Supporting information

NMR-Guided Discovery of Luvunga D: A Novel Propellane-Type Limonoid from *Luvunga scandens* That Functions as a Non-Classical Ferroptosis Inhibitor

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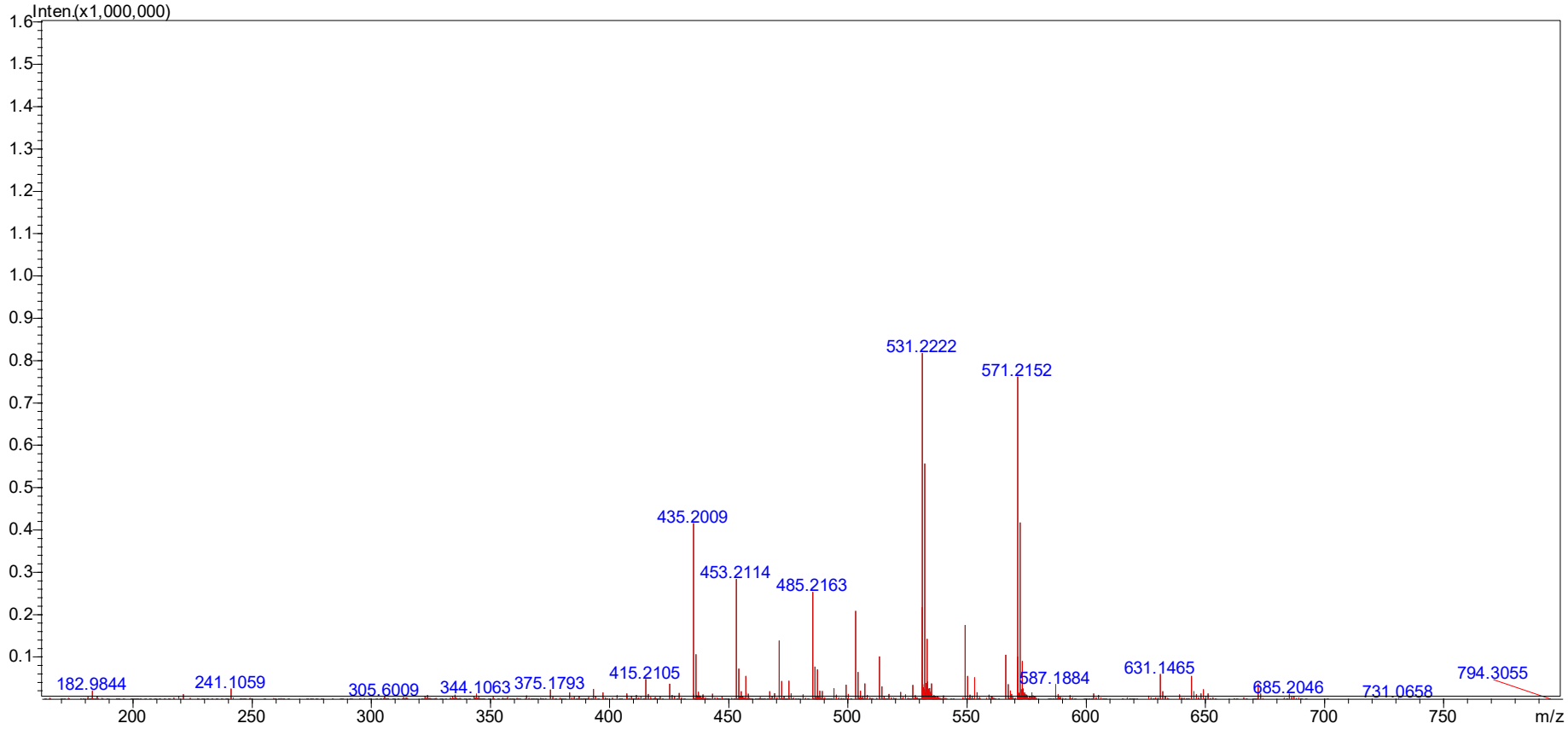


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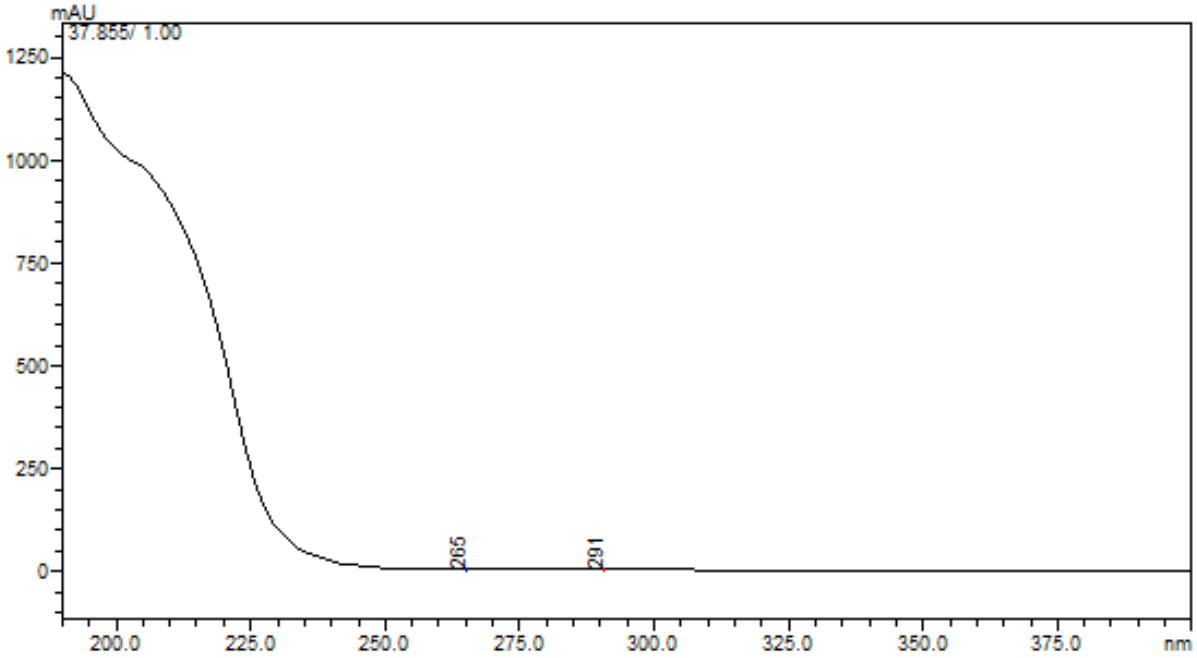


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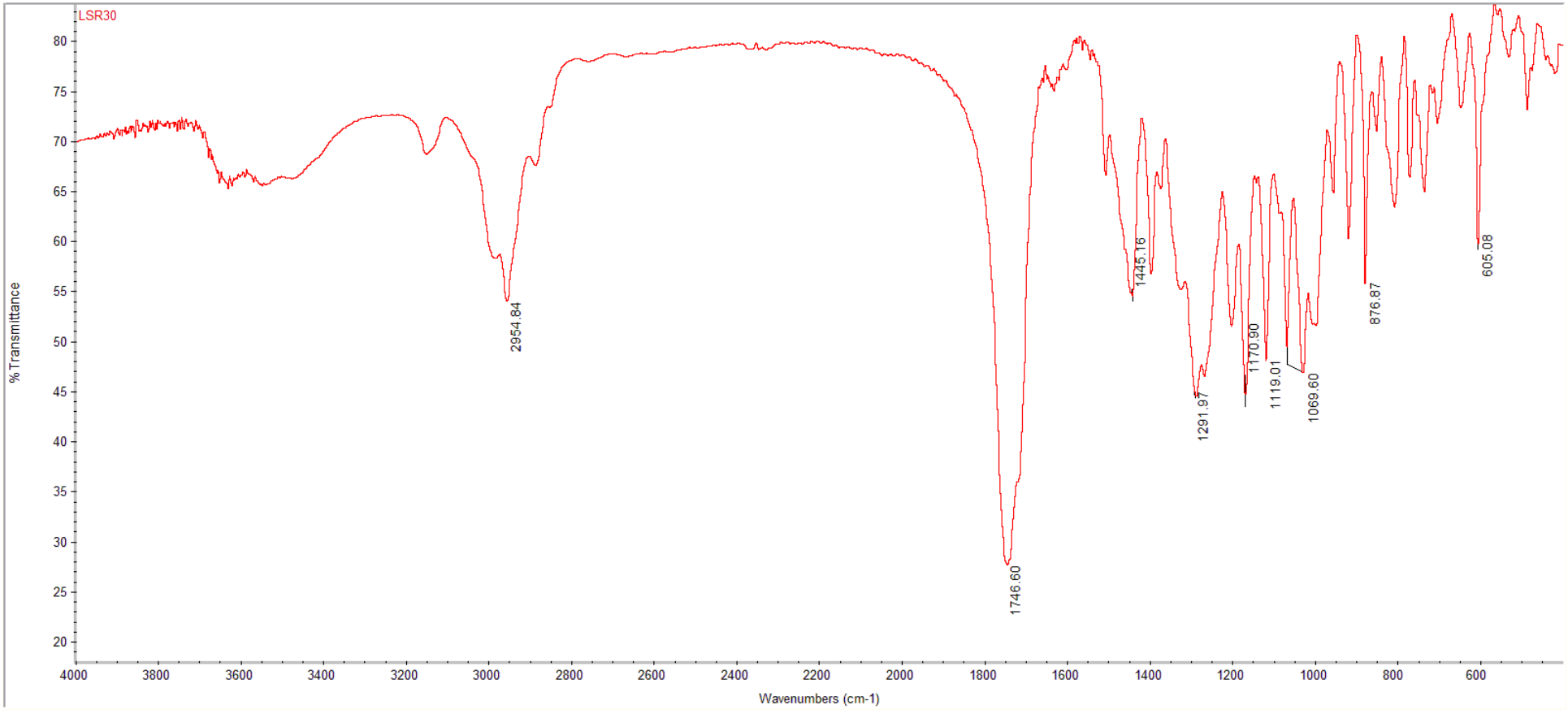


