

Supplementary data

Table of contents

Fig. S1. HR-DART-MS spectrum of compound **1**

Fig. S2. IR spectrum of compound **1**

Fig. S3. ^1H NMR spectrum of compound **1** (500 MHz, methanol- d_4)

Fig. S4. ^{13}C NMR spectrum of compound **1** (125 MHz, methanol- d_4)

Fig. S5. ^1H ^{13}C HSQC spectrum of compound **1**

Fig. S6. ^1H ^1H COSY spectrum of compound **1**

Fig. S7. ^1H ^{13}C HMBC spectrum of compound **1**

Fig. S8. ^1H ^1H NOESY spectrum of compound **1**

Fig. S9. HR-DART-MS spectrum of compound **2**

Fig. S10. IR spectrum of compound **2**

Fig. S11. ^1H NMR spectrum of compound **2** (500 MHz, methanol- d_4)

Fig. S12. ^{13}C NMR spectrum of compound **2** (125 MHz, methanol- d_4)

Fig. S13. ^1H ^{13}C HSQC spectrum of compound **2**

Fig. S14. ^1H ^1H COSY spectrum of compound **2**

Fig. S15. ^1H ^{13}C HMBC spectrum of compound **2**

Fig. S16. ^1H ^1H NOESY spectrum of compound **2**

Fig. S1. HR-DART-MS spectrum of compound **1**

Data:201027_PV1200_DV1950_300C

Sample Name:

Description:

Ionization Mode:ESI+

History:Determine m/z[Peak Detect[Centroid,25,Area];Correct Base[5.0%]];Correct Base[5.0%];Average(MS[1] 19....

Acquired:10/27/2020 12:53:36 PM

Operator:Administrator

Mass Calibration data:201027_2

Created:10/27/2020 3:51:06 PM

Created by:Administrator

Charge number:1

Tolerance:5.00(mmu)

Unsaturation Number:-1.5 .. 20.0 (Fraction:Both)

Element:¹²C:0 .. 100, ¹H:0 .. 200, ¹⁴N:1 .. 1, ¹⁶O:0 .. 10

Mass	Intensity	Relative Intensity	Calc. Mass	Mass Difference (mmu)	Possible Formula	Unsaturation Number
338.16009	78766.00	72.30	338.16036	-0.27	¹² C ₁₇ ¹ H ₂₄ ¹⁴ N ₁ ¹⁶ O ₆	6.5

