# Isolation of Lobane and Prenyleudesmane Diterpenoids from the Soft Coral *Lobophytum varium*

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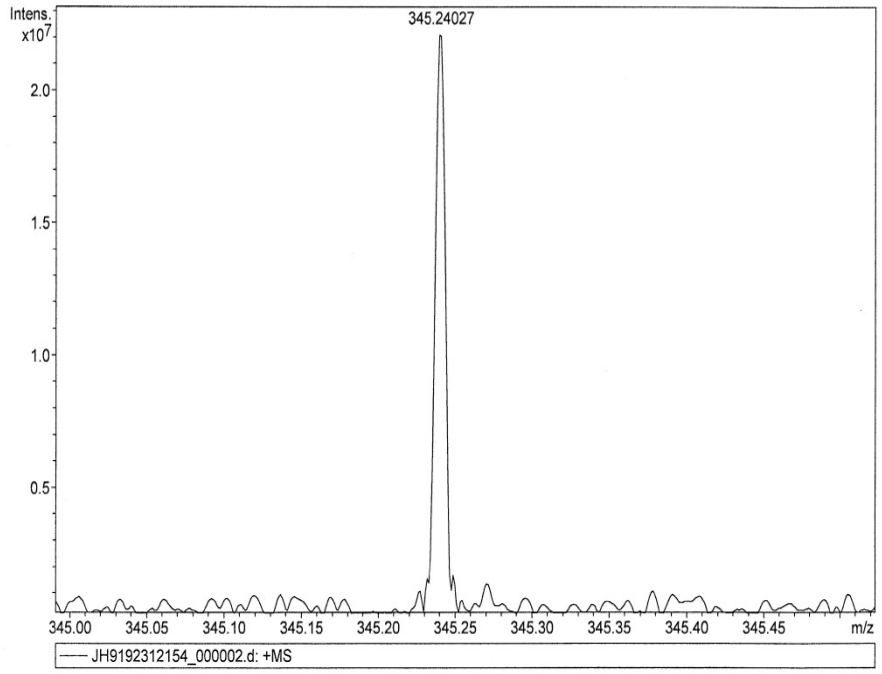
† These authors contributed equally to this work




| Meas. m/z | # | Formula | Score | m/z | err [mDa] | err [ppm] | mSigma | rdb | e⁻ Conf | N-Rule |
|---|---|---|---|---|---|---|---|---|---|---|
| 345.24027 | 1 | C 20 H 34 Na O 3 | 100.00 | 345.24002 | -0.25 | -0.73 | 18.4 | 3.5 | even | ok |

**Figure S1.** HRESIMS spectrum of **1**.

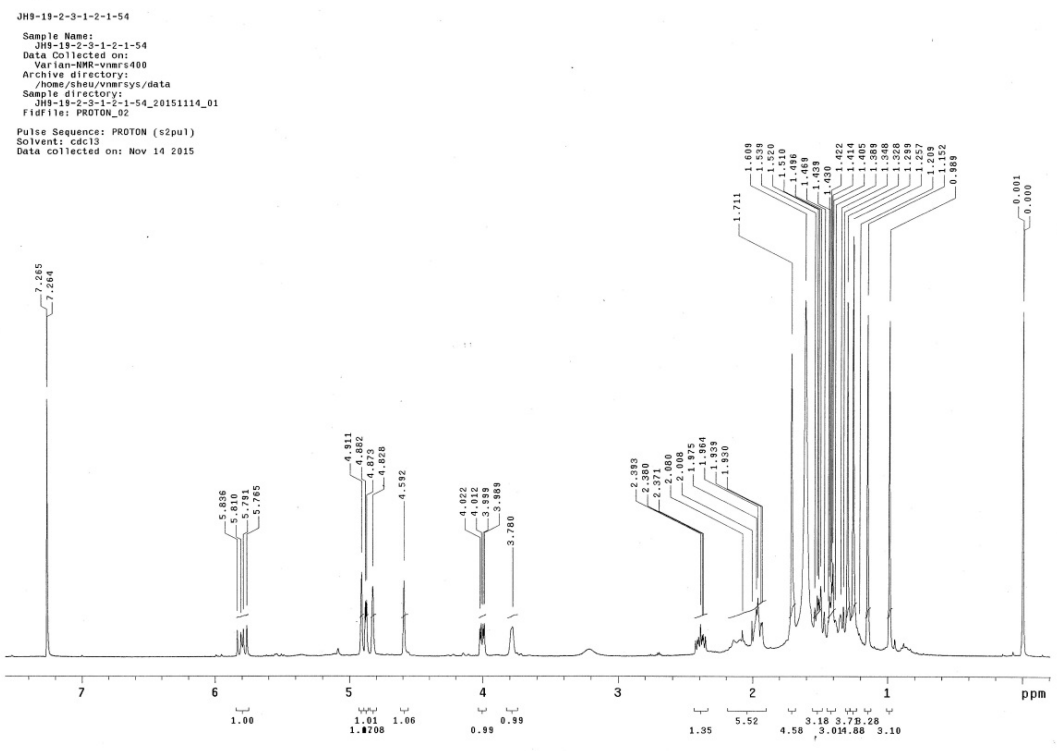



**Figure S2.** $^{1}$H NMR spectrum of **1** in $CDCl_3$ at 400 MHz

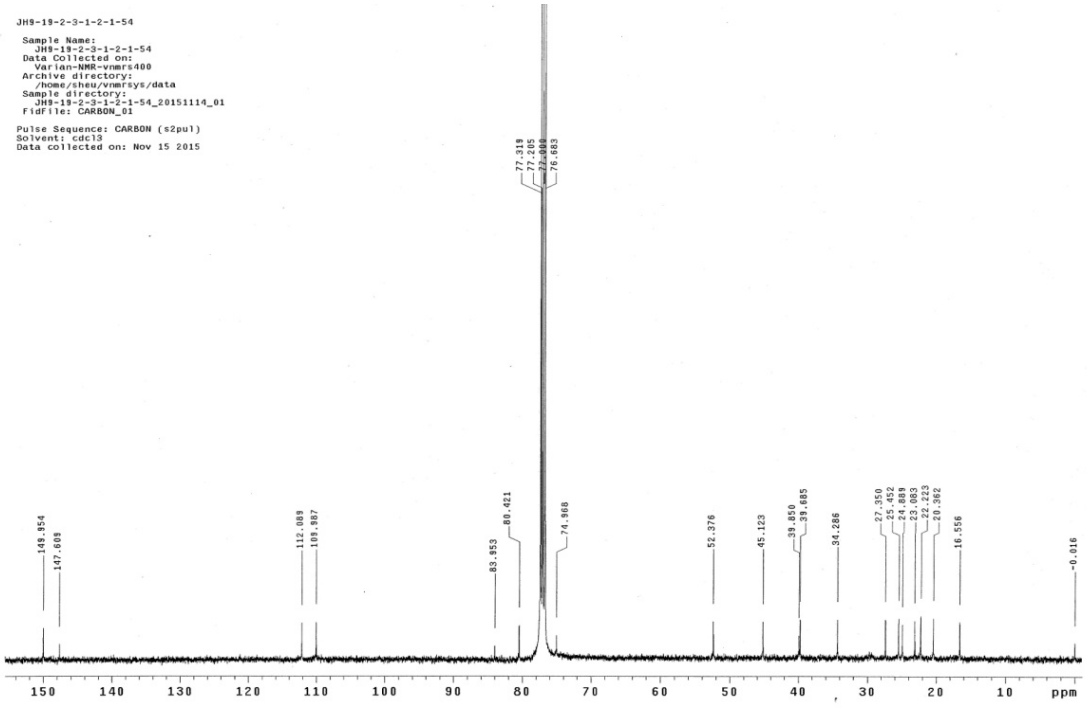



**Figure S3.** $^{13}$C NMR spectrum of **1** in $CDCl_3$ at 100 MHz.

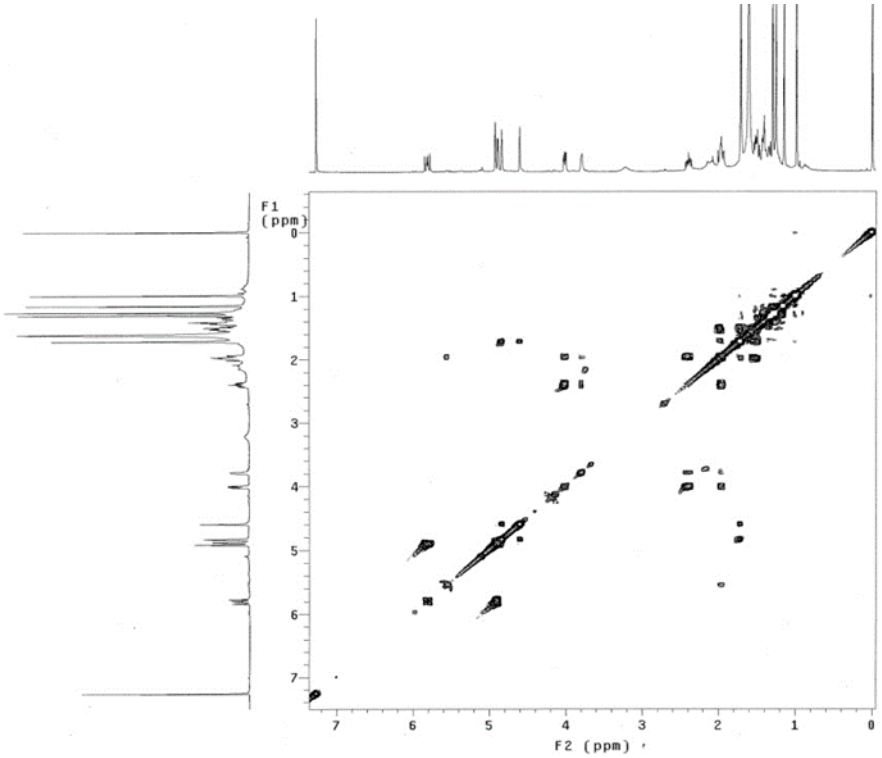



**Figure S4.** $^{1}$H-$^{1}$H COSY spectrum of **1** in $CDCl_3$.

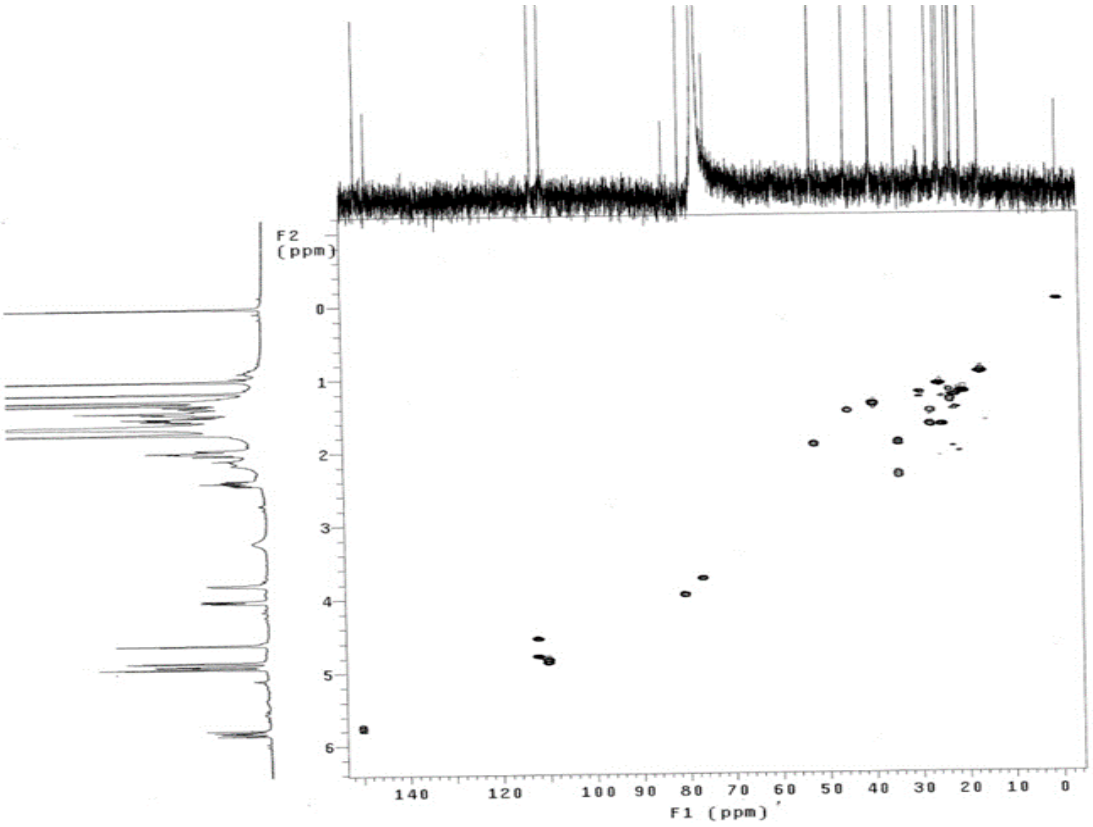



**Figure S5.** HSQC spectrum of **1** in $CDCl_3$.

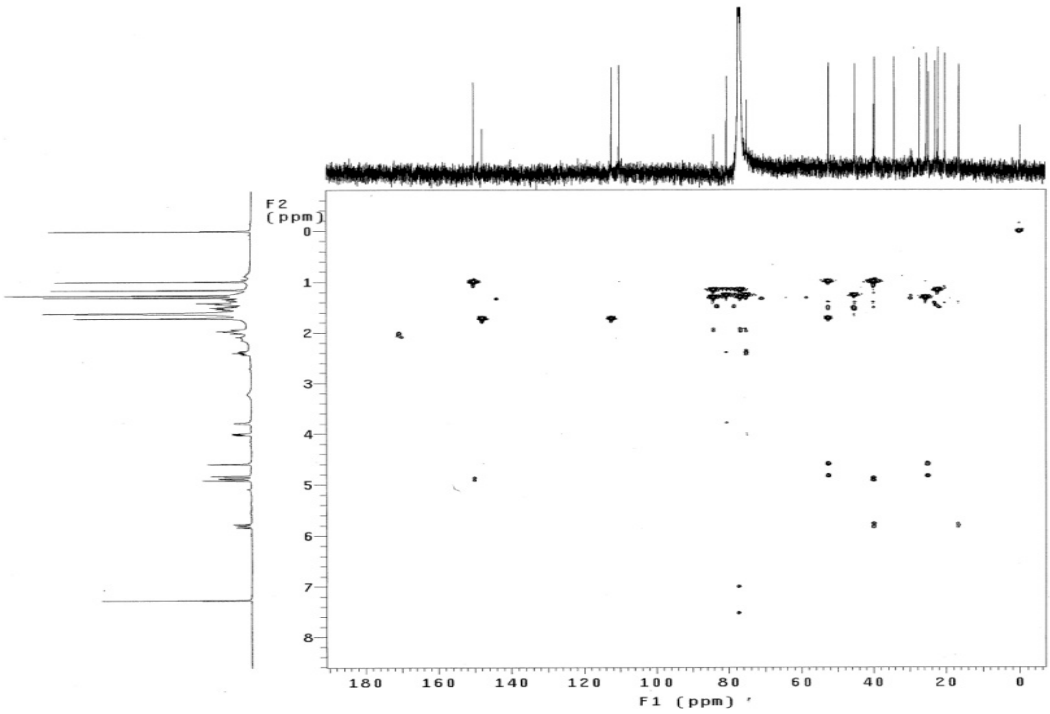



**Figure S6.** HMBC spectrum of **1** in $CDCl_3$.

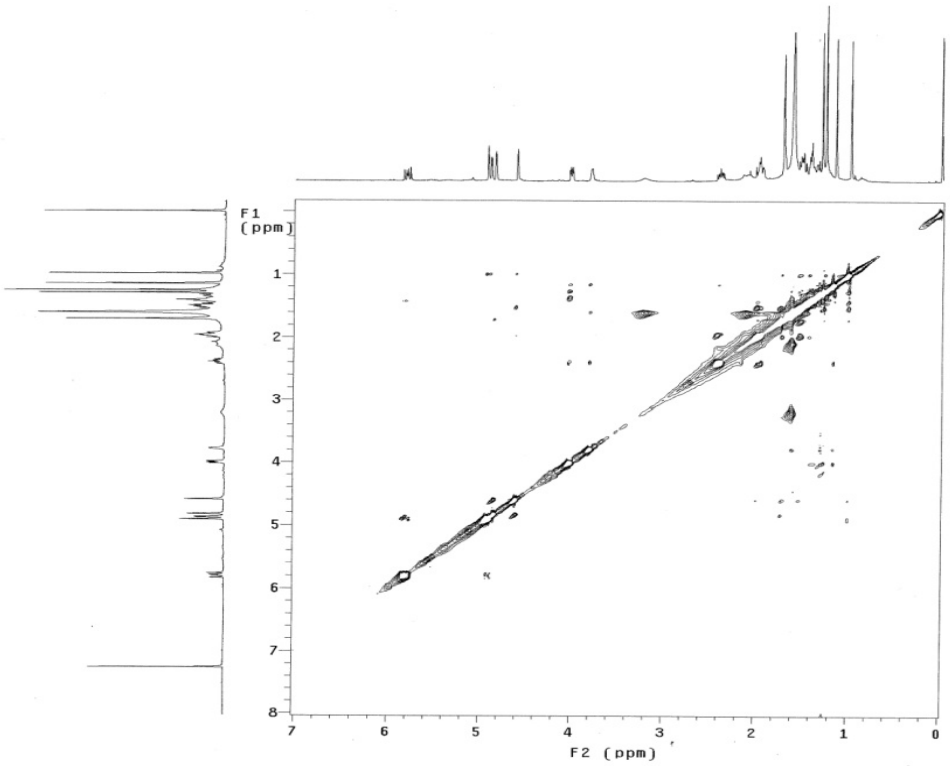



**Figure S7.** NOESY spectrum of **1** in $CDCl_3$.

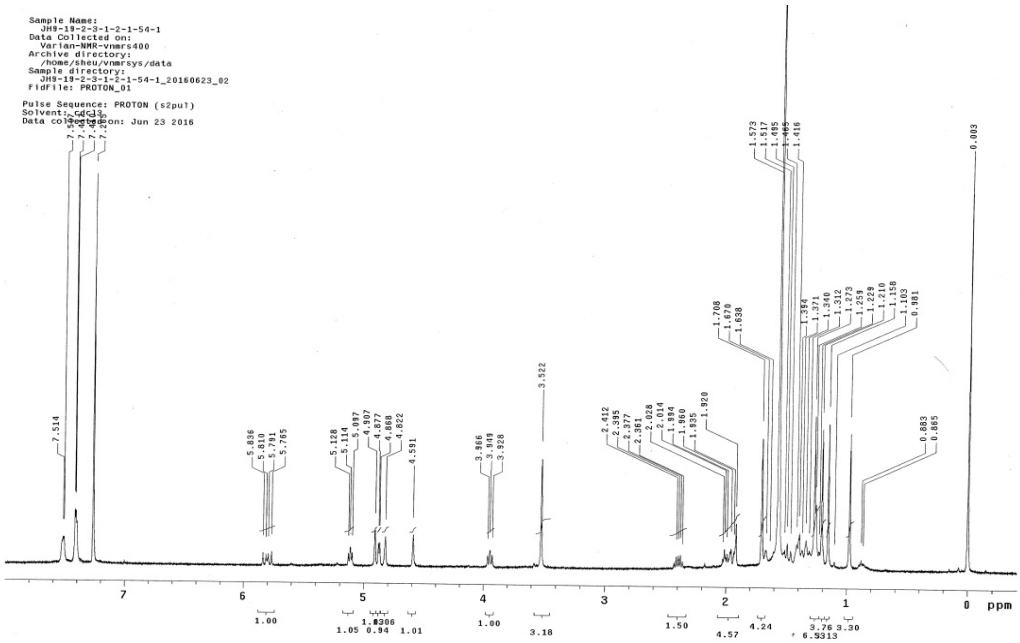



**Figure S8.** $^1$H NMR spectrum of (*S*)-MTPA ester of **1** (**1a)** in $CDCl_3$ at 400 MHz.

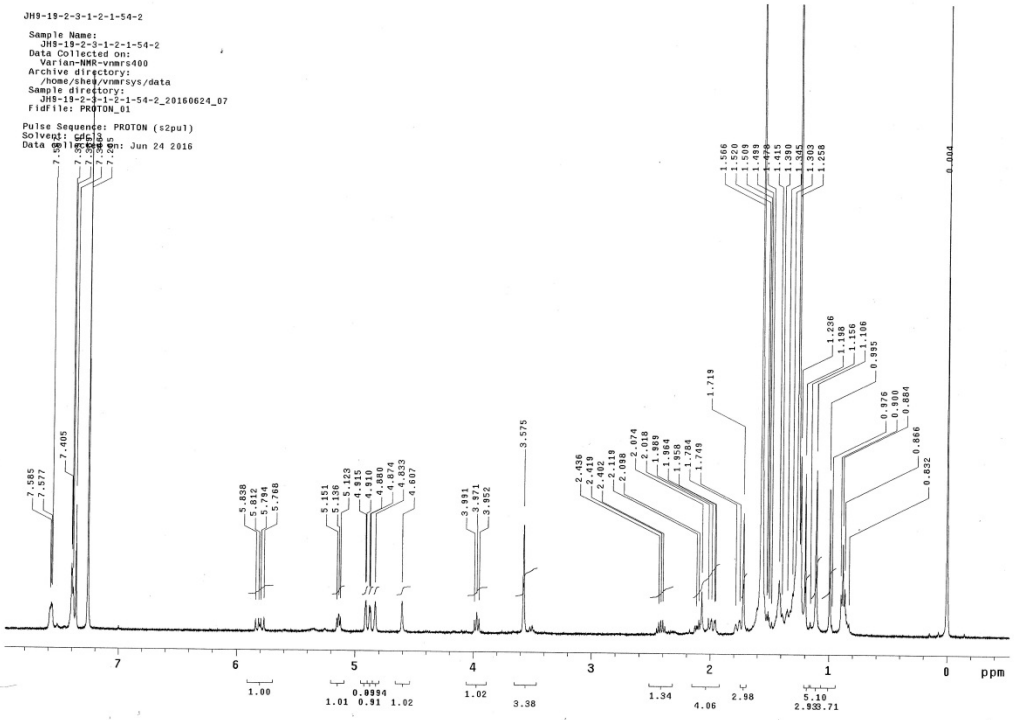
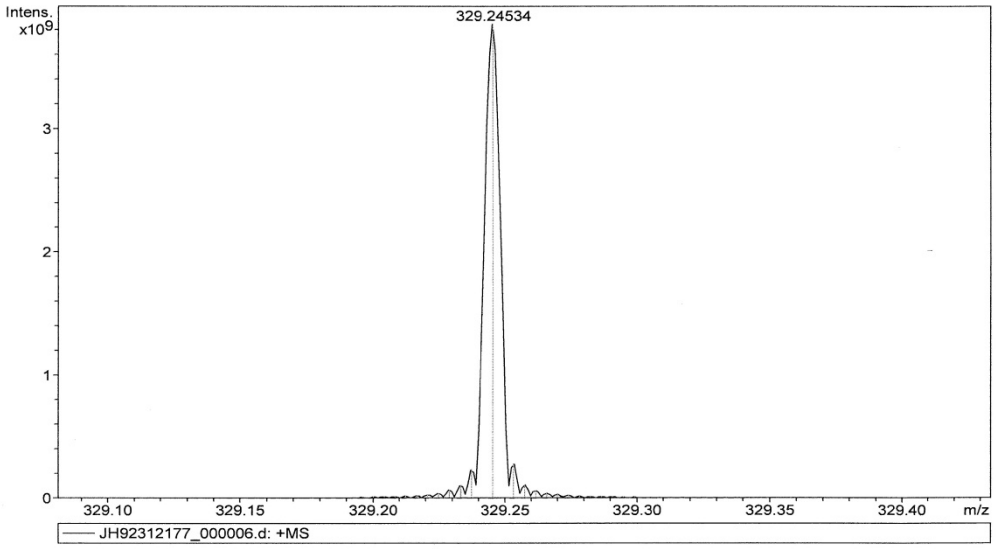



**Figure S9.** $^{1}$H NMR spectrum of (*R*)-MTPA ester of **1** (**1b)** in $CDCl_3$ at 400 MHz.

**Figure S10.** HRESIMS spectrum of **2**.




| Meas. m/z | # | Formula | Score | m/z | err [mDa] | err [ppm] | mSigma | rdb | e⁻ Conf | N-Rule |
|---|---|---|---|---|---|---|---|---|---|---|
| 329.24534 | 1 | C 20 H 34 Na O 2 | 100.00 | 329.24510 | -0.24 | -0.73 | 2.7 | 3.5 | even | ok |