Figure S 3. IR spectrum (film on KBr plates) of compound **3**

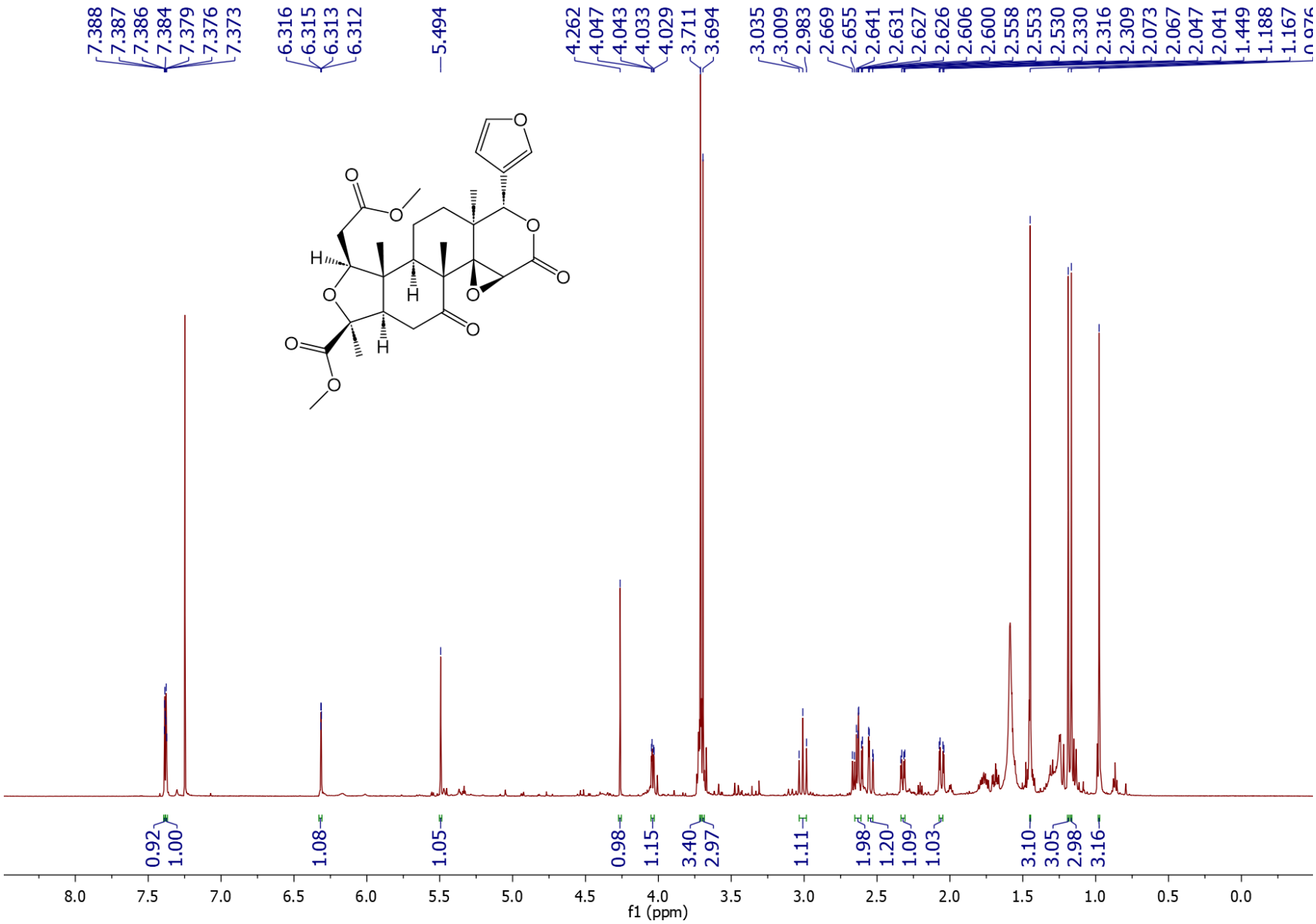


Figure S 4. ^{1}H-NMR (600 MHz) spectrum of compound **3** in $CDCl_3$

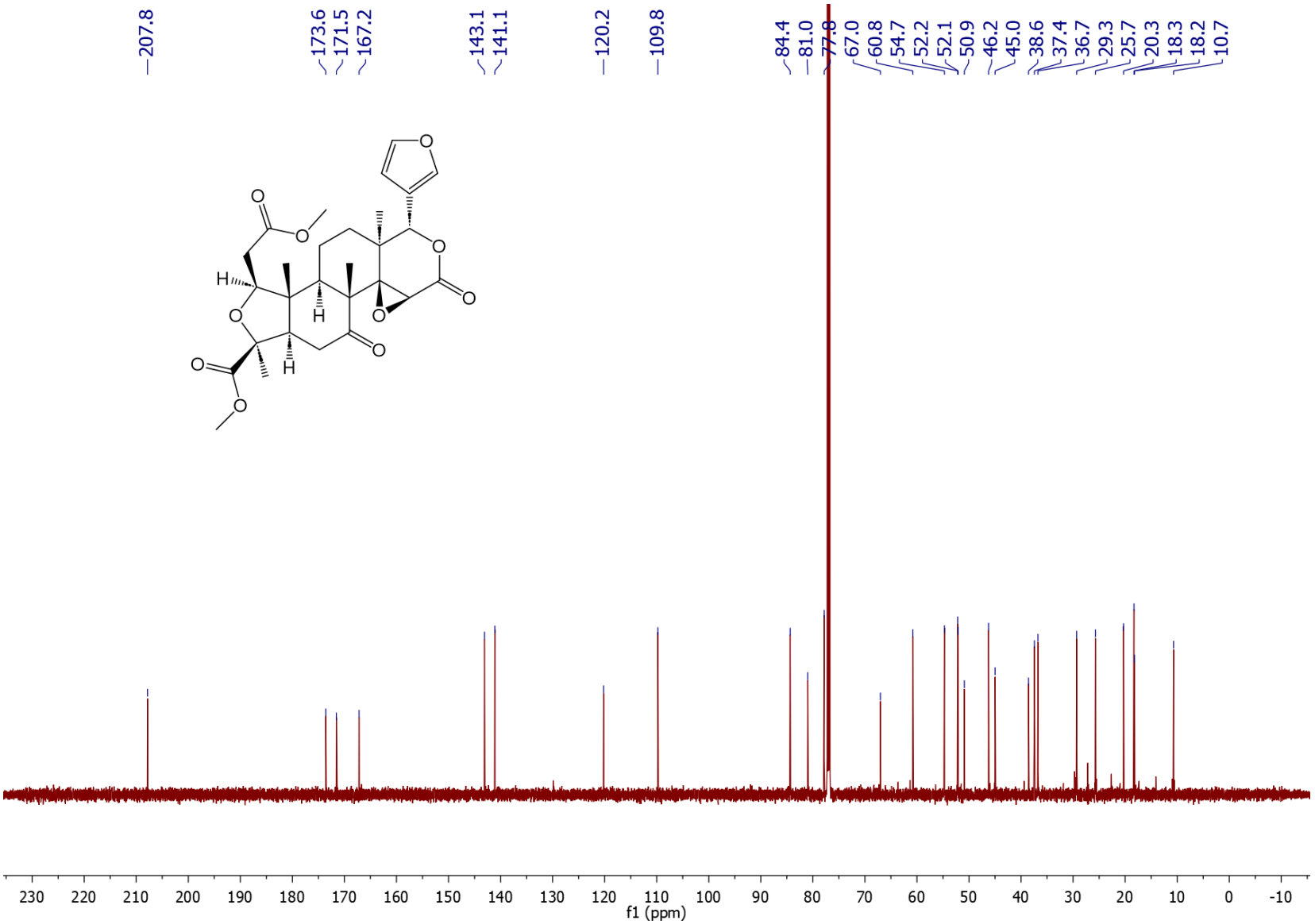


Figure S 5. ^{13}C-NMR (150 MHz) spectrum of compound **3** in $CDCl_3$

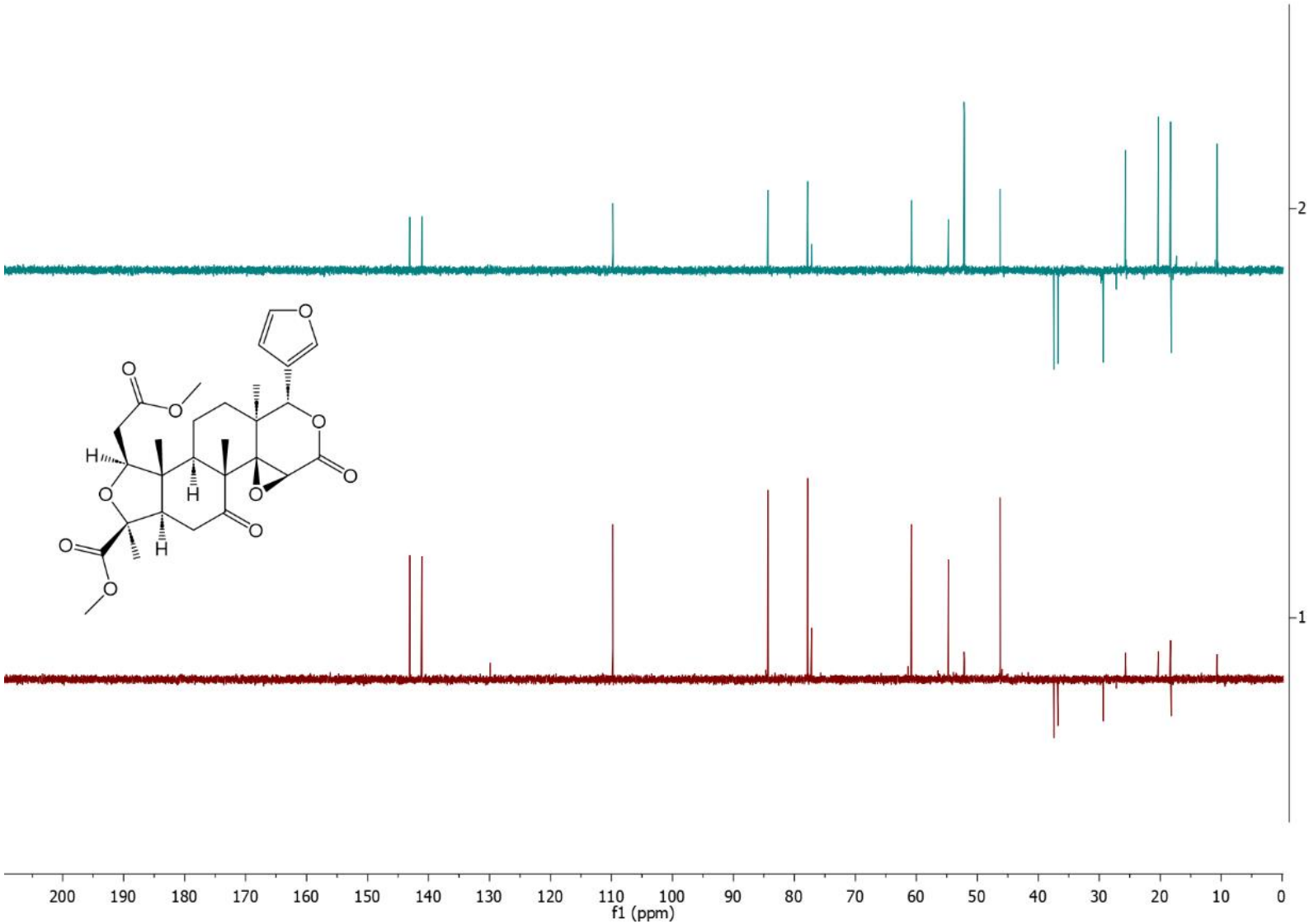


Figure S 6. DEPT-NMR (150 MHz) spectrum of compound **3** in $CDCl_3$

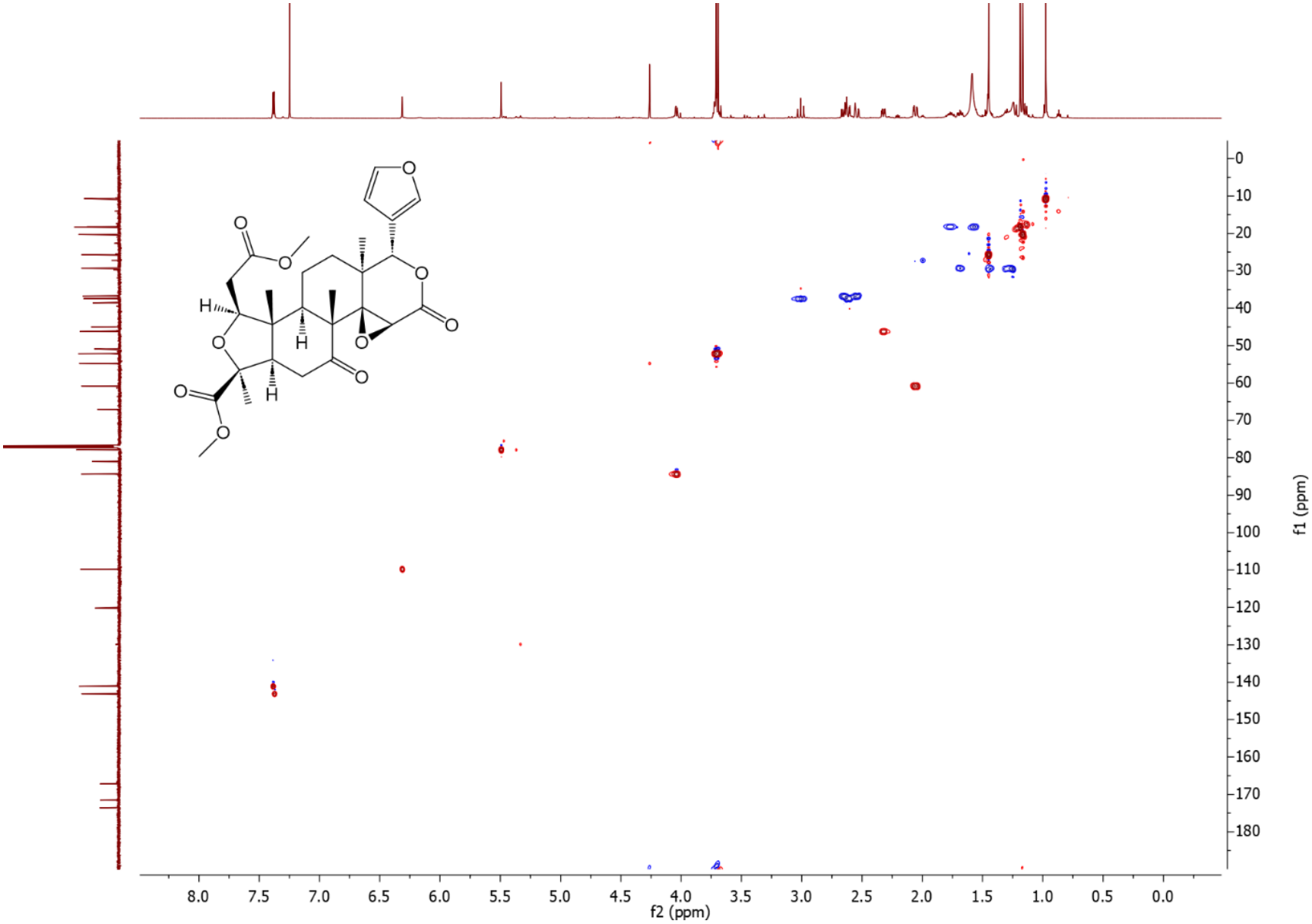


Figure S 7. HSQC spectrum of compound **3** in $CDCl_3$

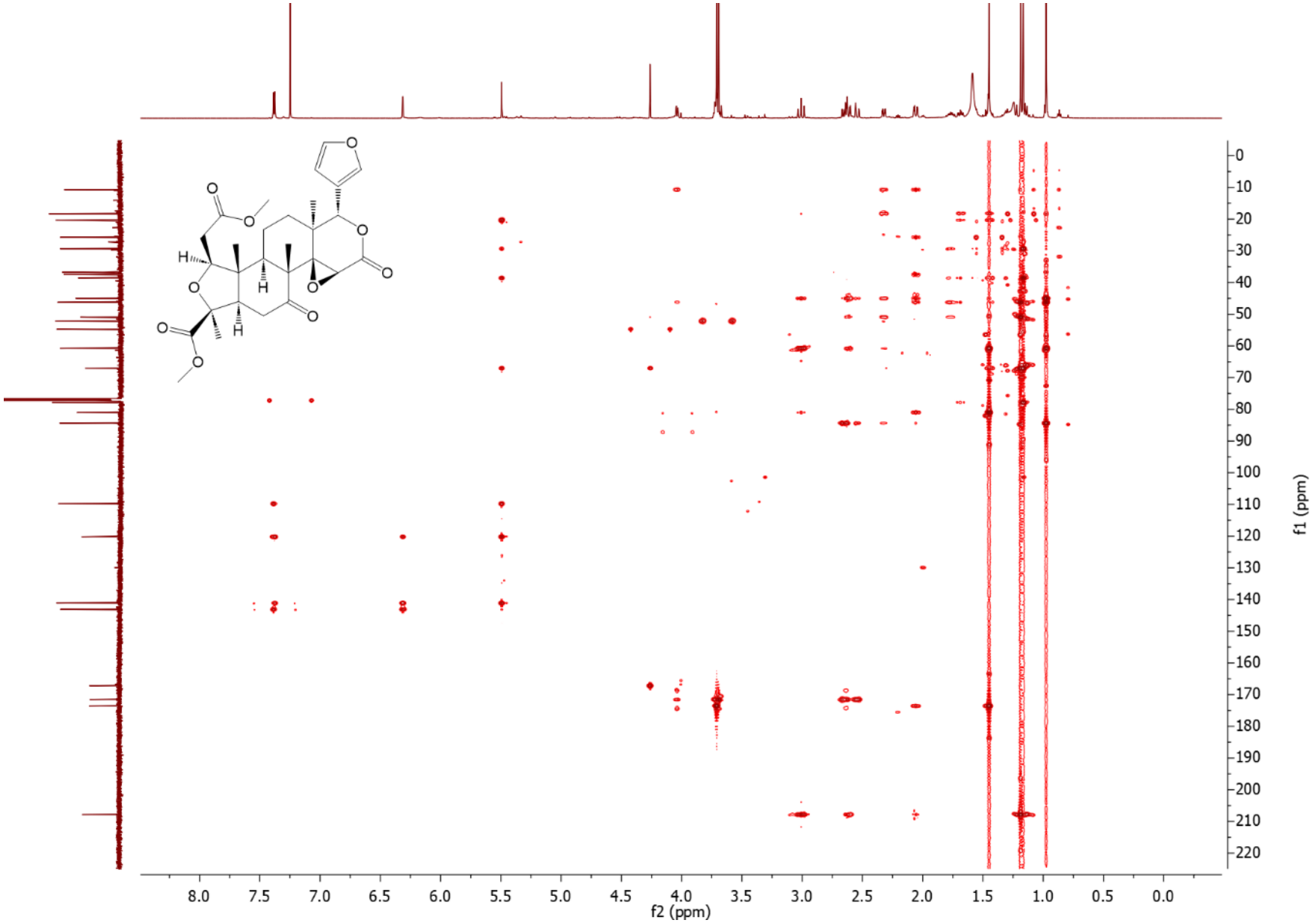


Figure S 8. HMBC spectrum of compound **3** in $CDCl_3$

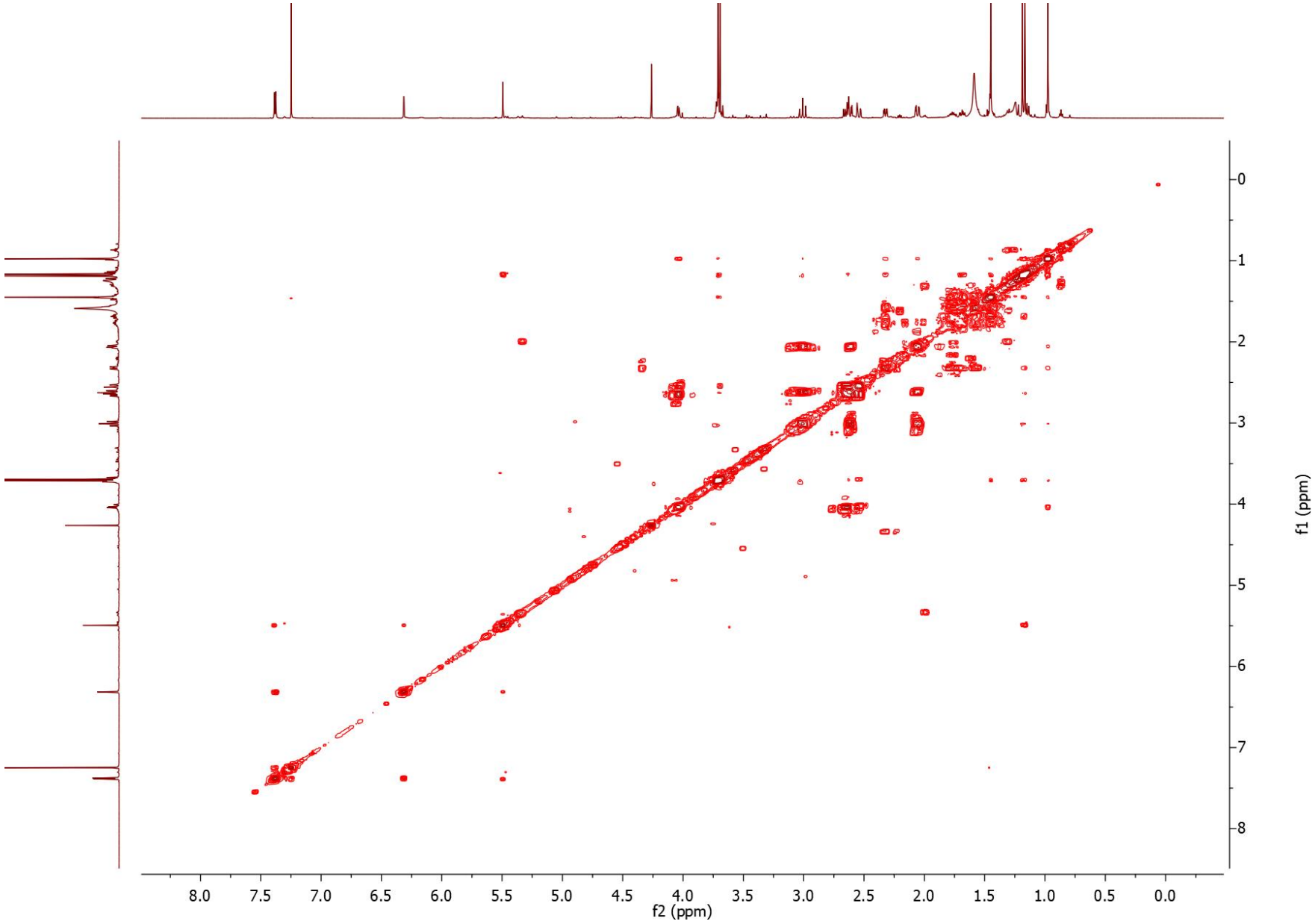