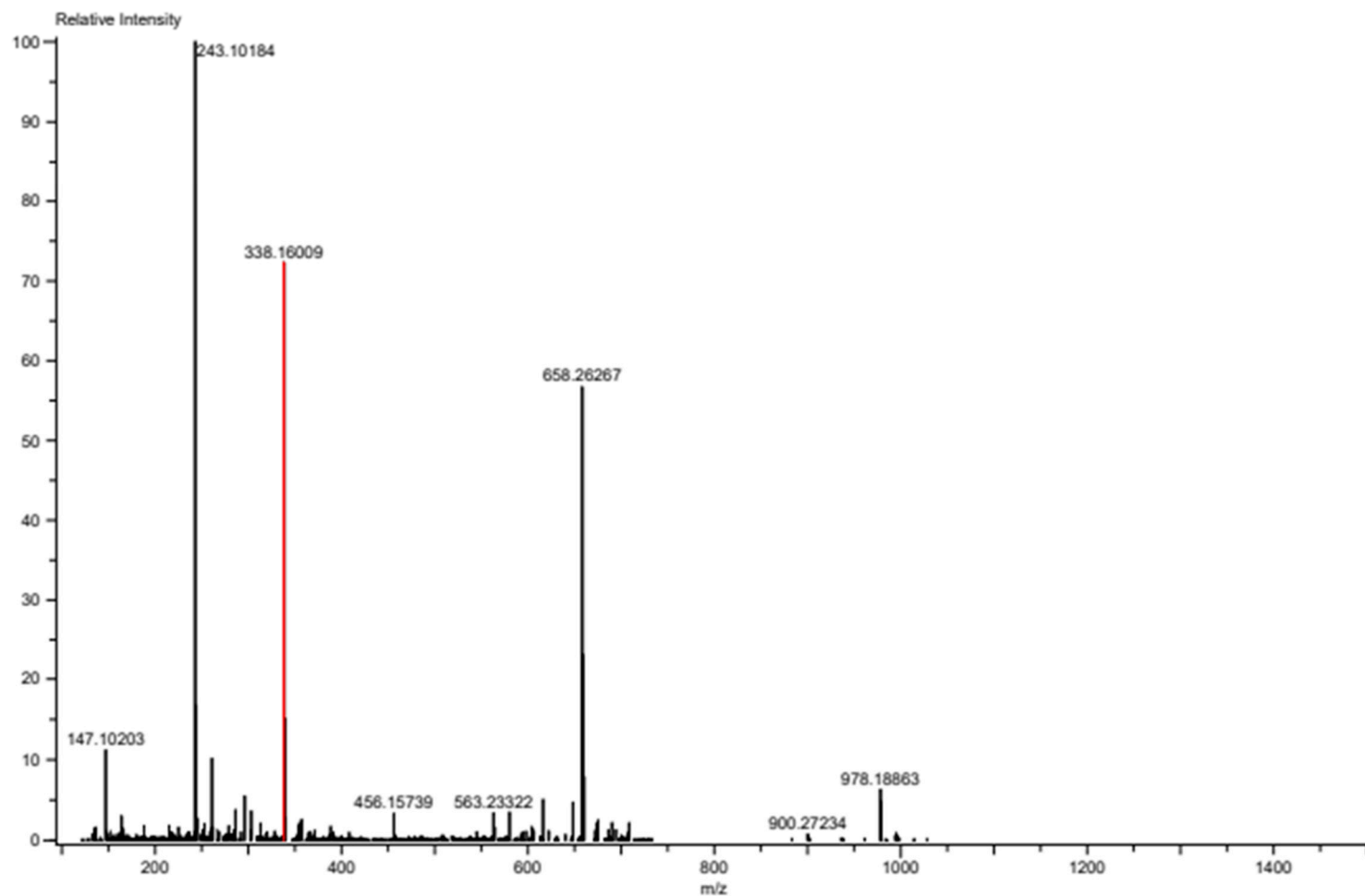


Fig. S2. IR spectrum of compound **1**

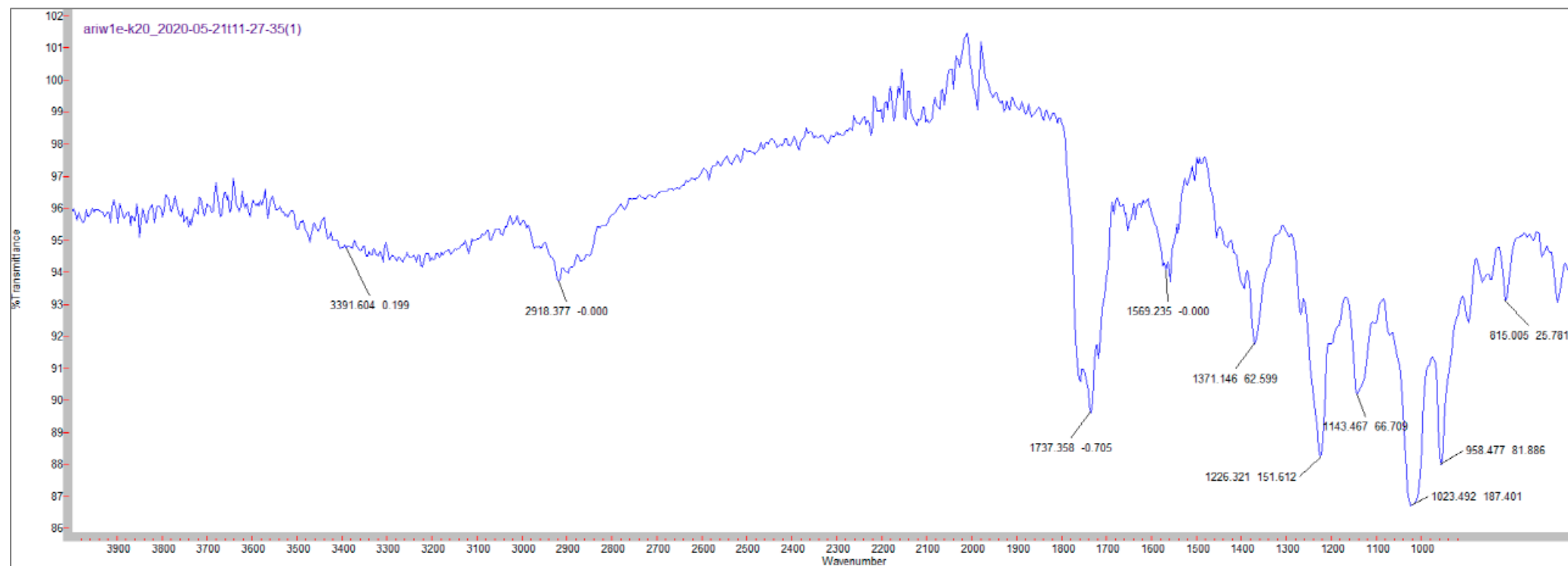


Fig. S3. ^1H NMR spectrum of compound **1** (500 MHz, methanol- d_4)

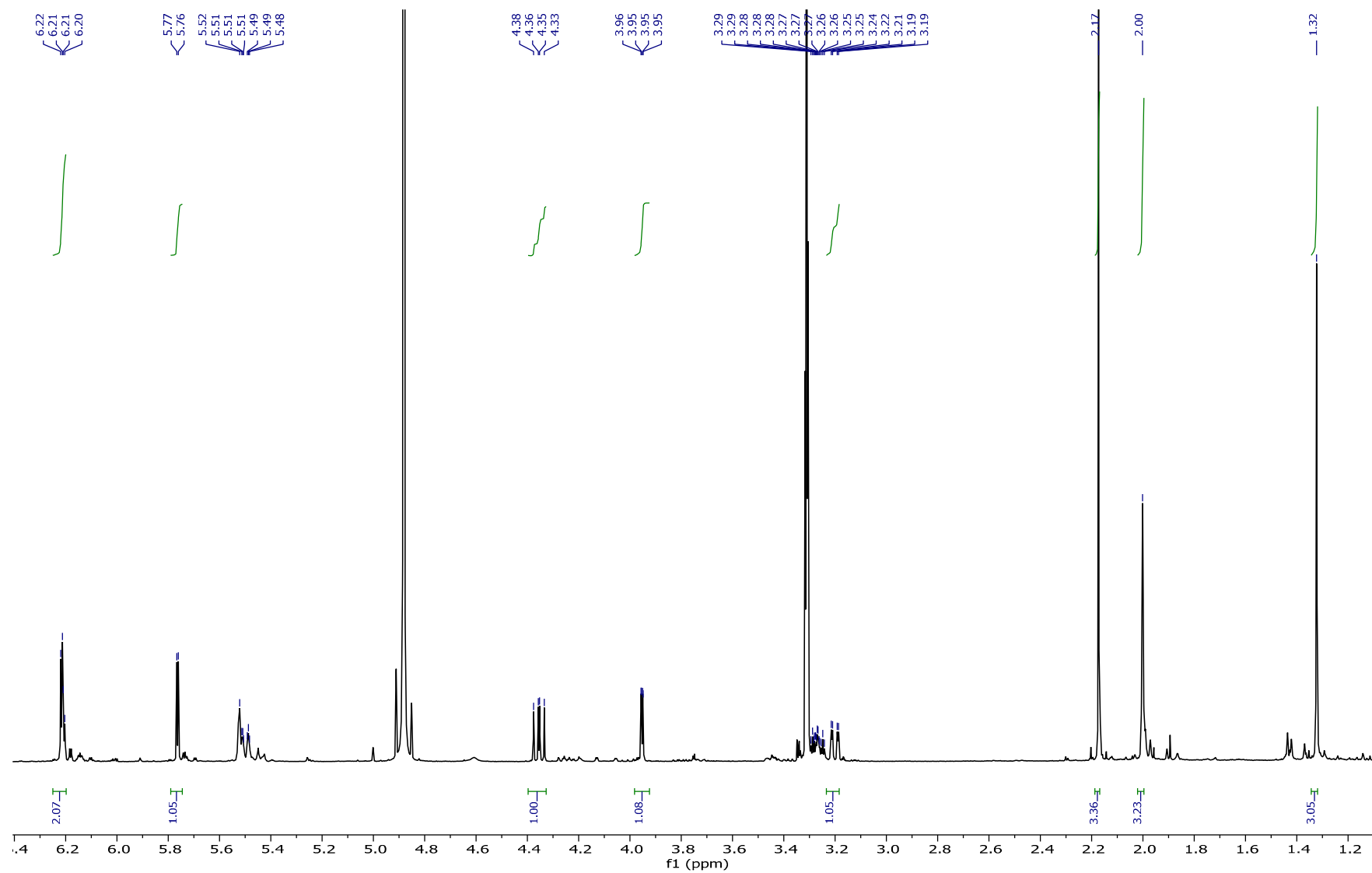


Fig. S4. ^{13}C NMR spectrum of compound **1** (125 MHz, methanol- d_4)