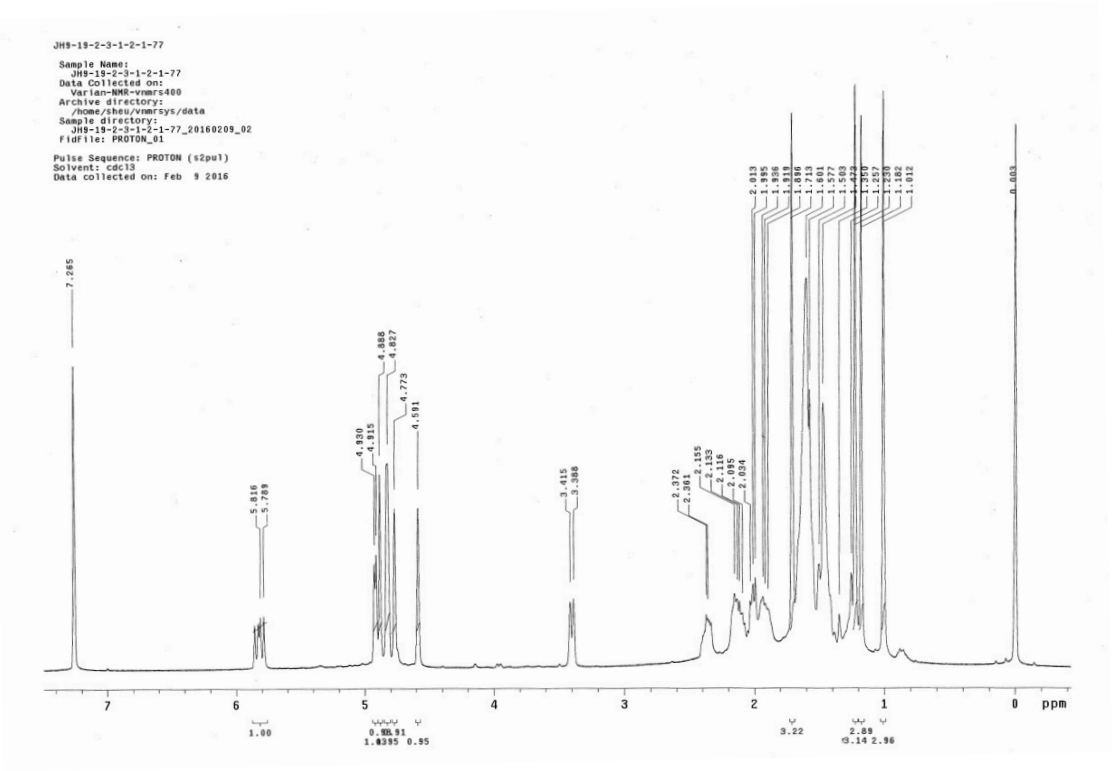



**Figure S11.** $^{1}$H NMR spectrum of **2** in $CDCl_3$ at 400 MHz.

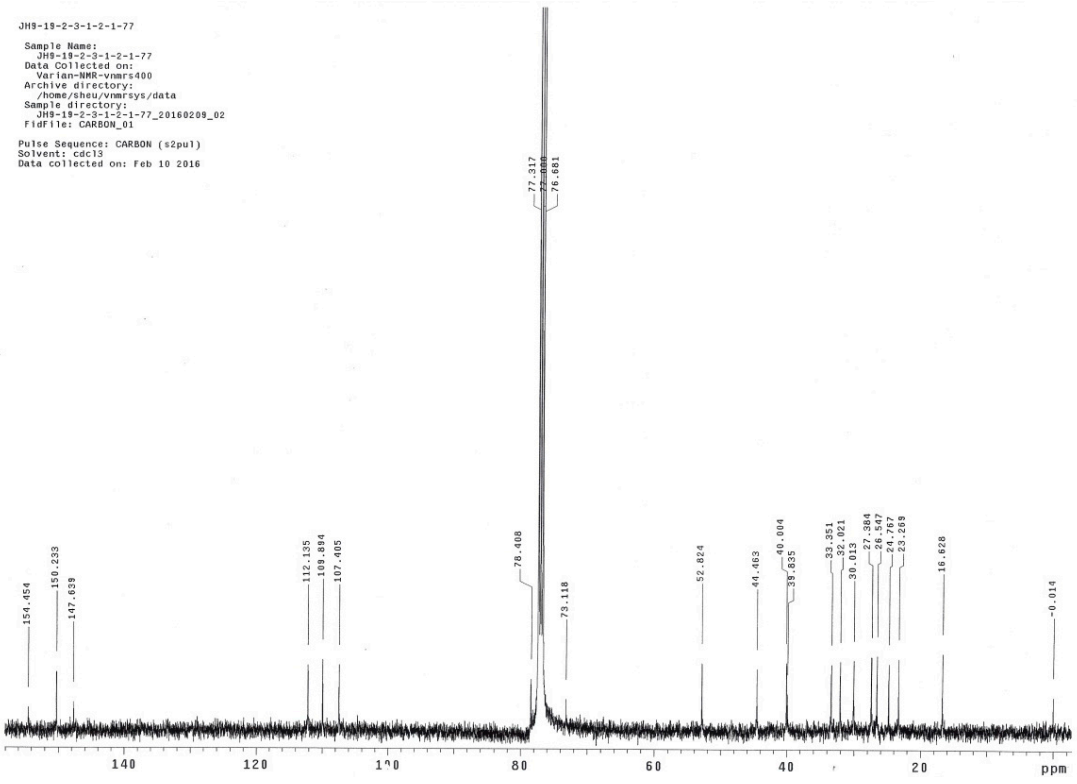



**Figure S12.** $^{13}$C NMR spectrum of **2** in $CDCl_3$ at 100 MHz.

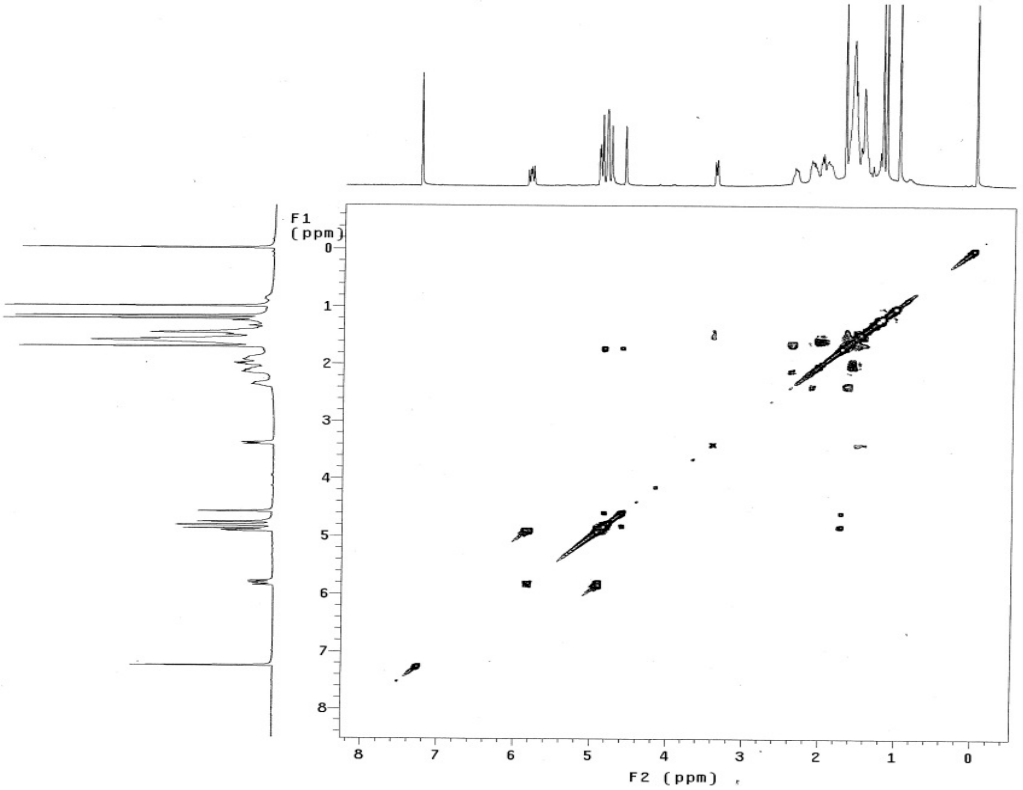



**Figure S13.** $^{1}$H-$^{1}$H COSY spectrum of **2** in $CDCl_3$..

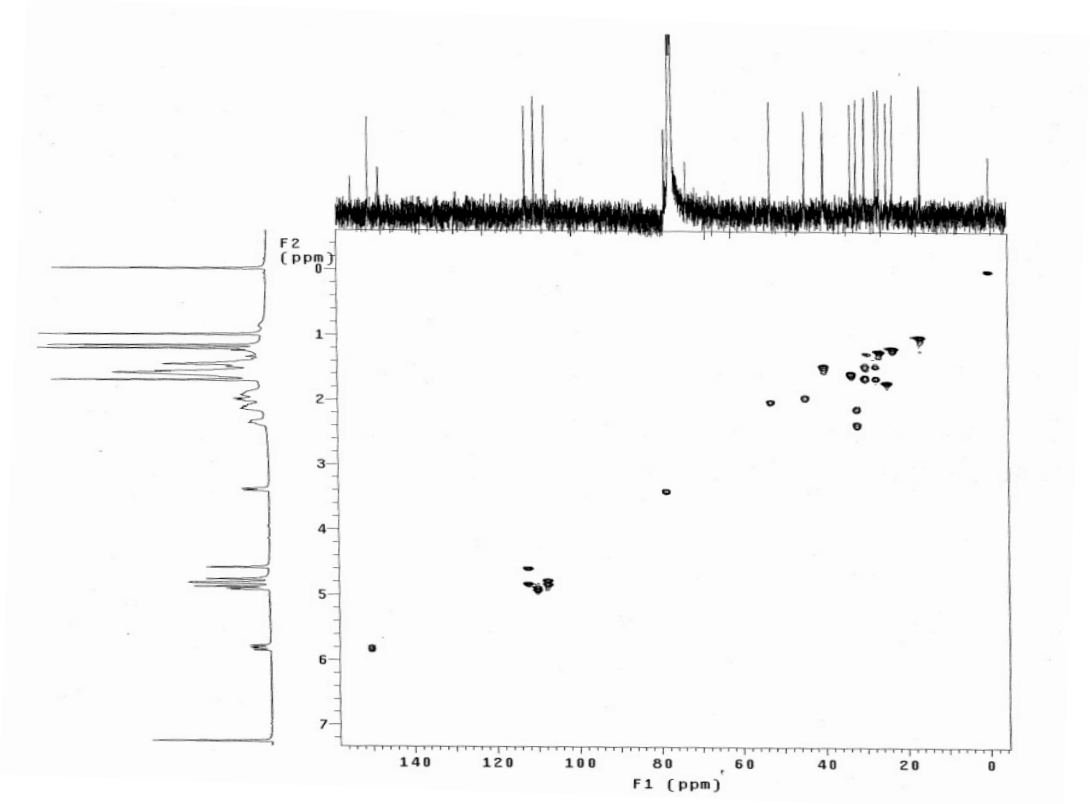



**Figure S14.** HSQC spectrum of **2** in $CDCl_3$.

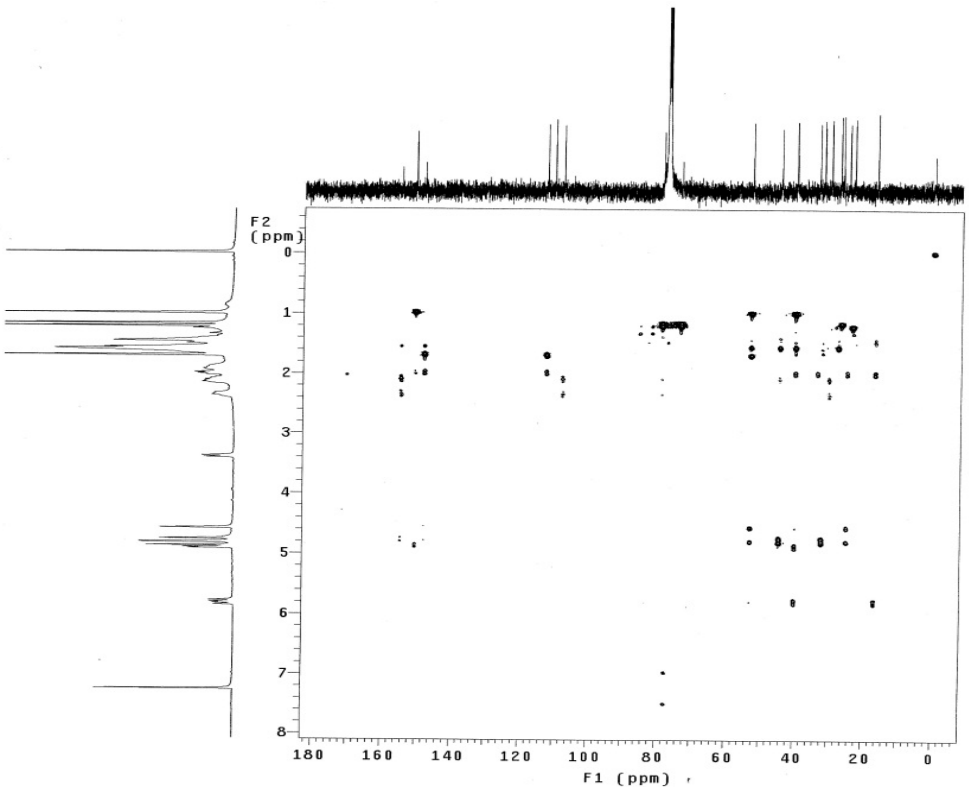



**Figure S15.** HMBC spectrum of **2** in $CDCl_3$.

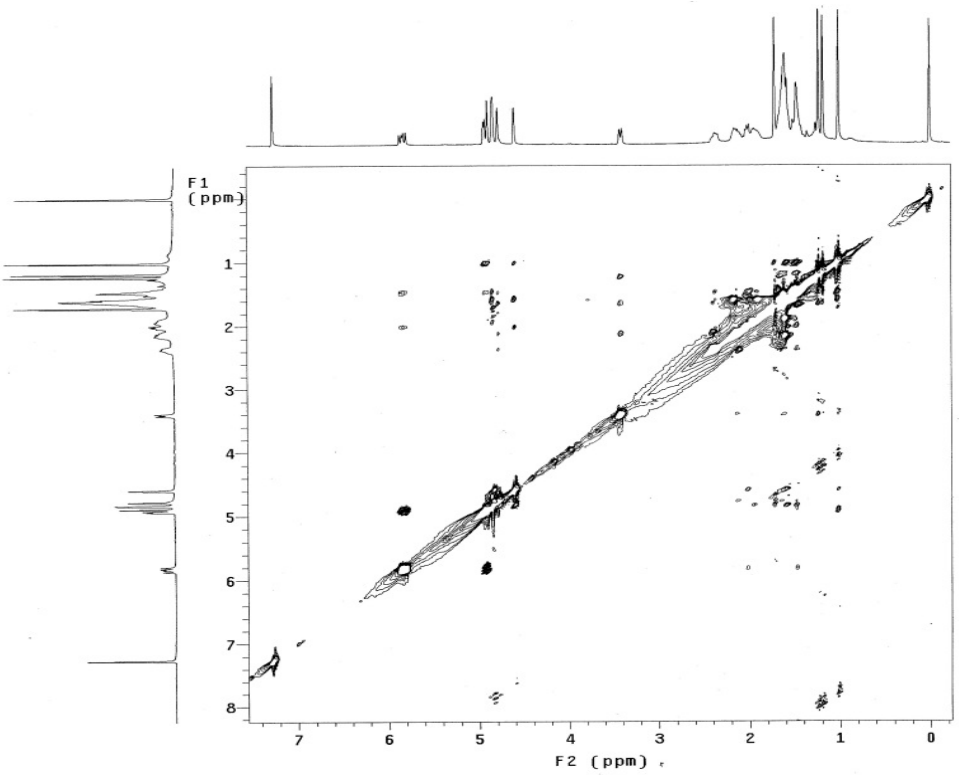
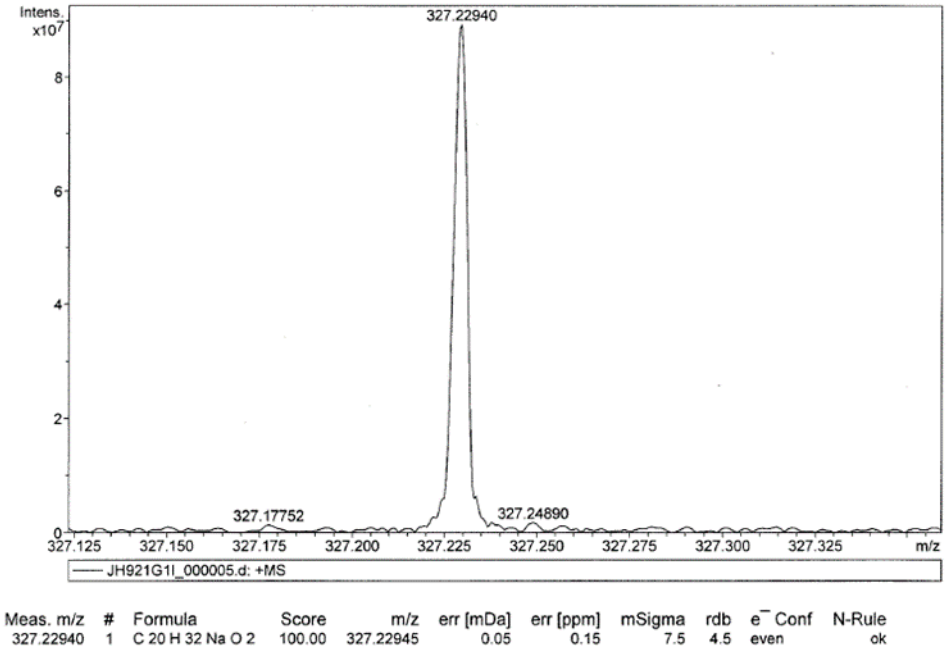



**Figure S16.** NOESY spectrum of **2** in $CDCl_3$.




| Meas. m/z | # | Formula | Score | m/z | err [mDa] | err [ppm] | mSigma | rdb | e⁻ Conf | N-Rule |
|---|---|---|---|---|---|---|---|---|---|---|
| 327.22940 | 1 | C 20 H 32 Na O 2 | 100.00 | 327.22945 | 0.05 | 0.15 | 7.5 | 4.5 | even | ok |