Figure S 9. ^{1}H-^{1}H-COSY spectrum of compound **3** in $CDCl_3$

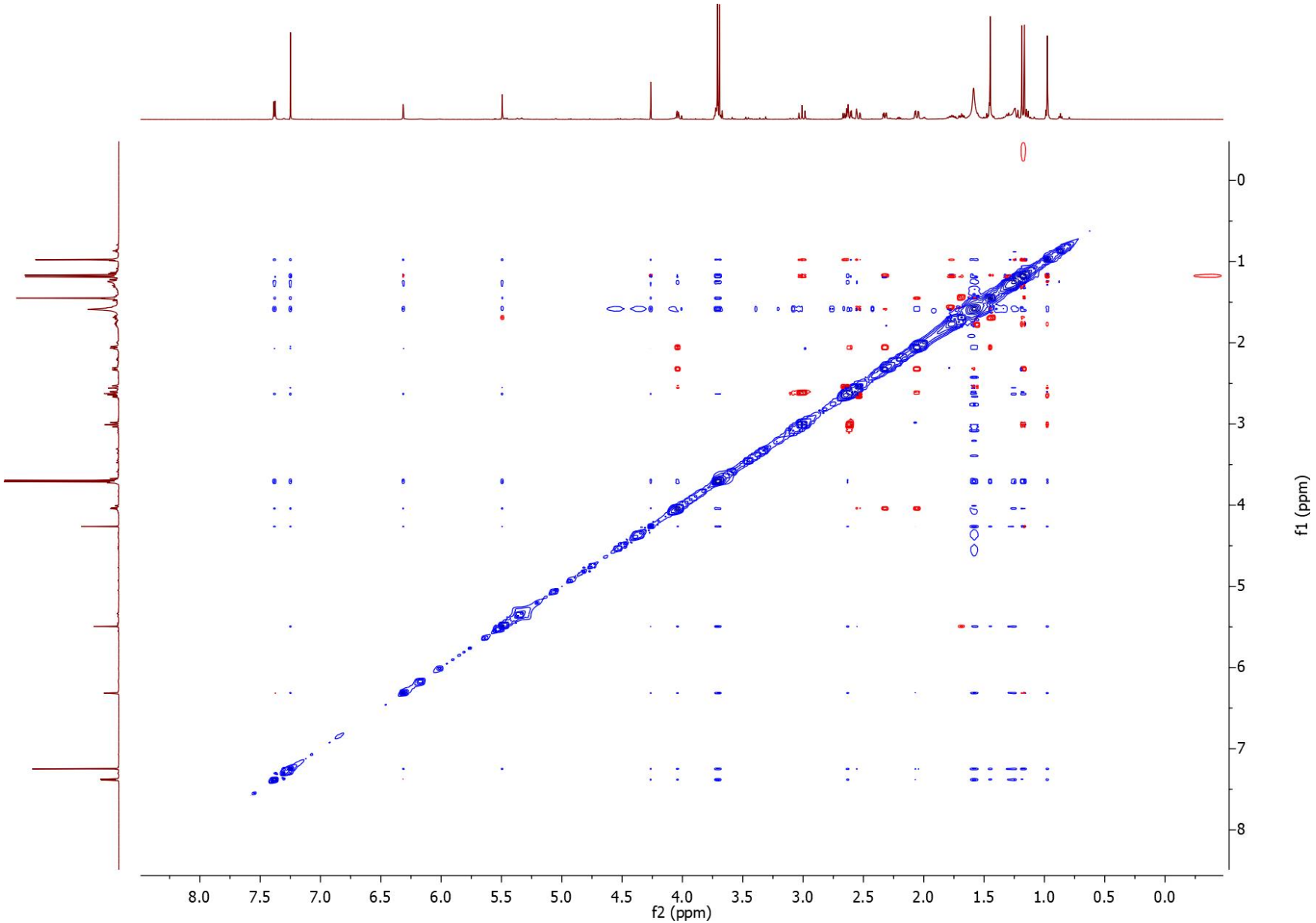


Figure S 10. ^{1}H-^{1}H-NOESY spectrum of compound **3** in $CDCl_3$

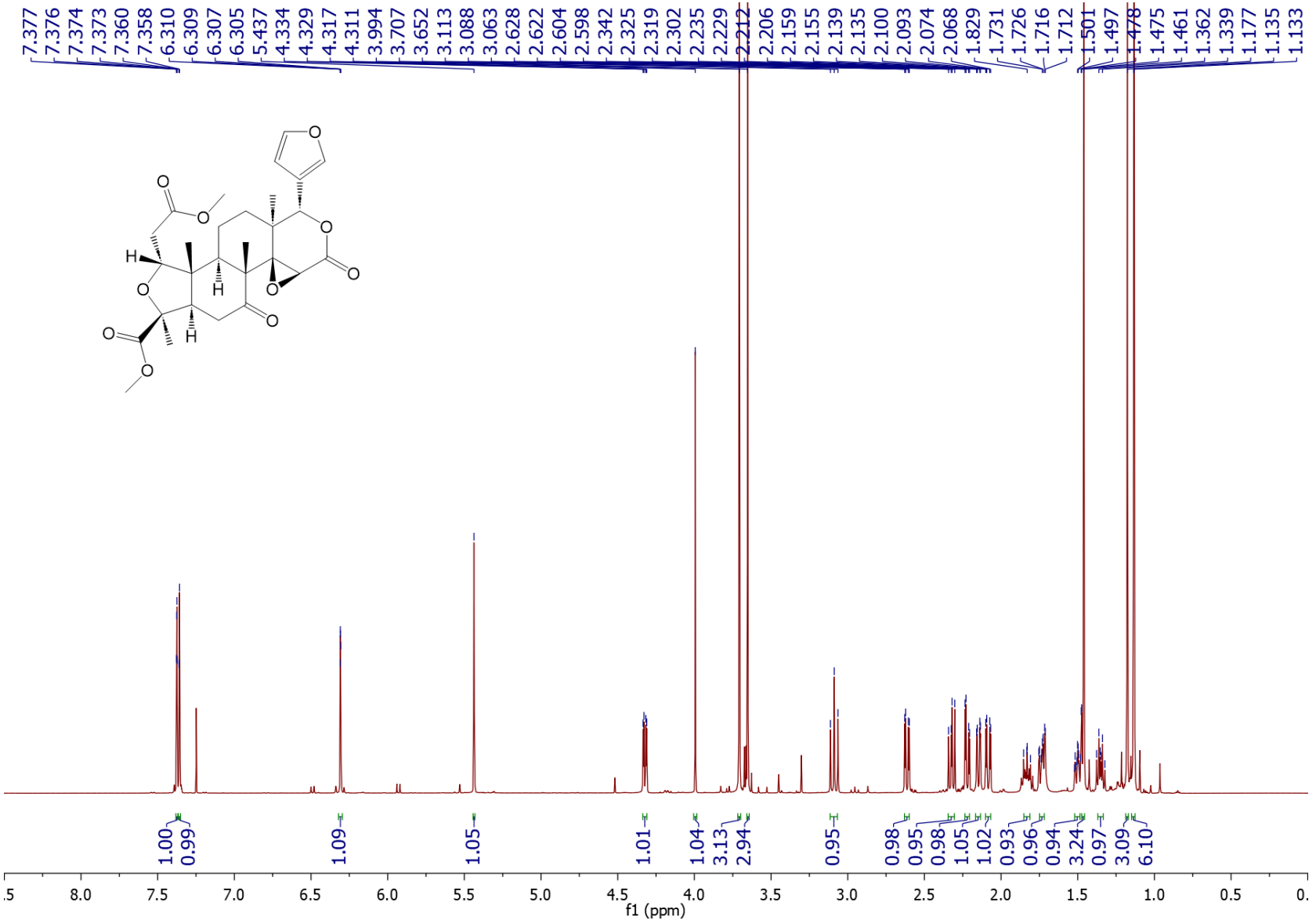


Figure S 11. ^{1}H-NMR (600 MHz) spectrum of compound **2** in $CDCl_3$

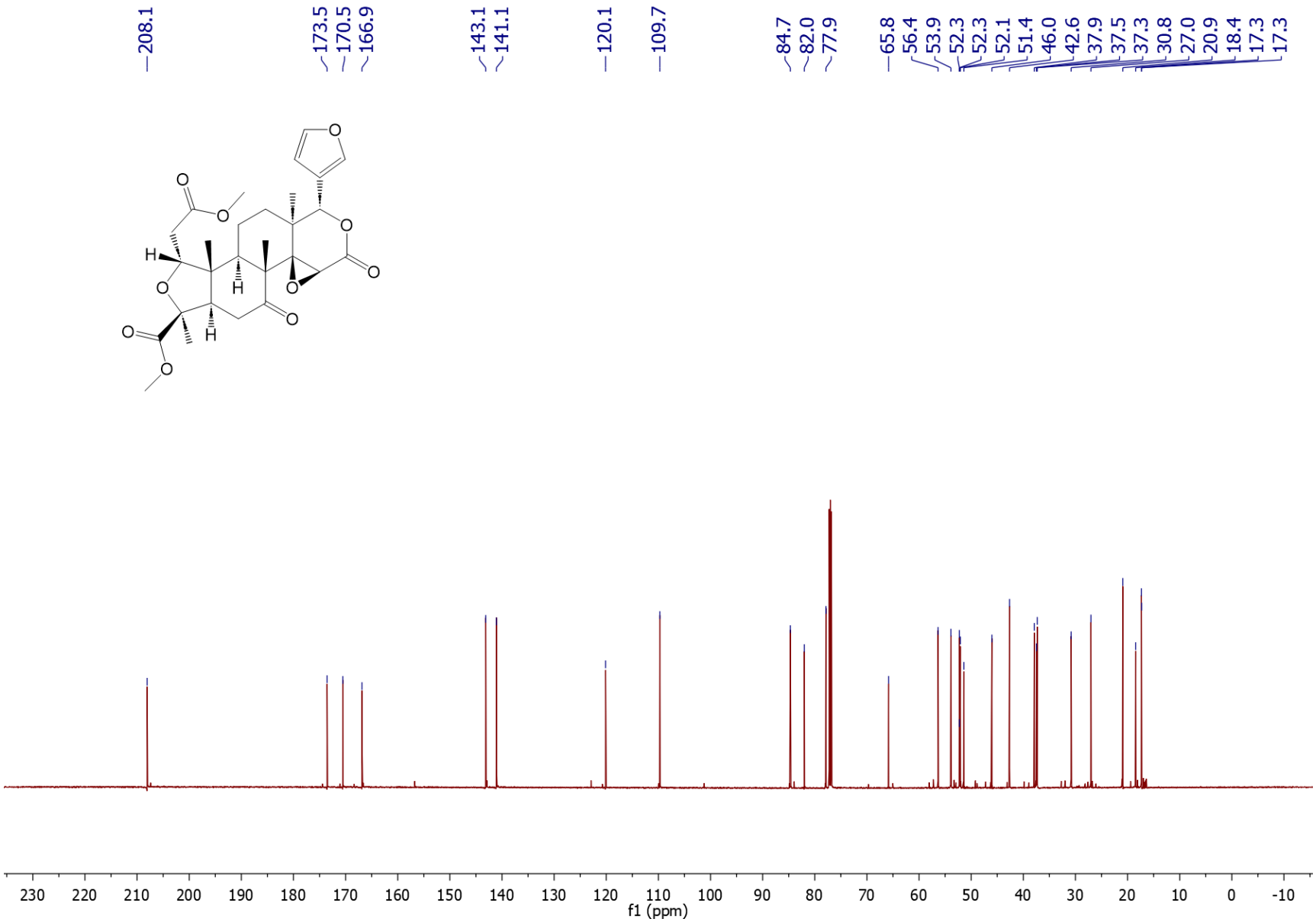


Figure S 12. ^{13}C-NMR (150 MHz) spectrum of compound **2** in $CDCl_3$

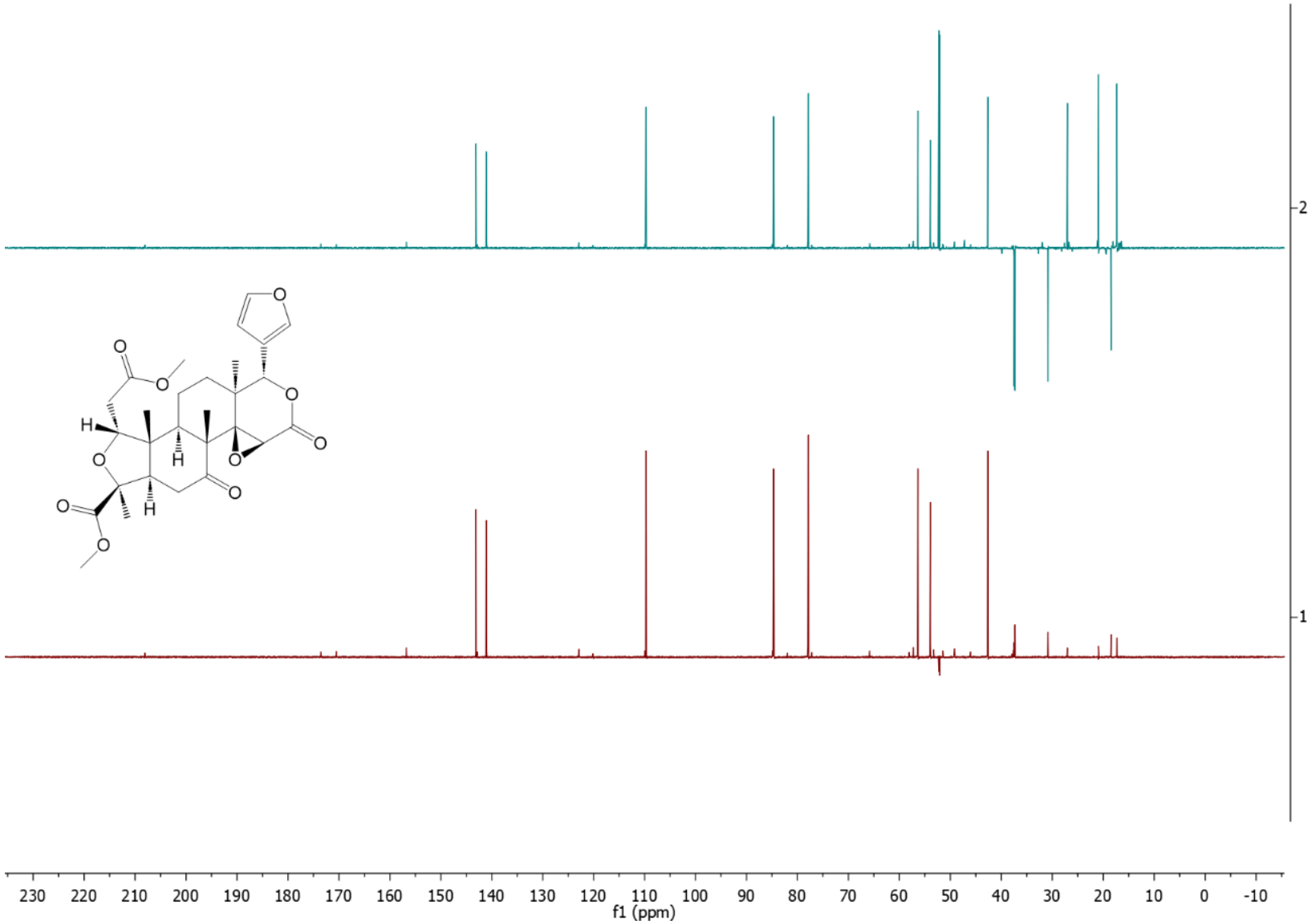


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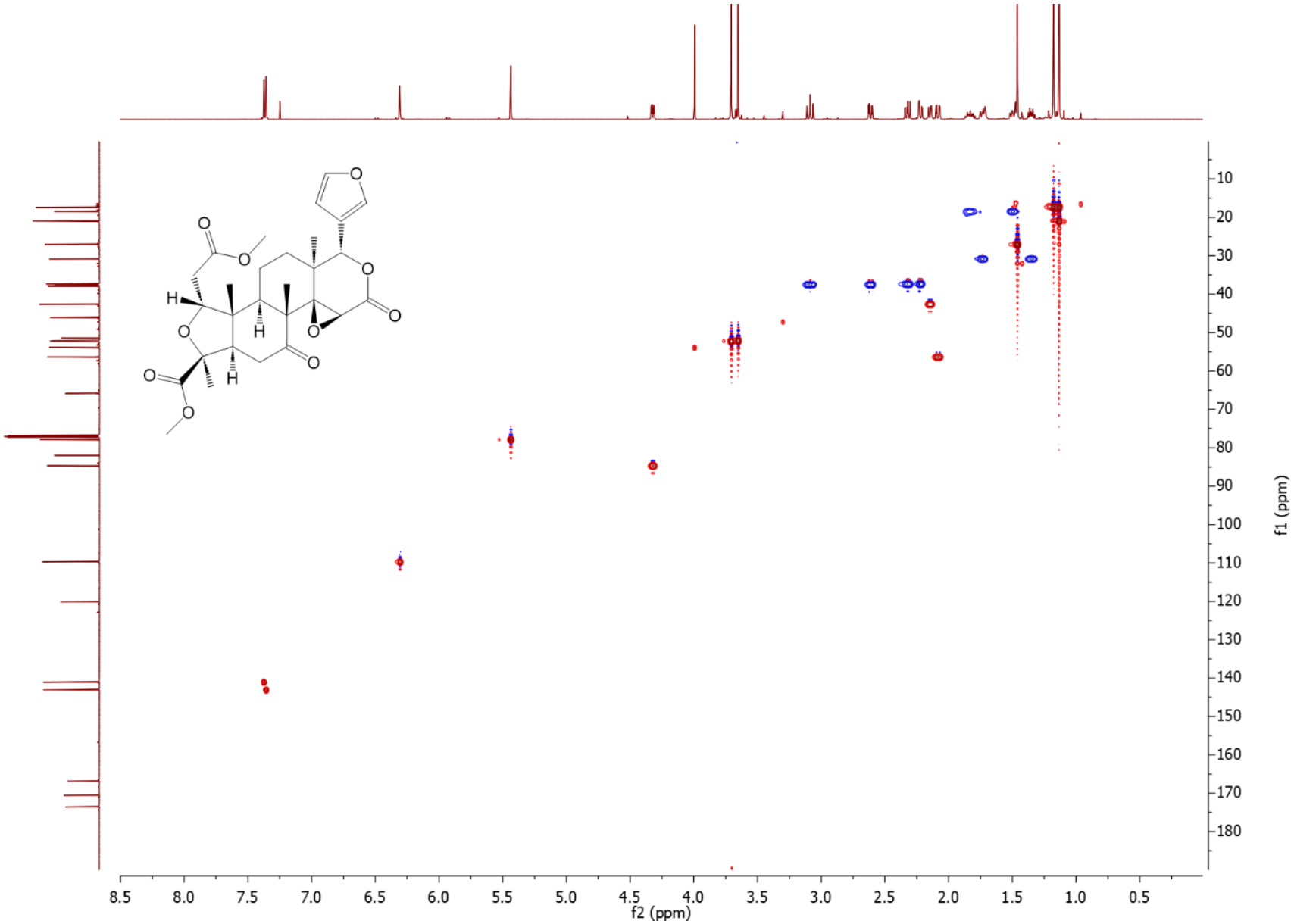


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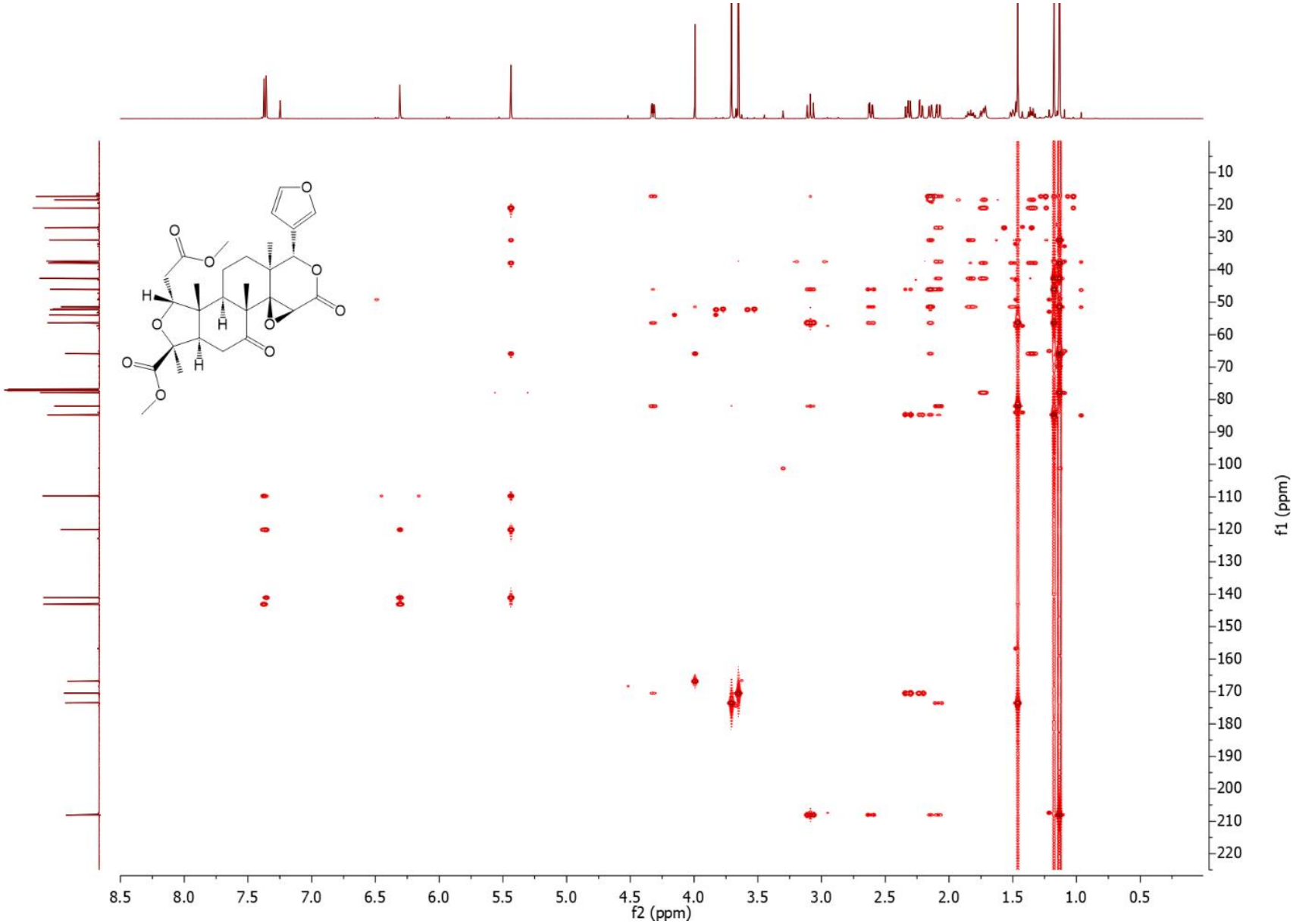