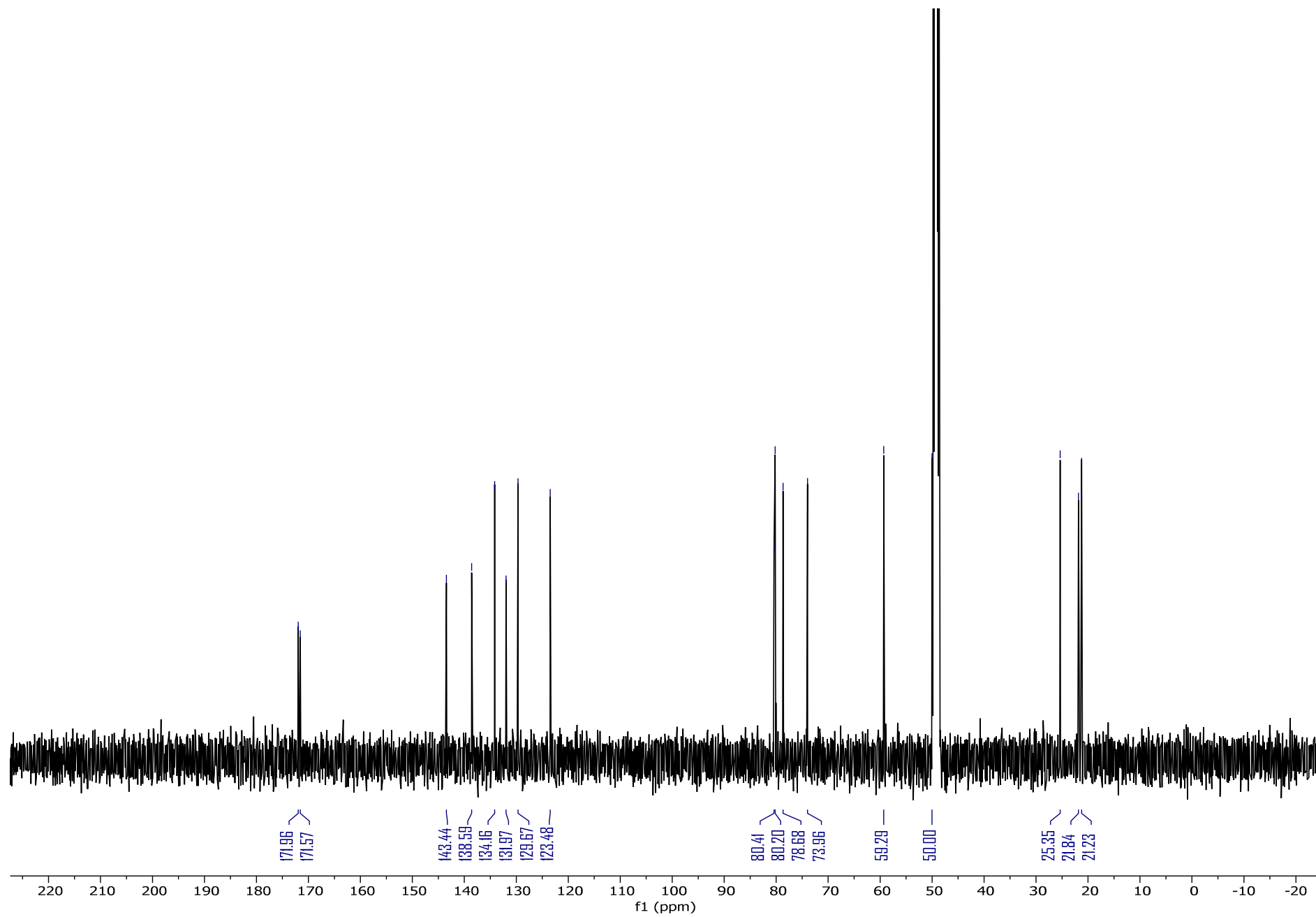


Fig. S5. ^1H ^{13}C HSQC spectrum of compound **1**

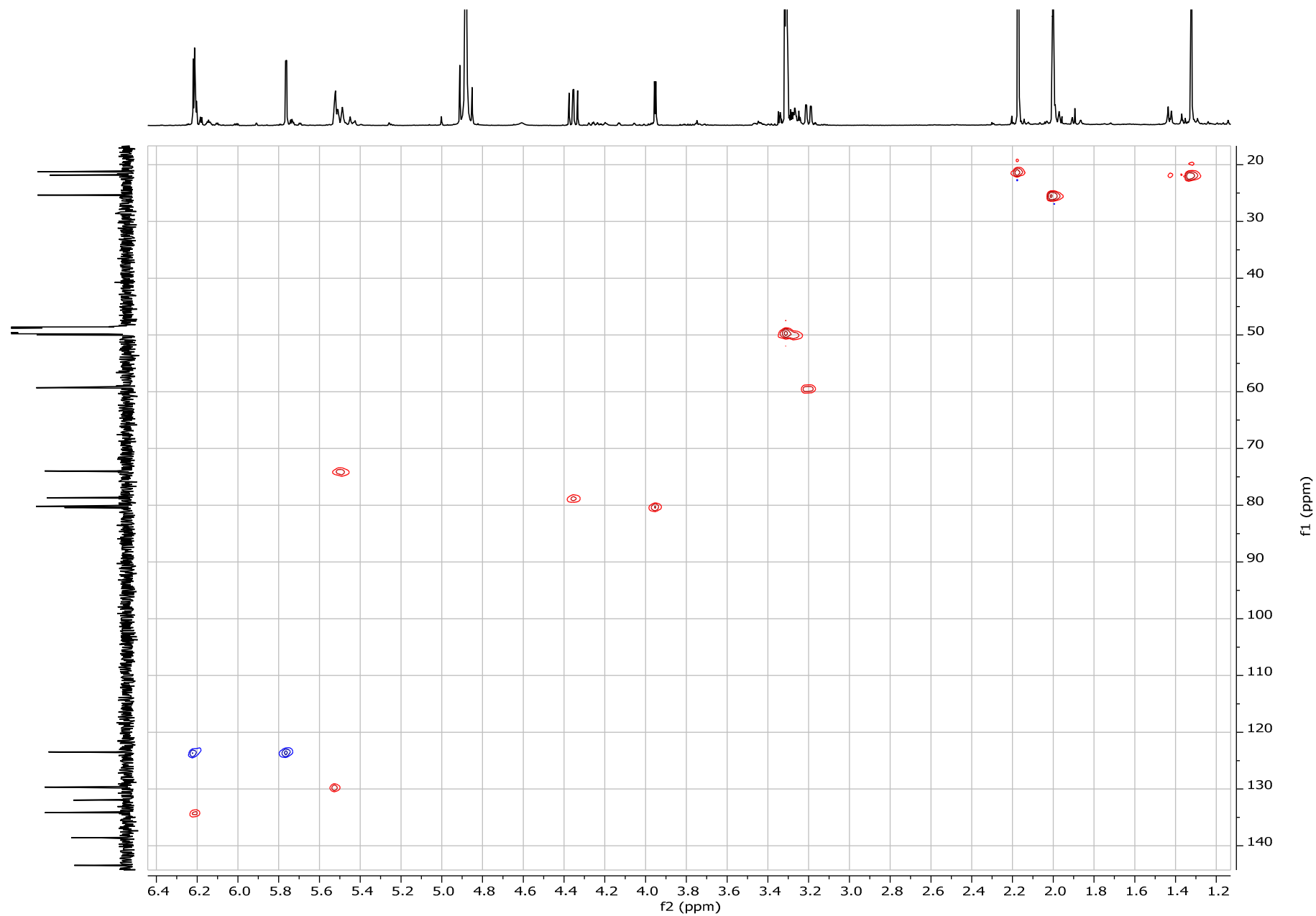


Fig. S6. ^1H ^1H COSY spectrum of compound **1**

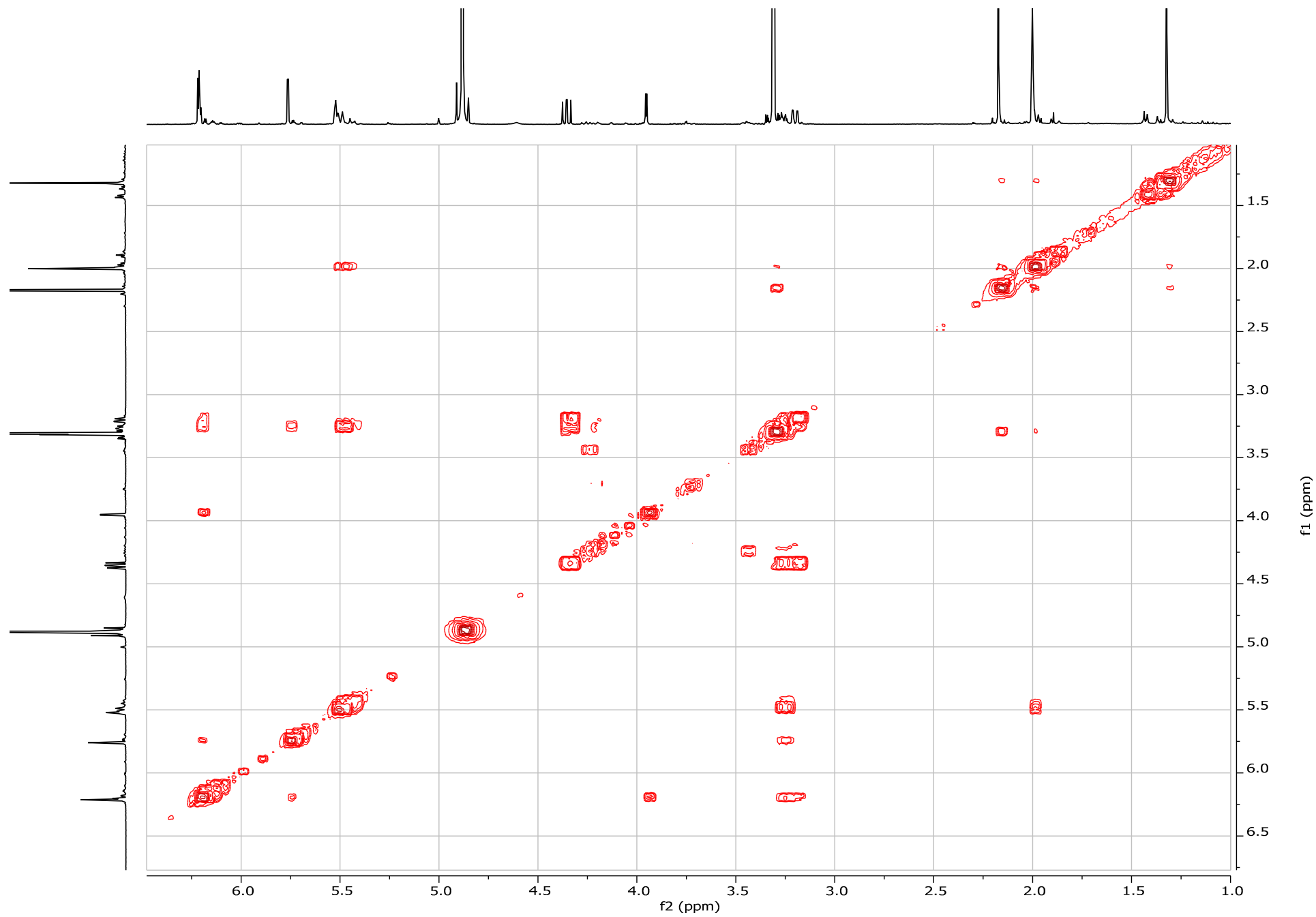


Fig. S7. ^1H ^{13}C HMBC spectrum of compound **1**

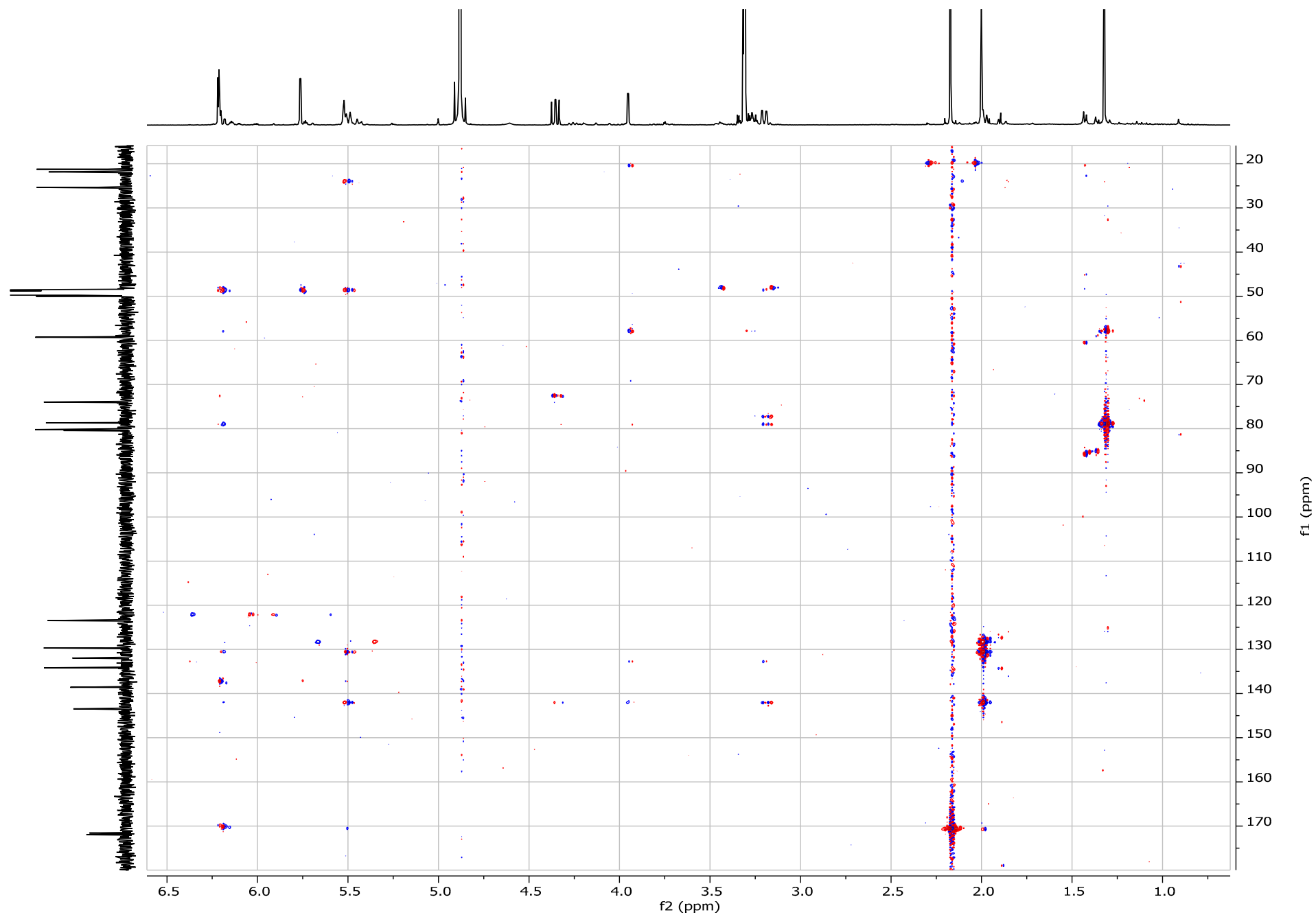


Fig. S8. ^1H ^1H NOESY spectrum of compound **1**