**Figure S17.** HRESIMS spectrum of **3**.

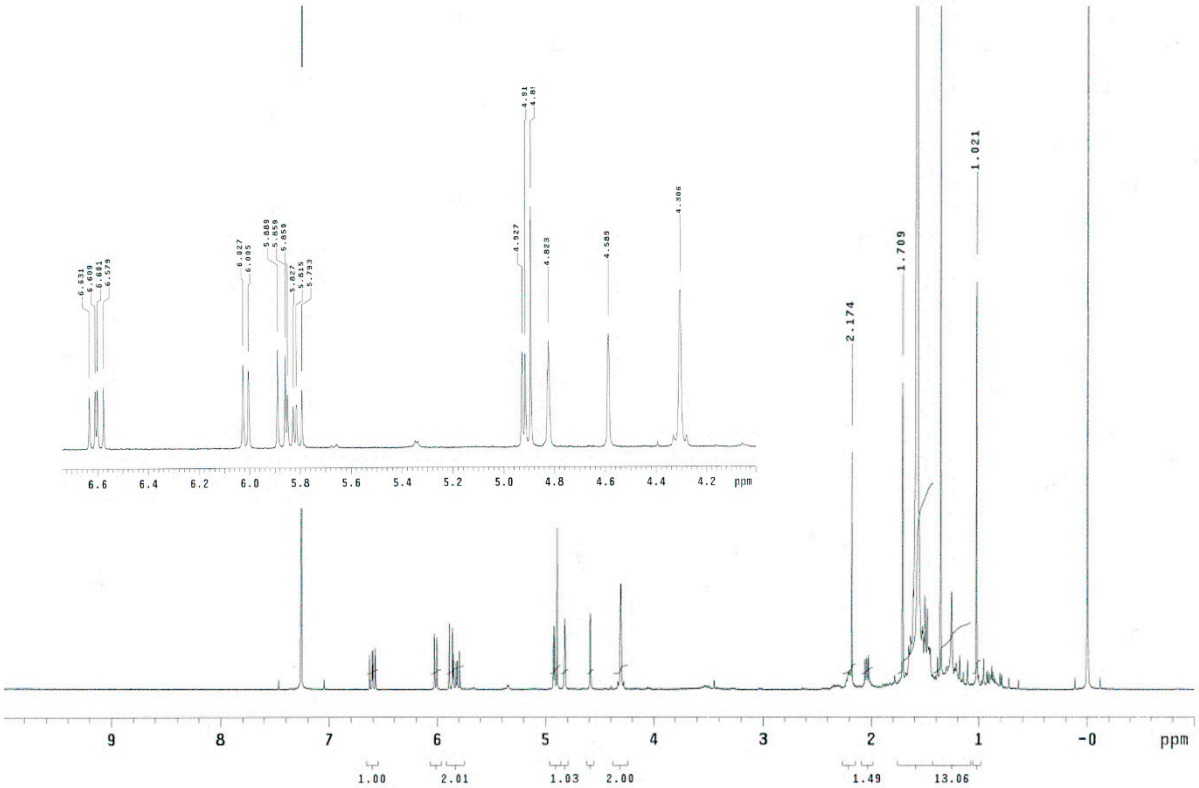



**Figure S18.** $^{1}$H NMR spectrum of **3** in $CDCl_3$ at 500 MHz.

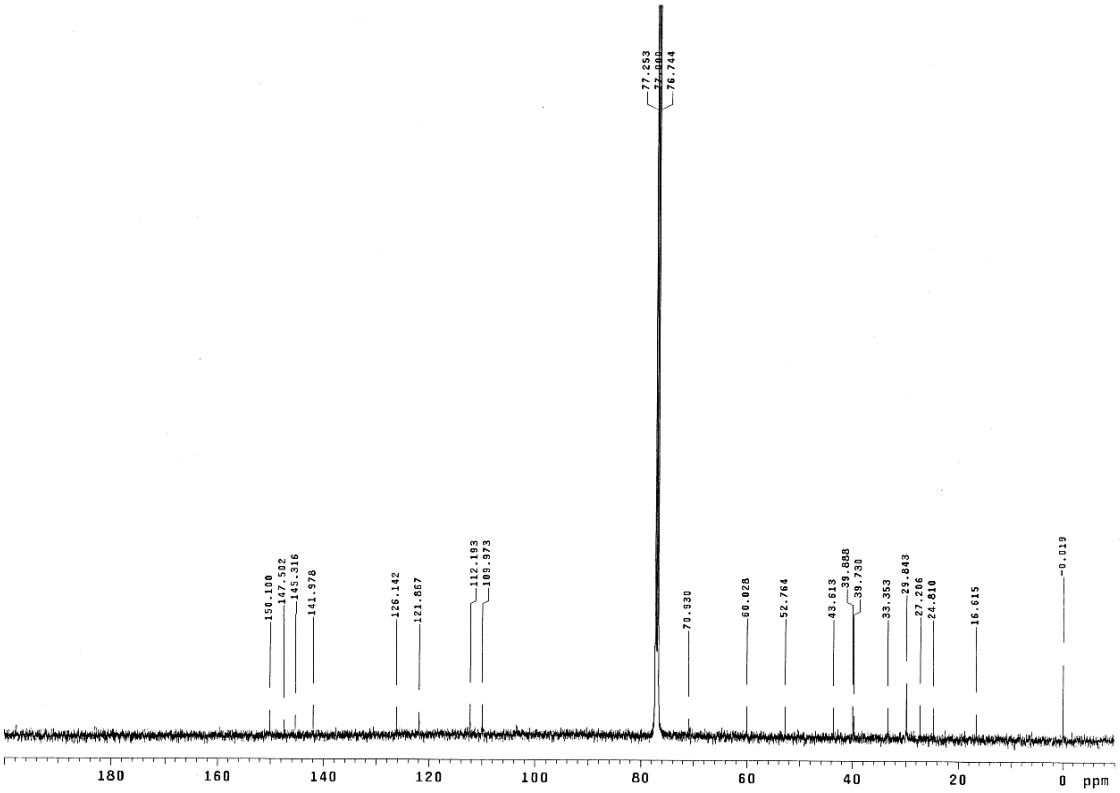



**Figure S19.** $^{13}C$ NMR spectrum of **3** in $CDCl_3$ at 125 MHz.

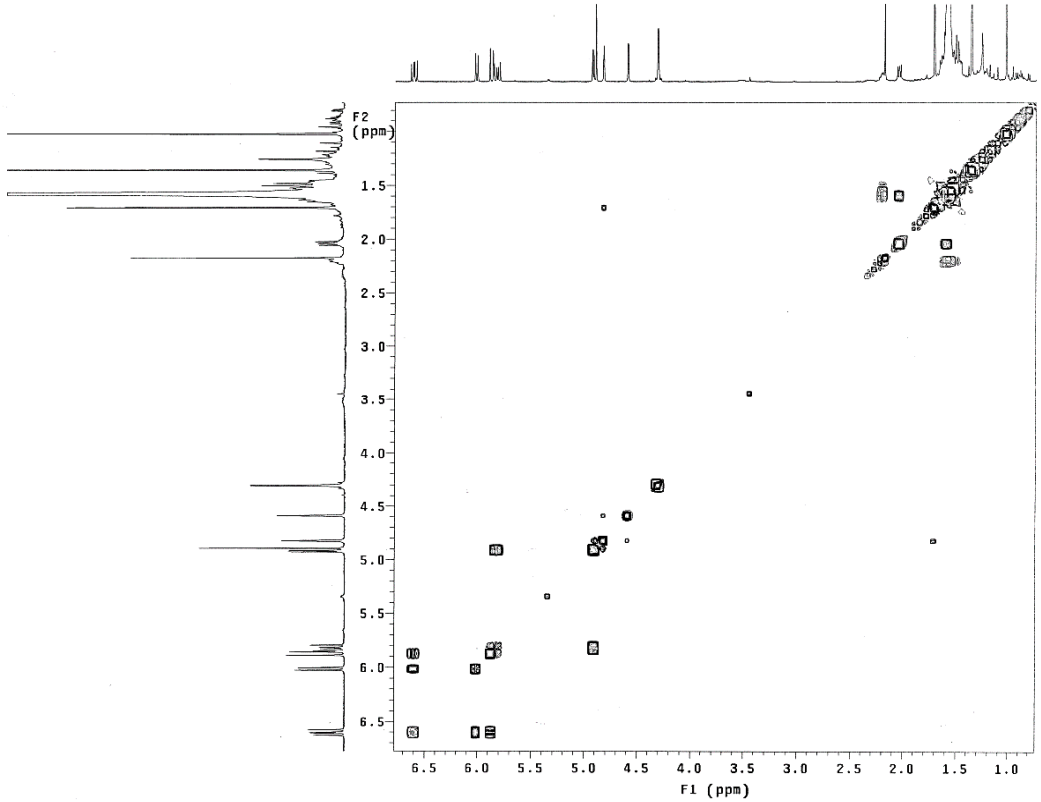



**Figure S20.** $^{1}H$-$^{1}H$ COSY spectrum of **3** in $CDCl_3$.

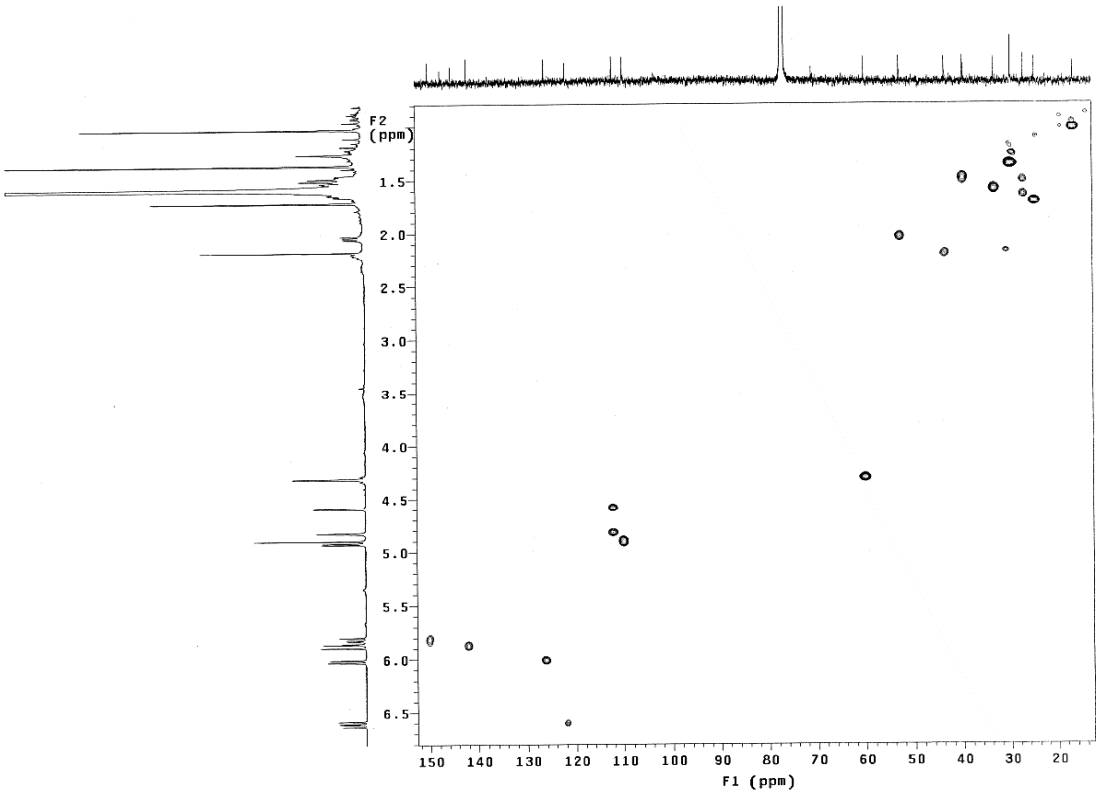



**Figure S21.** HSQC spectrum of **3** in $CDCl_3$.

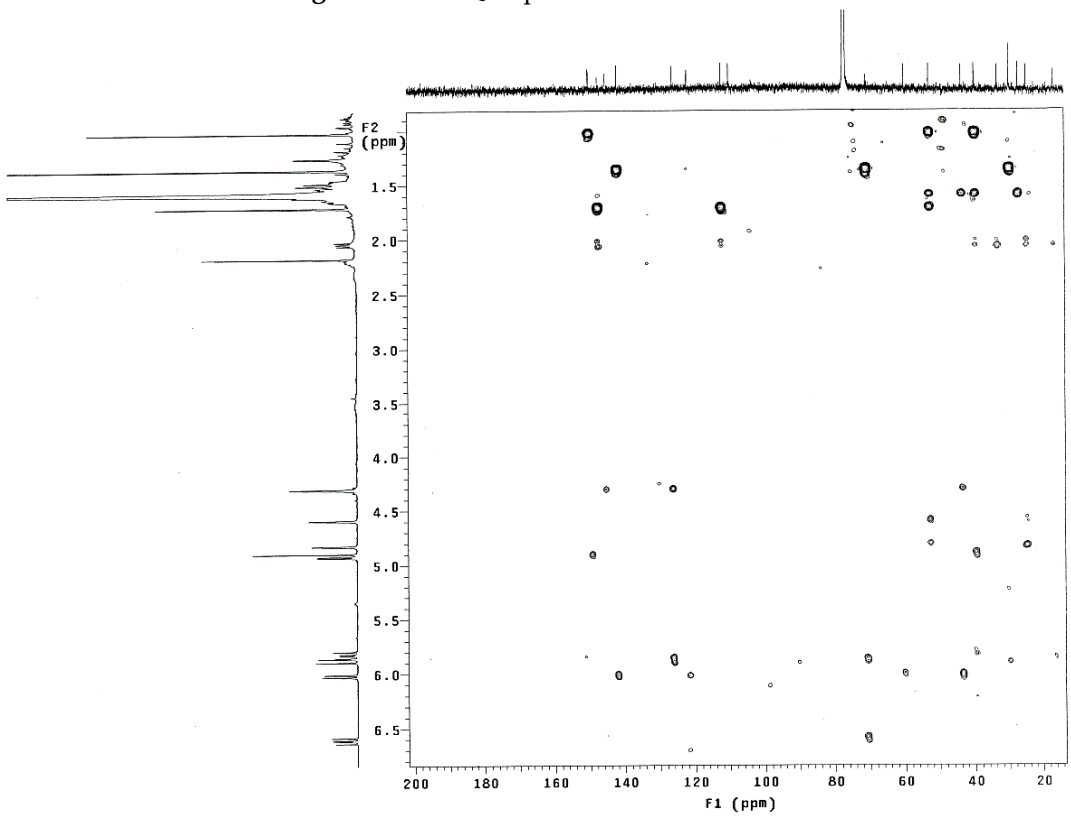



**Figure S22.** HMBC spectrum of **3** in $CDCl_3$.

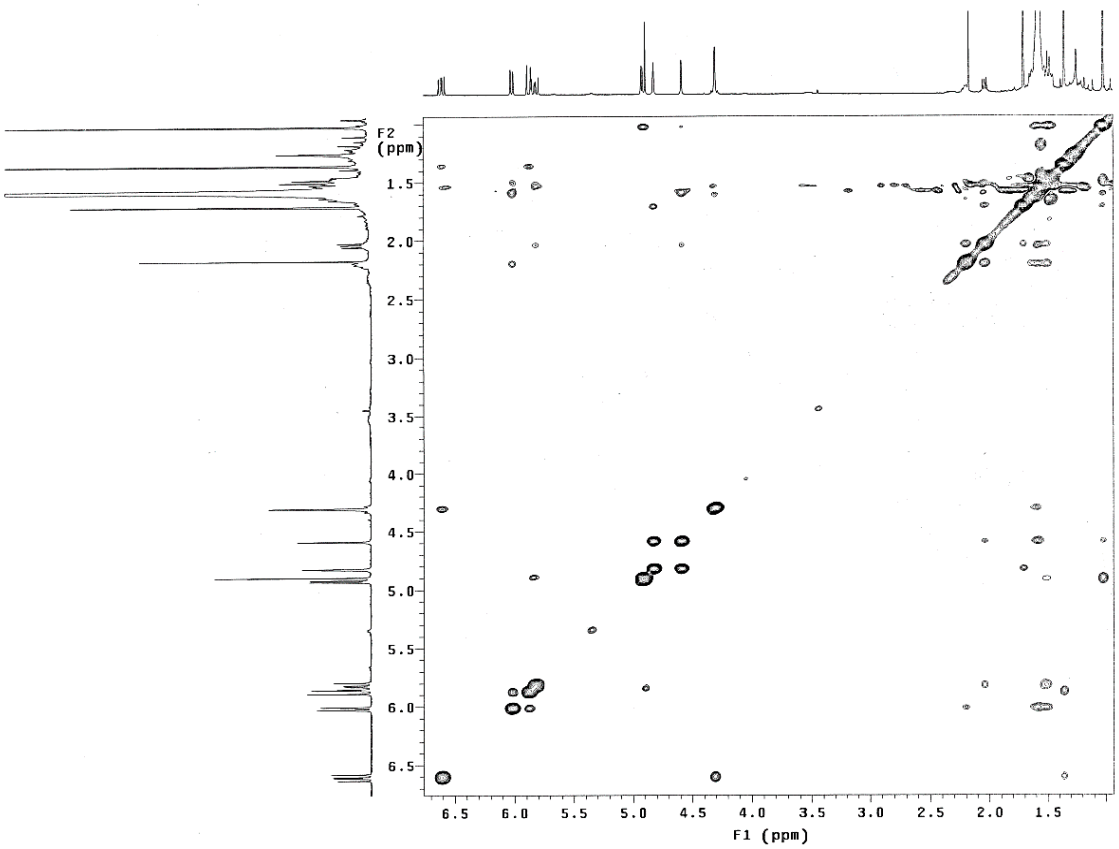
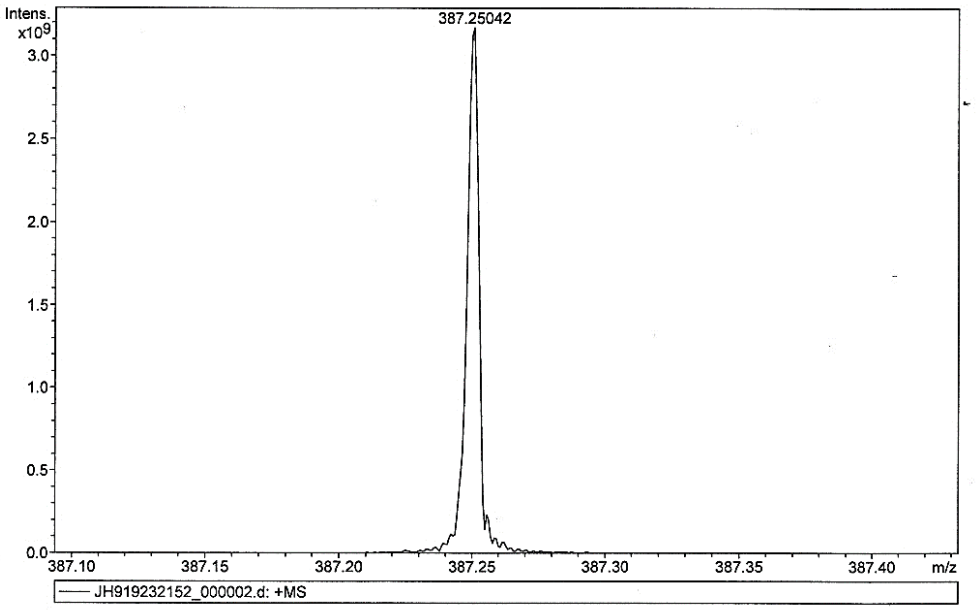



**Figure S23.** NOESY spectrum of **3** in $CDCl_3$.

**Figure S24.** HRESIMS spectrum of **4**.




| Meas. m/z | # | Formula | Score | m/z | err [mDa] | err [ppm] | mSigma | rdb | e⁻ Conf | N-Rule |
|---|---|---|---|---|---|---|---|---|---|---|
| 387.25042 | 1 | C 22 H 36 Na O 4 | 100.00 | 387.25058 | 0.16 | 0.41 | 7.4 | 4.5 | even | ok |

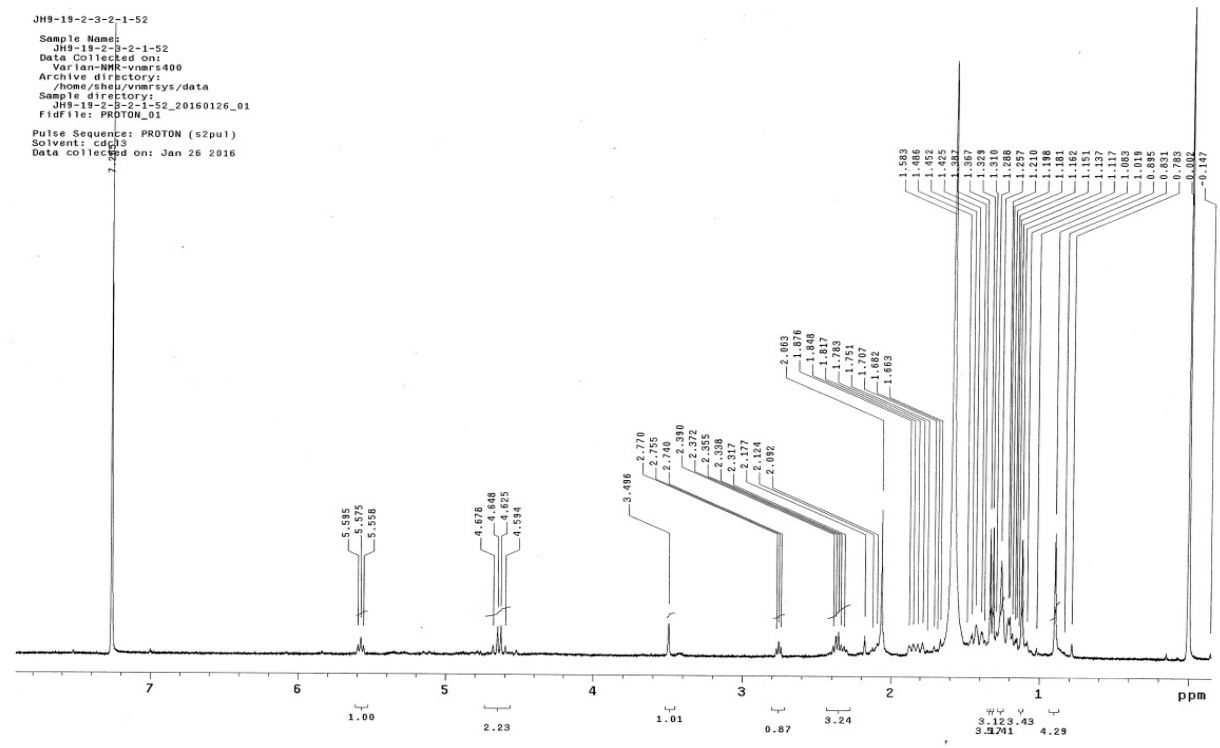



**Figure S25.** $^{1}$H NMR spectrum of **4** in $CDCl_3$ at 400 MHz.

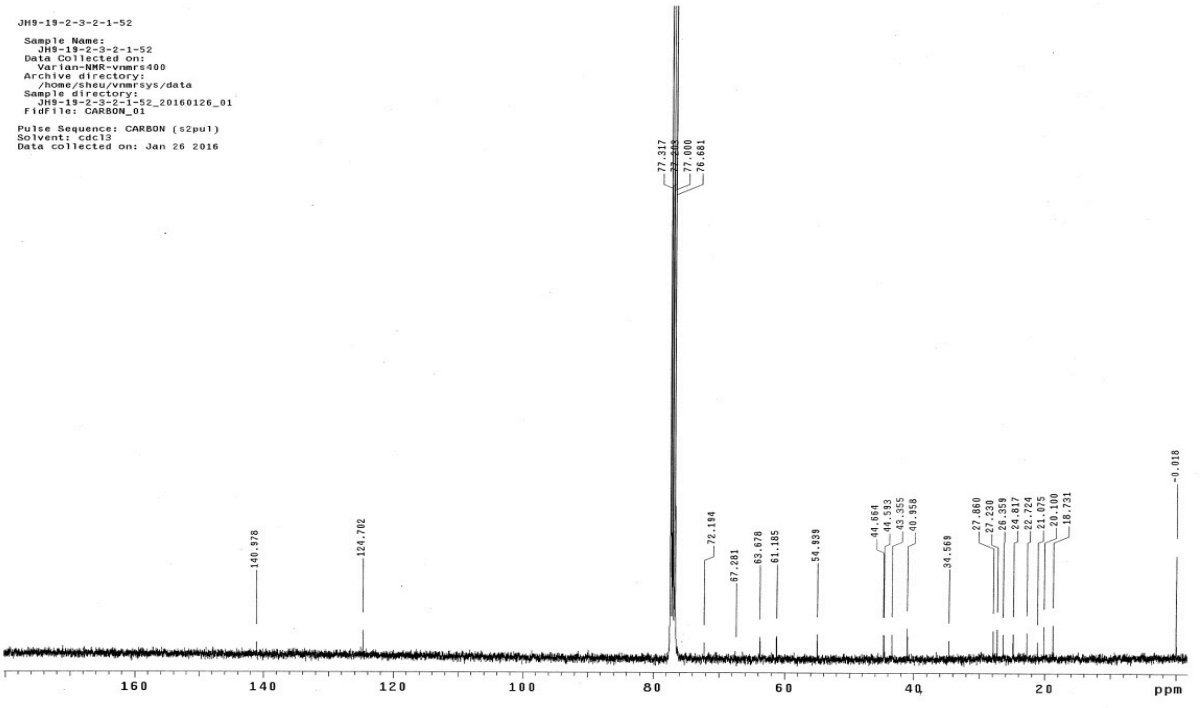



**Figure S26.** $^{13}$C NMR spectrum of **4** in $CDCl_3$ at 100 MHz.

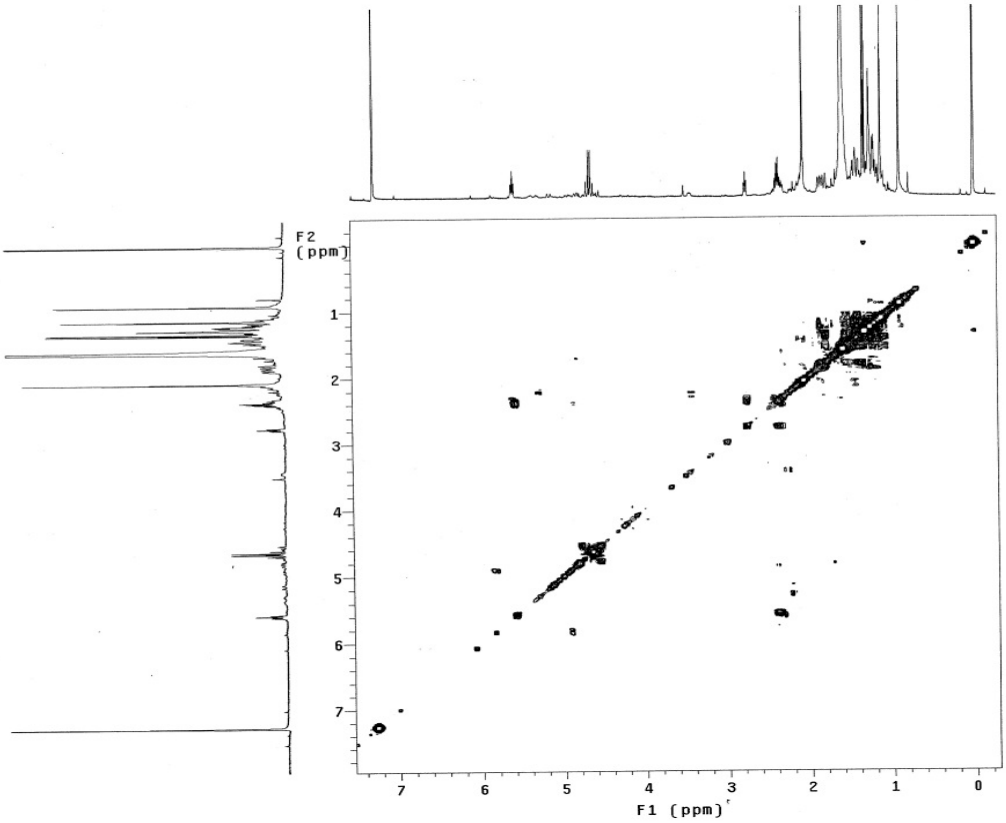



**Figure S27.** $^{1}H$-$^{1}H$ COSY spectrum of **4** in $CDCl_3$.

**Figure S28.** HSQC spectrum of **4** in $CDCl_3$.

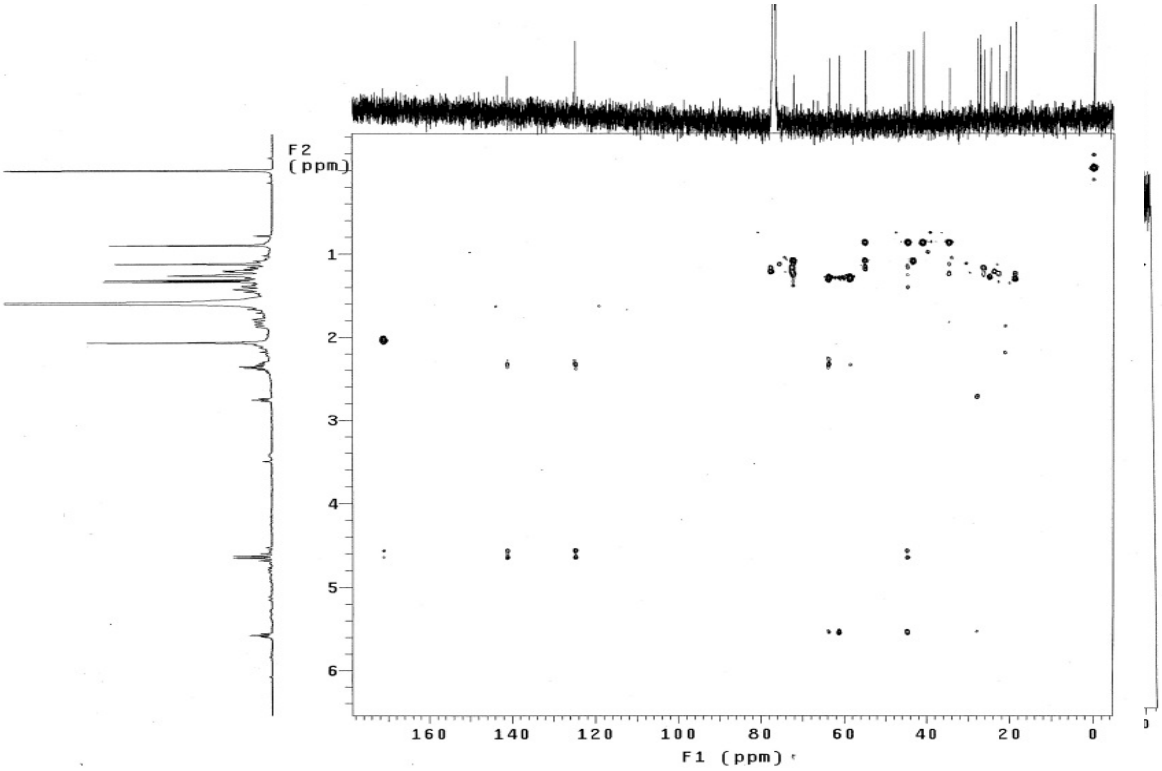



**Figure S29.** HMBC spectrum of **4** in $CDCl_3$.

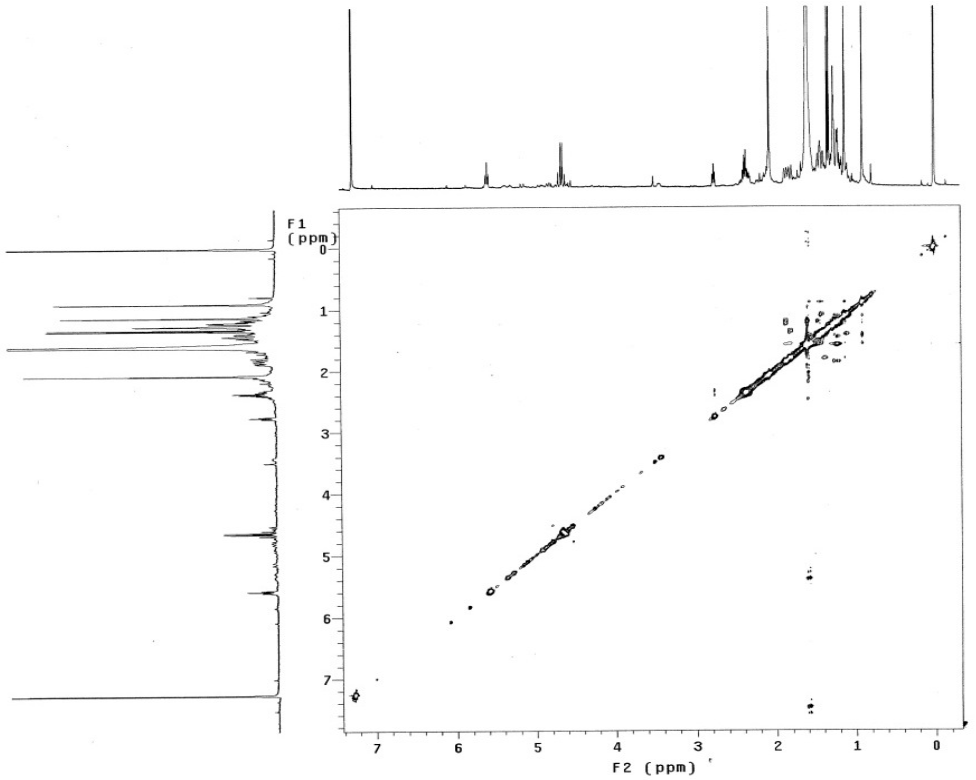
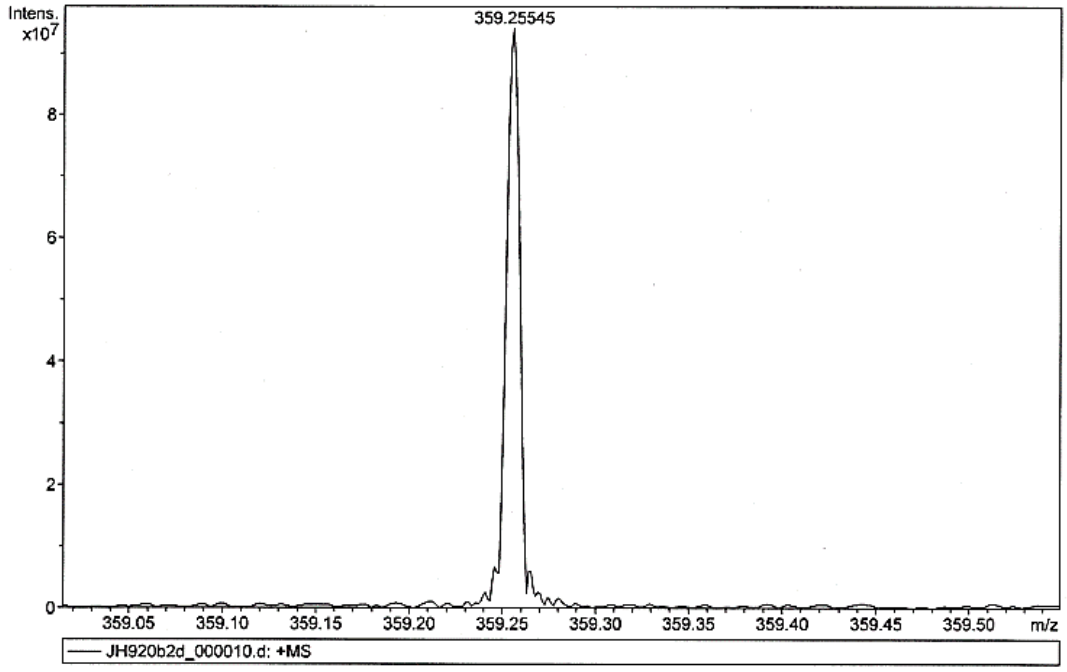



