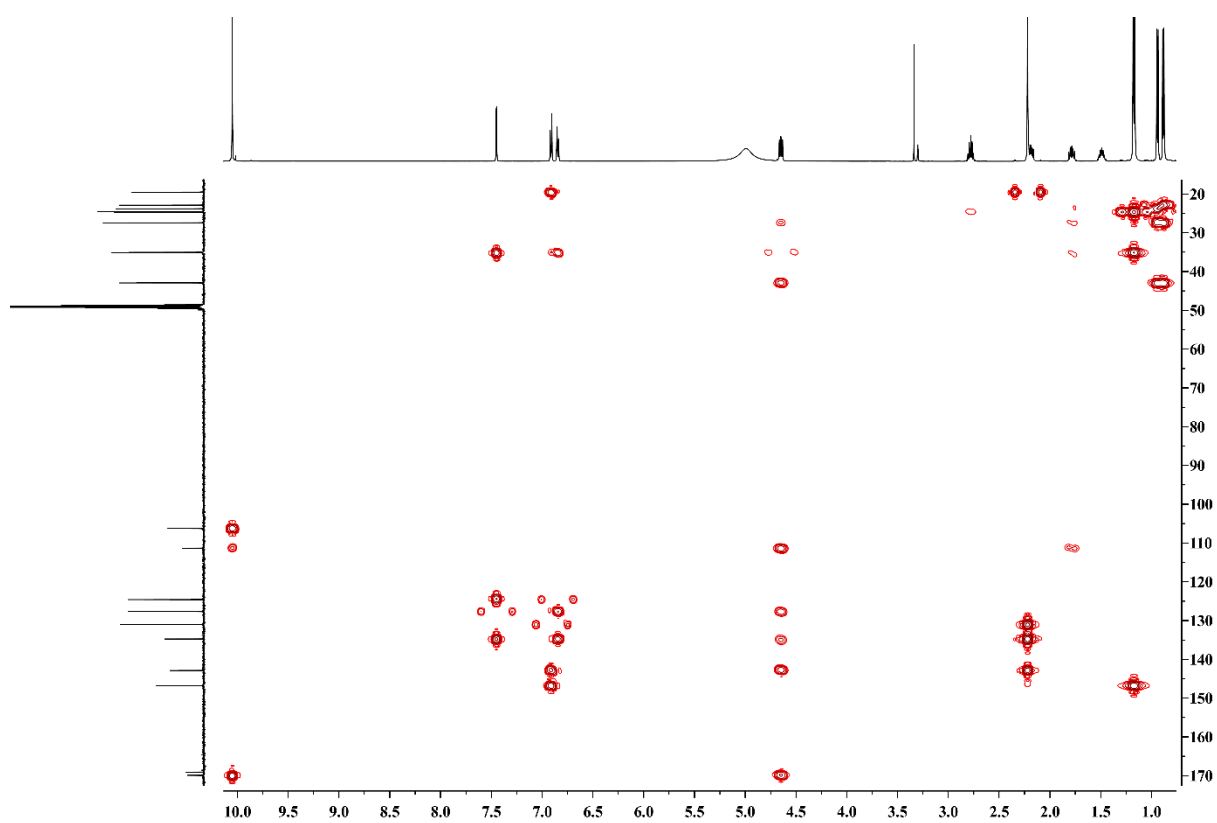


Figure S42 ^1H - ^1H COSY spectrum of **6**

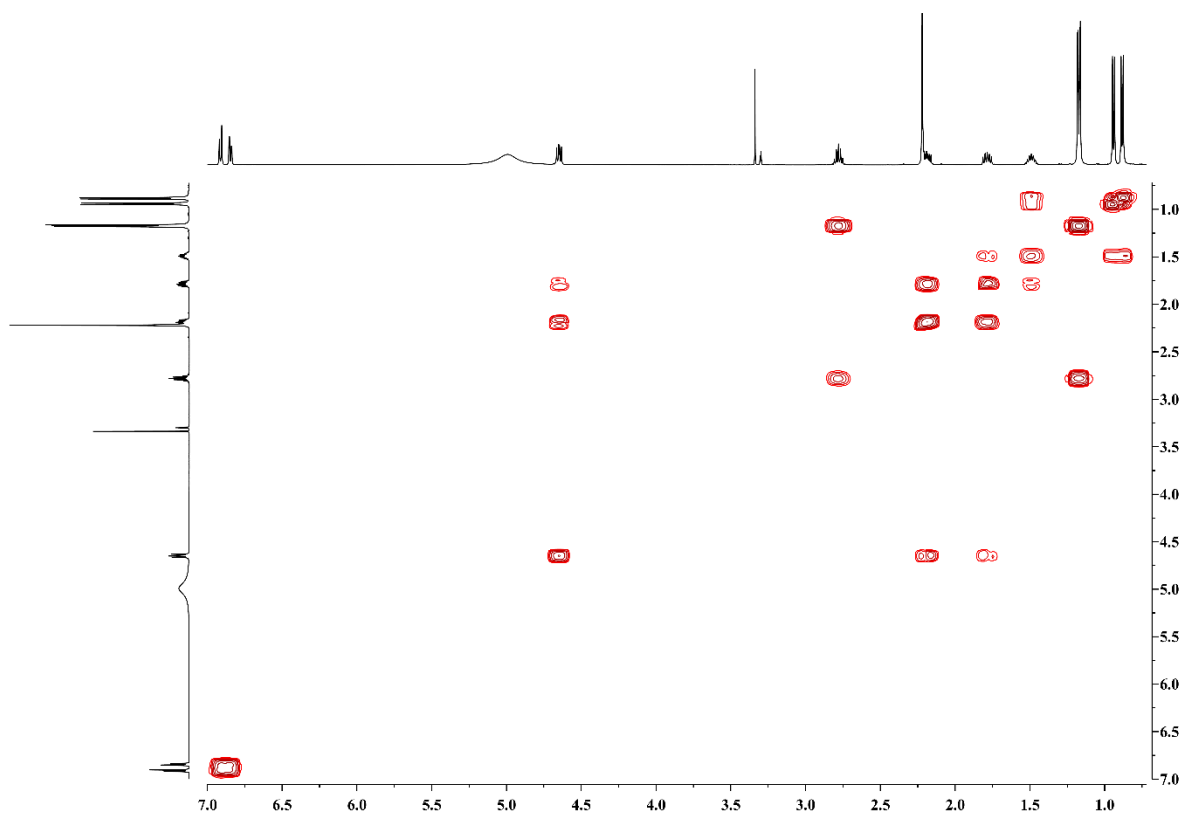
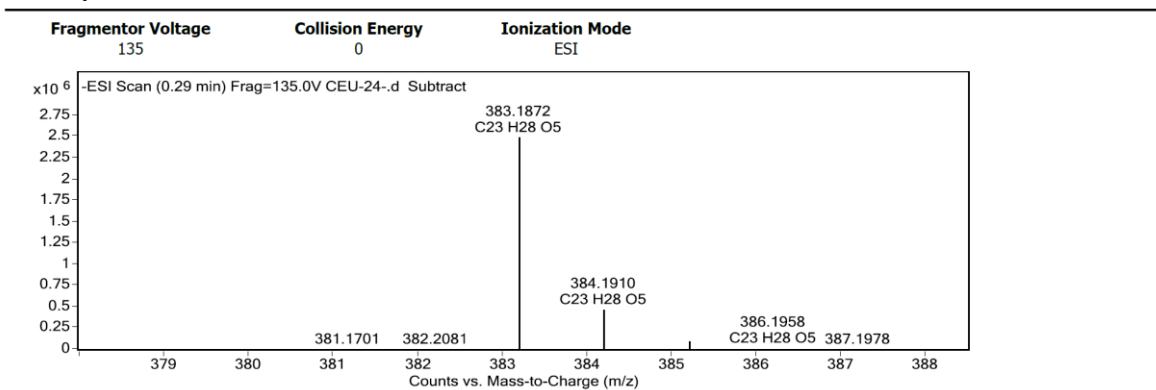


Figure S43 HRESIMS spectrum of **6**

User Spectra



Peak List

| m/z | z | Abund | Formula | Ion |
|-----------|---|------------|------------|--------|
| 383.1872 | 1 | 2490940.25 | C23 H28 O5 | (M-H)- |
| 384.191 | 1 | 467384.69 | C23 H28 O5 | (M-H)- |
| 385.1931 | 1 | 99076.27 | C23 H28 O5 | (M-H)- |
| 386.1958 | 1 | 14013.77 | C23 H28 O5 | (M-H)- |
| 397.2023 | 1 | 17099.75 | | |
| 399.1816 | 1 | 18213.43 | | |
| 429.2284 | 1 | 16047.94 | | |
| 761.4058 | 1 | 17920.81 | | |
| 1033.9879 | 1 | 29045.38 | | |
| 1034.9917 | 1 | 7714.88 | | |

Formula Calculator Element Limits

| Element | Min | Max |
|---------|-----|-----|
| C | 3 | 60 |
| H | 0 | 120 |
| O | 0 | 30 |

Formula Calculator Results

| Formula | CalculatedMass | CalculatedMz | Mz | Diff. (mDa) | Diff. (ppm) | DBE |
|------------|----------------|--------------|----------|-------------|-------------|---------|
| C23 H28 O5 | 384.1937 | 383.1864 | 383.1872 | -0.80 | -2.09 | 10.0000 |

Figure S44 ^1H NMR spectrum of **7** (500 MHz, CDCl_3)

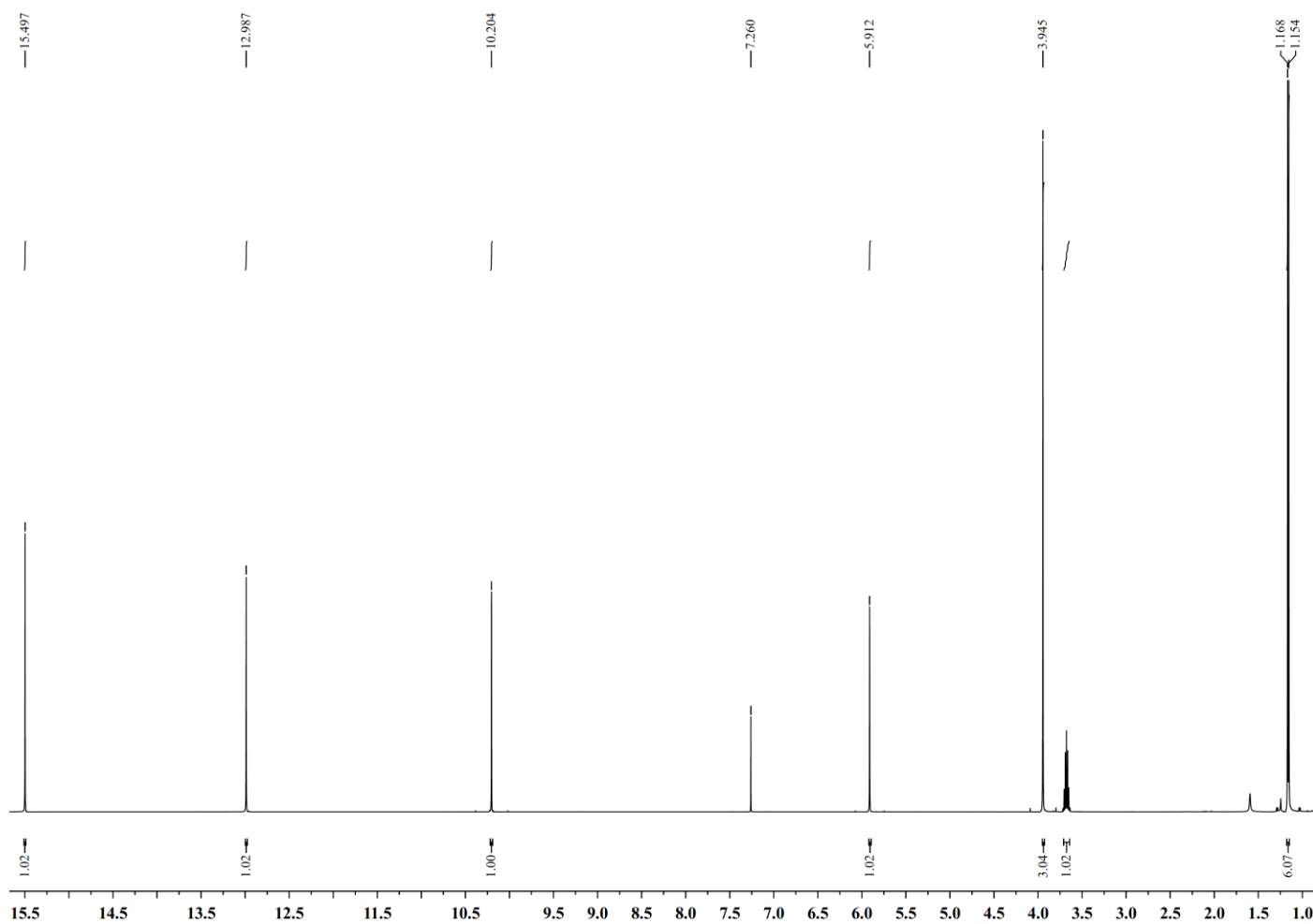


Figure S45 ^{13}C NMR spectrum of **7** (125 MHz, CDCl_3)

