Supporting Information for

The Depside Derivative Pericodepside Inhibits Cancer Cell Metastasis and Proliferation by Suppressing Epithelial−Mesenchymal Transition

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Figure S1: HRESIMS spectrum of compound **1**

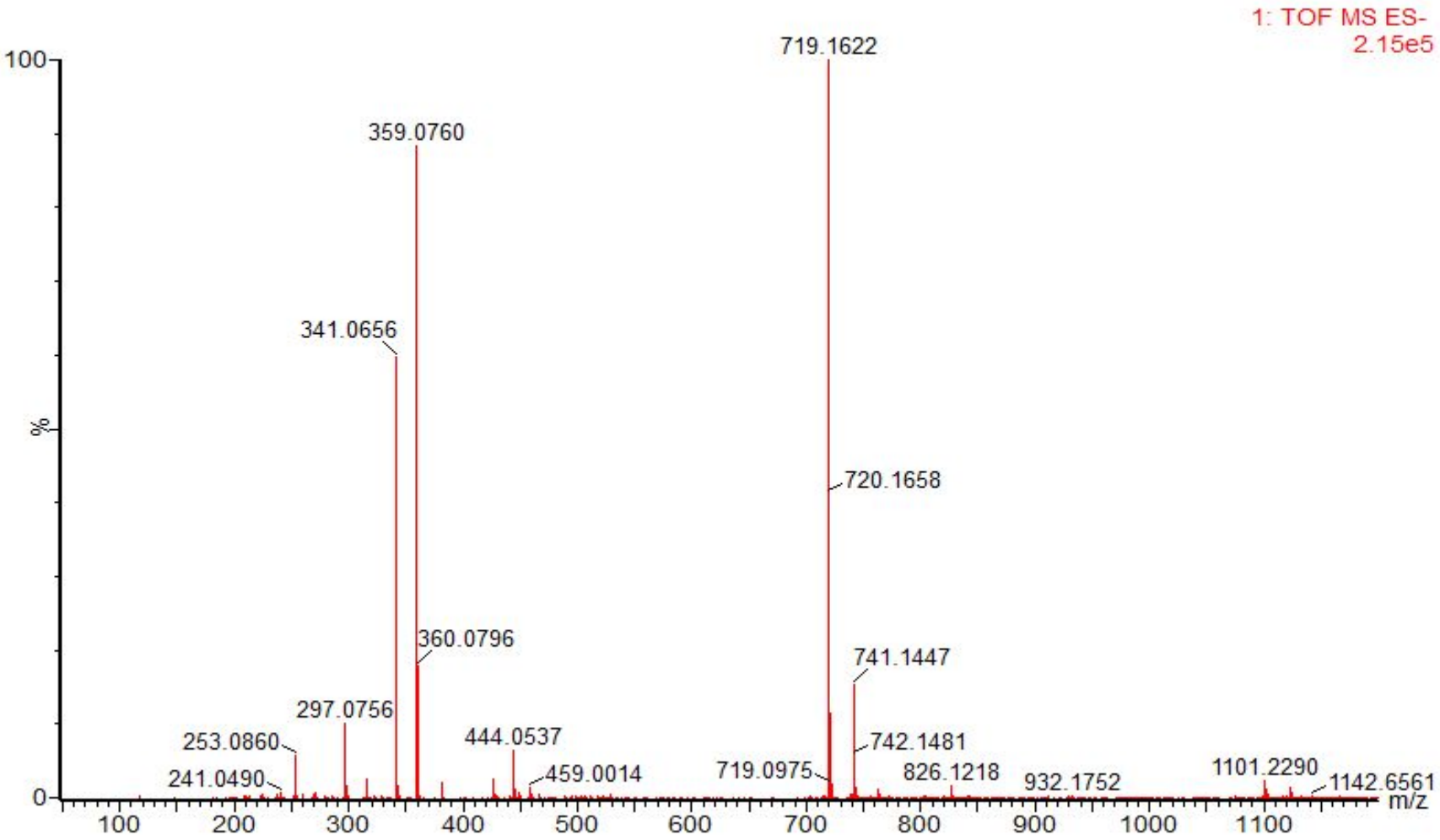


Figure S2: HRESIMS spectrum of compound **2**

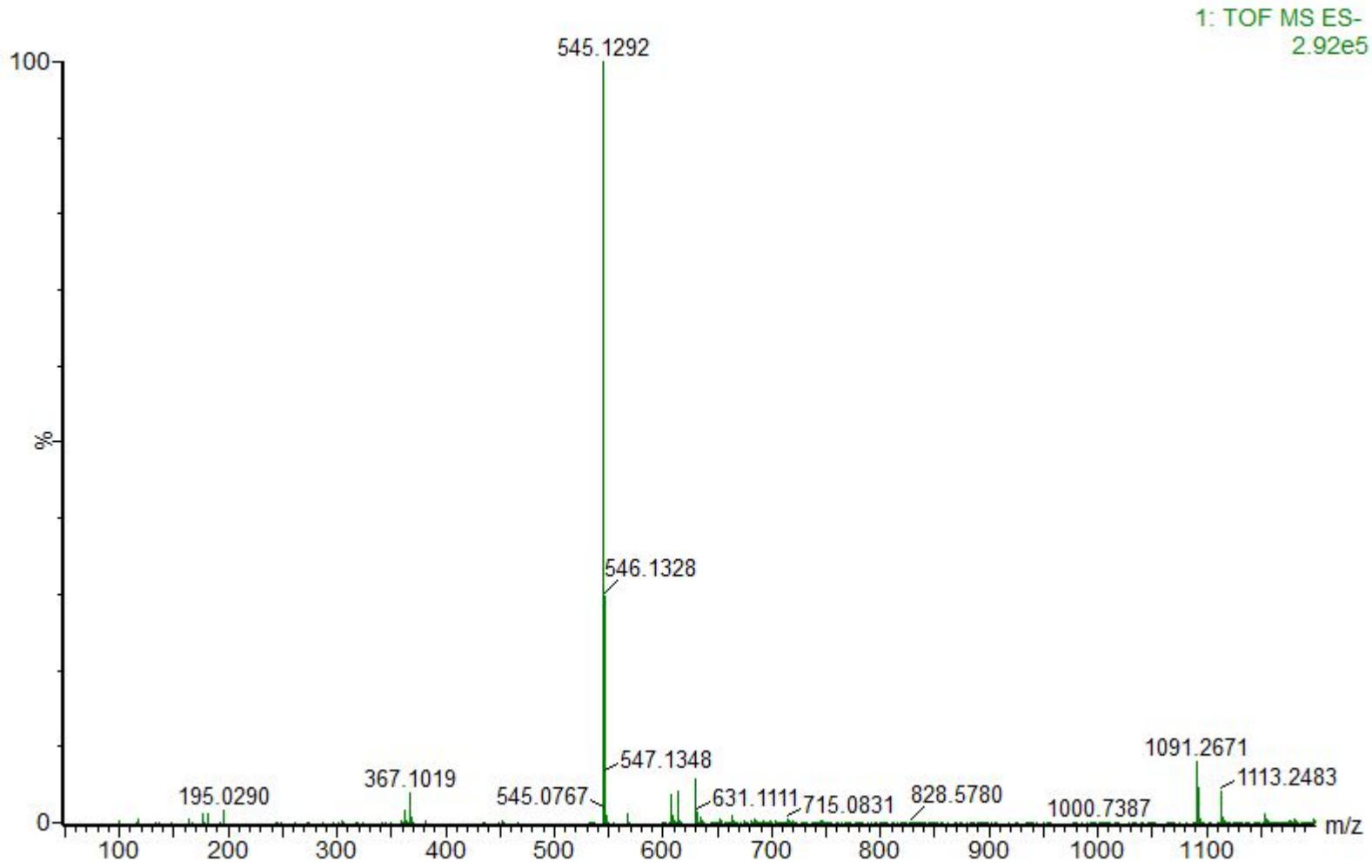


Figure S3: HPLC chromatogram of compound **2**. HPLC analysis employed a Shimadzu liquid chromatography system. Column: YMC-Pack ODS-A (column size, 150 × 4.6 mm; particle size, 5 μm; pore size, 12 nm; at 40 ℃). The UV-active metabolite was monitored at 254 nm by a diode array UV detector. The mobile phase consisted of distilled water/trifluoroacetic acid (99.9:0.1, v/v) for pump A and methanol/trifluoroacetic acid (99.9:0.1, v/v) for pump B. The mobile phase: a flow rate of 1.0 mL/min: 0–30 min, 20–100%; 30–40 min, 100%.