**Figure S30.** NOESY spectrum of **4** in $CDCl_3$.




| Meas. m/z | # | Formula | Score | m/z | err [mDa] | err [ppm] | mSigma | rdb | e⁻ Conf | N-Rule |
|---|---|---|---|---|---|---|---|---|---|---|
| 359.25545 | 1 | C 21 H 36 Na O 3 | 100.00 | 359.25567 | 0.22 | 0.61 | 0.6 | 3.5 | even | ok |

**Figure S31.** HRESIMS spectrum of **5a** and **5b**.

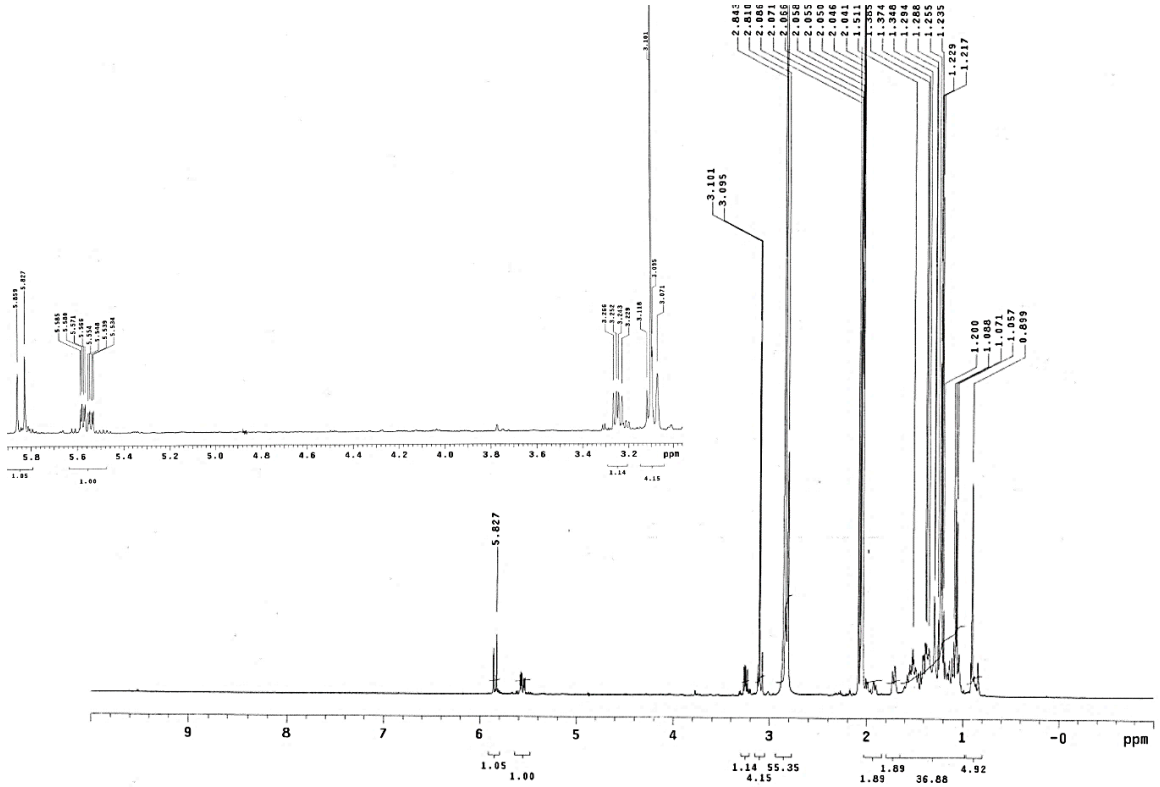


**Figure S32.** [1]H NMR spectrum of **5a** and **5b** in acetone-$d_6$ at 500 MHz.

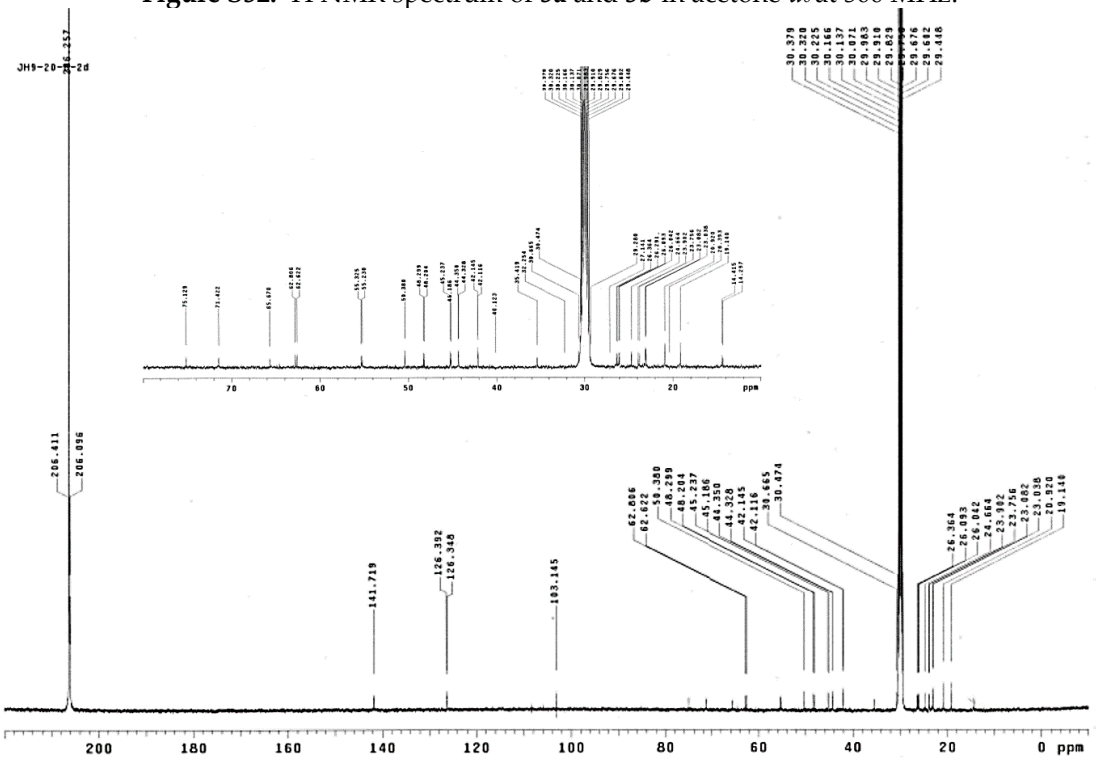


**Figure S33.** [13]C NMR spectrum of **5a** and **5b** in acetone-$d_6$ at 125 MHz.

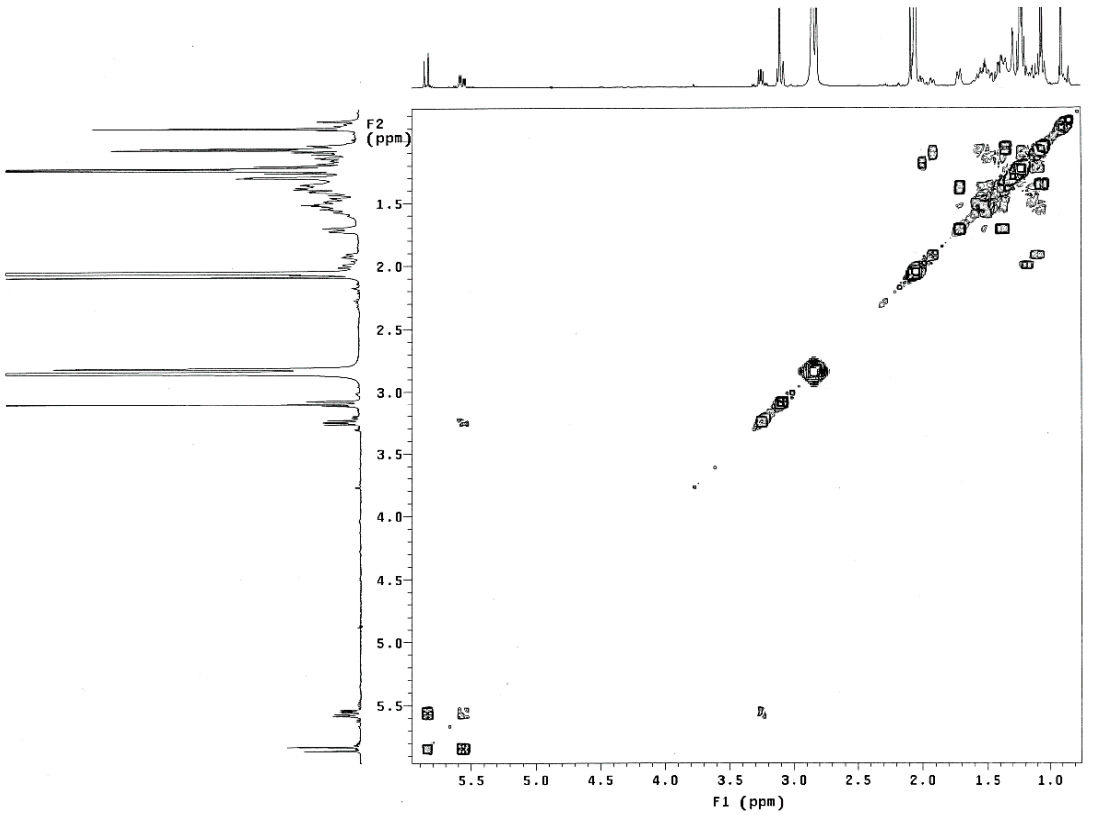



**Figure S34.** $^{1}$H-$^{1}$H COSY spectrum of **5a** and **5b** in acetone-$d_6$.

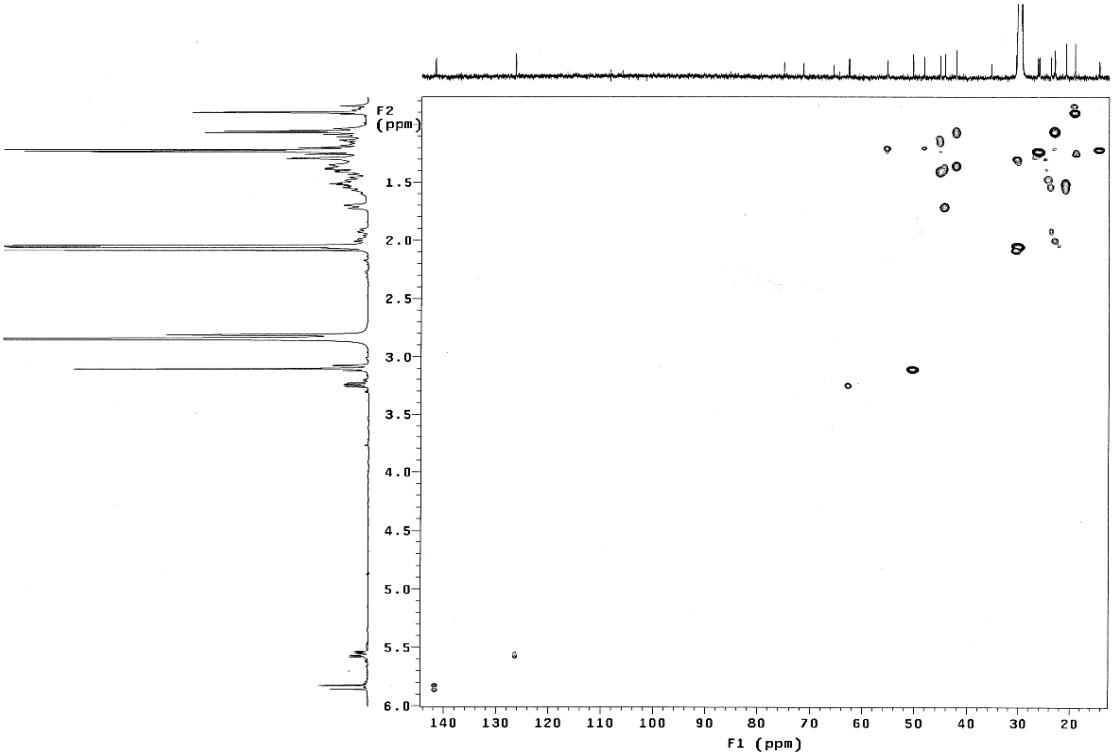



**Figure S35.** HSQC spectrum of **5a** and **5b** in acetone-$d_6$.

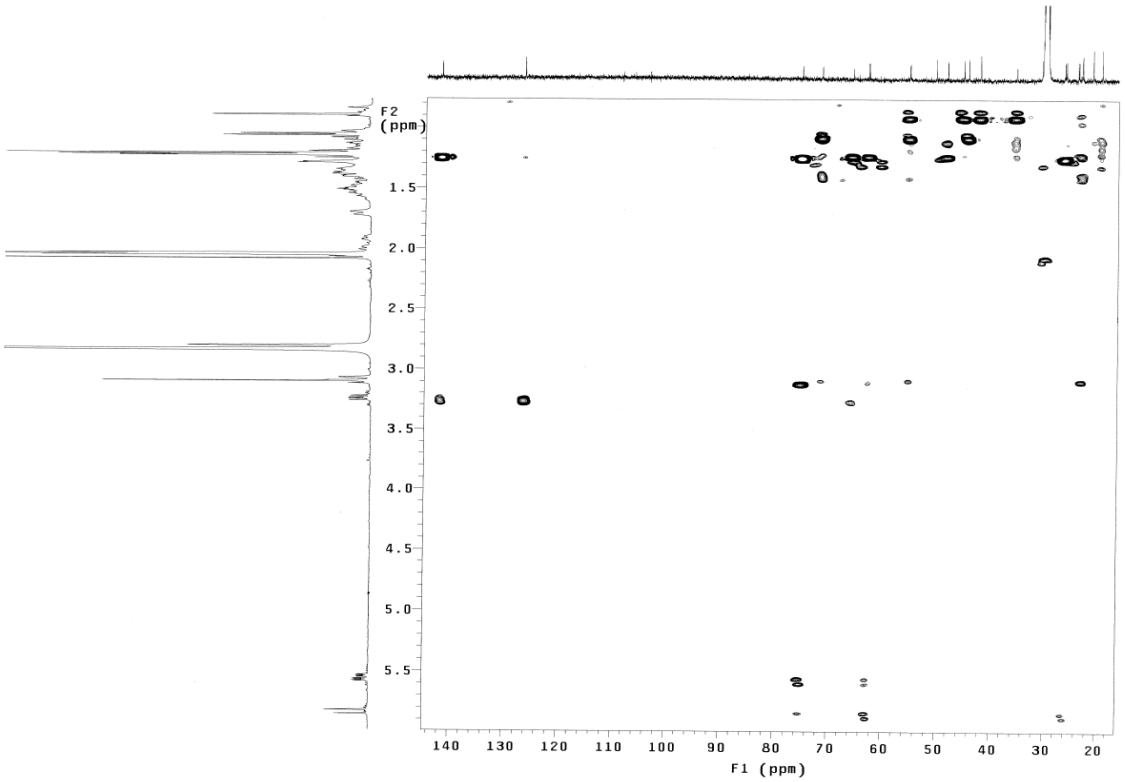



**Figure S36.** HMBC spectrum of **5a** and **5b** in acetone-$d_6$ .

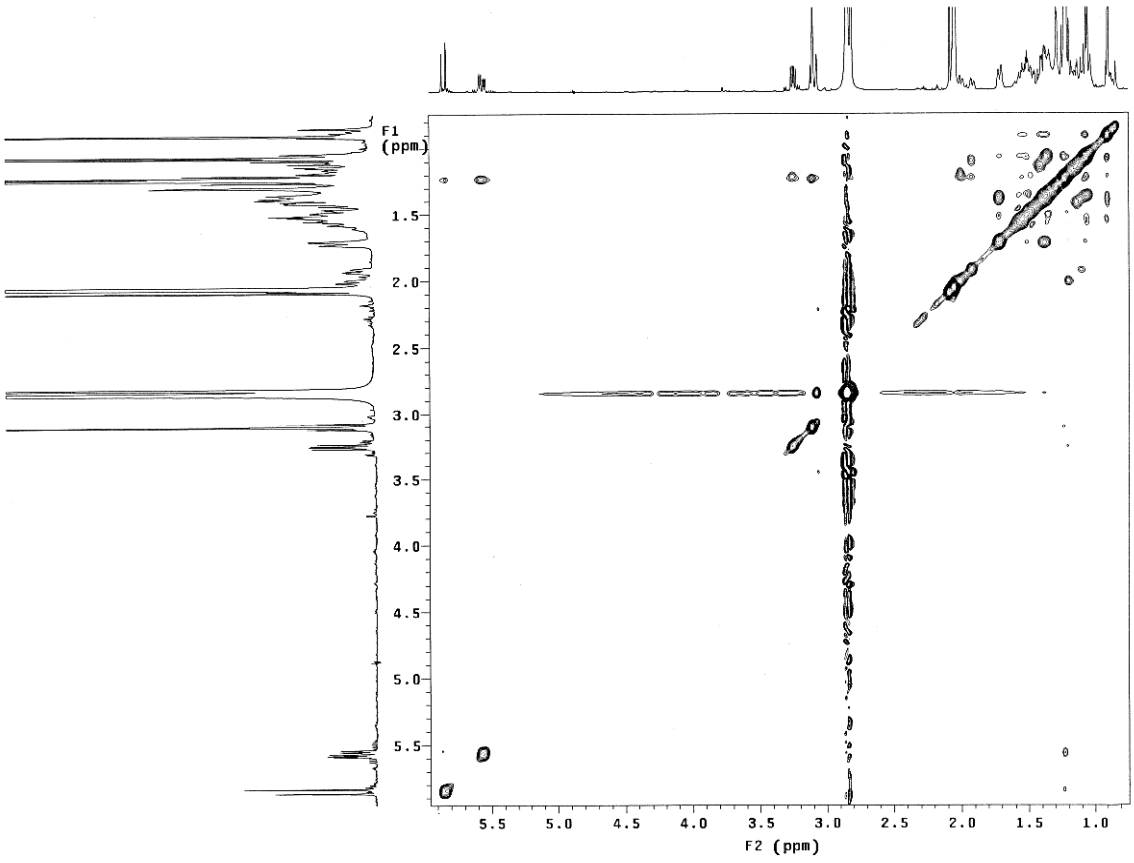
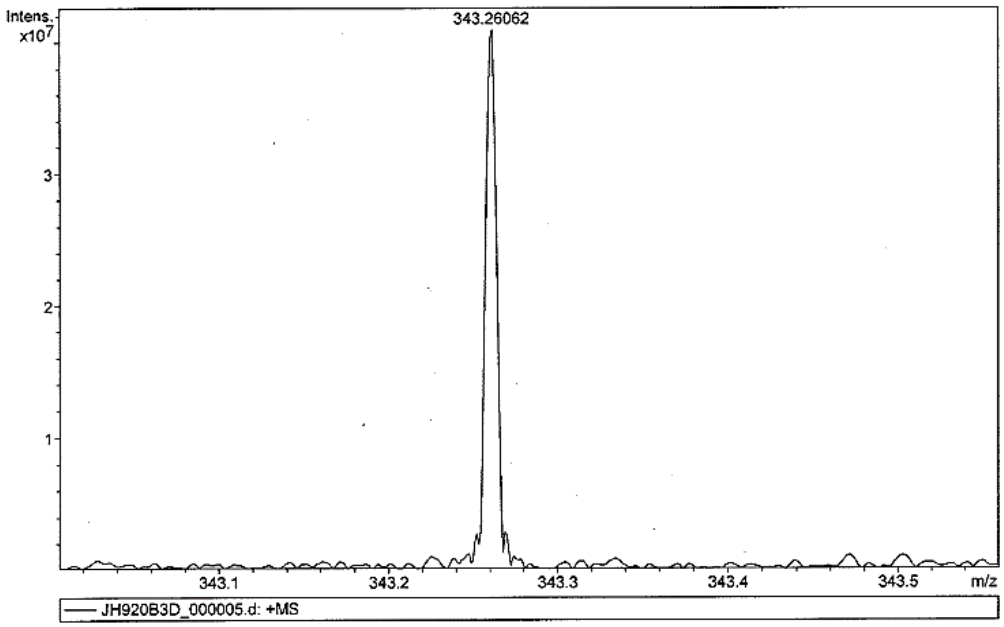



**Figure S37.** NOESY spectrum of **5a** and **5b** in acetone-$d_6$.




| Meas. m/z | # | Formula | Score | m/z | err [mDa] | err [ppm] | mSigma | rdb | e⁻ Conf | N-Rule |
|---|---|---|---|---|---|---|---|---|---|---|
| 343.26062 | 1 | C 21 H 36 Na O 2 | 100.00 | 343.26075 | 0.13 | 0.39 | 15.3 | 3.5 | even | ok |

