

Supplementary Materials

**Comprehensive metabolic profiling of euphorbiasteroid in rats by integrating
UPLC-Q/TOF-MS and NMR as well as microbial biotransformation**

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Figure S68. HMBC spectrum of compound **7** in CDCl₃

Figure S69. HSQC spectrum of compound **7** in CDCl₃

Figure S70. NOESY spectrum of compound **7** in CDCl₃

Figure S71. HR-ESI-MS spectrum of compound **8**

Figure S72. OR Valve of compound **8** in MeOH

Figure S73. UV spectrum of compound **8** in MeOH

Figure S74. CD spectrum of compound **8** in MeOH

Figure S75. ¹H NMR spectrum of compound **8** in CDCl₃

Figure S76. ¹³C NMR and DEPT spectrum of compound **8** in CDCl₃

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Figure S78. HMBC spectrum of compound **8** in CDCl₃

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Figure S99. ^{13}C NMR and DEPT spectrum of compound **11** in CDCl_3

Figure S100. ^1H - ^1H COSY spectrum of compound **11** in CDCl_3

Figure S101. HMBC spectrum of compound **11** in CDCl_3

Figure S102. HSQC spectrum of compound **11** in CDCl_3

Figure S103. NOESY spectrum of compound **11** in CDCl_3

Figure S104. HR-ESI-MS spectrum of compound **12**

Figure S105. OR valve of compound **12** in MeOH

Figure S106. UV spectrum of compound **12** in MeOH

Figure S107. CD spectrum of compound **12** in MeOH

Figure S108. ^1H NMR spectrum of compound **12** in CDCl_3

Figure S109. ^{13}C NMR and DEPT spectrum of compound **12** in CDCl_3

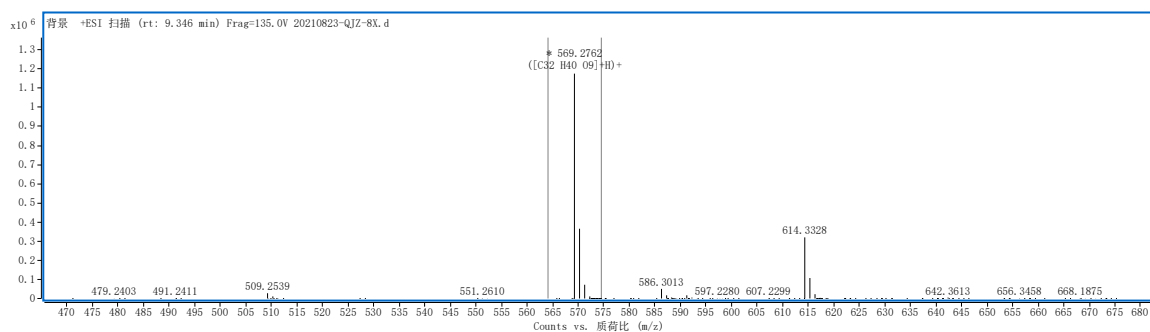
Figure S110. ^1H - ^1H COSY spectrum of compound **12** in CDCl_3

Figure S111. HMBC spectrum of compound **12** in CDCl_3

Figure S112. HSQC spectrum of compound **12** in CDCl_3

Figure S113. NOESY spectrum of compound **12** in CDCl_3

Table S1. Effects of metabolites on proliferation of four strains of human cells
(Inhibition rate %)



| Best | Formula(M) | Ion Formula | Tgt (m/z) | m/z | Diff (ppm) |
|------|--|--|-----------|----------|------------|
| TRUE | C ₃₂ H ₄₀ O ₉ | C ₃₂ H ₄₁ O ₉ | 569.2745 | 569.2762 | 2.99 |

Figure S1. HR-ESI-MS spectrum of compound **1**

Rudolph Research Analytical

Monday, 10/11/2021

This sample was measured on an Autopol VI, serial number 90079, manufactured by Rudolph Research Analytical, Hackettstown, NJ.

LotID : QJZ-8
Set Temperature : 20.0
Temp Corr : OFF

| n | Average | Std.Dev. | Maximum | Minimum | | | | | | |
|------|-----------|-------------|---------|---------|----------|-----|--------|-------|-------|---------|
| 6 | 116.102 | 0.0000 | 116.102 | 116.102 | | | | | | |
| S.No | Sample ID | Time | Result | Scale | OR ° Arc | WLG | Lg.mm | Conc. | Temp. | Comment |
| 1 | QJZ-8 | 10:45:38 AM | 116.102 | SR | 0.137 | 589 | 100.00 | 0.118 | 19.7 | |
| 2 | QJZ-8 | 10:45:45 AM | 116.102 | SR | 0.137 | 589 | 100.00 | 0.118 | 19.7 | |
| 3 | QJZ-8 | 10:45:53 AM | 116.102 | SR | 0.137 | 589 | 100.00 | 0.118 | 19.7 | |
| 4 | QJZ-8 | 10:46:00 AM | 116.102 | SR | 0.137 | 589 | 100.00 | 0.118 | 19.7 | |
| 5 | QJZ-8 | 10:46:08 AM | 116.102 | SR | 0.137 | 589 | 100.00 | 0.118 | 19.8 | |
| 6 | QJZ-8 | 10:46:15 AM | 116.102 | SR | 0.137 | 589 | 100.00 | 0.118 | 19.8 | |

Signature

Figure S2. OR valve of compound **1** in MeOH

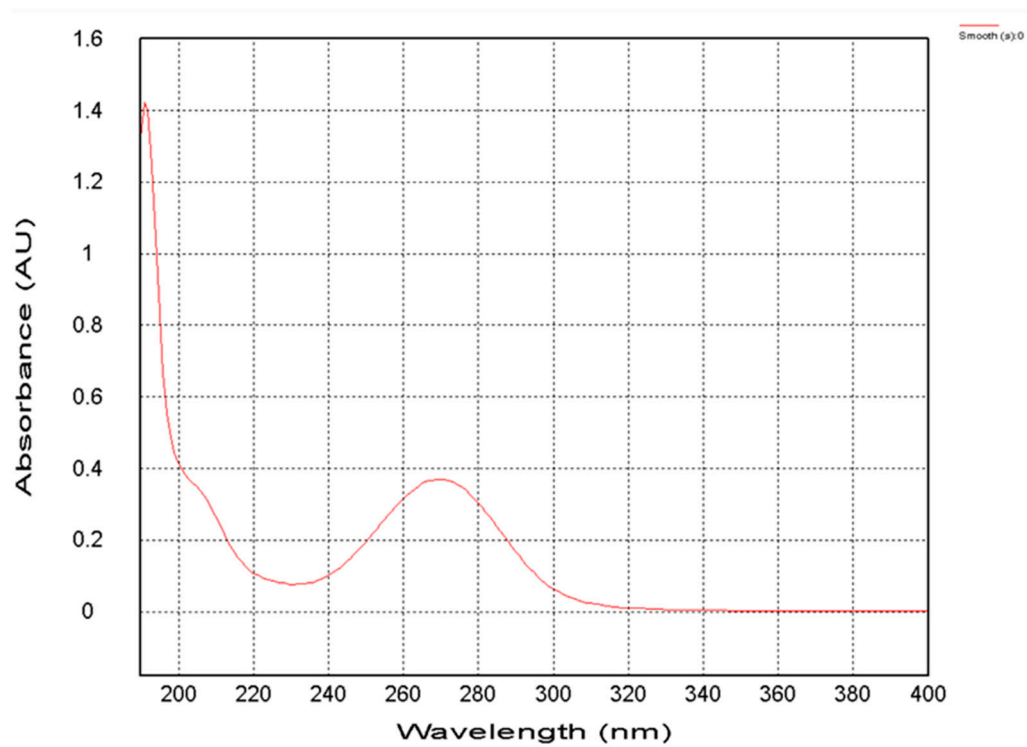


Figure S3. UV spectrum of compound **1** in MeOH

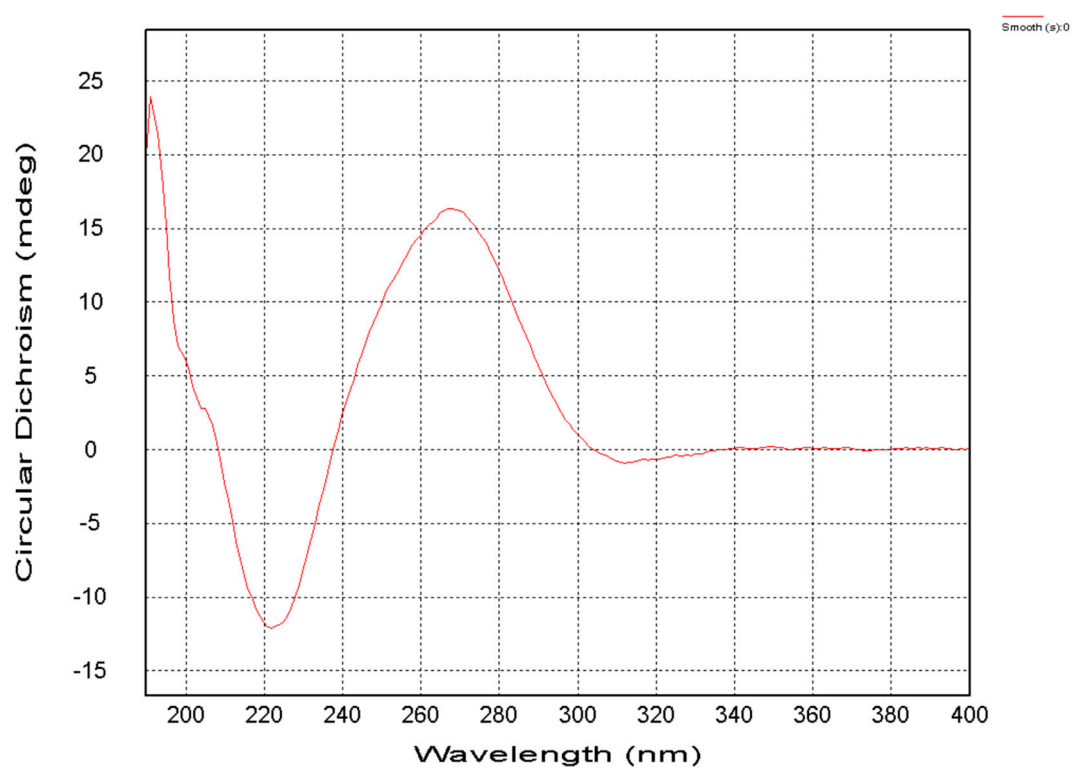


Figure S4. CD spectrum of compound **1** in MeOH

XSJ-QJZ-8 ^1H NMR (500 MHz, CDCl_3)

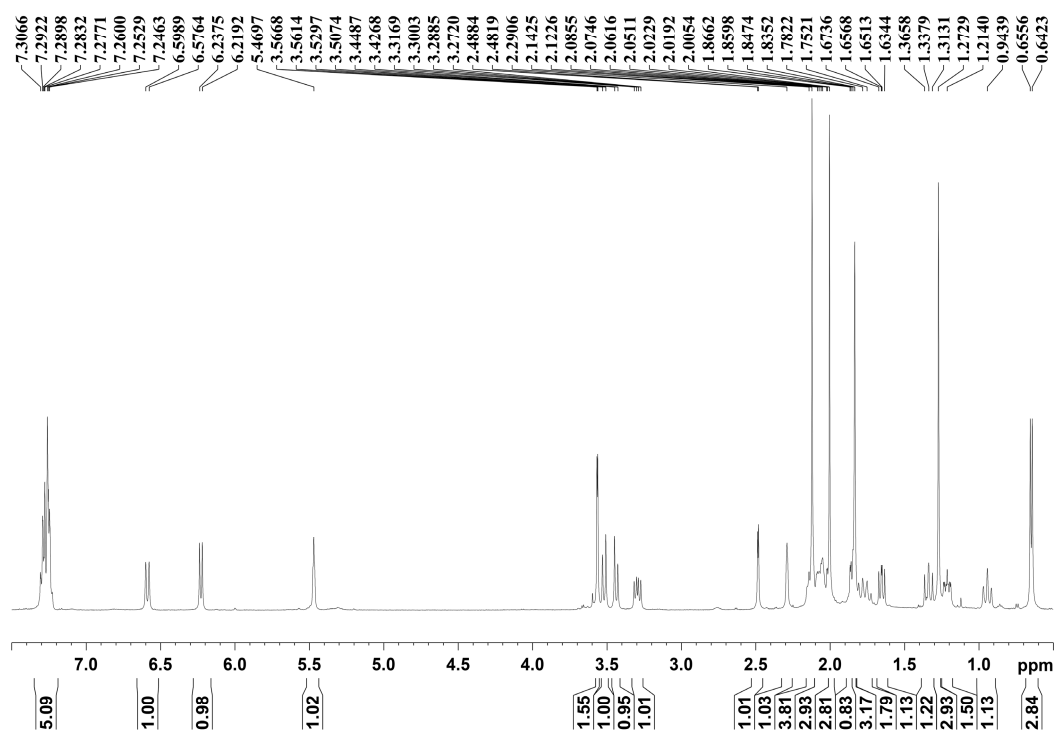


Figure S5. ^1H NMR spectrum of compound **1** in CDCl_3

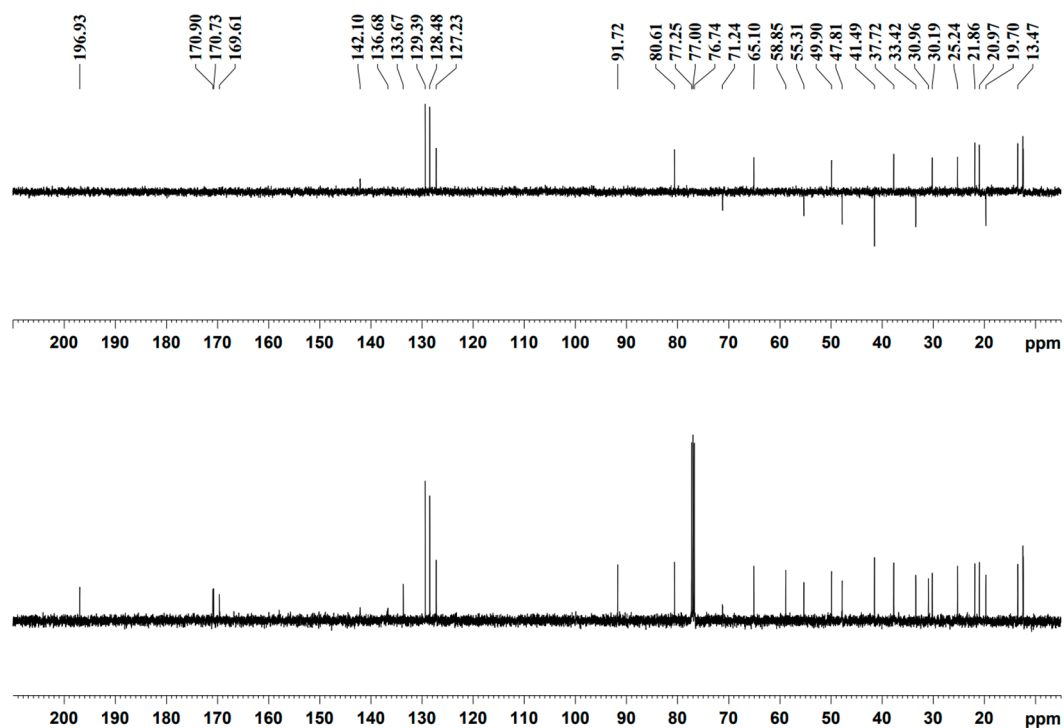


Figure S6. ^{13}C NMR and DEPT spectrum of compound **1** in CDCl_3

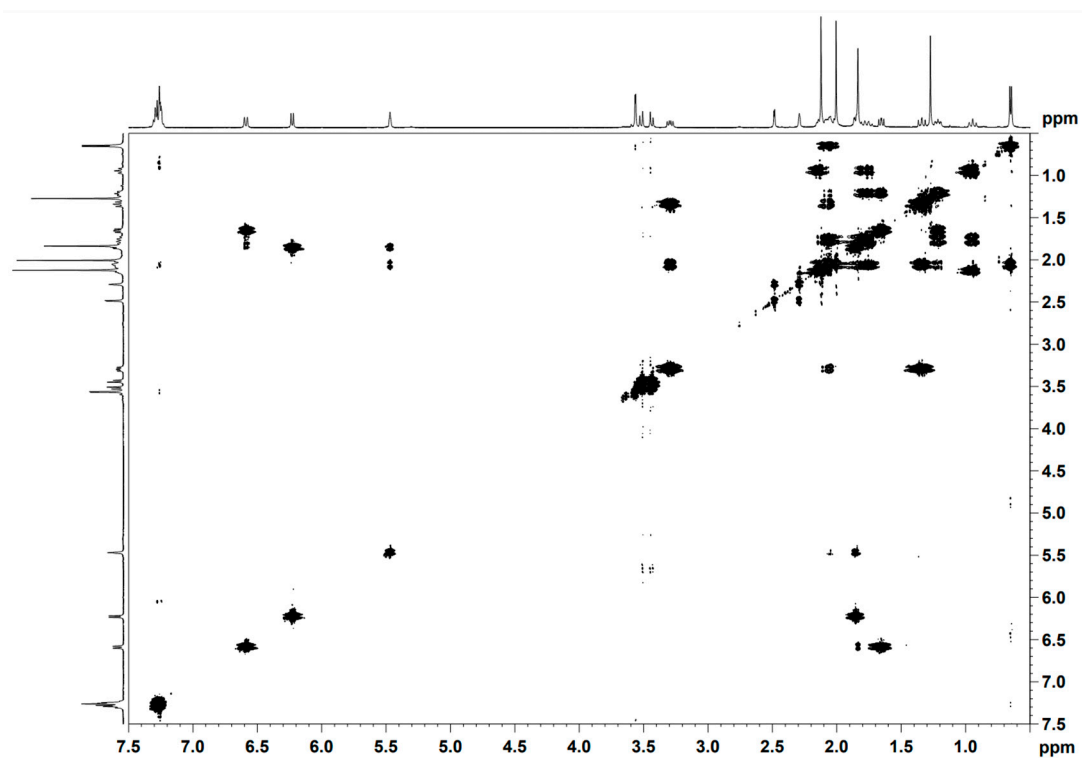


Figure S7. ^1H - ^1H COSY spectrum of compound **1** in CDCl_3

XSJ-QJZ-8 HMBC

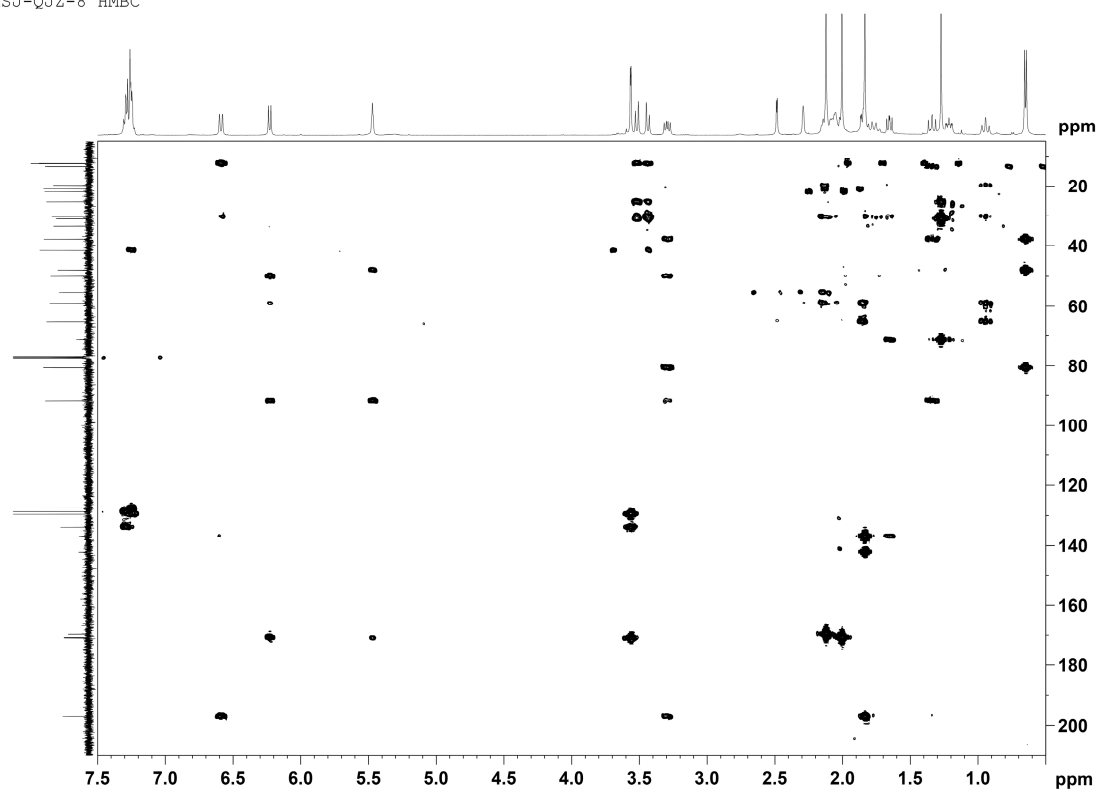


Figure S8. HMBC spectrum of compound **1** in CDCl_3

XSJ-QJZ-8 HSQC

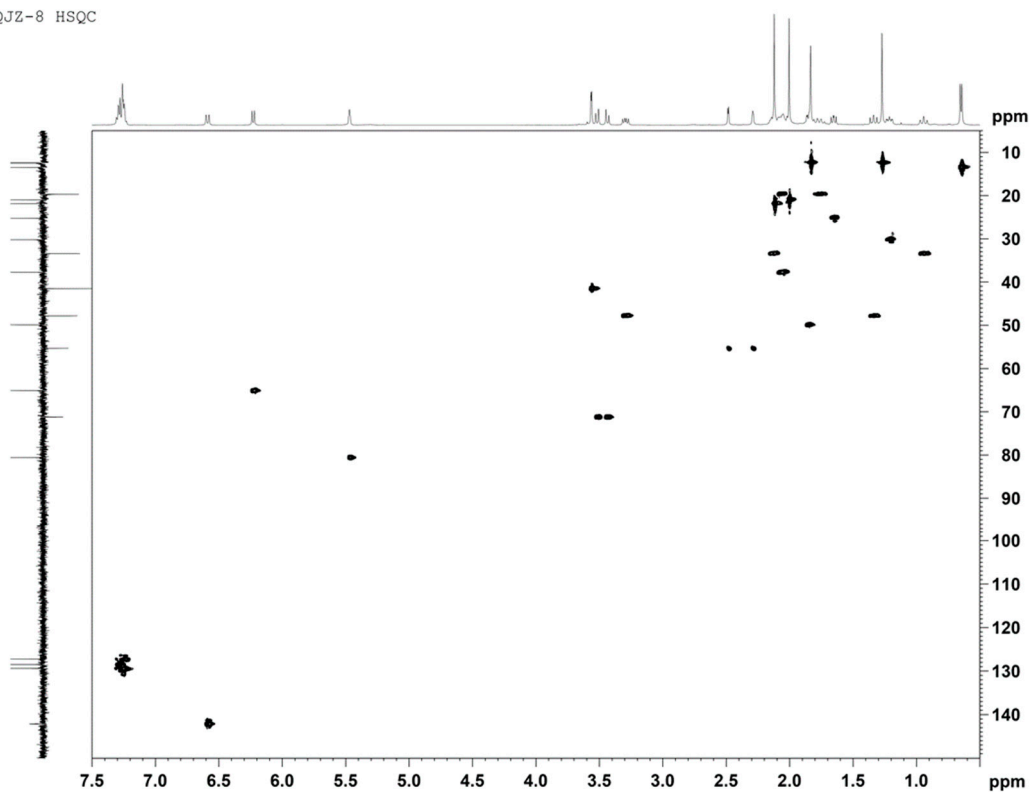


Figure S9. HSQC spectrum of compound **1** in CDCl₃

XSJ-QJZ-8 NOESY

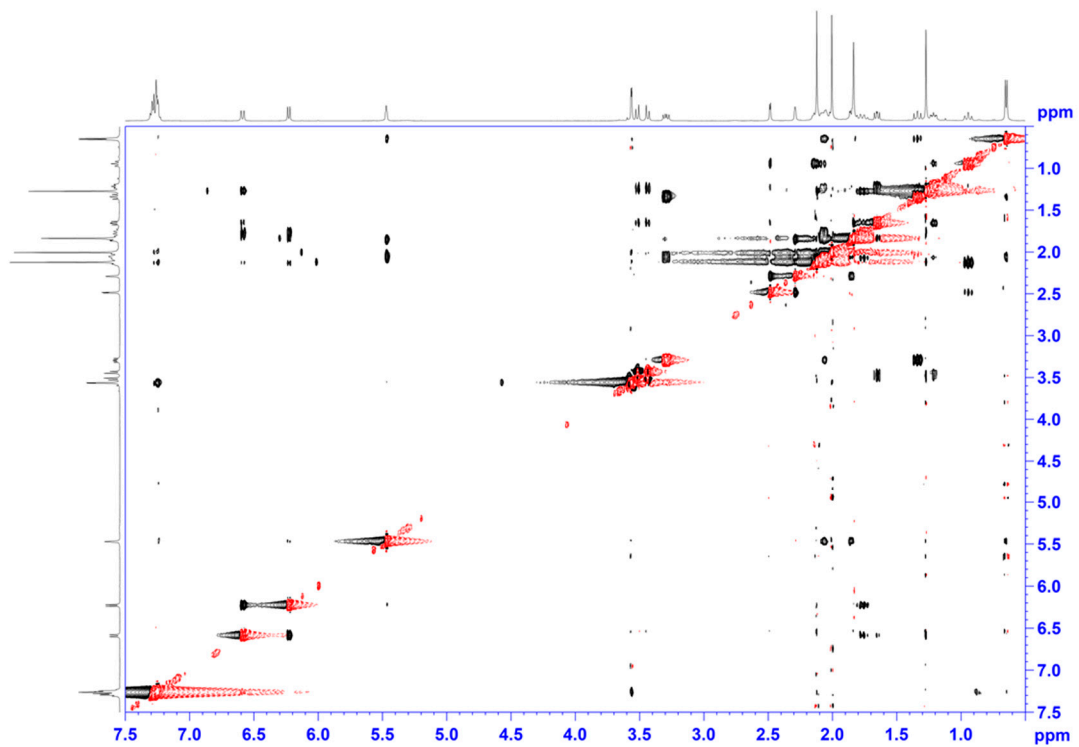
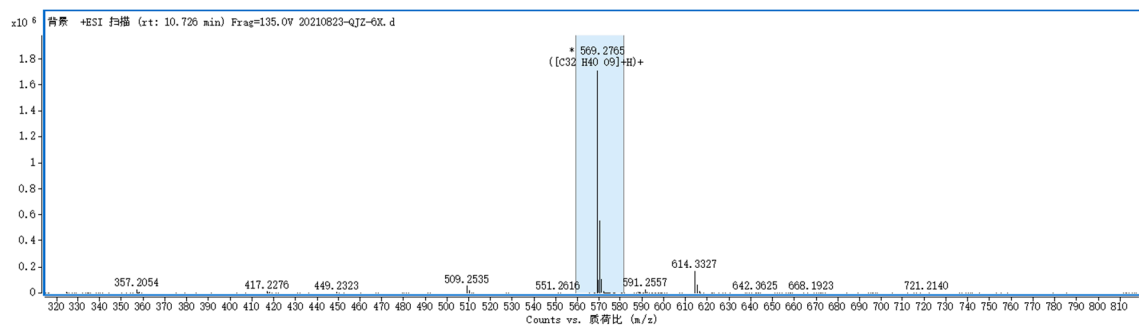


Figure S10. NOESY spectrum of compound **1** in CDCl₃



| Best | Formula(M) | Ion Formula | Tgt (m/z) | m/z | Diff (ppm) |
|------|--|--|-----------|----------|------------|
| TRUE | C ₃₂ H ₄₀ O ₉ | C ₃₂ H ₄₁ O ₉ | 569.2745 | 569.2765 | 3.51 |

Figure S11. HR-ESI-MS spectrum of compound **2**

Rudolph Research Analytical

Monday, 10/11/2021

This sample was measured on an Autopol VI, serial number 90079, manufactured by Rudolph Research Analytical, Hackettstown, NJ.