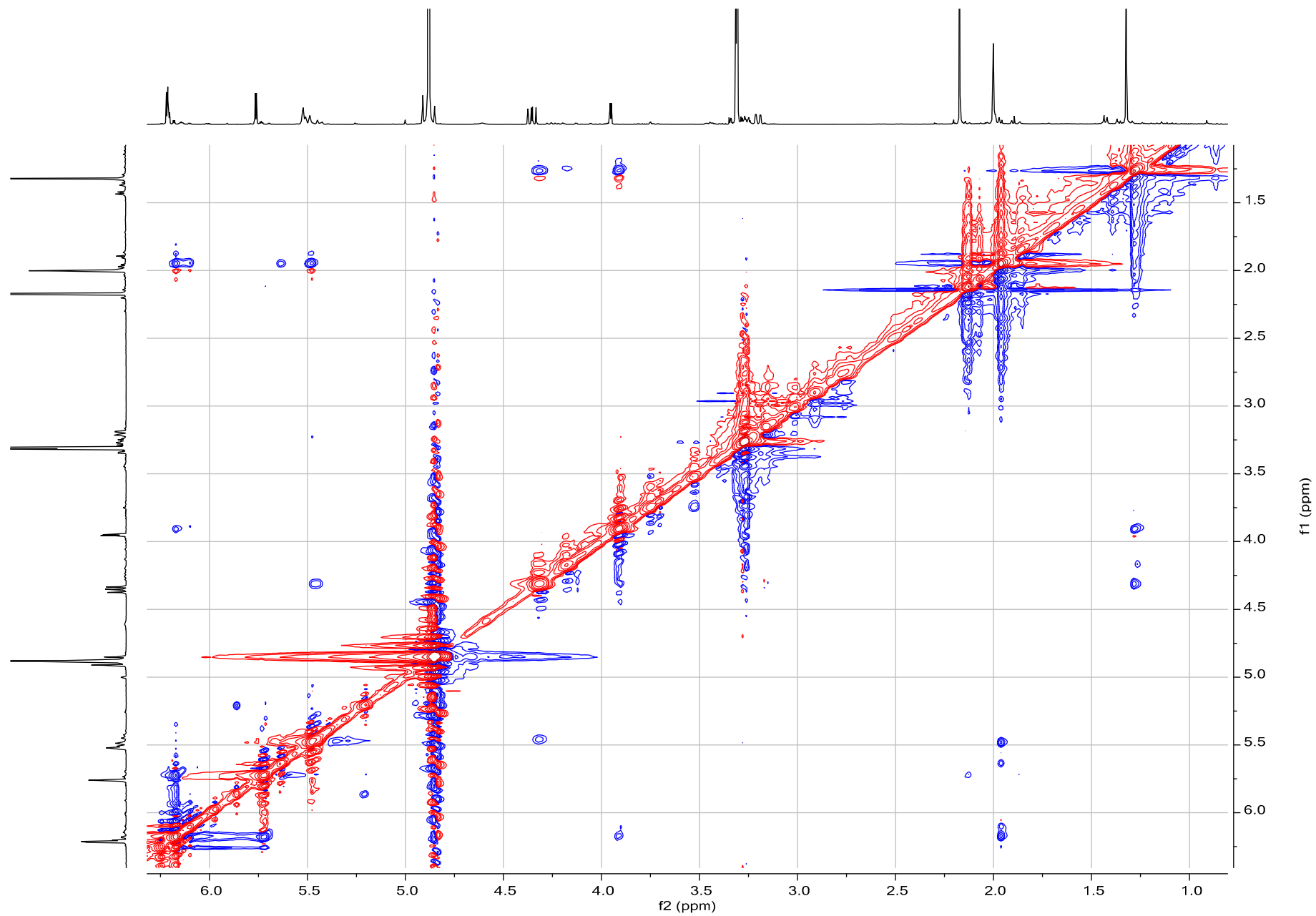


Fig. S9. HR-DART-MS spectrum of compound **2**

Data:201027_PV1200_DV1950_300C

Sample Name:

Description:

Ionization Mode:ESI+

History:Determine m/z[Peak Detect[Centroid,25,Area];Correct Base[5.0%];Correct Base[5.0%];Average(MS[1] 18....

Acquired:10/27/2020 12:53:36 PM

Operator:Administrator

Mass Calibration data:201027_2

Created:10/27/2020 3:48:40 PM

Created by:Administrator

Charge number:1

Tolerance:5.00(mmu)

Unsaturation Number:-1.5 .. 20.0 (Fraction:Both)

Element:¹²C:0 .. 100, ¹H:0 .. 200, ¹⁴N:1 .. 1, ¹⁶O:0 .. 10

Mass	Intensity	Relative Intensity	Calc. Mass	Mass Difference (mmu)	Possible Formula	Unsaturation Number
338.16007	62399.44	100.00	338.16036	-0.29	¹² C ₁₇ ¹ H ₂₄ ¹⁴ N ₁ ¹⁶ O ₆	6.5