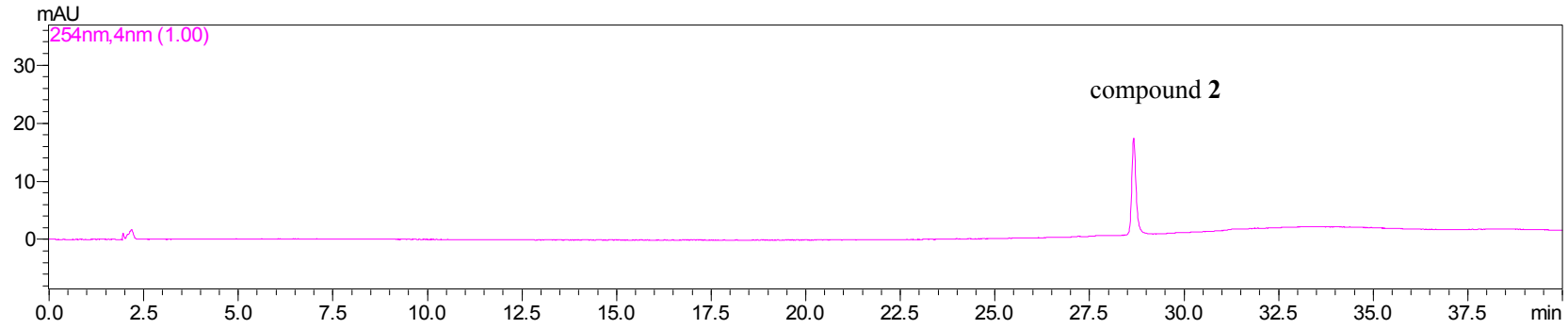
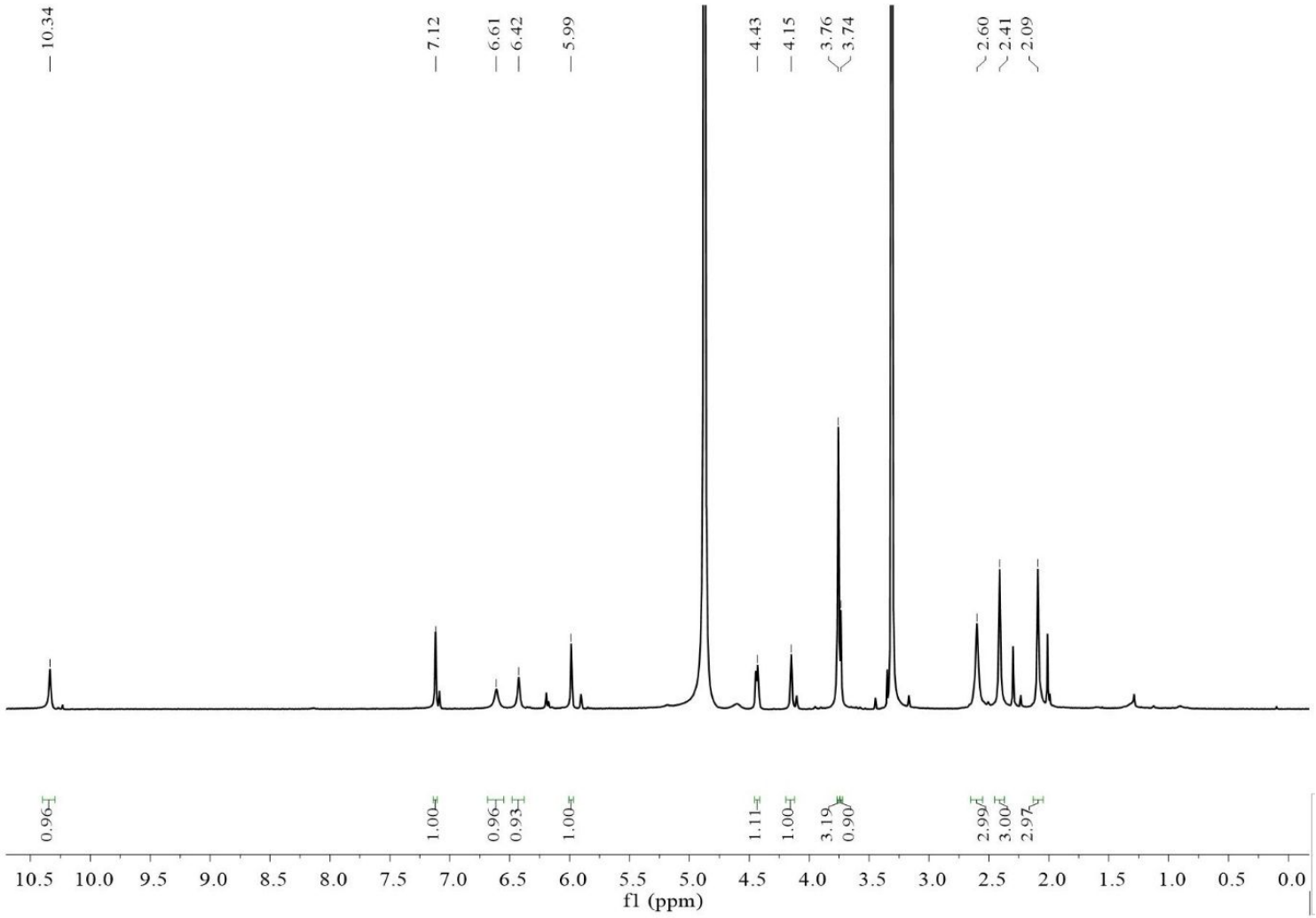


Figure S4: ^{1}H NMR spectrum of compound **2** in CD_3OD at 500MHz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7.12
6.61
6.42
5.99
4.43
4.15
3.76
3.74
2.60
2.41
2.09
0.96
1.00
0.96
0.93
1.00
1.11
1.00
3.19
0.90
2.99
3.00
2.97
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