LotID : QJZ-6
Set Temperature : 20.0
Temp Corr : OFF

| n | Average | Std.Dev. | Maximum | Minimum | | | | | | |
|------|-----------|-------------|---------|---------|----------|-----|--------|-------|-------|---------|
| 6 | 74.889 | 0.3140 | 75.333 | 74.667 | | | | | | |
| S.No | Sample ID | Time | Result | Scale | OR ° Arc | WLG | Lg.mm | Conc. | Temp. | Comment |
| 1 | QJZ-6 | 11:09:52 AM | 75.333 | SR | 0.113 | 589 | 100.00 | 0.150 | 19.7 | |
| 2 | QJZ-6 | 11:10:00 AM | 75.333 | SR | 0.113 | 589 | 100.00 | 0.150 | 19.7 | |
| 3 | QJZ-6 | 11:10:08 AM | 74.667 | SR | 0.112 | 589 | 100.00 | 0.150 | 19.7 | |
| 4 | QJZ-6 | 11:10:15 AM | 74.667 | SR | 0.112 | 589 | 100.00 | 0.150 | 19.8 | |
| 5 | QJZ-6 | 11:10:23 AM | 74.667 | SR | 0.112 | 589 | 100.00 | 0.150 | 19.8 | |
| 6 | QJZ-6 | 11:10:30 AM | 74.667 | SR | 0.112 | 589 | 100.00 | 0.150 | 19.8 | |

Signature

Figure S12. OR valve of compound **2** in MeOH

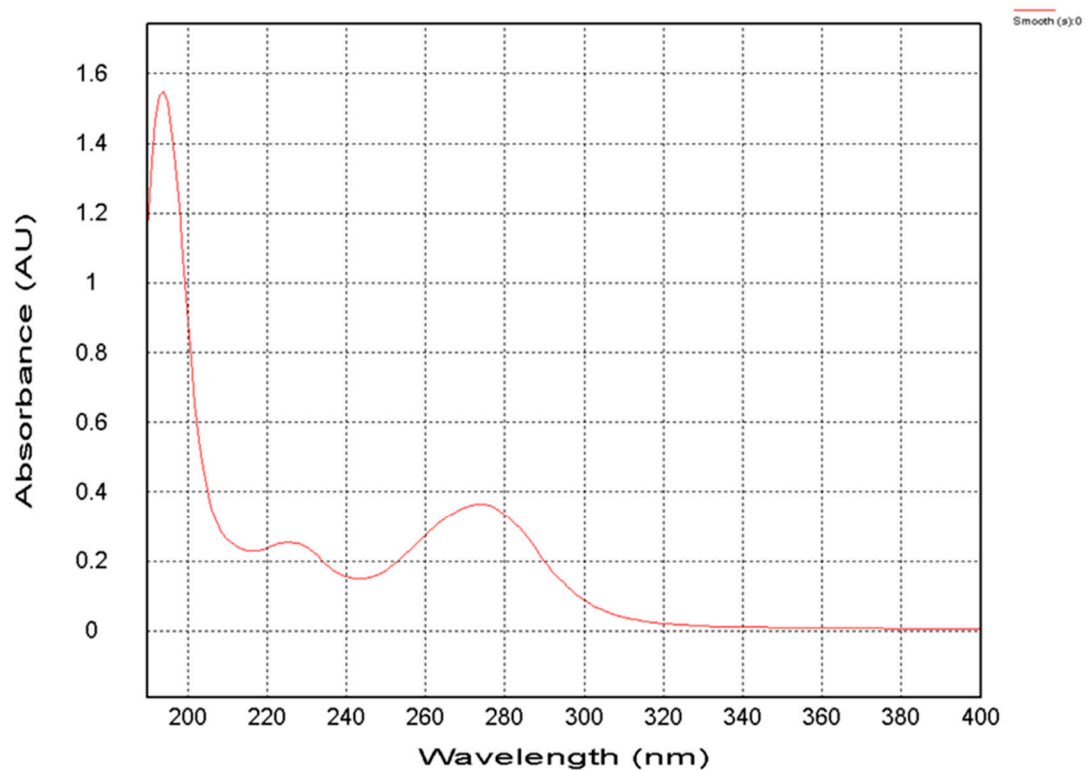


Figure S13. UV spectrum of compound **2** in MeOH

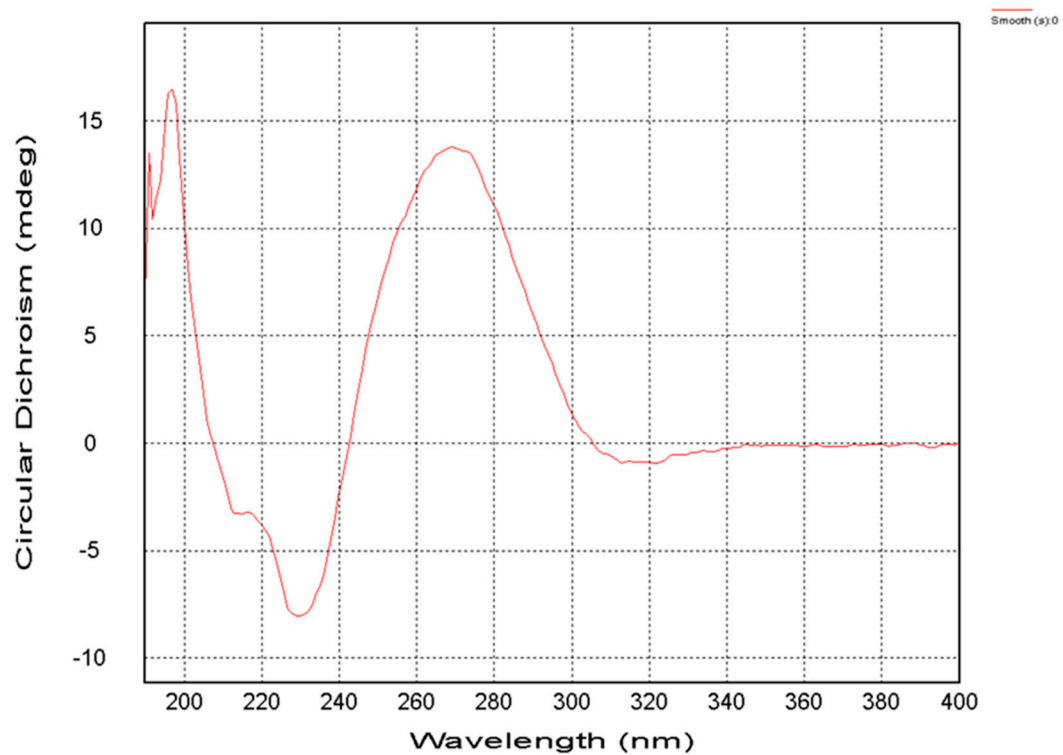


Figure S14. CD spectrum of compound **2** in MeOH

XSJ-QJZ-6 ^1H NMR (500 MHz, CDCl_3)

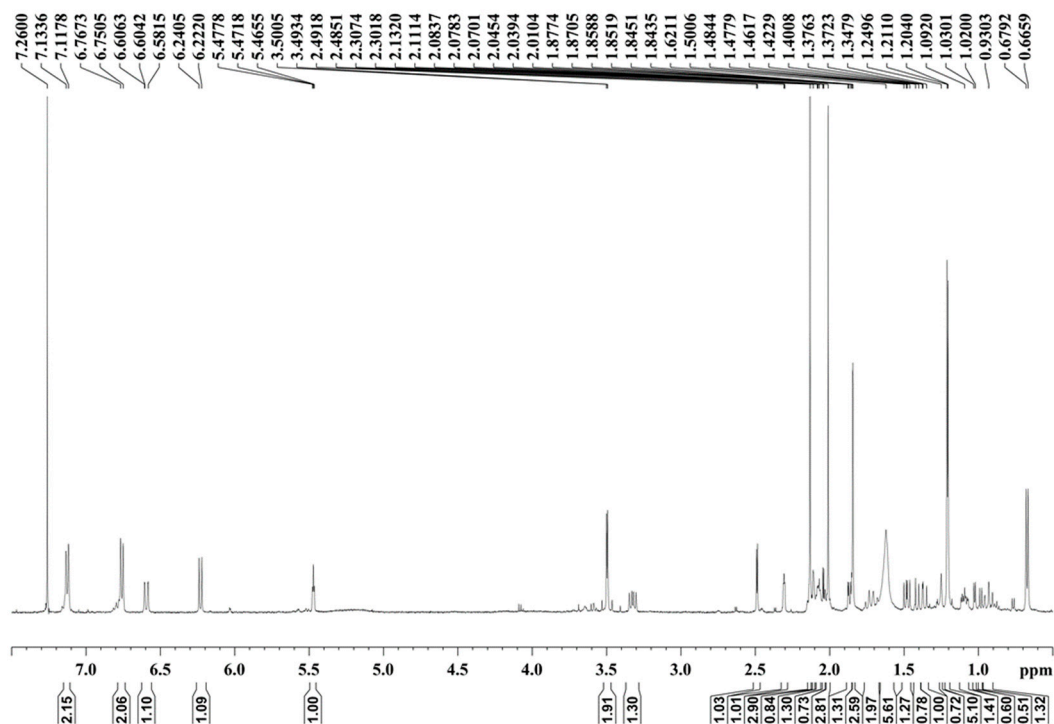


Figure S15. ^1H NMR spectrum of compound **2** in CDCl_3

XSJ-QJZ-6 ^{13}C and DEPT NMR (125 MHz, CDCl_3)

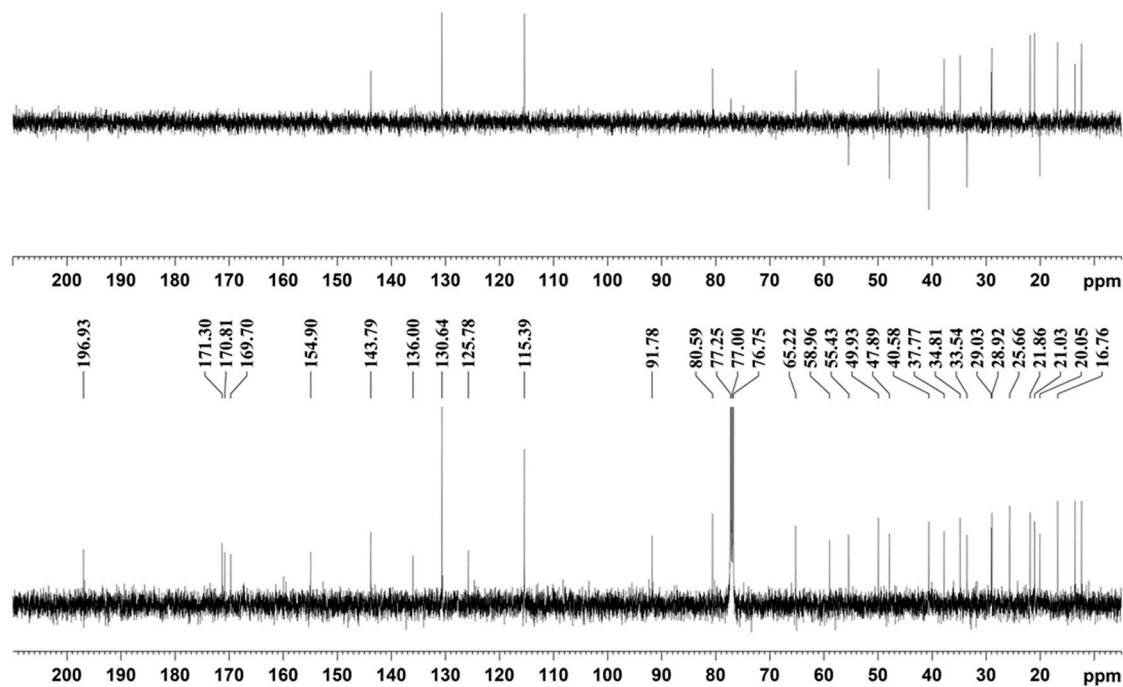


Figure S16. ^{13}C NMR and DEPT spectrum of compound **2** in CDCl_3

XSJ-QJZ-6 1H 1H COSY

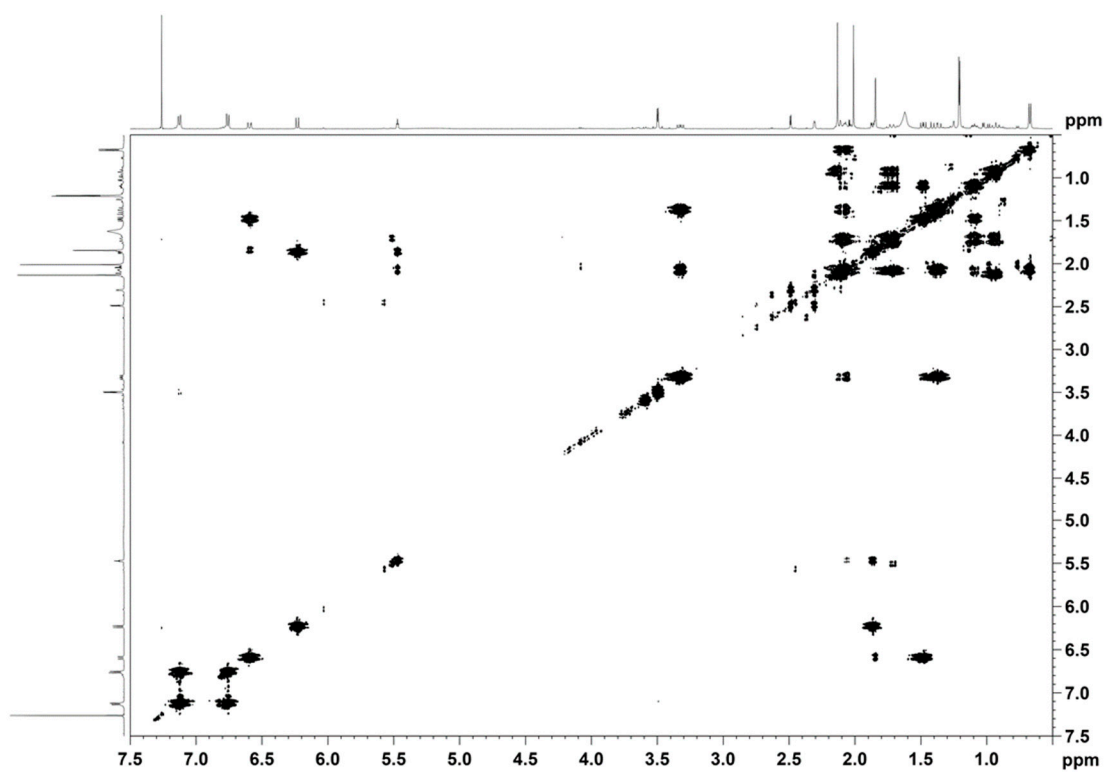


Figure S17. ^1H - ^1H COSY spectrum of compound **2** in CDCl_3

XSJ-QJZ-6 HMBC

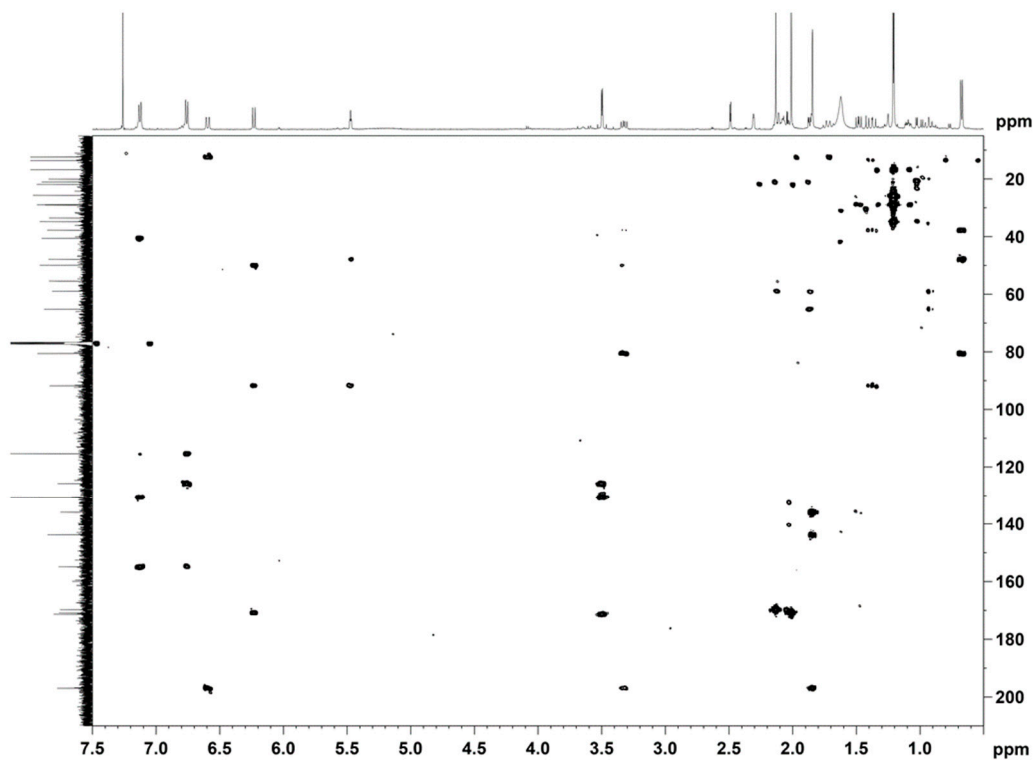


Figure S18. HMBC spectrum of compound **2** in CDCl_3

XSJ-QJZ-6 HSQC

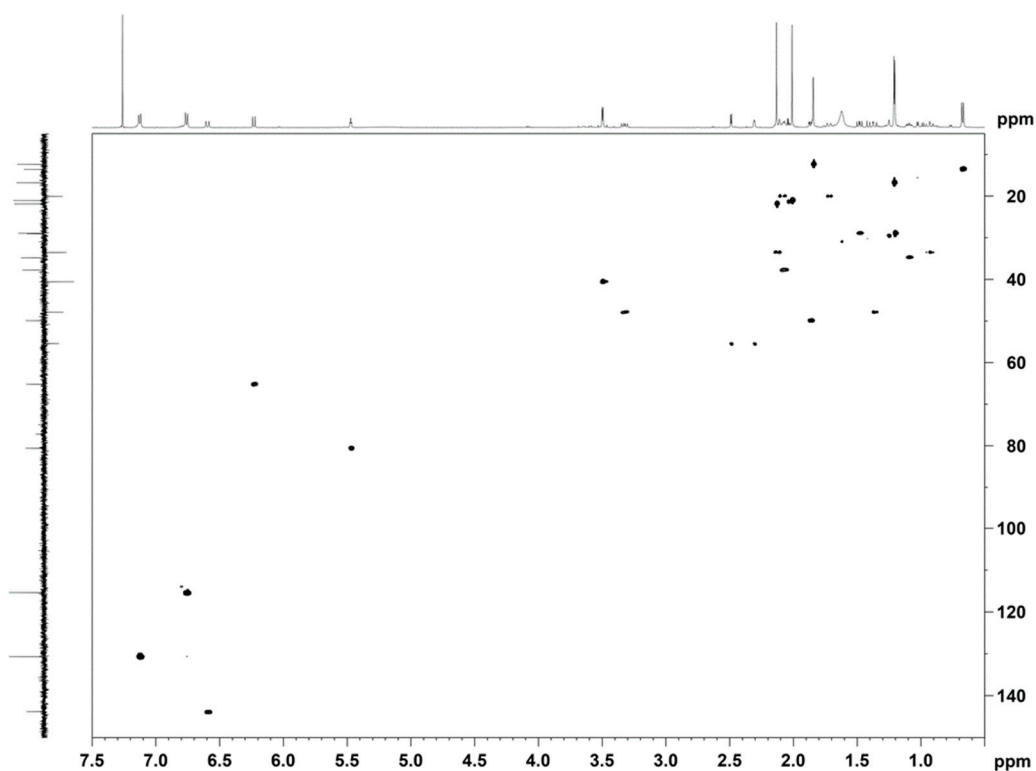


Figure S19. HSQC spectrum of compound **2** in CDCl₃

XSJ-QJZ-6 NOESY

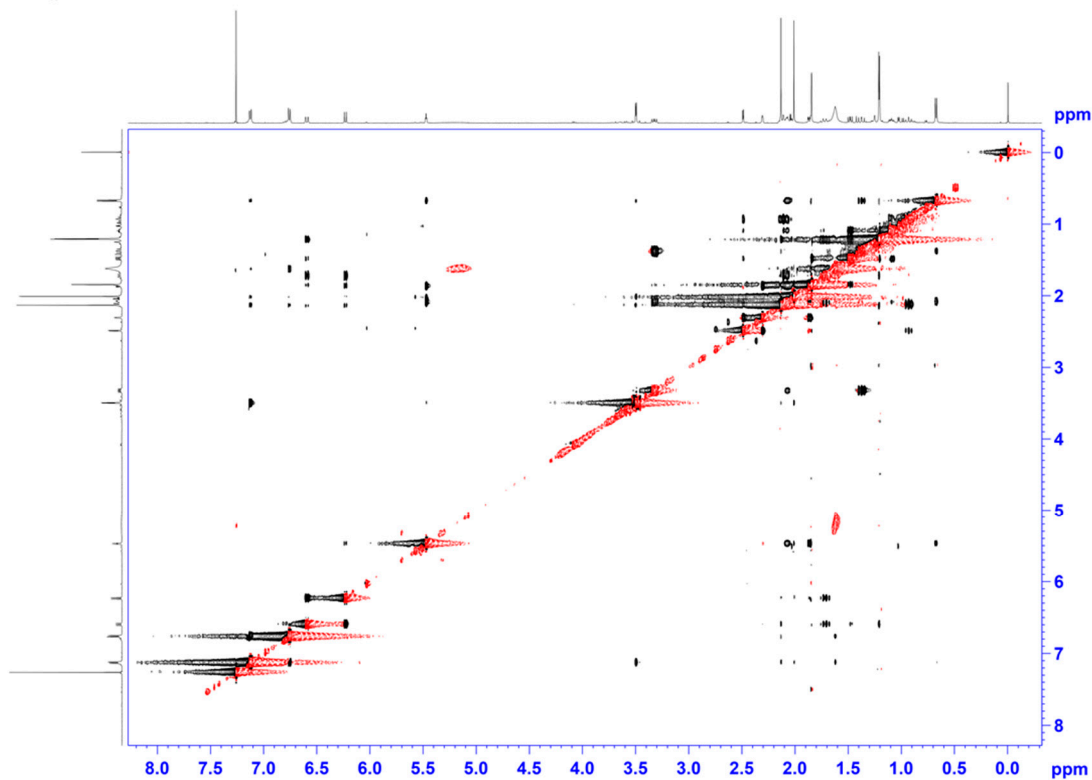
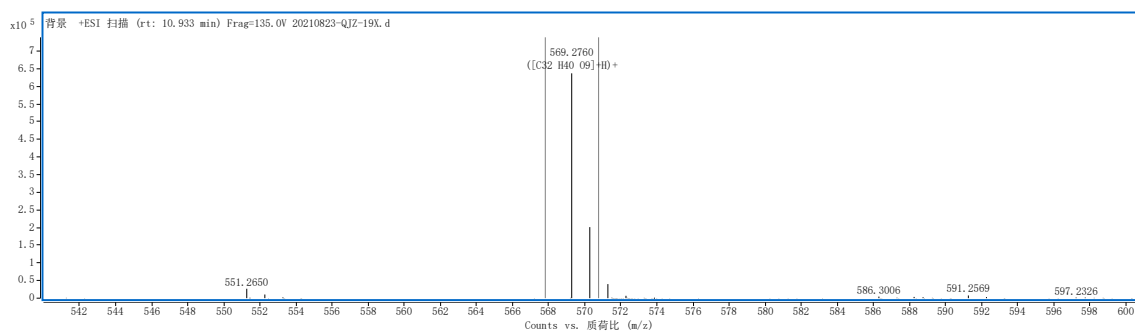


Figure S20. NOESY spectrum of compound **2** in CDCl₃



| Best | Formula(M) | Ion Formula | Tgt (m/z) | m/z | Diff (ppm) |
|------|--|--|-----------|----------|------------|
| TRUE | C ₃₂ H ₄₀ O ₉ | C ₃₂ H ₄₁ O ₉ | 569.2745 | 569.2760 | 2.63 |

Figure S21. HR-ESI-MS spectrum of compound **3**

Rudolph Research Analytical

Saturday, 10/09/2021

This sample was measured on an Autopol VI, serial number 90079, manufactured by Rudolph Research Analytical, Hackettstown, NJ.