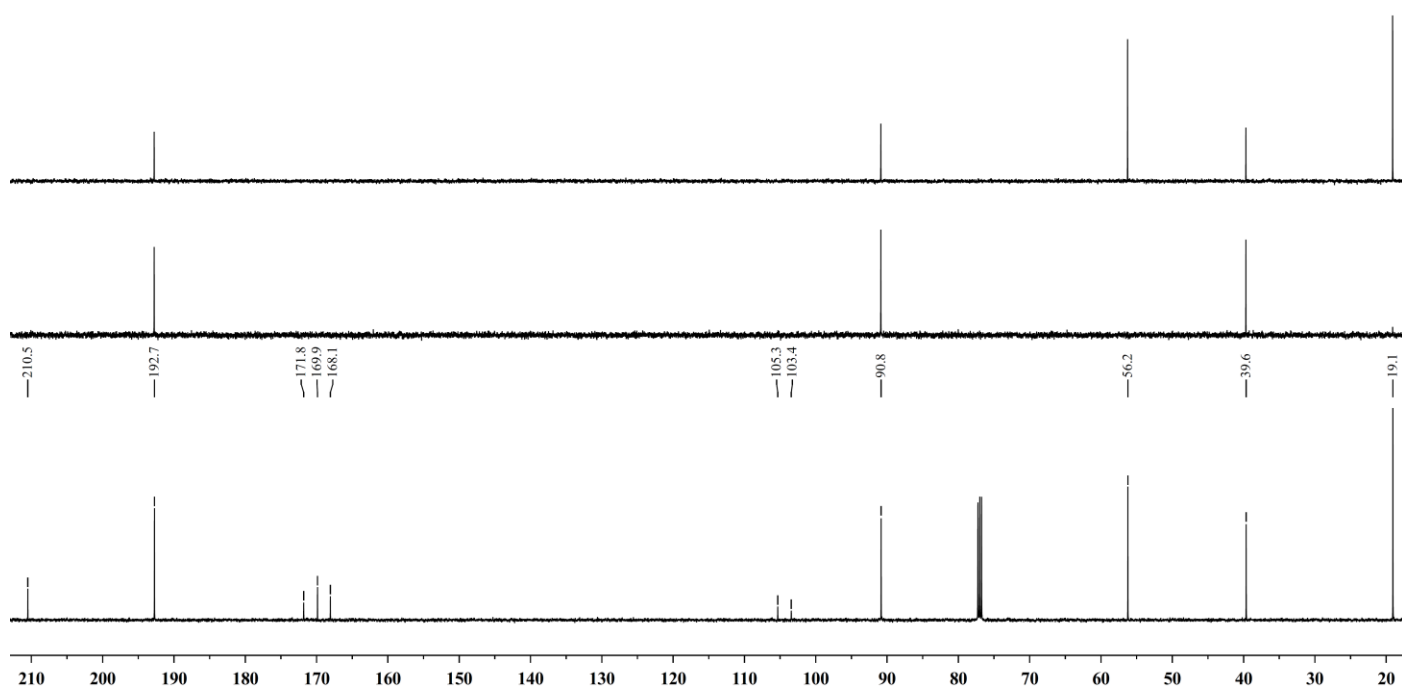


Figure S46 HSQC spectrum of 7

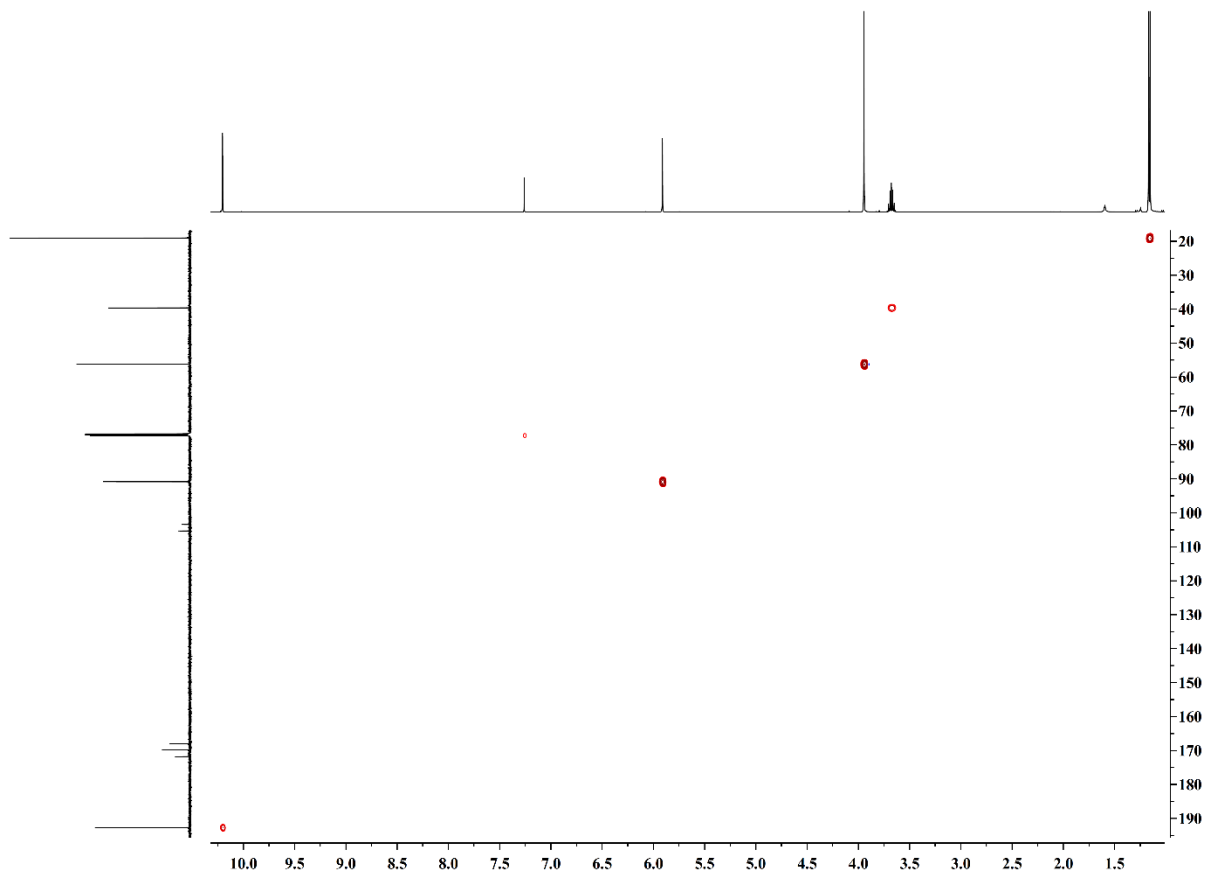


Figure S47 HMBC spectrum of 7

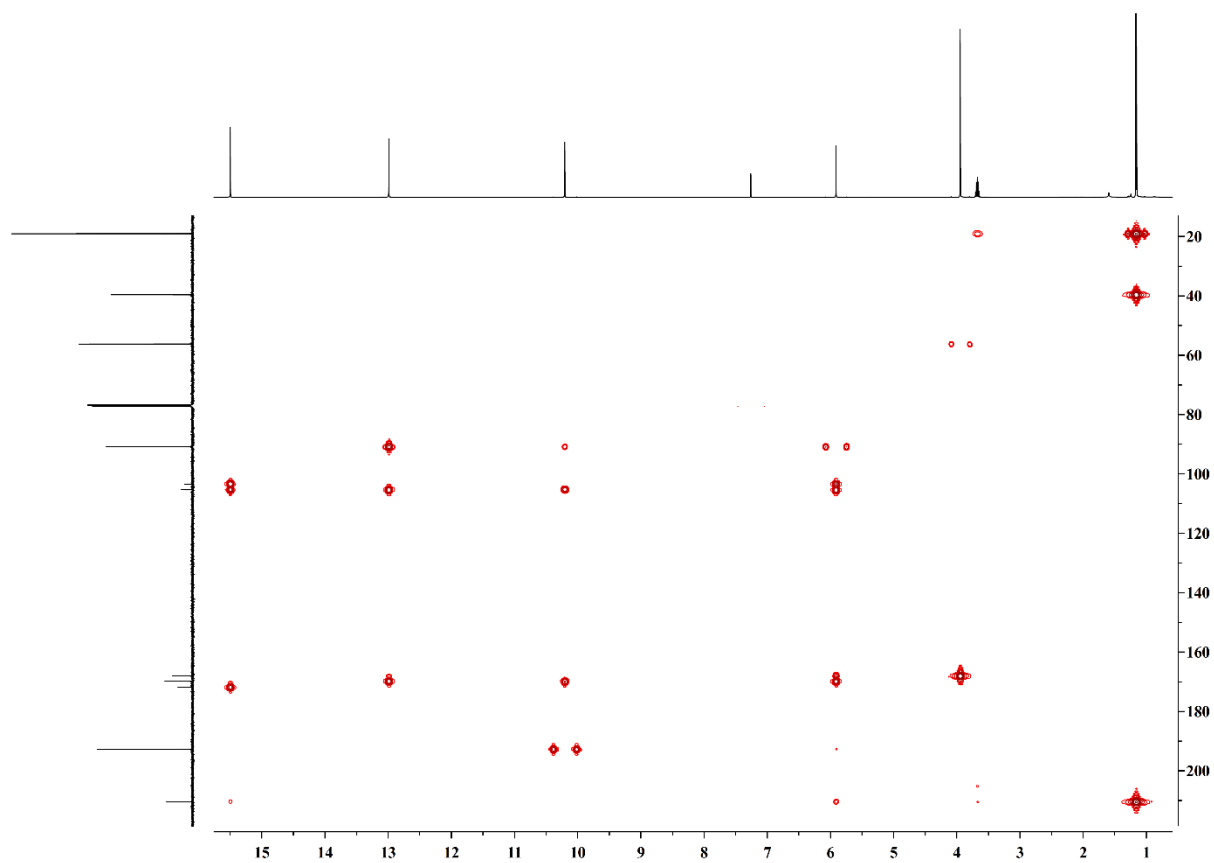


Figure S48 ^1H - ^1H COSY spectrum of 7

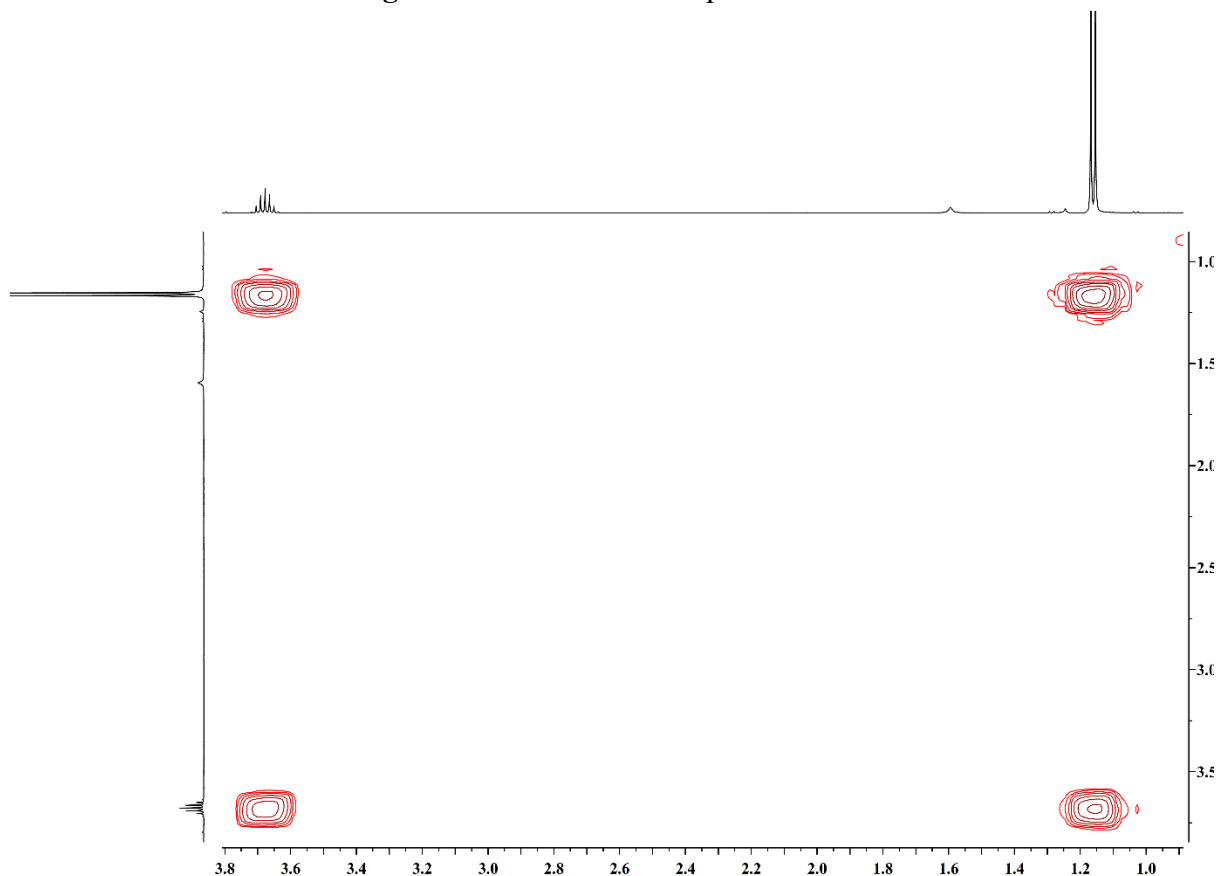
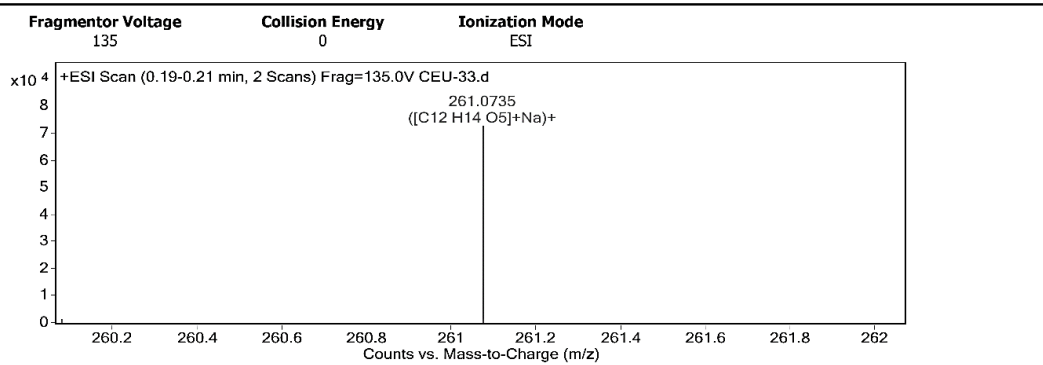


Figure S49 HRESIMS spectrum of 7

User Spectra



Peak List

| m/z | z | Abund | Formula | Ion |
|----------|---|----------|------------|---------|
| 258.0658 | 2 | 36301.57 | | |
| 261.0735 | 1 | 73119.33 | C12 H14 O5 | (M+Na)+ |
| 275.0896 | 1 | 34932.13 | | |
| 369.1196 | 2 | 30014.34 | | |
| 377.1088 | 2 | 75236.64 | | |
| 377.6105 | 2 | 30950.31 | | |
| 453.1687 | 2 | 28954.49 | | |
| 459.1694 | 2 | 33610.19 | | |

Formula Calculator Element Limits

| Element | Min | Max |
|---------|-----|-----|
| C | 3 | 60 |
| H | 0 | 120 |
| O | 0 | 30 |