Figure S5: ^{13}C NMR spectrum of compound **2** in CD_3OD at 125MHz

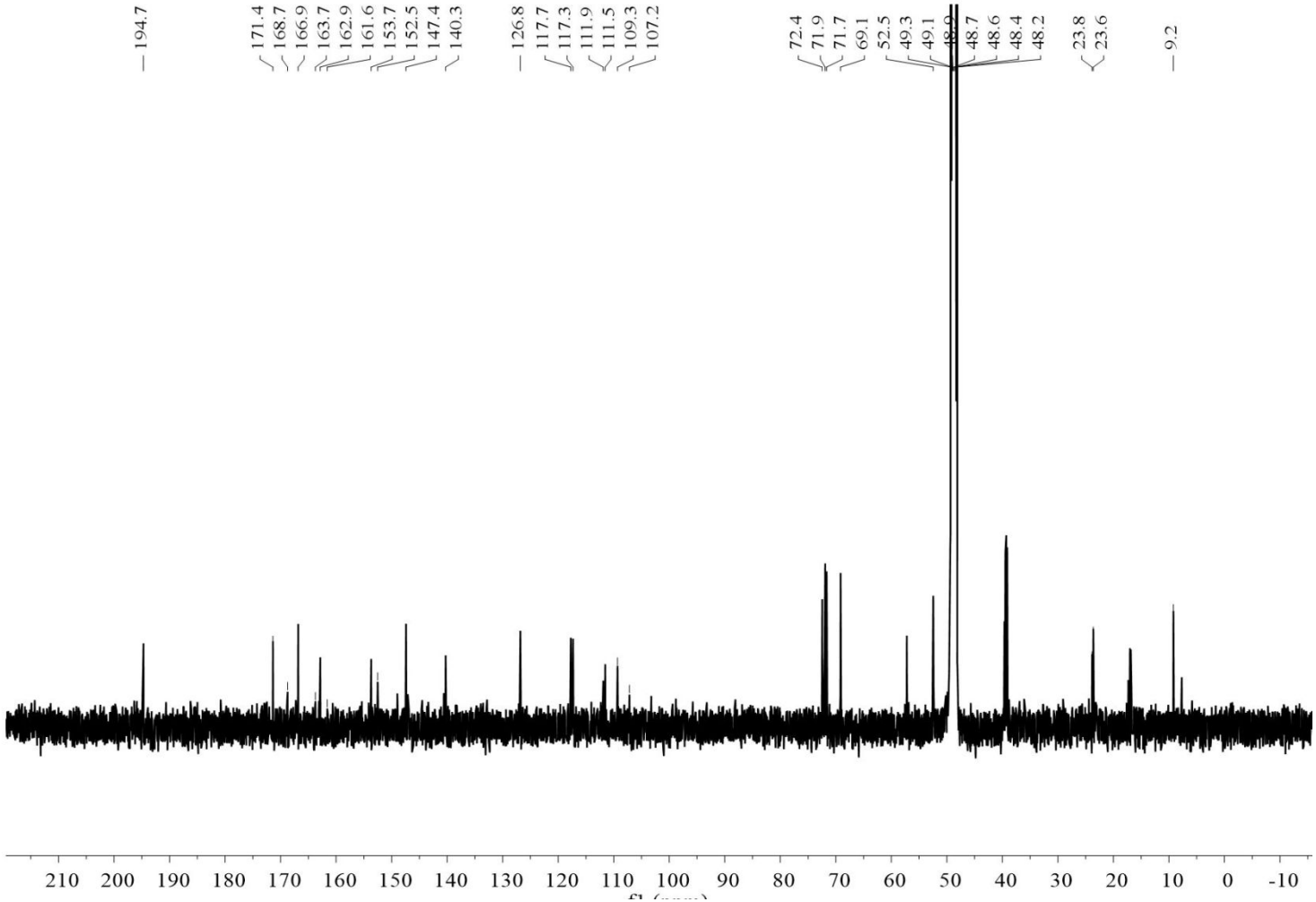


Figure S6: HSQC spectrum of compound **2** in CD_3OD

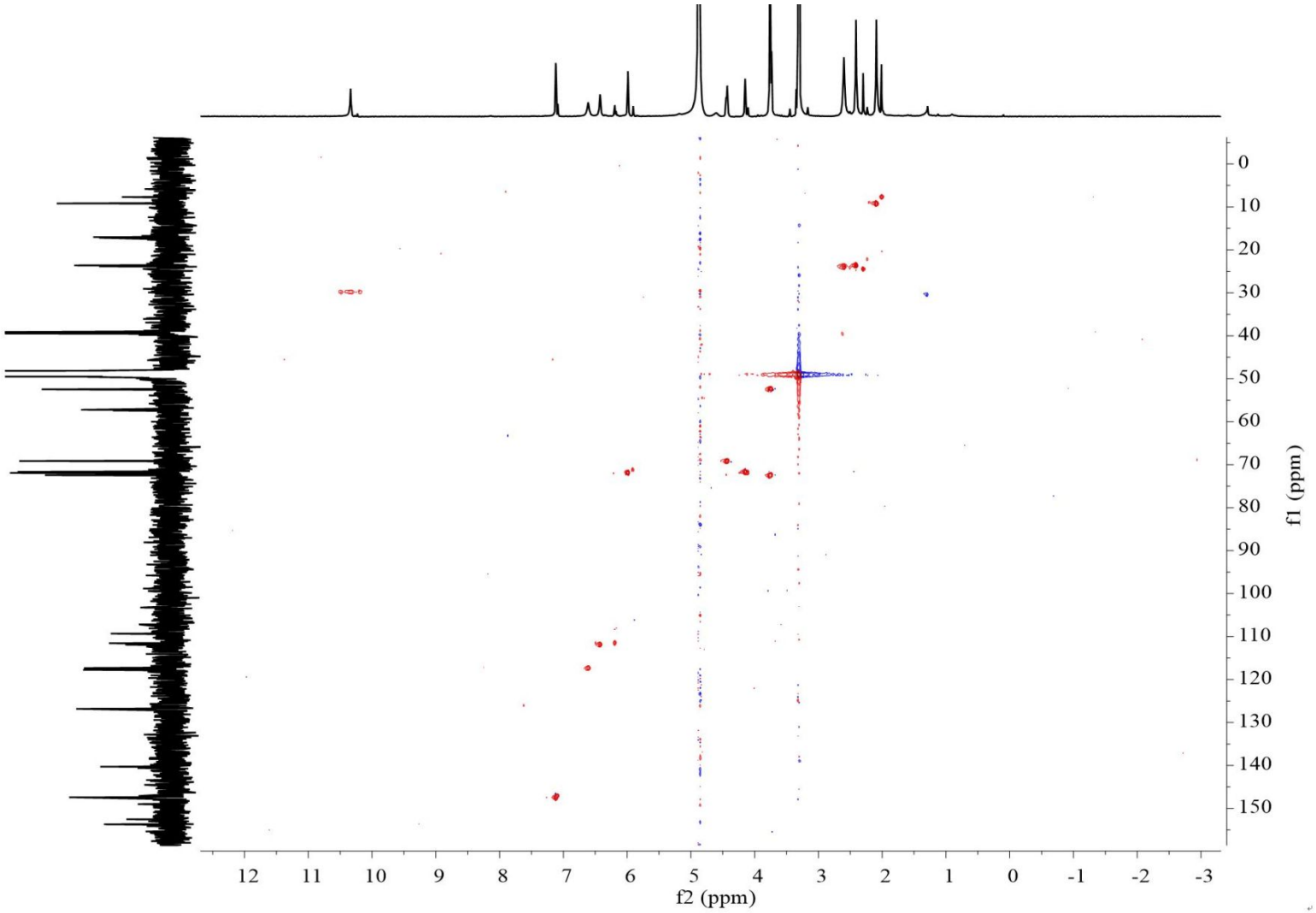


Figure S7: ^{1}H-^{1}H COSY spectrum of compound **2** in CD_3OD