LotID : QJZ-19
Set Temperature : 20.0
Temp Corr : OFF

| n | Average | Std.Dev. | Maximum | Minimum | | | | | | |
|------|-----------|-------------|---------|---------|----------|-----|--------|-------|-------|---------|
| 6 | 63.974 | 0.2866 | 64.615 | 63.846 | | | | | | |
| S.No | Sample ID | Time | Result | Scale | OR ° Arc | WLG | Lg.mm | Conc. | Temp. | Comment |
| 1 | QJZ-19 | 04:13:14 PM | 64.615 | SR | 0.084 | 589 | 100.00 | 0.130 | 19.7 | |
| 2 | QJZ-19 | 04:13:21 PM | 63.846 | SR | 0.083 | 589 | 100.00 | 0.130 | 19.7 | |
| 3 | QJZ-19 | 04:13:28 PM | 63.846 | SR | 0.083 | 589 | 100.00 | 0.130 | 19.7 | |
| 4 | QJZ-19 | 04:13:36 PM | 63.846 | SR | 0.083 | 589 | 100.00 | 0.130 | 19.7 | |
| 5 | QJZ-19 | 04:13:43 PM | 63.846 | SR | 0.083 | 589 | 100.00 | 0.130 | 19.7 | |
| 6 | QJZ-19 | 04:13:51 PM | 63.846 | SR | 0.083 | 589 | 100.00 | 0.130 | 19.8 | |

Signature

Figure S22. OR value of compound **3** in MeOH

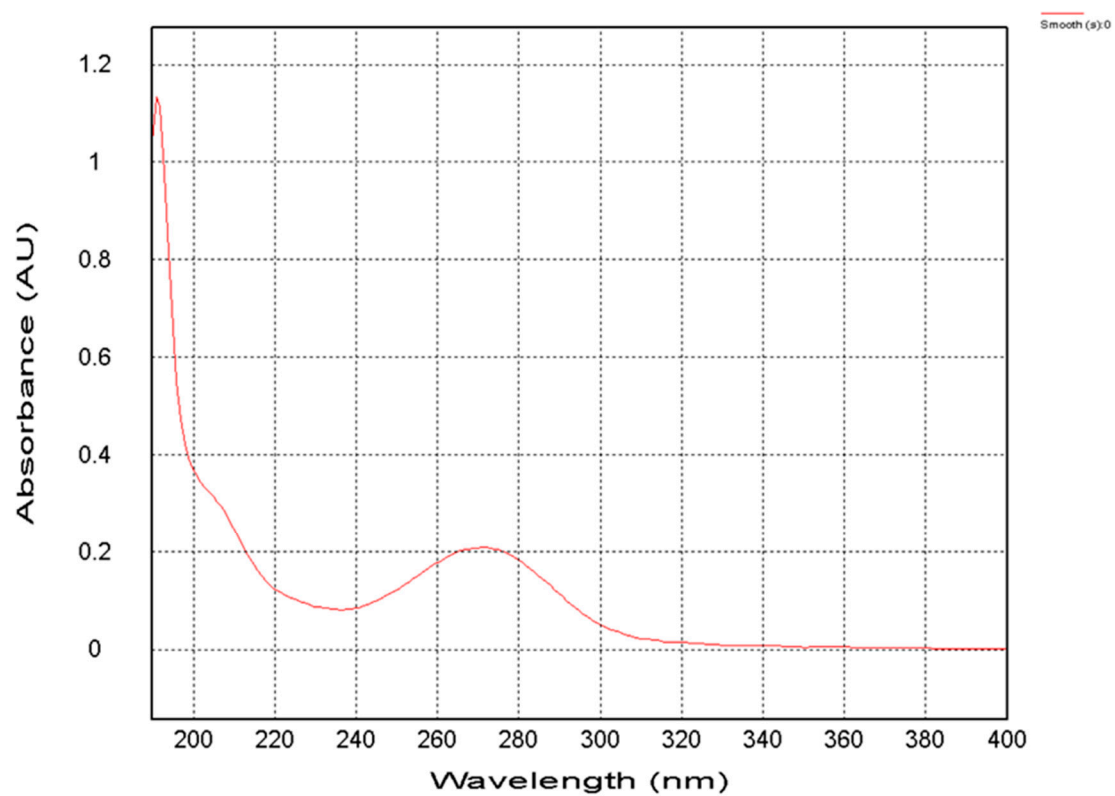


Figure S23. UV spectrum of compound **3** in MeOH

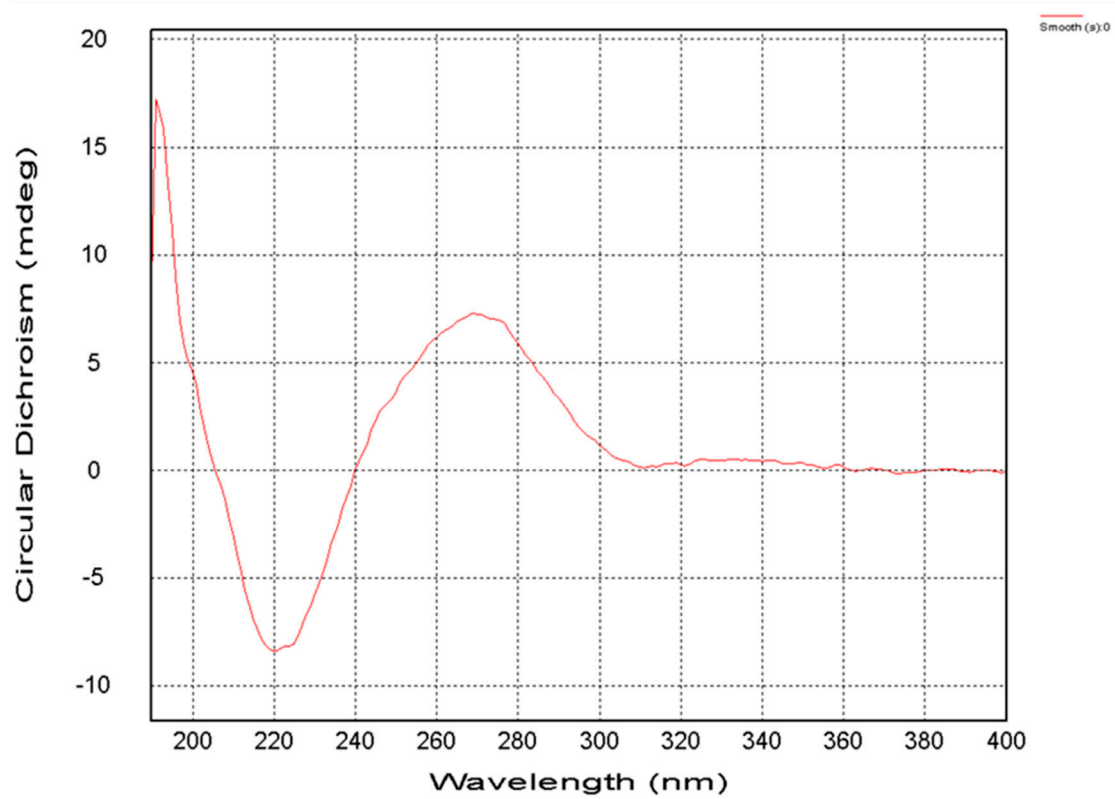


Figure S24. CD spectrum of compound **3** in MeOH

XSJ-QJZ-19 ^1H NMR (500 MHz, CDCl_3)

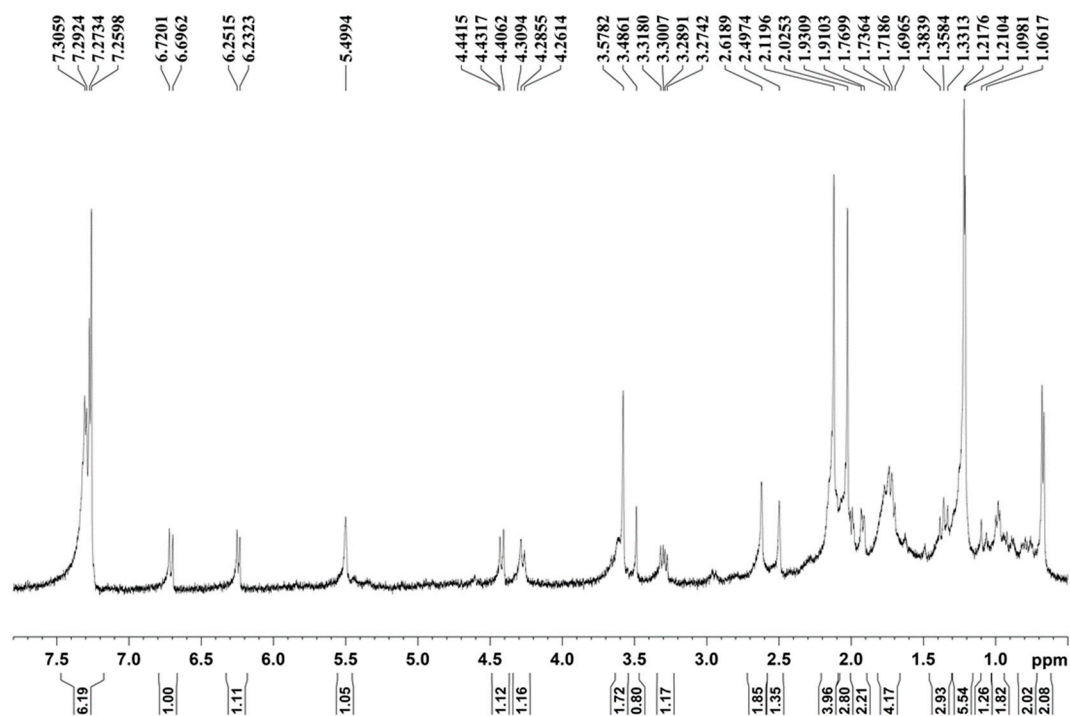


Figure S25. ^1H NMR spectrum of compound **3** in CDCl_3

XSJ-QJZ-19 ^{13}C and DEPT NMR (125 MHz, CDCl_3)

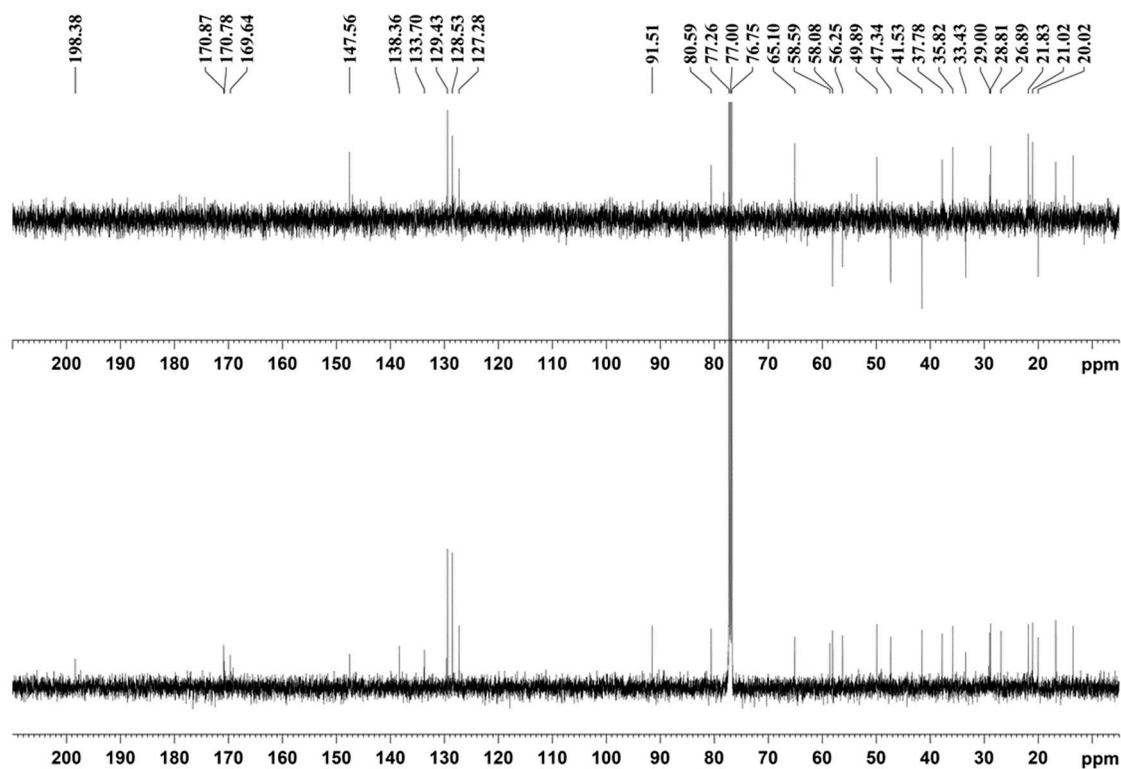


Figure S26. ^{13}C NMR and DEPT spectrum of compound **3** in CDCl_3

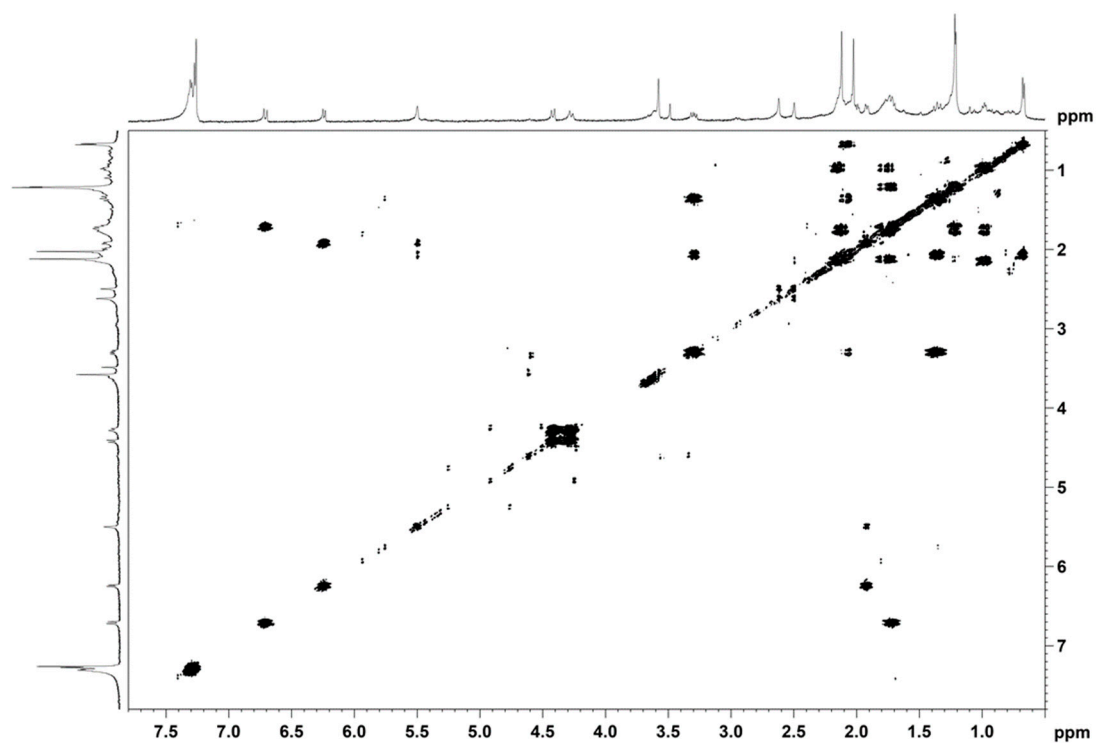


Figure S27. ^1H - ^1H COSY spectrum of compound **3** in CDCl_3

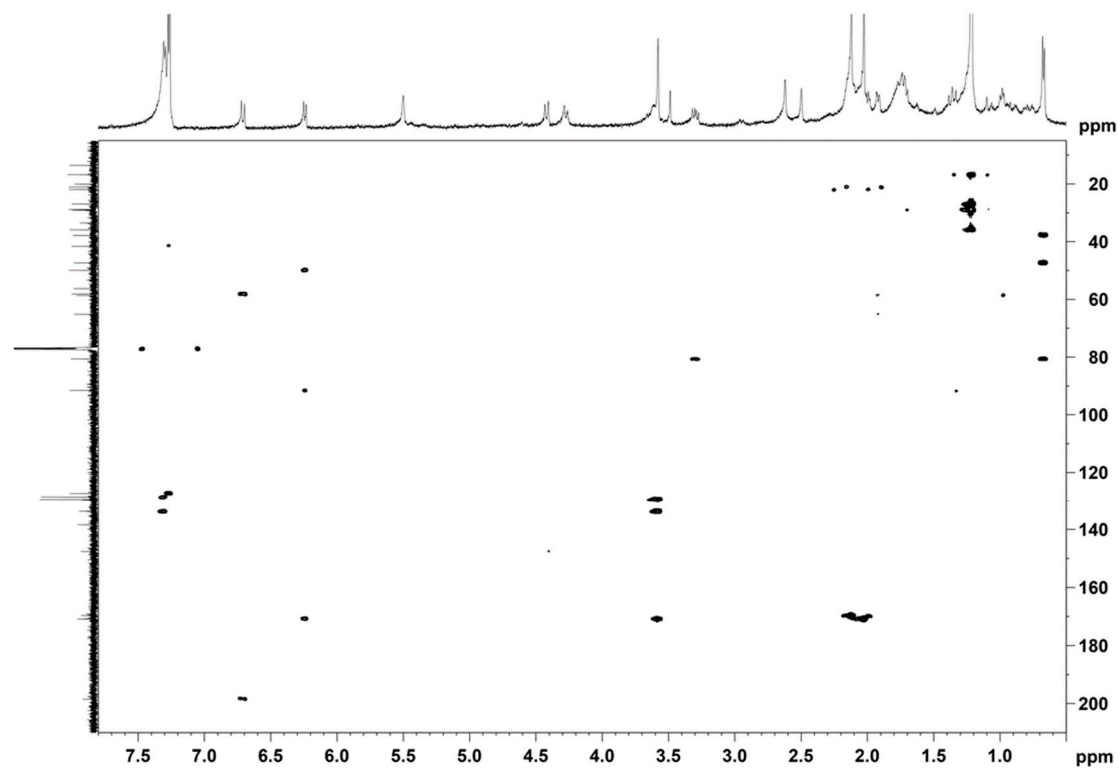


Figure S28. HMBC spectrum of compound **3** in CDCl_3

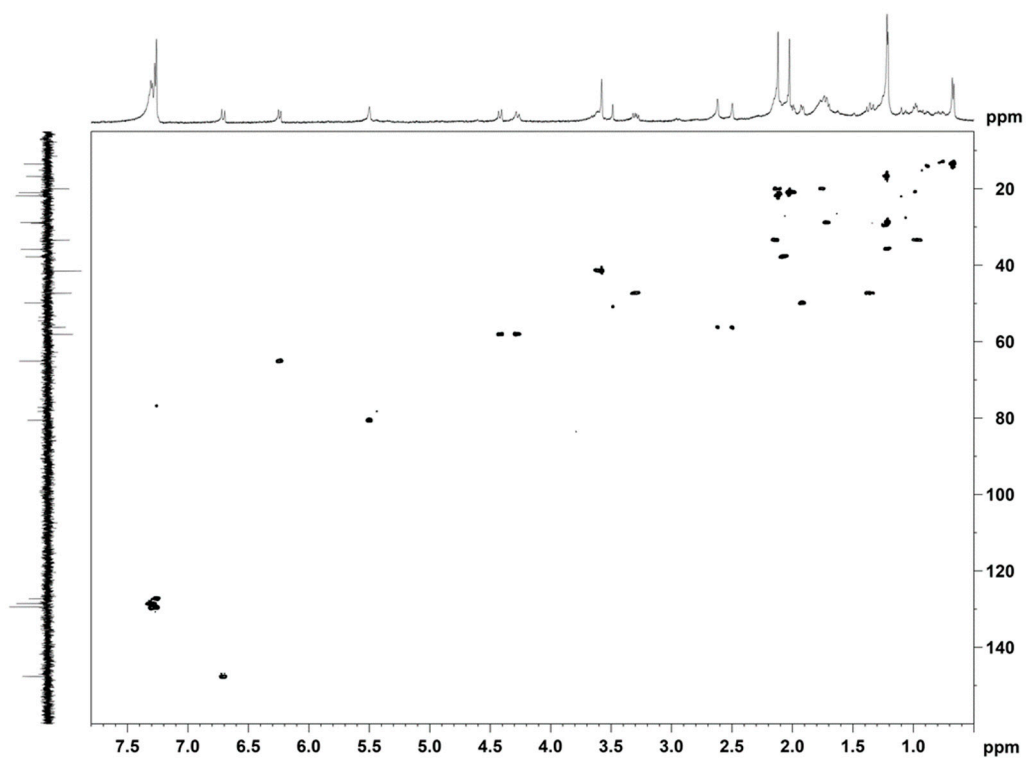


Figure S29. HSQC spectrum of compound **3** in CDCl₃

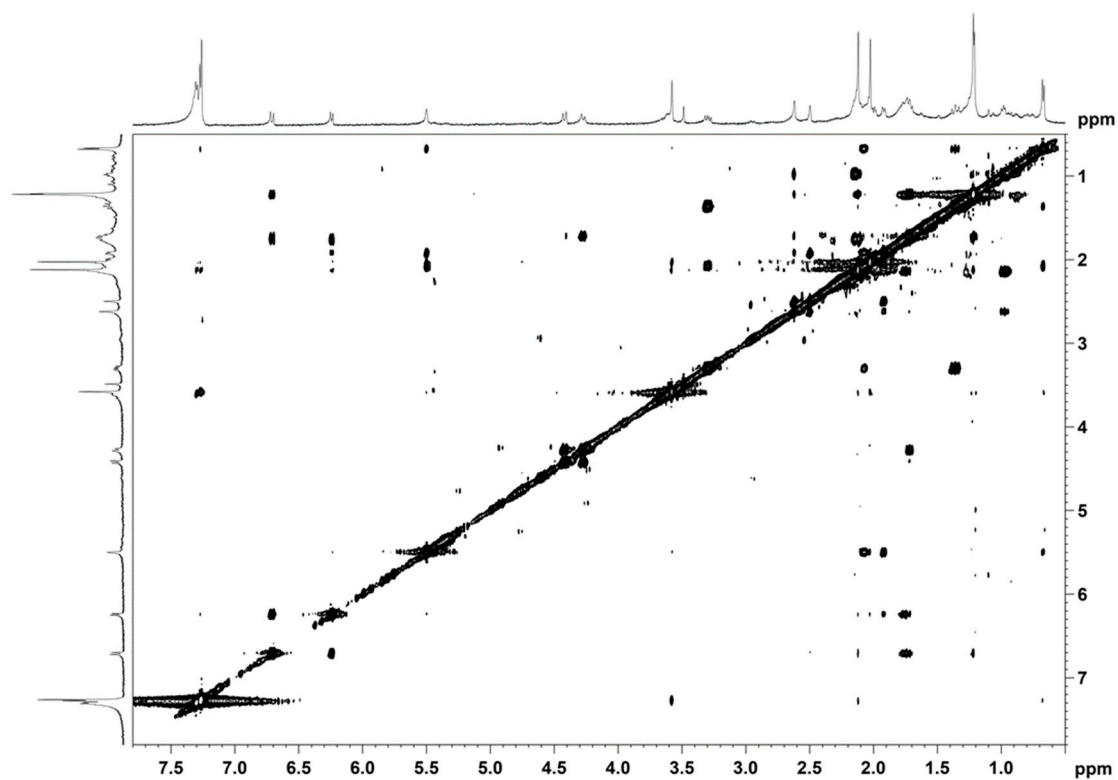
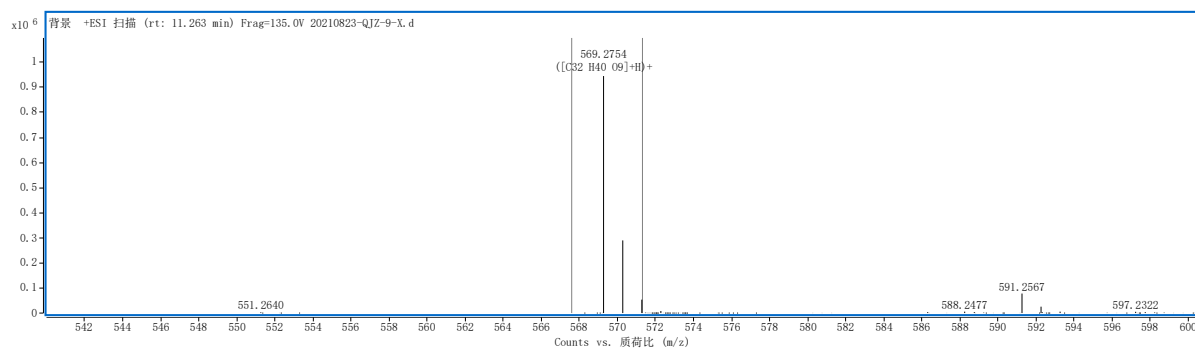


Figure S30. NOESY spectrum of compound **3** in CDCl₃



| Best | Formula(M) | Ion Formula | Tgt (m/z) | m/z | Diff (ppm) |
|------|--|--|-----------|----------|------------|
| TRUE | C ₃₂ H ₄₀ O ₉ | C ₃₂ H ₄₁ O ₉ | 569.2745 | 569.2754 | 1.58 |

Figure S31. HR-ESI-MS spectrum of compound **4**

Rudolph Research Analytical

Monday, 10/11/2021

This sample was measured on an Autopol VI, serial number 90079, manufactured by Rudolph Research Analytical, Hackettstown, NJ.

LotID : QJZ-9
Set Temperature : 20.0
Temp Corr : OFF

| n | Average | Std.Dev. | Maximum | Minimum | | | | | | |
|------|-----------|-------------|---------|---------|----------|-----|--------|-------|-------|---------|
| 6 | 70.000 | 0.4000 | 70.400 | 69.600 | | | | | | |
| S.No | Sample ID | Time | Result | Scale | OR ° Arc | WLG | Lg.mm | Conc. | Temp. | Comment |
| 1 | QJZ-9 | 10:32:39 AM | 69.600 | SR | 0.087 | 589 | 100.00 | 0.125 | 20.2 | |
| 2 | QJZ-9 | 10:32:47 AM | 69.600 | SR | 0.087 | 589 | 100.00 | 0.125 | 20.1 | |
| 3 | QJZ-9 | 10:32:54 AM | 69.600 | SR | 0.087 | 589 | 100.00 | 0.125 | 20.1 | |
| 4 | QJZ-9 | 10:33:01 AM | 70.400 | SR | 0.088 | 589 | 100.00 | 0.125 | 20.1 | |
| 5 | QJZ-9 | 10:33:09 AM | 70.400 | SR | 0.088 | 589 | 100.00 | 0.125 | 20.0 | |
| 6 | QJZ-9 | 10:33:20 AM | 70.400 | SR | 0.088 | 589 | 100.00 | 0.125 | 20.0 | |

Signature _____

Figure S32. OR value of compound **4** in MeOH

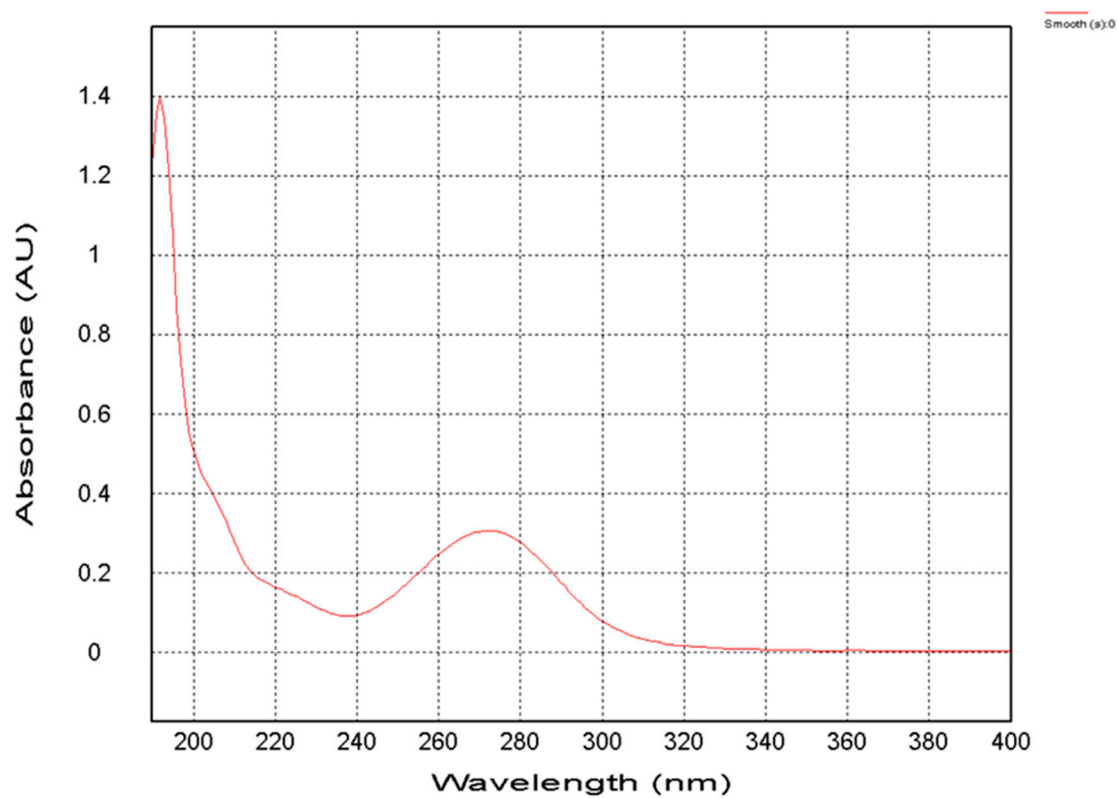


Figure S33. UV spectrum of compound 4 in MeOH

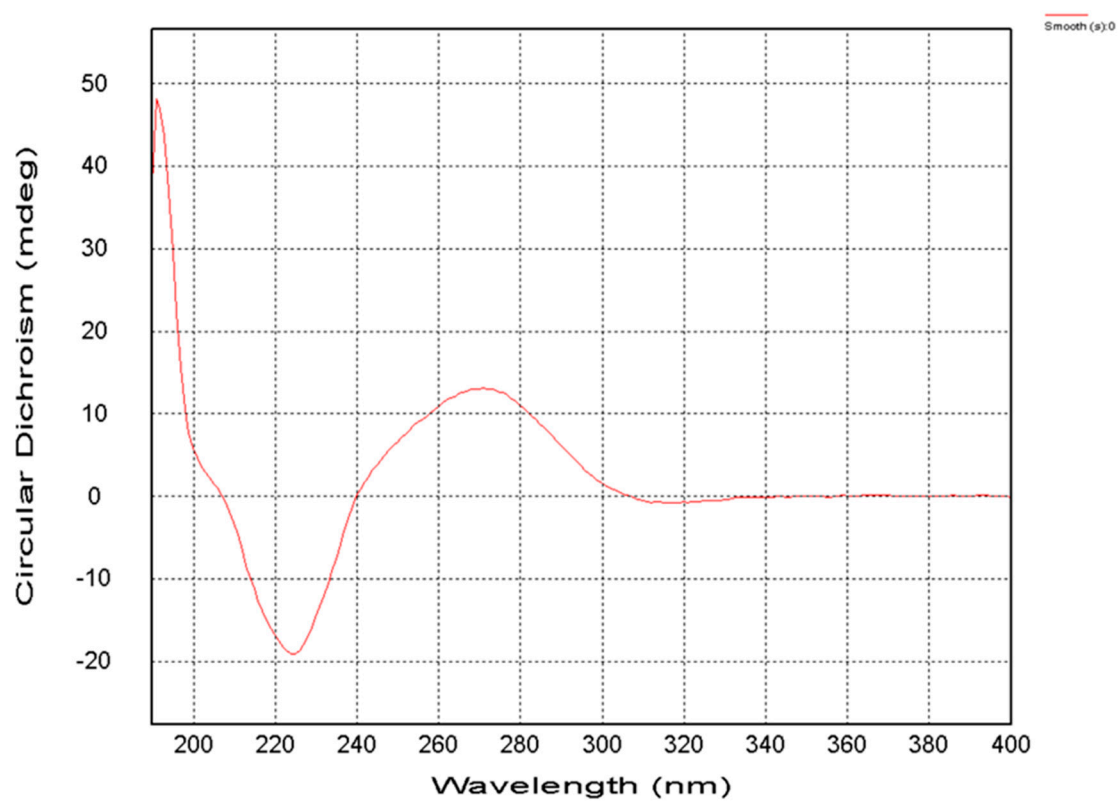


Figure S34. CD spectrum of compound 4 in MeOH

XSJ-QJZ-9 ¹H NMR (500 MHz, CDCl₃)