**Figure S38.** HRESIMS spectrum of **6**.

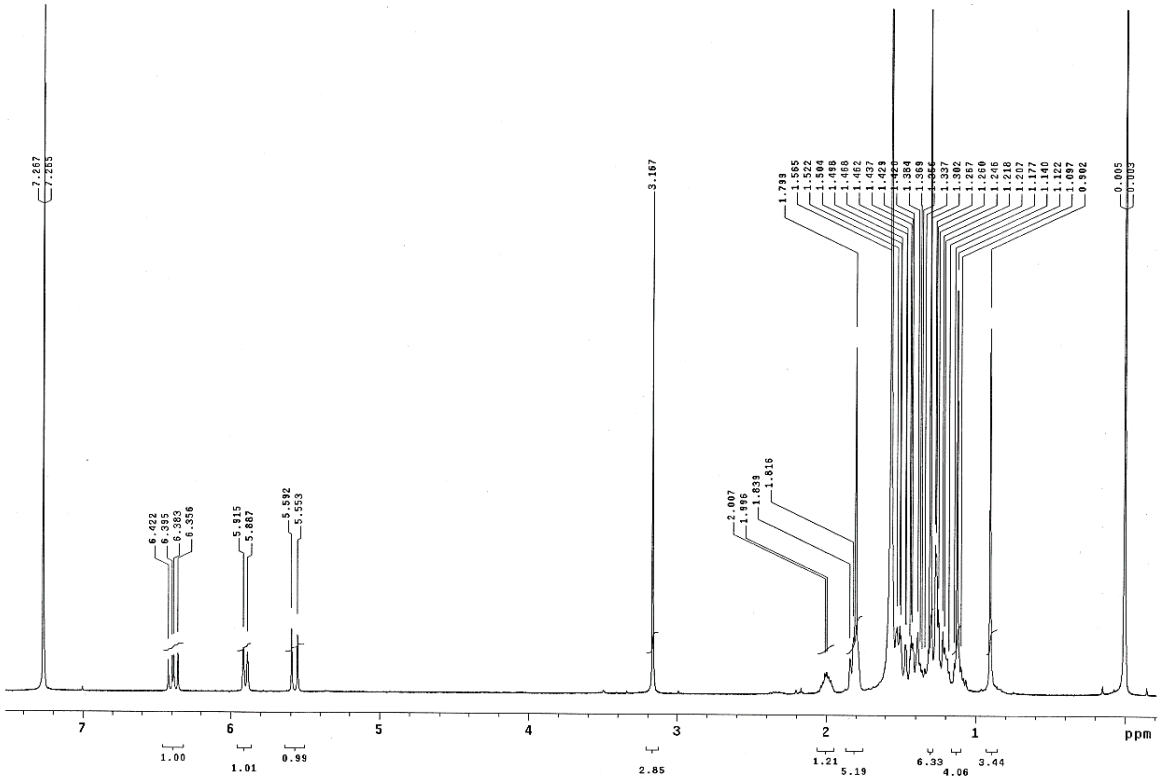



**Figure S39.** $^{1}$H NMR spectrum of **6** in $CDCl_3$ at 400 MHz.

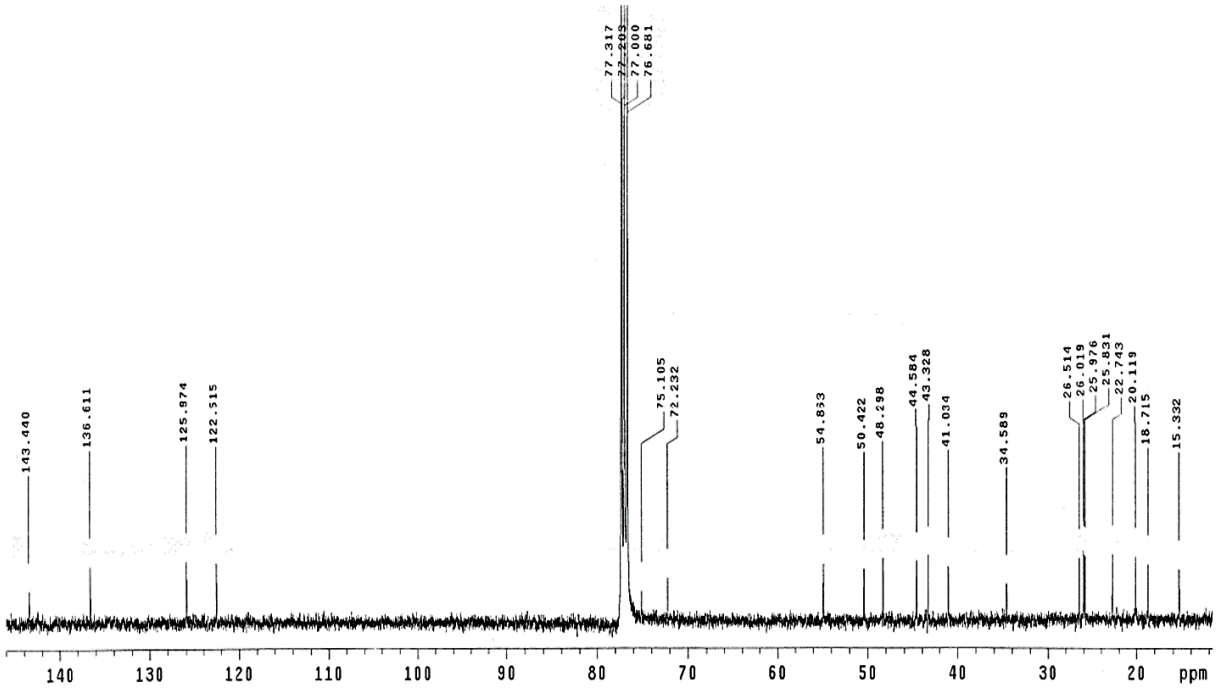



**Figure S40.** $^{13}C$ NMR spectrum of **6** in $CDCl_3$ at 100 MHz.

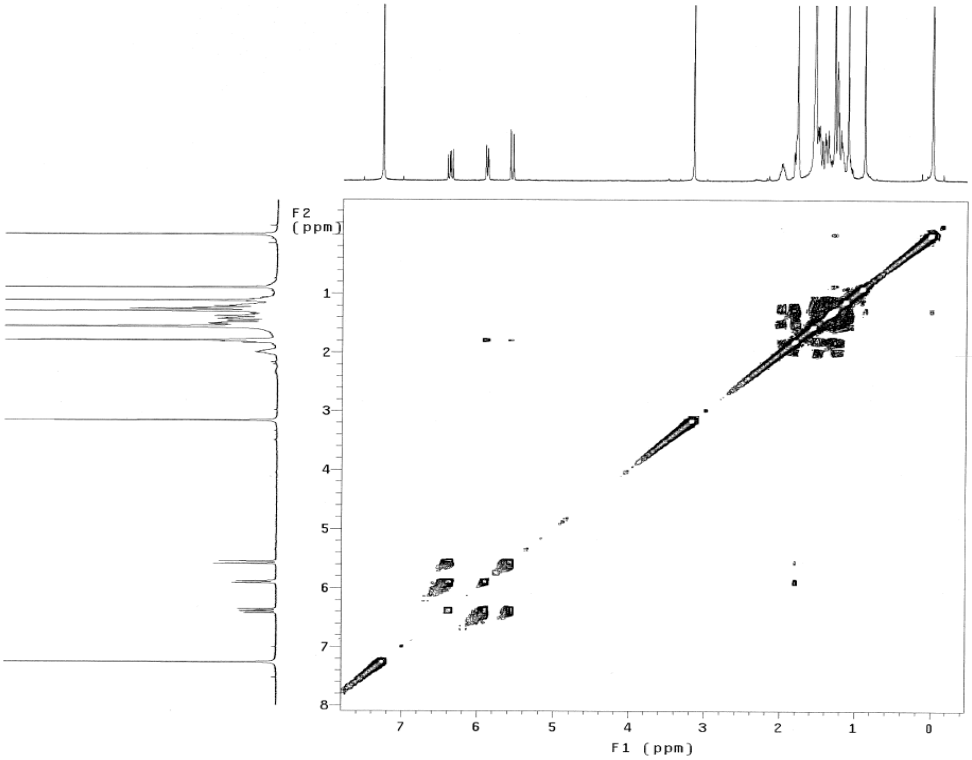



**Figure S41.** $^{1}H$-$^{1}H$ COSY spectrum of **6** in $CDCl_3$.

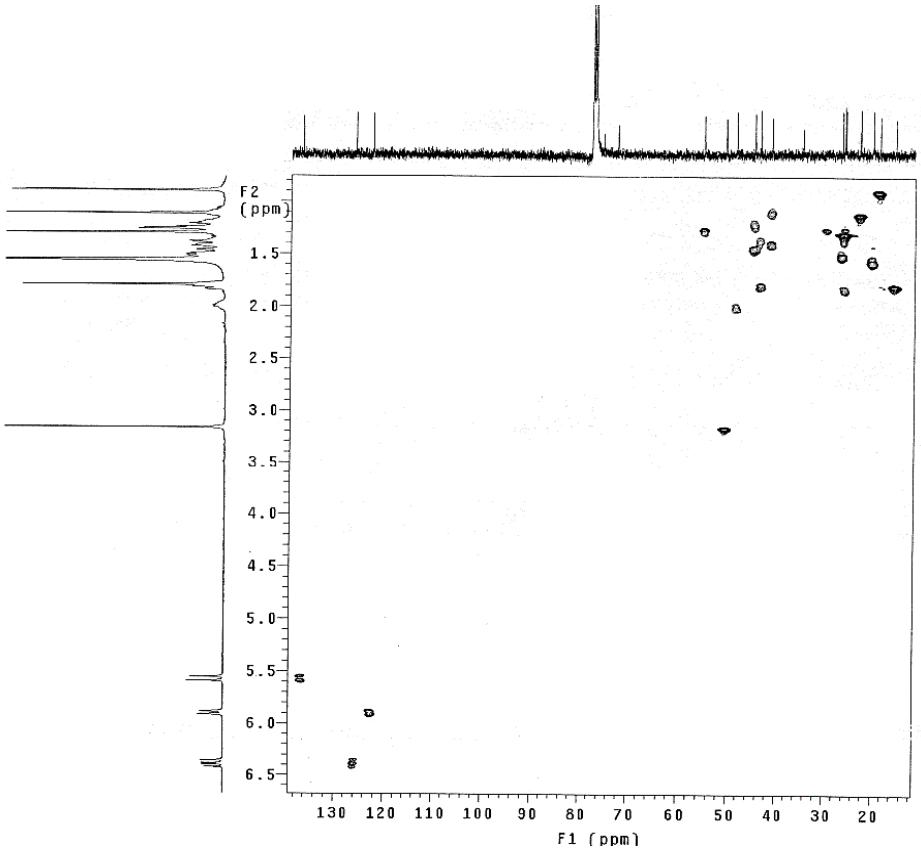



**Figure S42.** HSQC spectrum of **6** in $CDCl_3$.

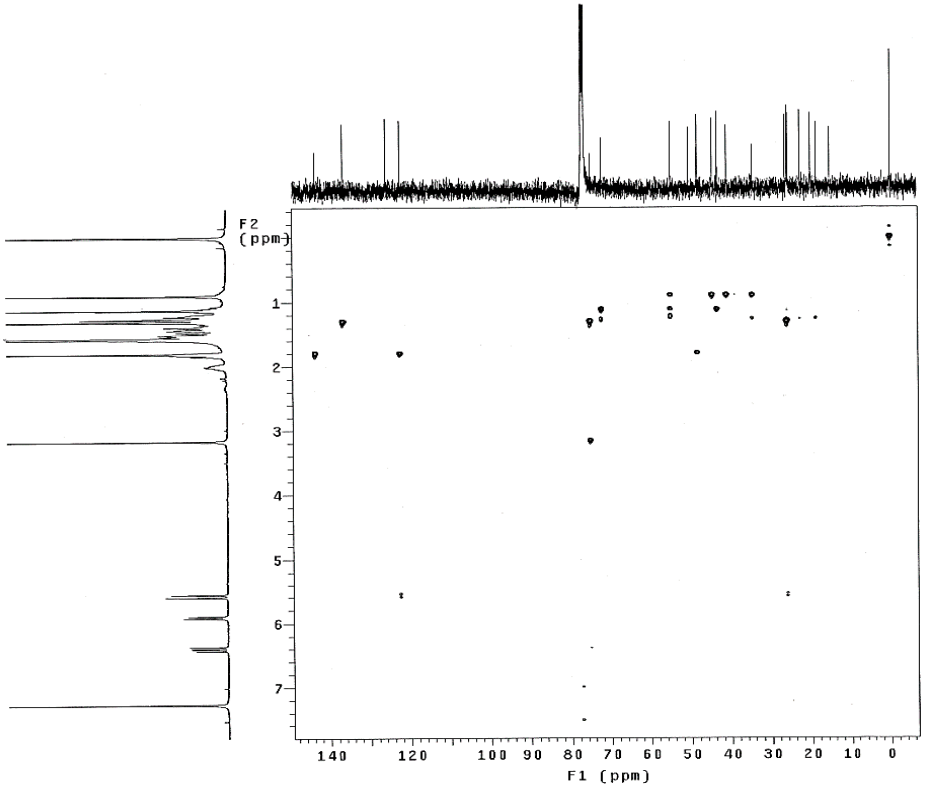



**Figure S43.** HMBC spectrum of **6** in $CDCl_3$.

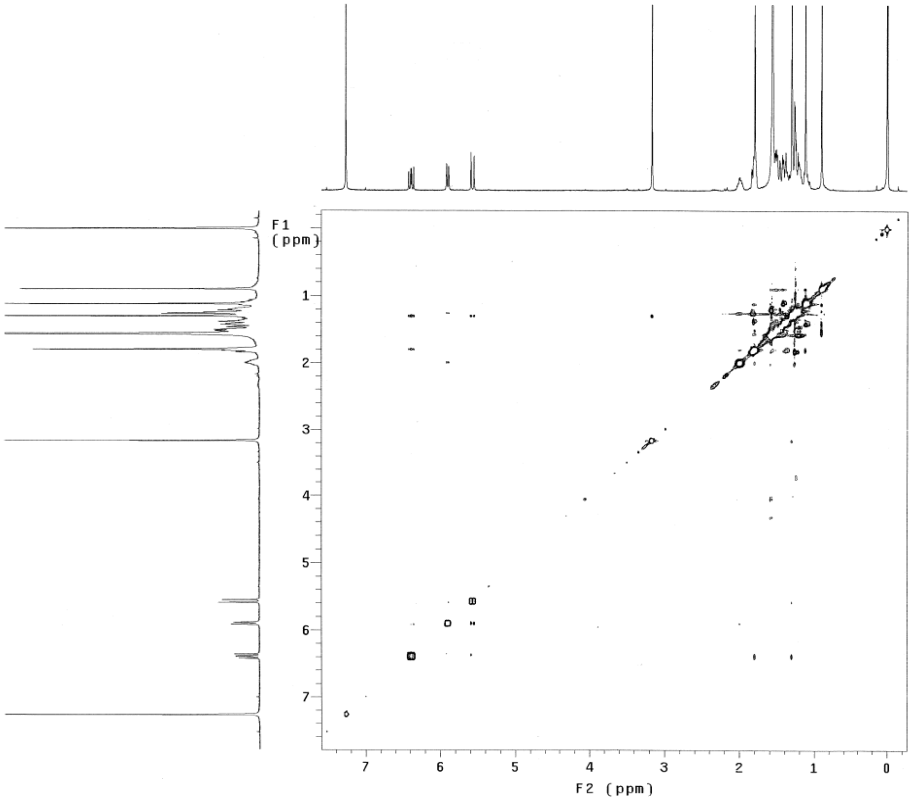
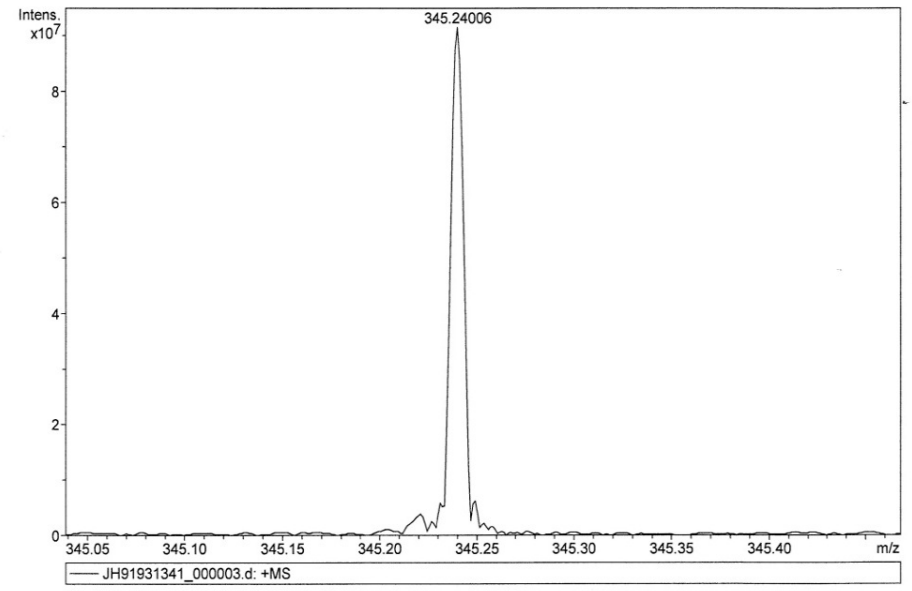



**Figure S44.** NOESY spectrum of **6** in $CDCl_3$.




| Meas. m/z | # | Formula | Score | m/z | err [mDa] | err [ppm] | mSigma | rdb | e⁻ Conf | N-Rule |
|---|---|---|---|---|---|---|---|---|---|---|
| 345.24006 | 1 | C 20 H 34 Na O 3 | 100.00 | 345.24002 | -0.05 | -0.14 | 4.3 | 3.5 | even | ok |

**Figure S45.** HRESIMS spectrum of **7**.

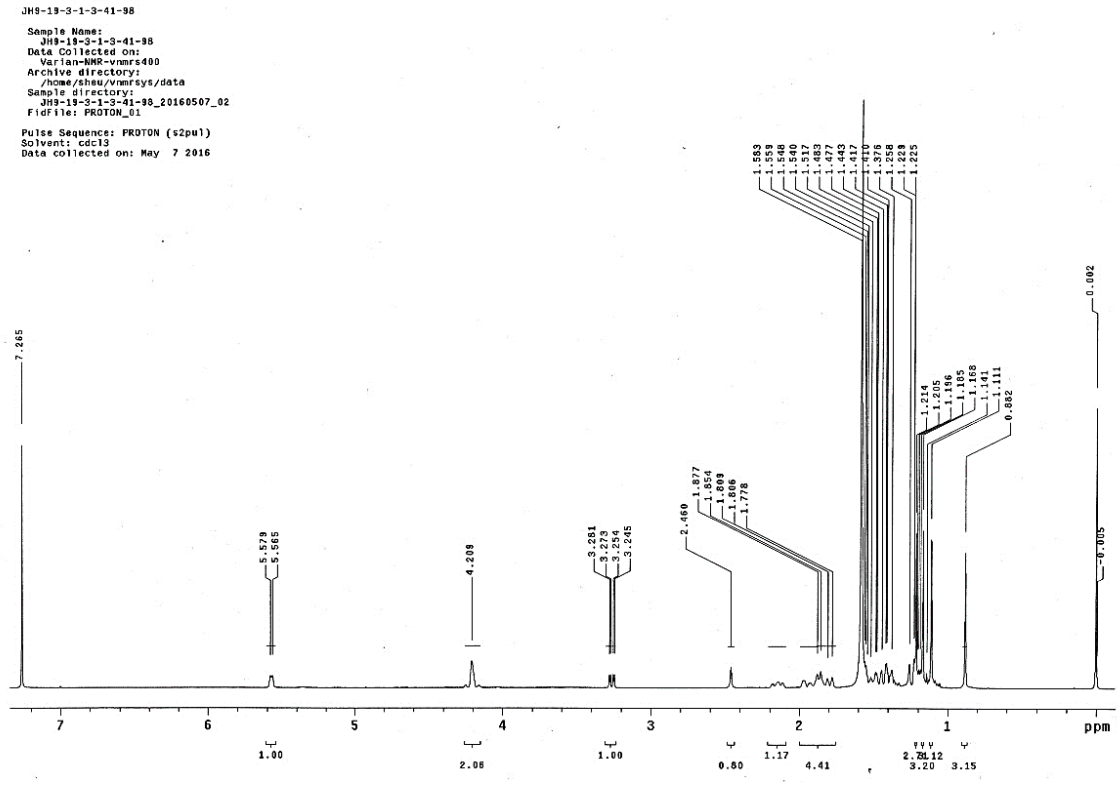



**Figure S46.** $^{1}$H NMR spectrum of **7** in $CDCl_3$ at 400 MHz.

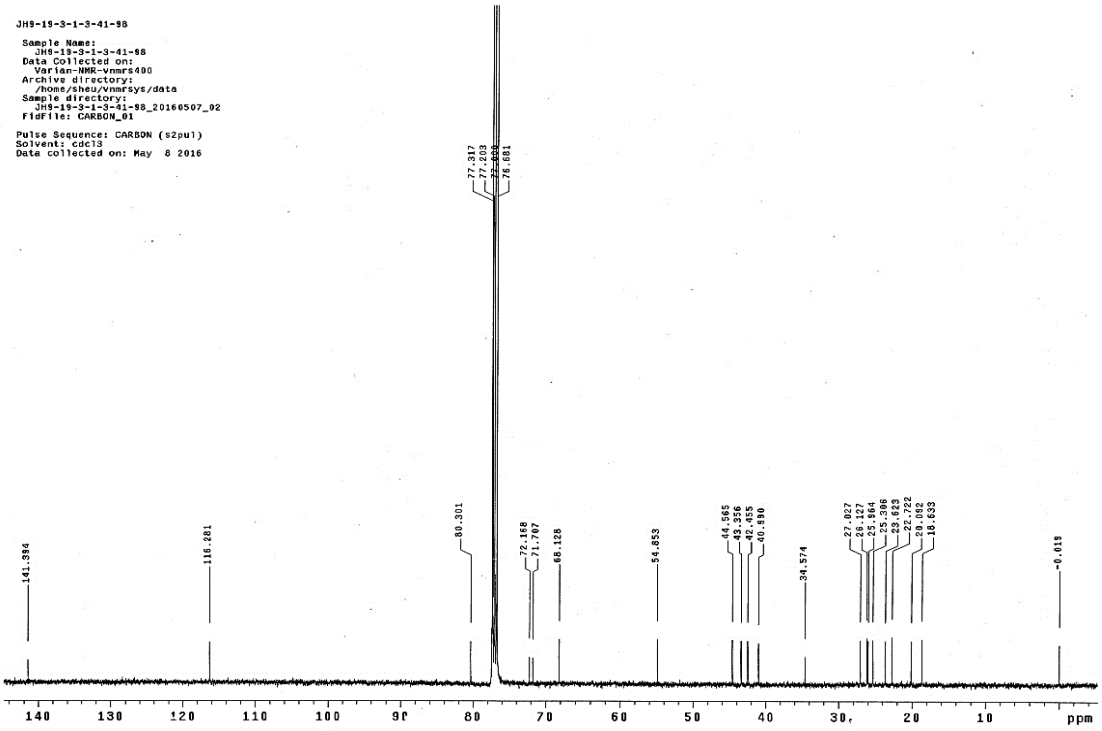
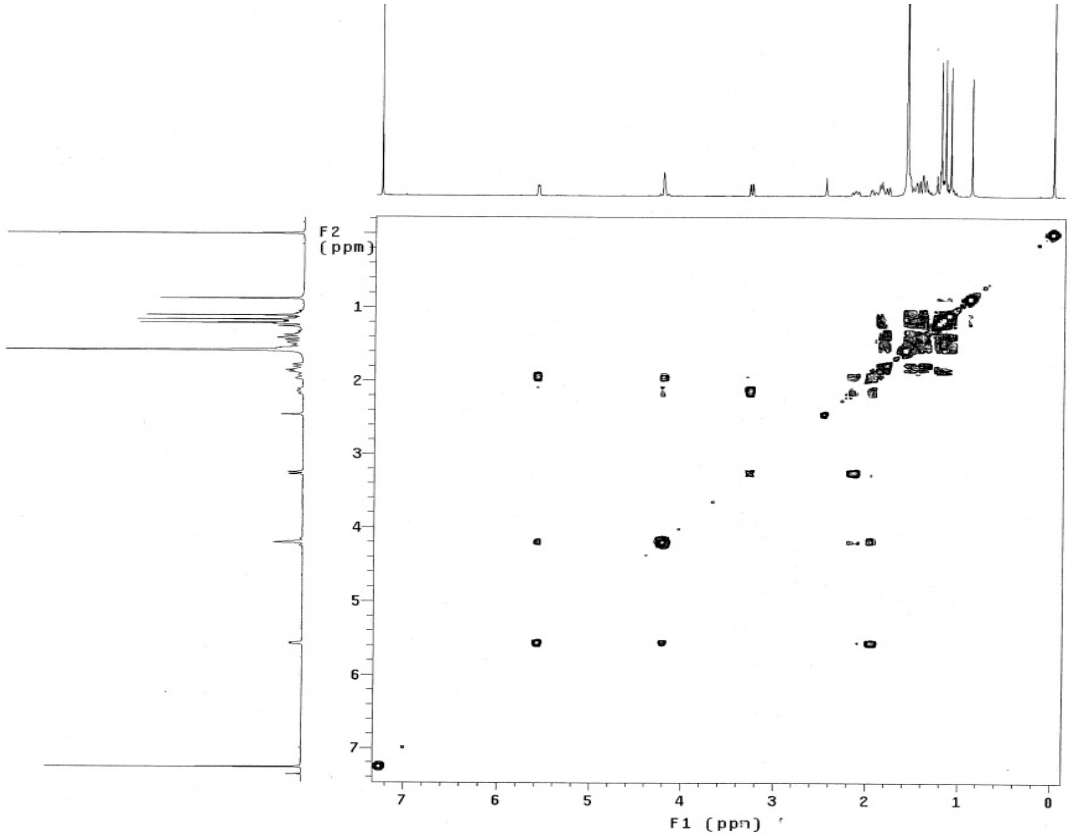