Figure S 15. HMBC spectrum of compound **2** in $CDCl_3$

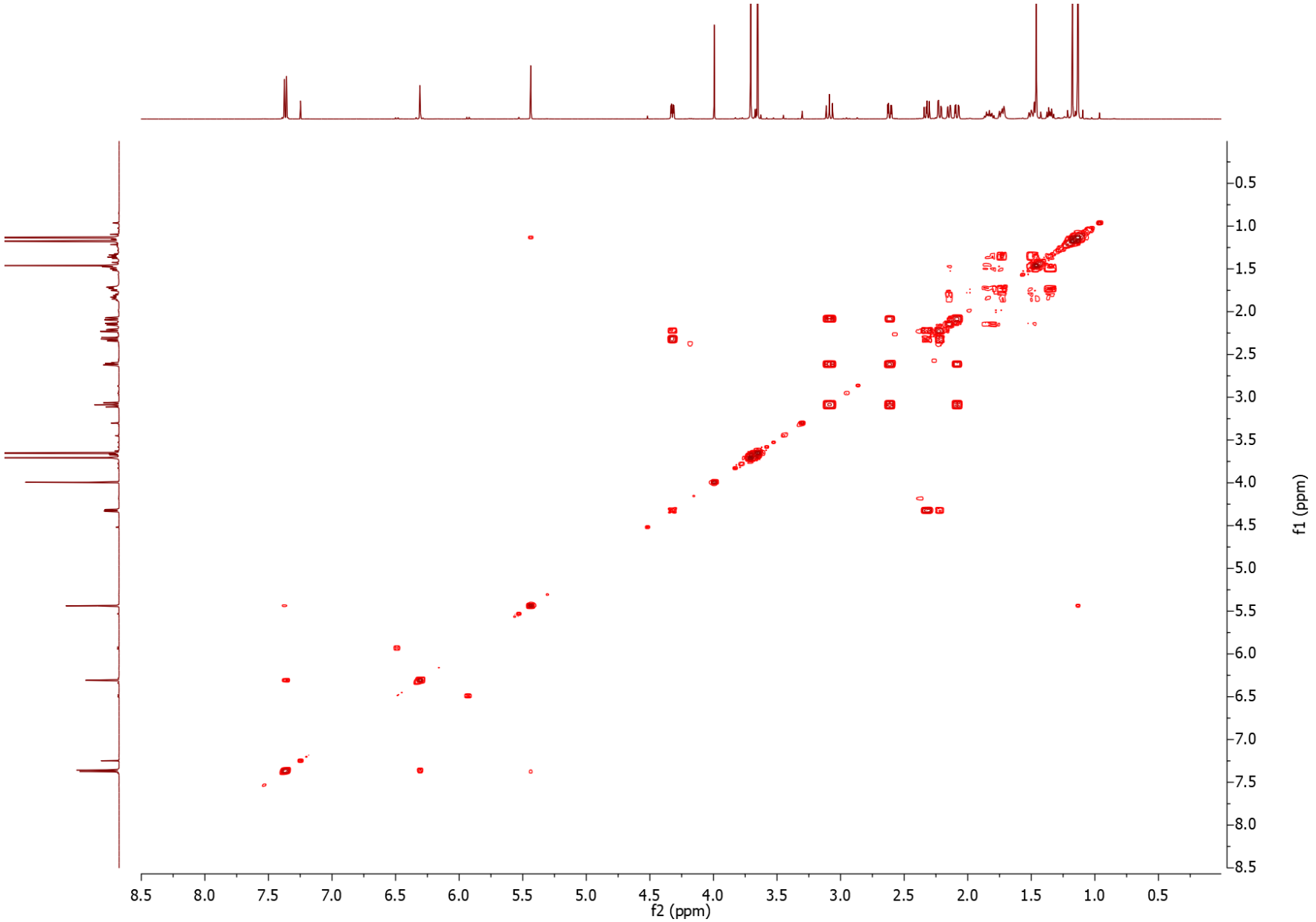


Figure S 16. ^{1}H-^{1}H-COSY spectrum of compound **2** in $CDCl_3$

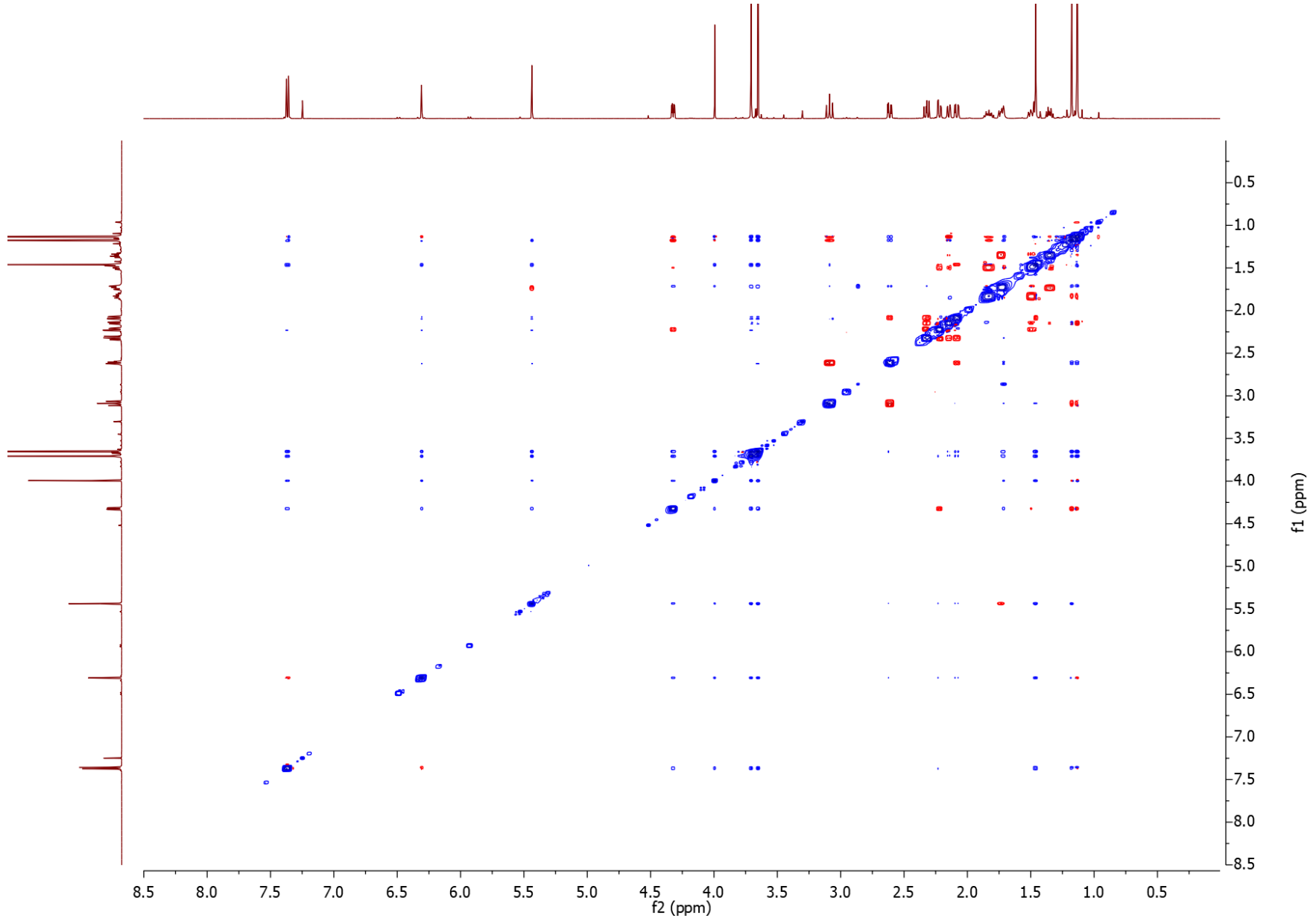


Figure S 17. ^{1}H-^{1}H-NOESY spectrum of compound **2** in $CDCl_3$

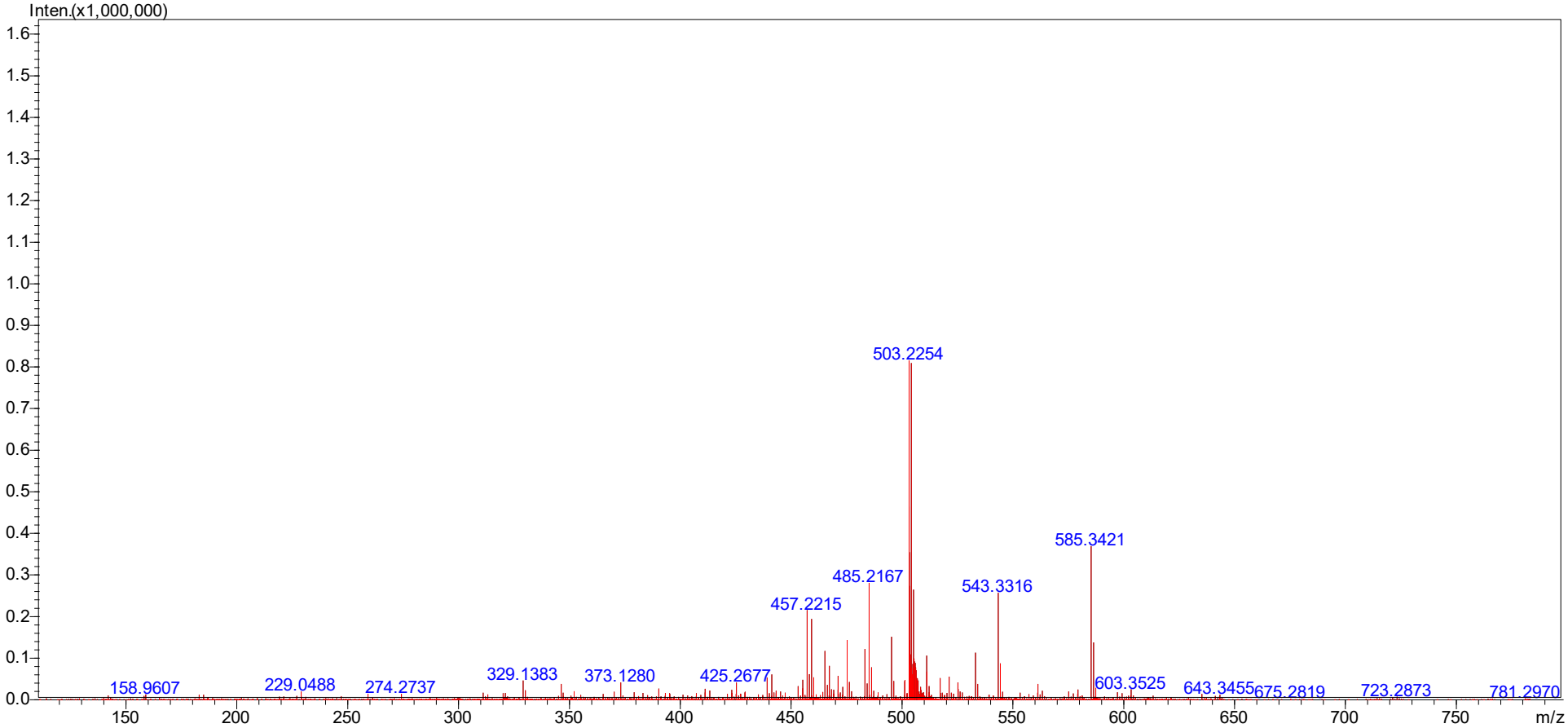


Figure S 18. HR-ESI-MS spectrum of compound **4**

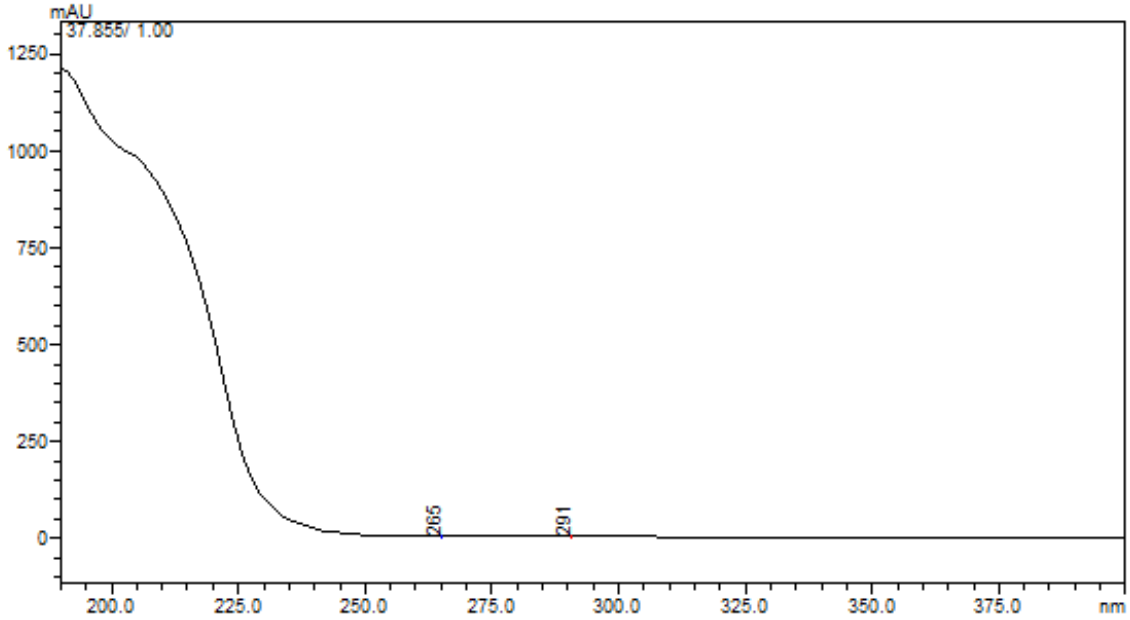


Figure S 19. UV spectrum of compound **4** in methanol

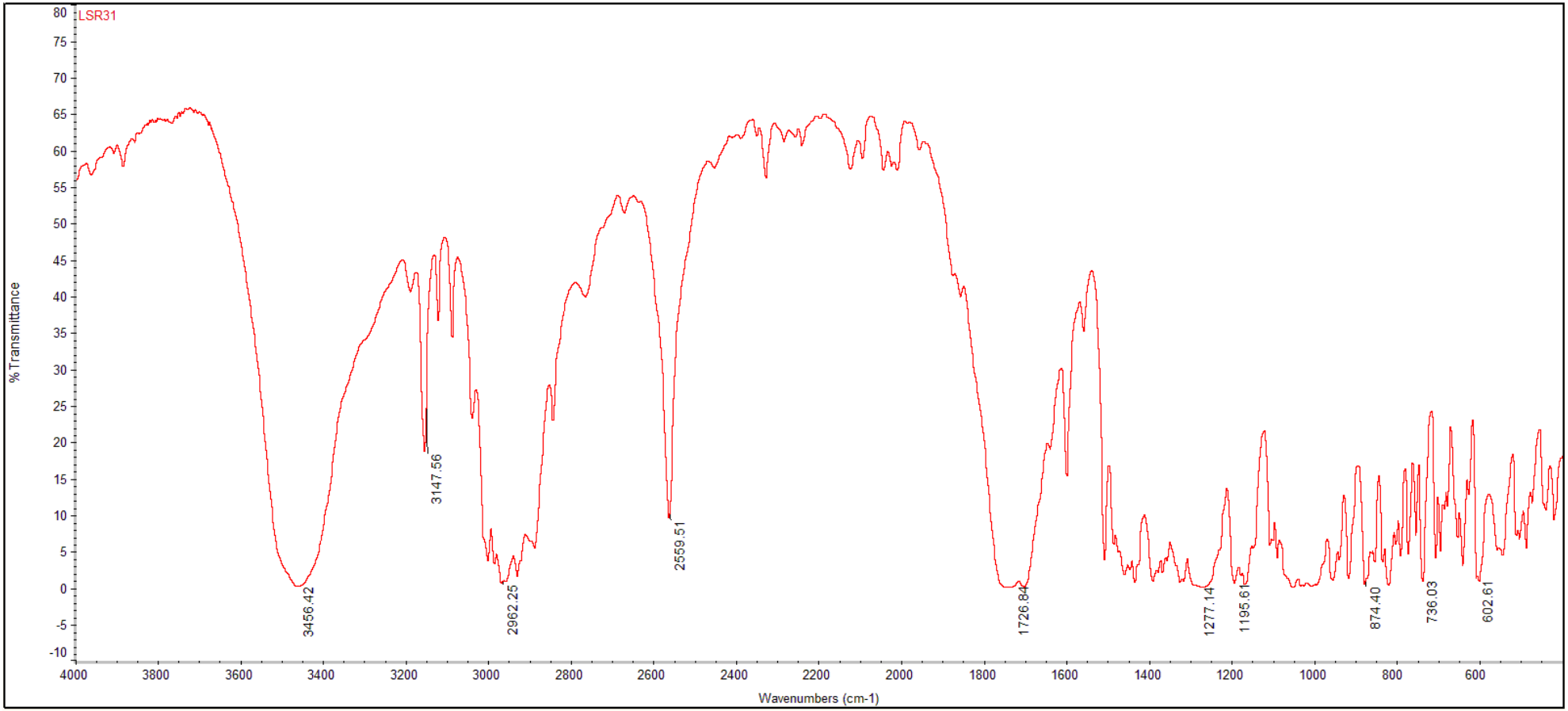


Figure S 20. IR spectrum (film on KBr plates) of compound **4**

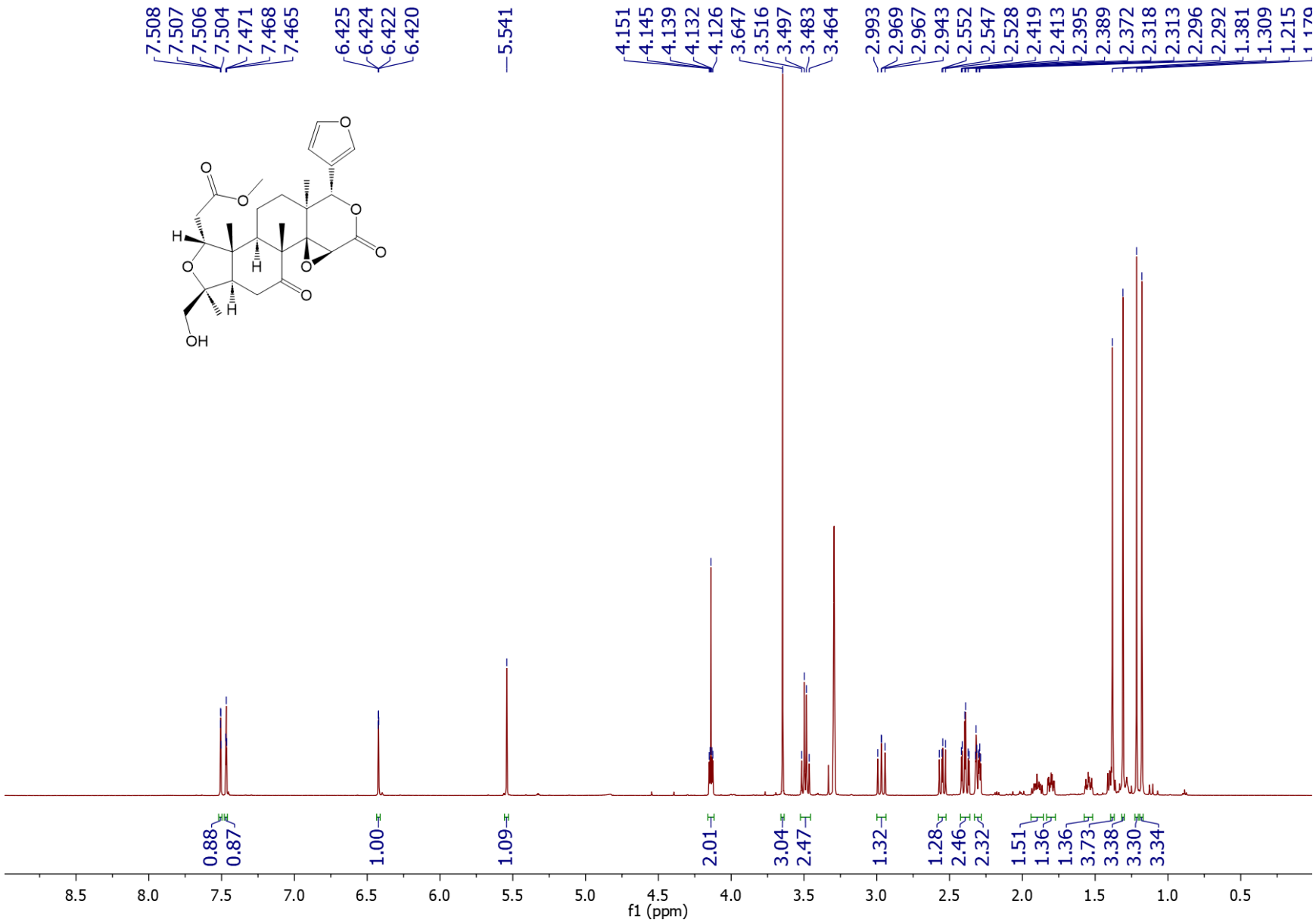


Figure S 21. ^{1}H-NMR (600 MHz) spectrum of compound **4** in CD_3OD

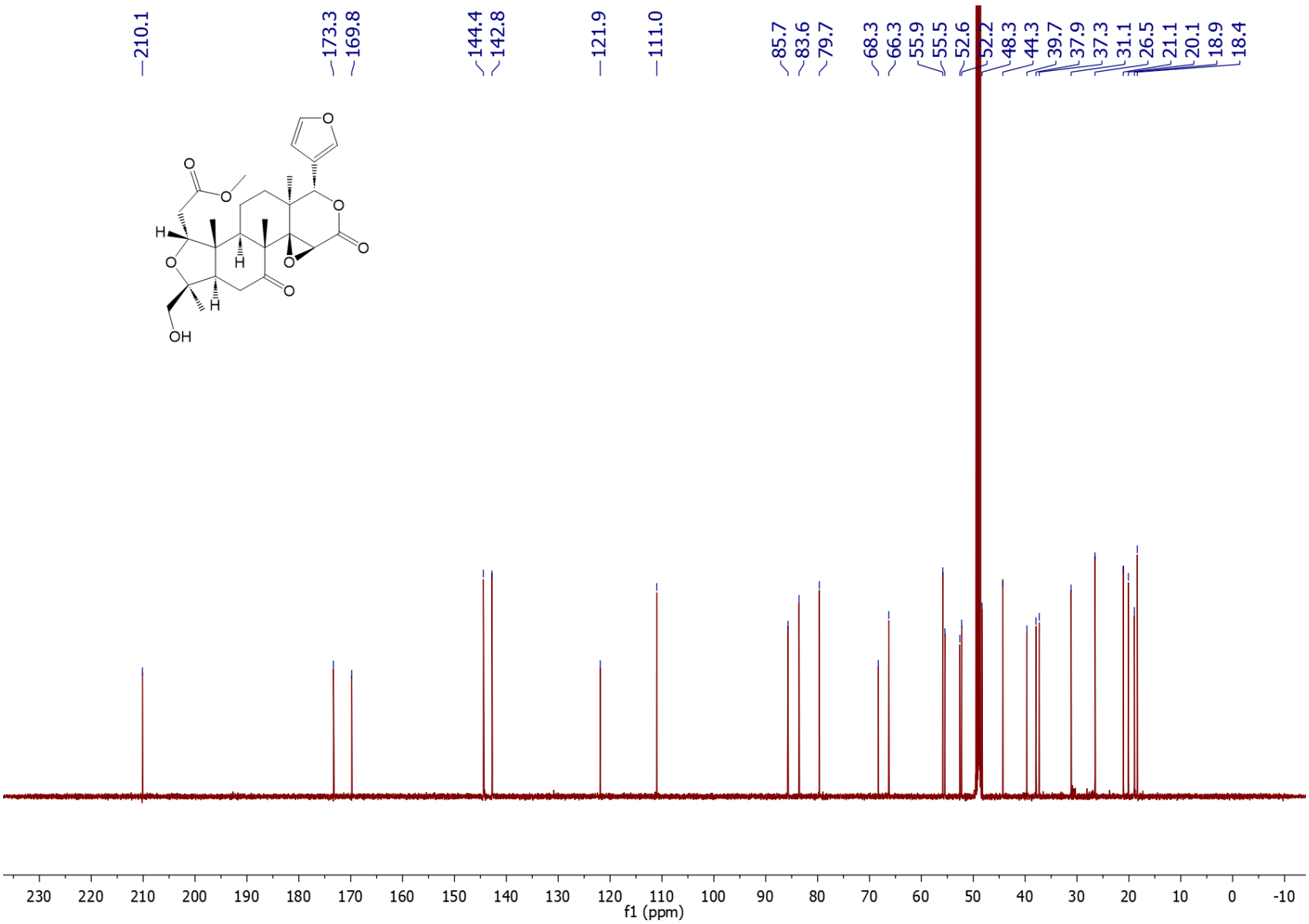


Figure S 22. ^{13}C-NMR (150 MHz) spectrum of compound **4** in CD_3OD

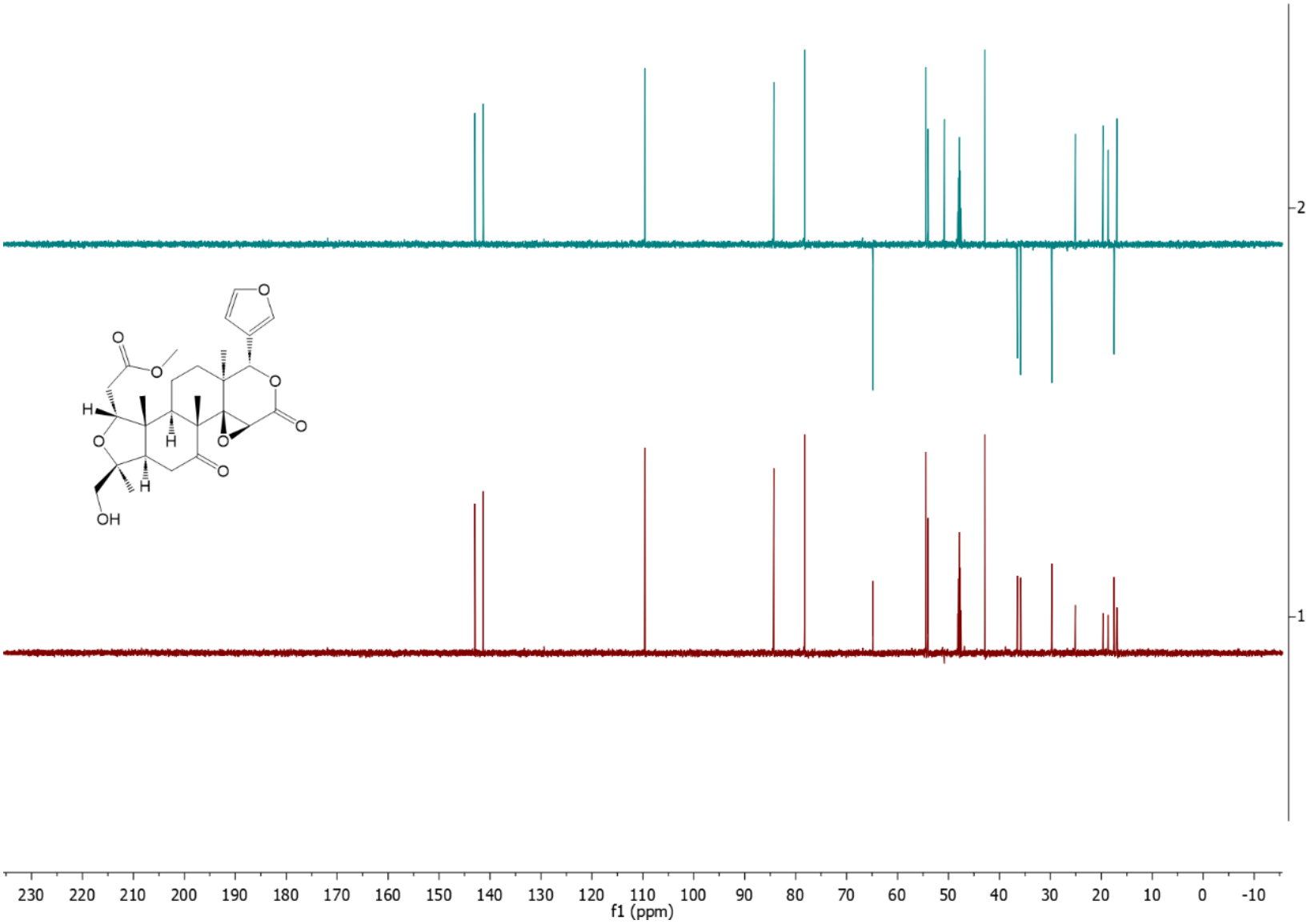


Figure S 23. DEPT-NMR (150 MHz) spectrum of compound **4** in CD_3OD

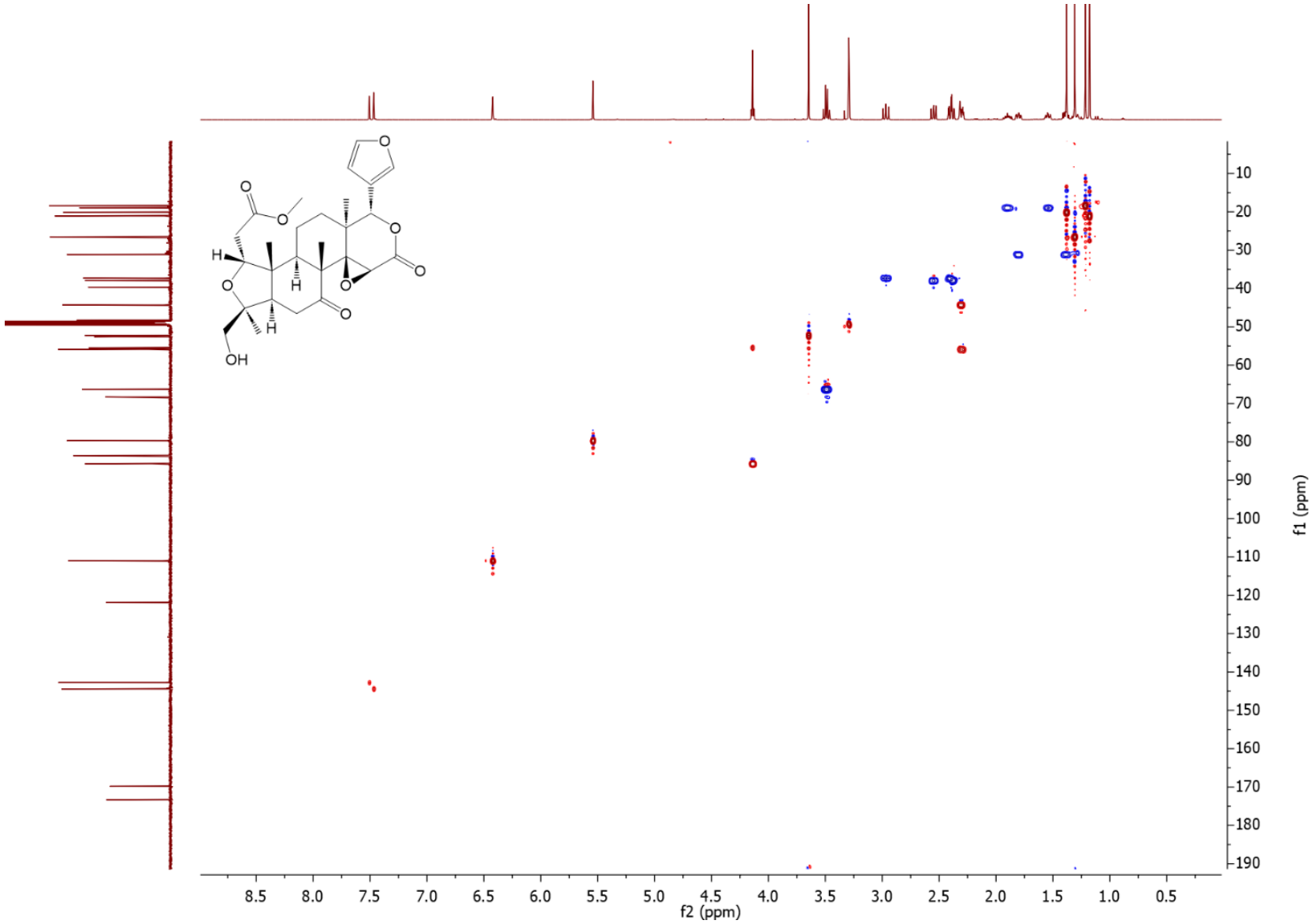


Figure S 24. HSQC spectrum of compound **4** in CD_3OD

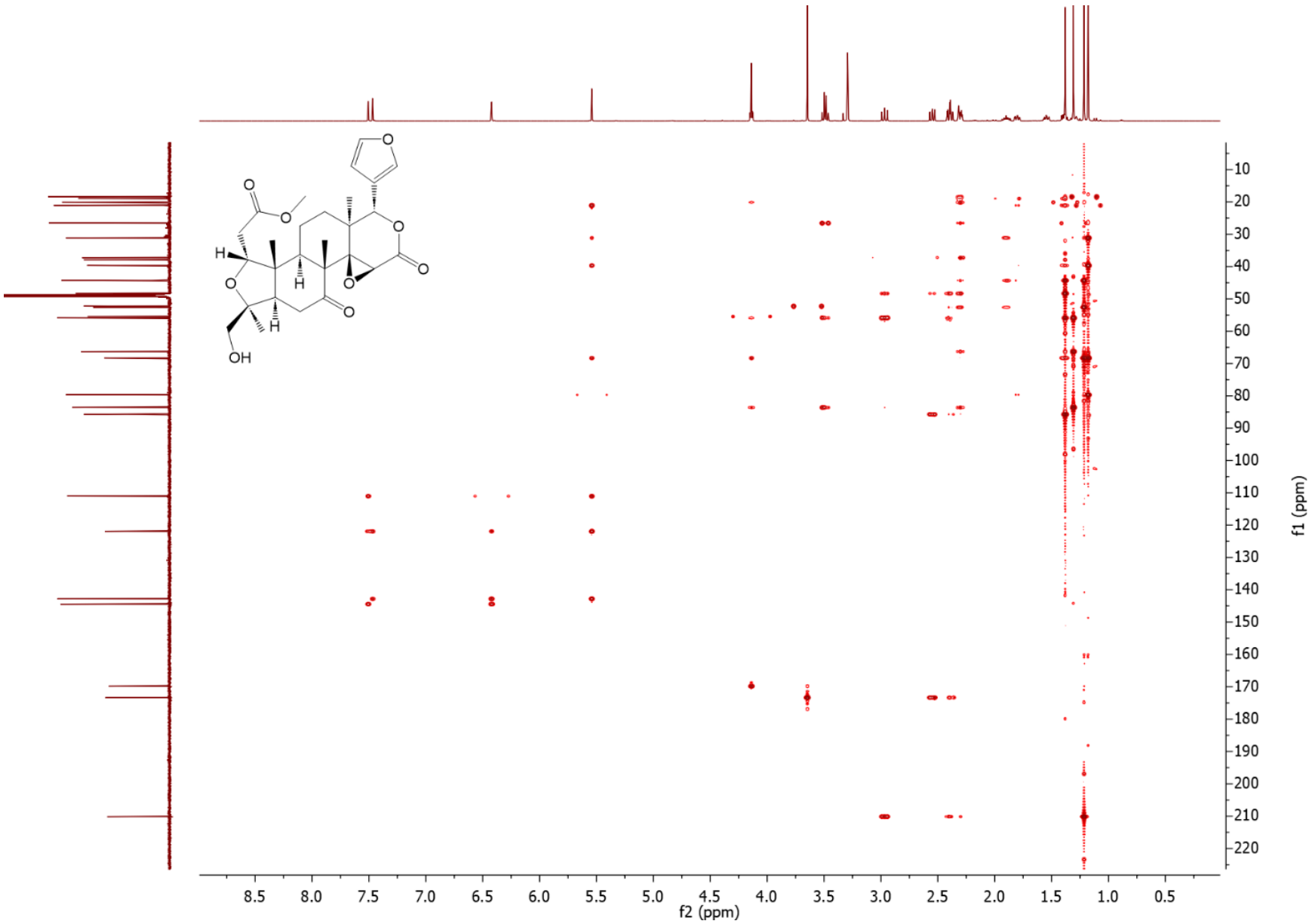


Figure S 25. HMBC spectrum of compound **4** in CD_3OD

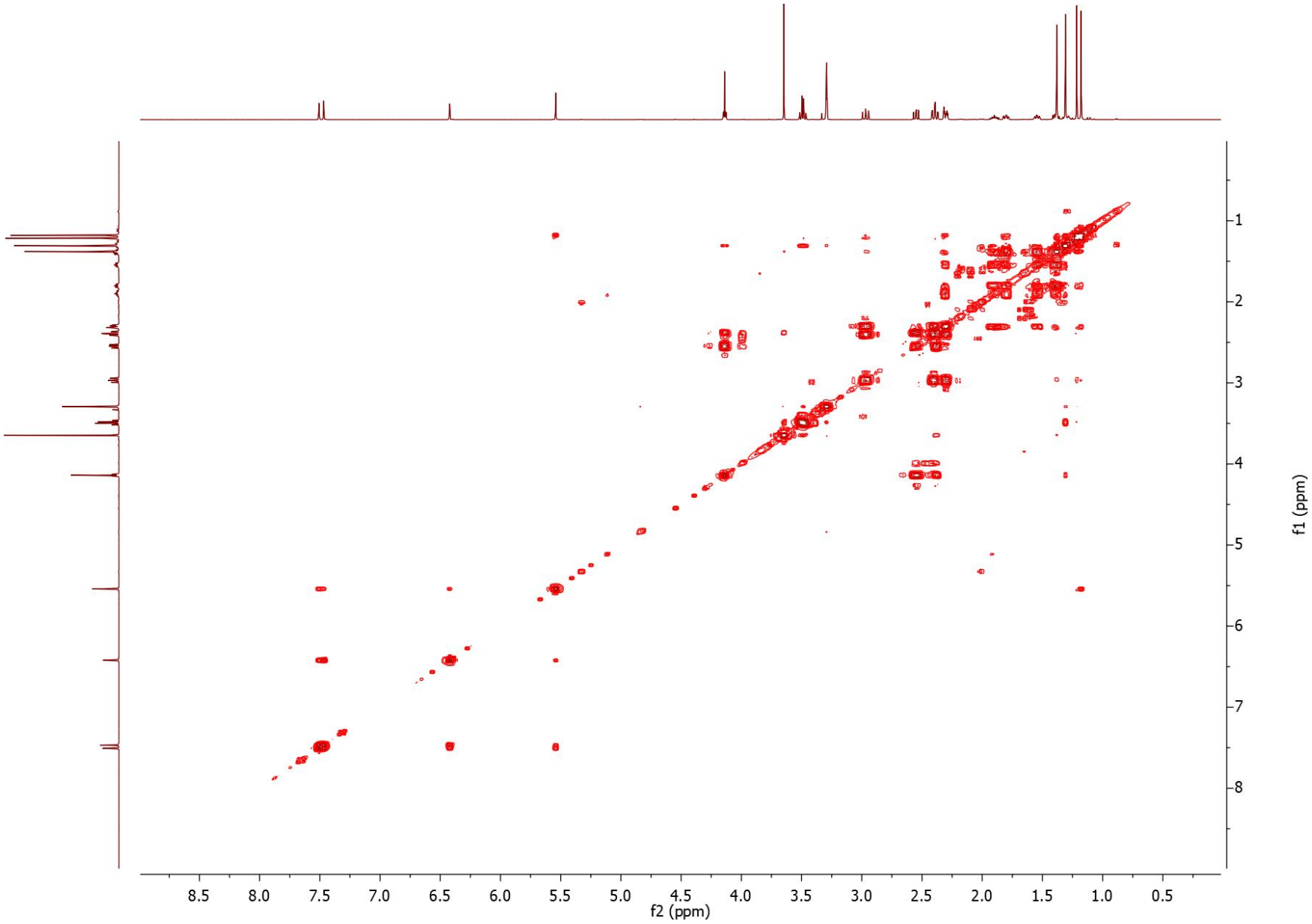


Figure S 26. ^{1}H-^{1}H-COSY spectrum of compound **4** in CD_3OD

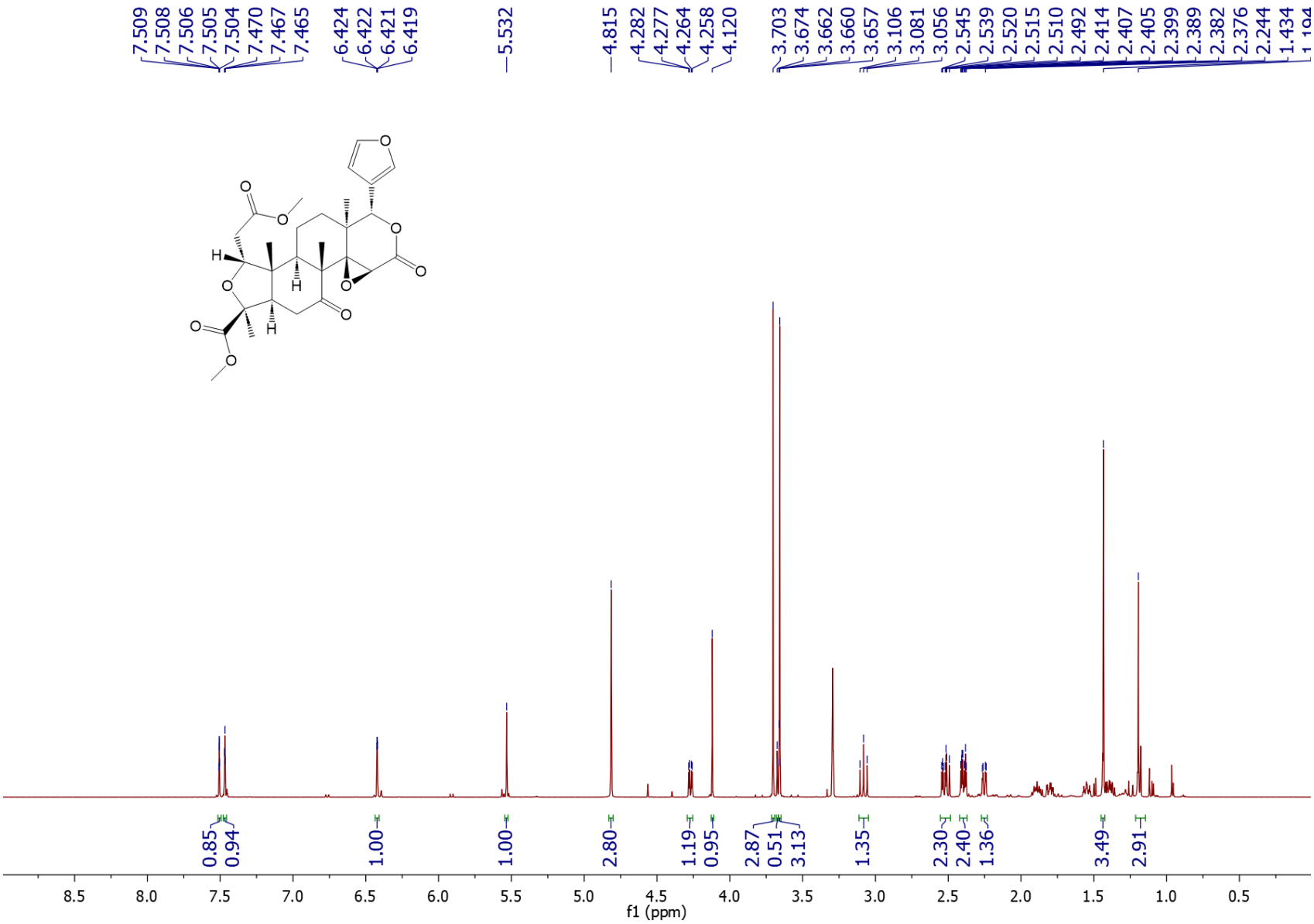


Figure S 27. ^{1}H-NMR (600 MHz) spectrum of compound **2** in CD_3OD

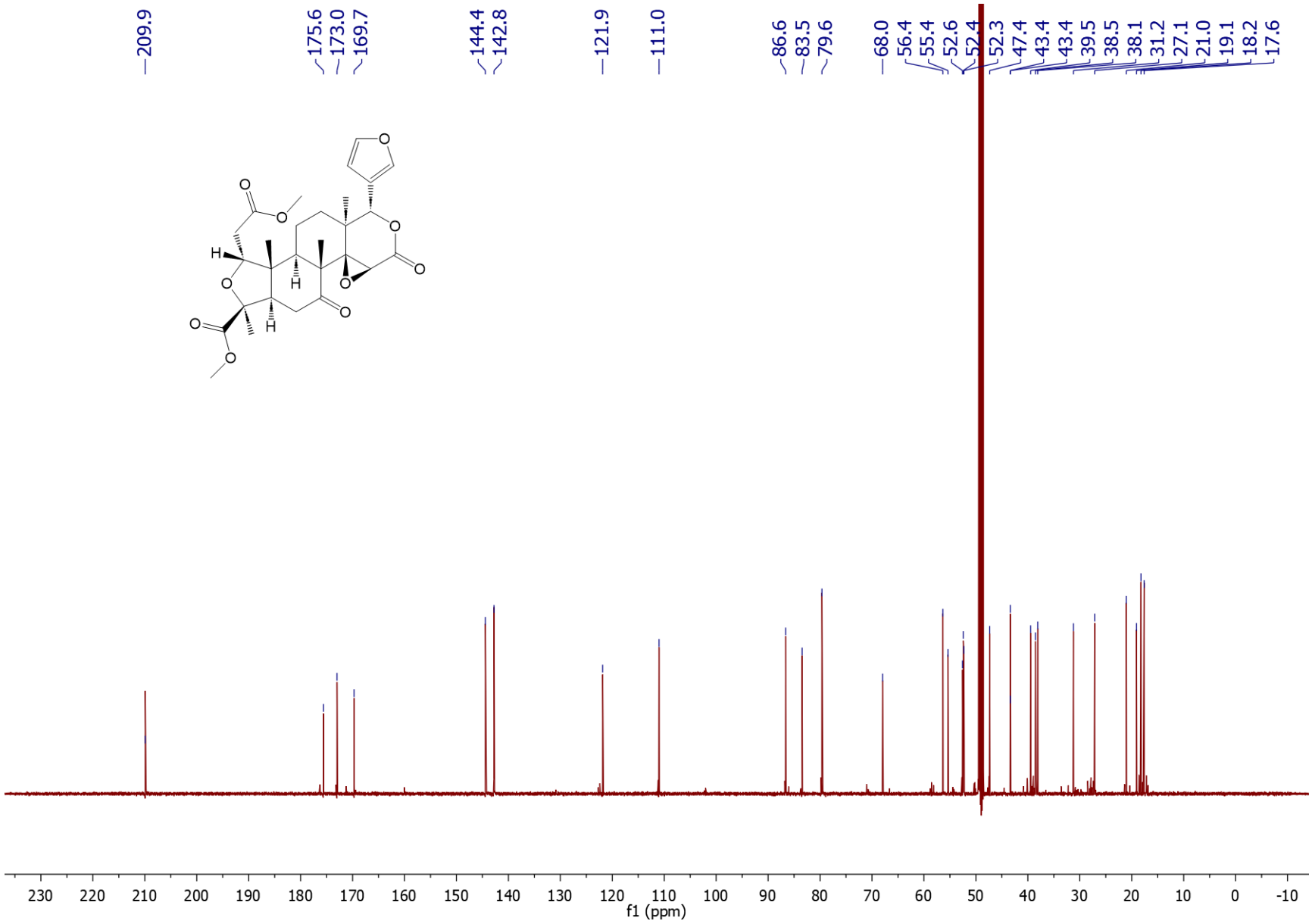