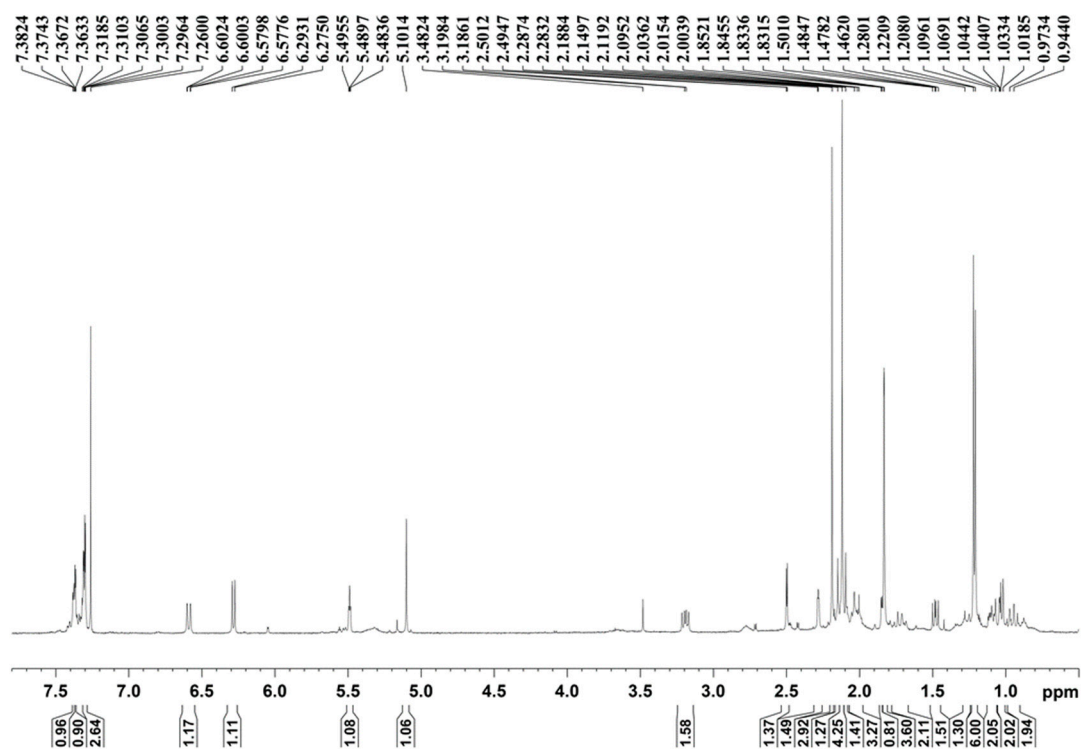


Figure S35. ¹H NMR spectrum of compound **4** in CDCl₃

XSJ-QJZ-9 C13 and DEPT NMR (125 MHz, CDCl₃)

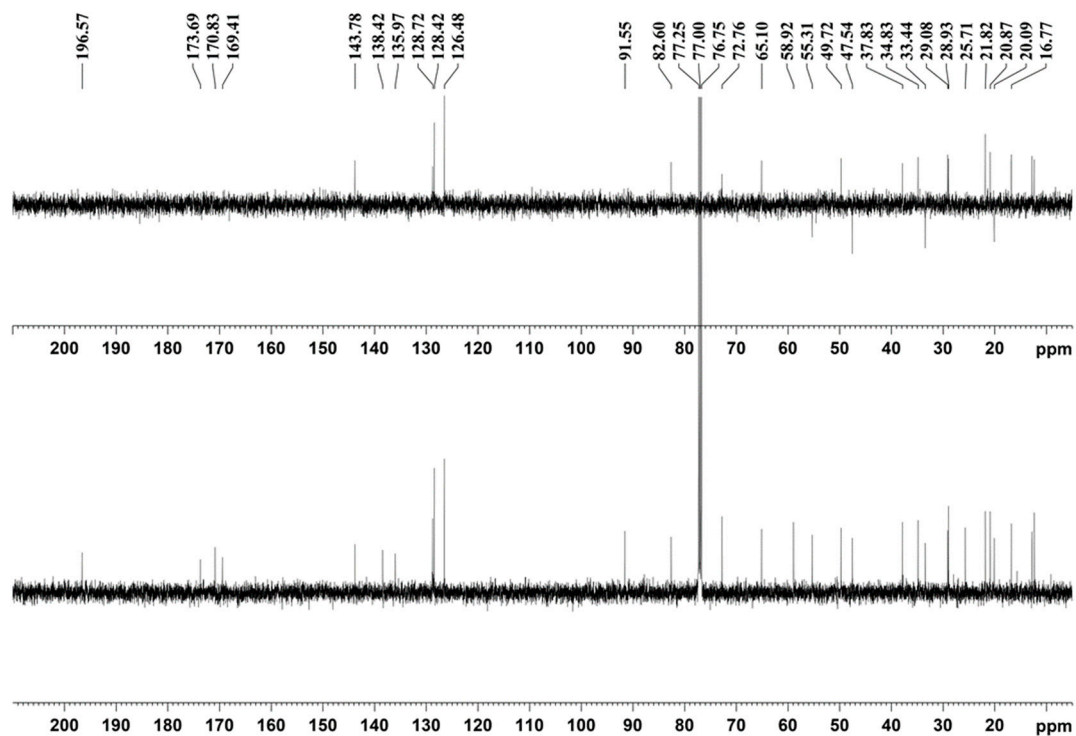


Figure S36. ¹³C NMR and DEPT spectrum of compound **4** in CDCl₃

XSJ-QJZ-9 1H 1H COSY

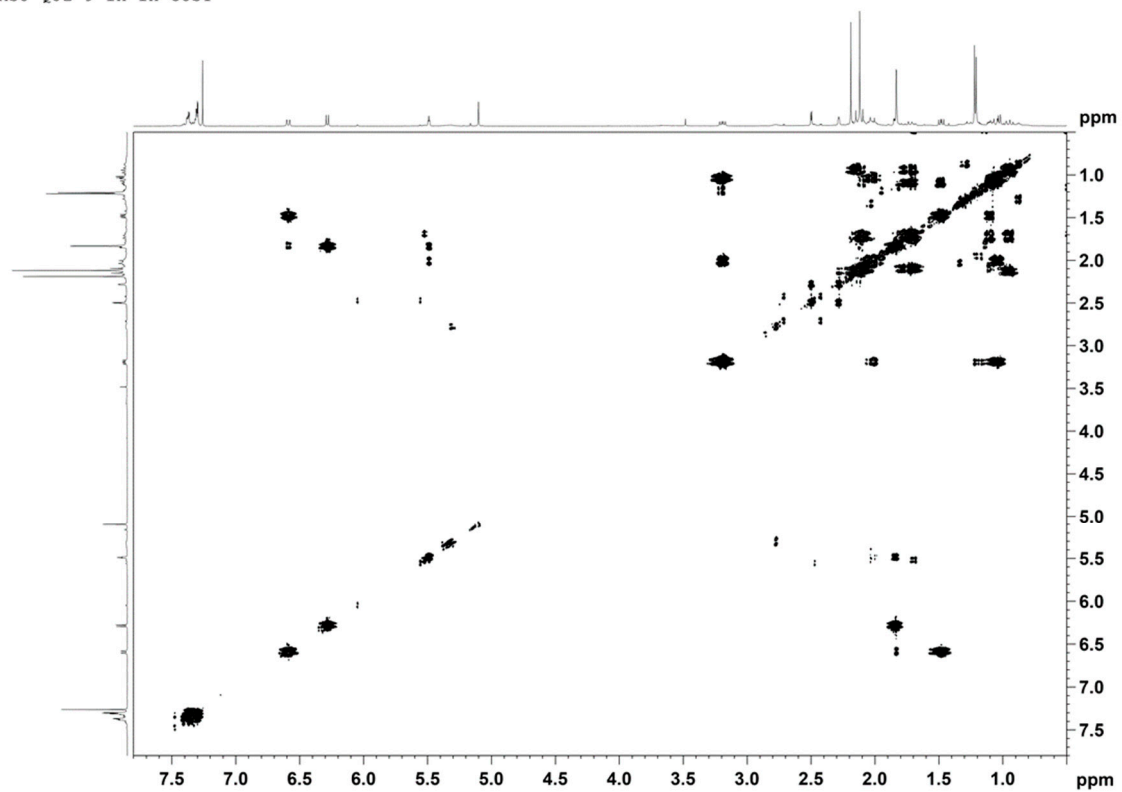


Figure S37. ¹H-¹H COSY spectrum of compound **4** in CDCl₃

XSJ-QJZ-9 HMBC

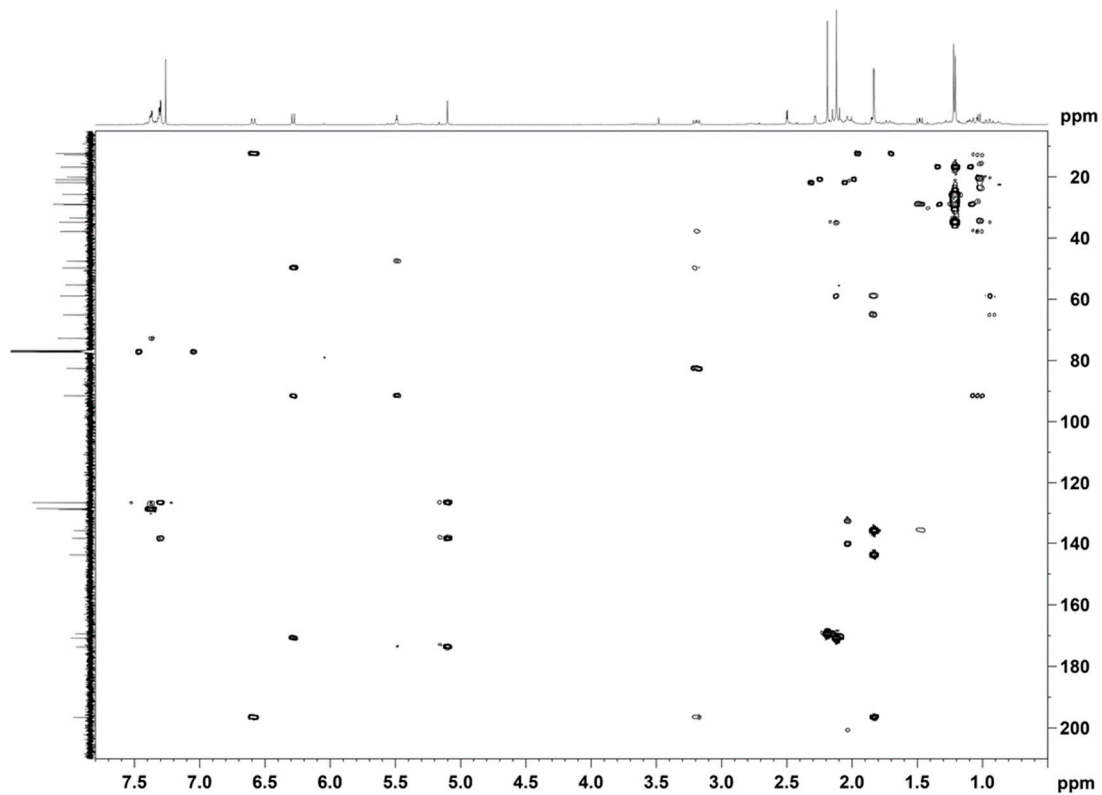


Figure S38. HMBC spectrum of compound **4** in CDCl₃

XSJ-QJZ-9 HSQC

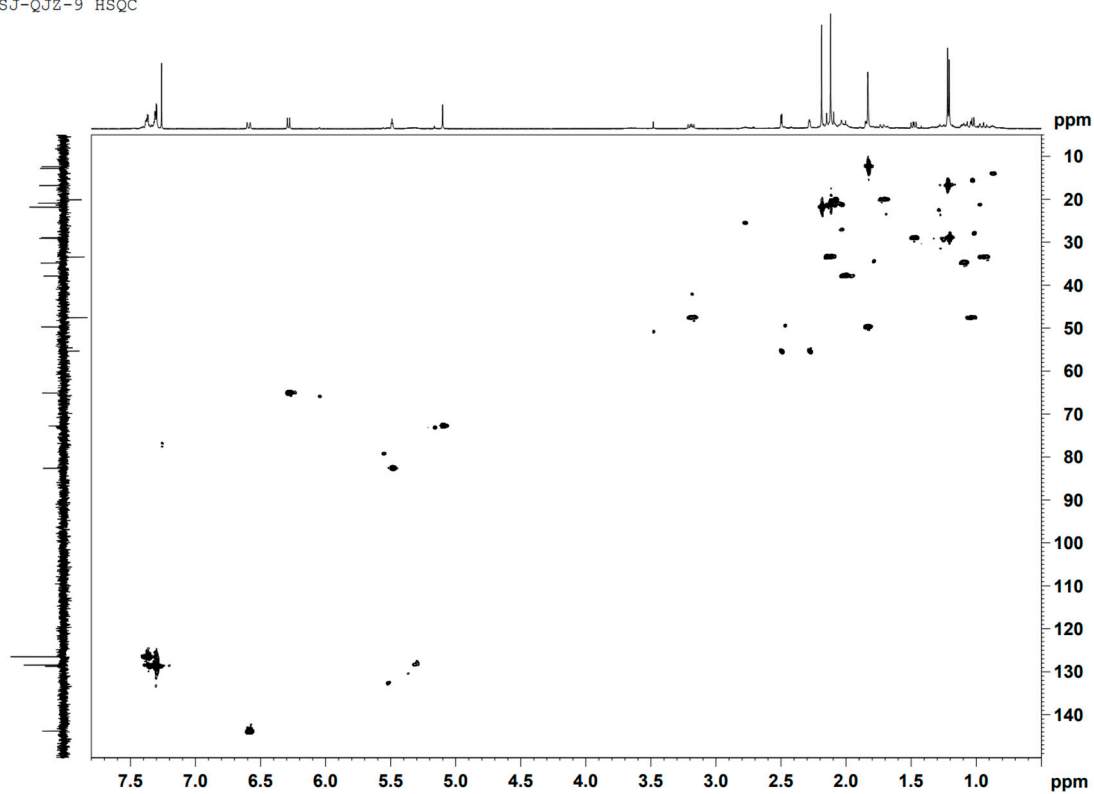


Figure S39. HSQC spectrum of compound **4** in CDCl₃

XSJ-QJZ-9 NOESY

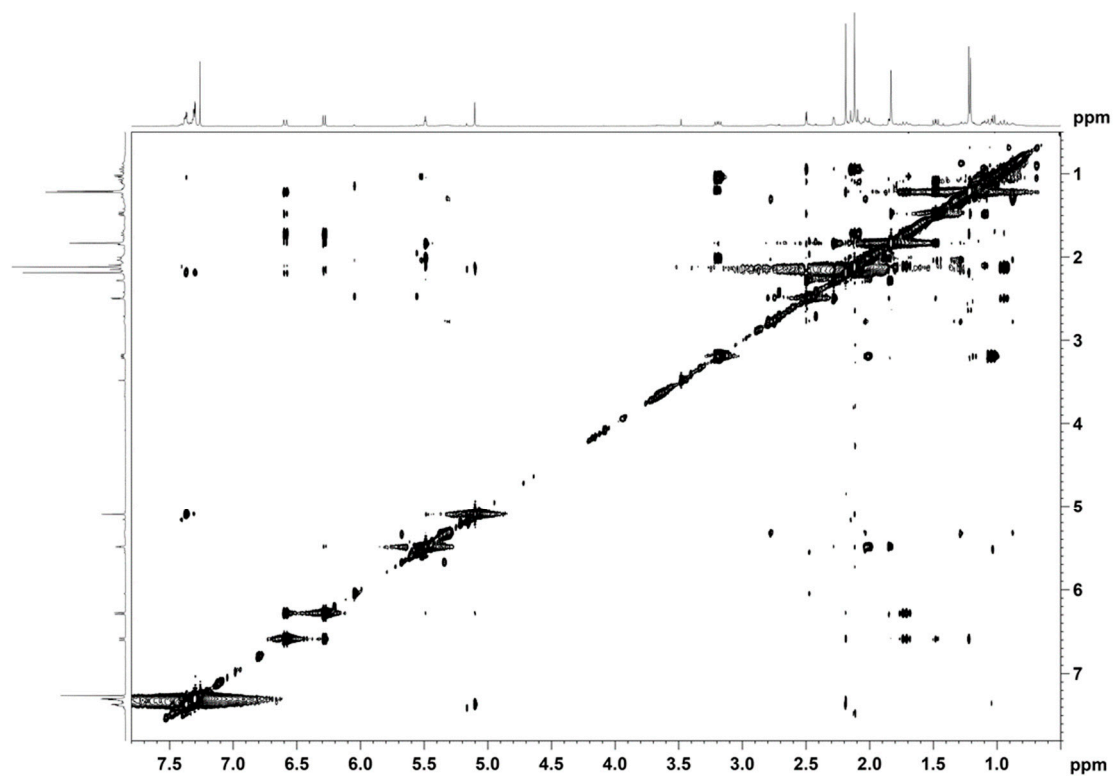
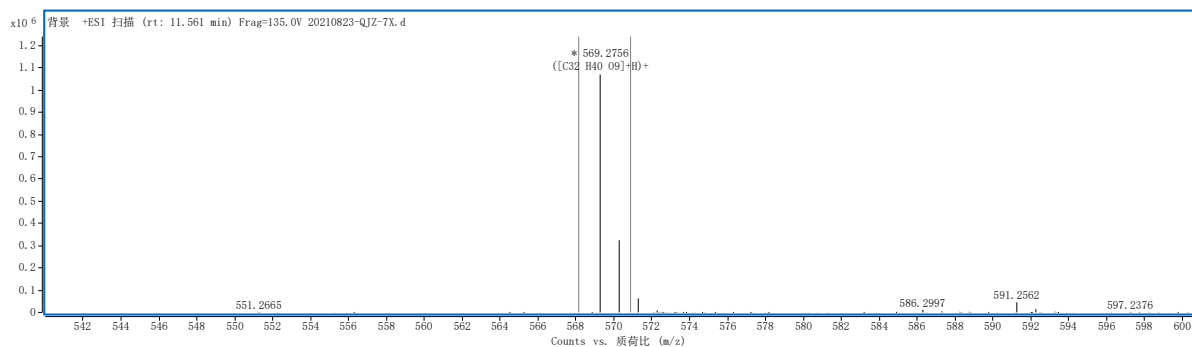


Figure S40. NOESY spectrum of compound **4** in CDCl₃



| Best | Formula(M) | Ion Formula | Tgt (m/z) | m/z | Diff (ppm) |
|------|--|--|-----------|----------|------------|
| TRUE | C ₃₂ H ₄₀ O ₉ | C ₃₂ H ₄₁ O ₉ | 569.2745 | 569.2756 | 1.93 |

Figure S41. HR-ESI-MS spectrum of compound **5**

Rudolph Research Analytical

Monday, 10/11/2021

This sample was measured on an Autopol VI, serial number 90079, manufactured by Rudolph Research Analytical, Hackettstown, NJ.

LotID : QJZ-7
Set Temperature : 20.0
Temp Corr : OFF

| n | Average | Std.Dev. | Maximum | Minimum | | | | | | |
|------|-----------|-------------|---------|---------|----------|-----|--------|-------|-------|---------|
| 6 | 112.654 | 0.4365 | 112.963 | 112.037 | | | | | | |
| S.No | Sample ID | Time | Result | Scale | OR ° Arc | WLG | Lg.mm | Conc. | Temp. | Comment |
| 1 | QJZ-7 | 10:58:17 AM | 112.037 | SR | 0.121 | 589 | 100.00 | 0.108 | 20.1 | |
| 2 | QJZ-7 | 10:58:25 AM | 112.037 | SR | 0.121 | 589 | 100.00 | 0.108 | 20.1 | |
| 3 | QJZ-7 | 10:58:32 AM | 112.963 | SR | 0.122 | 589 | 100.00 | 0.108 | 20.1 | |
| 4 | QJZ-7 | 10:58:40 AM | 112.963 | SR | 0.122 | 589 | 100.00 | 0.108 | 20.0 | |
| 5 | QJZ-7 | 10:58:47 AM | 112.963 | SR | 0.122 | 589 | 100.00 | 0.108 | 20.0 | |
| 6 | QJZ-7 | 10:58:54 AM | 112.963 | SR | 0.122 | 589 | 100.00 | 0.108 | 20.0 | |

Signature

Figure S42. OR value of compound **5** in MeOH

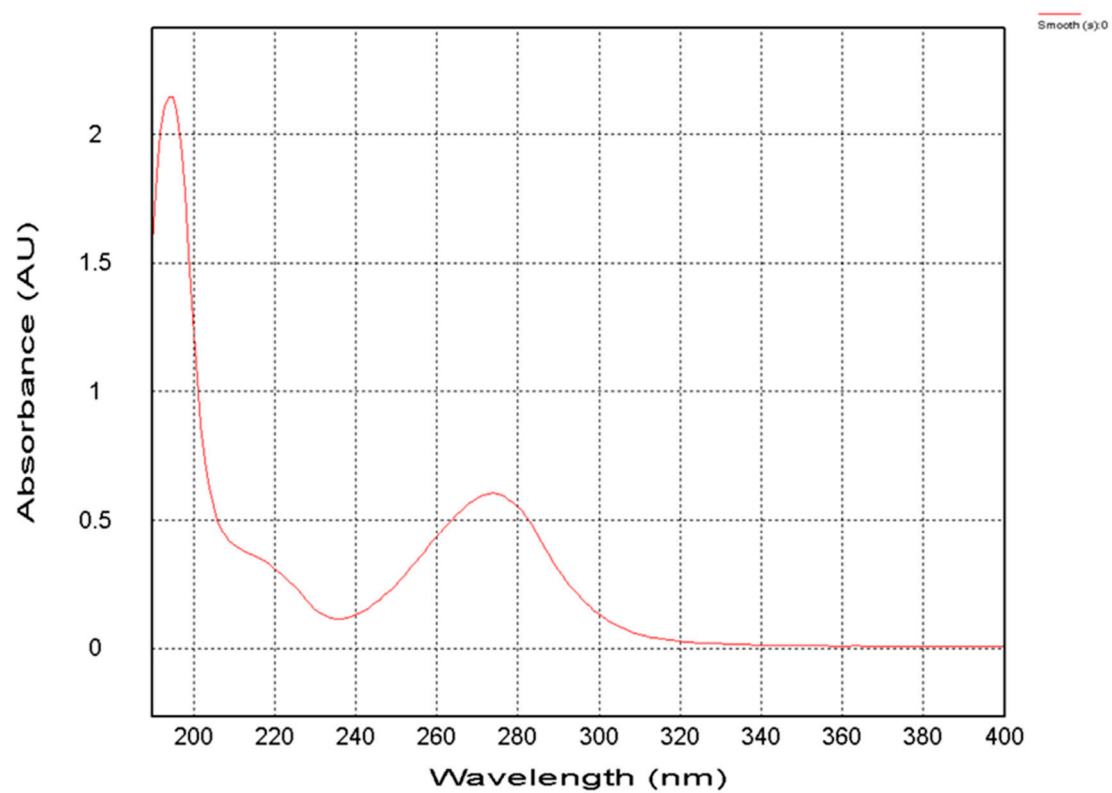


Figure S43. UV spectrum of compound **5** in MeOH

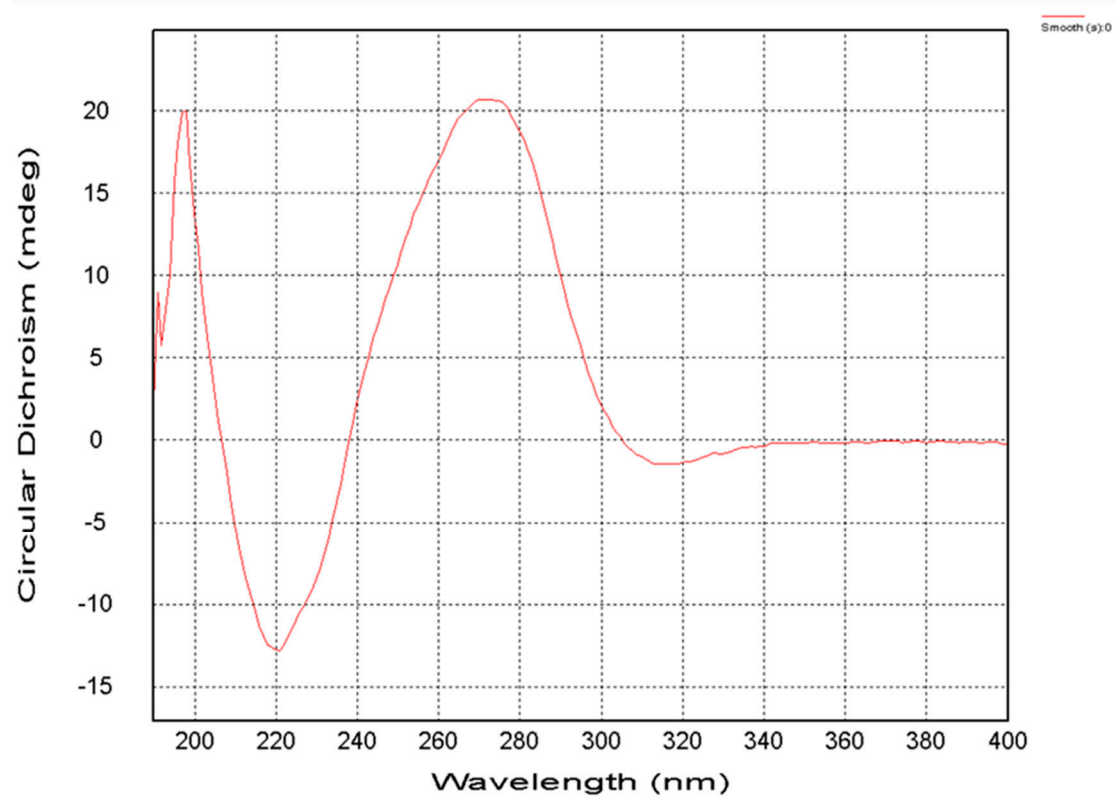


Figure S44. CD spectrum of compound **5** in MeOH

XSJ-QJZ-7 ^1H NMR (500 MHz, CDCl_3)