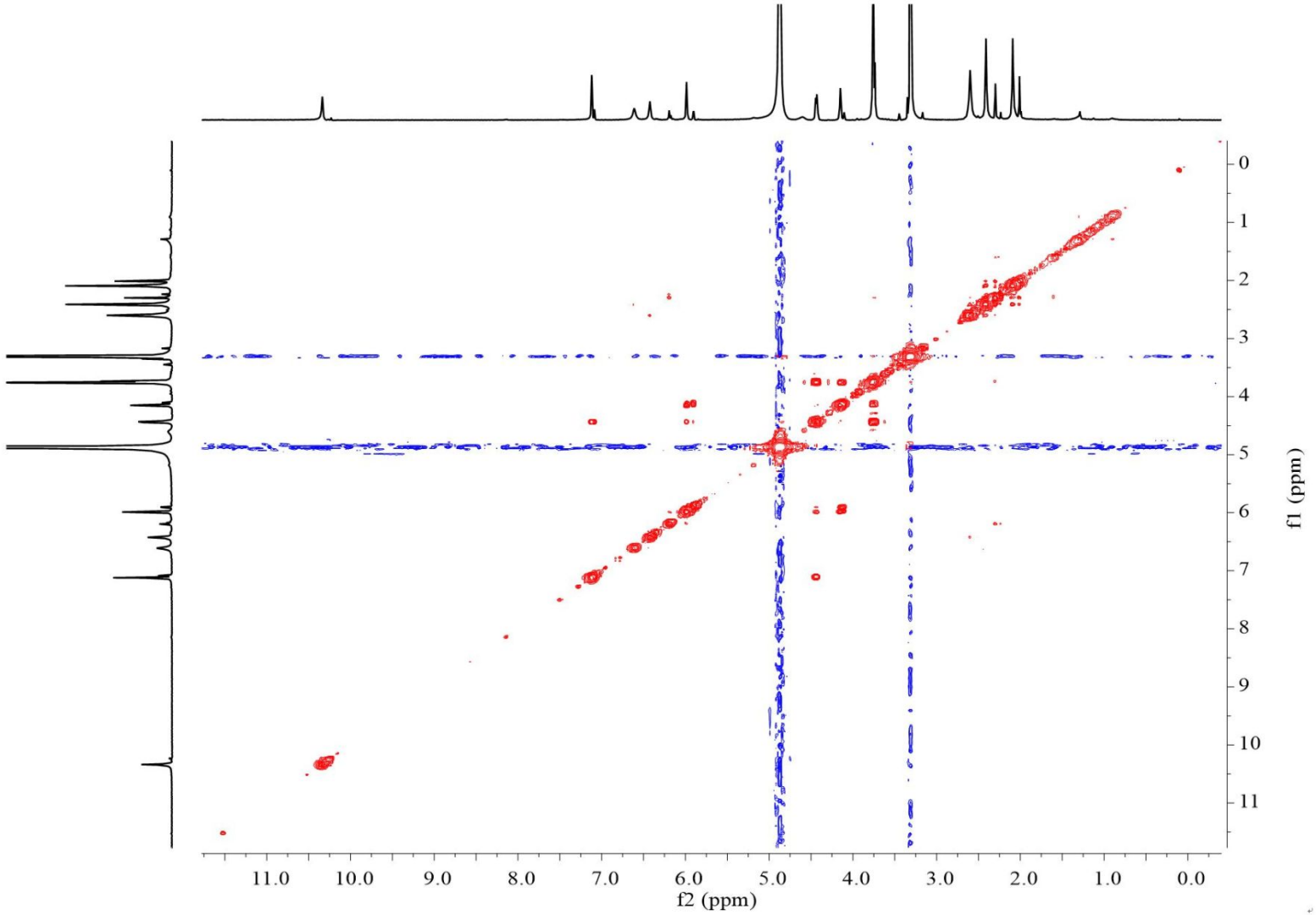


Figure S8: HMBC spectrum of compound **2** in CD_3OD

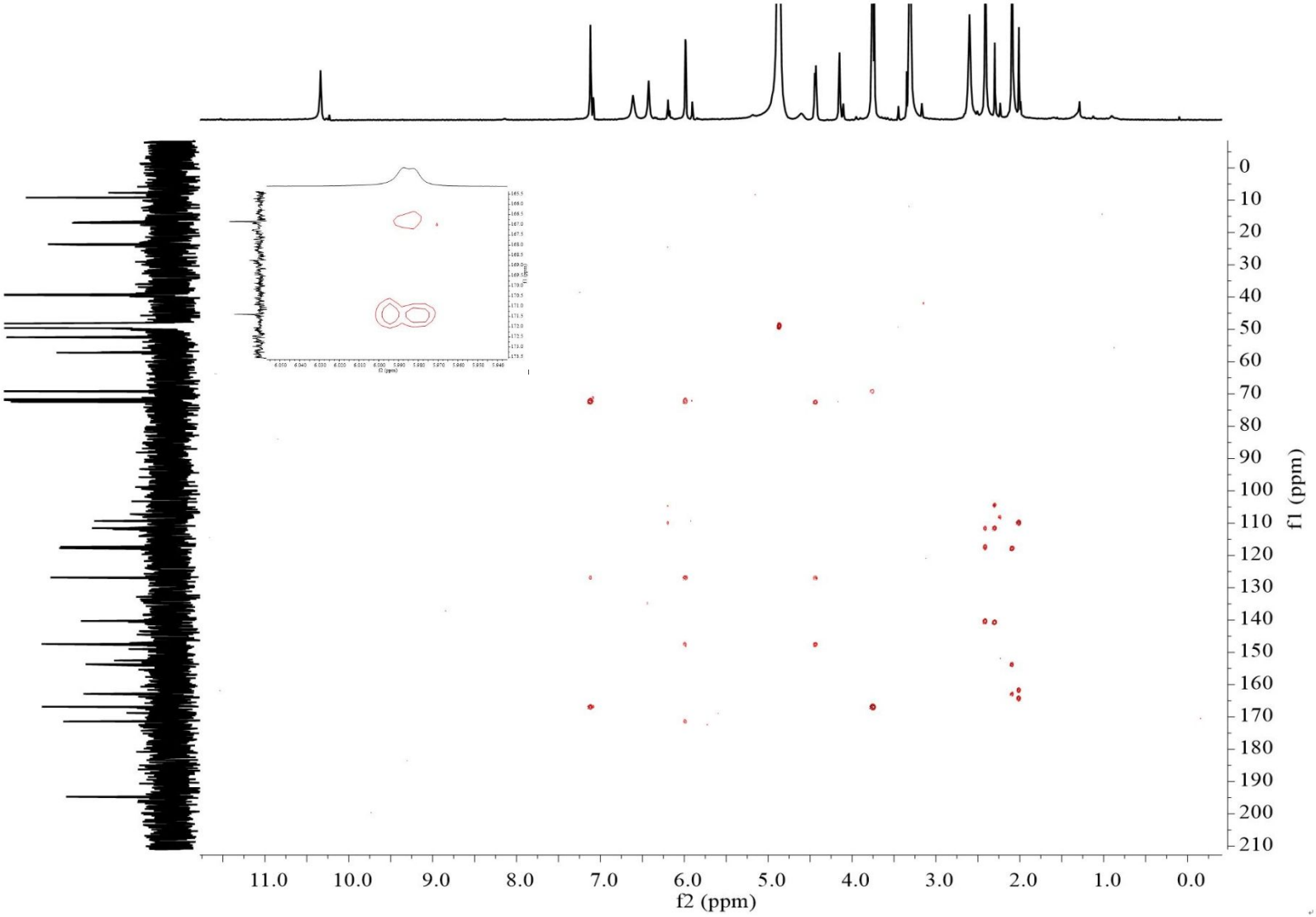


Figure S9: [1]H NMR spectrum of compound **2** in DMSO-d_6 at 400MHz

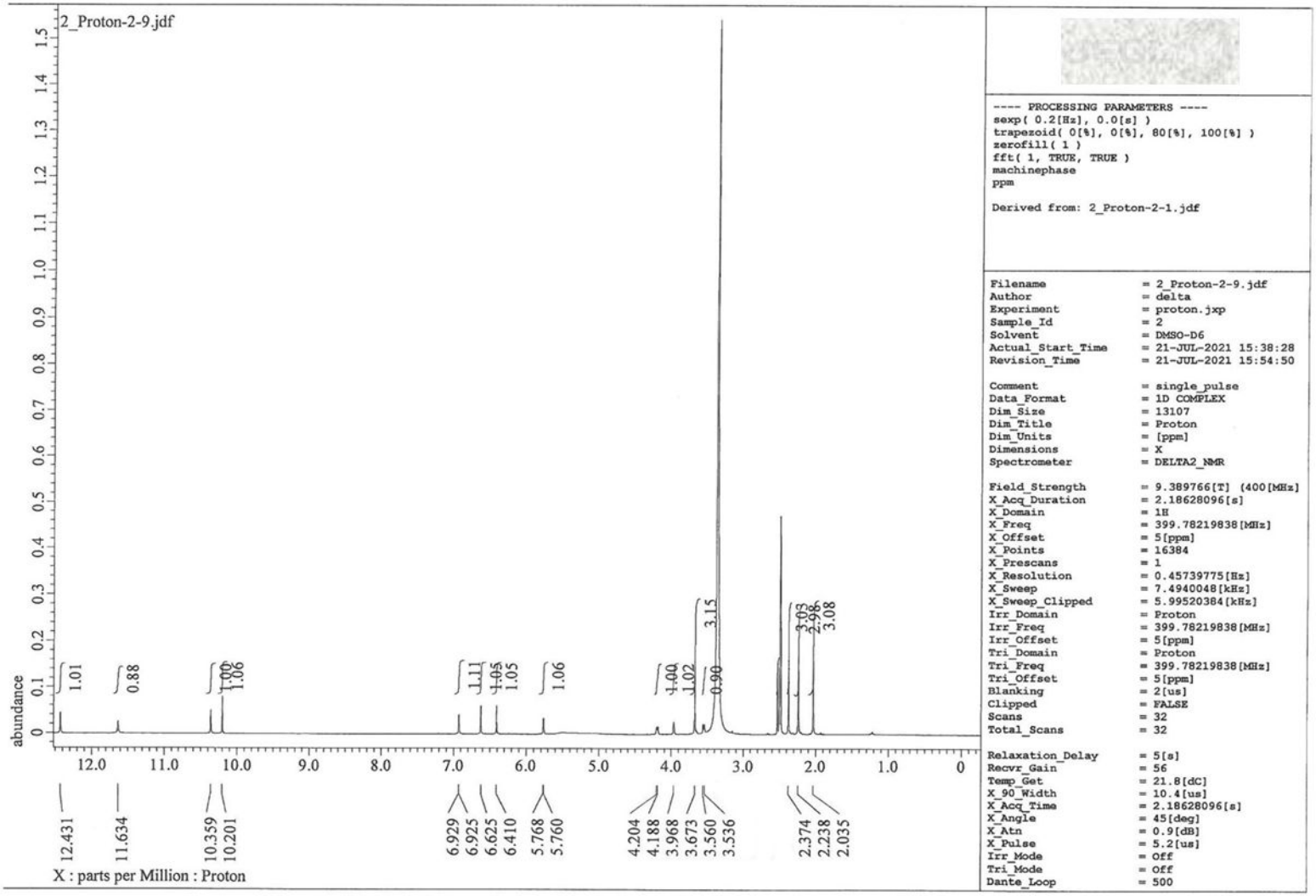