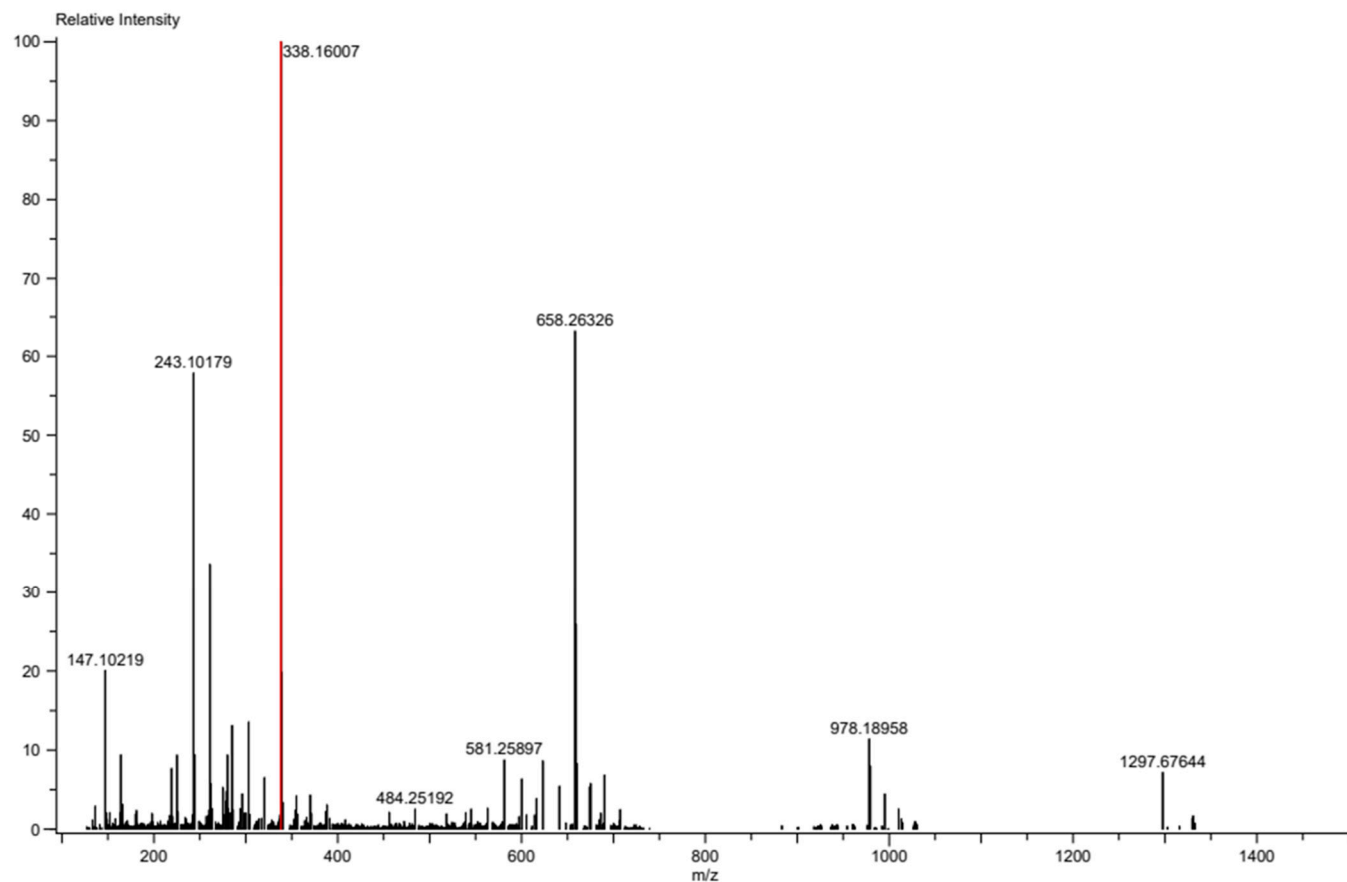


Fig. S10. IR spectrum of compound **2**

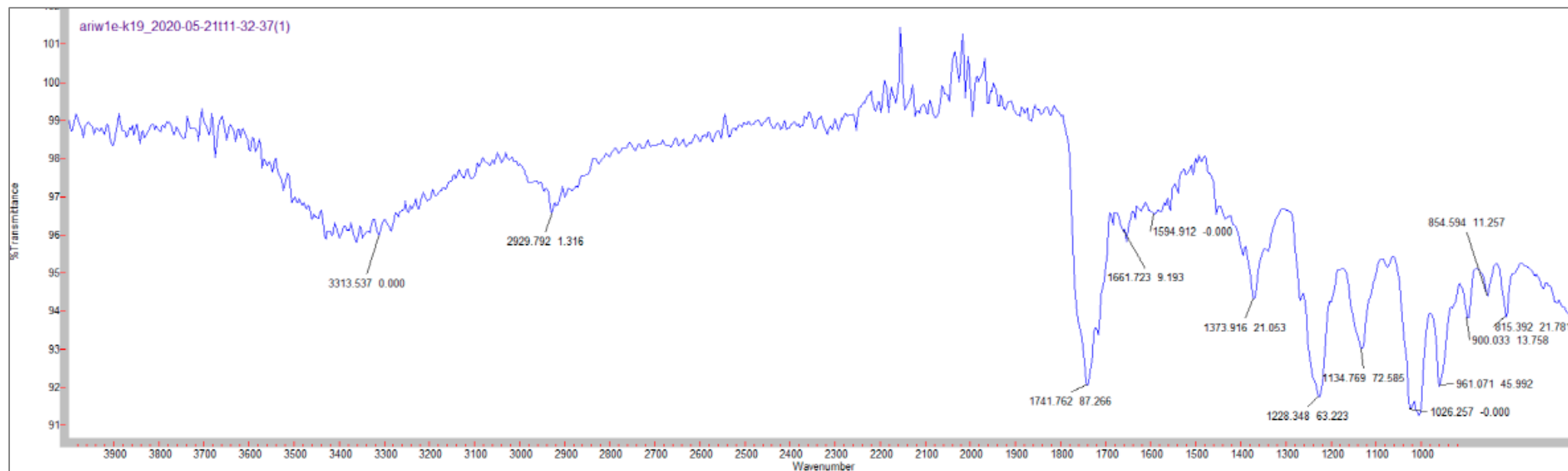


Fig. S11. ^1H NMR spectrum of compound **2** (500 MHz, methanol- d_4)

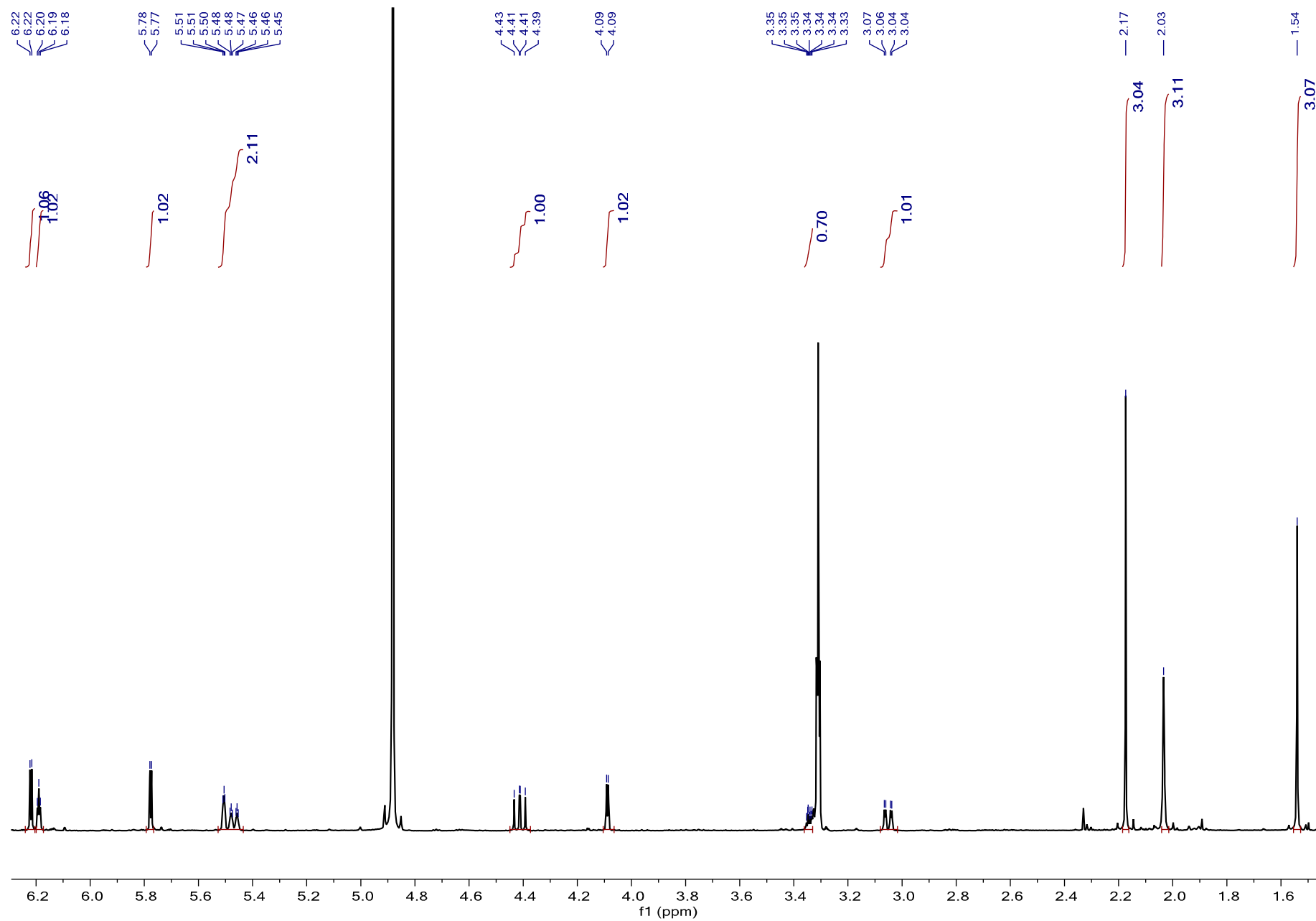


Fig. S12. ^{13}C NMR spectrum of compound **2** (125 MHz, methanol- d_4)