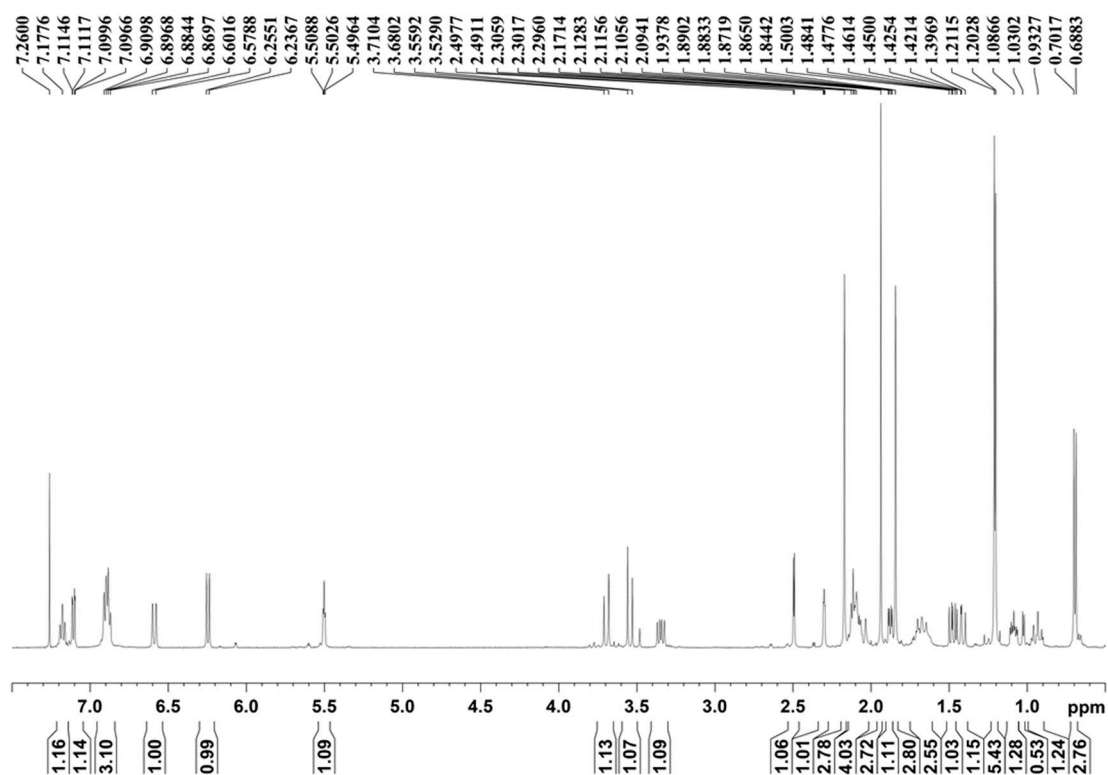


Figure S45. ^1H NMR spectrum of compound **5** in CDCl_3

XSJ-QJZ-7 ^{13}C and DEPT NMR (125 MHz, CDCl_3)

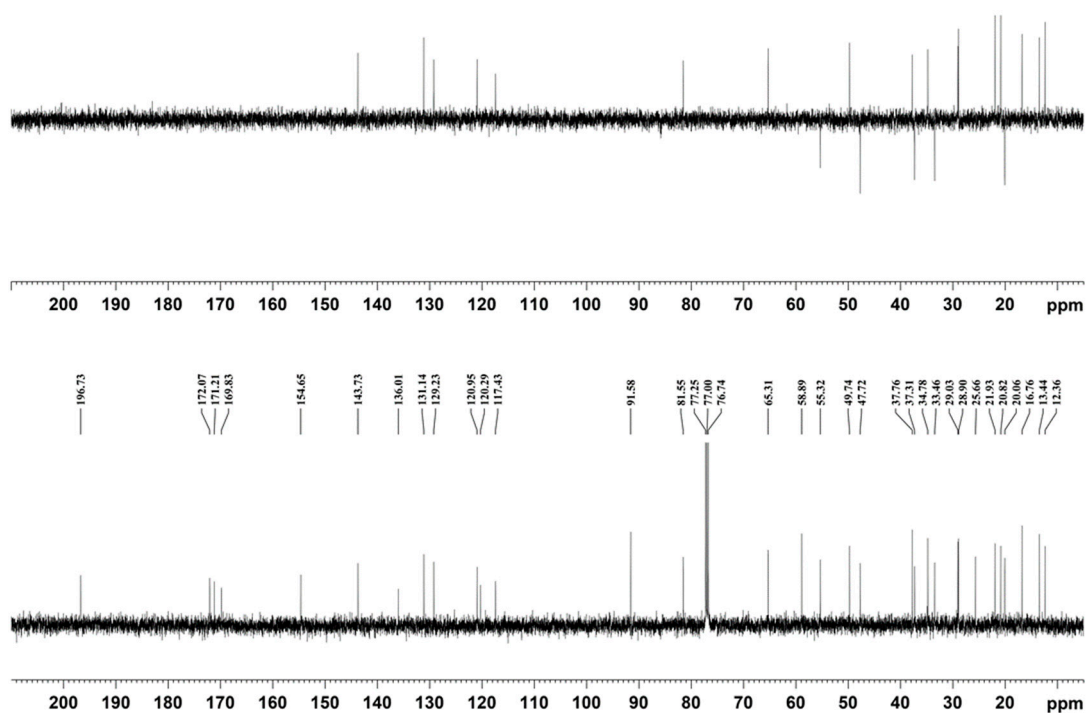


Figure S46. ^{13}C NMR and DEPT spectrum of compound **5** in CDCl_3

XSJ-QJZ-7 ^1H ^1H COSY

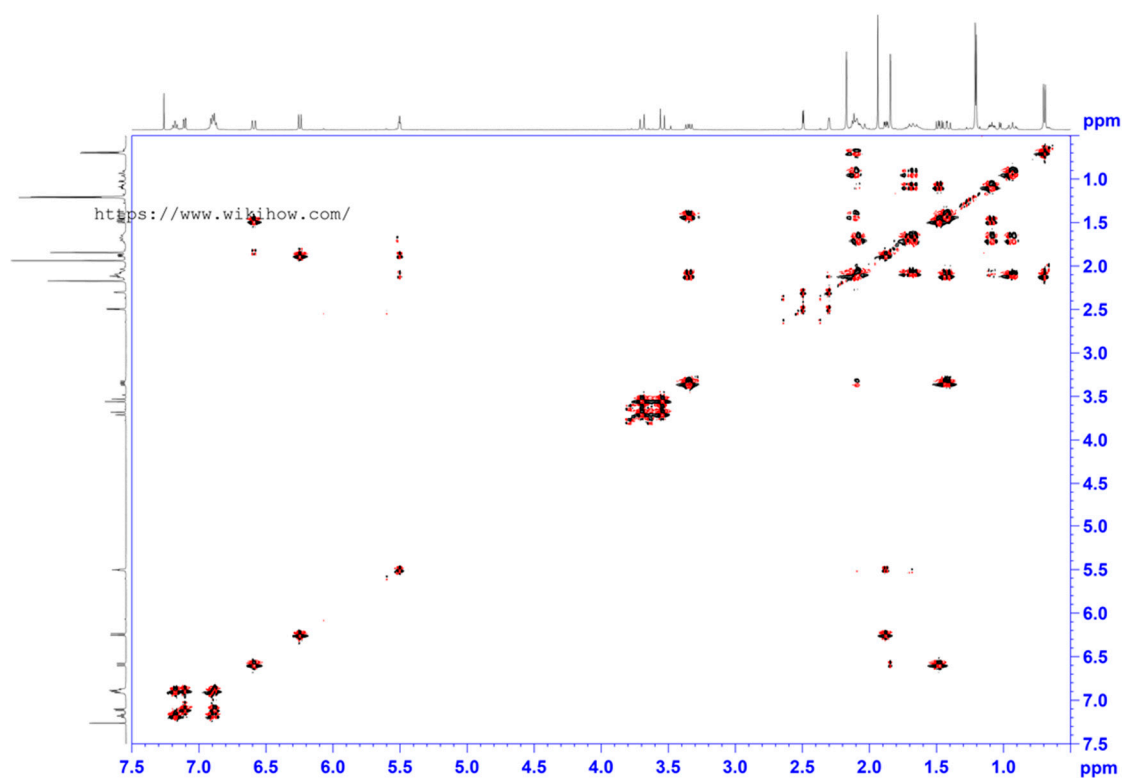


Figure S47. ^1H - ^1H COSY spectrum of compound **5** in CDCl_3

XSJ-QJZ-7 HMBC

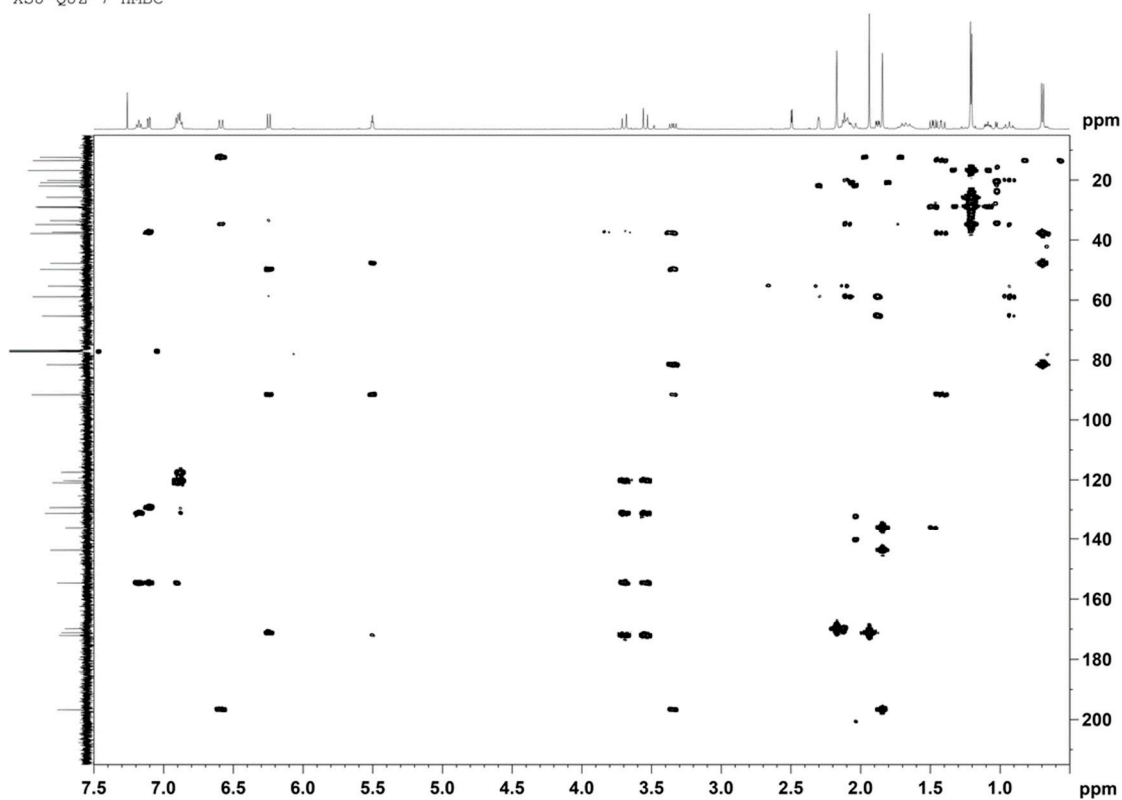
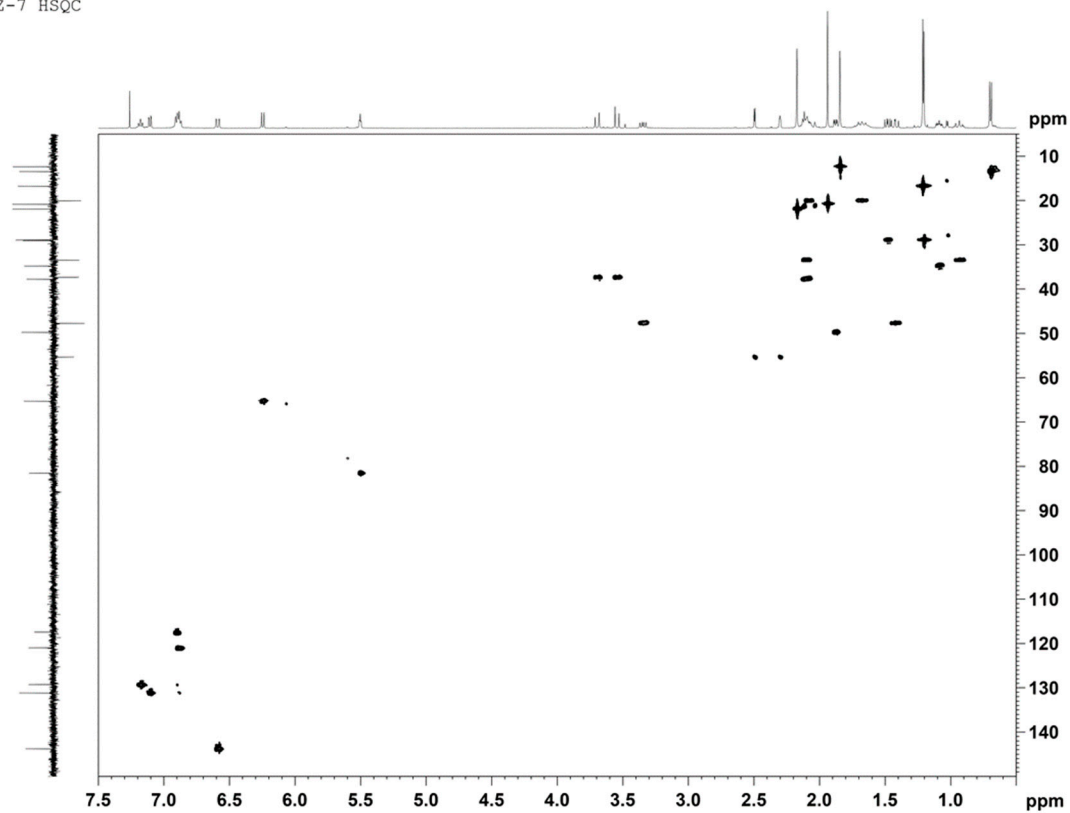
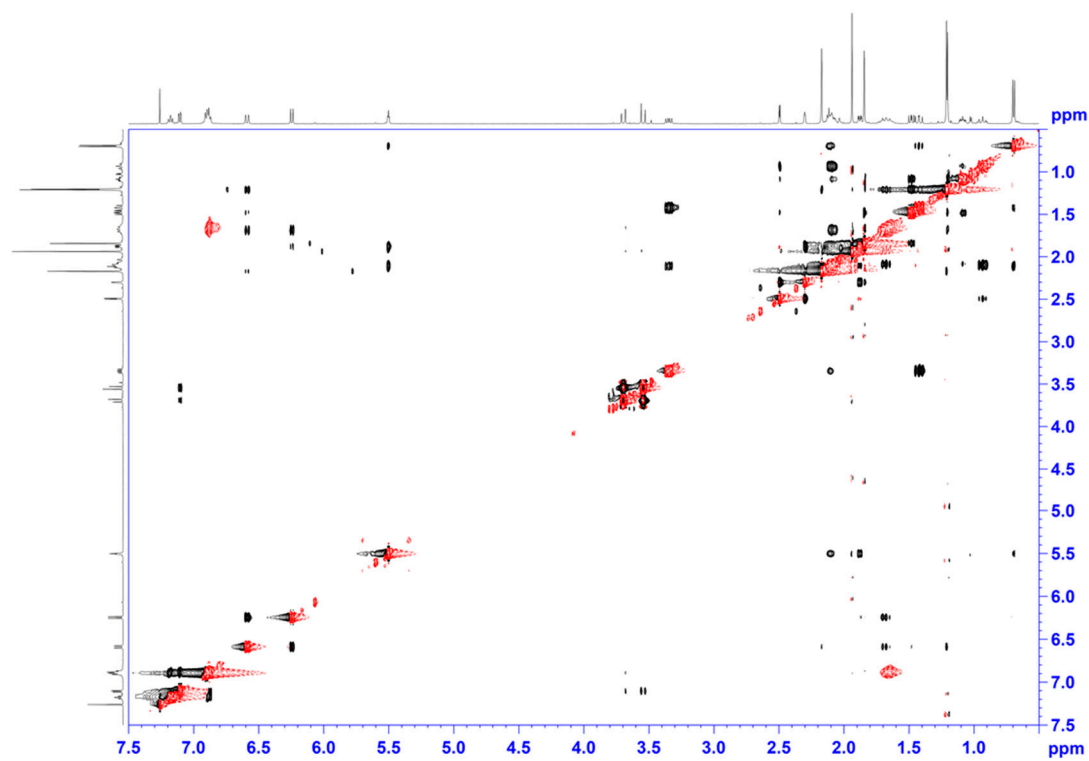
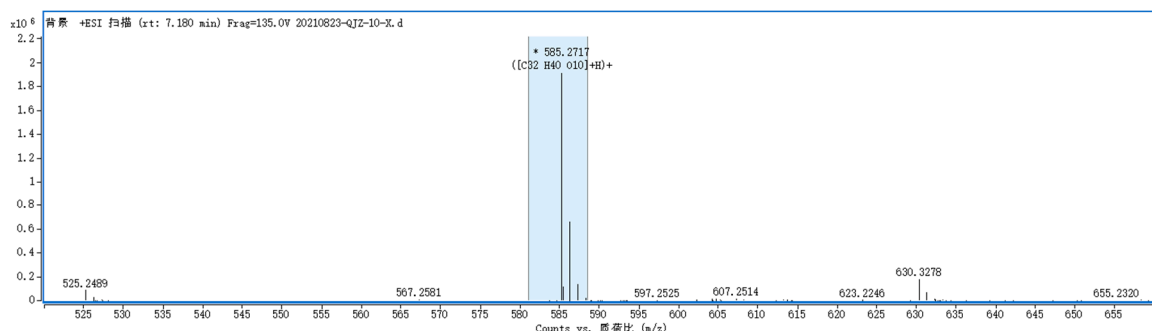


Figure S48. HMBC spectrum of compound **5** in CDCl_3

Figure S49. HSQC spectrum of compound **5** in CDCl₃Figure S50. NOESY spectrum of compound **5** in CDCl₃



| Best | Formula(M) | Ion Formula | Tgt (m/z) | m/z | Diff (ppm) |
|------|---|---|-----------|----------|------------|
| TRUE | C ₃₂ H ₄₀ O ₁₀ | C ₃₂ H ₄₁ O ₁₀ | 585.2694 | 585.2717 | 3.93 |

Figure S51. HR-ESI-MS spectrum of compound **6**

Rudolph Research Analytical

Monday, 10/11/2021

This sample was measured on an Autopol VI, serial number 90079, manufactured by Rudolph Research Analytical, Hackettstown, NJ.

LotID : QJZ-10
Set Temperature : 20.0
Temp Corr : OFF

| n | Average | Std.Dev. | Maximum | Minimum | | | | | | |
|------|-----------|-------------|---------|---------|----------|-----|--------|-------|-------|---------|
| 6 | 87.143 | 0.4760 | 87.619 | 86.667 | | | | | | |
| S.No | Sample ID | Time | Result | Scale | OR ° Arc | WLG | Lg.mm | Conc. | Temp. | Comment |
| 1 | QJZ-10 | 10:17:24 AM | 86.667 | SR | 0.091 | 589 | 100.00 | 0.105 | 20.3 | |
| 2 | QJZ-10 | 10:17:32 AM | 86.667 | SR | 0.091 | 589 | 100.00 | 0.105 | 20.2 | |
| 3 | QJZ-10 | 10:17:39 AM | 87.619 | SR | 0.092 | 589 | 100.00 | 0.105 | 20.2 | |
| 4 | QJZ-10 | 10:17:47 AM | 86.667 | SR | 0.091 | 589 | 100.00 | 0.105 | 20.2 | |
| 5 | QJZ-10 | 10:17:54 AM | 87.619 | SR | 0.092 | 589 | 100.00 | 0.105 | 20.1 | |
| 6 | QJZ-10 | 10:18:02 AM | 87.619 | SR | 0.092 | 589 | 100.00 | 0.105 | 20.1 | |

Signature

Figure S52. OR value of compound **6** in MeOH

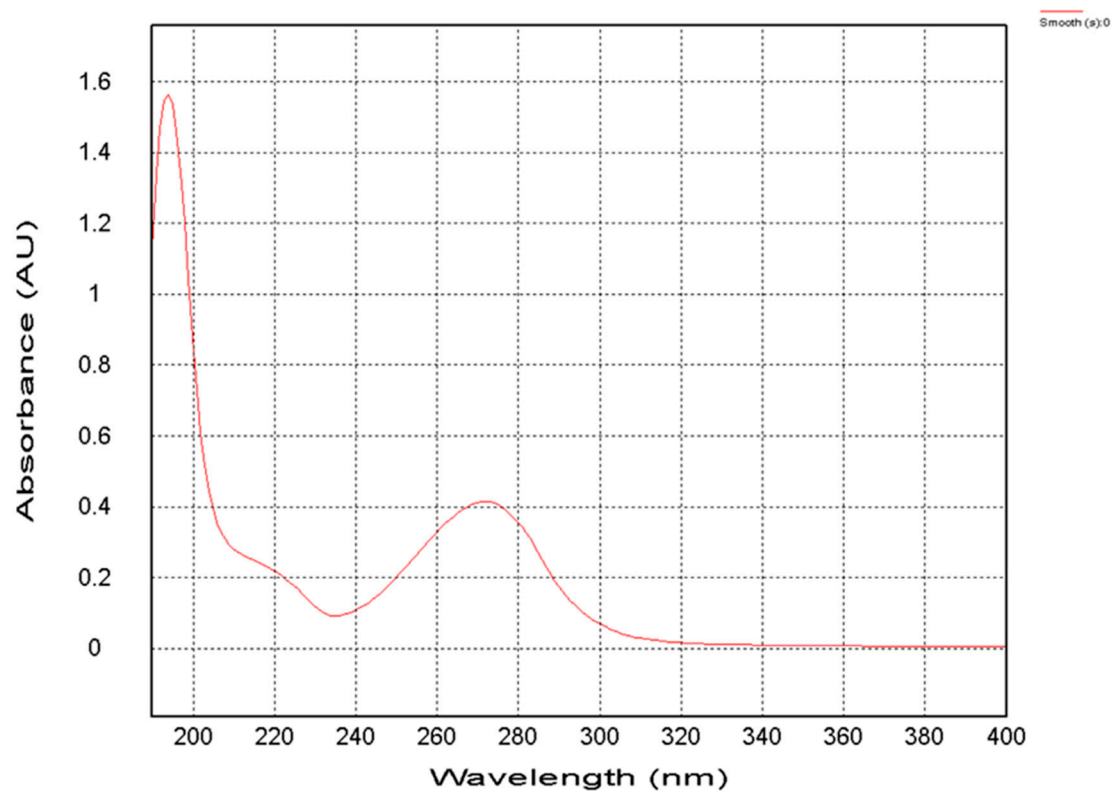


Figure S53. UV spectrum of compound **6** in MeOH

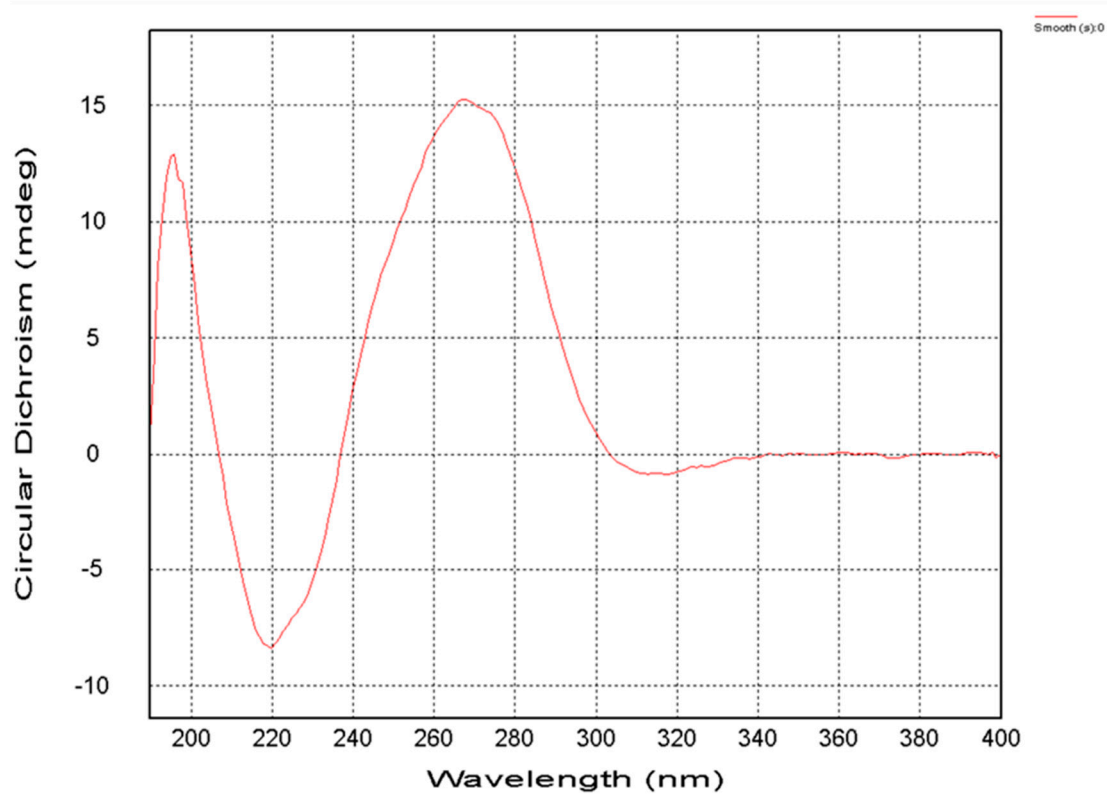


Figure S54. CD spectrum of compound **6** in MeOH

XSJ-QJZ-10 ^1H NMR (500 MHz, CD_3COCD_3)