Formula Calculator Results

| Formula | CalculatedMass | CalculatedMz | Mz | Diff. (mDa) | Diff. (ppm) | DBE |
|------------|----------------|--------------|----------|-------------|-------------|--------|
| C12 H14 O5 | 238.0841 | 261.0733 | 261.0735 | -0.20 | -0.77 | 6.0000 |

Figure S50 ^1H NMR spectrum of **8** (600 MHz, acetone- d_6)

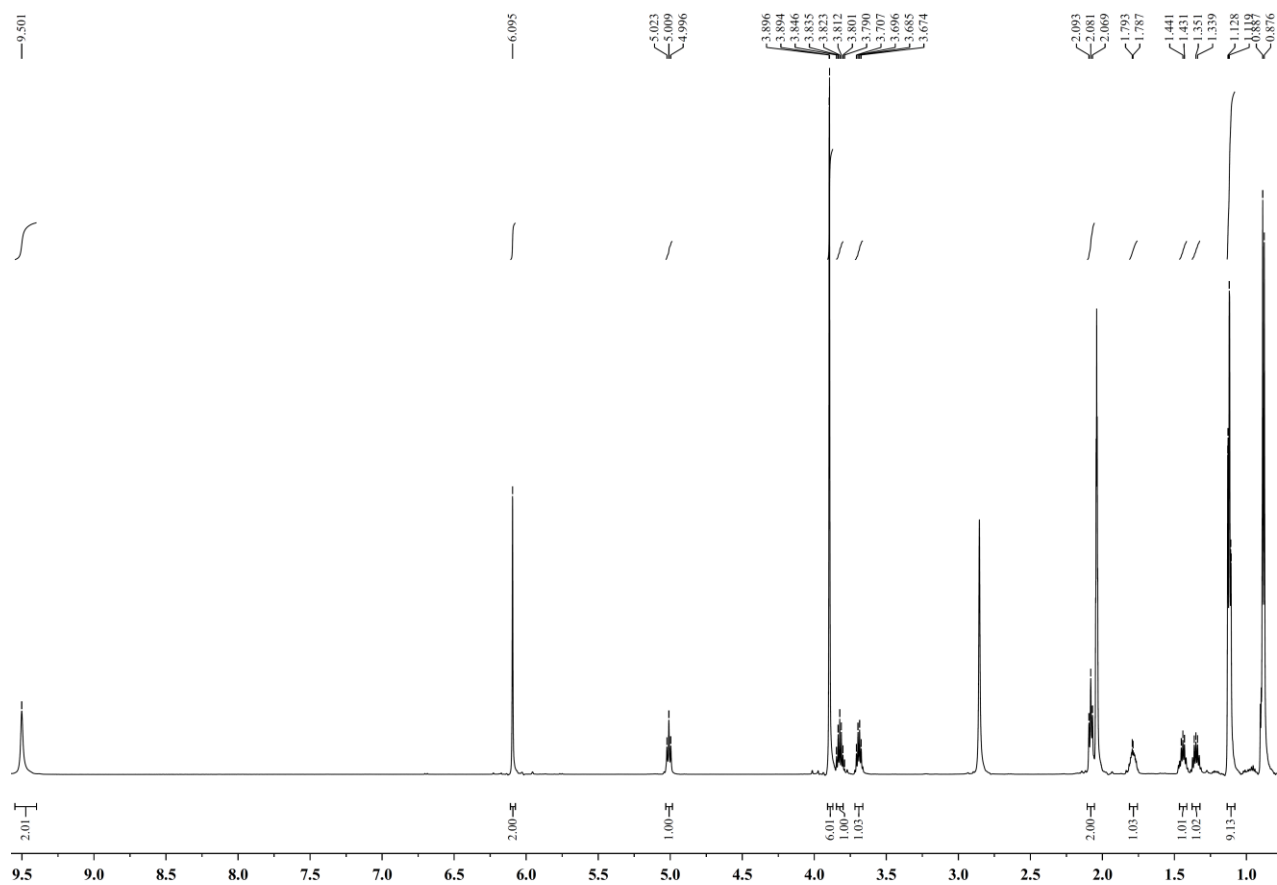


Figure S51 ^{13}C NMR spectrum of **8** (150 MHz, acetone- d_6)