Figure S 28. ^{13}C-NMR (150 MHz) spectrum of compound **2** in CD_3OD

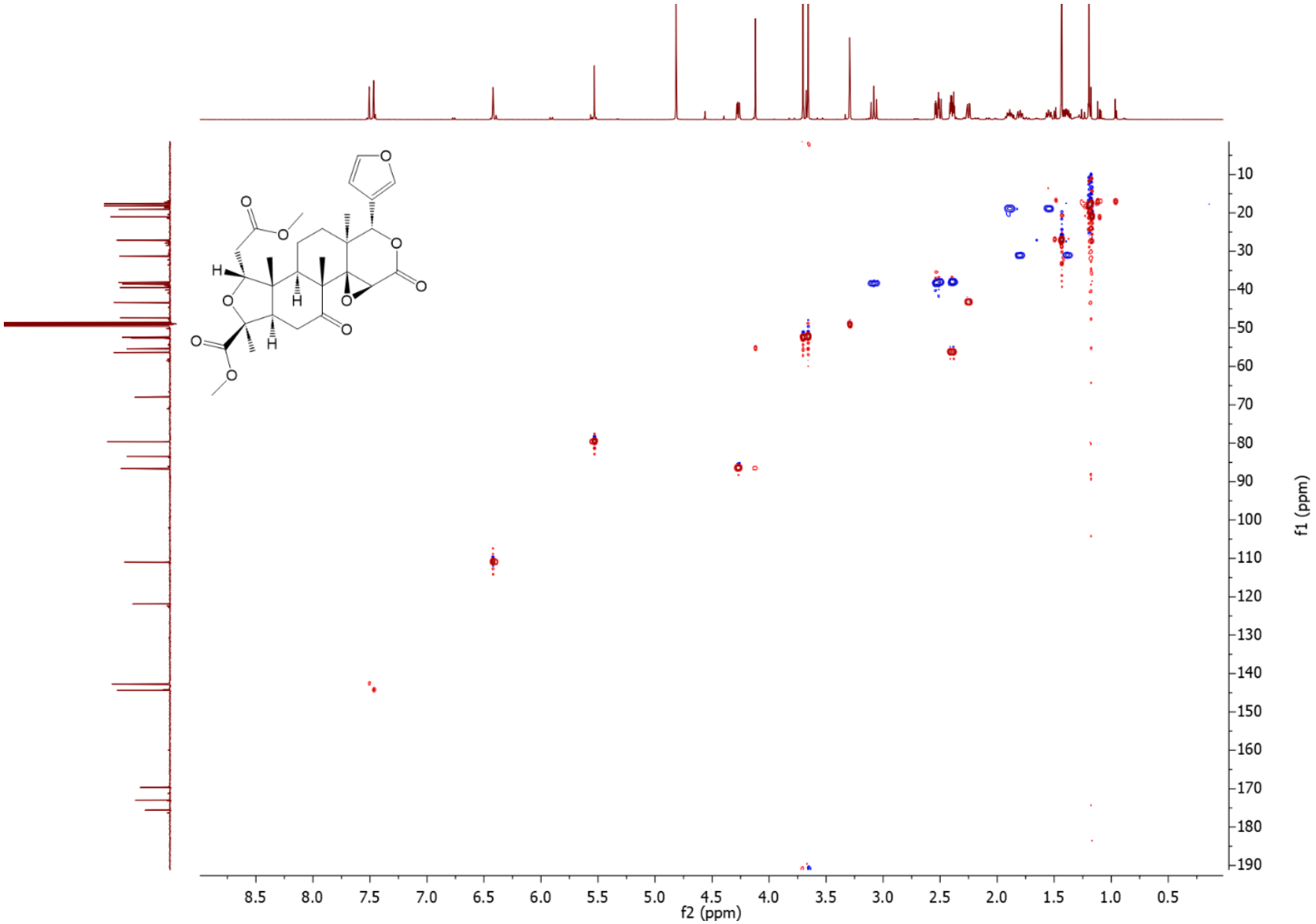


Figure S 29. HSQC spectrum of compound **2** in CD_3OD

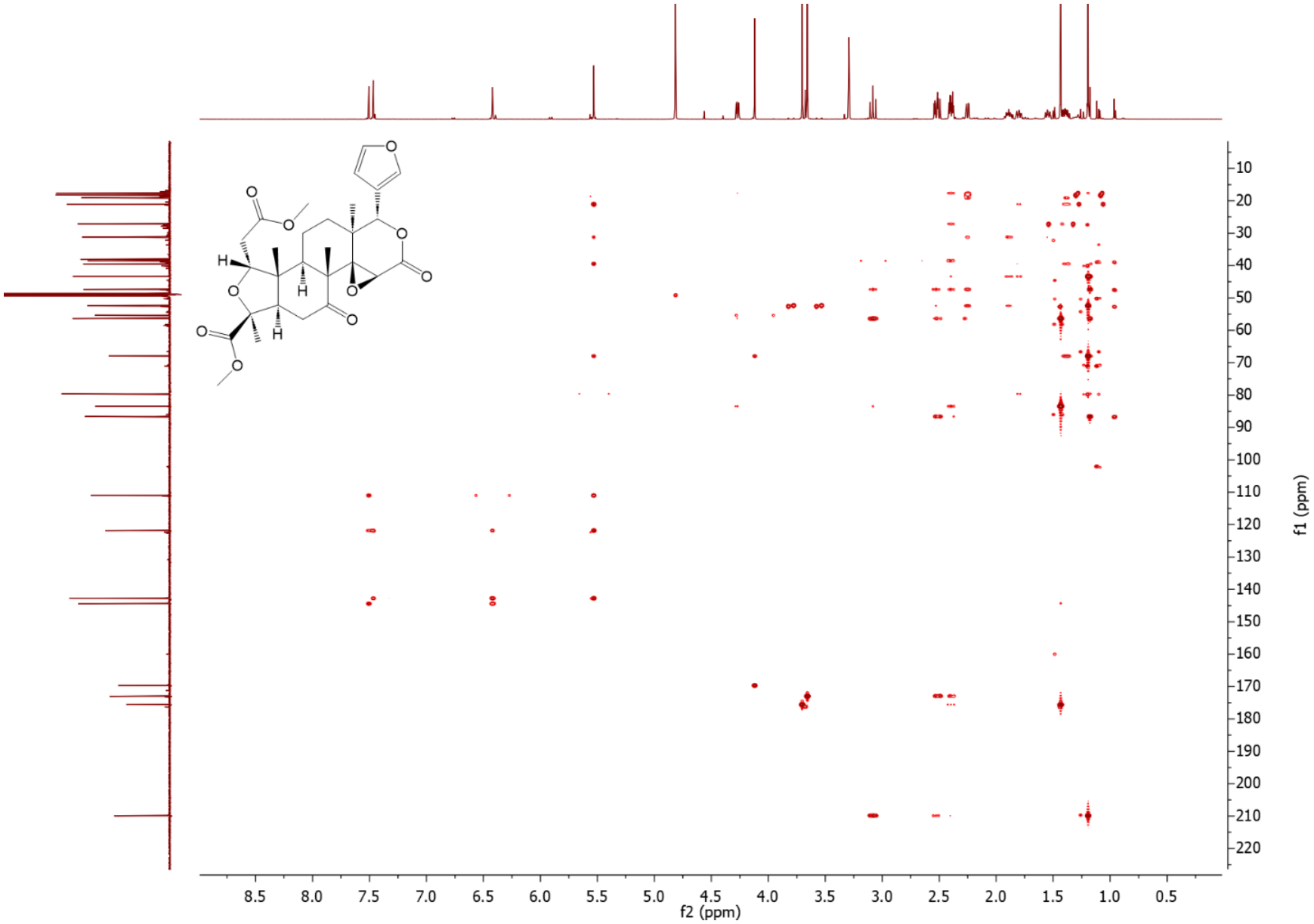


Figure S 30. HMBC spectrum of compound **2** in CD_3OD

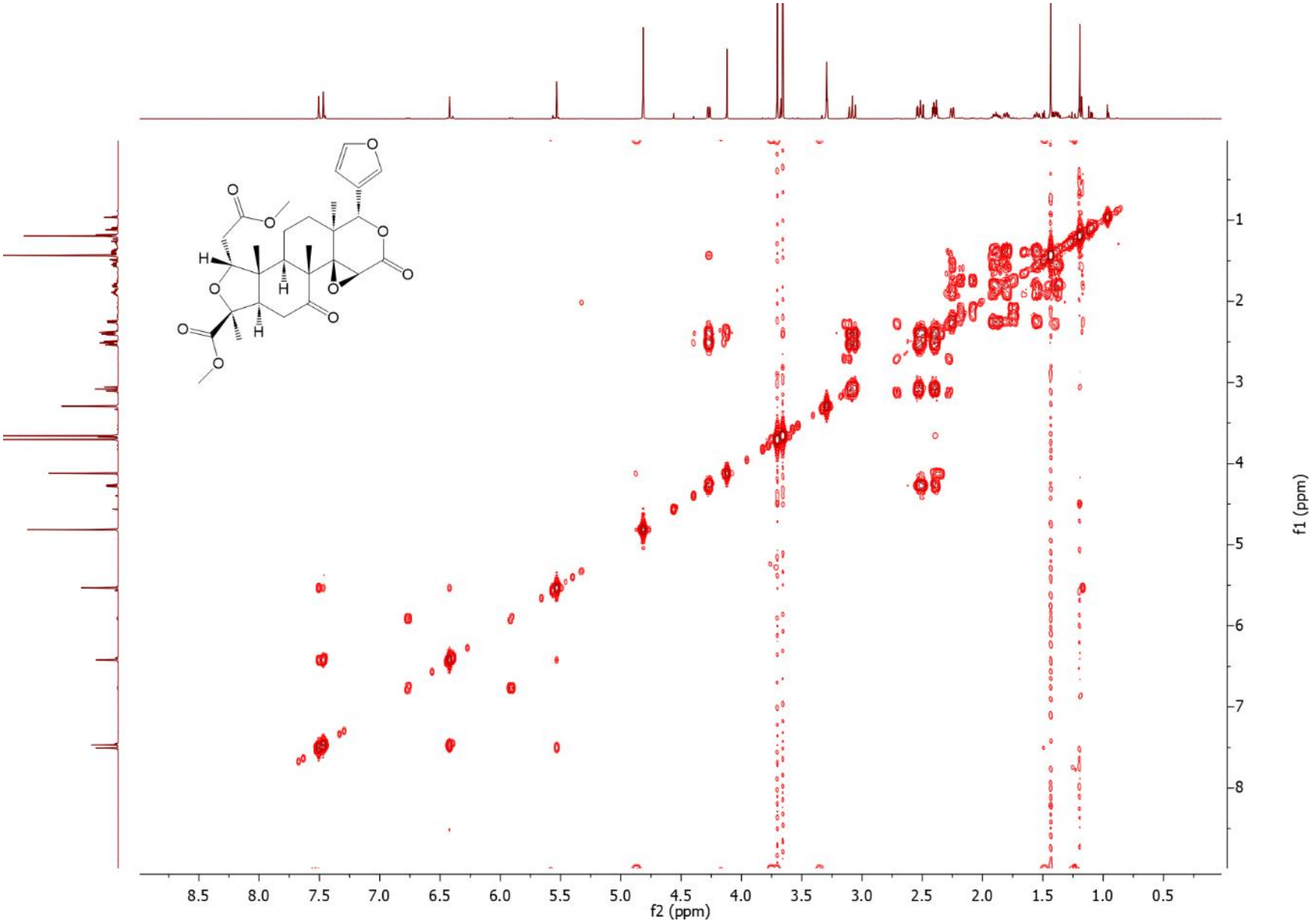


Figure S 31. ^{1}H-^{1}H-COSY spectrum of compound **2** in CD_3OD

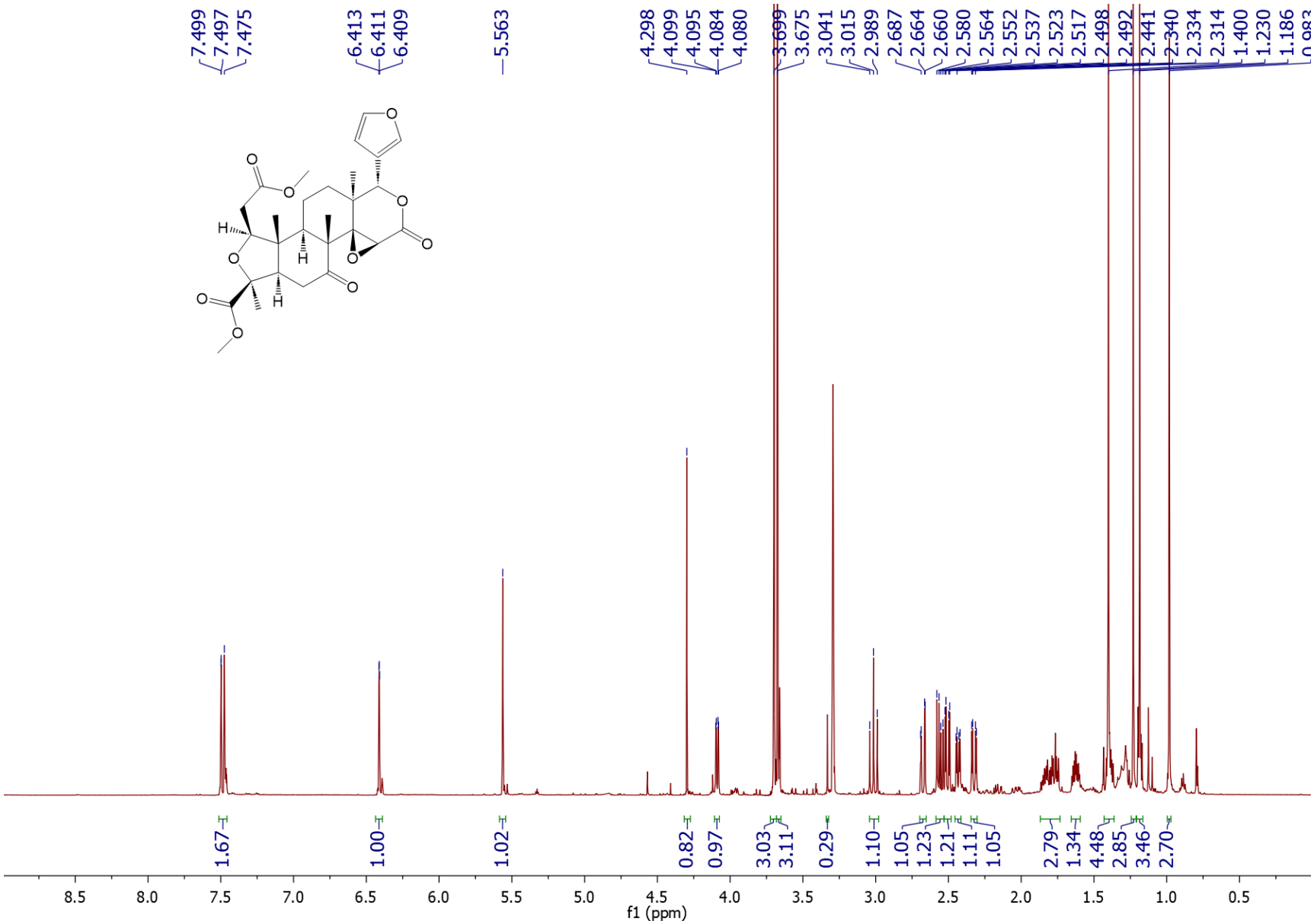


Figure S 32. ^{1}H-NMR (600 MHz) spectrum of compound **3** in CD_3OD

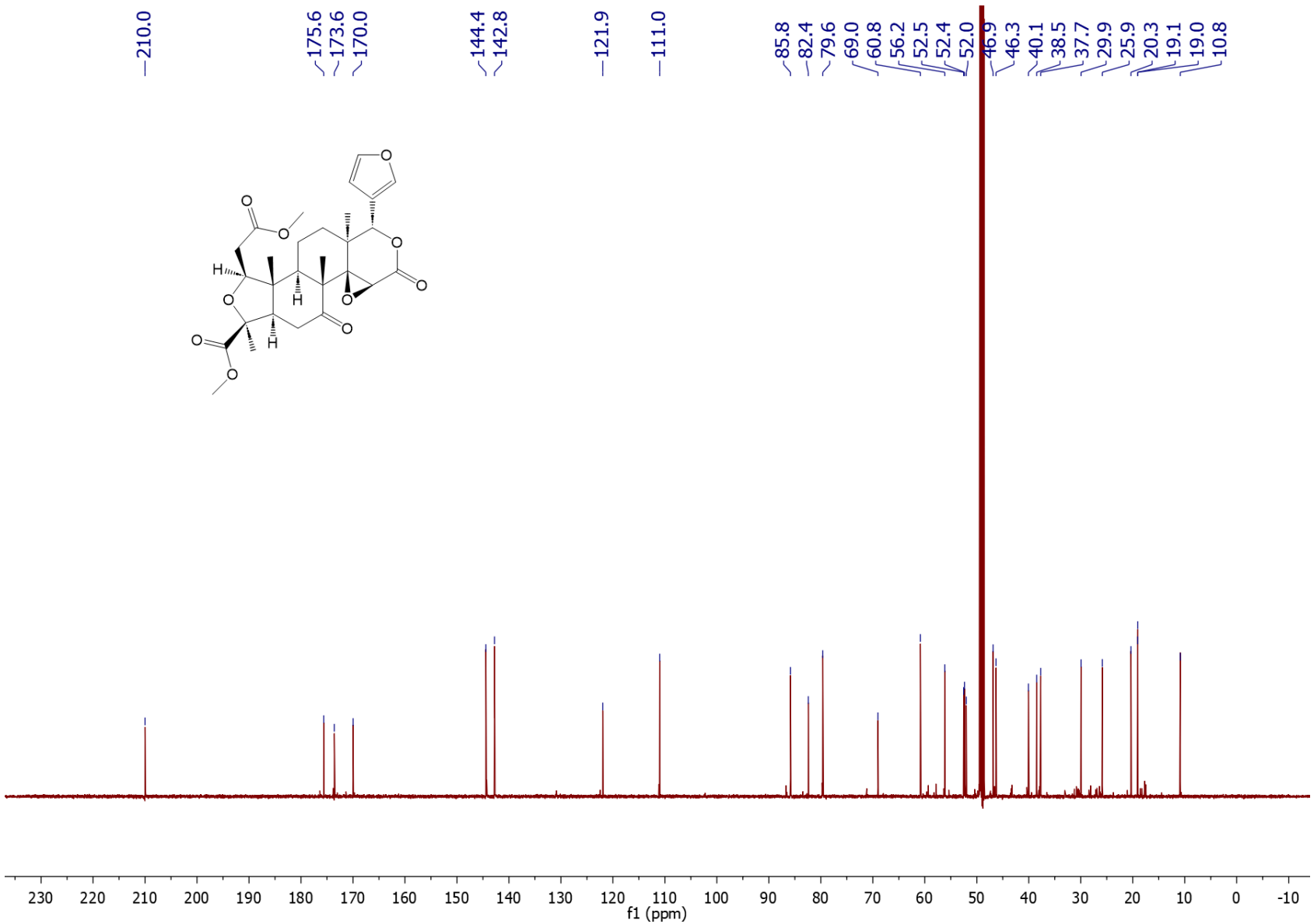


Figure S 33. ^{13}C-NMR (150 MHz) spectrum of compound **3** in CD_3OD

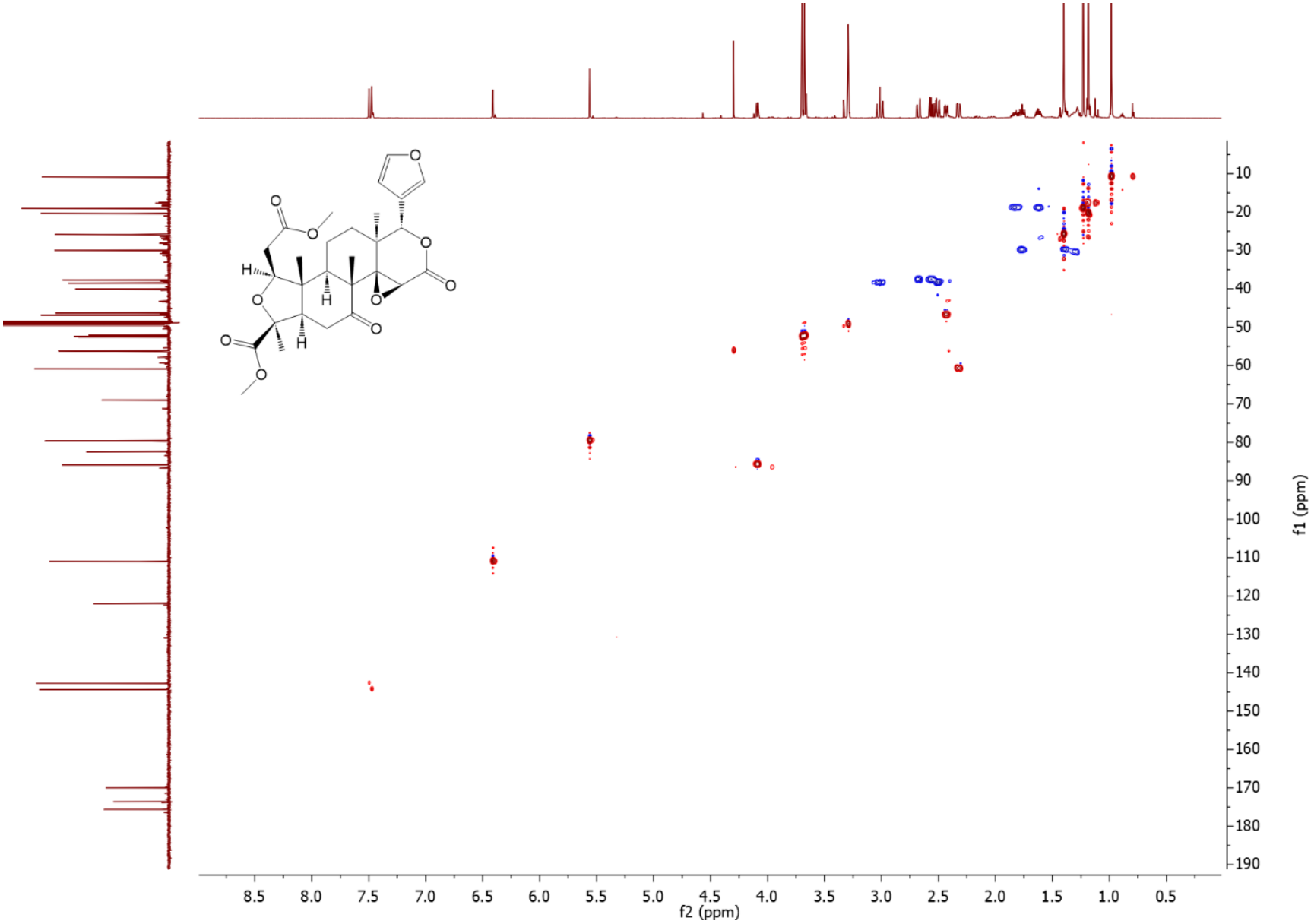


Figure S 34. HSQC spectrum of compound **3** in CD_3OD

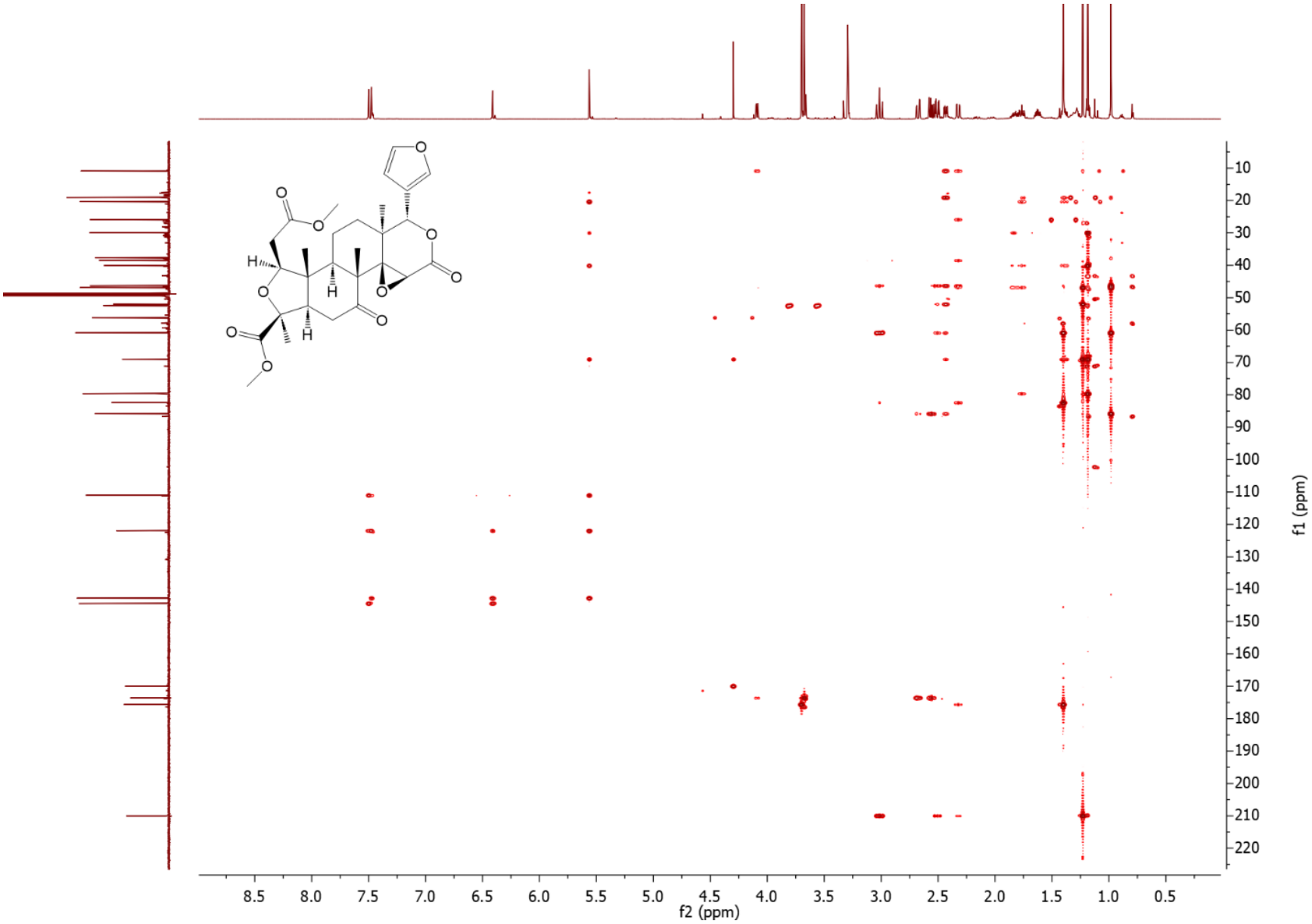


Figure S 35. HMBC spectrum of compound **3** in CD_3OD

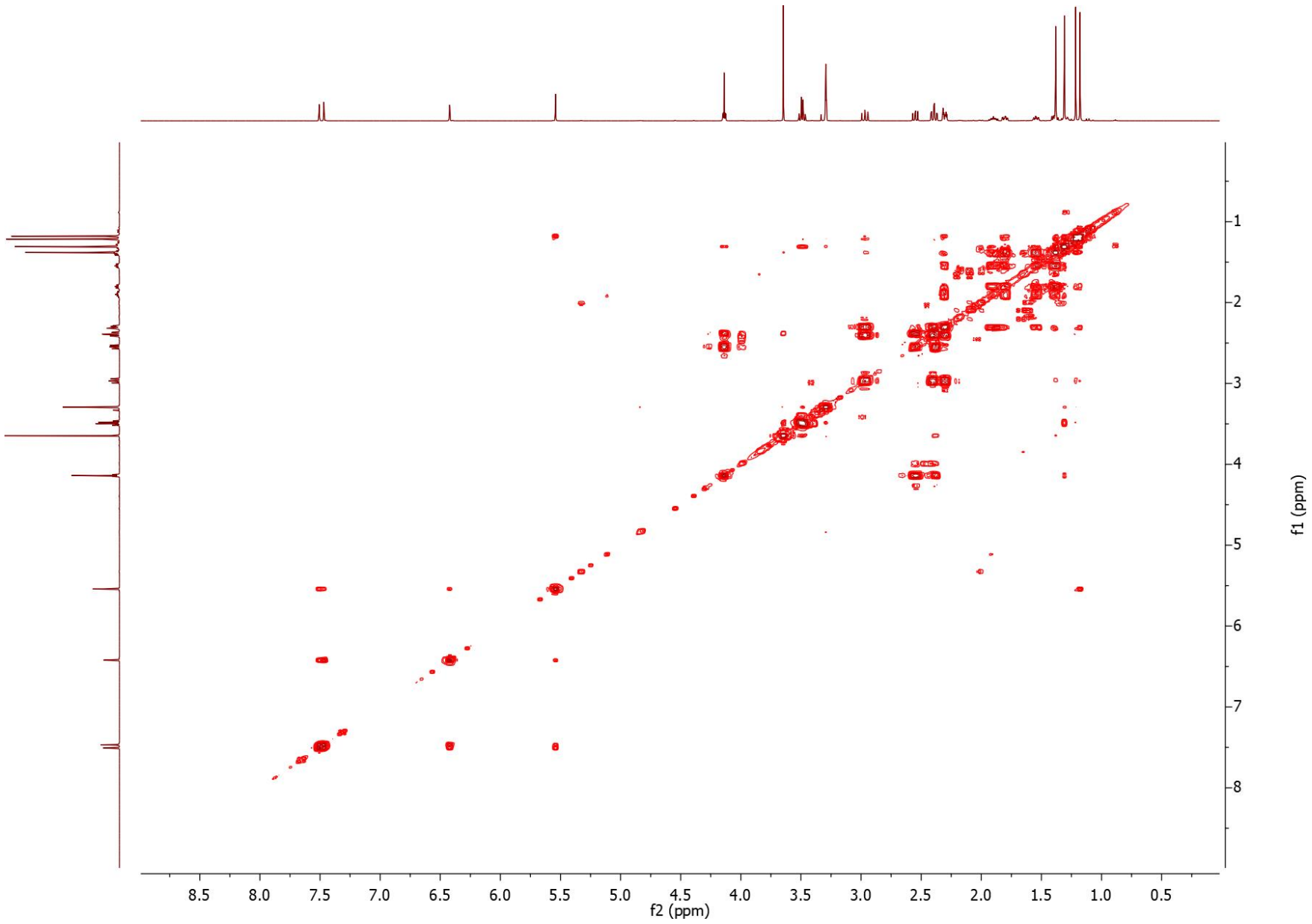


Figure S 36. ^{1}H-^{1}H-COSY spectrum of compound **3** in CD_3OD

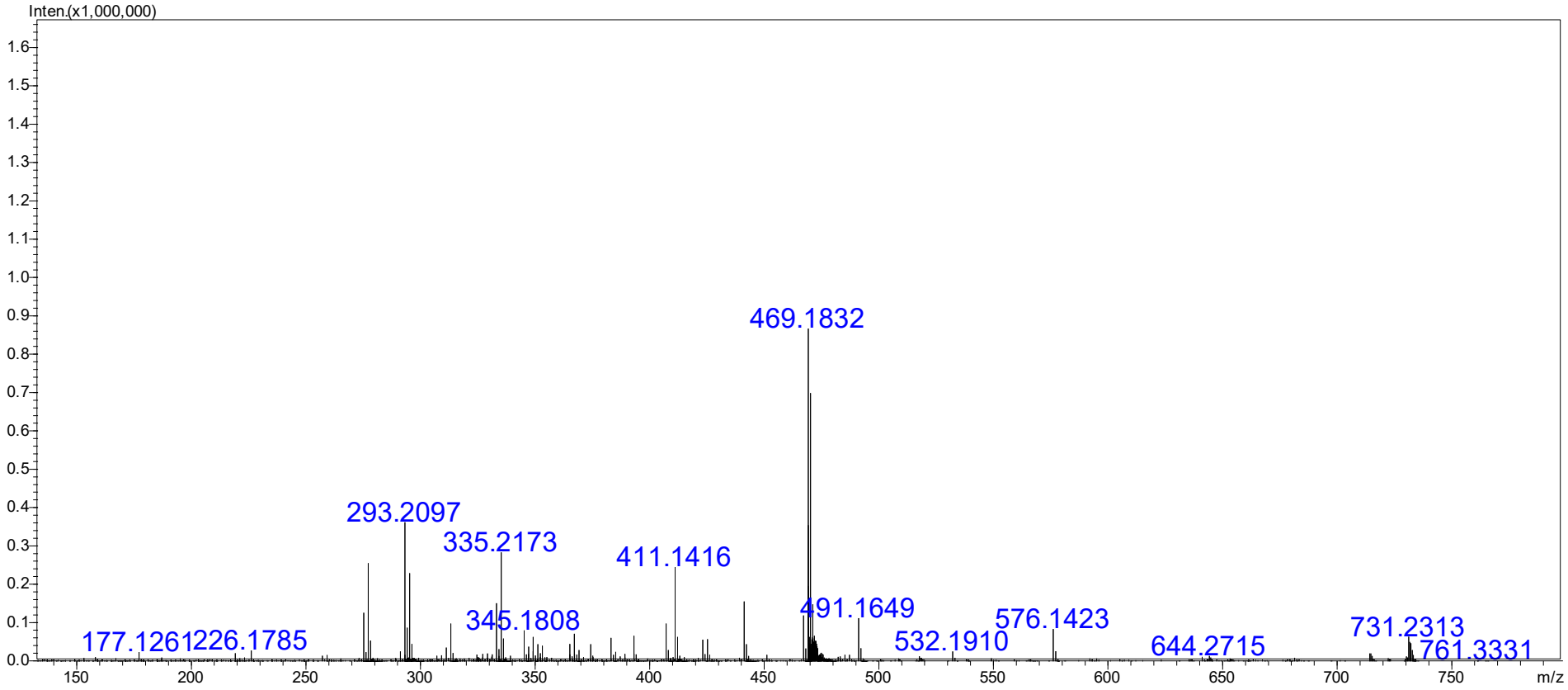


Figure S 37. HR-ESI-MS spectrum of compound **8**

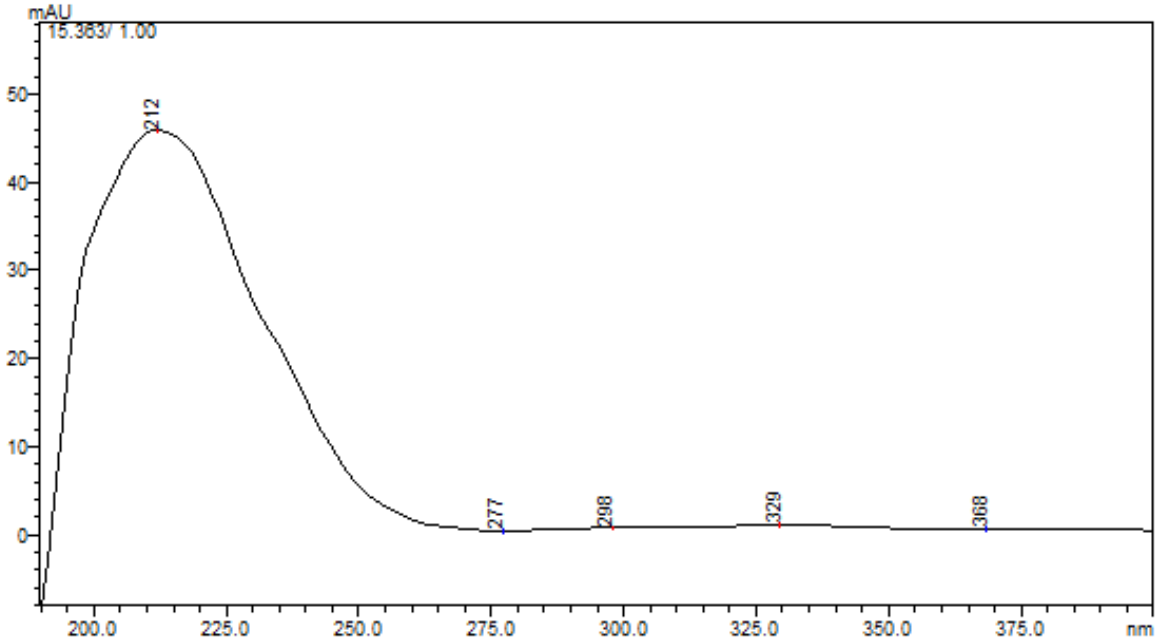


Figure S 38. UV spectrum of compound **8** in methanol

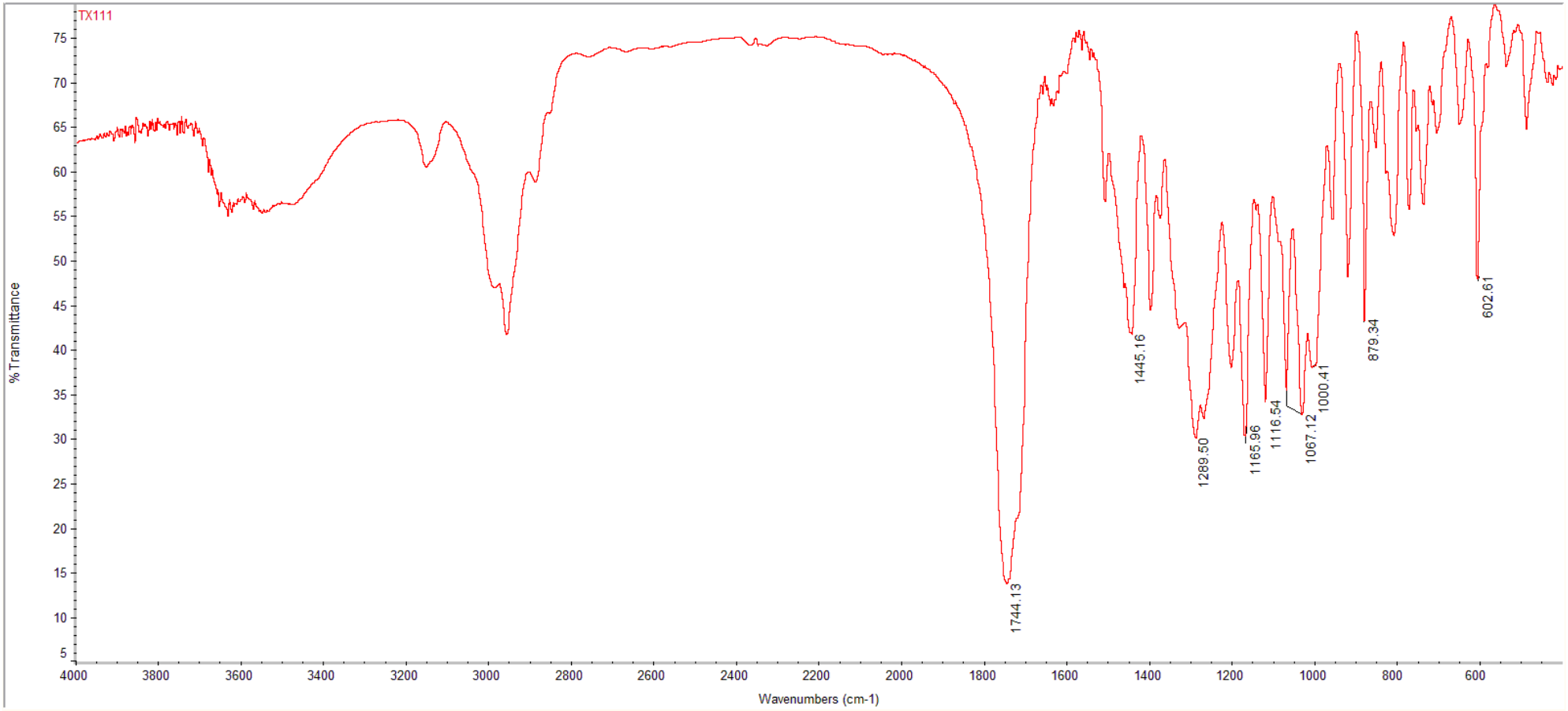


Figure S 39. IR spectrum (film on KBr plates) of compound **8**

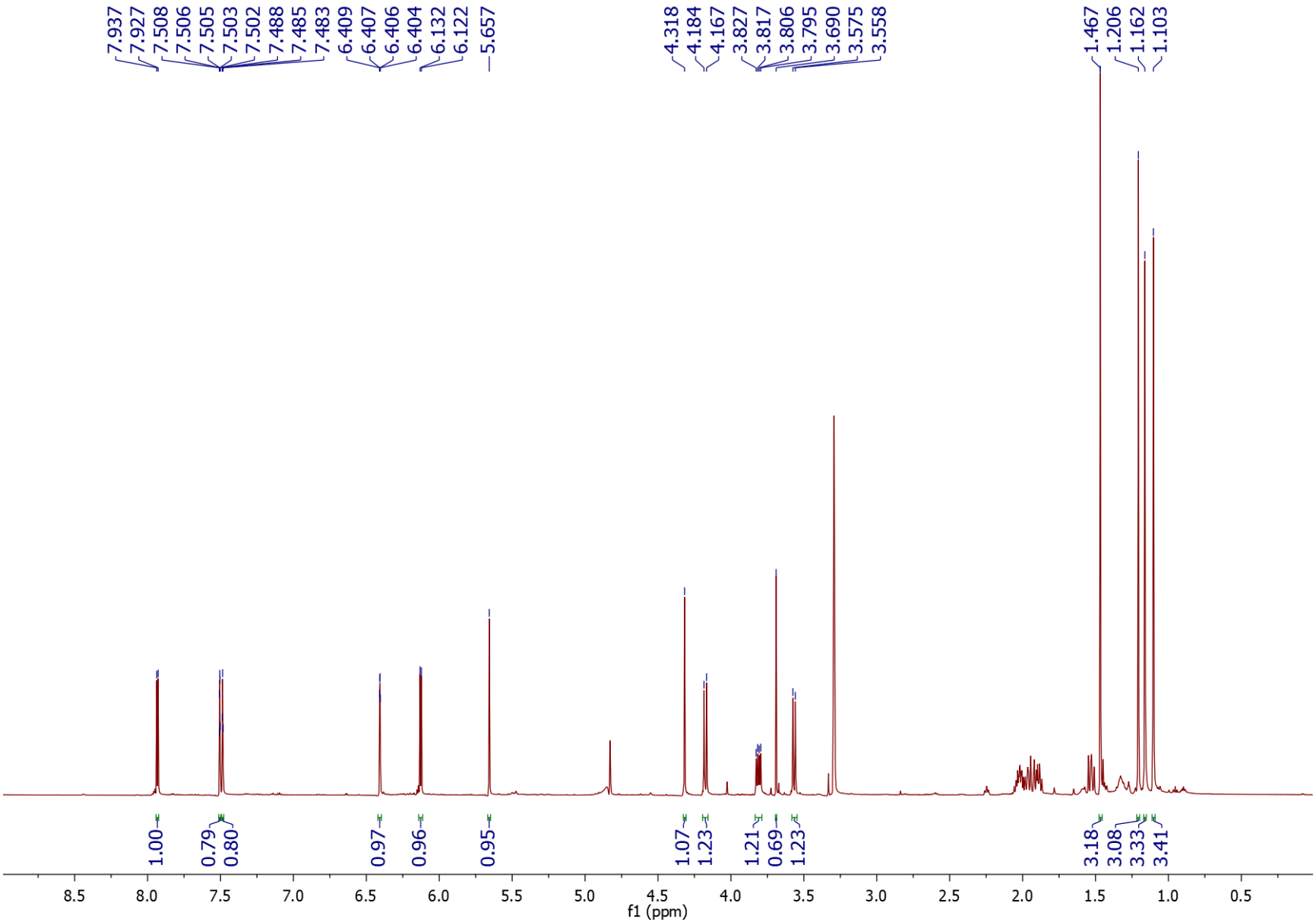


Figure S 40. ^{1}H-NMR (600 MHz) spectrum of compound **8** in CD_3OD

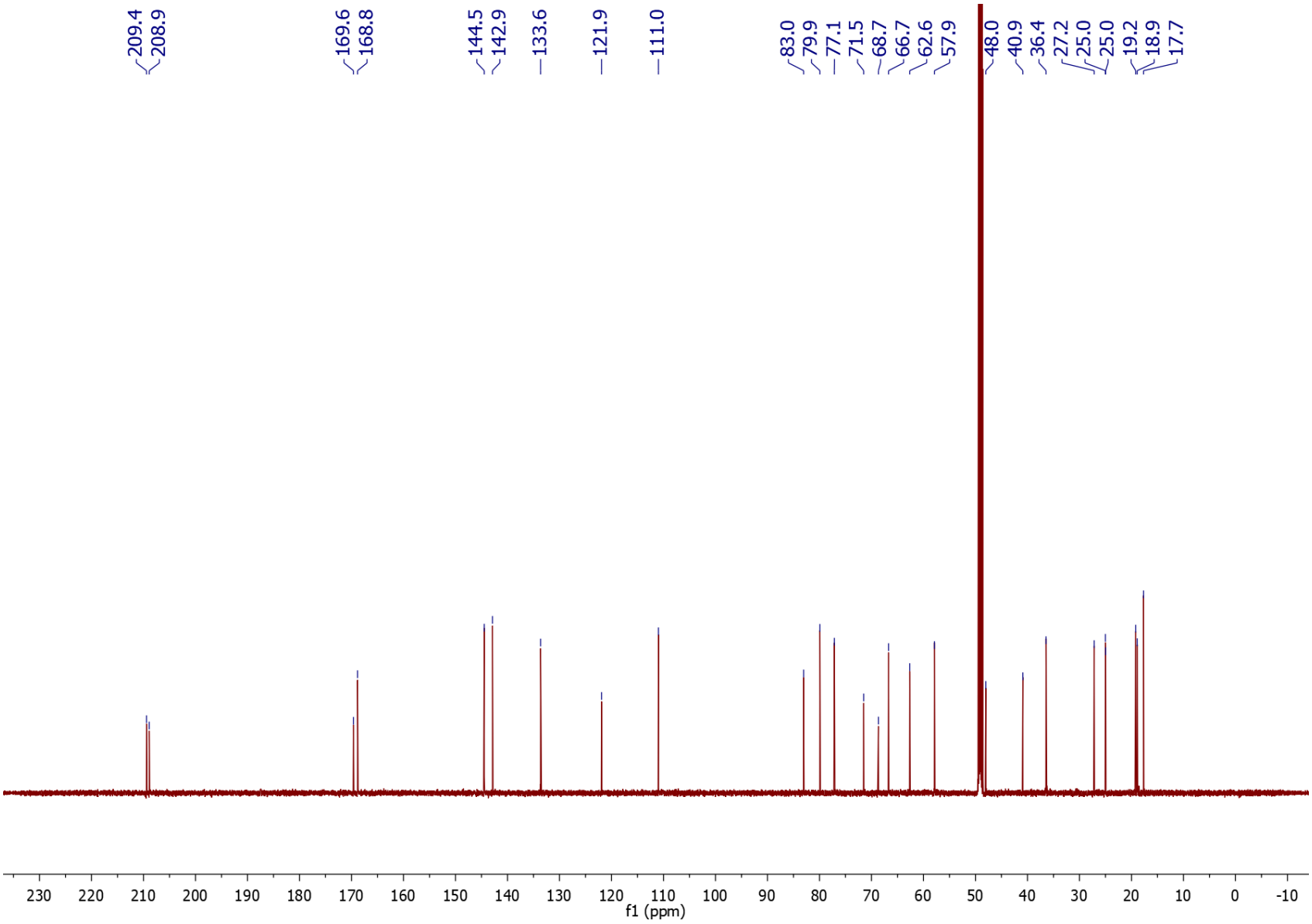


Figure S 41. ^{13}C-NMR (150 MHz) spectrum of compound **8** in CD_3OD