**Figure S47.** $^{13}C$ NMR spectrum of **7** in $CDCl_3$ at 100 MHz.

**Figure S48.** $^{1}H$-$^{1}H$ COSY spectrum of **7** in $CDCl_3$.



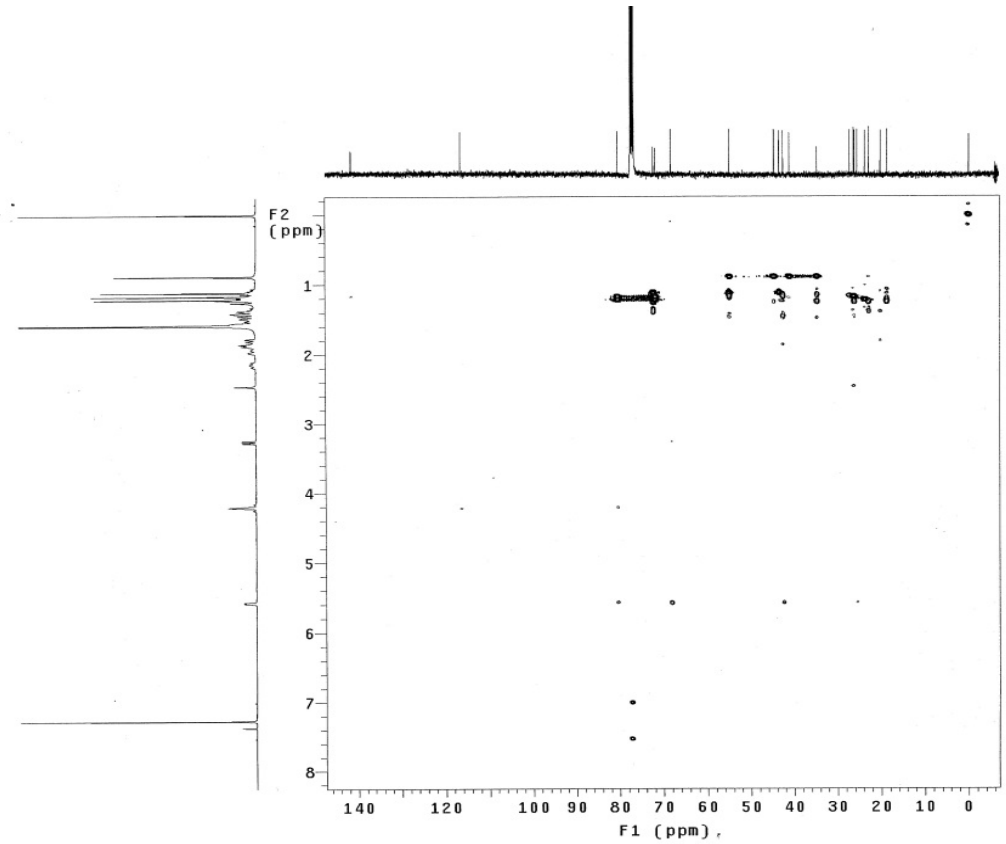



**Figure S49.** HSQC spectrum of **7** in $CDCl_3$.

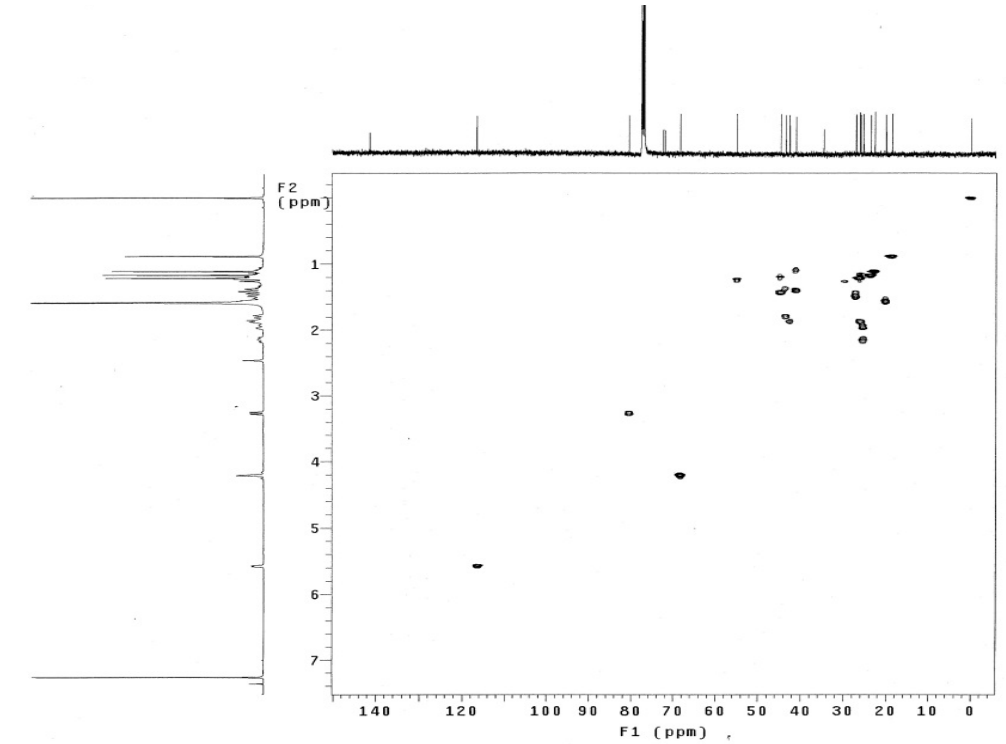



**Figure S50.** HMBC spectrum of **7** in $CDCl_3$.

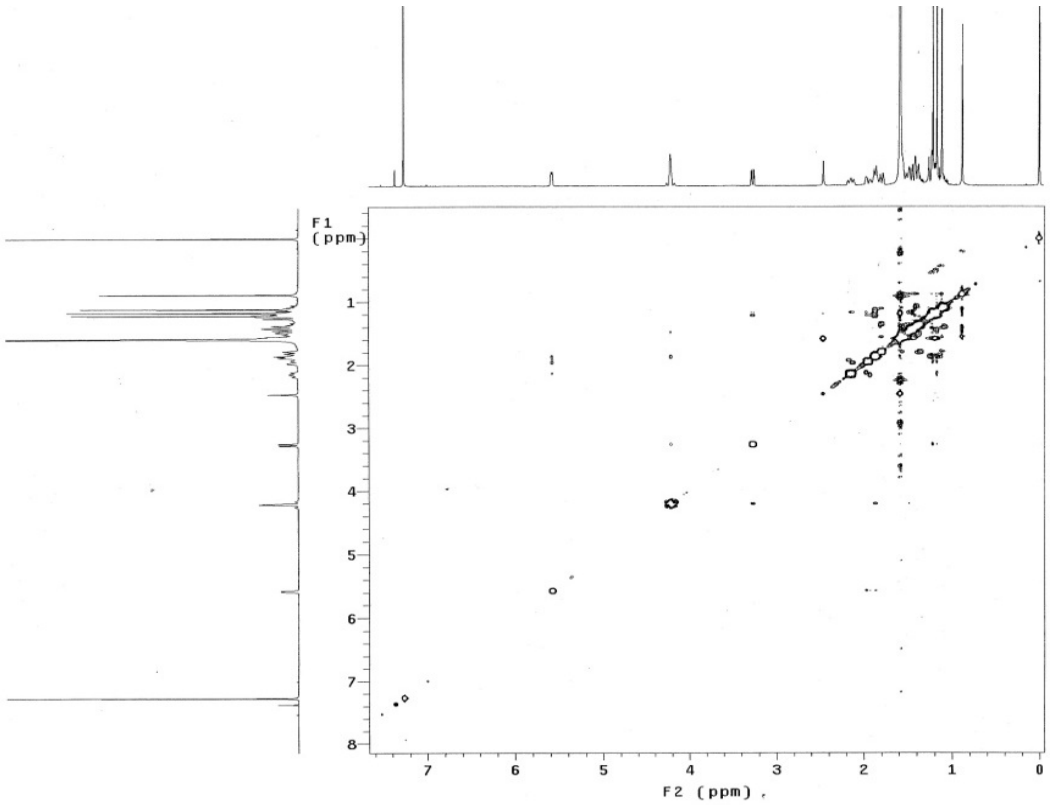
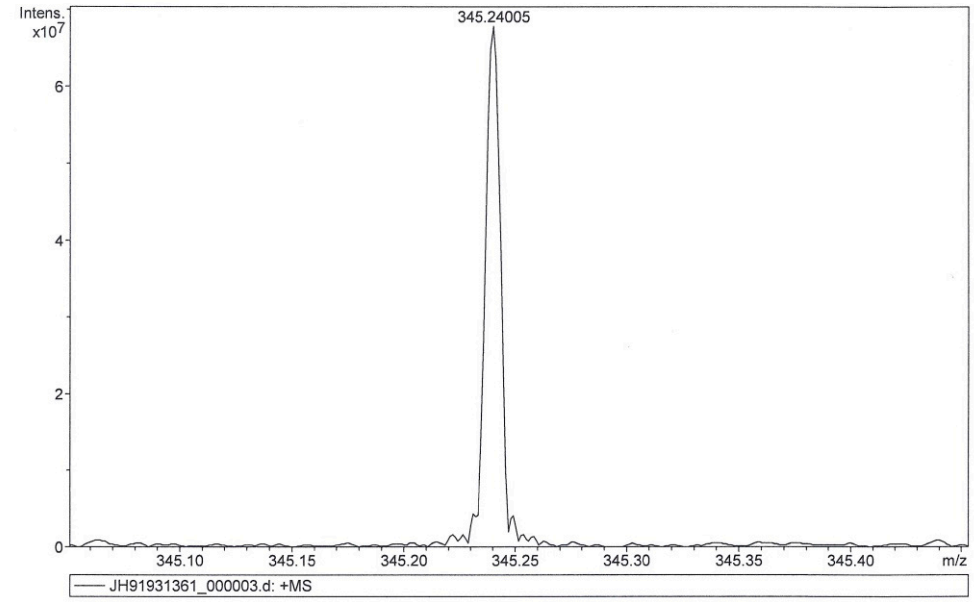



**Figure S51.** NOESY spectrum of **7** in $CDCl_3$.




| Meas. m/z | # | Formula | Score | m/z | err [mDa] | err [ppm] | mSigma | rdb | e¯ Conf | N-Rule |
|---|---|---|---|---|---|---|---|---|---|---|
| 345.24005 | 1 | C 20 H 34 Na O 3 | 100.00 | 345.24002 | -0.04 | -0.11 | 13.3 | 3.5 | even | ok |

**Figure S52.** HRESIMS spectrum of **8**.

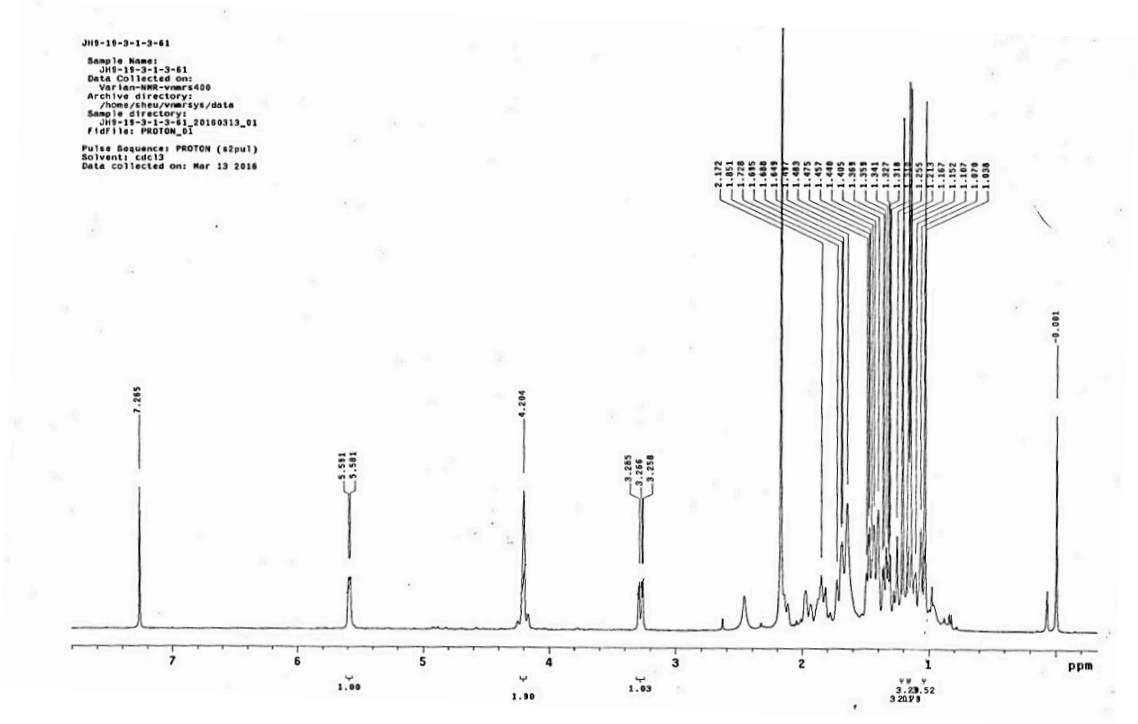



**Figure S53.** $^{1}$H NMR spectrum of **8** in $CDCl_3$ at 400 MHz.

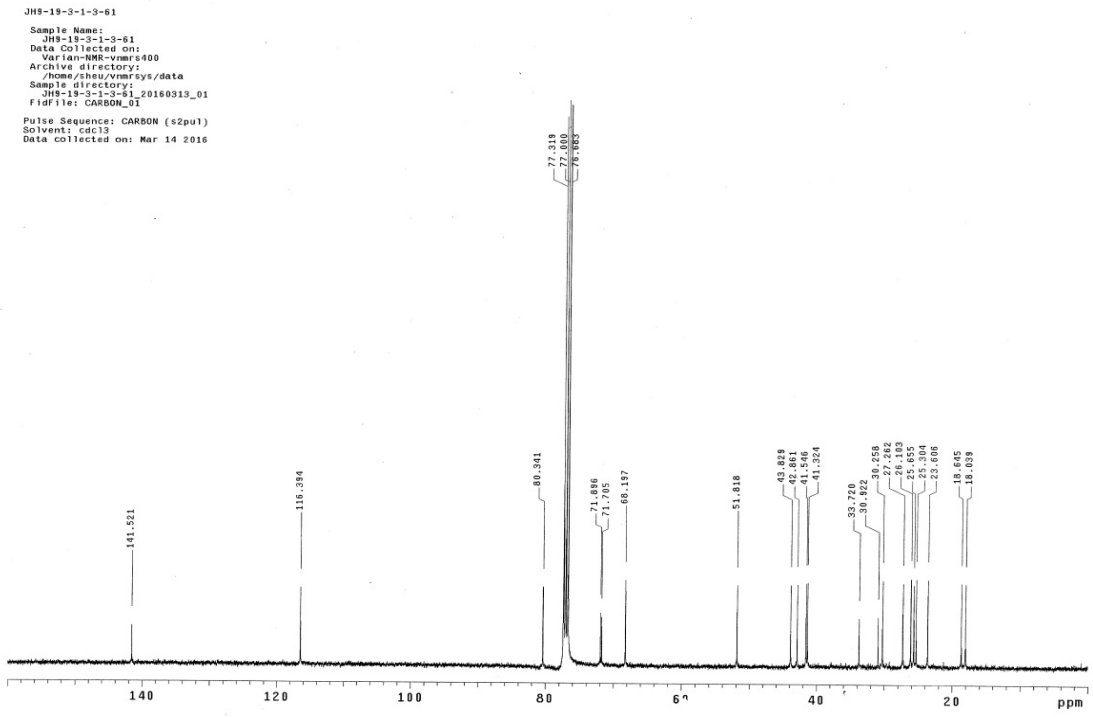



**Figure S54.** $^{13}$C NMR spectrum of **8** in $CDCl_3$ at 100 MHz.

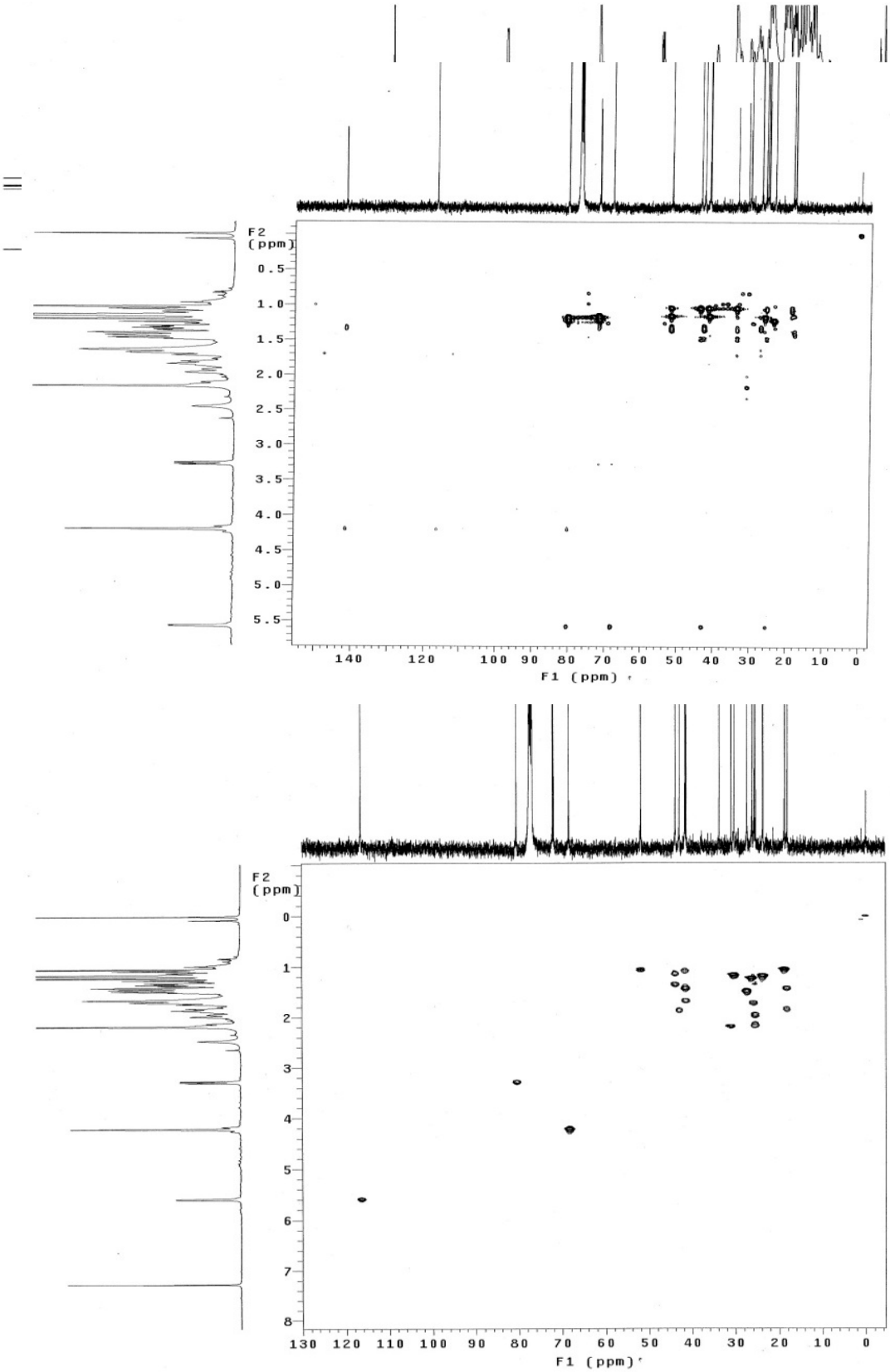
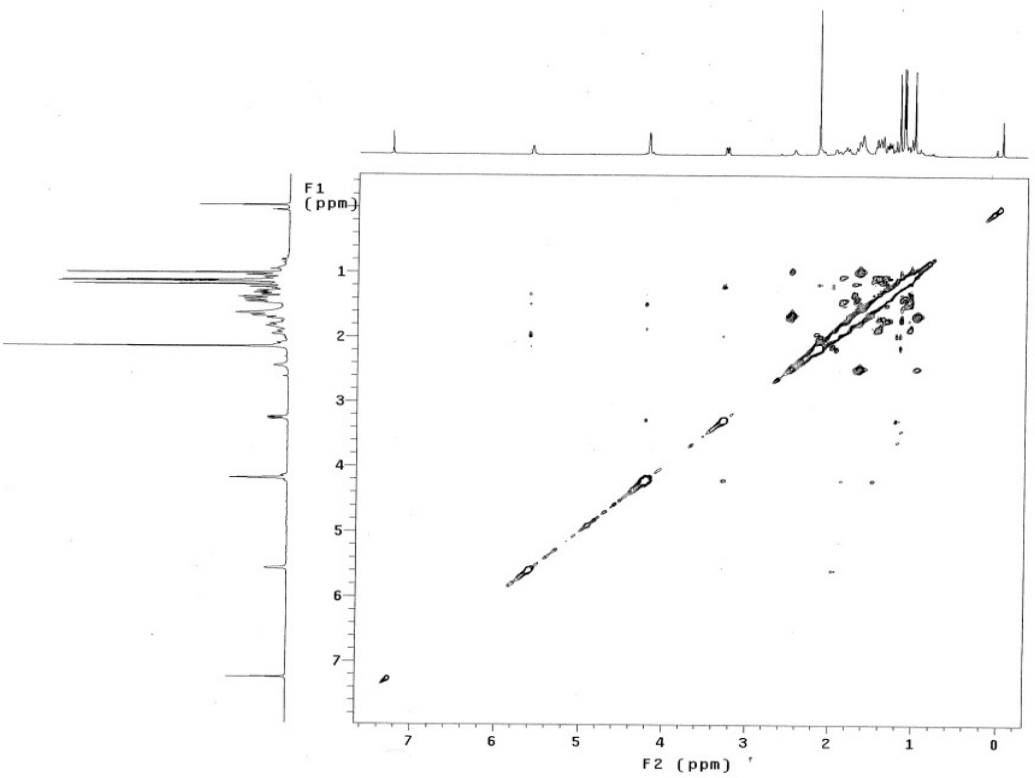


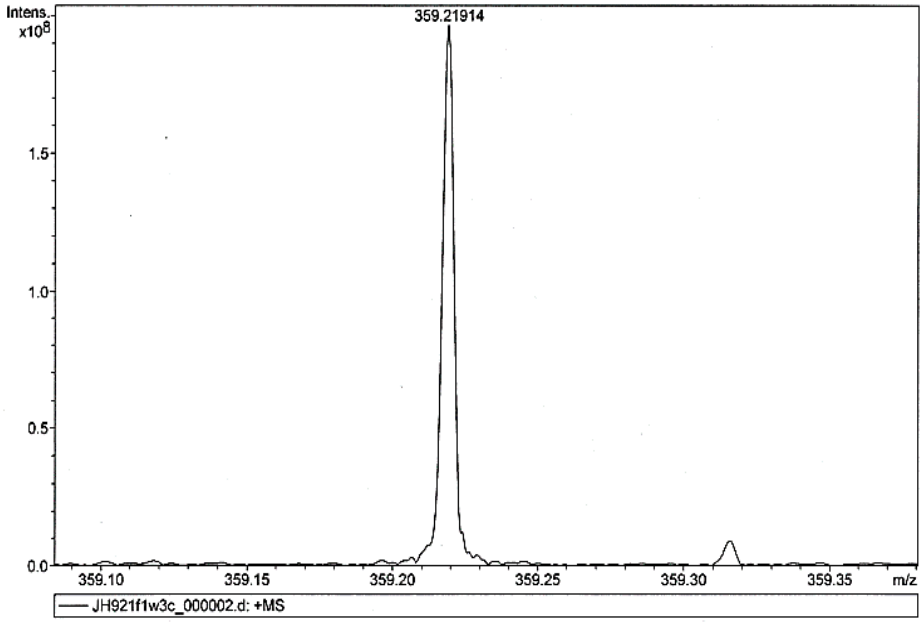

**Figure S55.** $^{1}H$-$^{1}H$ COSY spectrum of **8** in $CDCl_3$.

**Figure S56.** HSQC spectrum of **8** in $CDCl_3$.

**Figure S57.** HMBC spectrum of **8** in $CDCl_3$.

**Figure S58.** NOESY spectrum of **8** in $CDCl_3$.




| Meas. m/z | # | Formula | Score | m/z | err [mDa] | err [ppm] | mSigma | rdb | e⁻ Conf | N-Rule |
|---|---|---|---|---|---|---|---|---|---|---|
| 359.21914 | 1 | C 20 H 32 Na O 4 | 100.00 | 359.21928 | 0.14 | 0.40 | 9.4 | 4.5 | even | ok |