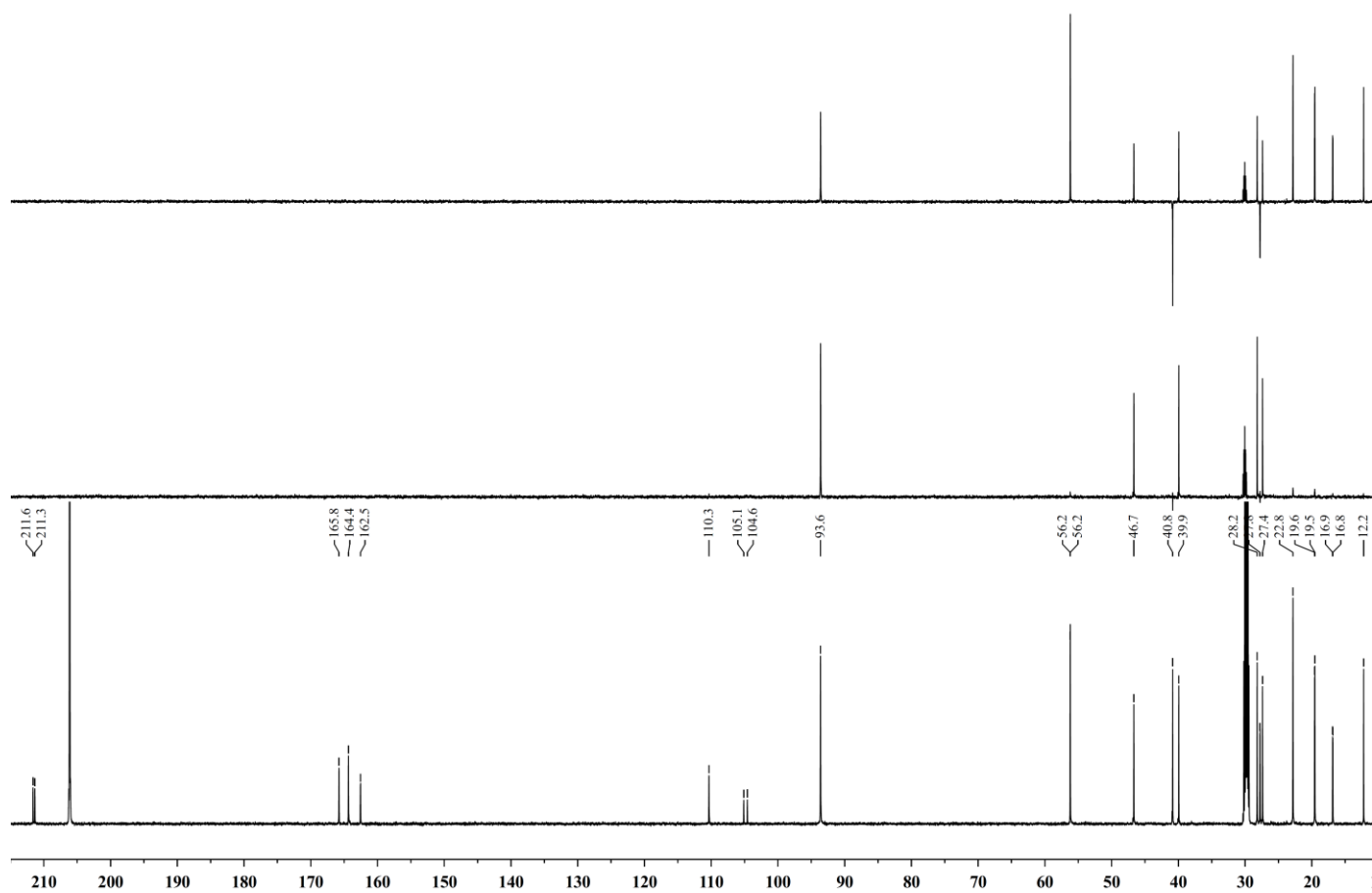


Figure S52 HSQC spectrum of **8**

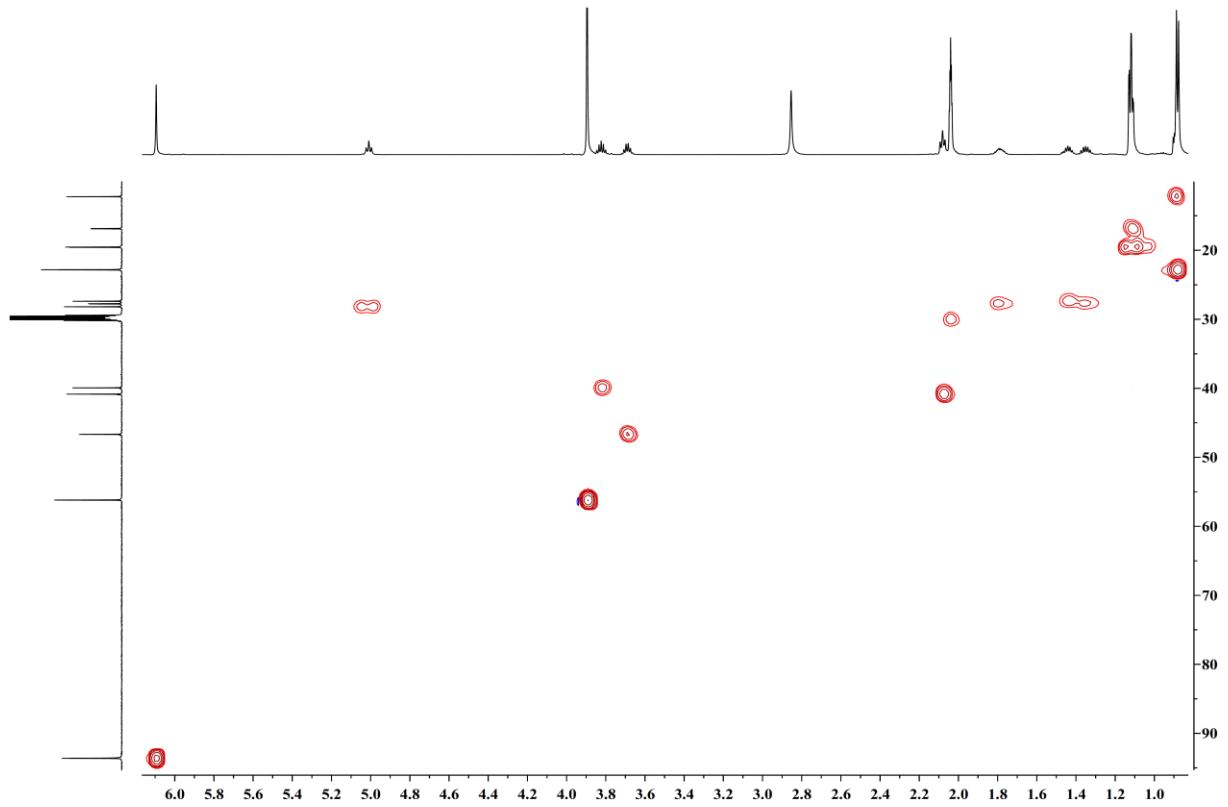


Figure S53 HMBC spectrum of **8**

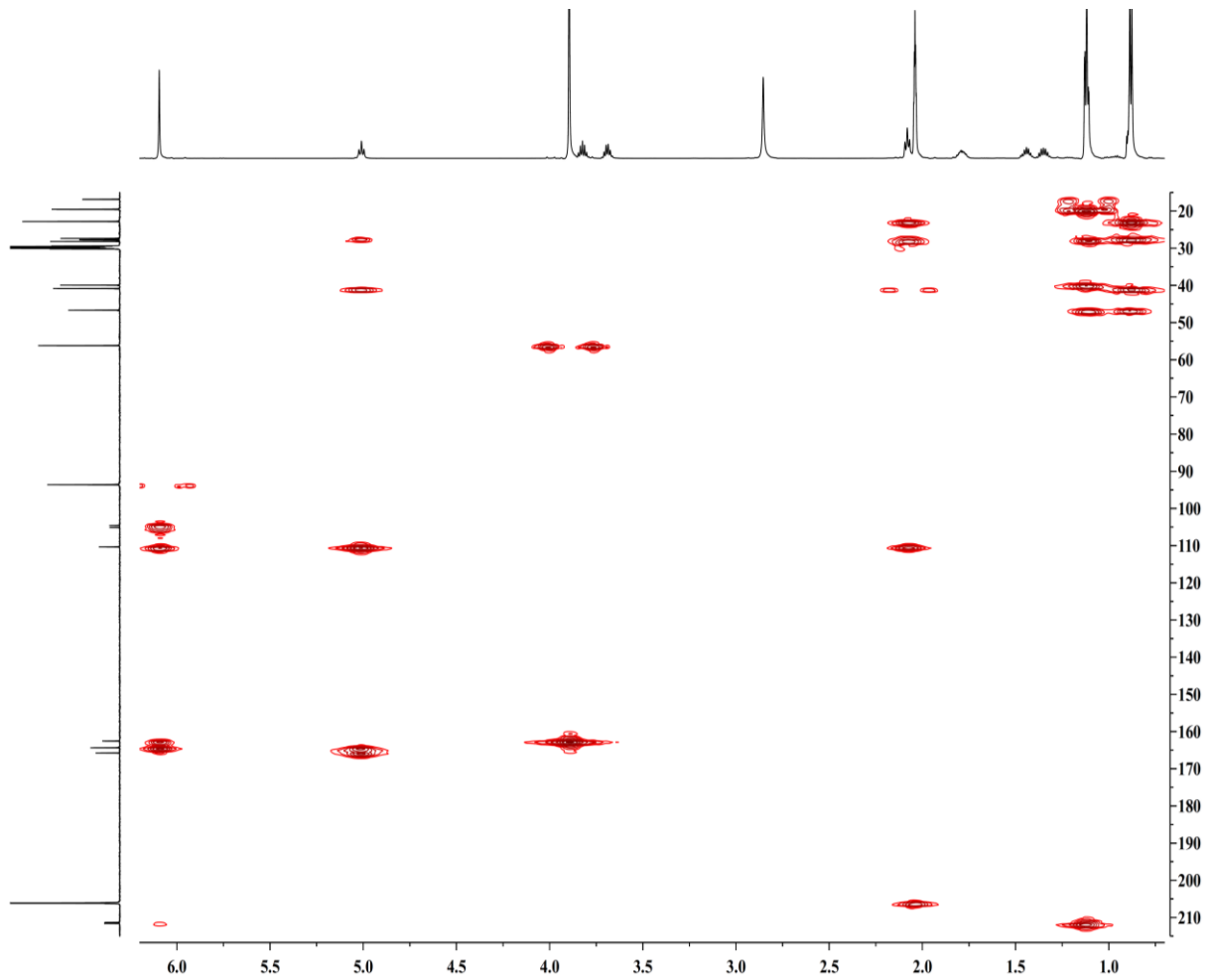


Figure S54 ^1H - ^1H COSY spectrum of **8**

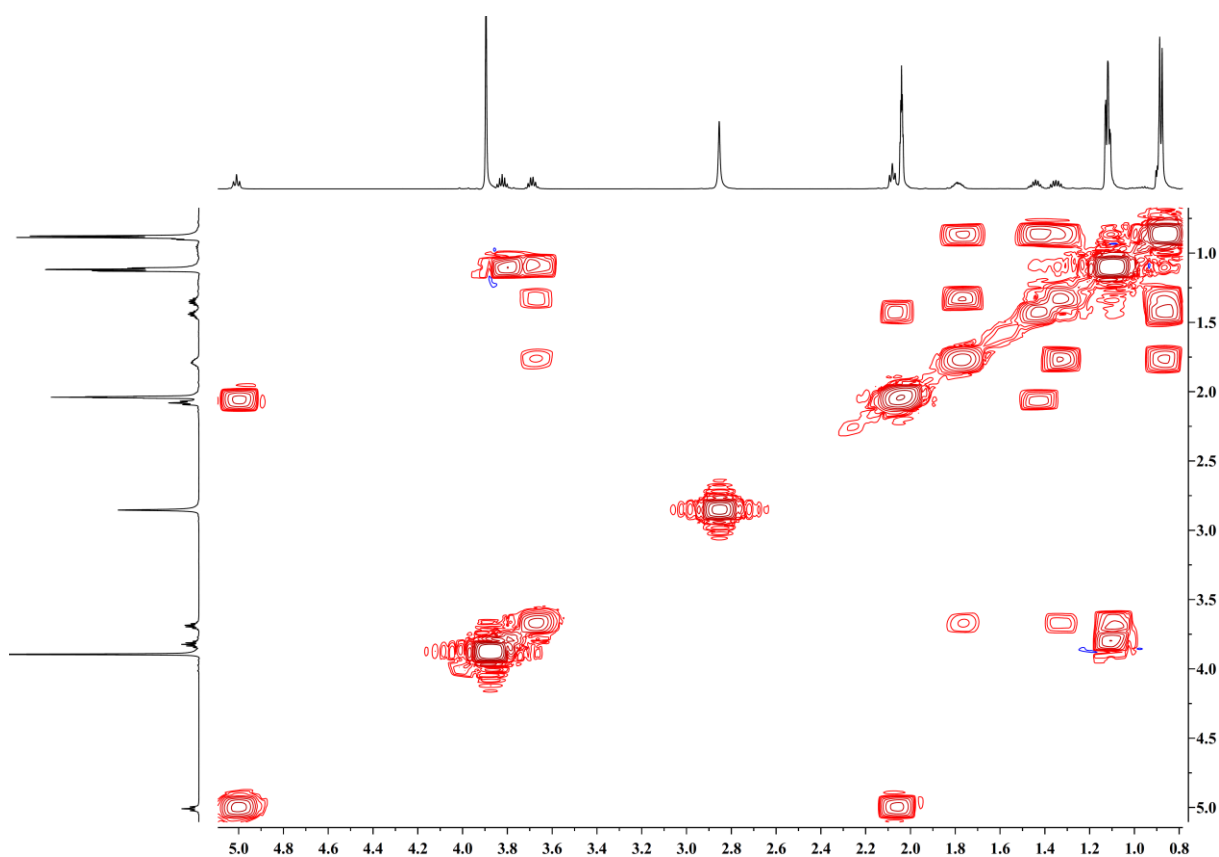
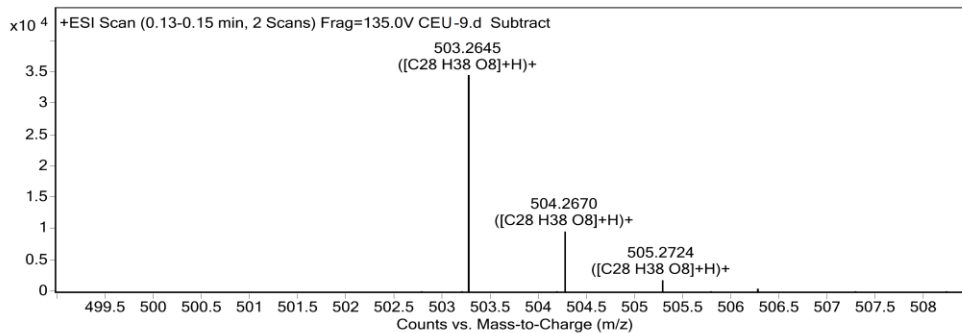


Figure S55 HRESIMS spectrum of **8**

User Spectra

Fragmentor Voltage: 135 Collision Energy: 0 Ionization Mode: ESI



Peak List

| <i>m/z</i> | <i>z</i> | Abund | Formula | Ion |
|------------|----------|----------|--|--------------------|
| 279.1594 | 1 | 8301.38 | | |
| 291.6231 | 2 | 4067.44 | | |
| 293.1746 | 1 | 8516.72 | | |
| 437.1949 | 1 | 2613.73 | | |
| 453.1675 | 1 | 3175.68 | | |
| 503.2645 | 1 | 34652.38 | C ₂₈ H ₃₈ O ₈ | (M+H) ⁺ |
| 504.267 | 1 | 9774.65 | C ₂₈ H ₃₈ O ₈ | (M+H) ⁺ |
| 525.2465 | 1 | 8340.53 | | |
| 526.2508 | 1 | 2471.41 | | |
| 1027.5058 | 1 | 4077.35 | | |

Formula Calculator Element Limits

| Element | Min | Max |
|---------|-----|-----|
| C | 3 | 120 |
| H | 0 | 240 |
| O | 0 | 30 |

Formula Calculator Results

| Formula | CalculatedMass | CalculatedMz | Mz | Diff. (mDa) | Diff. (ppm) | DBE |
|--|----------------|--------------|----------|-------------|-------------|---------|
| C ₂₈ H ₃₈ O ₈ | 502.2567 | 503.2639 | 503.2645 | -0.60 | -1.19 | 10.0000 |

Figure S56 ^1H NMR spectrum of **9** (600 MHz, CDCl_3)

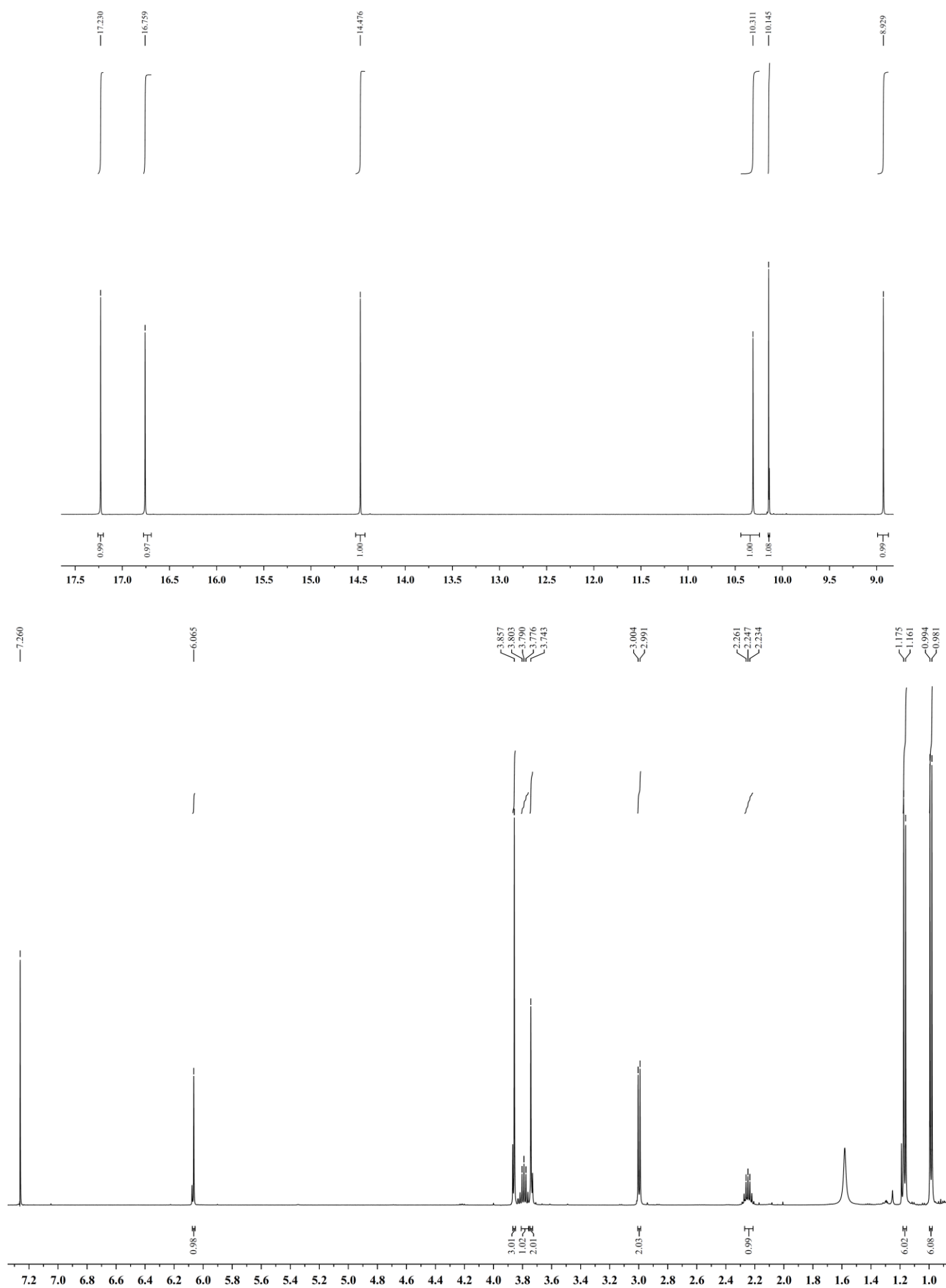


Figure S57 ^{13}C NMR spectrum of **9** (150 MHz, CDCl_3)