Figure S10: ^{13}C NMR spectrum of compound **2** in DMSO-d_6 at 100MHz

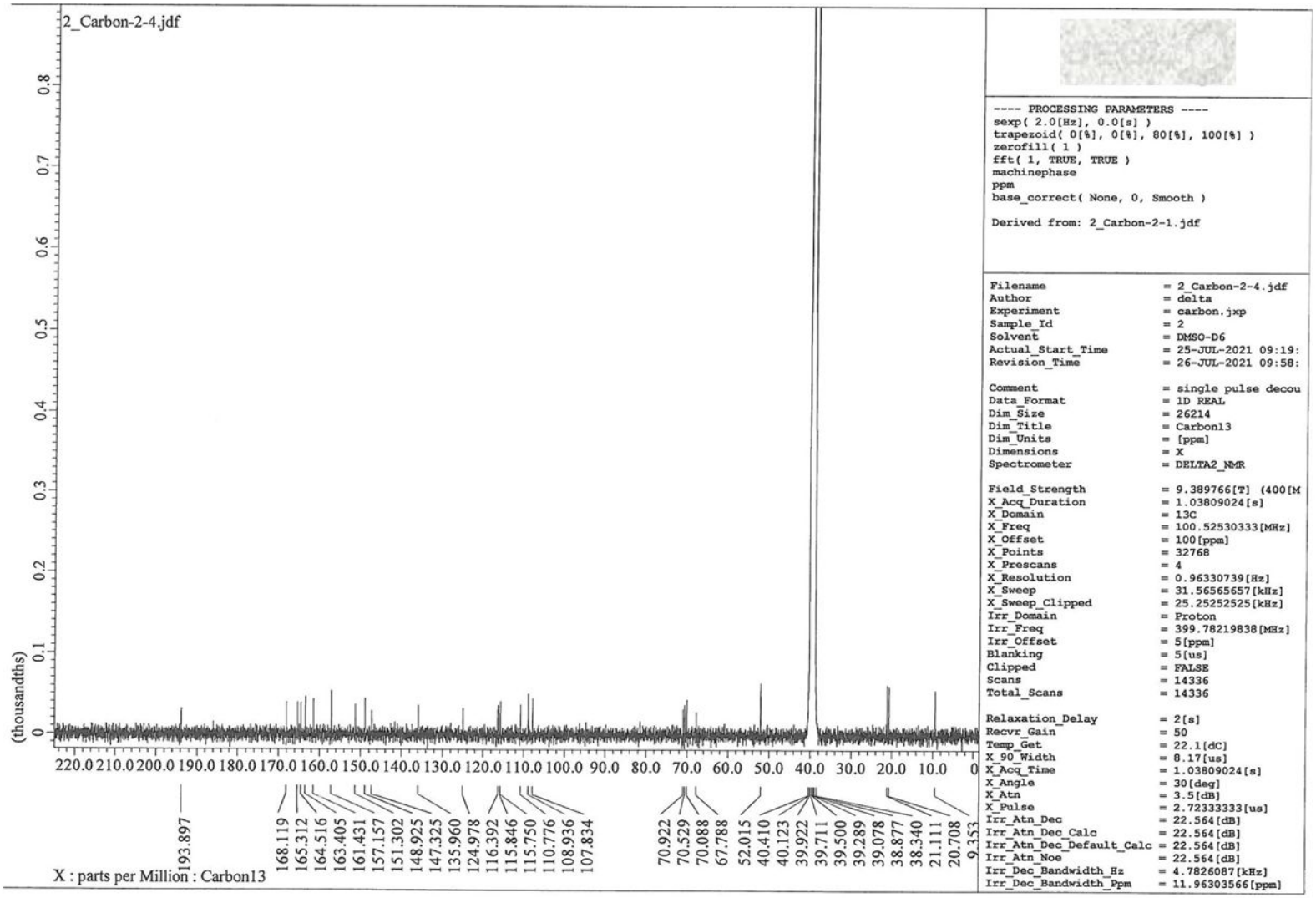


Figure S11: HSQC spectrum of compound **2** in DMSO-d_6

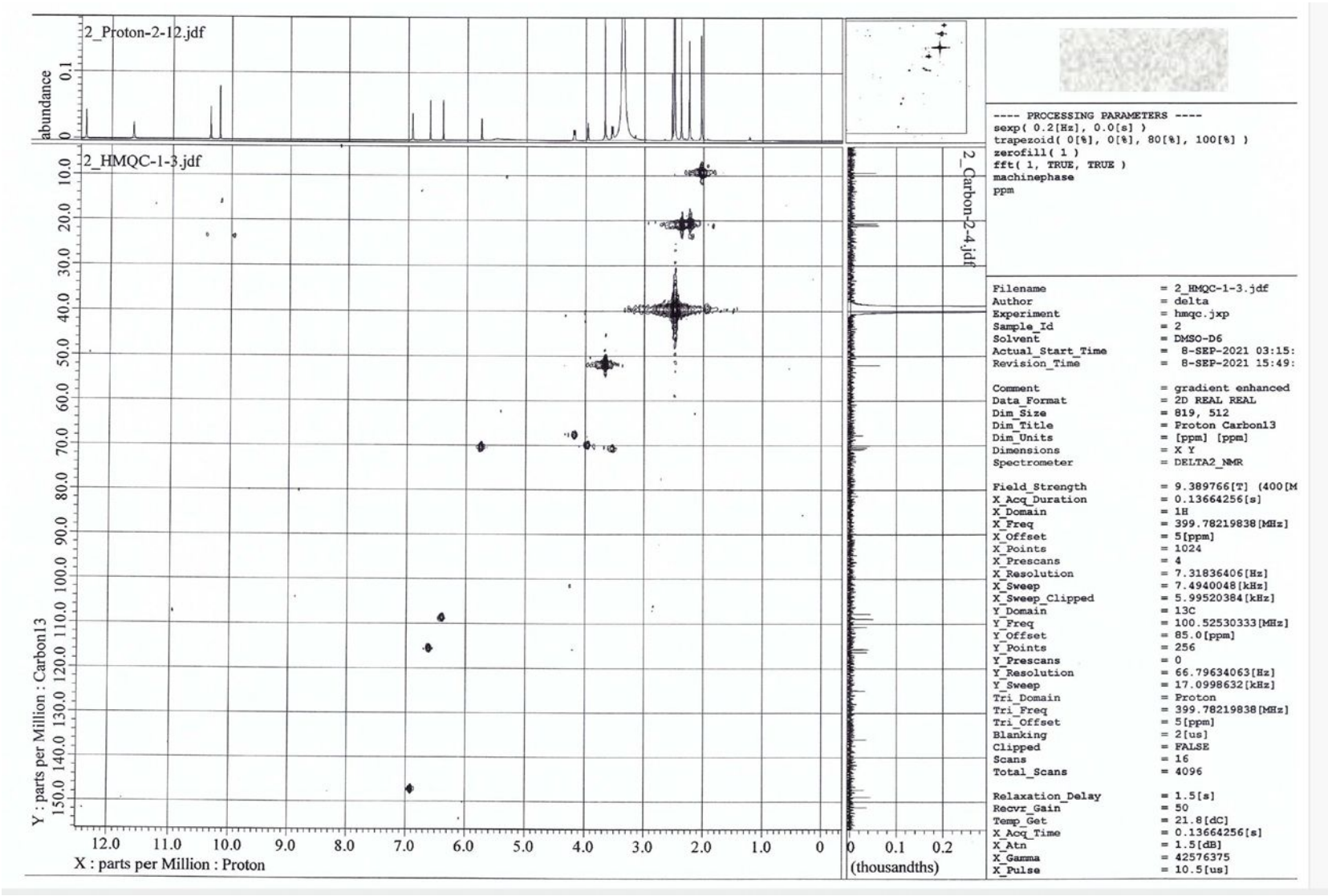
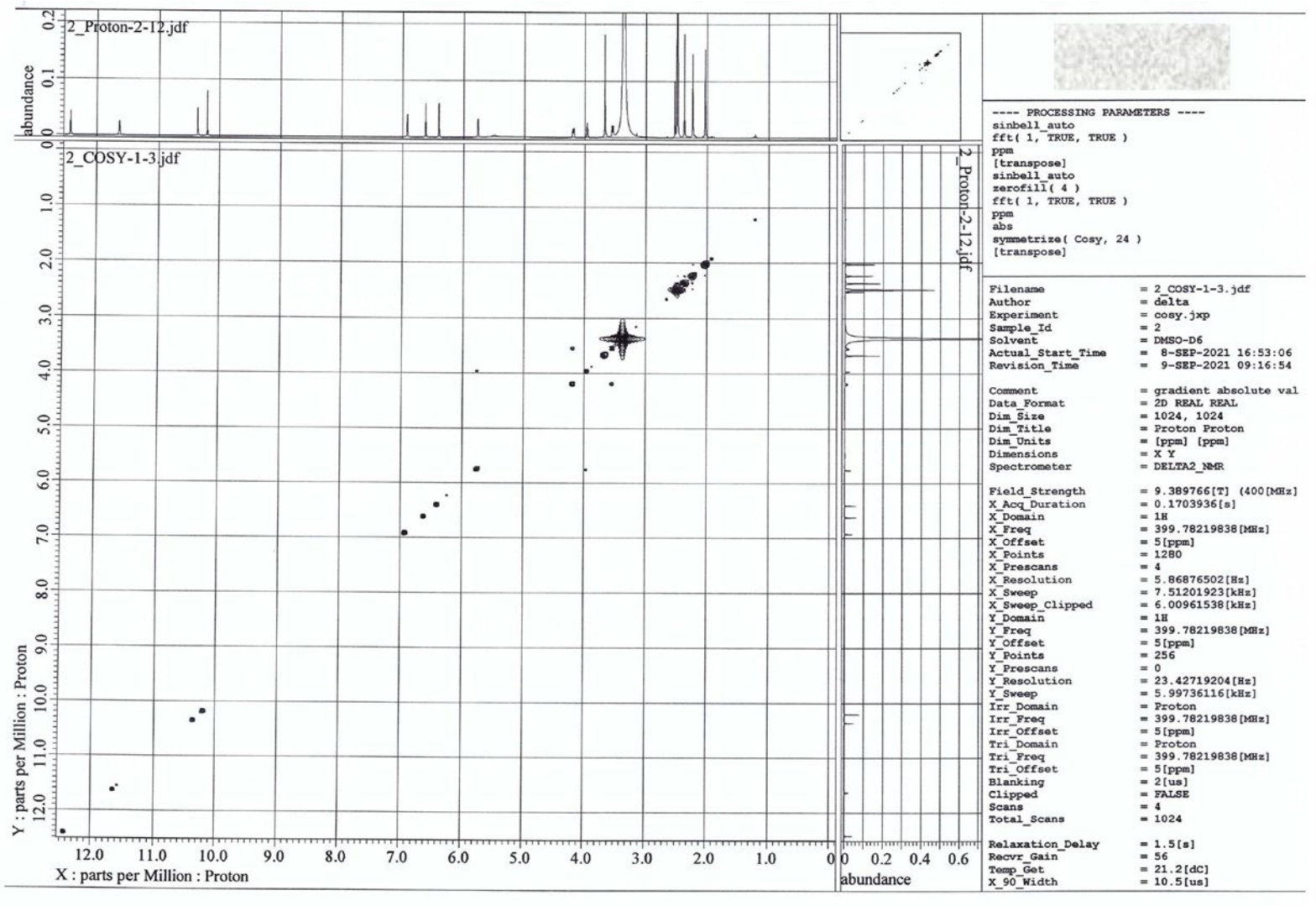
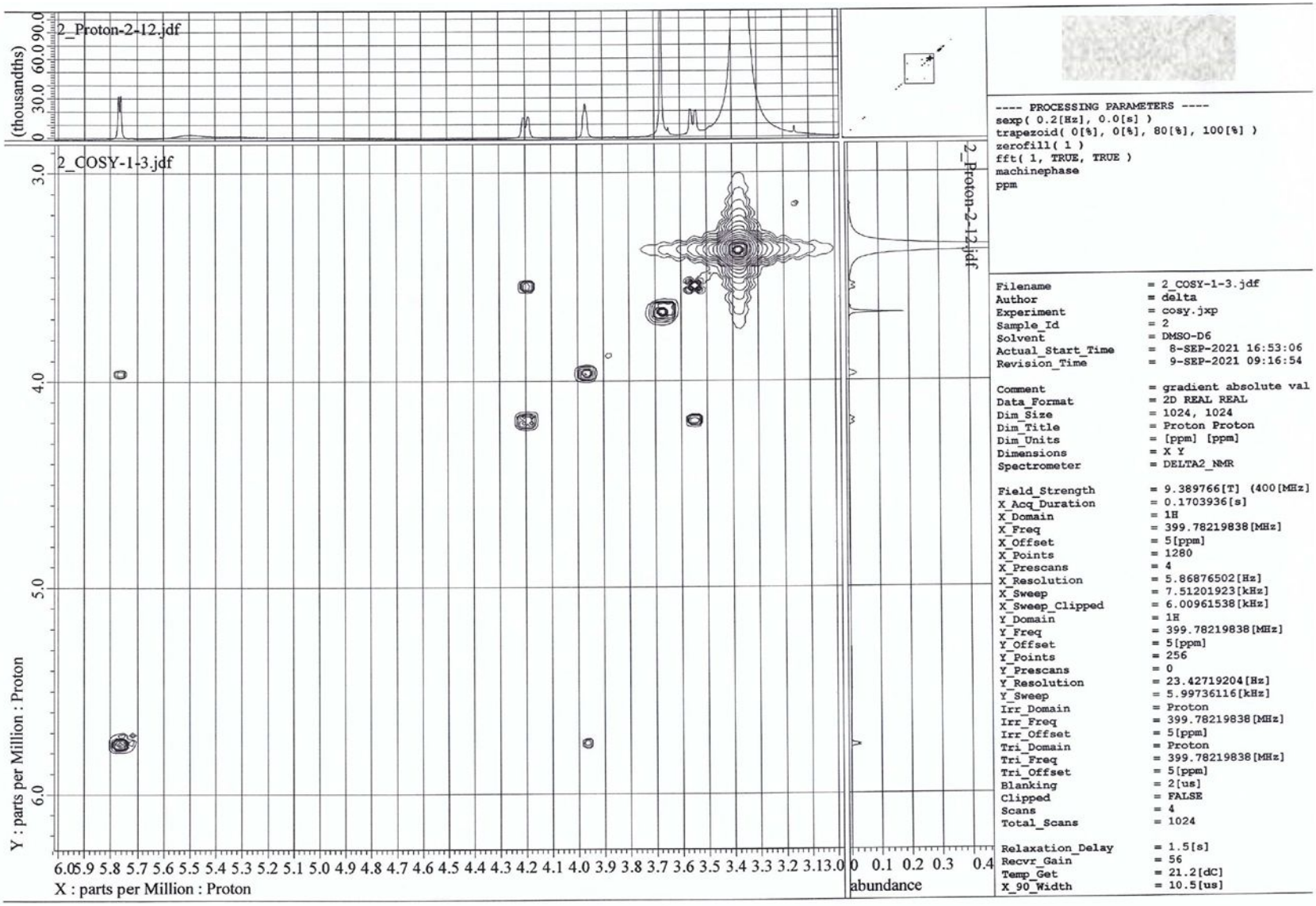