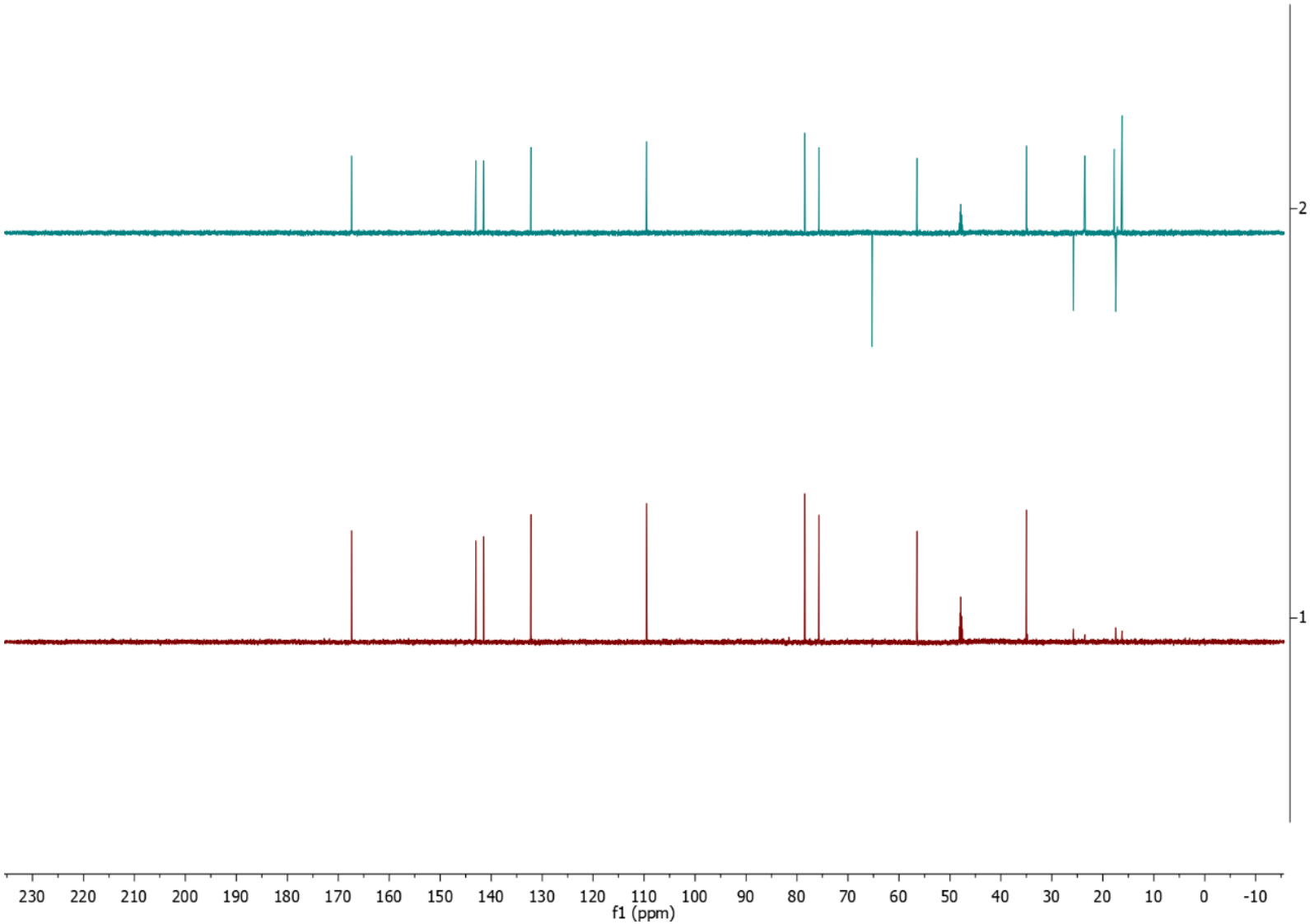


Figure S 42. DEPT-NMR (150 MHz) spectrum of compound **8** in CD_3OD

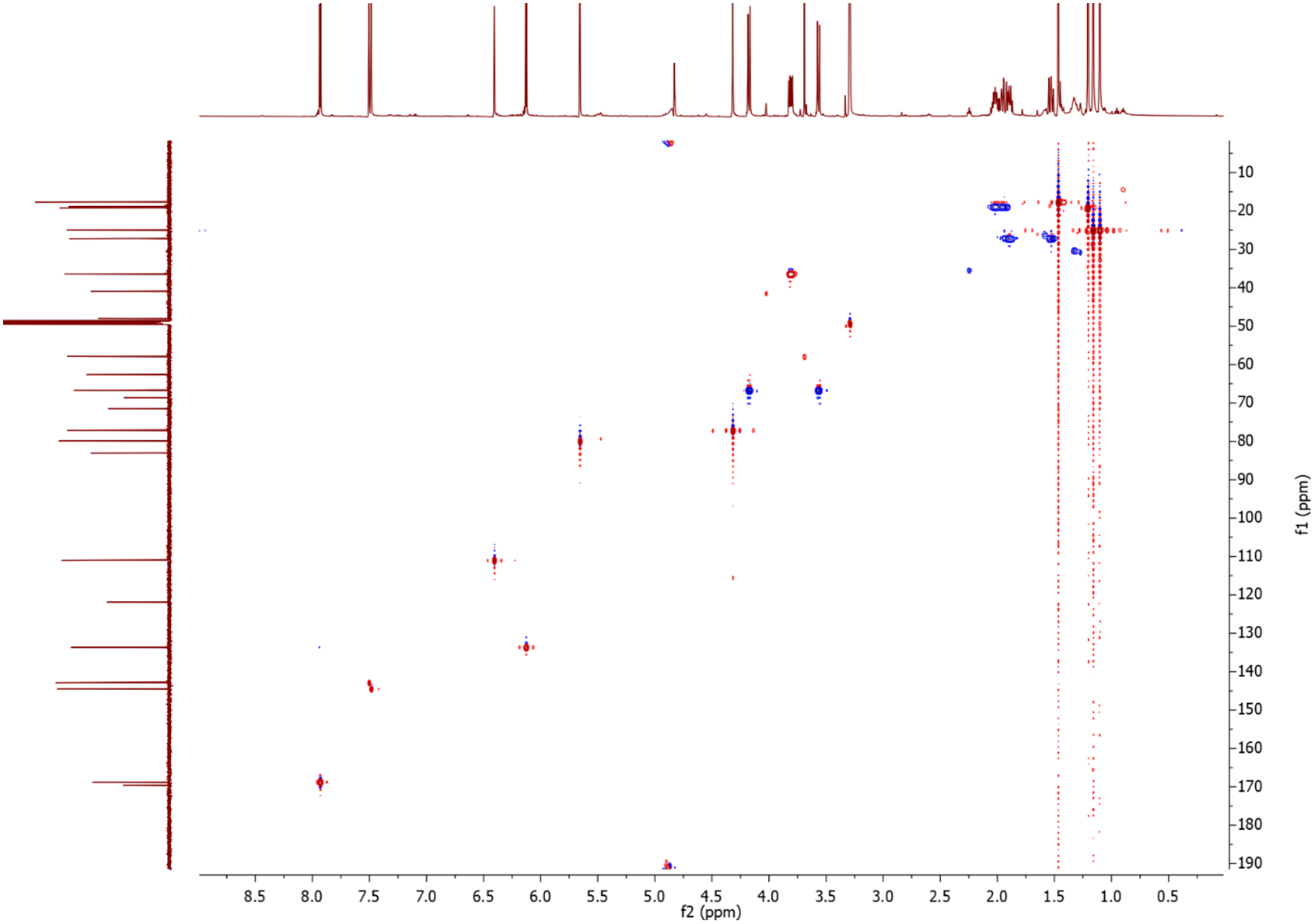


Figure S 43. HSQC spectrum of compound **8** in CD_3OD

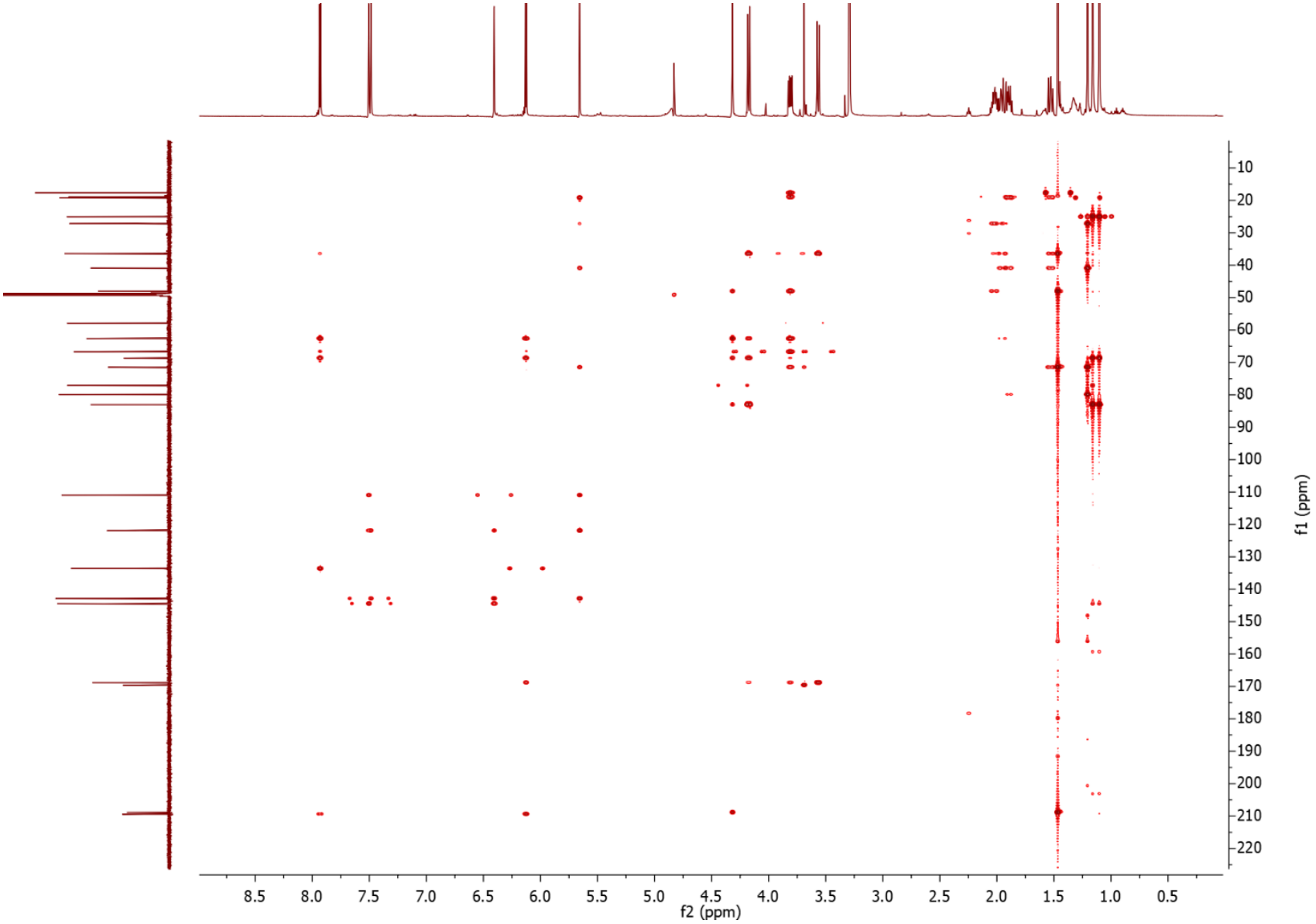


Figure S 44. HMBC spectrum of compound **8** in CD_3OD

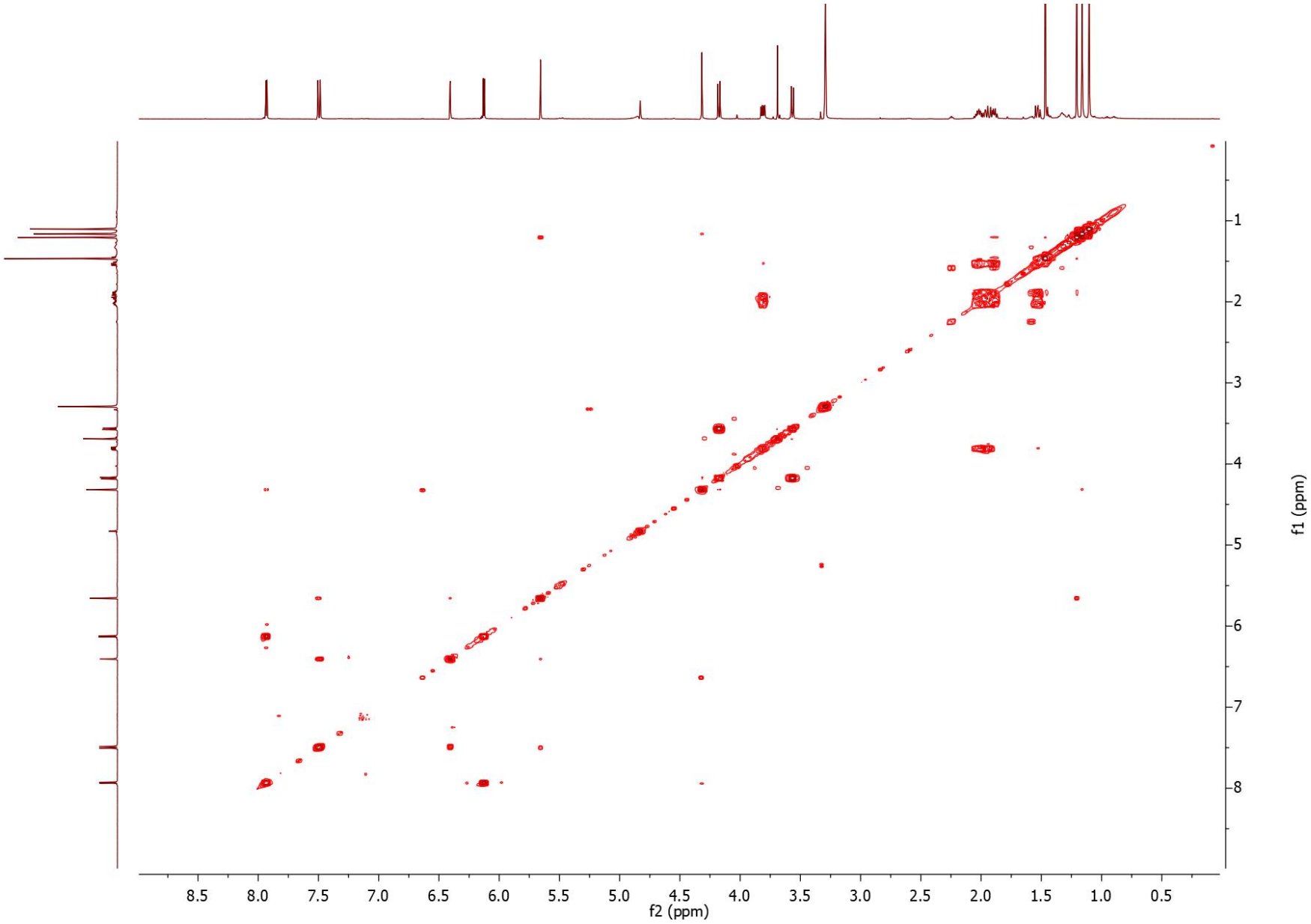


Figure S 45. ^{1}H-^{1}H-COSY spectrum of compound **8** in CD_3OD

Table S 1. Crystal data and experimental details for compound **4**

Crystal data		
Empirical formula	C27 H34 O9	
Formula weight	502.54	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 7.8196(2) Å	α= 90°.
	b = 10.6277(3) Å	β= 90°.
	c = 28.4548(8) Å	γ = 90°.
Volume	2364.72(11) $Å^3$	
Z	4	
F(000)	1072	
Density (calculated)	1.412 Mg/m^3	
Wavelength	1.54178 Å	
Cell parameters reflections used	9189	
Theta range for Cell parameters	3.11 to 72.11°.	
Absorption coefficient	0.877 mm^{-1}	
Temperature	100(2) K	
Crystal size	0.150 x 0.150 x 0.100 mm^3	
Data collection		
Diffractometer	Bruker AXS D8 VENTURE, PhotonIII_C28	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.0000 and 0.579373	
No. of measured reflections	24152	
No. of independent reflections	4641 [R(int) = 0.0448]	
No. of observed [I>2_igma(I)]	4610	

Completeness to theta = 67.679°	100.0 %
Theta range for data collection	3.106 to 72.100°.
Refinement	