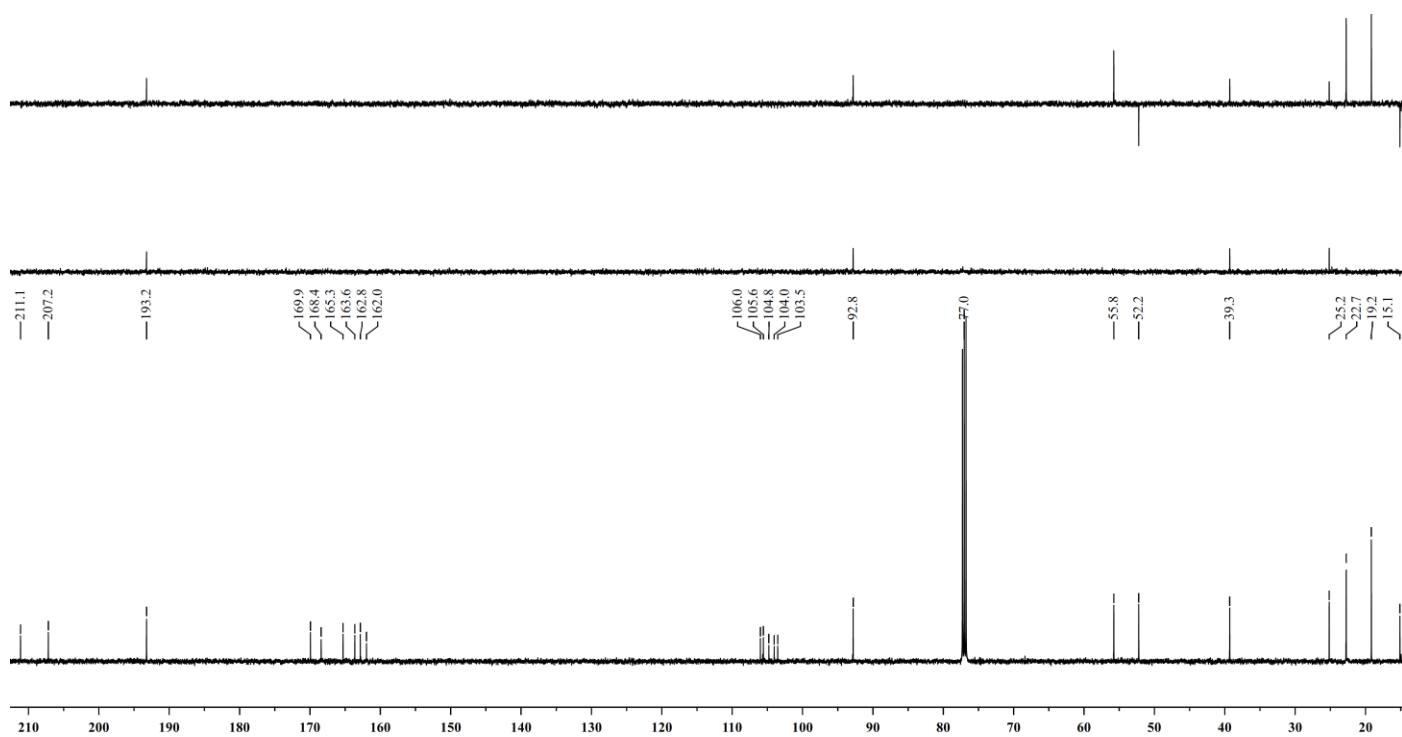


Figure S58 HSQC spectrum of **9**

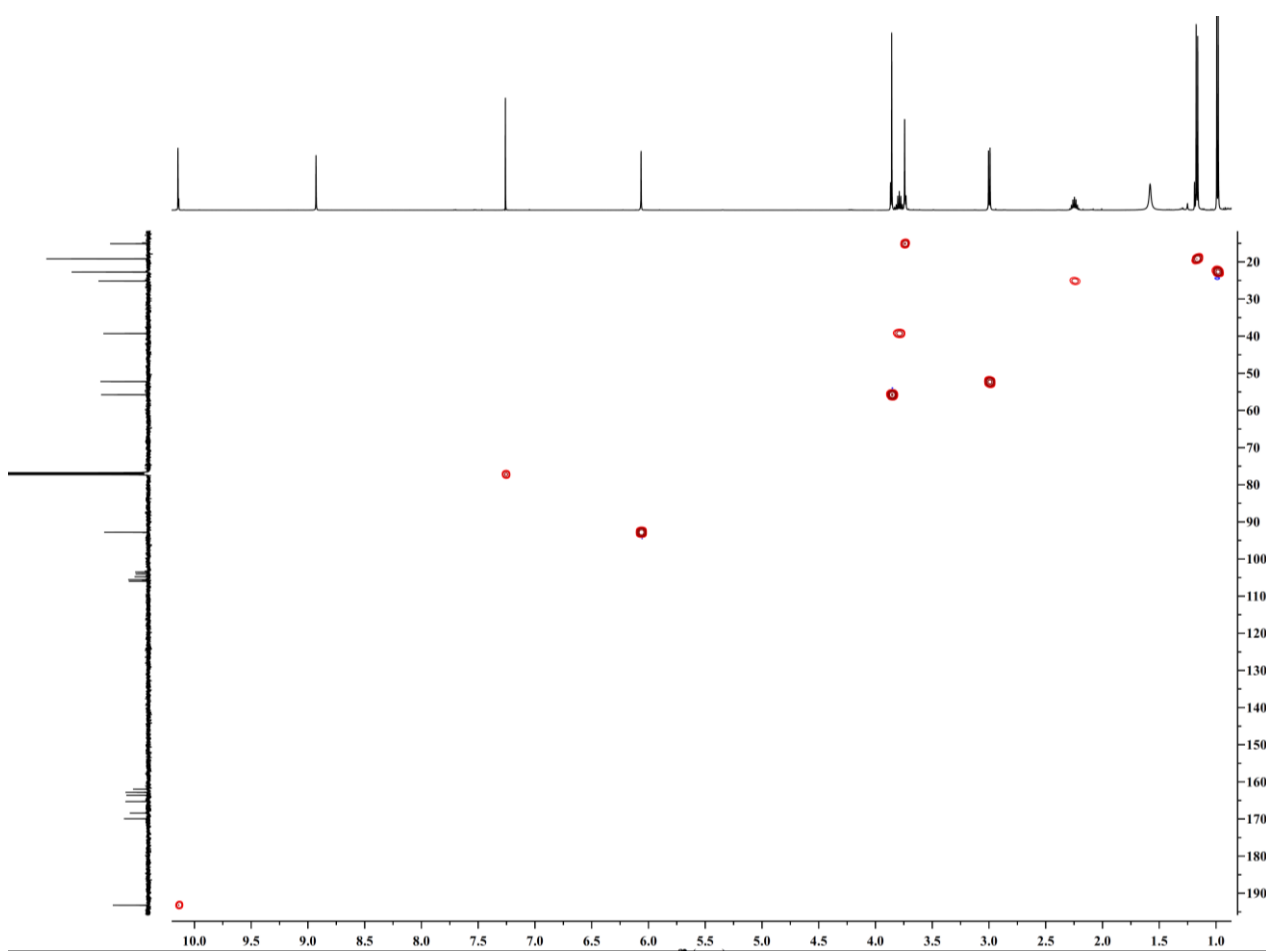


Figure S59 HMBC spectrum of **9**

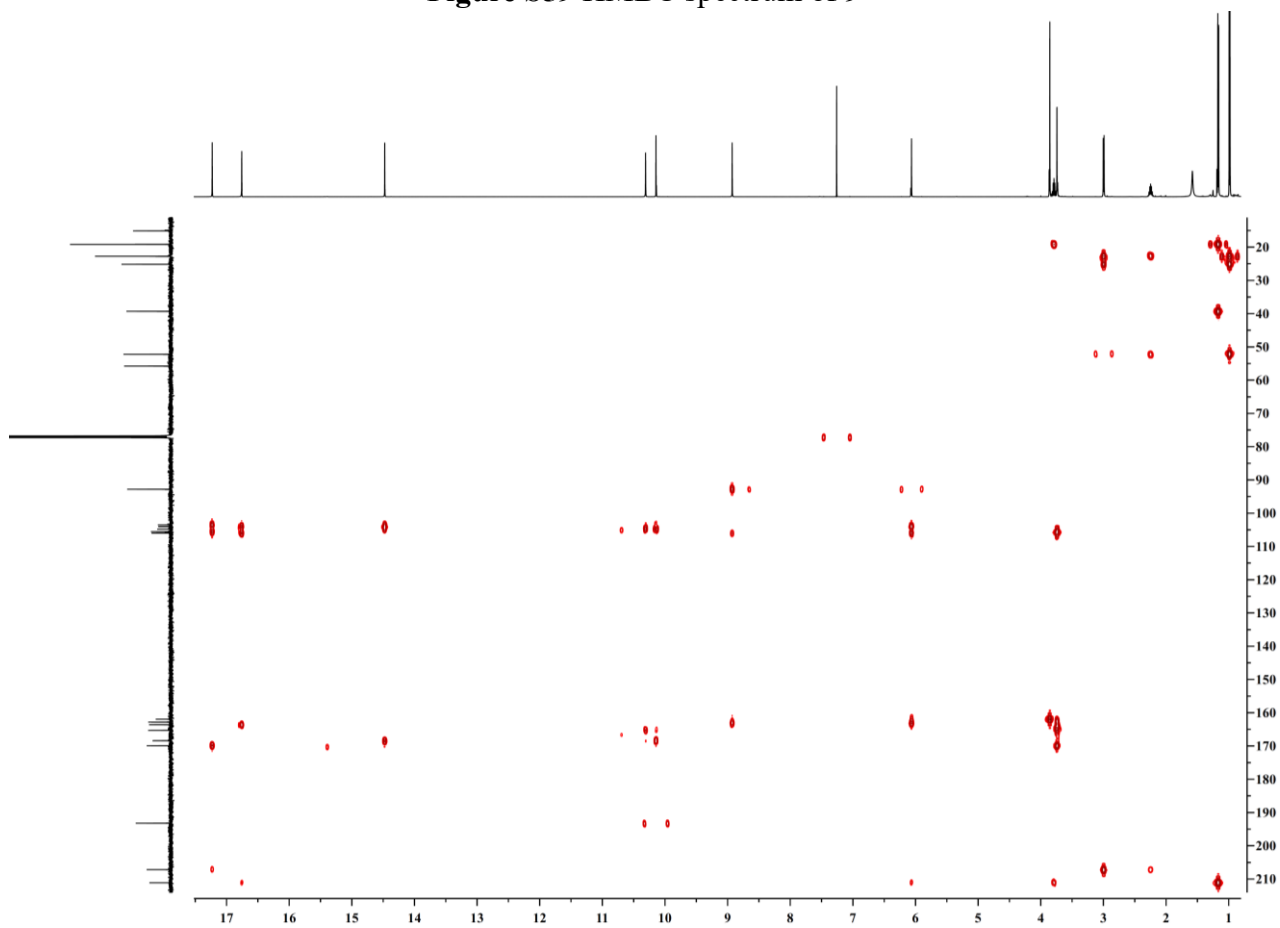


Figure S60 ^1H - ^1H COSY spectrum of **9**

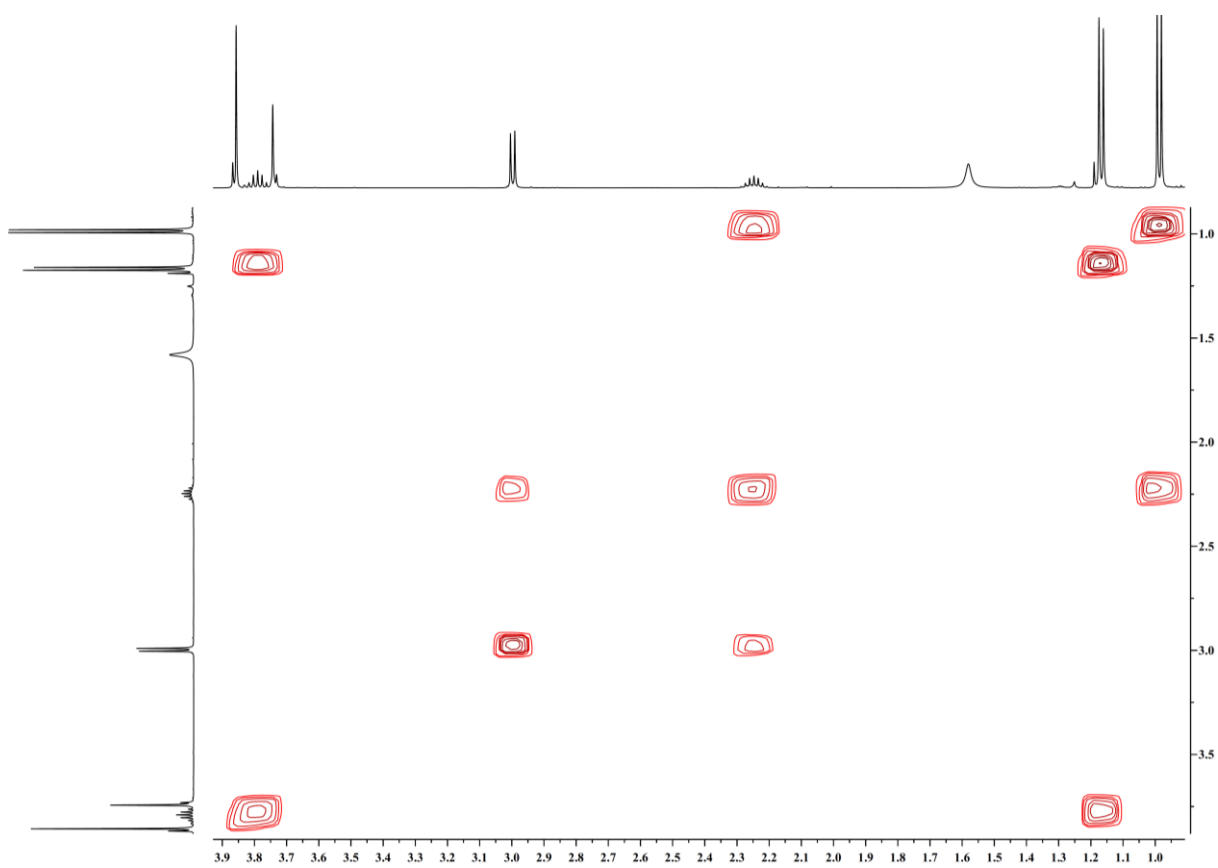
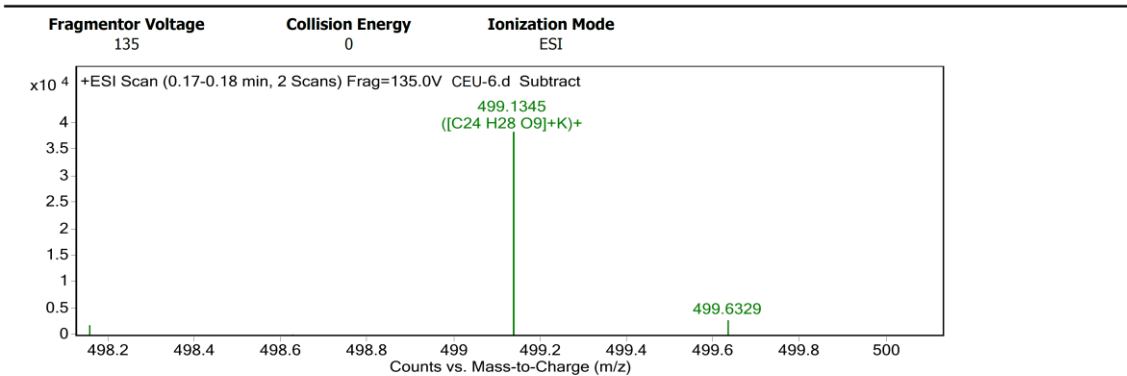


Figure S61 HRESIMS spectrum of **9**

User Spectra



Peak List

| m/z | z | Abund | Formula | Ion |
|----------|---|----------|--|--------------------|
| 299.1114 | 1 | 56808.45 | | |
| 301.1416 | 1 | 35021.72 | | |
| 315.0855 | 1 | 90959.04 | | |
| 317.1157 | 1 | 68790.2 | | |
| 499.1345 | 1 | 38546.86 | C ₂₄ H ₂₈ O ₉ | (M+K) ⁺ |
| 540.1553 | 1 | 19467.76 | | |
| 575.233 | 1 | 21283.24 | | |
| 658.433 | 1 | 26975.96 | | |

Formula Calculator Element Limits

| Element | Min | Max |
|---------|-----|-----|
| C | 3 | 60 |
| H | 0 | 120 |
| O | 0 | 10 |

Formula Calculator Results

| Formula | CalculatedMass | CalculatedMz | Mz | Diff. (mDa) | Diff. (ppm) | DBE |
|--|----------------|--------------|----------|-------------|-------------|---------|
| C ₂₄ H ₂₈ O ₉ | 460.1733 | 499.1365 | 499.1345 | 2.00 | 4.01 | 11.0000 |