Figure S12: ^{1}H-^{1}H COSY spectrum of compound **2** in DMSO-d_6

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(thousandths)
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2_COSY-1-3.jdf
3.0
4.0
5.0
6.0
Y : parts per Million : Proton
6.0 5.9 5.8 5.7 5.6 5.5 5.4 5.3 5.2 5.1 5.0 4.9 4.8 4.7 4.6 4.5 4.4 4.3 4.2 4.1 4.0 3.9 3.8 3.7 3.6 3.5 3.4 3.3 3.2 3.1 3.0
X : parts per Million : Proton
2_Proton-2-12.jdf
0 0.1 0.2 0.3 0.4
abundance
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trapezoid(0[%], 0[%], 80[%], 100[%])
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fft(1, TRUE, TRUE)
machinephase
ppm
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X_Prescans = 4
X_Resolution = 5.86876502[Hz]
X_Sweep = 7.51201923[kHz]
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Y_Domain = 1H
Y_Freq = 399.78219838[MHz]
Y_Offset = 5[ppm]
Y_Points = 256
Y_Prescans = 0
Y_Resolution = 23.42719204[Hz]
Y_Sweep = 5.99736116[kHz]
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Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
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Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
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Total_Scans = 1024
Relaxation_Delay = 1.5[s]
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Temp_Get = 21.2[dC]
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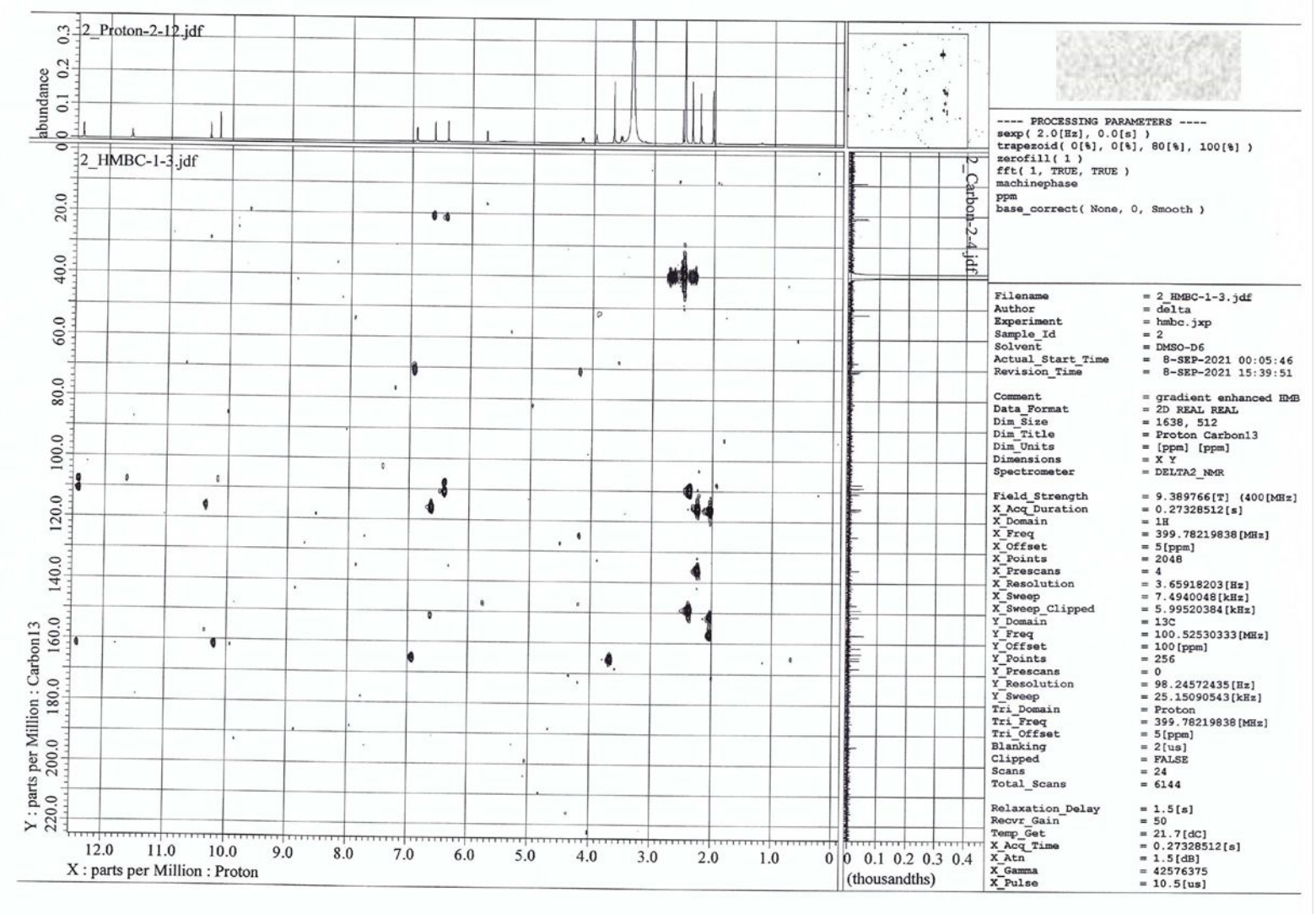
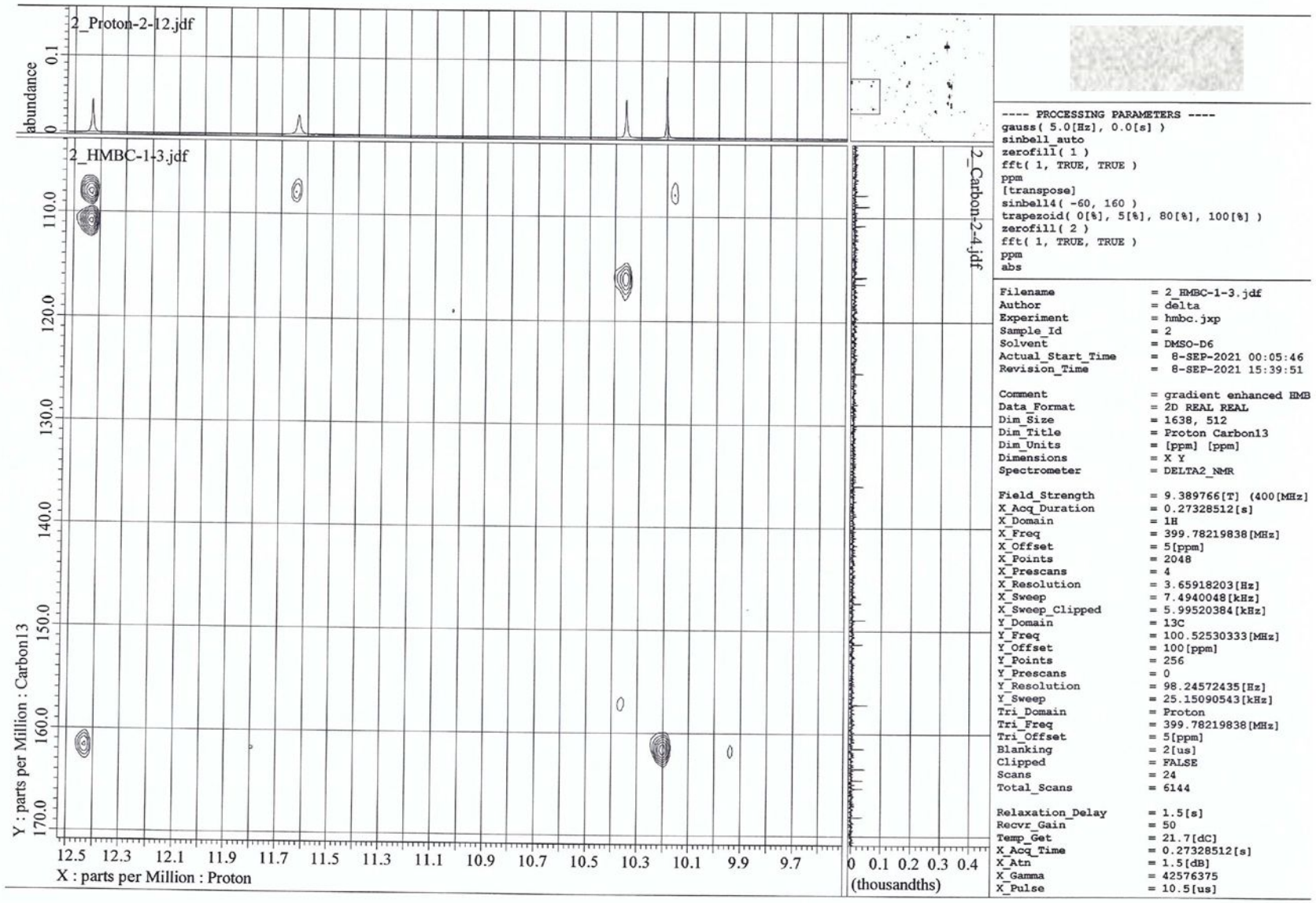
Figure S13: HMBC spectrum of compound **2** in DMSO-d_6