**Figure S59.** HRESIMS spectrum of **9**.

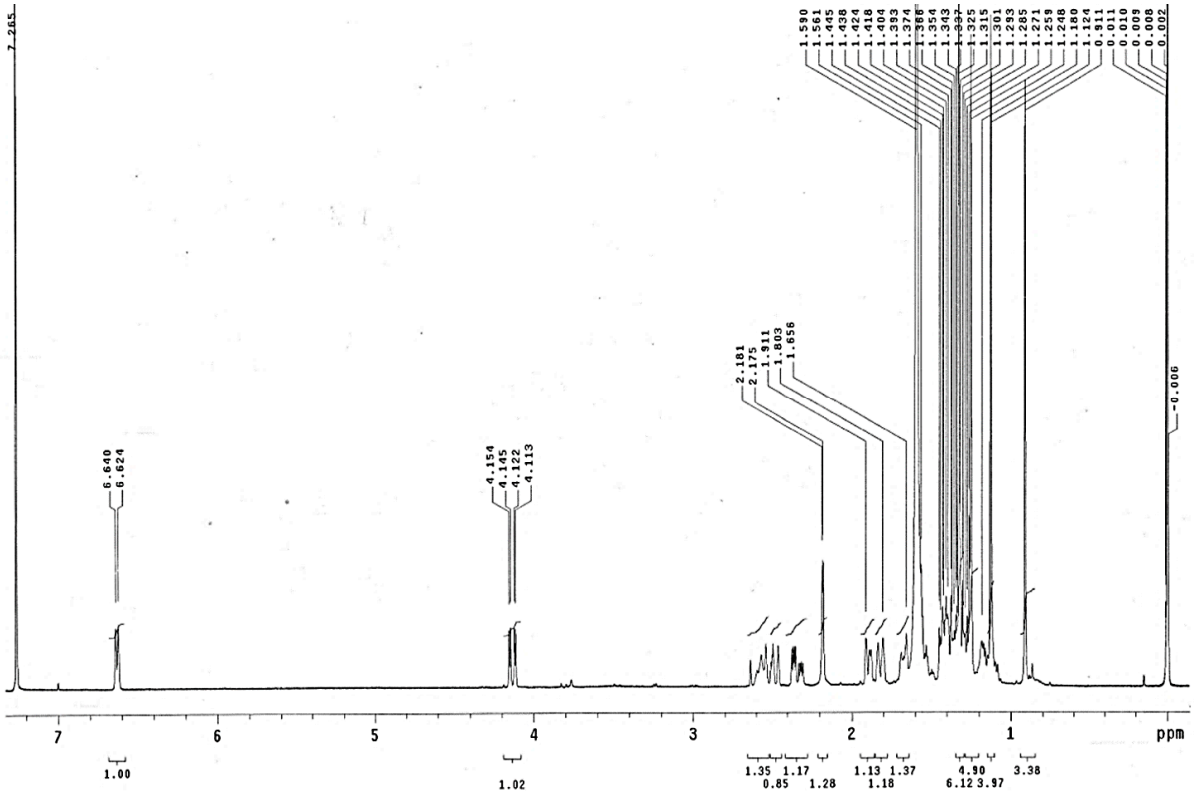


**Figure S60.** $^{1}$H NMR spectrum of **9** in $CDCl_3$ at 400 MHz.

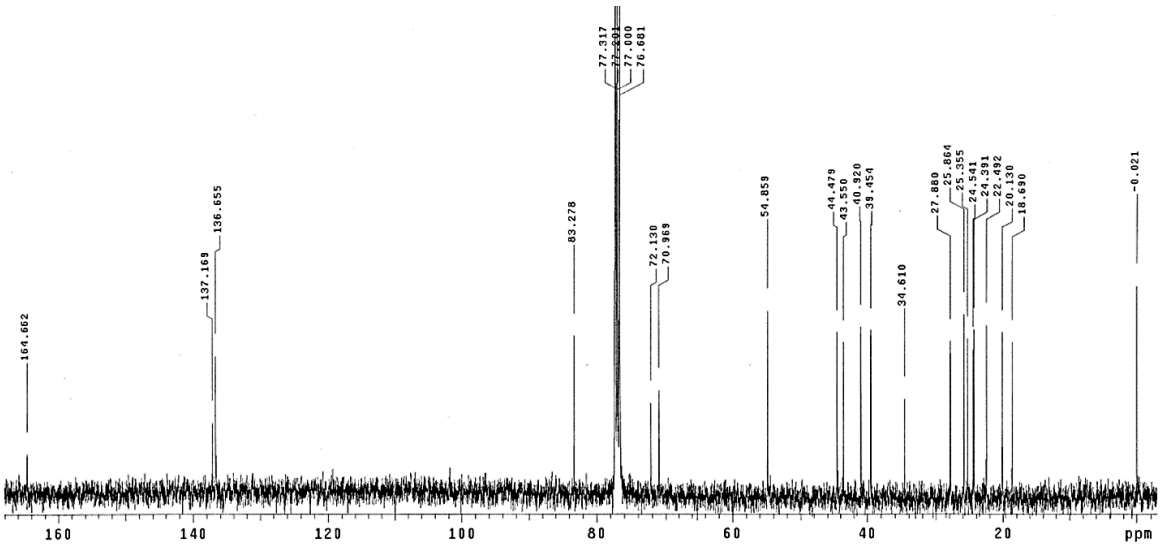


**Figure S61.** $^{13}$C NMR spectrum of **9** in $CDCl_3$ at 100 MHz.

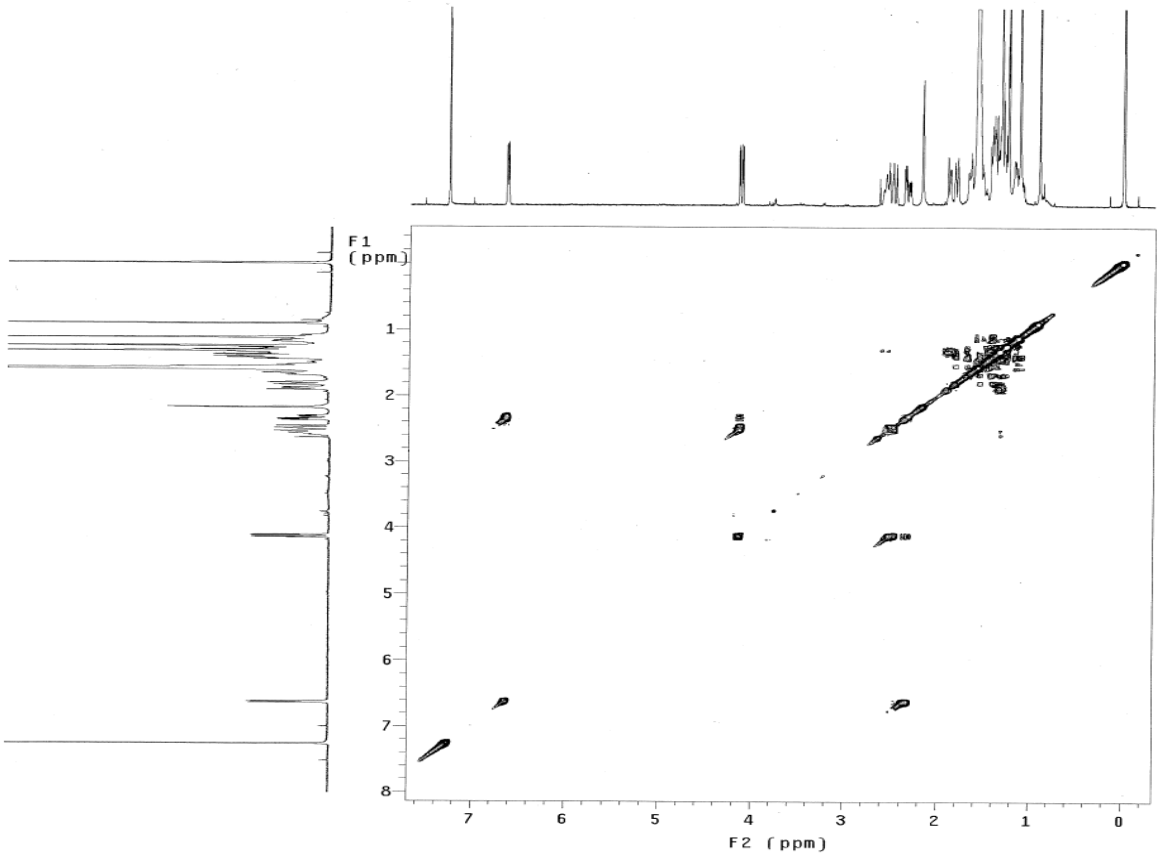



**Figure S62.** $^{1}H$-$^{1}H$ COSY spectrum of **9** in $CDCl_3$.

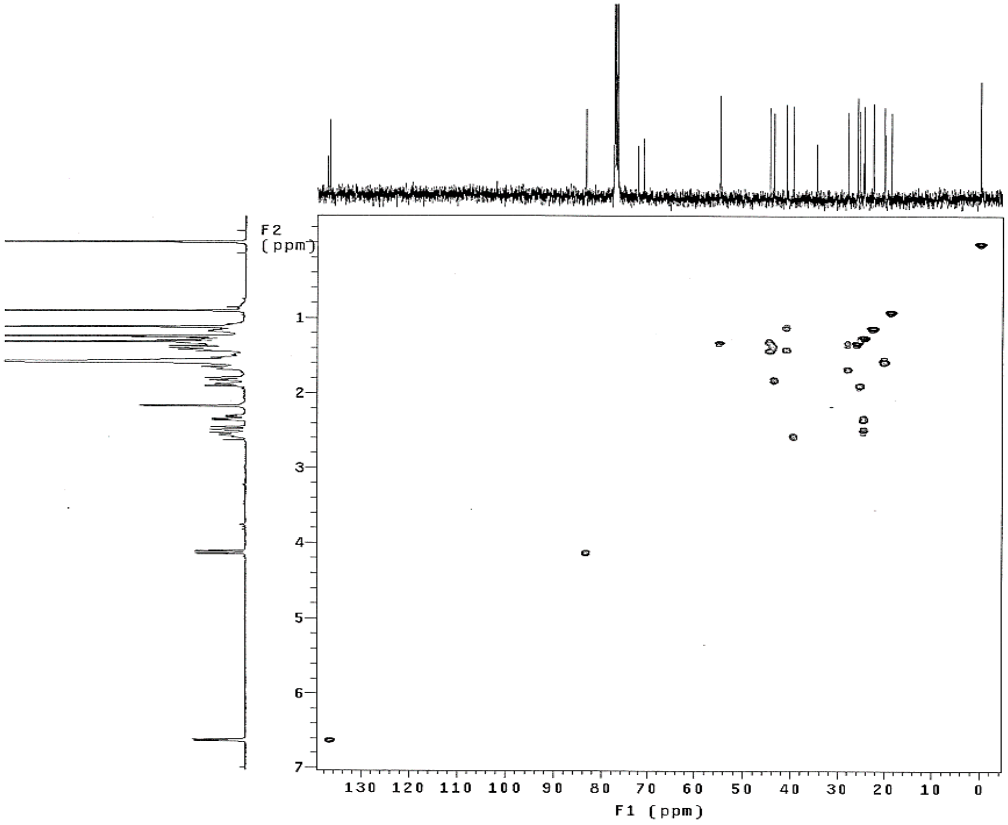



**Figure S63.** HSQC spectrum of **9** in $CDCl_3$.

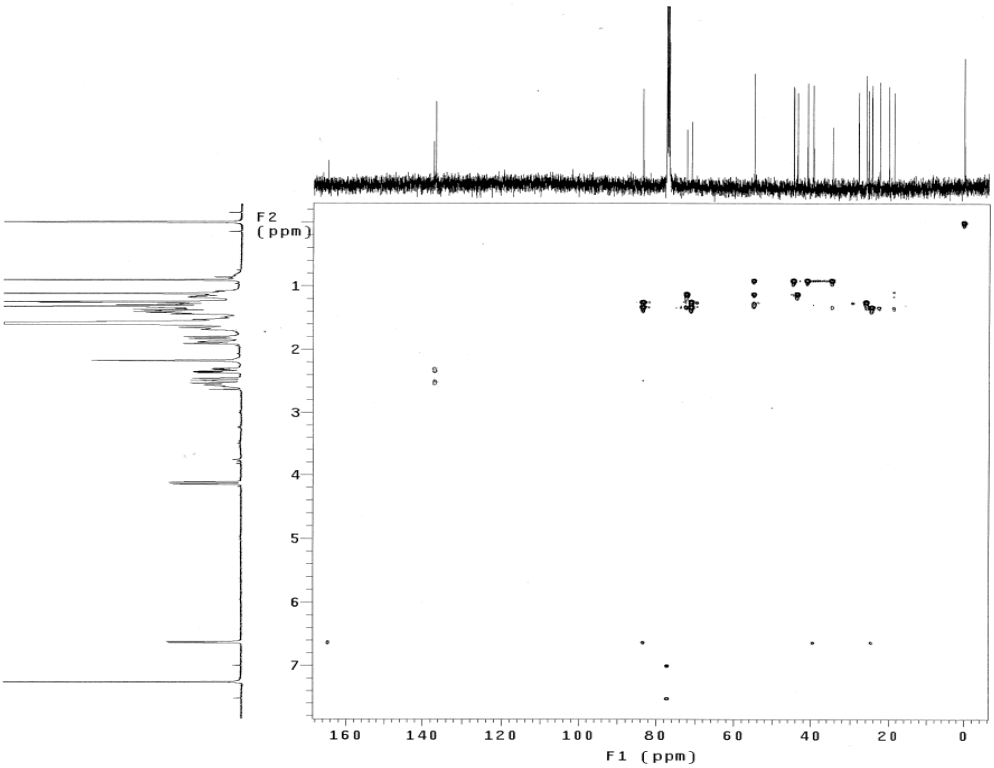



**Figure S64.** HMBC spectrum of **9** in $CDCl_3$.

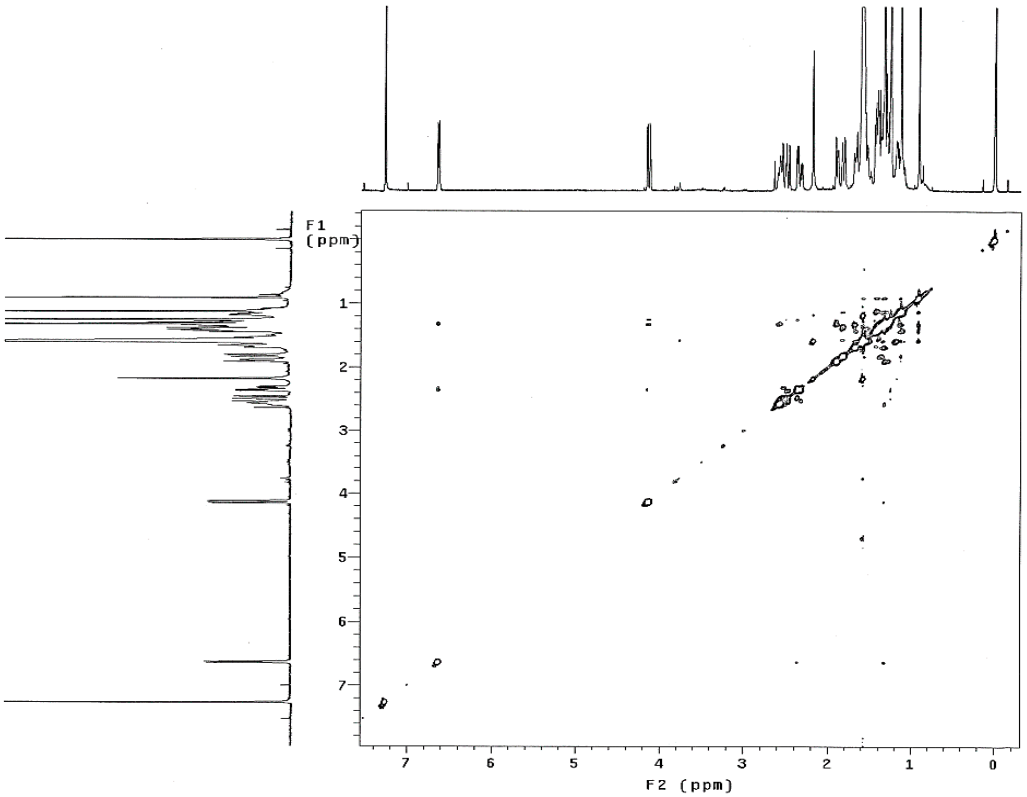
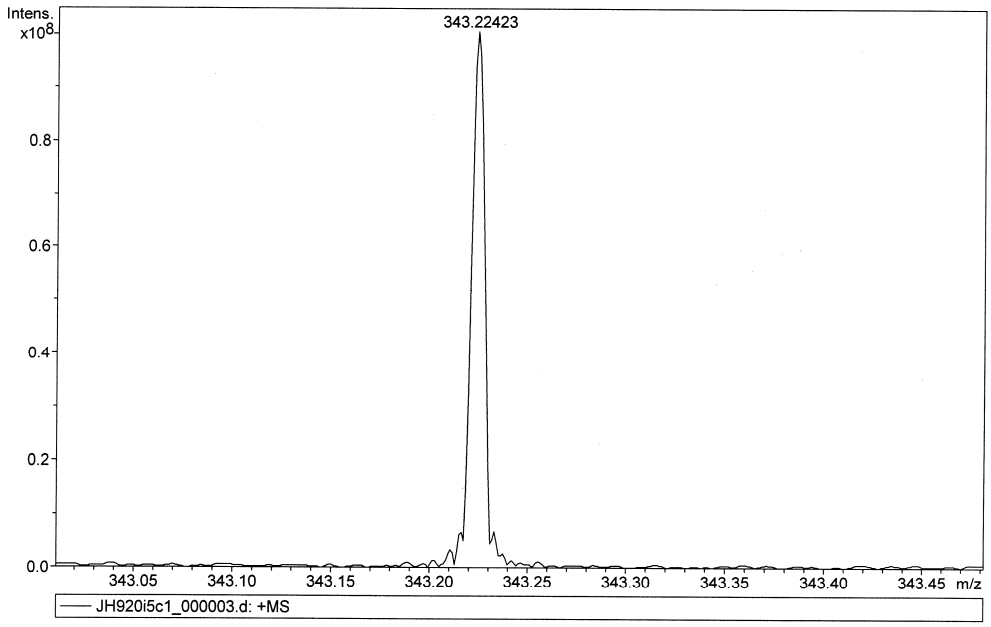



**Figure S65.** NOESY spectrum of **9** in $CDCl_3$.




| Meas. m/z | # | Formula | Score | m/z | err [mDa] | err [ppm] | mSigma | rdb | e⁻ Conf | N-Rule |
|---|---|---|---|---|---|---|---|---|---|---|
| 343.22423 | 1 | C 20 H 32 Na O 3 | 100.00 | 343.22437 | 0.13 | 0.39 | 17.0 | 4.5 | even | ok |