Figure S62 ¹H NMR (600 MHz, pyridine-*d*₅) spectrum of **10** and **11**

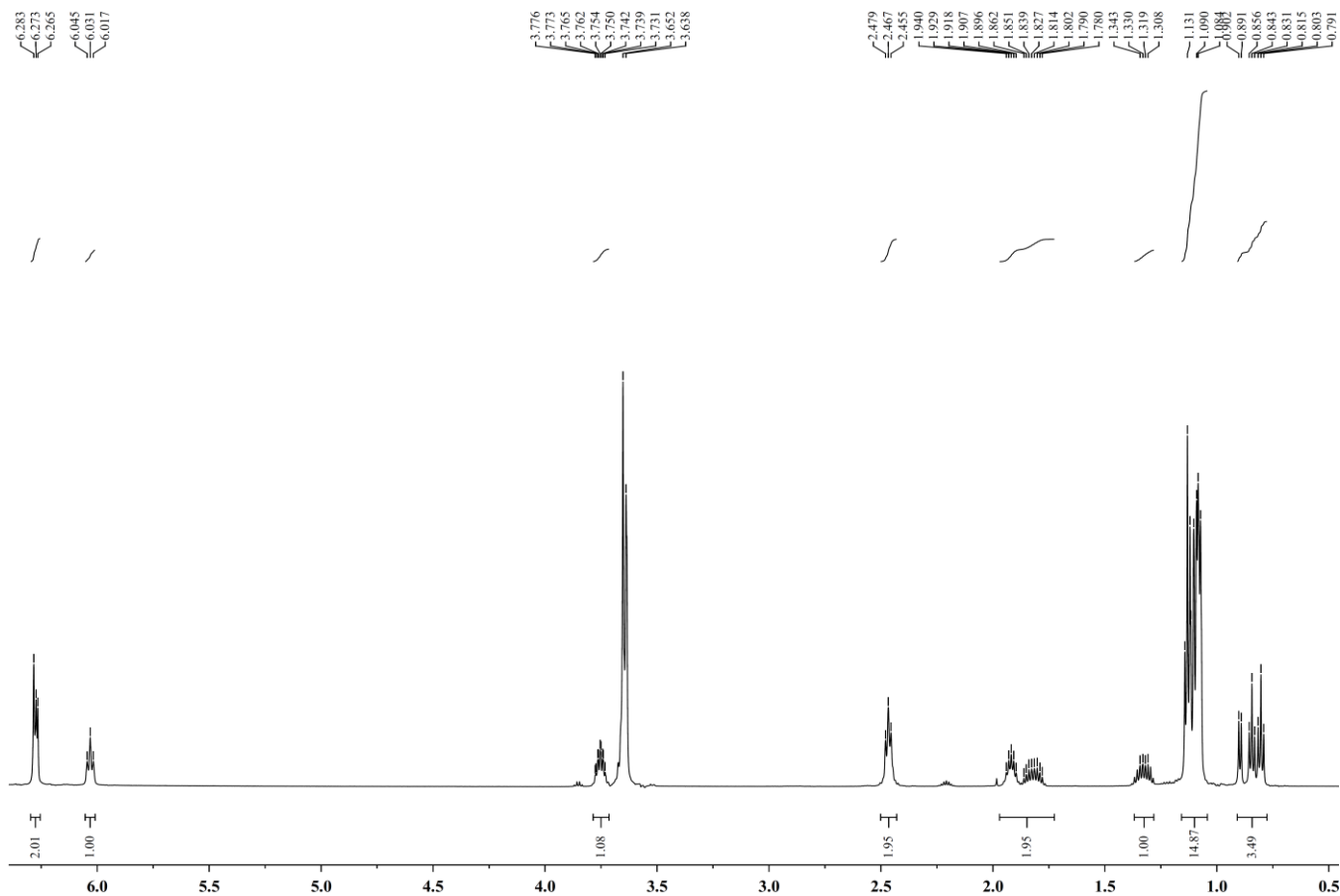


Figure S63 ^{13}C NMR (150 MHz, pyridine- d_5) spectrum of **10** and **11**

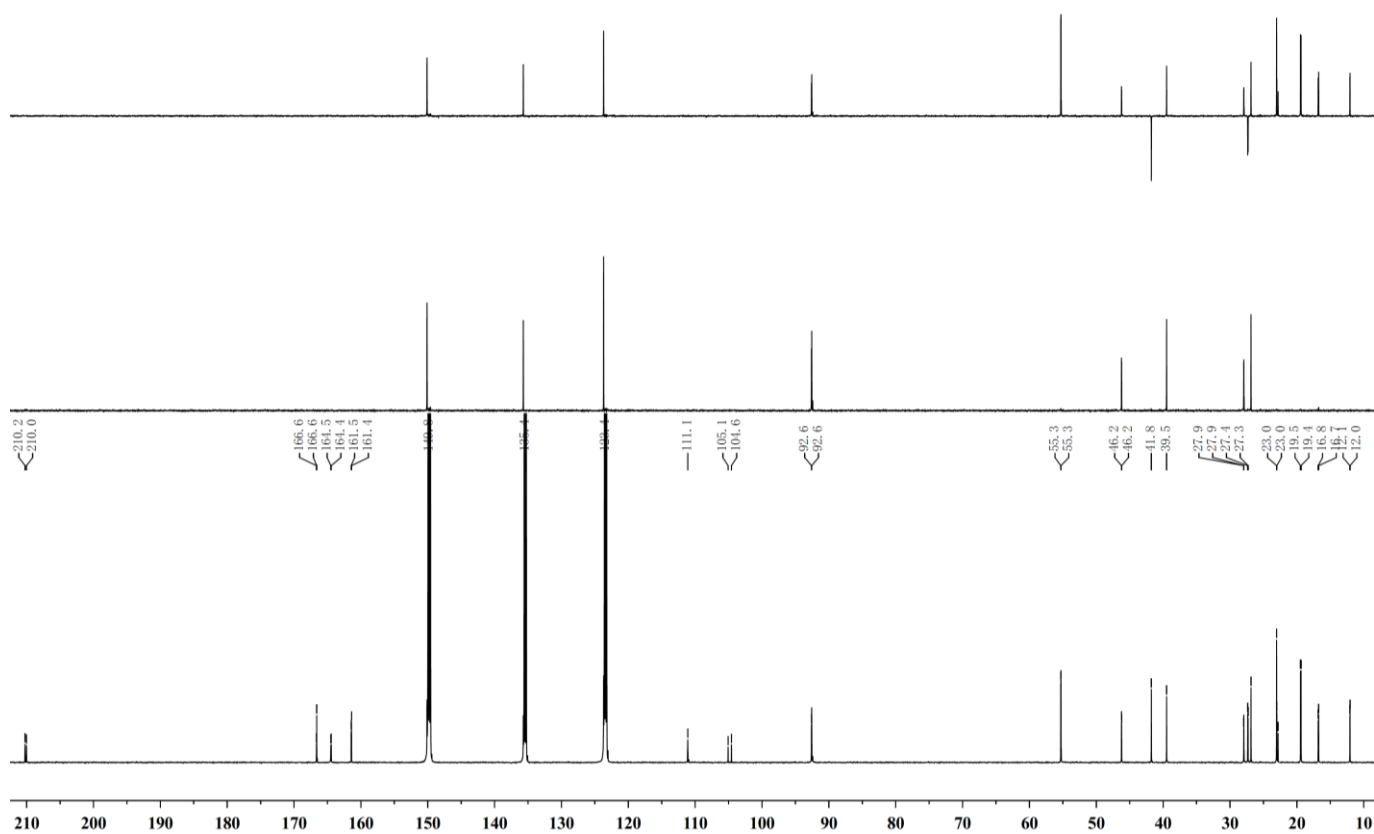


Figure S64 HSQC spectrum of the mixture **10** and **11**

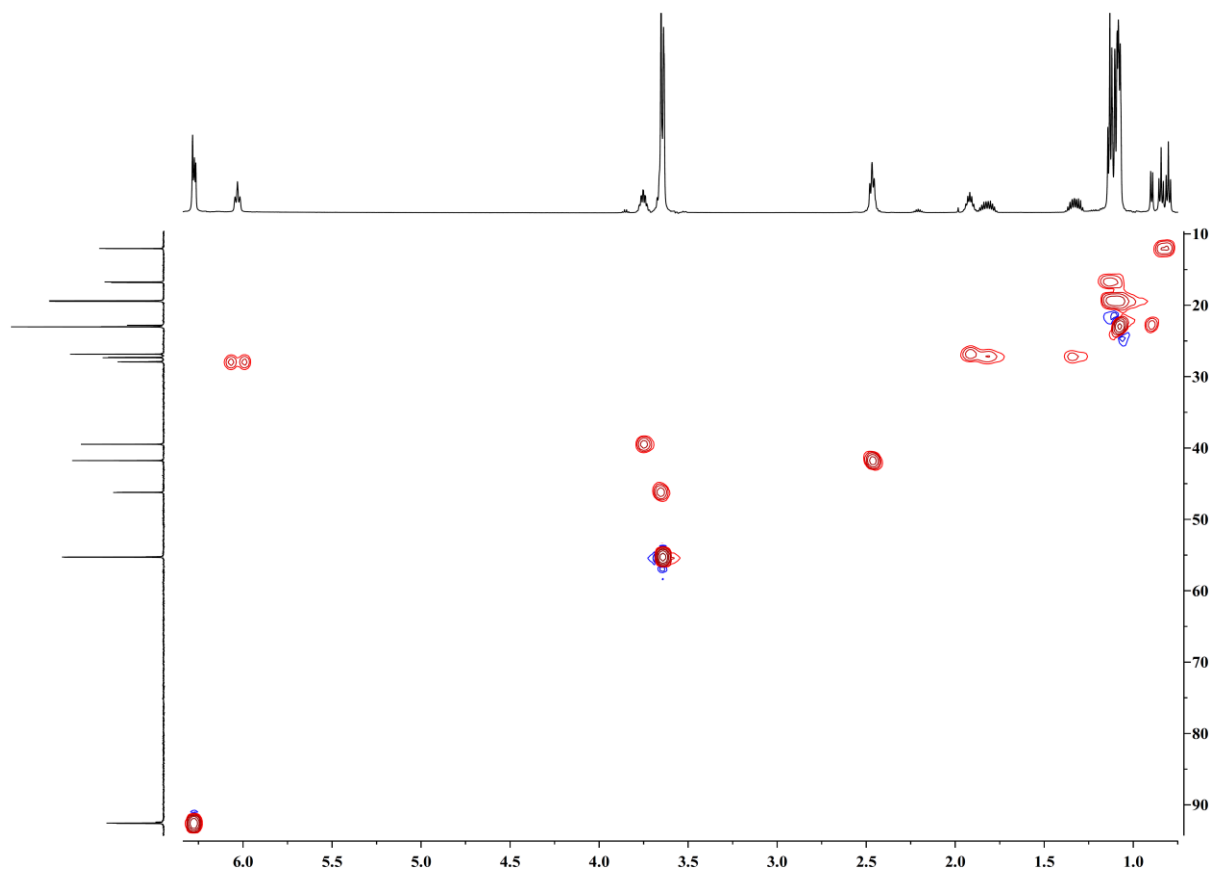


Figure S65 HMBC spectrum of the mixture **10** and **11**

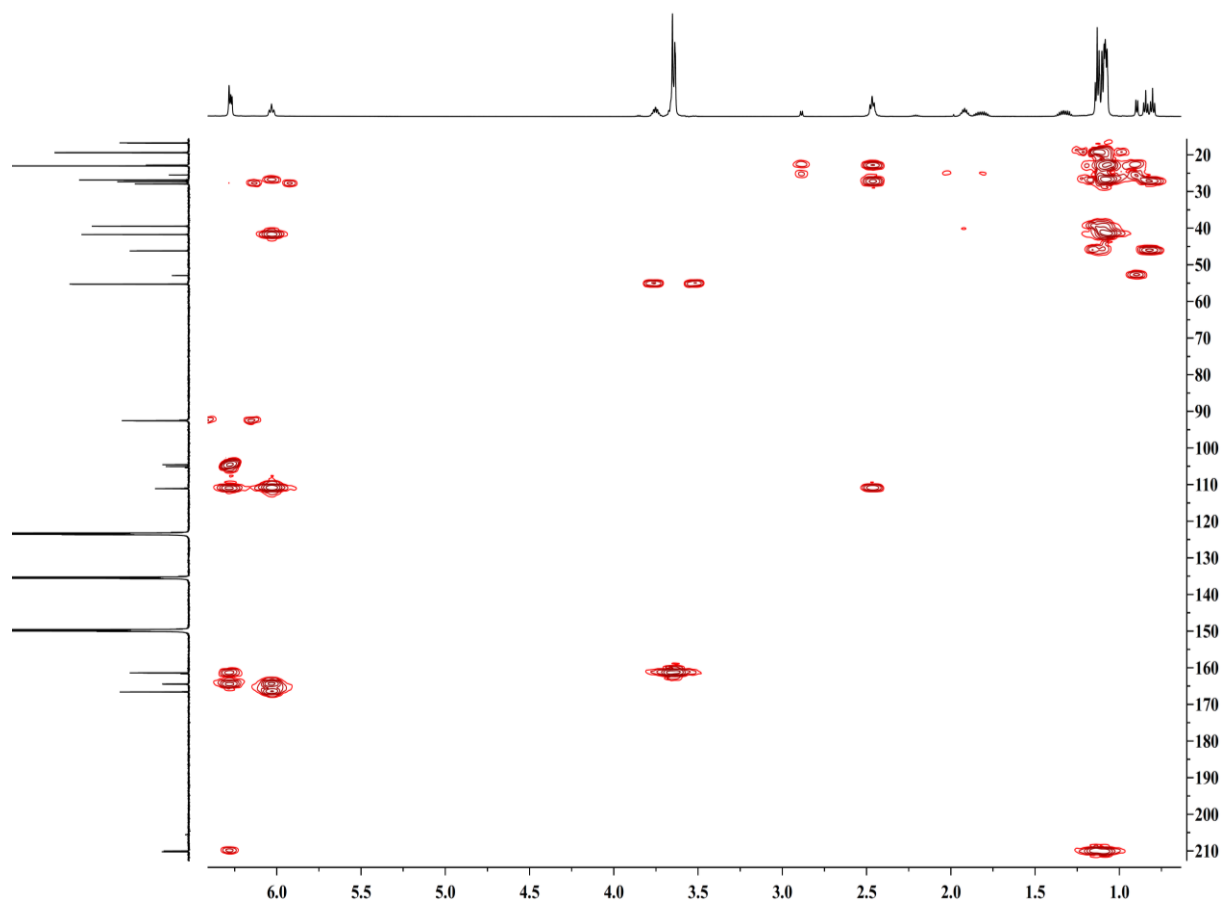


Figure S66 ^1H - ^1H COSY spectrum of the mixture **10** and **11**

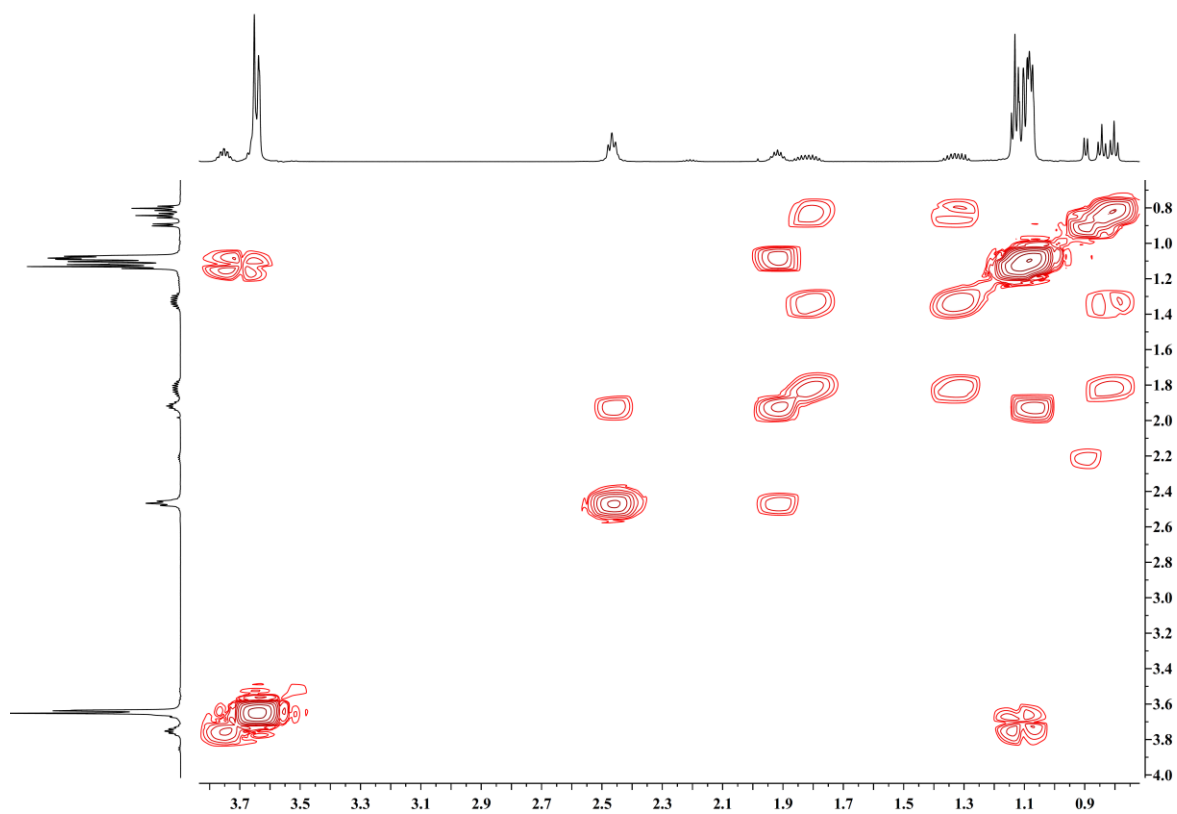
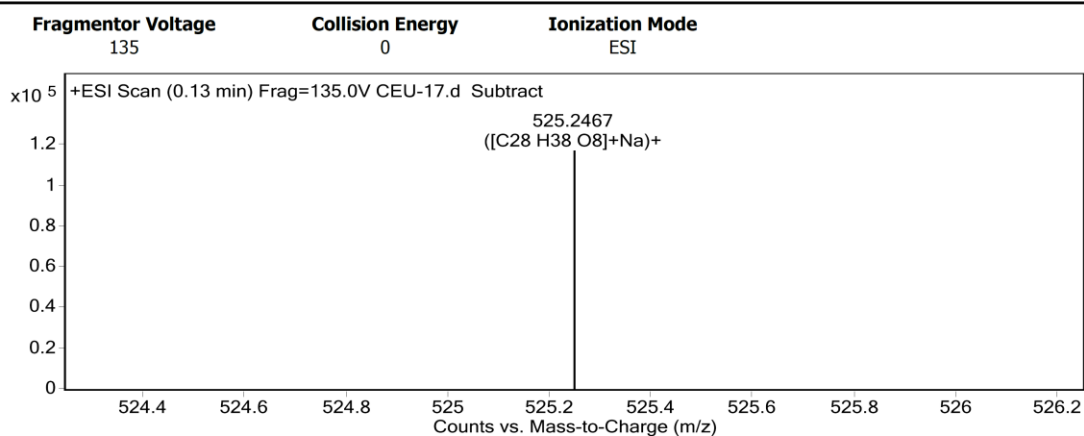


Figure S67 HRESIMS spectrum of the mixture 10 and 11

User Spectra



Peak List

| m/z | z | Abund | Formula | Ion |
|-----------|---|-----------|------------|---------|
| 279.1591 | 1 | 22184.19 | | |
| 293.1745 | 1 | 22731.09 | | |
| 503.2642 | 1 | 46258.4 | | |
| 525.2467 | 1 | 117672.32 | C28 H38 O8 | (M+Na)+ |
| 526.2497 | 1 | 33675.64 | C28 H38 O8 | (M+Na)+ |
| 541.2205 | 1 | 54502.98 | | |
| 542.2235 | 1 | 15409.3 | | |
| 1027.5037 | 1 | 23117.11 | | |

Formula Calculator Element Limits