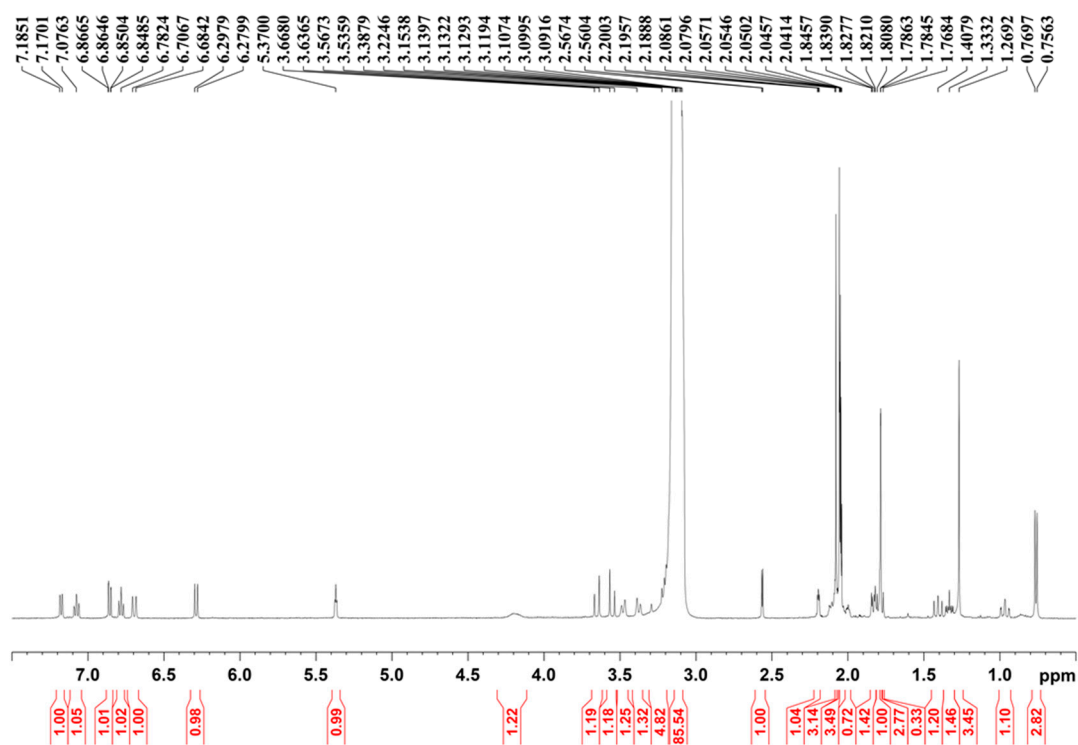


Figure S55. ^1H NMR spectrum of compound **6** in $\text{C}_3\text{D}_6\text{O}$

XSJ-QJZ-10 ^{13}C and DEPT NMR (125 MHz, CD_3COCD_3)

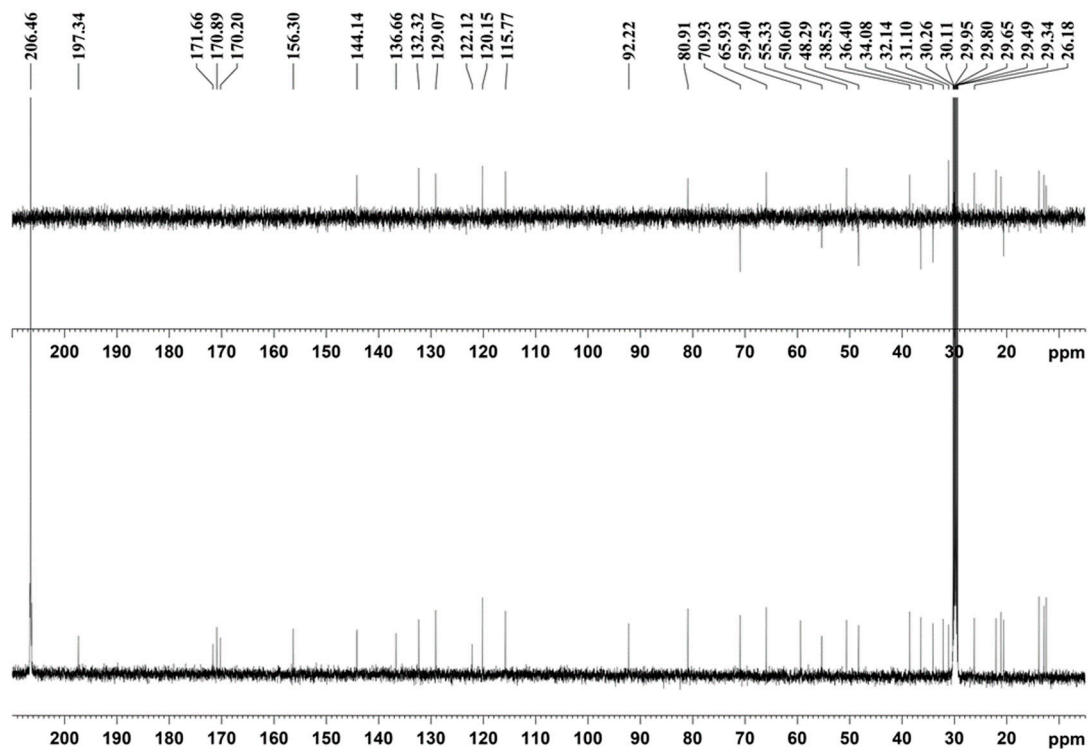


Figure S56. ^{13}C NMR and DEPT spectrum of compound **6** in $\text{C}_3\text{D}_6\text{O}$

XSJ-QJZ-10 1H 1H COSY

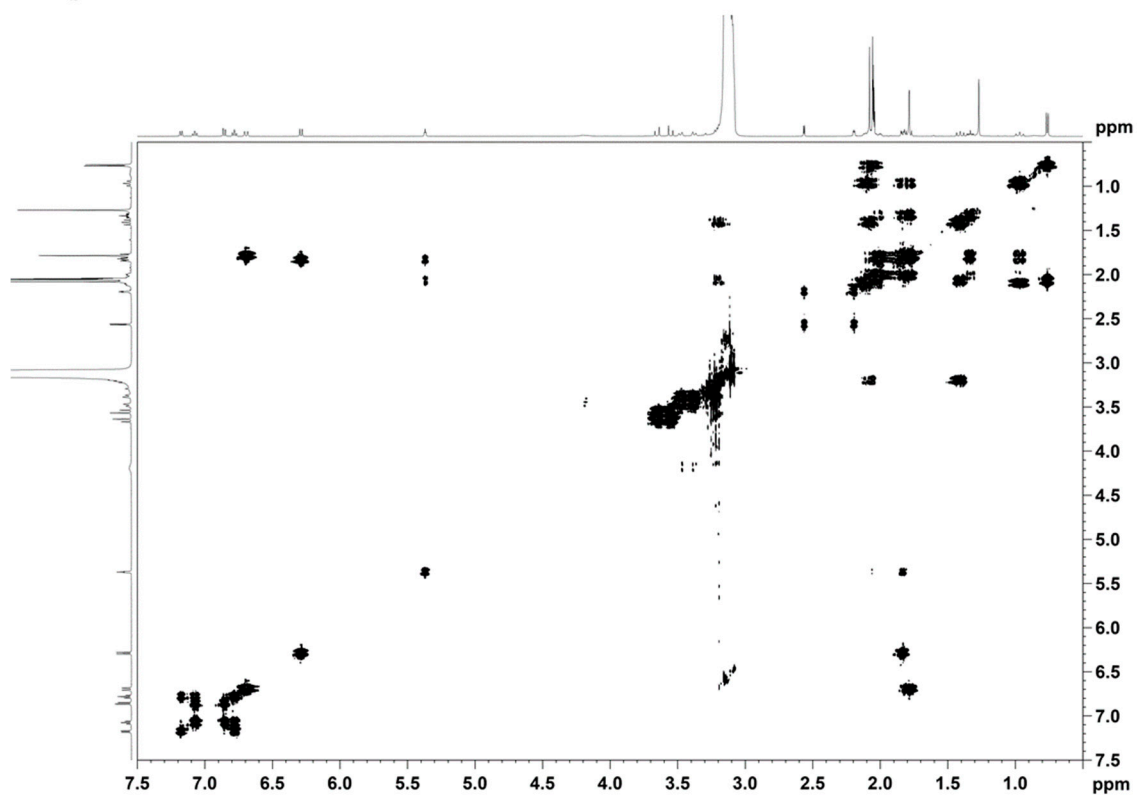


Figure S57. ^1H - ^1H NMR spectrum of compound **6** in $\text{C}_3\text{D}_6\text{O}$

XSJ-QJZ-10 HMBC

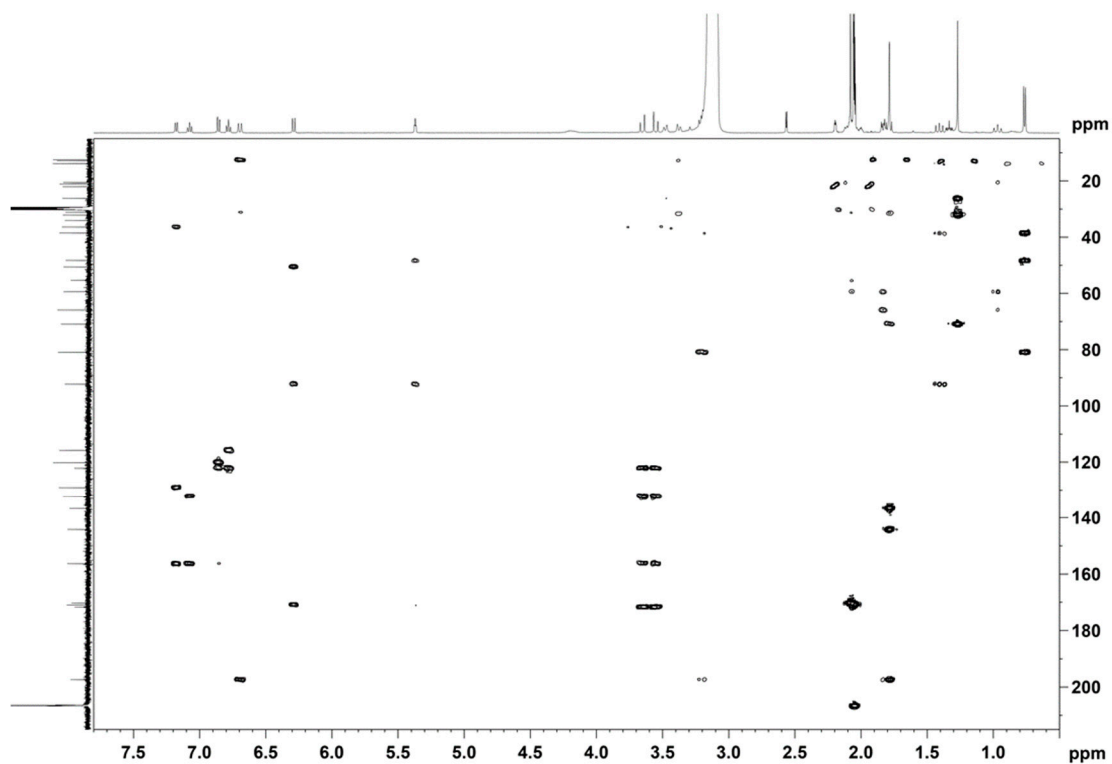


Figure S58. HMBC spectrum of compound **6** in $\text{C}_3\text{D}_6\text{O}$

XSJ-QJZ-10 HSQC

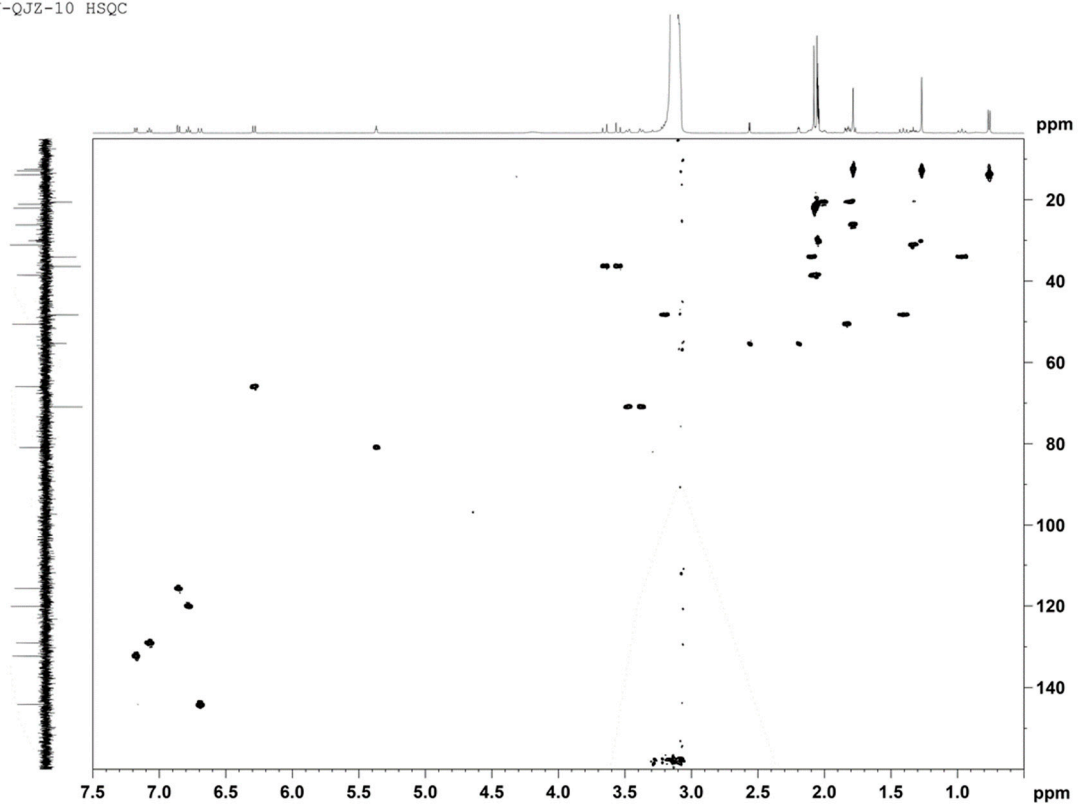


Figure S59. HSQC spectrum of compound **6** in C₃D₆O

XSJ-QJZ-10 NOESY

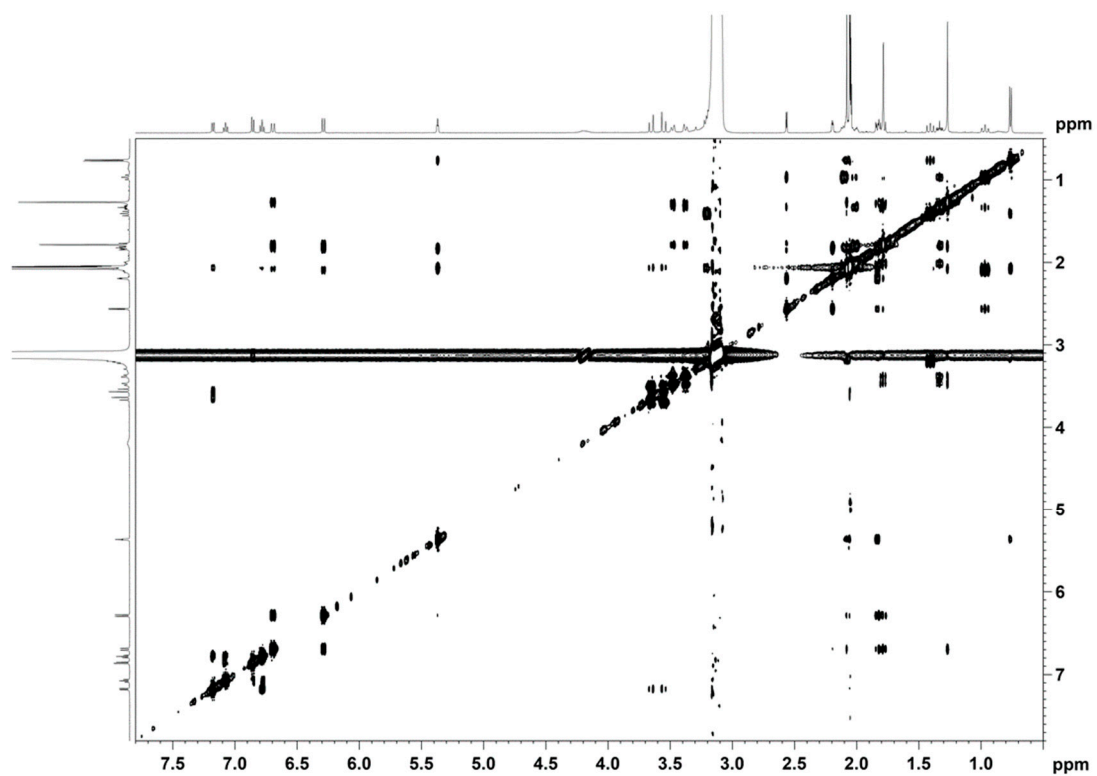
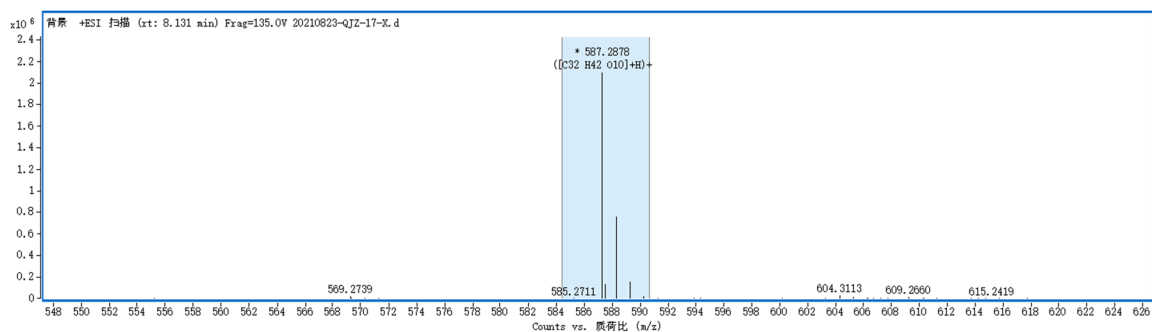


Figure S60. NOESY spectrum of compound **6** in C₃D₆O



| Best | Formula(M) | Ion Formula | Tgt (m/z) | m/z | Diff (ppm) |
|------|---|---|-----------|----------|------------|
| TRUE | C ₃₂ H ₄₂ O ₁₀ | C ₃₂ H ₄₃ O ₁₀ | 587.2851 | 587.2878 | 4.59 |

Figure S61. HR-ESI-MS spectrum of compound 7

Rudolph Research Analytical

Saturday, 10/09/2021

This sample was measured on an Autopol VI, serial number 90079, manufactured by Rudolph Research Analytical, Hackettstown, NJ.

LotID : QJZ-17
Set Temperature : 20.0
Temp Corr : OFF

| n | Average | Std.Dev. | Maximum | Minimum | | | | | | |
|------|-----------|-------------|---------|---------|----------|-----|--------|-------|-------|---------|
| 6 | 60.000 | 0.0000 | 60.000 | 60.000 | | | | | | |
| S.No | Sample ID | Time | Result | Scale | OR ° Arc | WLG | Lg.mm | Conc. | Temp. | Comment |
| 1 | QJZ-17 | 04:36:50 PM | 60.000 | SR | 0.102 | 589 | 100.00 | 0.170 | 19.7 | |
| 2 | QJZ-17 | 04:36:57 PM | 60.000 | SR | 0.102 | 589 | 100.00 | 0.170 | 19.7 | |
| 3 | QJZ-17 | 04:37:05 PM | 60.000 | SR | 0.102 | 589 | 100.00 | 0.170 | 19.7 | |
| 4 | QJZ-17 | 04:37:12 PM | 60.000 | SR | 0.102 | 589 | 100.00 | 0.170 | 19.7 | |
| 5 | QJZ-17 | 04:37:20 PM | 60.000 | SR | 0.102 | 589 | 100.00 | 0.170 | 19.8 | |
| 6 | QJZ-17 | 04:37:27 PM | 60.000 | SR | 0.102 | 589 | 100.00 | 0.170 | 19.8 | |

Signature

Figure S62. OR value of compound 7 in MeOH

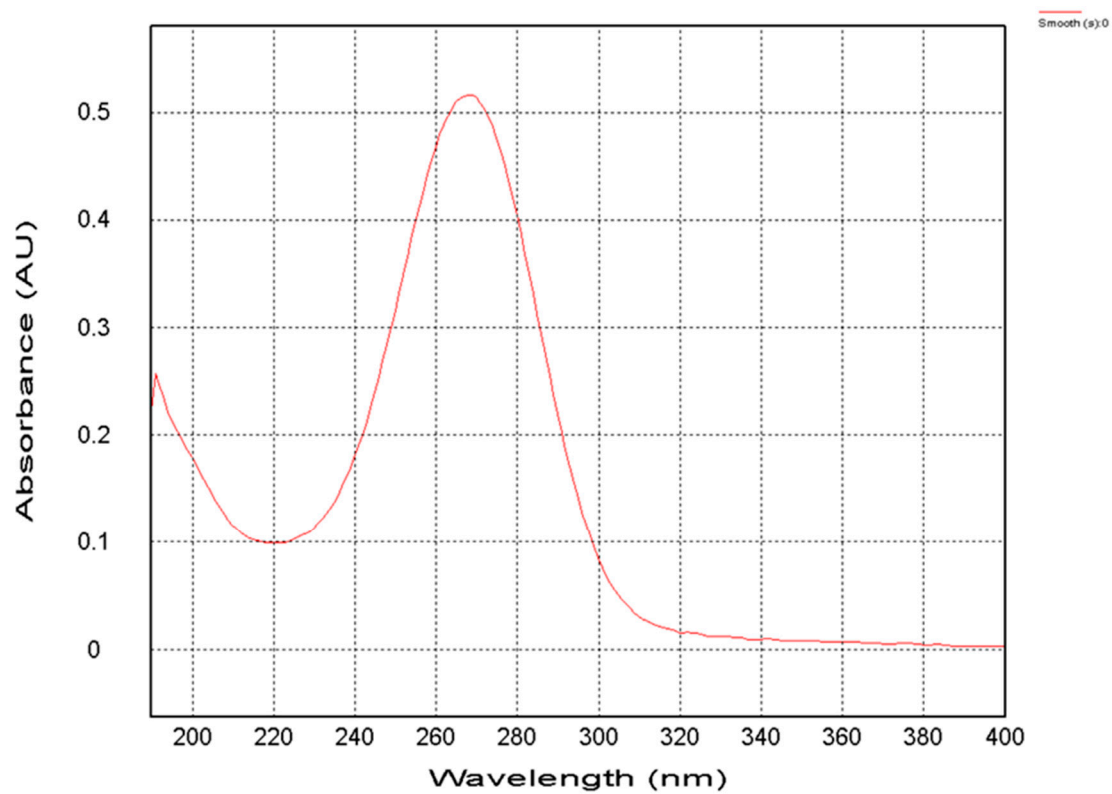


Figure S63. UV spectrum of compound 7 in MeOH

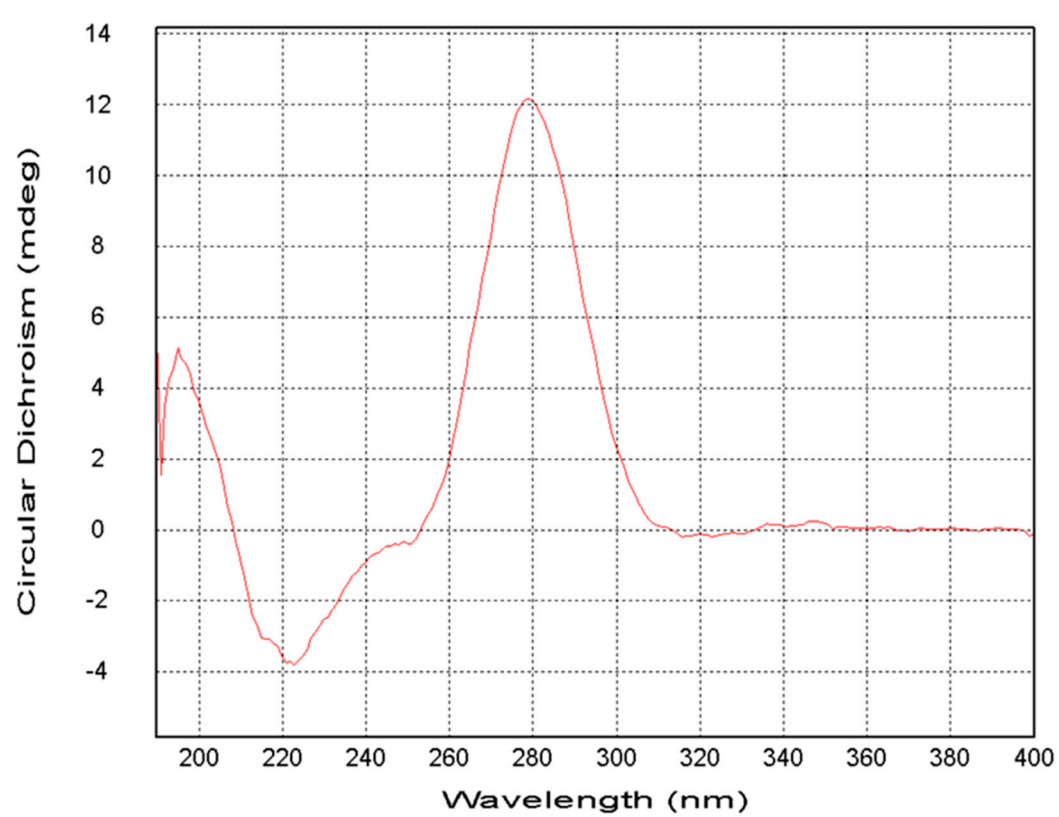


Figure S64. CD spectrum of compound 7 in MeOH

XSJ-QJZ-17 ^1H NMR (500 MHz, CDCl_3)

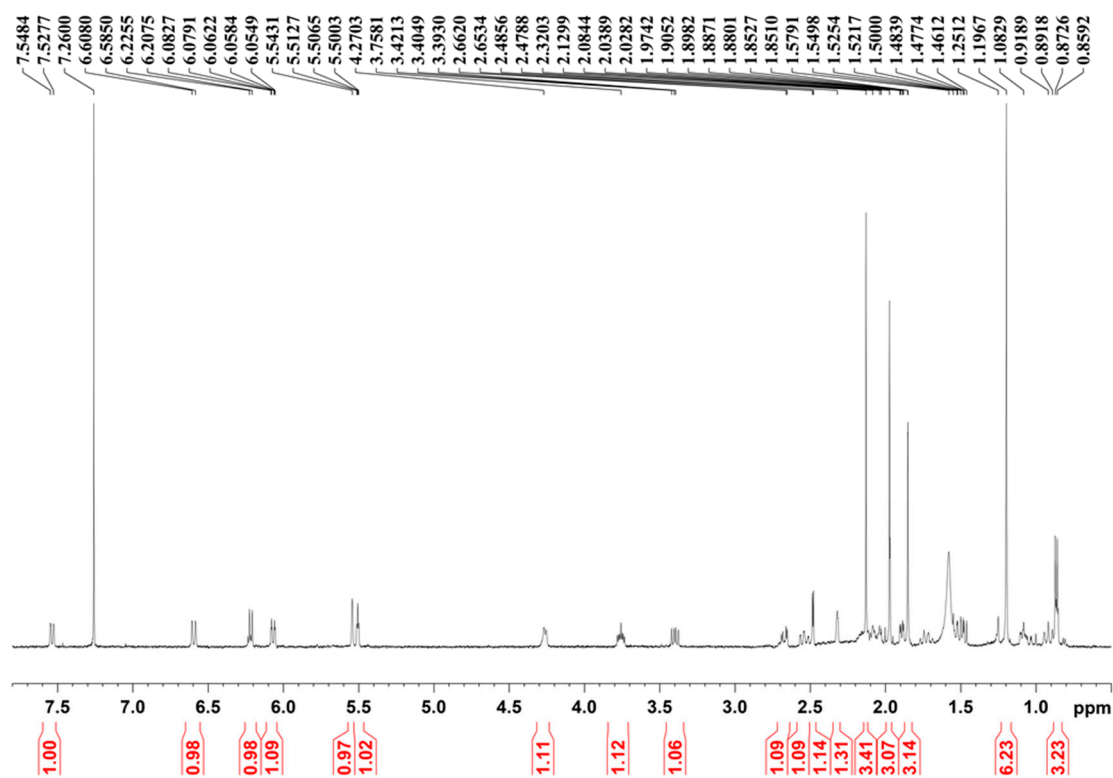


Figure S65. ^1H NMR spectrum of compound 7 in CDCl_3

XSJ-QJZ-17 ^{13}C and DEPT NMR (125 MHz, CDCl_3)