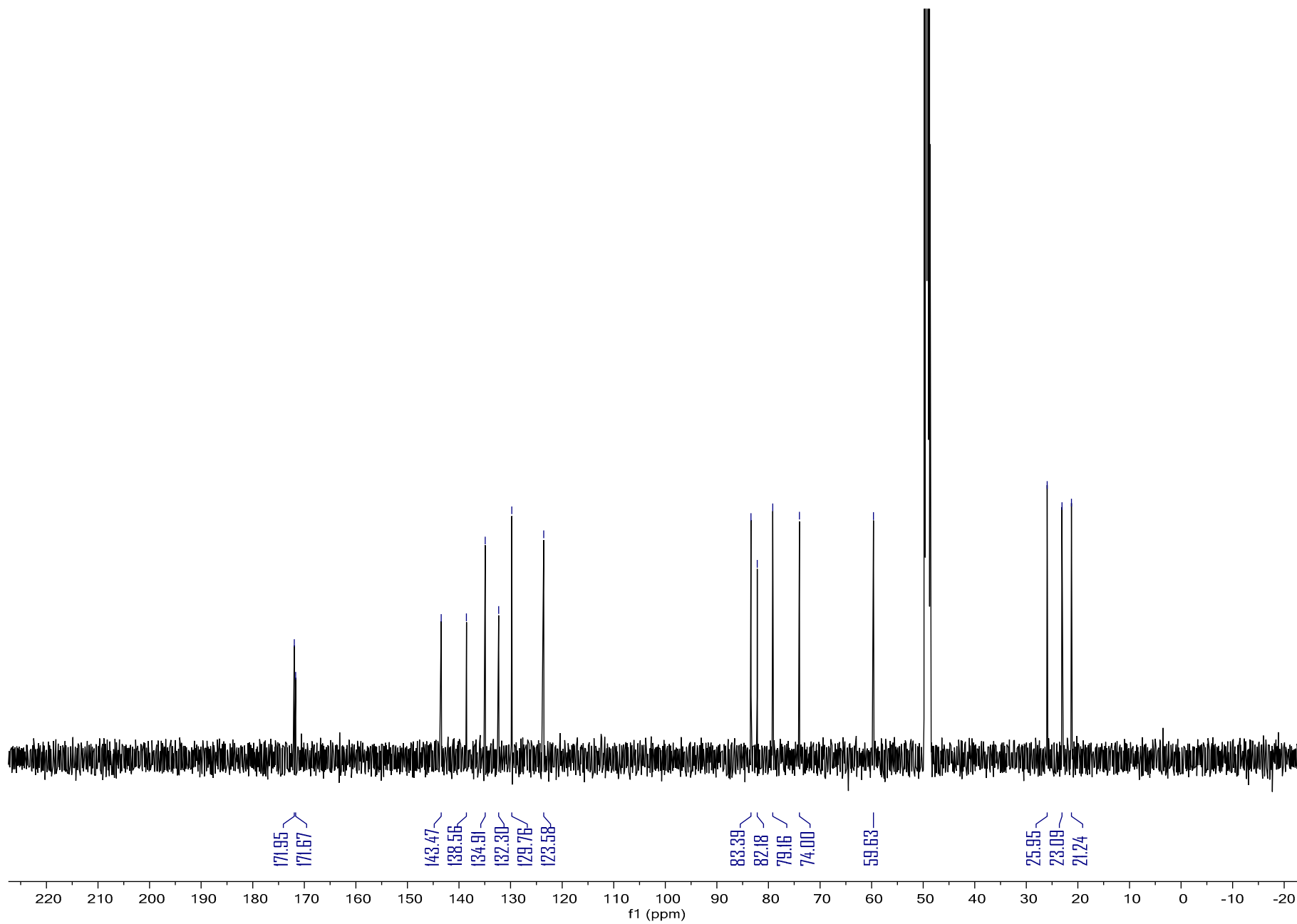


Fig. S13. ^1H ^{13}C HSQC spectrum of compound **2**

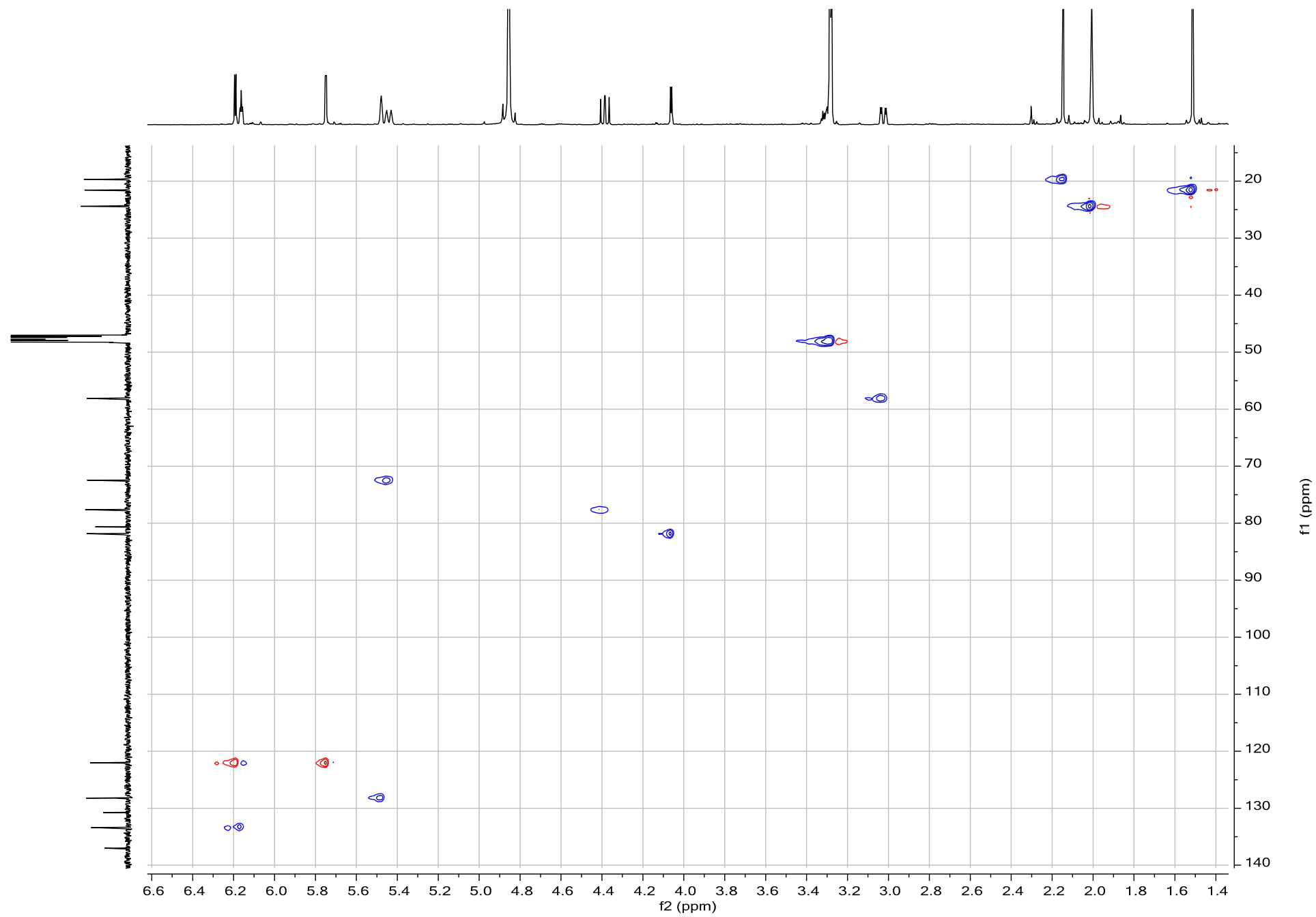


Fig. S14. ^1H ^1H COSY spectrum of compound **2**