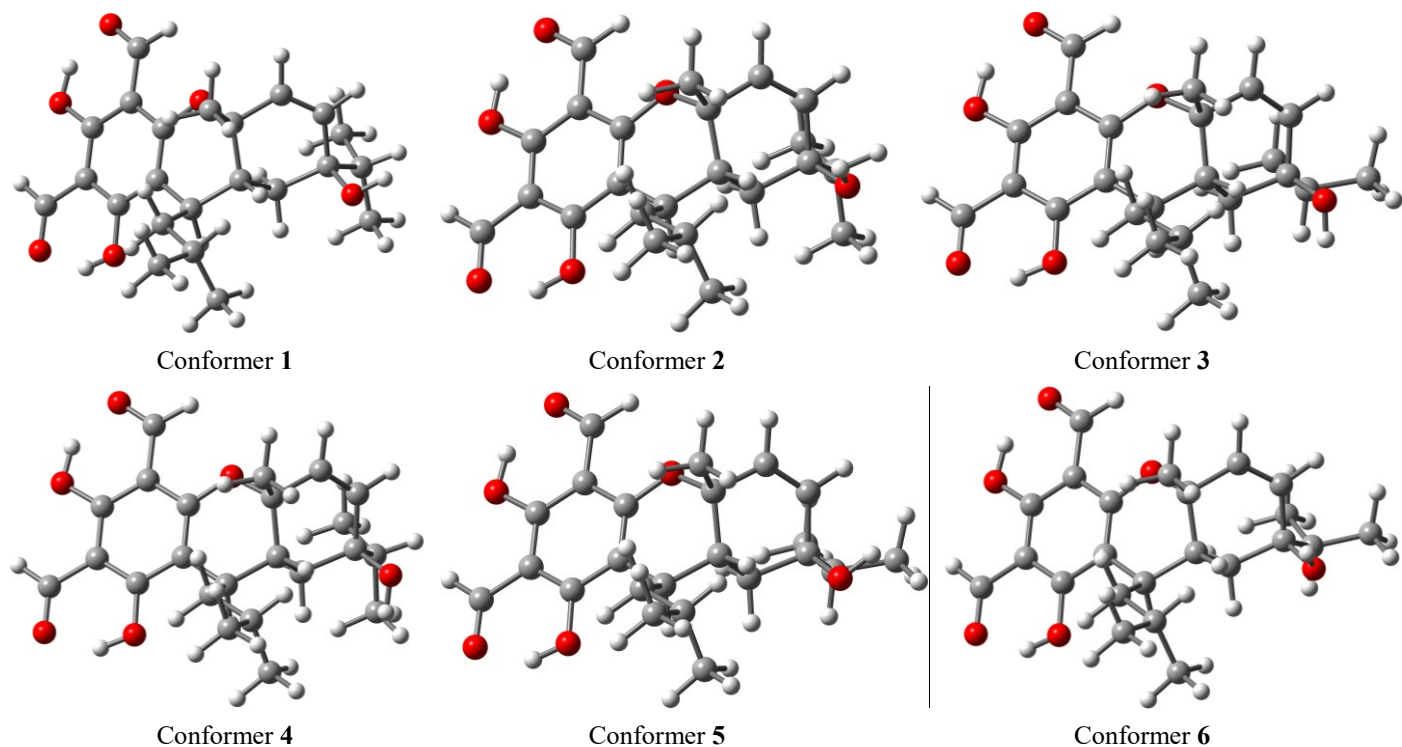
| Element | Min | Max |
|---------|-----|-----|
| C | 3 | 60 |
| H | 0 | 120 |
| O | 0 | 30 |

Formula Calculator Results

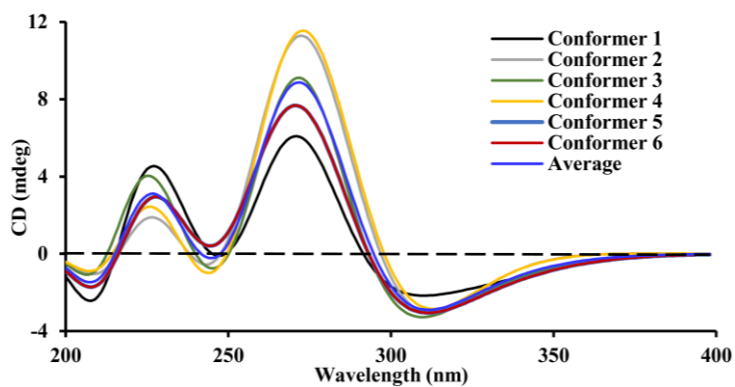
| Formula | CalculatedMass | CalculatedMz | Mz | Diff. (mDa) | Diff. (ppm) | DBE |
|------------|----------------|--------------|----------|-------------|-------------|---------|
| C28 H38 O8 | 502.2567 | 525.2459 | 525.2467 | -0.80 | -1.52 | 10.0000 |

ECD computational data of 2–6 and 9

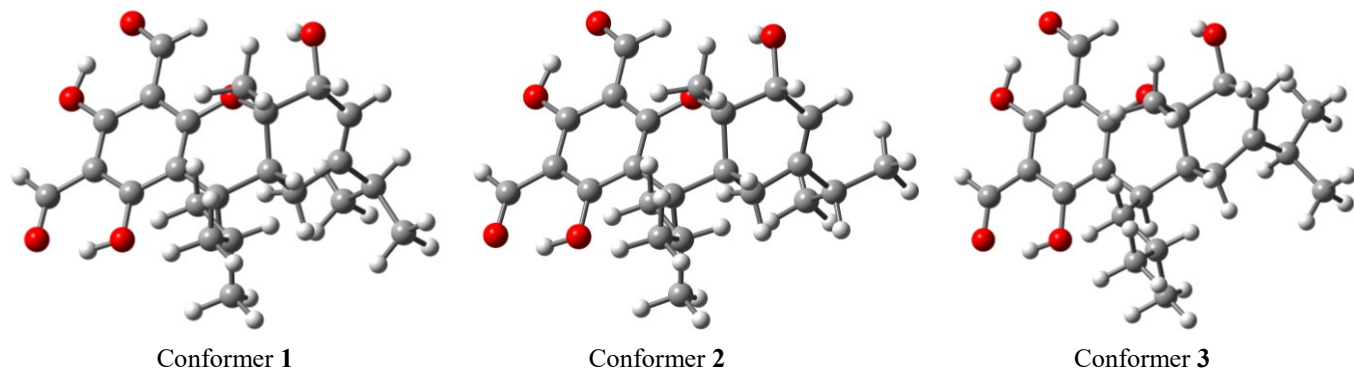
Computational data of (1*R*,4*R*,6*R*,9'*R*)-2

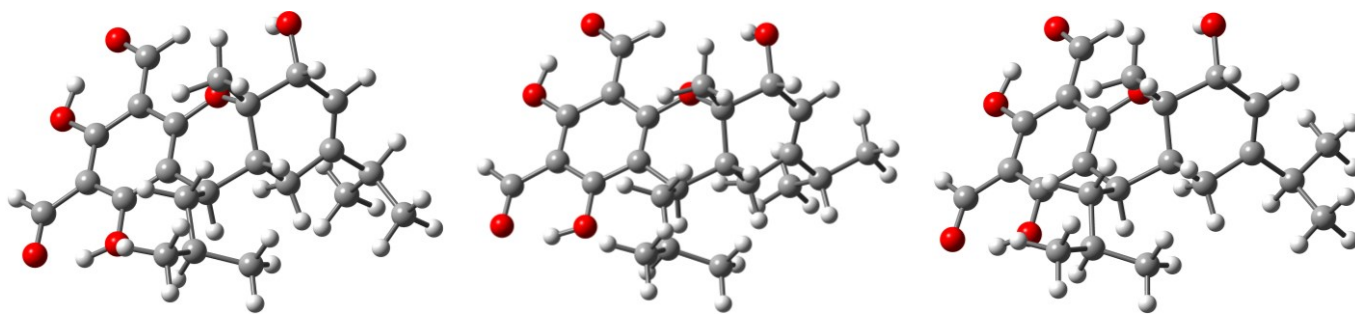


| No. | Distribution (%) | Relative Energy (kcal/mol) | No. | Distribution (%) | Relative Energy (kcal/mol) |
|-------------|------------------|----------------------------|-------------|------------------|----------------------------|
| Conformer 1 | 33.1633 | 0.0000 | Conformer 4 | 10.7445 | 0.6678 |
| Conformer 2 | 16.6238 | 0.4092 | Conformer 5 | 8.6848 | 0.7939 |
| Conformer 3 | 12.4021 | 0.5828 | Conformer 6 | 7.0969 | 0.9135 |