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0.1
2_HMBC-1-3.jdf
2_Carbon-2-4.jdf
110.0
120.0
130.0
140.0
150.0
160.0
170.0
Y : parts per Million : Carbon13
12.5 12.3 12.1 11.9 11.7 11.5 11.3 11.1 10.9 10.7 10.5 10.3 10.1 9.9 9.7
X : parts per Million : Proton
0 0.1 0.2 0.3 0.4
(thousandths)
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[transpose]
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fft(1, TRUE, TRUE)
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X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 2048
X_Prescans = 4
X_Resolution = 3.65918203[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Y_Domain = 13C
Y_Freq = 100.52530333[MHz]
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Y_Sweep = 25.15090543[kHz]
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Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
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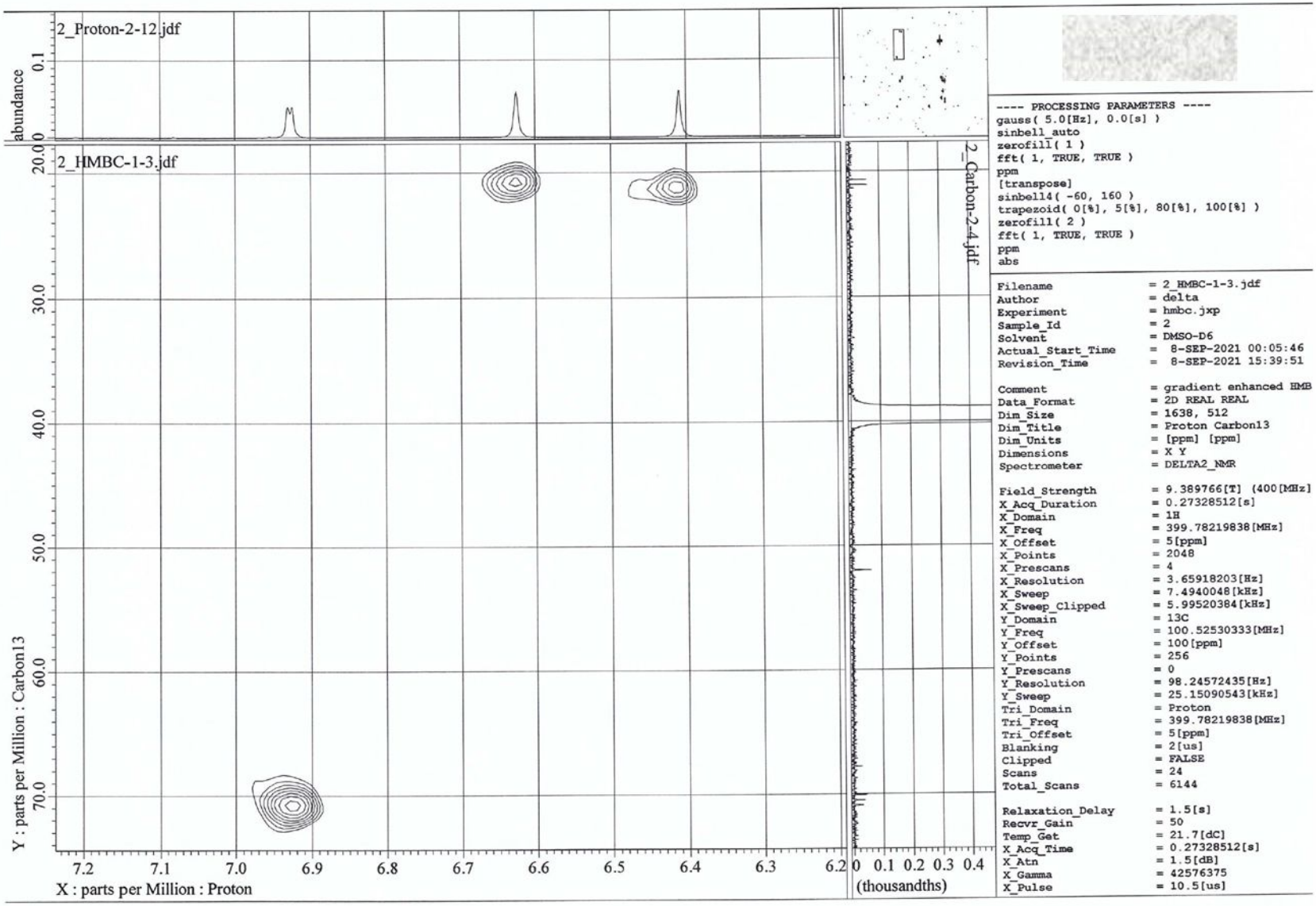
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abundance
0.1
0
2_HMBC-1-3.jdf
20.0
30.0
40.0
50.0
60.0
70.0
Y : parts per Million : Carbon13
7.2
7.1
7.0
6.9
6.8
6.7
6.6
6.5
6.4
6.3
6.2
X : parts per Million : Proton
2_Carbon-2-4.jdf
0
0.1
0.2
0.3
0.4
(thousandths)
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zerofill(2)
fft(1, TRUE, TRUE)
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Experiment = hmbc.jxp
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X_Freq = 399.78219838[MHz]
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X_Points = 2048
X_Prescans = 4
X_Resolution = 3.65918203[Hz]
X_Sweep = 7.4940048[kHz]
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Y_Freq = 100.52530333[MHz]
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Y_Points = 256
Y_Prescans = 0
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Tri_Freq = 399.78219838[MHz]
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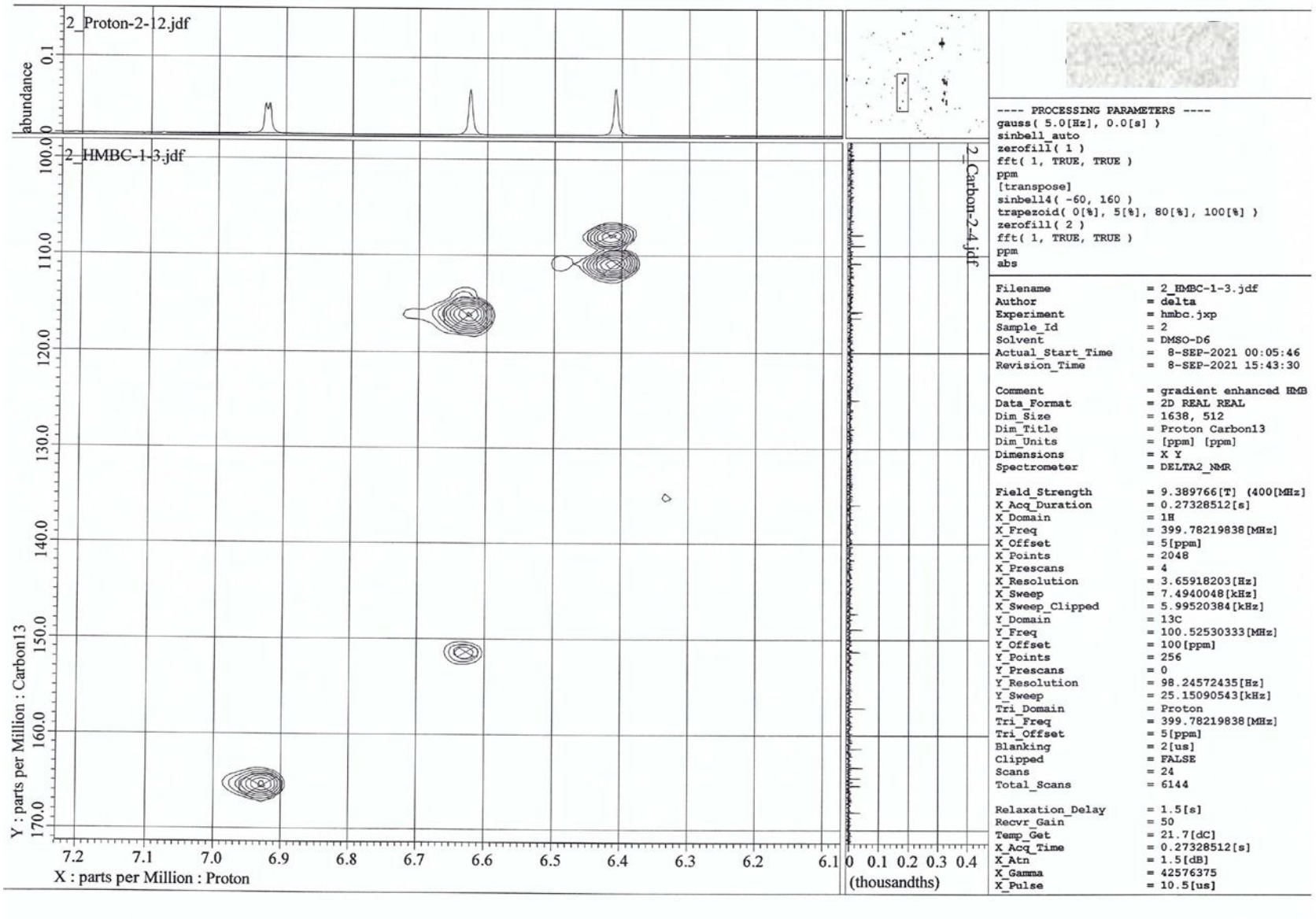
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0.1
0
2_HMBC-1-3.jdf
100.0
110.0
120.0
130.0
140.0
150.0
160.0
170.0
Y : parts per Million : Carbon13
7.2
7.1
7.0
6.9
6.8
6.7
6.6
6.5
6.4
6.3
6.2
6.1
X : parts per Million : Proton