Final R indices [I>2sigma(I)]	R1 = 0.0310, wR2 = 0.0816
R indices (all data)	R1 = 0.0311, wR2 = 0.0818
Goodness-of-fit on F^2	1.049
No. of reflections	4641
No. of parameters	349
No. of restraints	0
Absolute structure parameter	0.00(5)
Largest diff. peak and hole	0.203 and -0.276 e.$Å^{-3}$

Table S 2. Optical Rotation of compound **3**

3

[Data Information]
Creation Date 2025/4/26 02.35 p.m

[Measurement Information]
Instrument Name P-2000
Model Name P-2000
Serial No. A062461232
Polarizer Dichrom
Faraday Cell Flint Glass

Accessory RSC-200
Accessory S/N B045761260

Light Source Na
Monitor wavelength 589 nm
D.I.T. 5 sec
No. of cycle 5
Cycle interval 2 sec
Temp. Monitor Cell
Temp. Corr. Factor None
Aperture (S) 3.0 nm
Aperture (L) Auto
Mode Specific O.R.
Path Length 50 nm
Cencentration 1.83 w/v%
Water content of sample 0%
Factor 1

No.	Sample Name	Measurement Date	PMT Voltage[V]	Temperature[C]	Optical Rotation Monitor	Specific O.R.
1	3			24.00	0.0101	-49.5848
2	3	2025/4/26 02.35 p.m	312	24.00	0.0140	-49.8785
3	3	2025/4/26 02.35 p.m	399	24.00	0.0071	-49.8245
4	3	2025/4/26 02.35 p.m	389	24.00	0.0137	-49.8970
5	3	2025/4/26 02.35 p.m	356	24.00	0.0138	-49.7787
6	3	2025/4/26 02.35 p.m	382	24.00	0.0116	-49.6752

Table S 3. Optical Rotation of compound **4**

4

[Data Information]
Creation Date 2025/4/26 02.50 p.m

[Measurement Information]
Instrument Name P-2000
Model Name P-2000
Serial No. A062461232