Computational data of (1*S*,2*R*,6*R*,9'*R*)-3



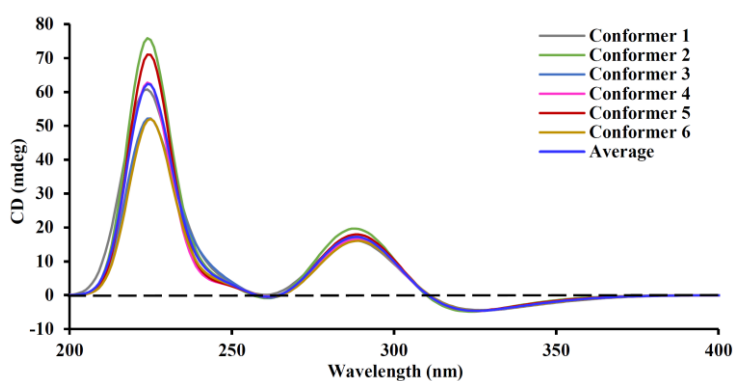


Conformer 4

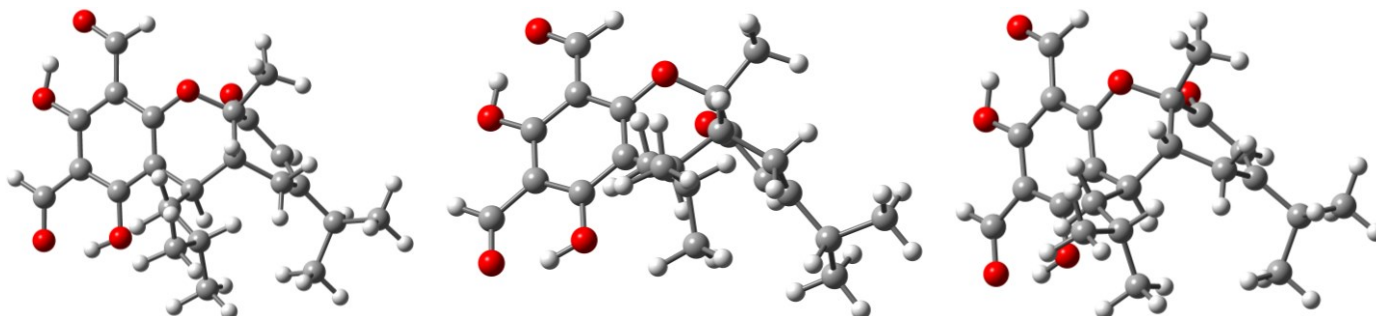
Conformer 5

Conformer 6

| No. | Distribution (%) | Relative Energy (kcal/mol) | No. | Distribution (%) | Relative Energy (kcal/mol) |
|-------------|------------------|----------------------------|-------------|------------------|----------------------------|
| Conformer 1 | 34.1493 | 0.0000 | Conformer 4 | 12.2541 | 0.6072 |
| Conformer 2 | 20.3125 | 0.3125 | Conformer 5 | 7.2280 | 0.9200 |
| Conformer 3 | 17.4926 | 0.3964 | Conformer 6 | 6.2769 | 1.0036 |



Computational data of (1*S*,6*R*,9'*R*)-4

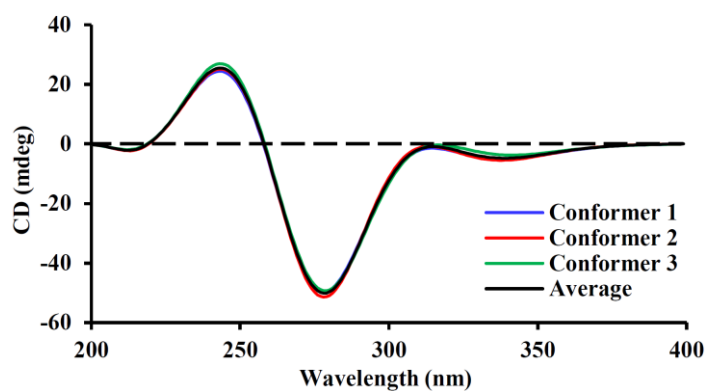


Conformer 1

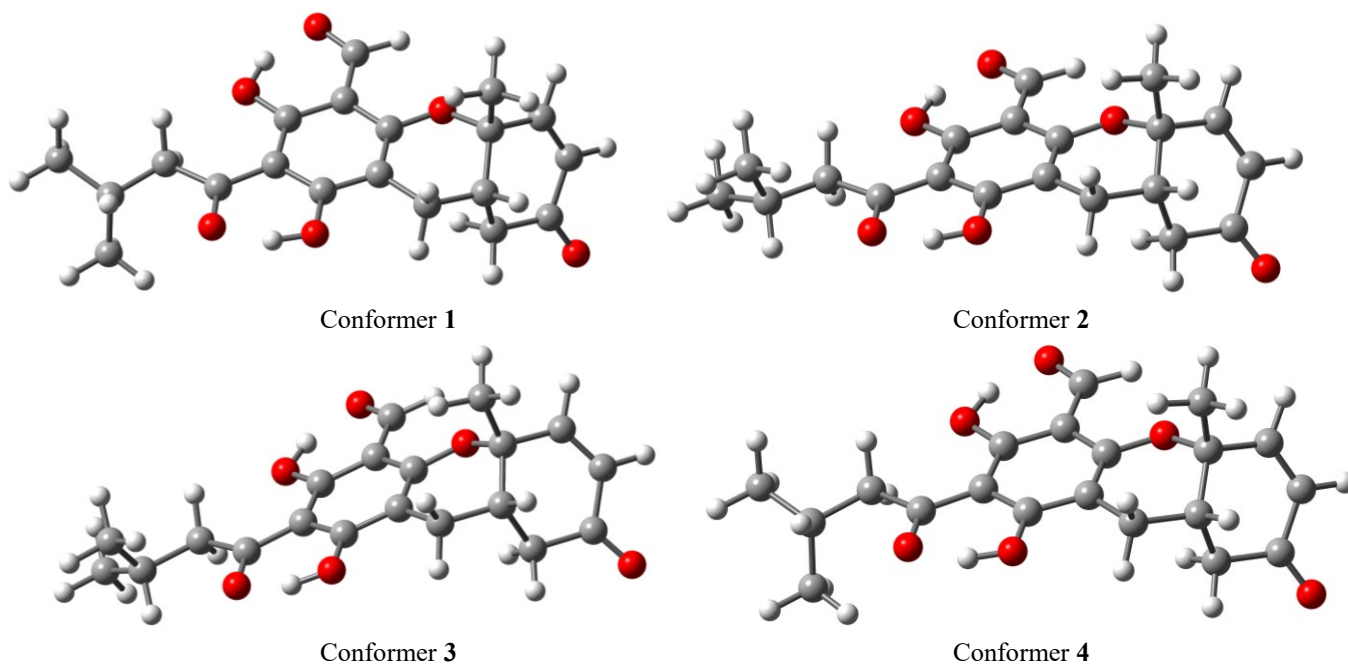
Conformer 2

Conformer 3

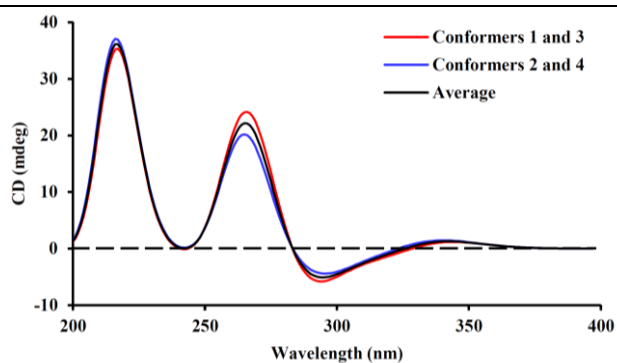
| No. | Distribution (%) | Relative Energy (kcal/mol) |
|-------------|------------------|----------------------------|
| Conformer 1 | 45.1622 | 0.0000 |
| Conformer 2 | 20.0367 | 0.4815 |
| Conformer 3 | 19.1046 | 0.5097 |



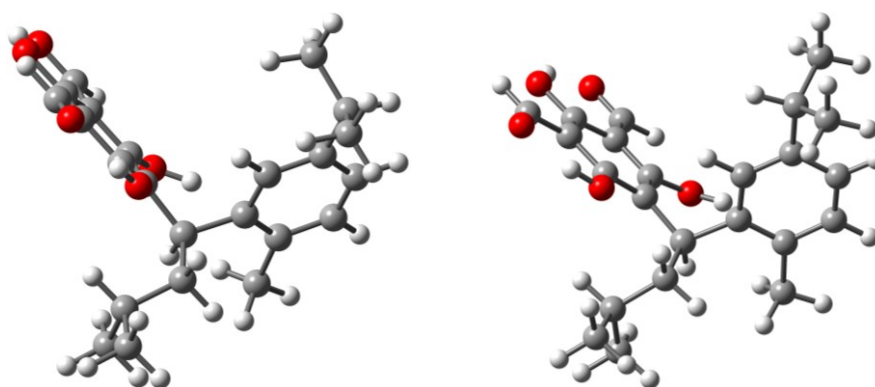
Computational data of (1*S*,6*S*)-5



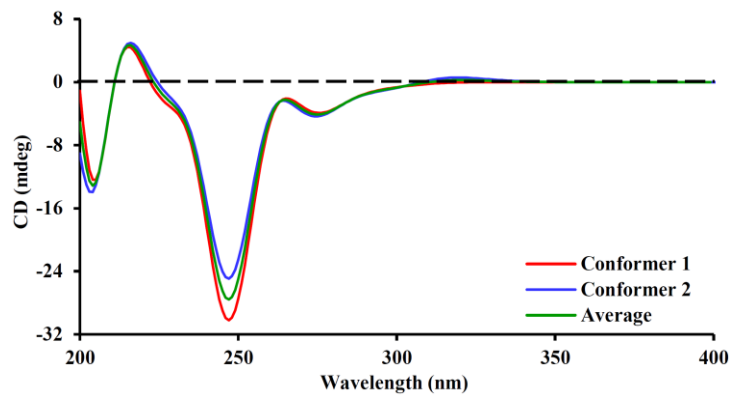
| No. | Distribution (%) | Relative Energy (kcal/mol) | No. | Distribution (%) | Relative Energy (kcal/mol) |
|-------------|------------------|----------------------------|-------------|------------------|----------------------------|
| Conformer 1 | 33.5606 | 0.0000 | Conformer 3 | 9.6010 | 0.7415 |
| Conformer 2 | 29.2783 | 0.0809 | Conformer 4 | 8.7216 | 0.7984 |



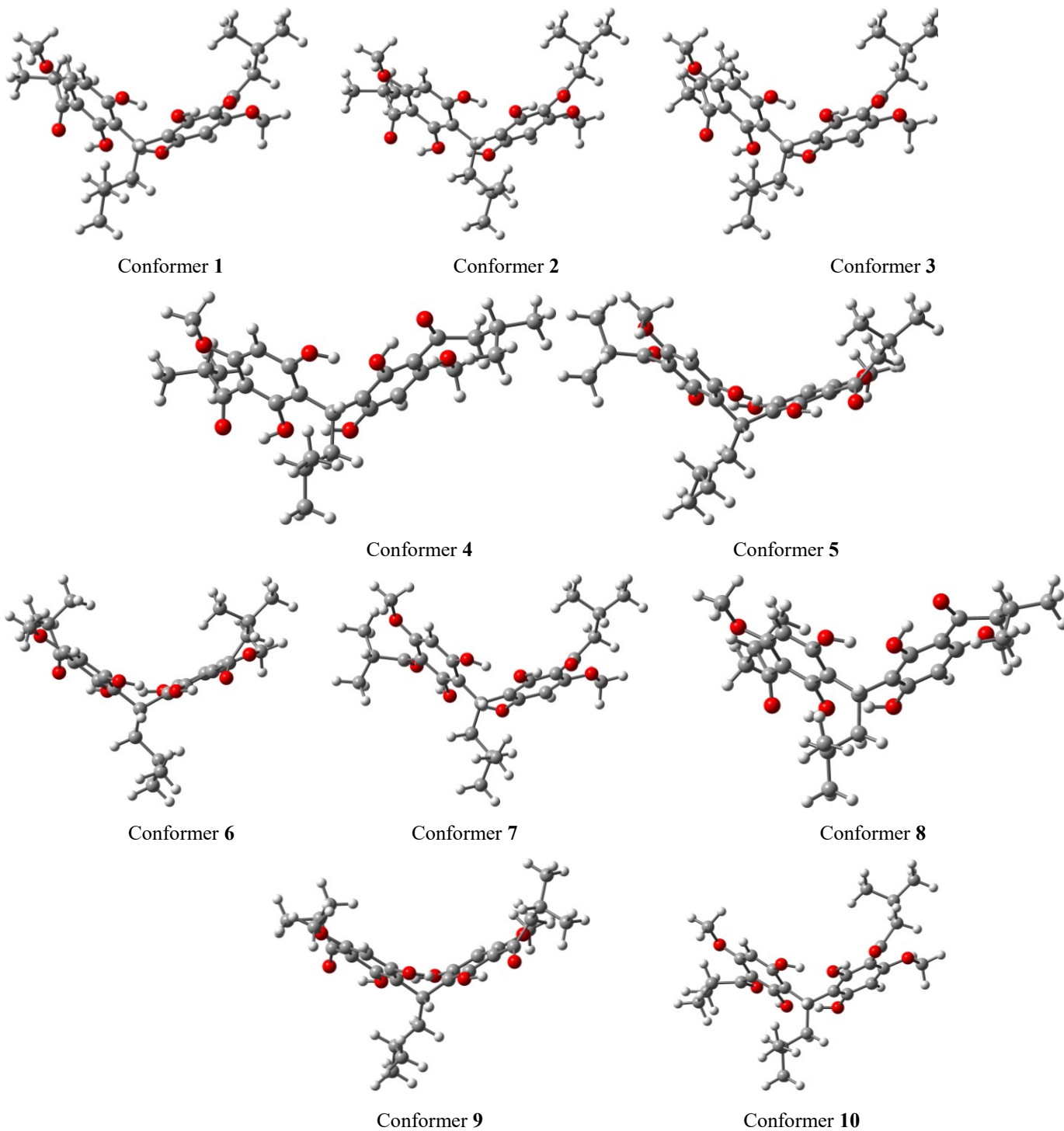
Computational data of (9'*R*)-6



| No. | Distribution (%) | Relative Energy (kcal/mol) |
|-------------|------------------|----------------------------|
| Conformer 1 | 55.2162 | 0.0000 |
| Conformer 2 | 36.4902 | 0.2454 |



Computational data of (1''S)-8



| No. | Distribution (%) | Relative Energy (kcal/mol) | No. | Distribution (%) | Relative Energy (kcal/mol) |
|-------------|------------------|----------------------------|--------------|------------------|----------------------------|
| Conformer 1 | 12.8695 | 0.0000 | Conformer 6 | 5.1513 | 0.5425 |
| Conformer 2 | 10.5966 | 0.1151 | Conformer 7 | 4.7548 | 0.5899 |
| Conformer 3 | 6.2867 | 0.4245 | Conformer 8 | 3.0025 | 0.8623 |
| Conformer 4 | 6.1767 | 0.4349 | Conformer 9 | 2.8001 | 0.9037 |
| Conformer 5 | 5.2207 | 0.5346 | Conformer 10 | 2.6472 | 0.9369 |