**Figure S66.** HRESIMS spectrum of **10**.

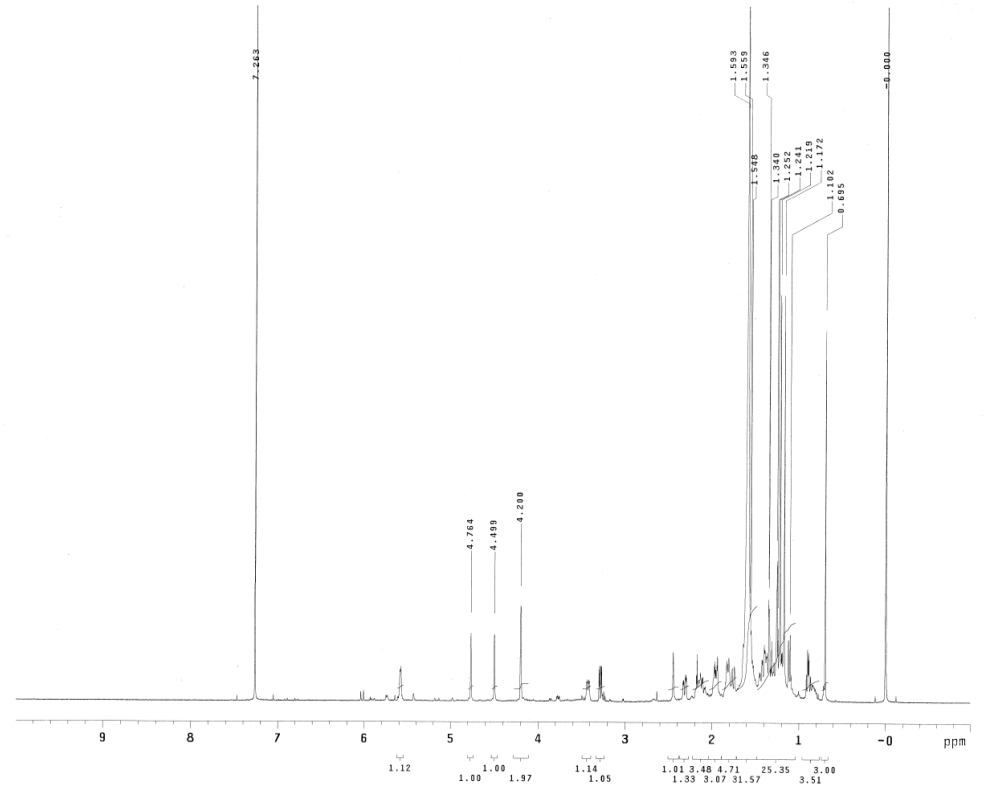



**Figure S67.** $^{1}$H NMR spectrum of **10** in $CDCl_3$ at 500 MHz.

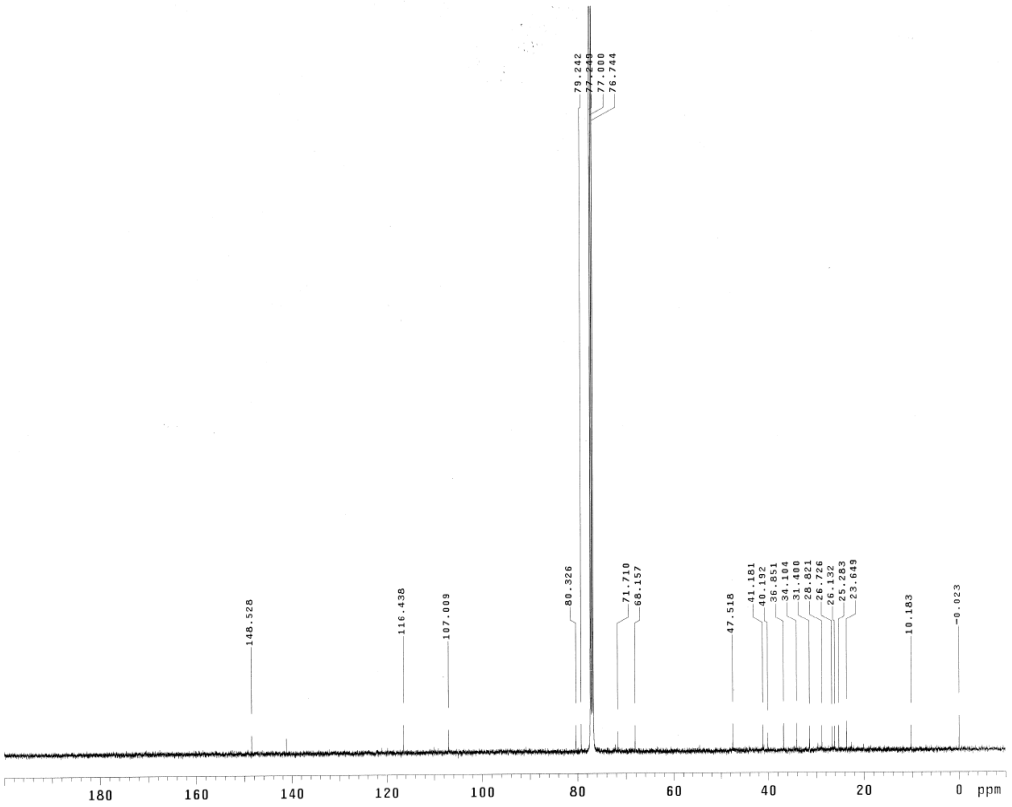



**Figure S68.** $^{13}$C NMR spectrum of **10** in $CDCl_3$ at 125 MHz.

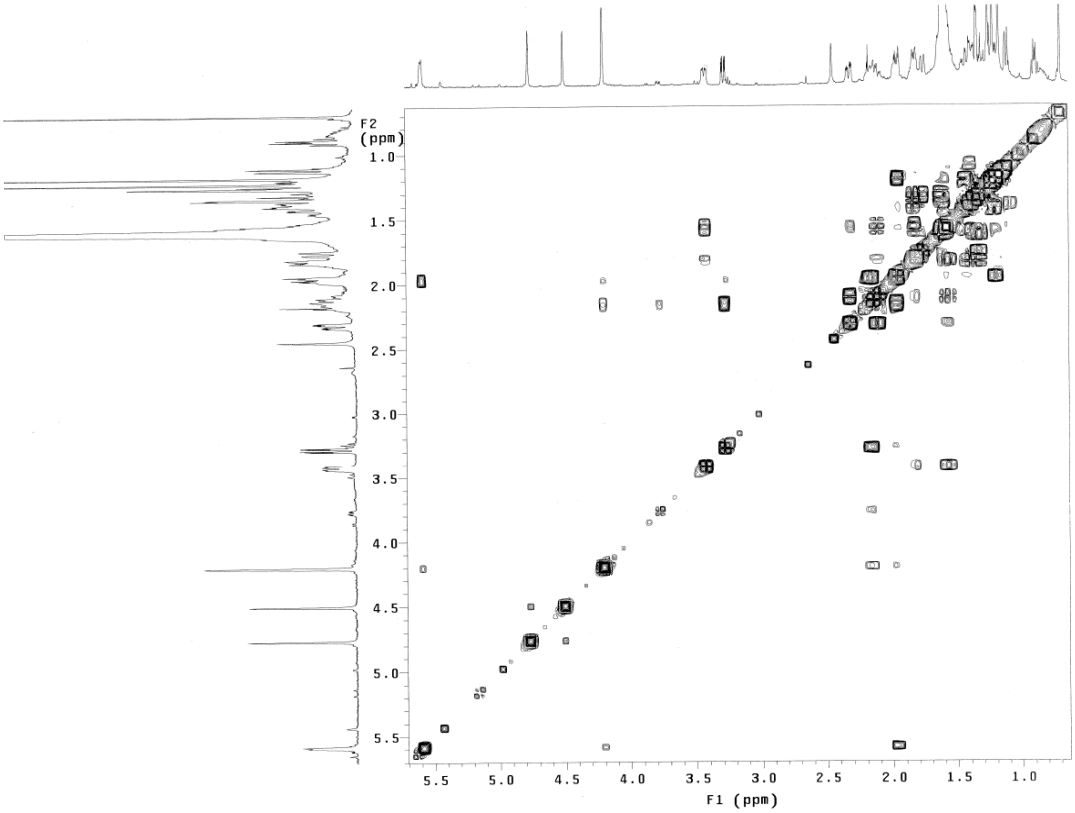



**Figure S69.** $^{1}$H-$^{1}$H COSY spectrum of **10** in $CDCl_3$.

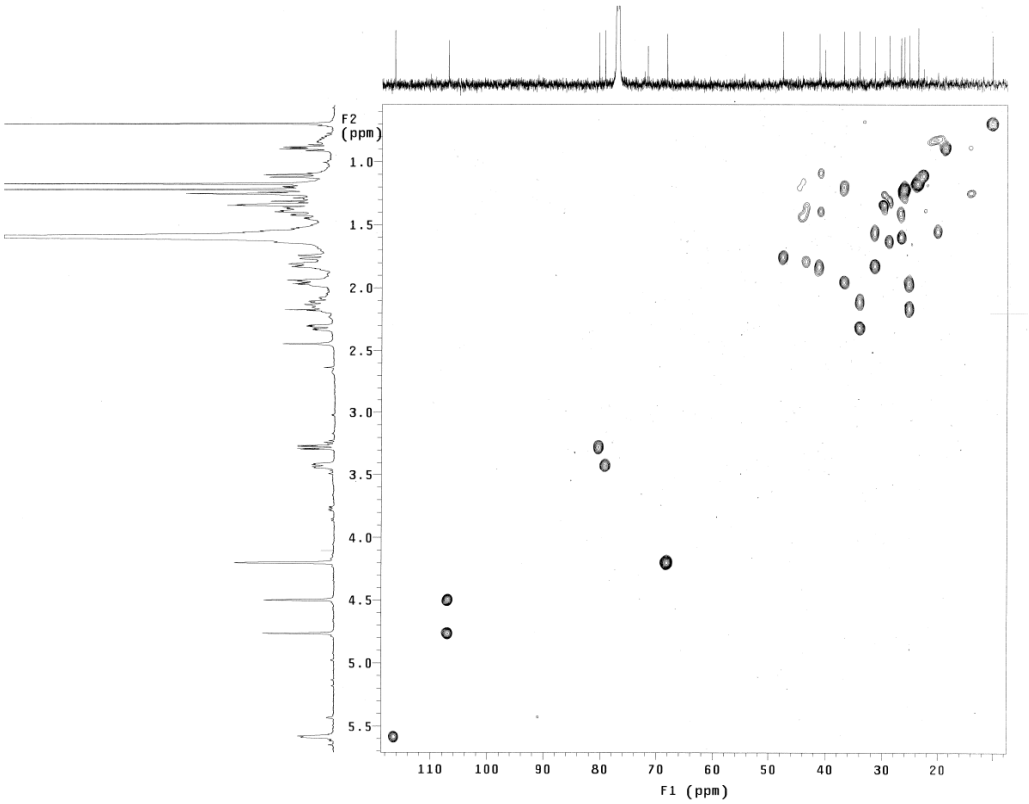



**Figure S70.** HSQC spectrum of **10** in $CDCl_3$.

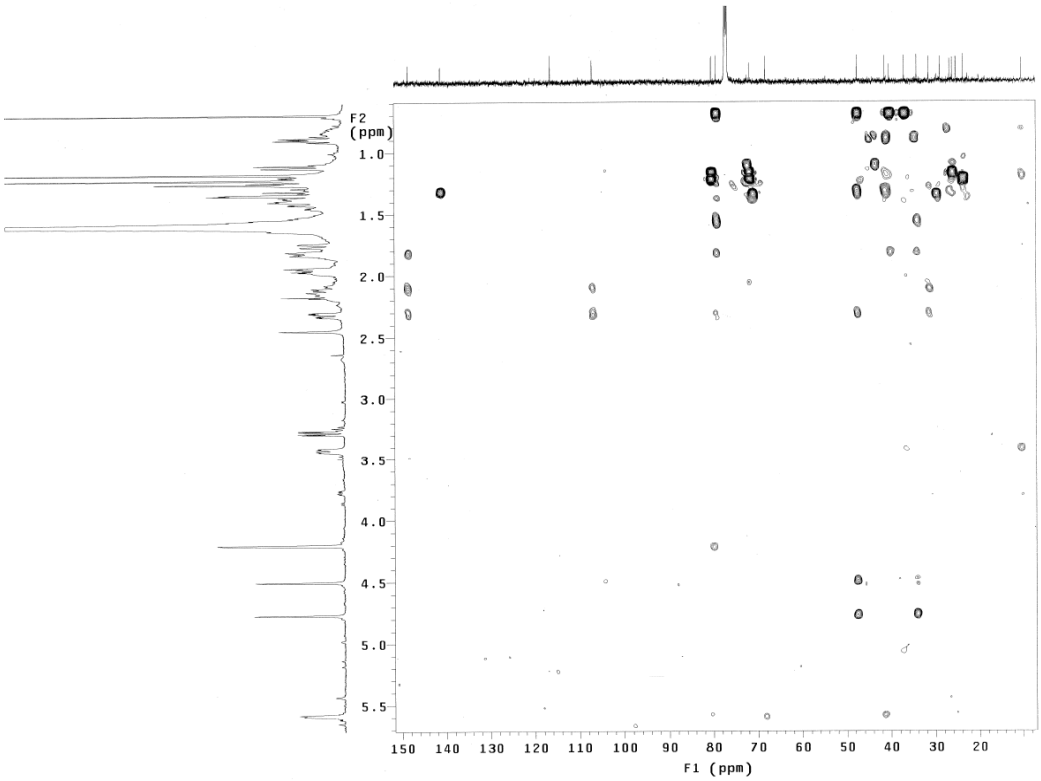



**Figure S71.** HMBC spectrum of **10** in $CDCl_3$.

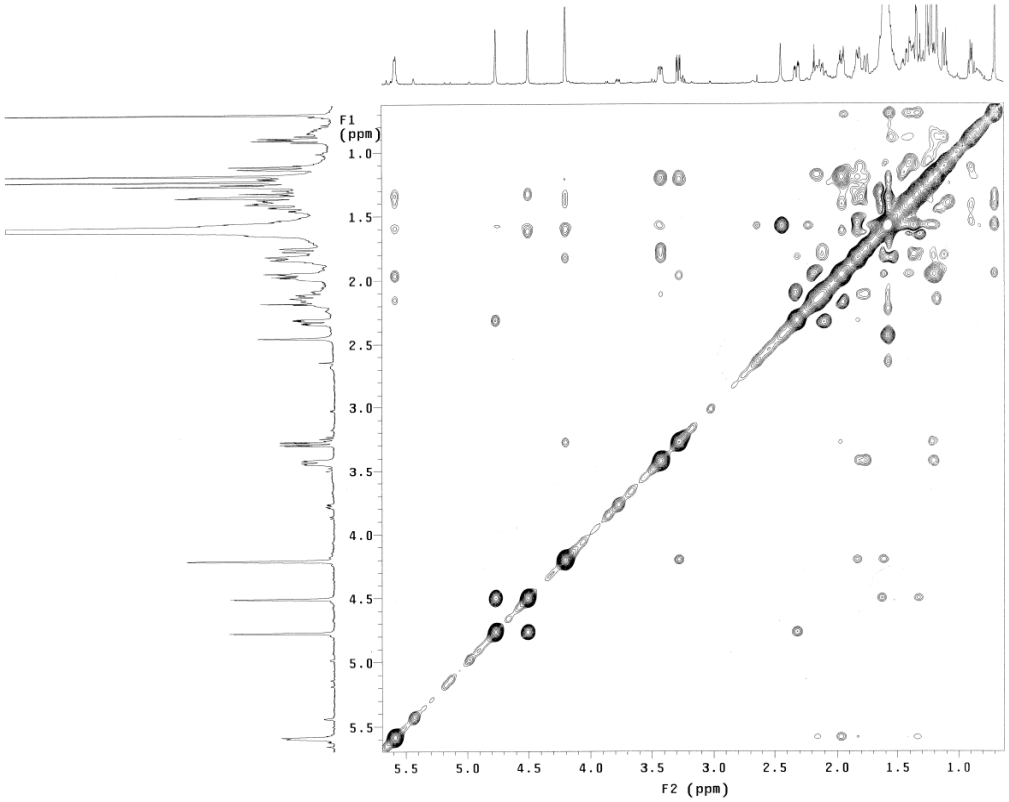
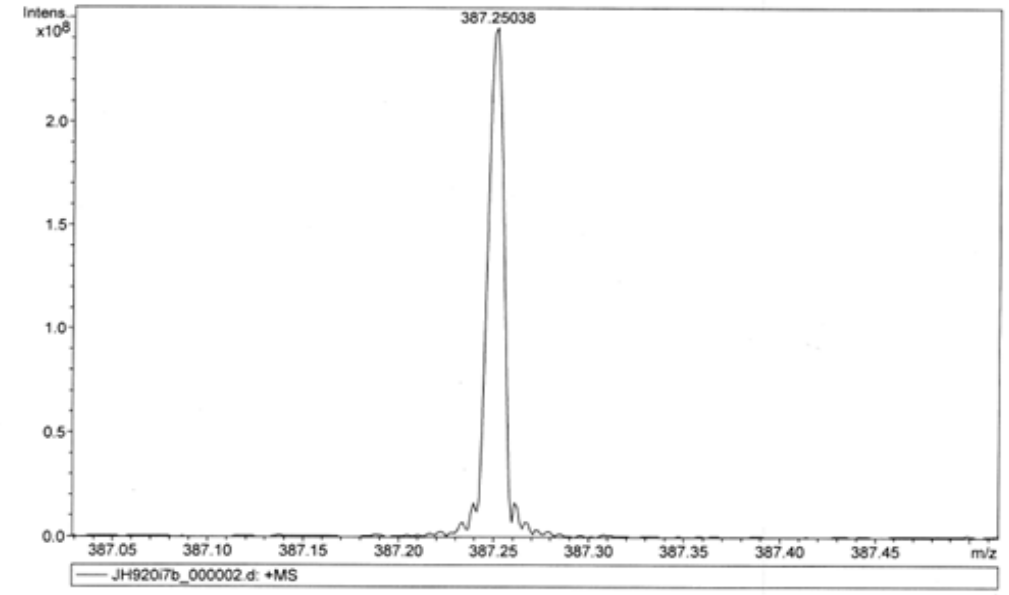



**Figure S72.** NOESY spectrum of **10** in $CDCl_3$.




| Meas. m/z | # | Formula | Score | m/z | err [mDa] | err [ppm] | mSigma | rdb | e⁻ Conf | N-Rule |
|---|---|---|---|---|---|---|---|---|---|---|
| 387.25038 | 1 | C 22 H 36 Na O 4 | 100.00 | 387.25058 | 0.20 | 0.51 | 4.2 | 4.5 | even | ok |

**Figure S73.** HRESIMS spectrum of **11**.

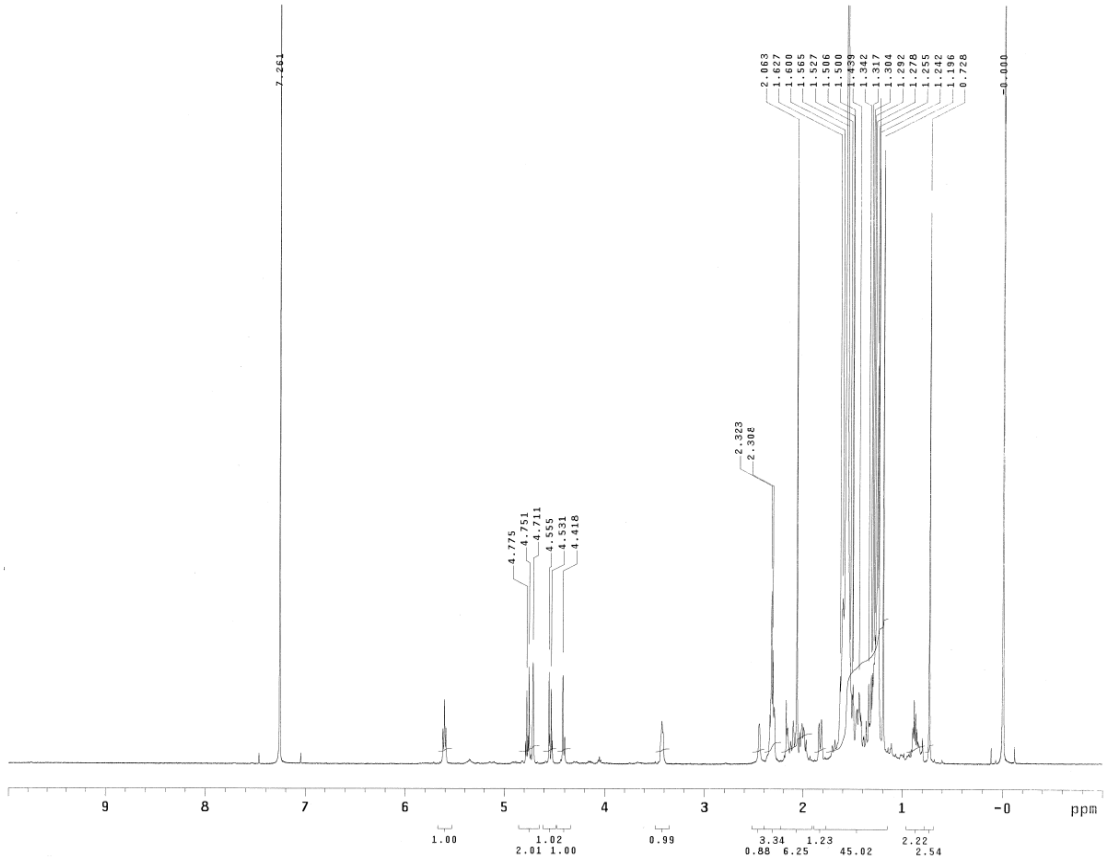



**Figure S74.** $^{1}$H NMR spectrum of **11** in $CDCl_3$ at 500 MHz.

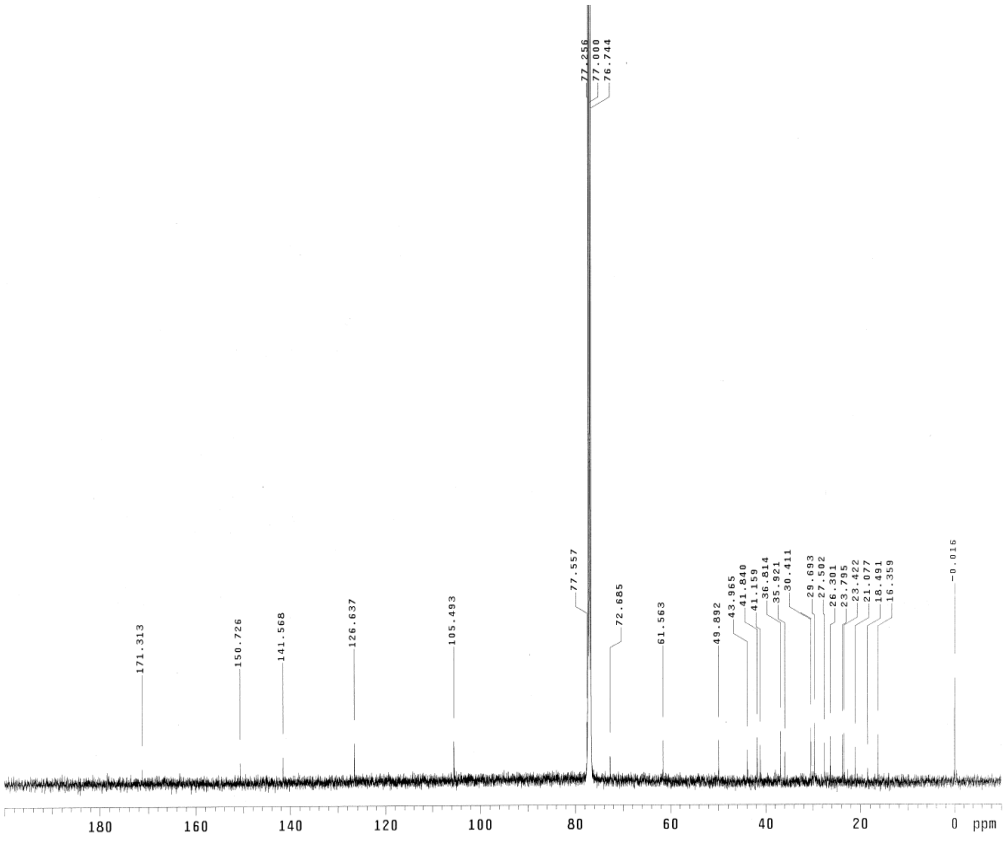



**Figure S75.** $^{13}$C NMR spectrum of **11** in $CDCl_3$ at 125 MHz.

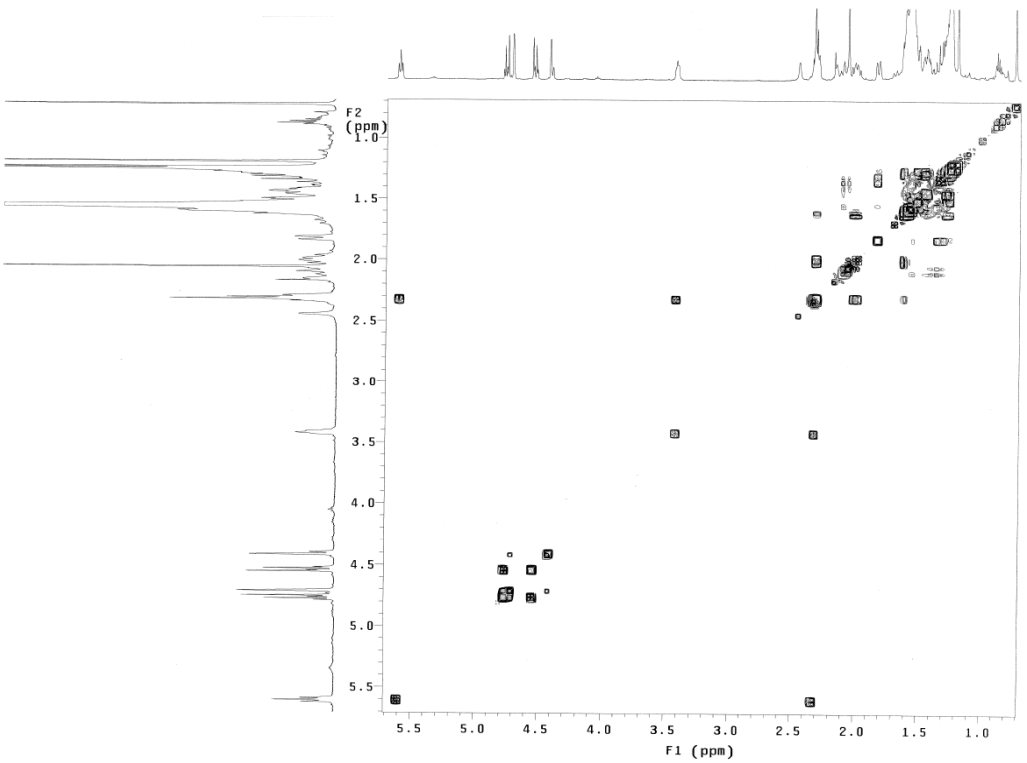



**Figure S76.** $^{1}$H-$^{1}$H COSY spectrum of **11** in $CDCl_3$.

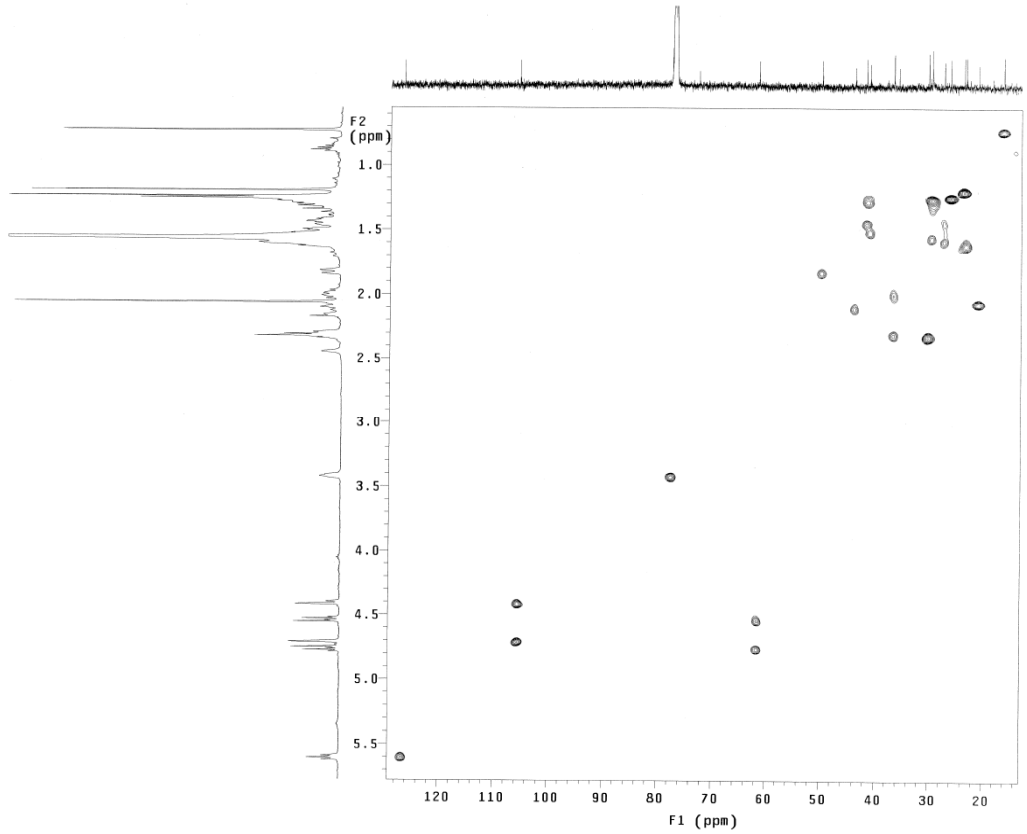



**Figure S77.** HSQC spectrum of **11** in $CDCl_3$.

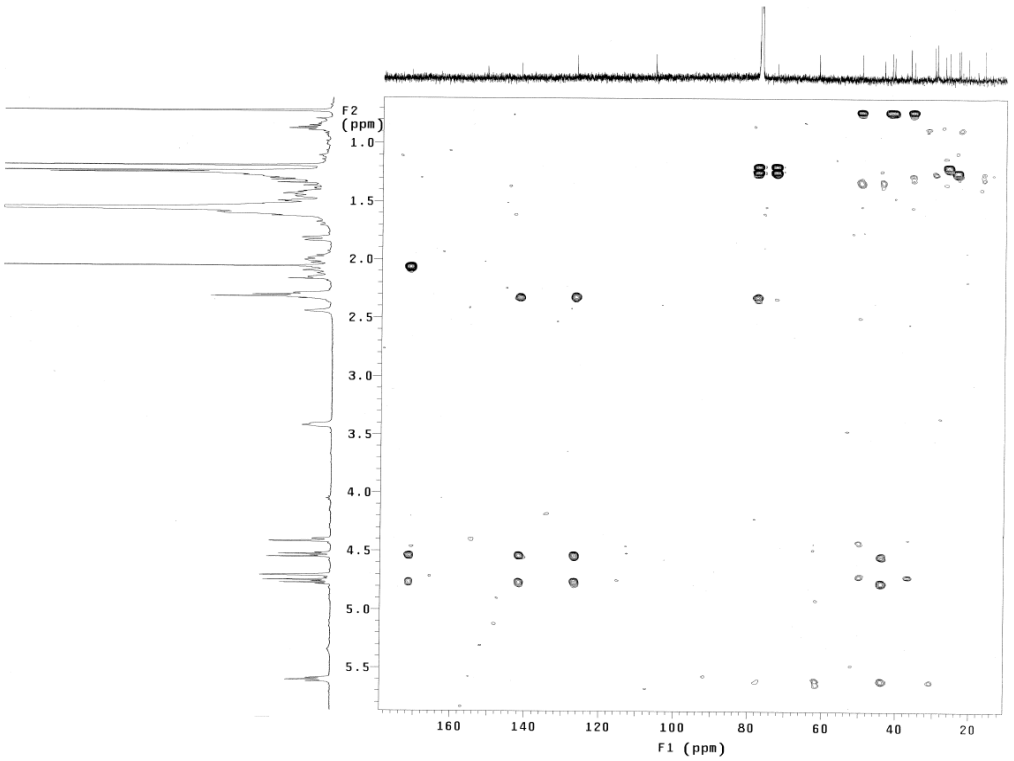



**Figure S78.** HMBC spectrum of **11** in $CDCl_3$.

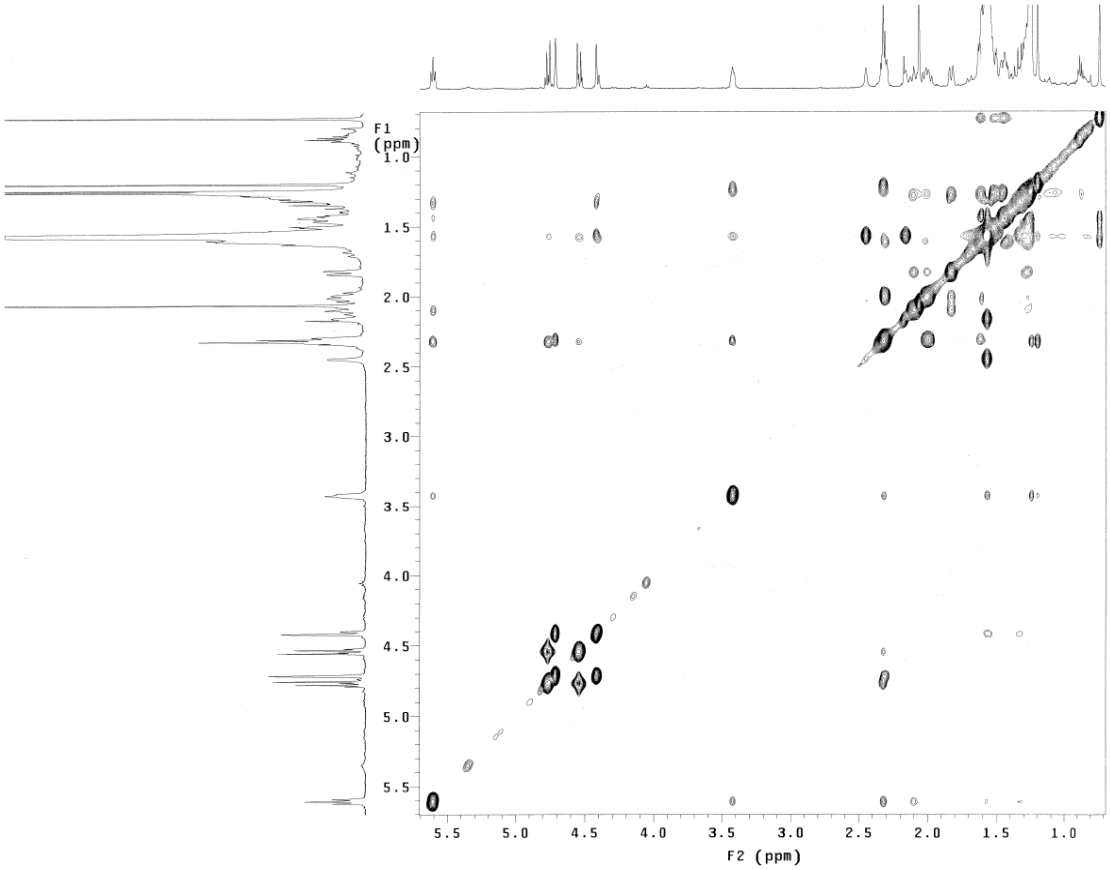



**Figure S79.** NOESY spectrum of **11** in $CDCl_3$.