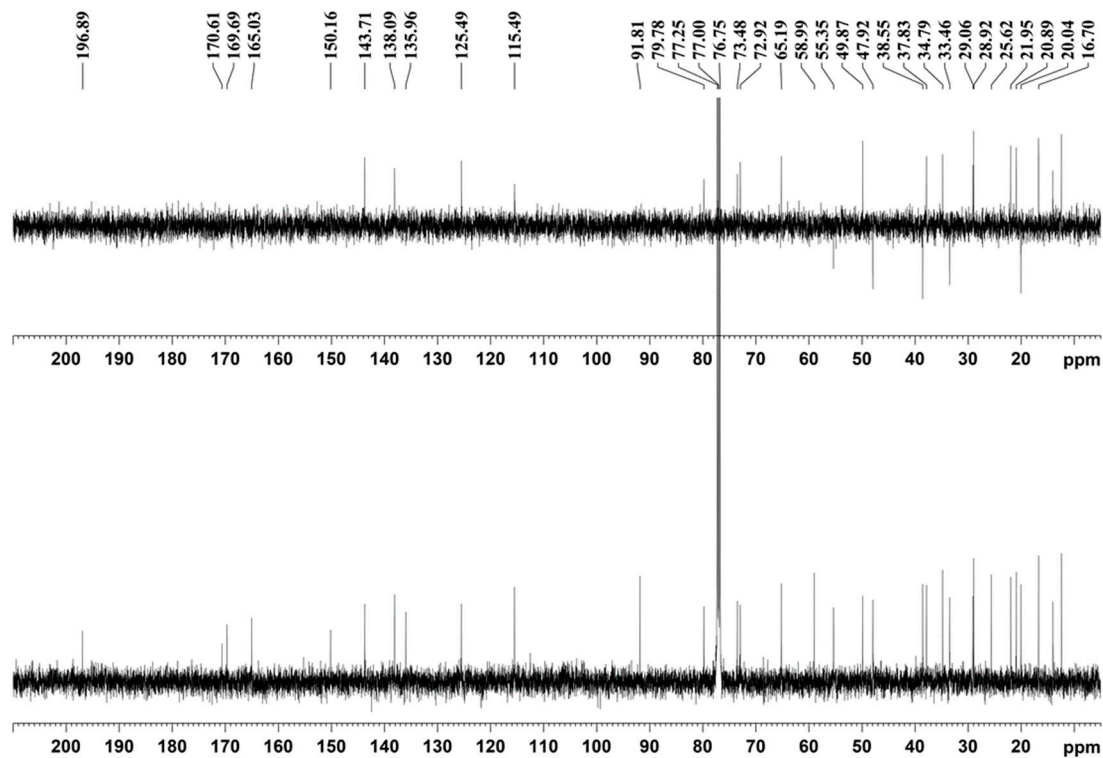


Figure S66. ^{13}C NMR and DEPT spectrum of compound 7 in CDCl_3

XSJ-QJZ-17 1H 1H COSY

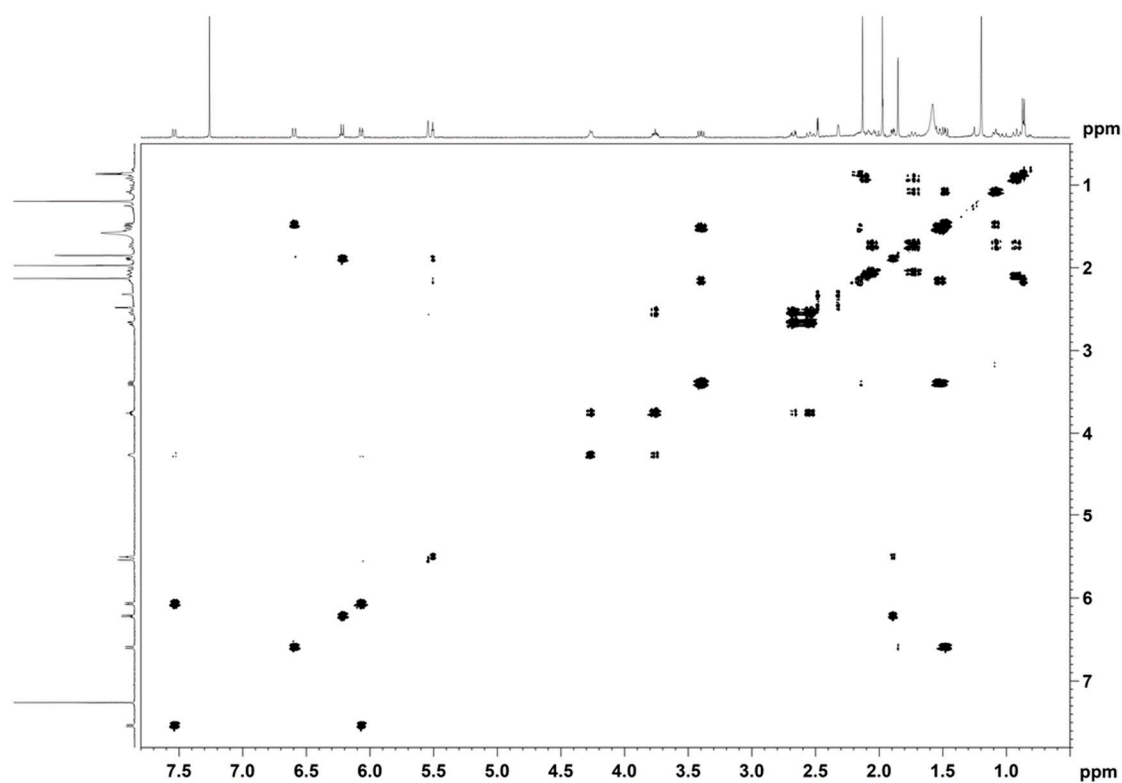


Figure S67. ^1H - ^1H NMR spectrum of compound **7** in CDCl_3

XSJ-QJZ-17 HMBC

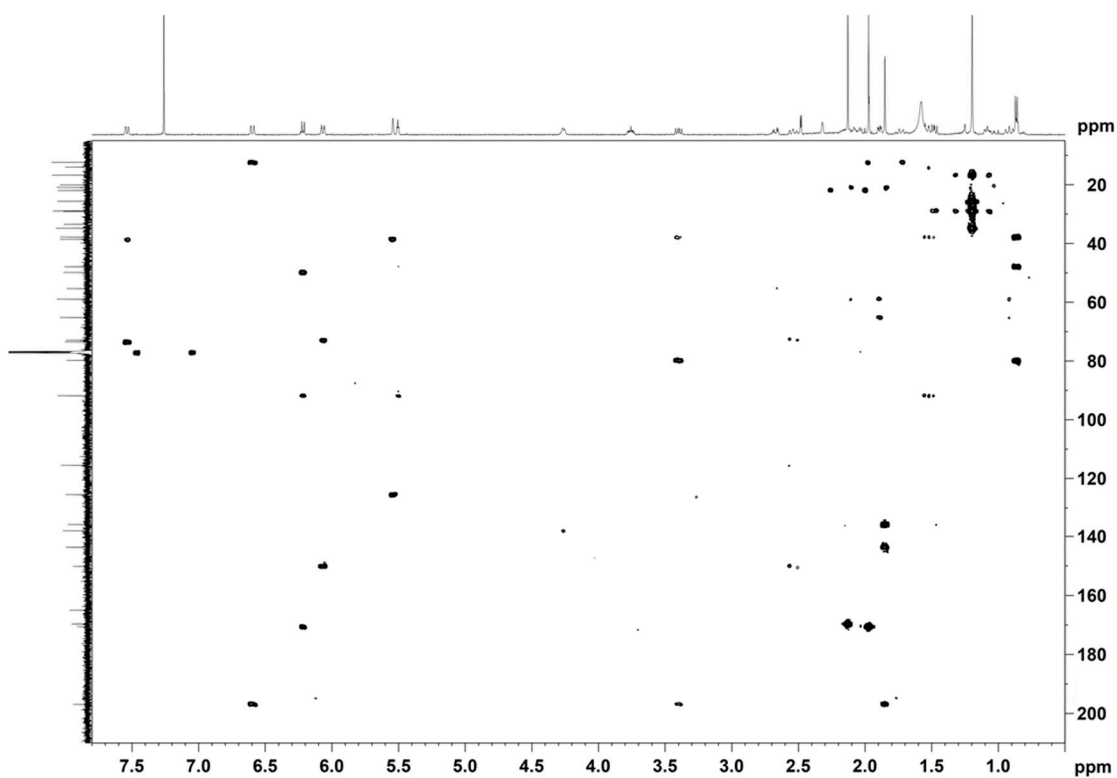


Figure S68. HMBC spectrum of compound **7** in CDCl_3

XSJ-QJZ-17 HSQC

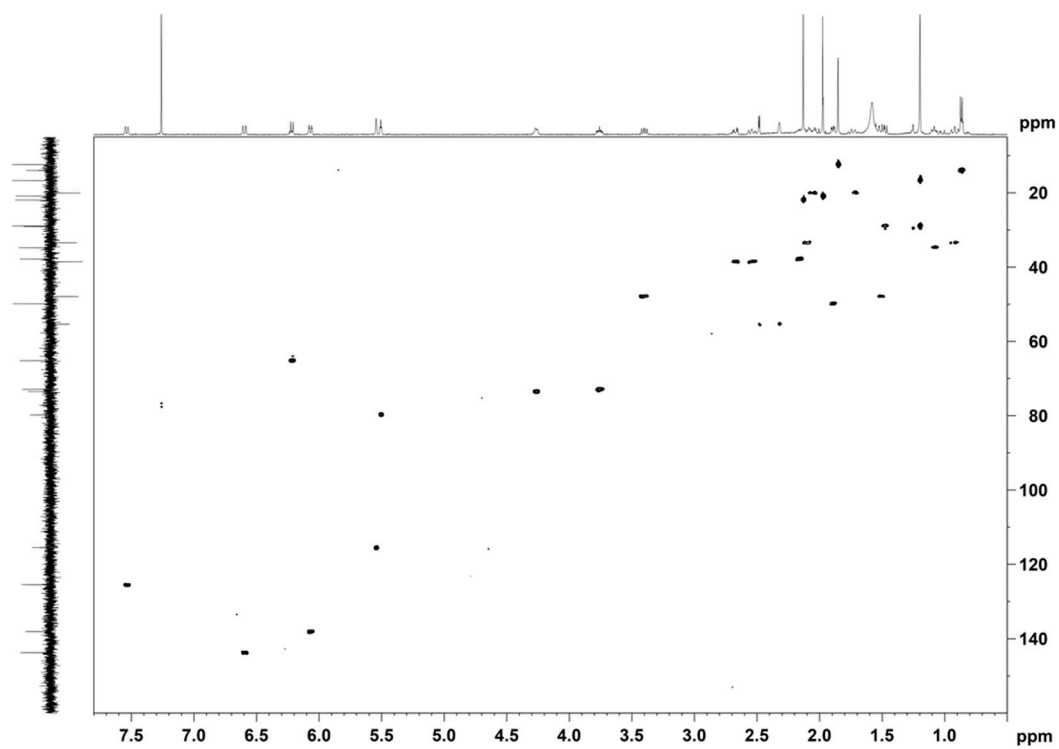


Figure S69. HSQC spectrum of compound **7** in CDCl₃

XSJ-QJZ-17 NOESY

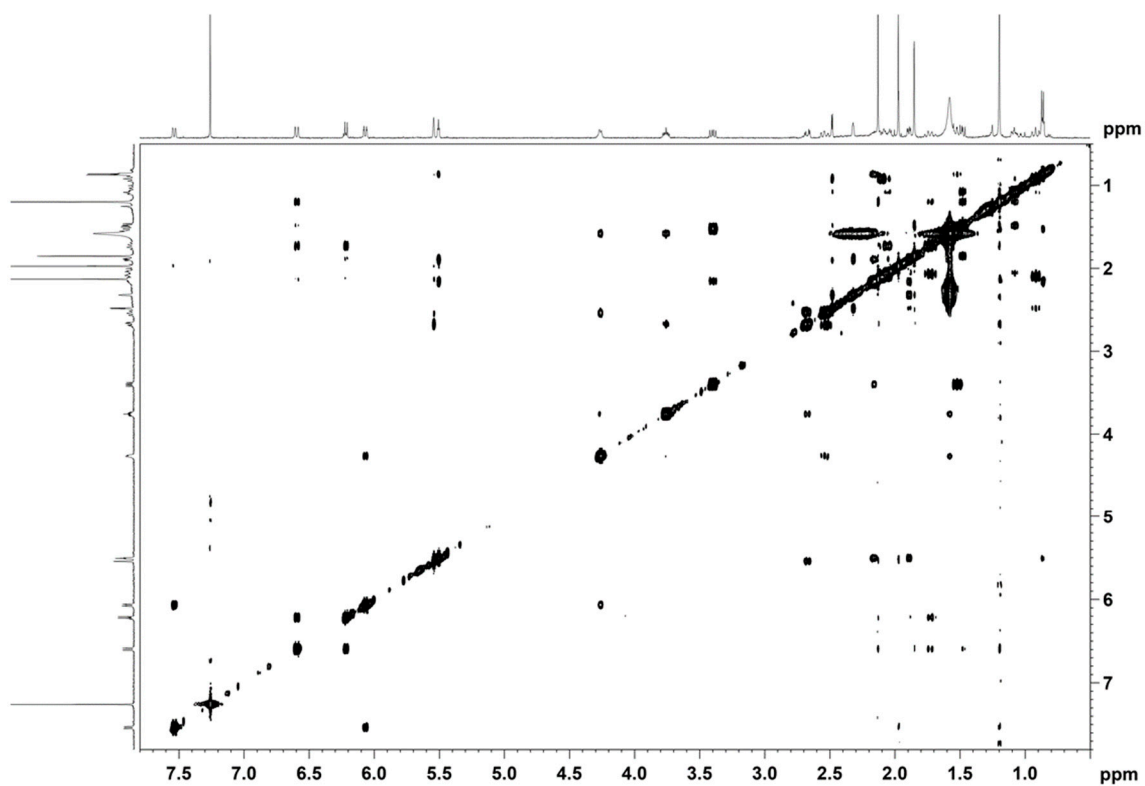
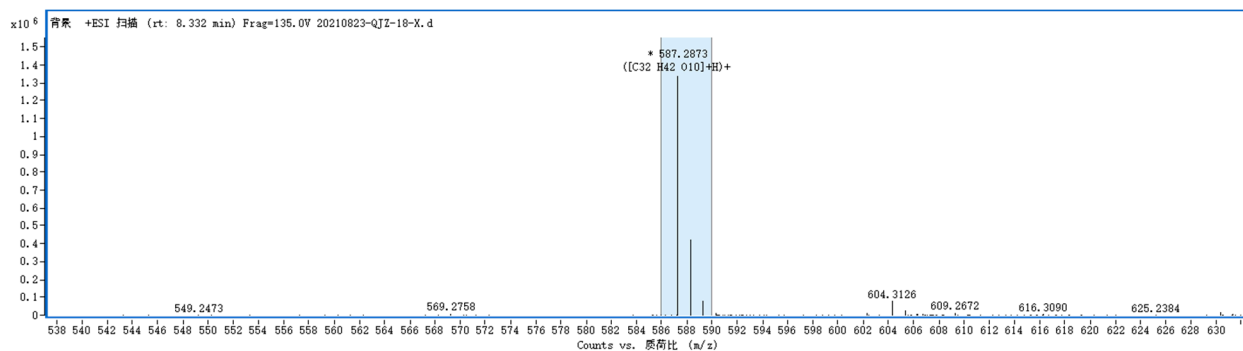


Figure S70. NOESY spectrum of compound **7** in CDCl₃



| Best | Formula(M) | Ion Formula | Tgt (m/z) | m/z | Diff (ppm) |
|------|---|---|-----------|----------|------------|
| TRUE | C ₃₂ H ₄₂ O ₁₀ | C ₃₂ H ₄₃ O ₁₀ | 587.2851 | 587.2873 | 3.75 |

Figure S71. HR-ESI-MS spectrum of compound **8**

Rudolph Research Analytical

Saturday, 10/09/2021

This sample was measured on an Autopol VI, serial number 90079, manufactured by Rudolph Research Analytical, Hackettstown, NJ.

LotID : QJZ-18
Set Temperature : 20.0
Temp Corr : OFF

| n | Average | Std.Dev. | Maximum | Minimum | | | | | | |
|------|-----------|-------------|---------|---------|----------|-----|--------|-------|-------|---------|
| 6 | 90.833 | 0.0000 | 90.833 | 90.833 | | | | | | |
| S.No | Sample ID | Time | Result | Scale | OR ° Arc | WLG | Lg.mm | Conc. | Temp. | Comment |
| 1 | QJZ-18 | 04:25:19 PM | 90.833 | SR | 0.109 | 589 | 100.00 | 0.120 | 20.2 | |
| 2 | QJZ-18 | 04:25:27 PM | 90.833 | SR | 0.109 | 589 | 100.00 | 0.120 | 20.1 | |
| 3 | QJZ-18 | 04:25:34 PM | 90.833 | SR | 0.109 | 589 | 100.00 | 0.120 | 20.1 | |
| 4 | QJZ-18 | 04:25:42 PM | 90.833 | SR | 0.109 | 589 | 100.00 | 0.120 | 20.1 | |
| 5 | QJZ-18 | 04:25:49 PM | 90.833 | SR | 0.109 | 589 | 100.00 | 0.120 | 20.1 | |
| 6 | QJZ-18 | 04:25:56 PM | 90.833 | SR | 0.109 | 589 | 100.00 | 0.120 | 20.0 | |

Signature

Figure S72. OR value of compound **8** in MeOH

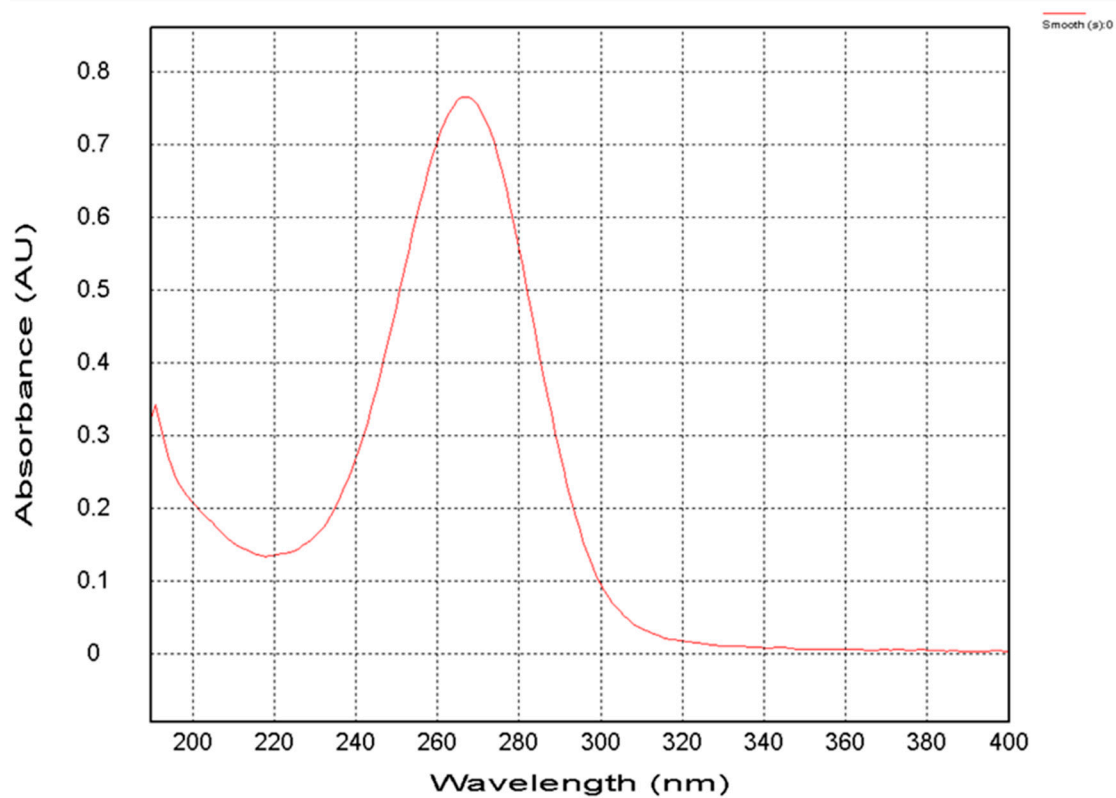


Figure S73. UV spectrum of compound **8** in MeOH

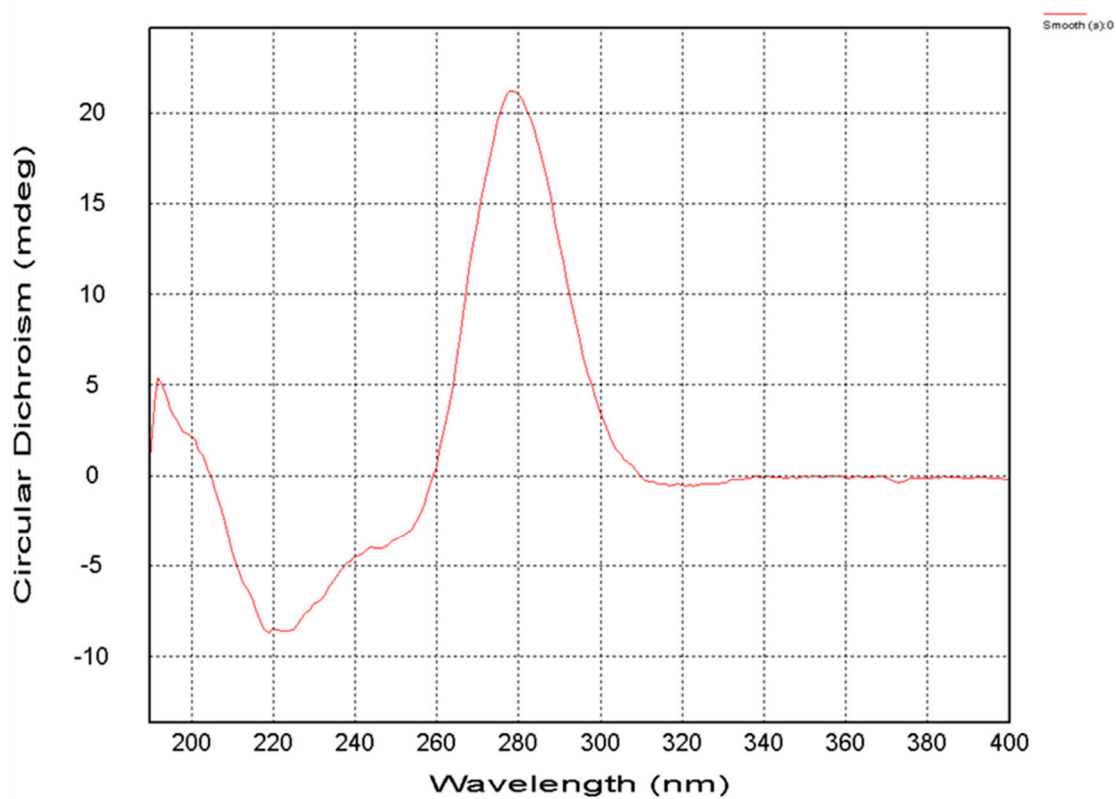


Figure S74. CD spectrum of compound **8** in MeOH

XSJ-QJZ-18 ¹H NMR (500 MHz, CDCl₃)

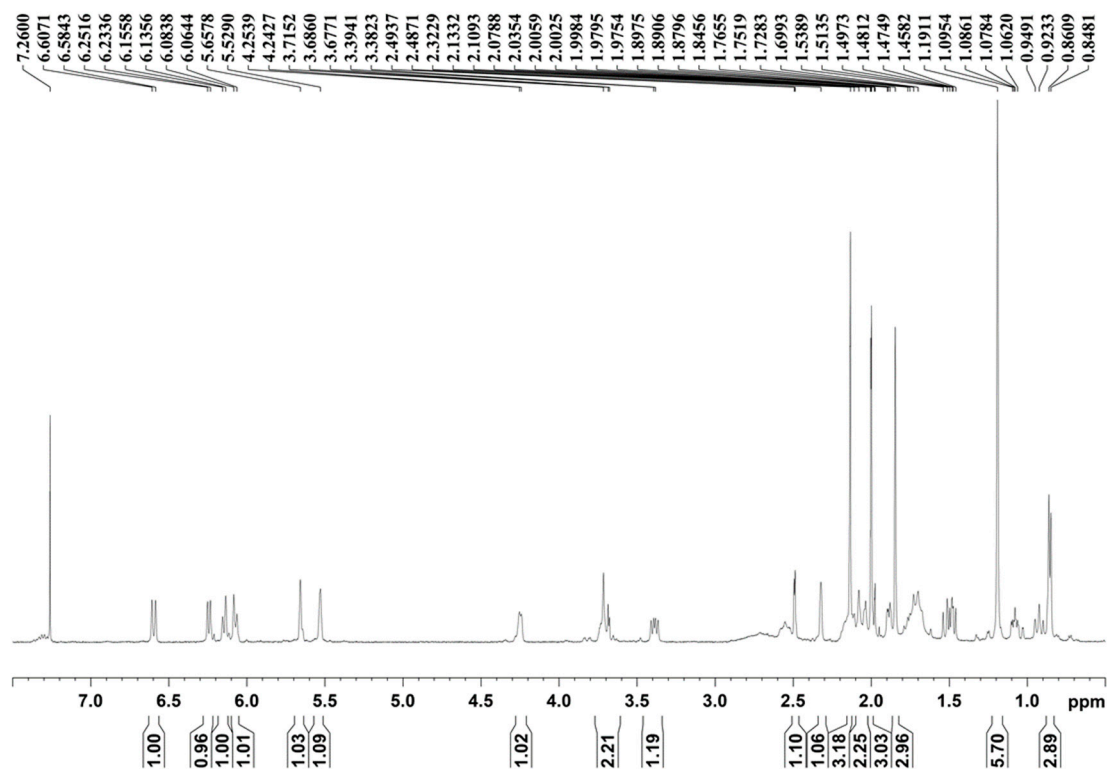


Figure S75. ¹H NMR spectrum of compound **8** in CDCl₃

XSJ-QJZ-18 C13 and DEPT NMR (125 MHz, CDCl₃)