2_Carbon-2-4.jdf
0 0.1 0.2 0.3 0.4
(thousandths)
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zerofill(2)
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X_Sweep_Clipped = 5.99520384[kHz]
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Y_Freq = 100.52530333[MHz]
Y_Offset = 100[ppm]
Y_Points = 256
Y_Prescans = 0
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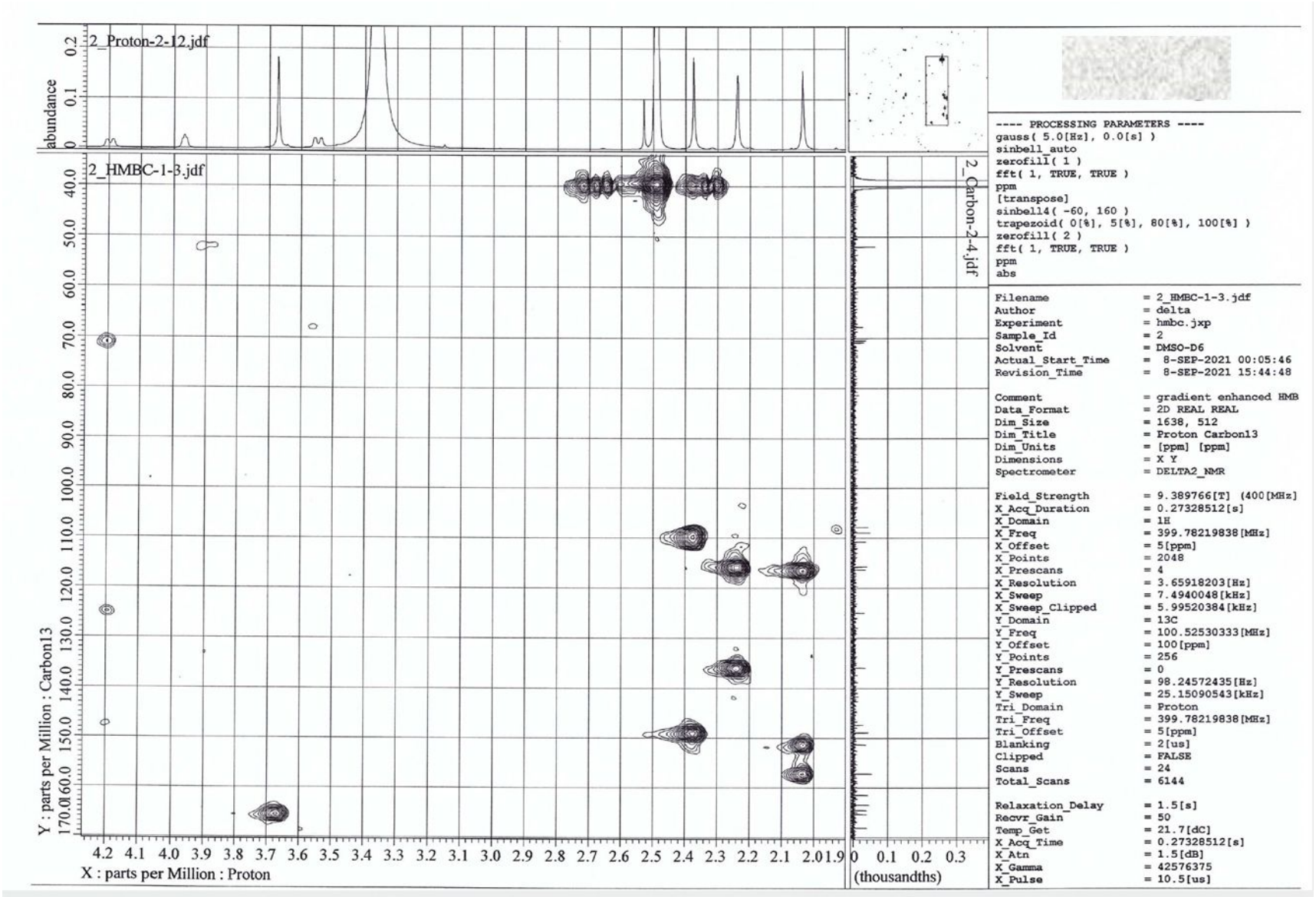
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abundance
2_HMBC-1-3.jdf
2_Carbon-2-4.jdf
Y : parts per Million : Carbon13
X : parts per Million : Proton
(thousandths)
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[transpose]
sinbell4(-60, 160)
trapezoid(0[%], 5[%], 80[%], 100[%])
zerofill(2)
fft(1, TRUE, TRUE)
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X_Offset = 5[ppm]
X_Points = 2048
X_Prescans = 4
X_Resolution = 3.65918203[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Y_Domain = 13C
Y_Freq = 100.52530333[MHz]
Y_Offset = 100[ppm]
Y_Points = 256
Y_Prescans = 0
Y_Resolution = 98.24572435[Hz]
Y_Sweep = 25.15090543[kHz]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 24
Total_Scans = 6144
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Temp_Get = 21.7[dC]
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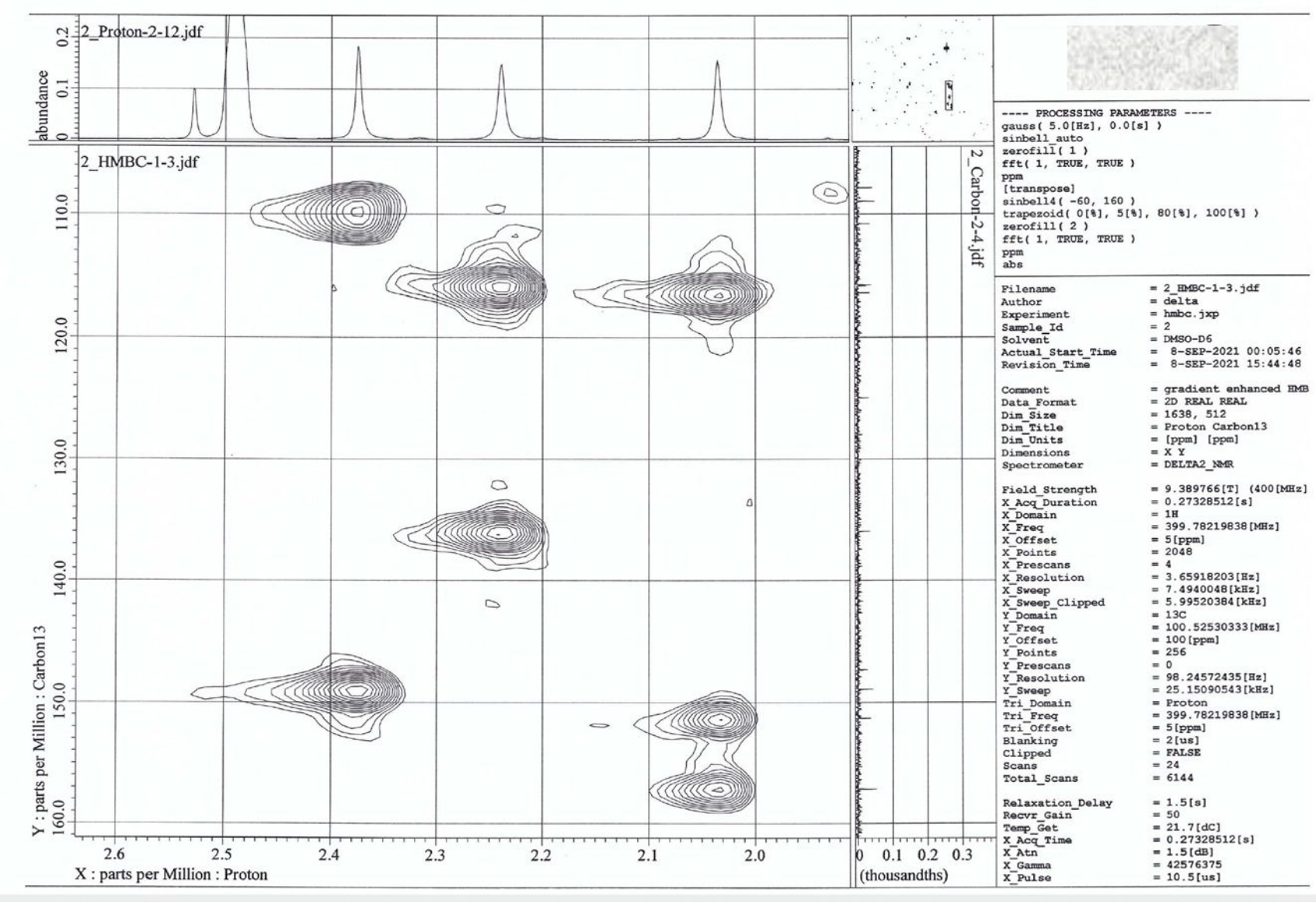
X_Gamma = 42576375
X_Pulse = 10.5[us]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abundance
0
0.1
0.2
2_HMBC-1-3.jdf
2_Carbon-2-4.jdf
Y : parts per Million : Carbon13
110.0
120.0
130.0
140.0
150.0
160.0
2.6
2.5
2.4
2.3
2.2
2.1
2.0
X : parts per Million : Proton
0
0.1
0.2
0.3
(thousandths)
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X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 2048
X_Prescans = 4
X_Resolution = 3.65918203[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Y_Domain = 13C
Y_Freq = 100.52530333[MHz]
Y_Offset = 100[ppm]
Y_Points = 256
Y_Prescans = 0
Y_Resolution = 98.24572435[Hz]
Y_Sweep = 25.15090543[kHz]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 24
Total_Scans = 6144
Relaxation_Delay = 1.5[s]
Recvr_Gain = 50
Temp_Get = 21.7[dC]
X_Acq_Time = 0.27328512[s]
X_Atn = 1.5[dB]
X_Gamma = 42576375
X_Pulse = 10.5[us]