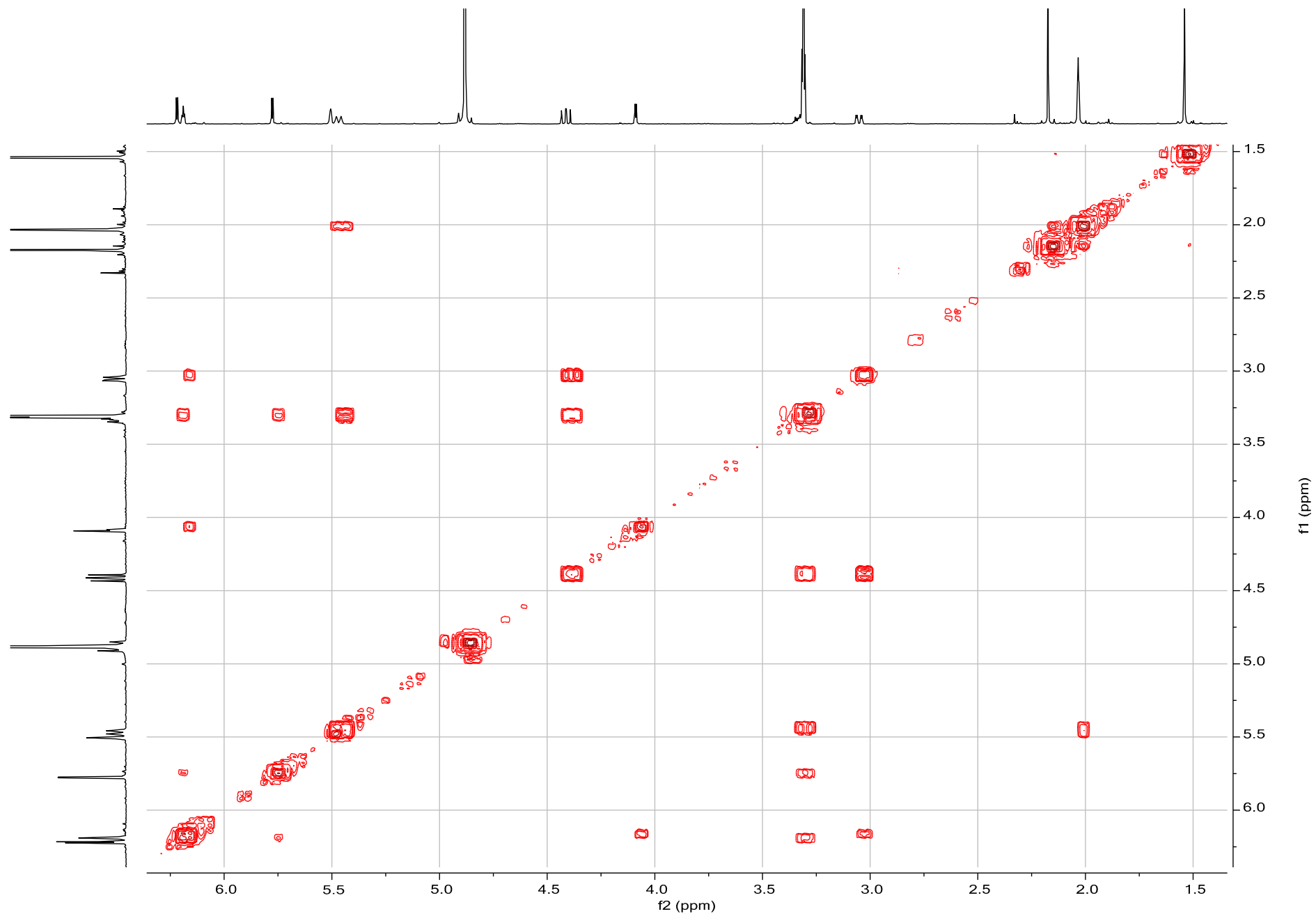


Fig. S15. ^1H ^{13}C HMBC spectrum of compound 2

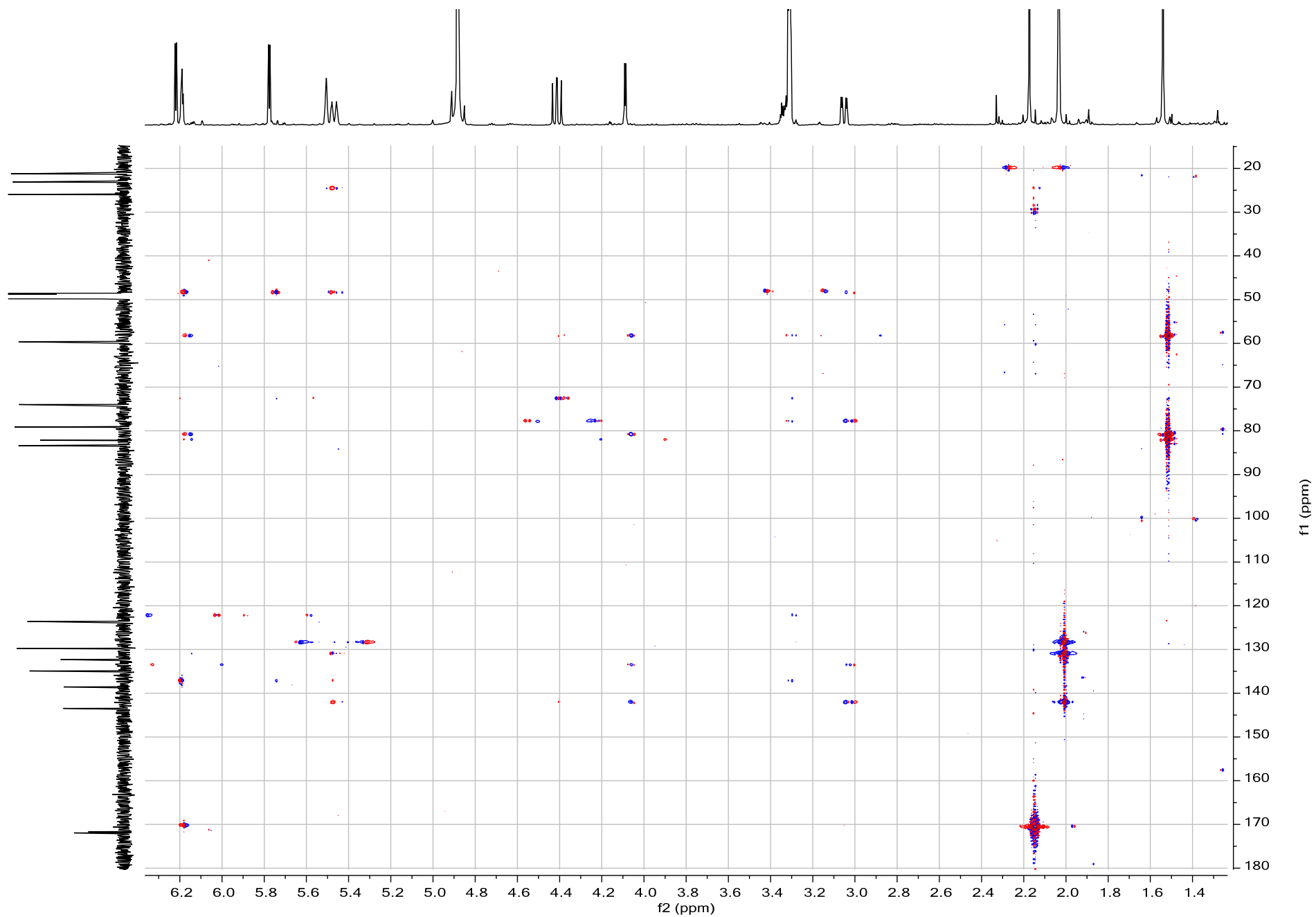


Fig. S16. ^1H ^1H NOESY spectrum of compound 2