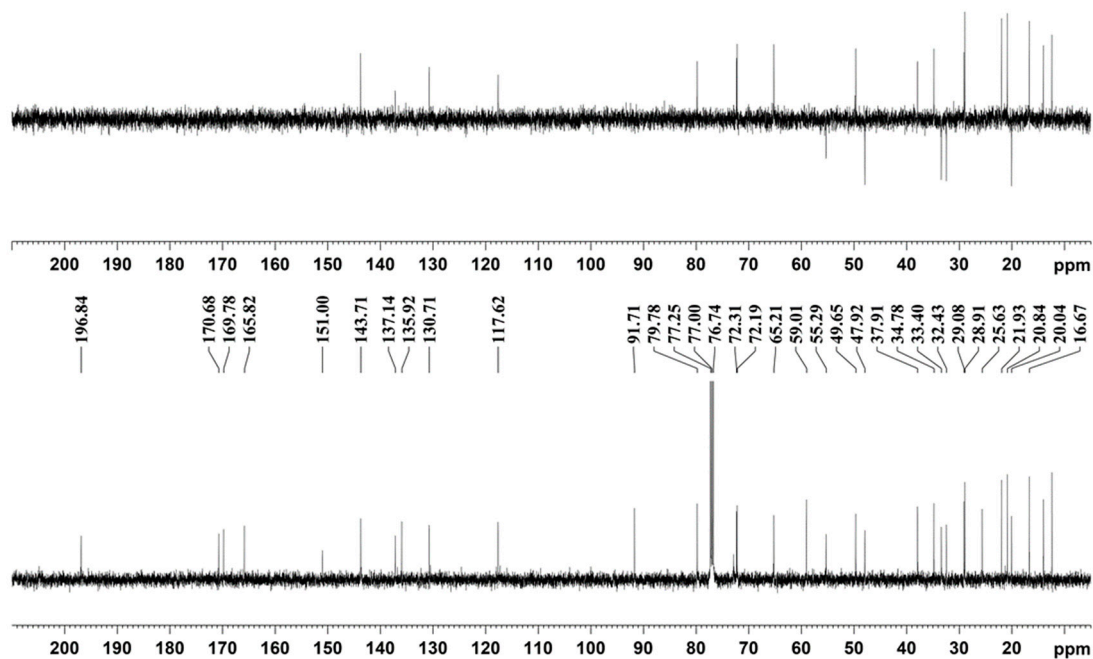


Figure S76. ¹³C NMR and DEPT spectrum of compound **8** in CDCl₃

XSJ-QJZ-18 1H 1H COSY

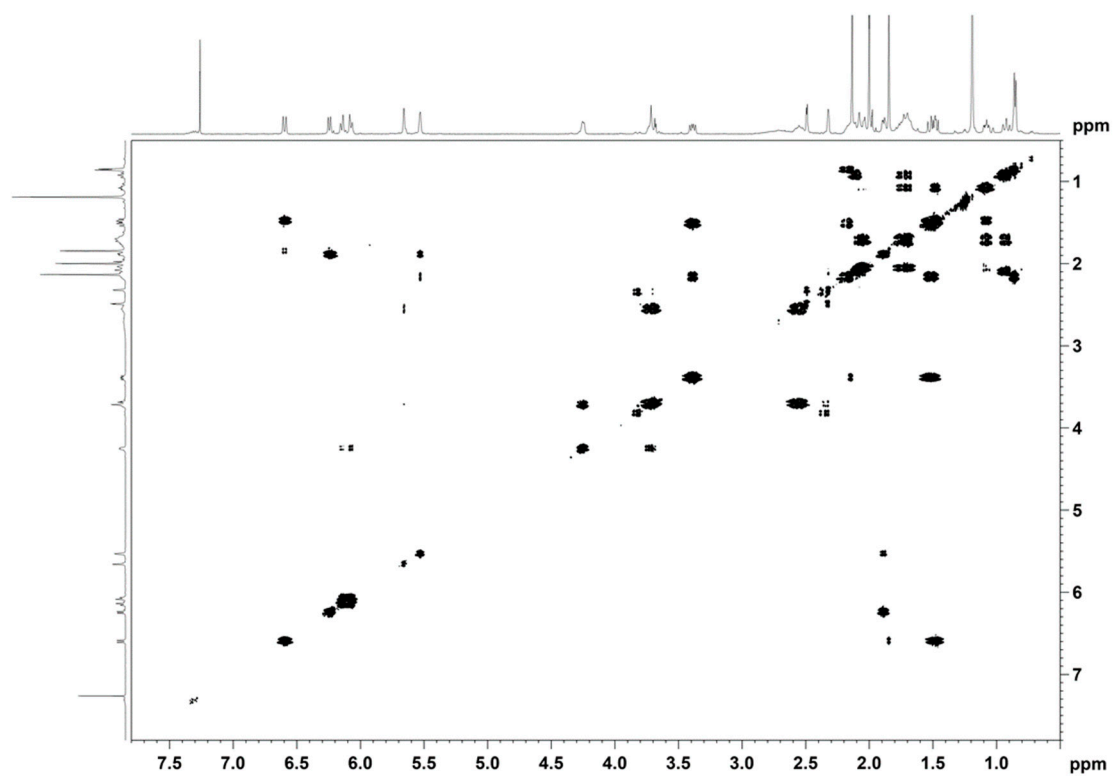


Figure S77. ¹H-¹H NMR spectrum of compound **8** in CDCl₃

XSJ-QJZ-18 HMBC

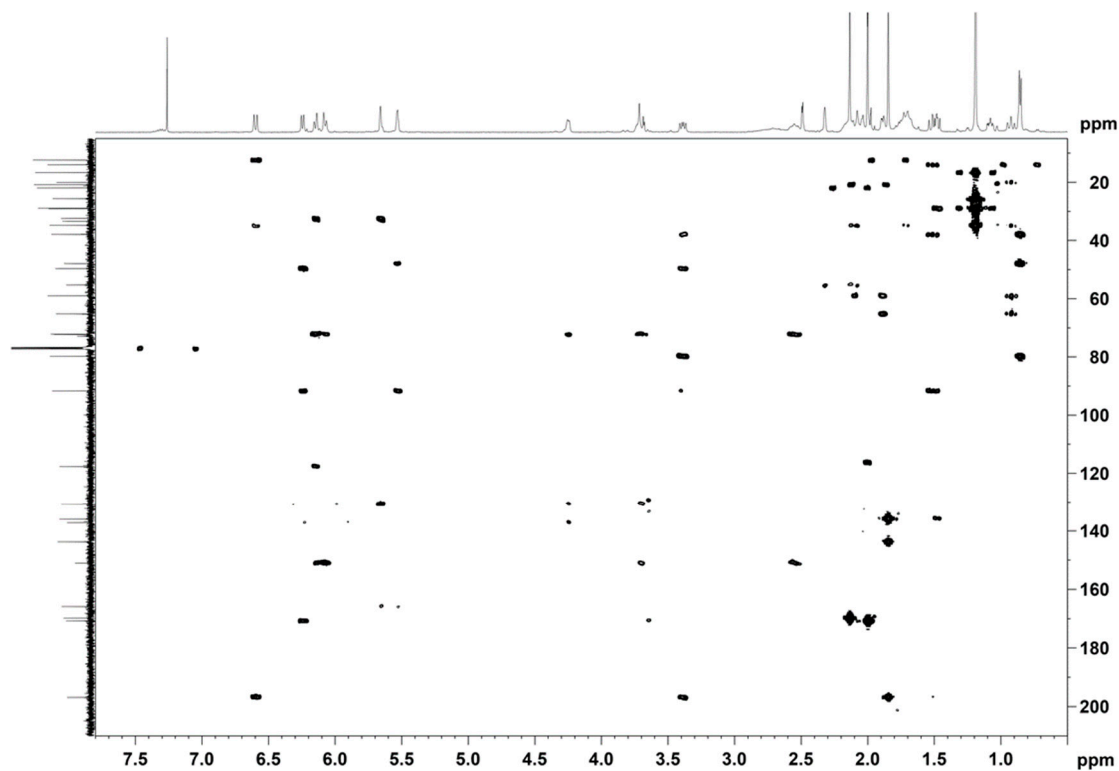


Figure S78. HMBC spectrum of compound **8** in CDCl₃

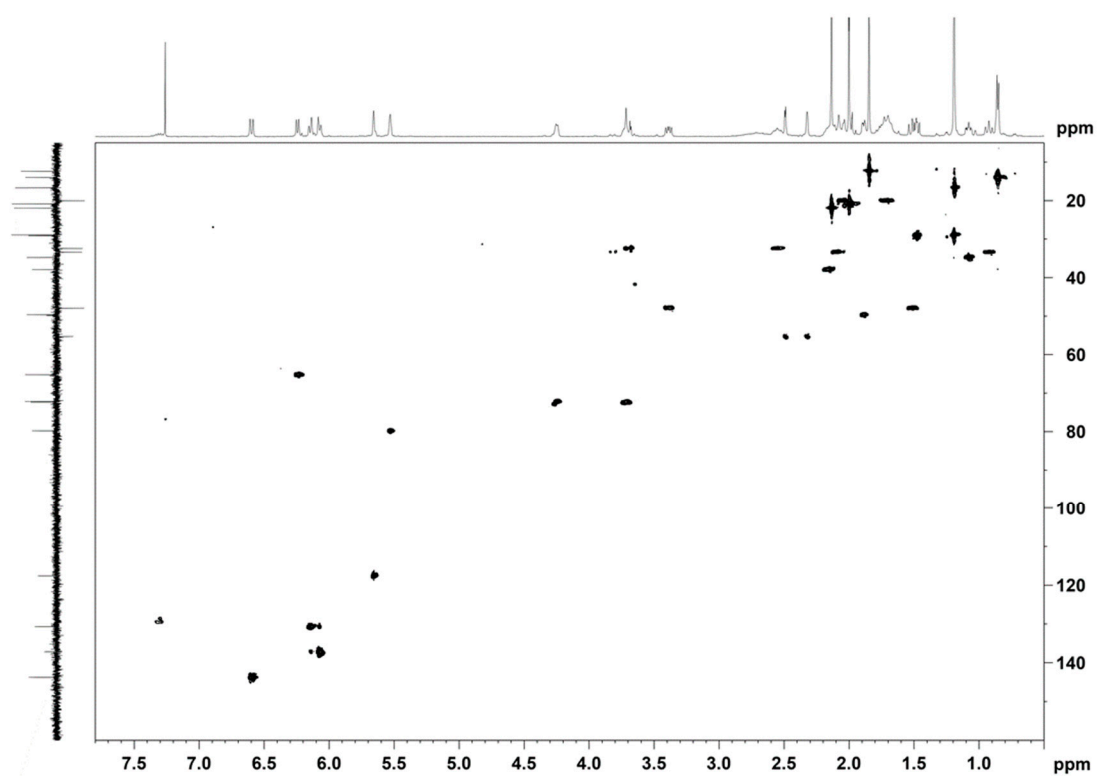


Figure S79. HSQC spectrum of compound **8** in CDCl₃

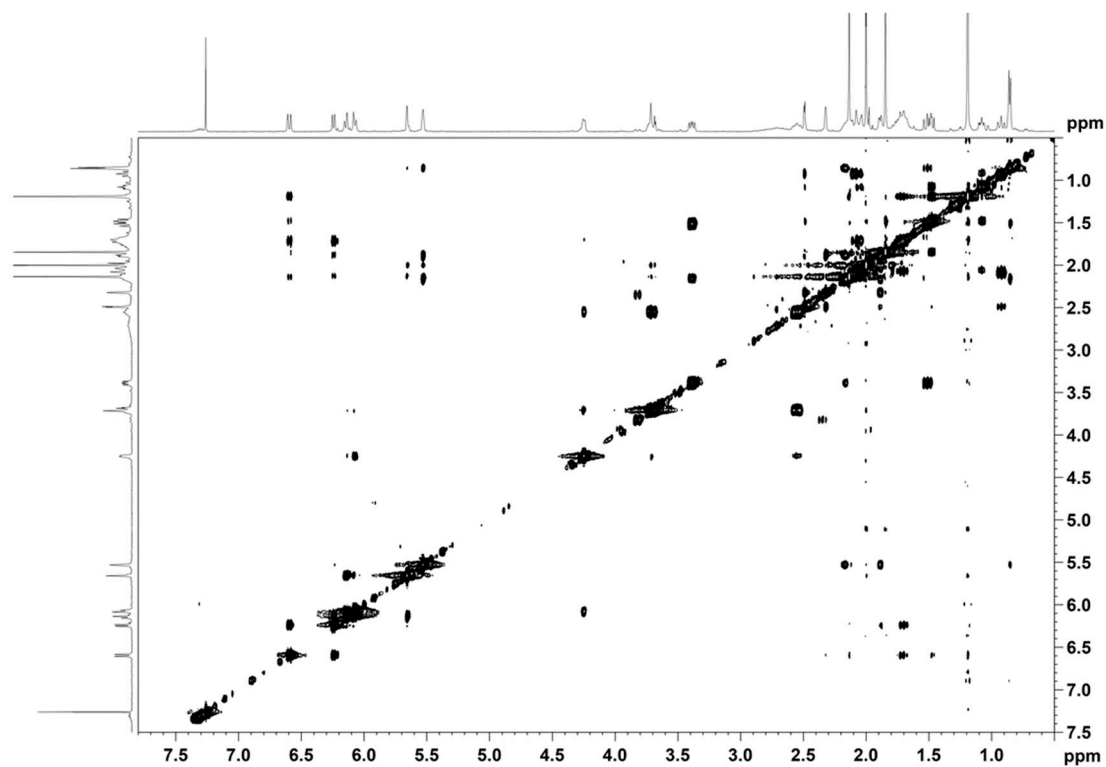
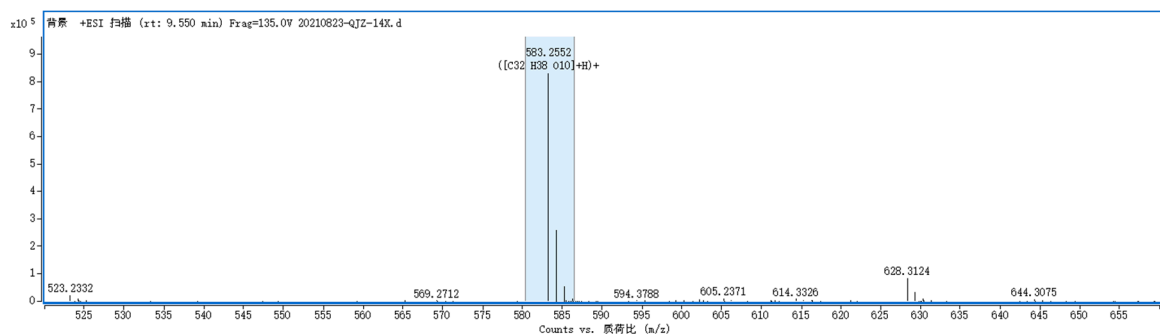


Figure S80. NOESY spectrum of compound **8** in CDCl₃



| Best | Formula(M) | Ion Formula | Tgt (m/z) | m/z | Diff (ppm) |
|------|---|---|-----------|----------|------------|
| TRUE | C ₃₂ H ₃₈ O ₁₀ | C ₃₂ H ₃₉ O ₁₀ | 583.2538 | 583.2552 | 2.40 |

Figure S81. HRESIMS spectrum of compound **9**

Rudolph Research Analytical

Saturday, 10/09/2021

This sample was measured on an Autopol VI, serial number 90079, manufactured by Rudolph Research Analytical, Hackettstown, NJ.

LotID : QJZ-14
Set Temperature : 20.0
Temp Corr : OFF

| n | Average | Std.Dev. | Maximum | Minimum | | | | | | |
|------|-----------|-------------|---------|---------|----------|-----|--------|-------|-------|---------|
| 6 | 77.778 | 0.3833 | 78.049 | 77.236 | | | | | | |
| S.No | Sample ID | Time | Result | Scale | OR ° Arc | WLG | Lg.mm | Conc. | Temp. | Comment |
| 1 | QJZ-14 | 04:47:14 PM | 77.236 | SR | 0.095 | 589 | 100.00 | 0.123 | 20.1 | |
| 2 | QJZ-14 | 04:47:22 PM | 78.049 | SR | 0.096 | 589 | 100.00 | 0.123 | 20.1 | |
| 3 | QJZ-14 | 04:47:29 PM | 77.236 | SR | 0.095 | 589 | 100.00 | 0.123 | 20.1 | |
| 4 | QJZ-14 | 04:47:37 PM | 78.049 | SR | 0.096 | 589 | 100.00 | 0.123 | 20.0 | |
| 5 | QJZ-14 | 04:47:45 PM | 78.049 | SR | 0.096 | 589 | 100.00 | 0.123 | 20.0 | |
| 6 | QJZ-14 | 04:47:52 PM | 78.049 | SR | 0.096 | 589 | 100.00 | 0.123 | 20.0 | |

Signature

Figure S82. OR value of compound **9** in MeOH

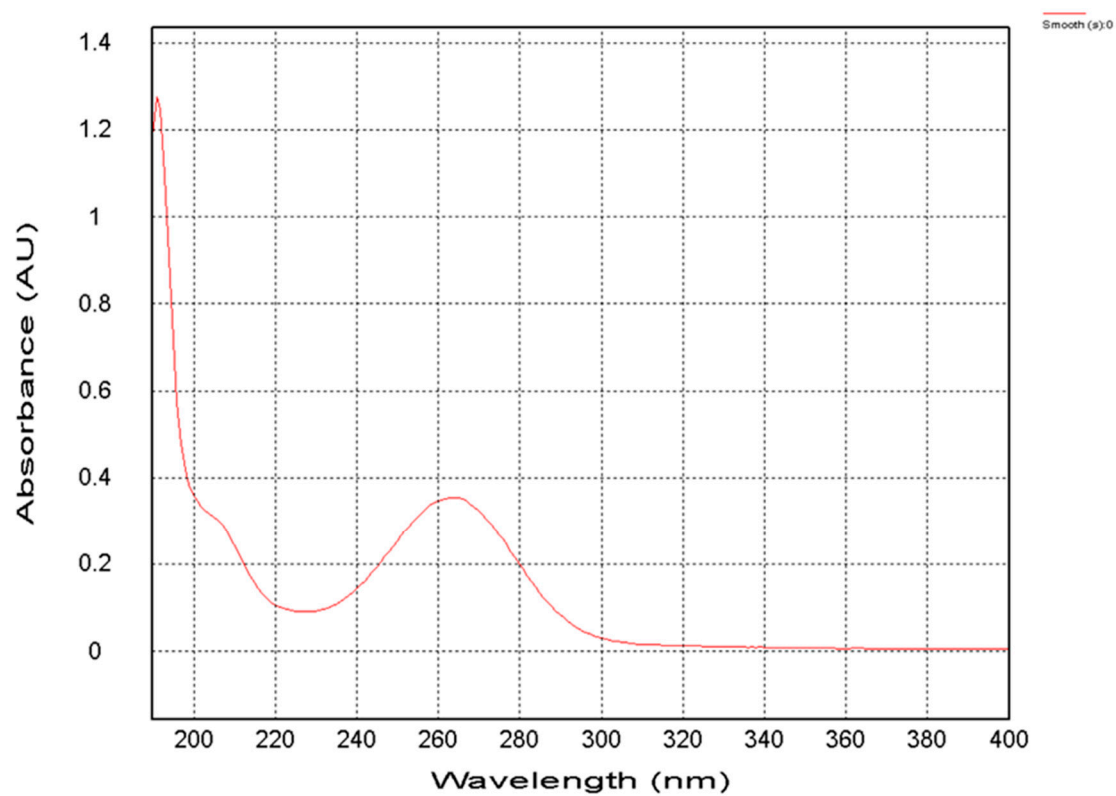


Figure S83. UV spectrum of compound **9** in MeOH

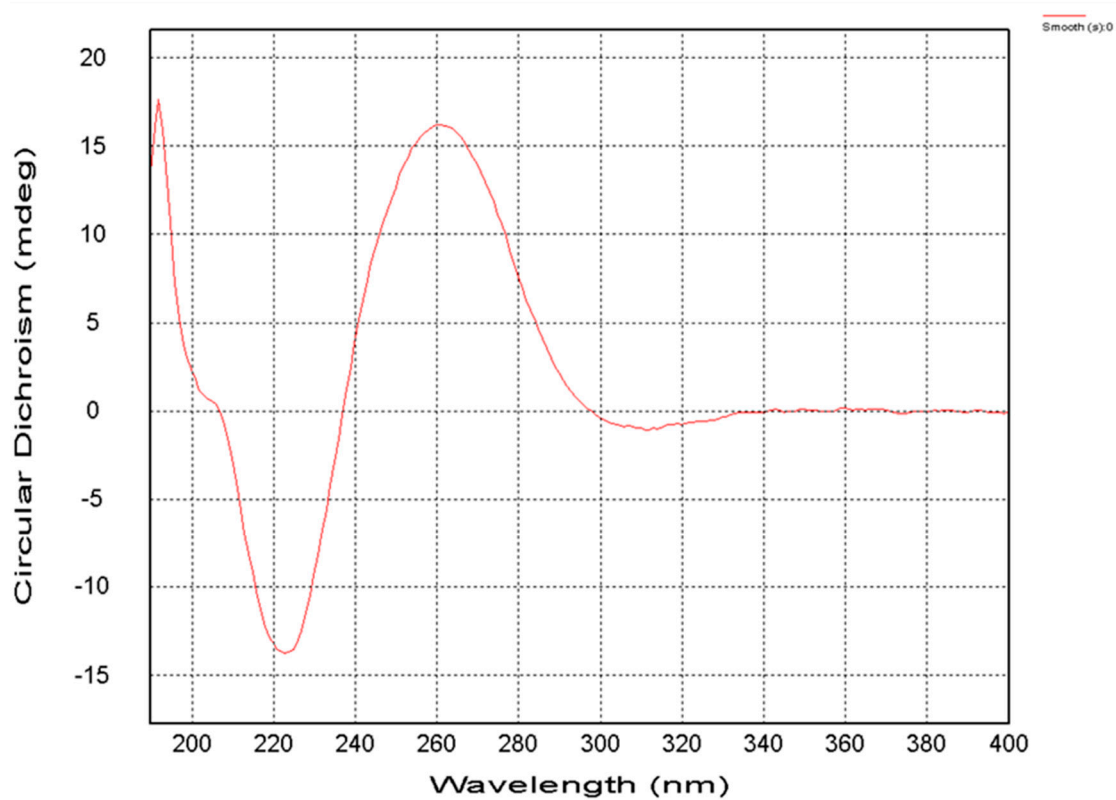


Figure S84. CD spectrum of compound **9** in MeOH

XSJ-QJZ-14 ^1H NMR (500 MHz, CDCl_3)

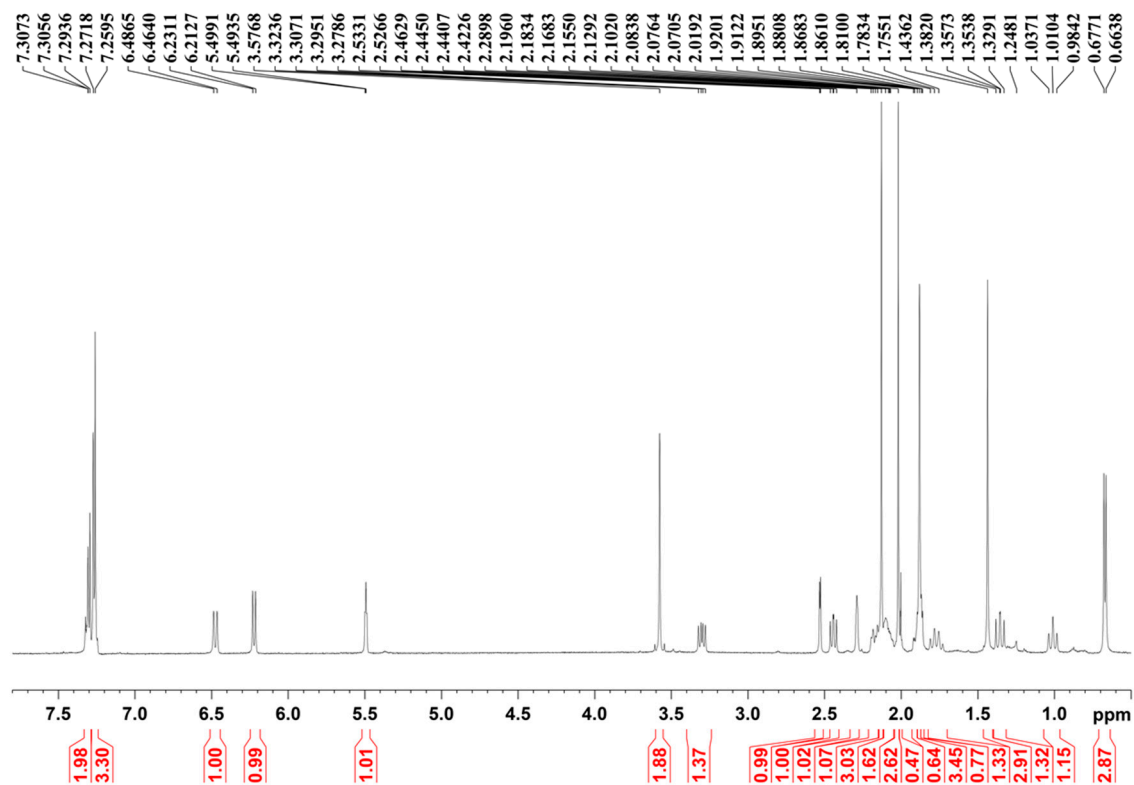


Figure S85. ^1H NMR spectrum of compound **9** in CDCl_3

XSJ-QJZ-14 ^{13}C and DEPT NMR (125 MHz, CDCl_3)

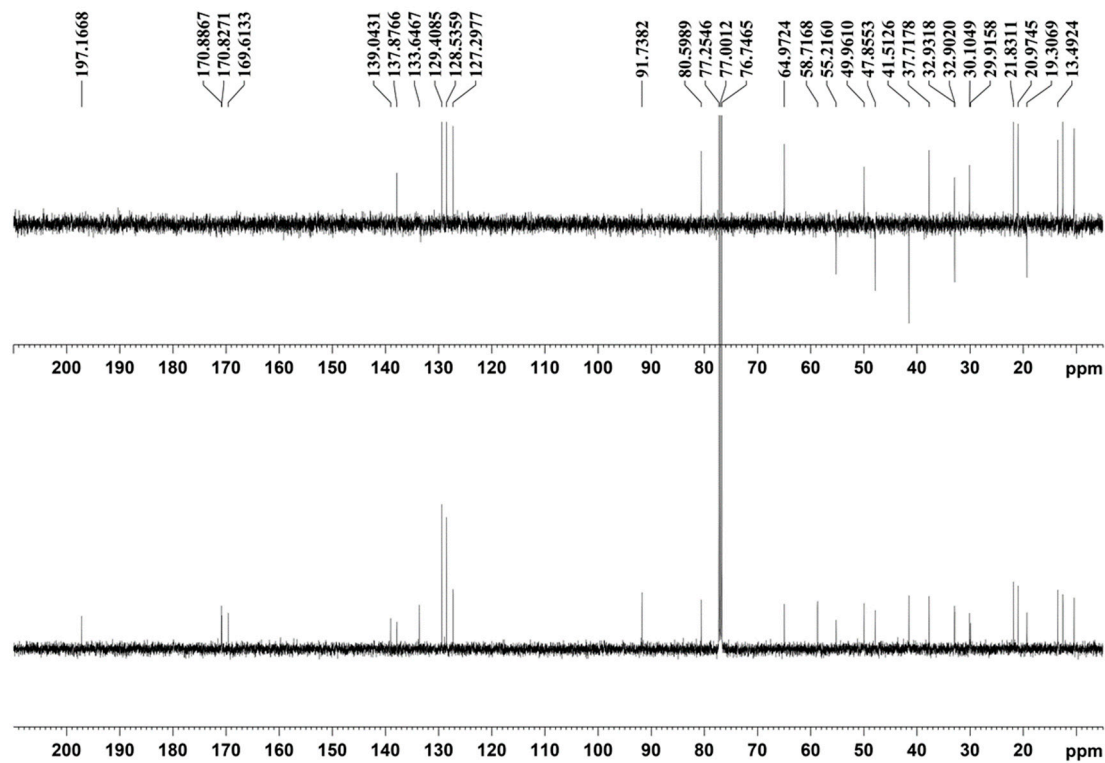


Figure S86. ^{13}C NMR and DEPT spectrum of compound **9** in CDCl_3