Polarizer Dichrom
Faraday Cell Flint Glass

Accessory RSC-200
Accessory S/N B045761260

Light Source Na
Monitor wavelength 589 nm
D.I.T. 5 sec
No. of cycle 5
Cycle interval 2 sec
Temp. Monitor Cell
Temp. Corr. Factor None
Aperture (S) 3.0 nm
Aperture (L) Auto
Mode Specific O.R.
Path Length 50 nm
Cencentration 1.83 w/v%
Water content of sample 0%
Factor 1

No.	Sample Name	Measurement Date	PMT Voltage[V]	Temperature[C]	Optical Rotation Monitor	Specific O.R.
1	4			24.00	0.0124	-31.4691
2	4	2025/4/26 02.50 p.m	328	24.00	0.0091	-31.1887
3	4	2025/4/26 02.50 p.m	344	24.00	0.0077	-31.6874
4	4	2025/4/26 02.50 p.m	293	24.00	0.0074	-31.5258
5	4	2025/4/26 02.50 p.m	393	24.00	0.0028	-31.1547
6	4	2025/4/26 02.50 p.m	374	24.00	0.0088	-31.6896

Table S 4. Optical Rotation of compound **8**

8

[Data Information]
Creation Date 2025/4/26 03.24 p.m

[Measurement Information]
Instrument Name P-2000
Model Name P-2000
Serial No. A062461232
Polarizer Dichrom
Faraday Cell Flint Glass

Accessory RSC-200
Accessory S/N B045761260

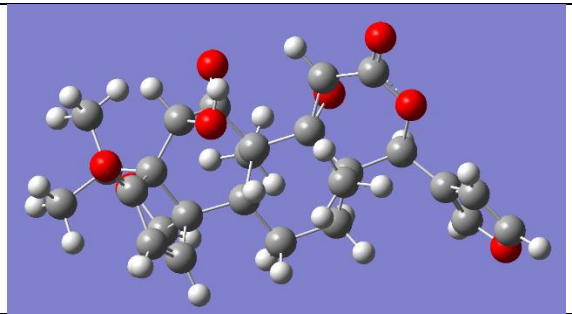
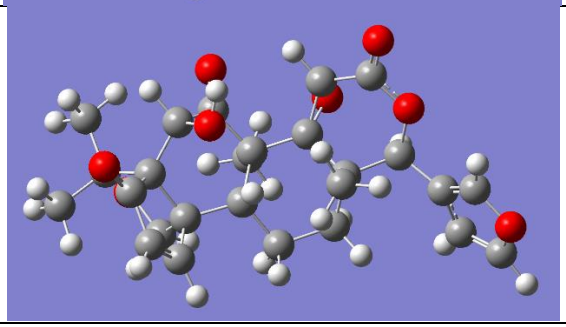
Light Source Na
Monitor wavelength 589 nm
D.I.T. 5 sec
No. of cycle 5
Cycle interval 2 sec
Temp. Monitor Cell
Temp. Corr. Factor None
Aperture (S) 3.0 nm
Aperture (L) Auto
Mode Specific O.R.
Path Length 50 nm
Cencentration 1.83 w/v%
Water content of sample 0%
Factor 1

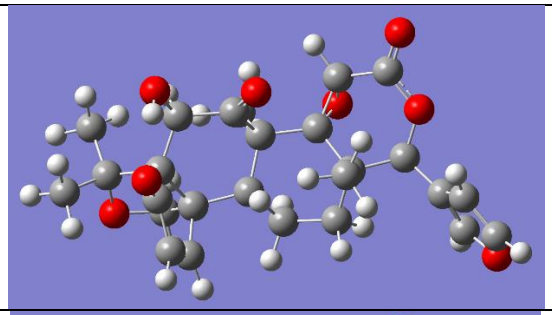
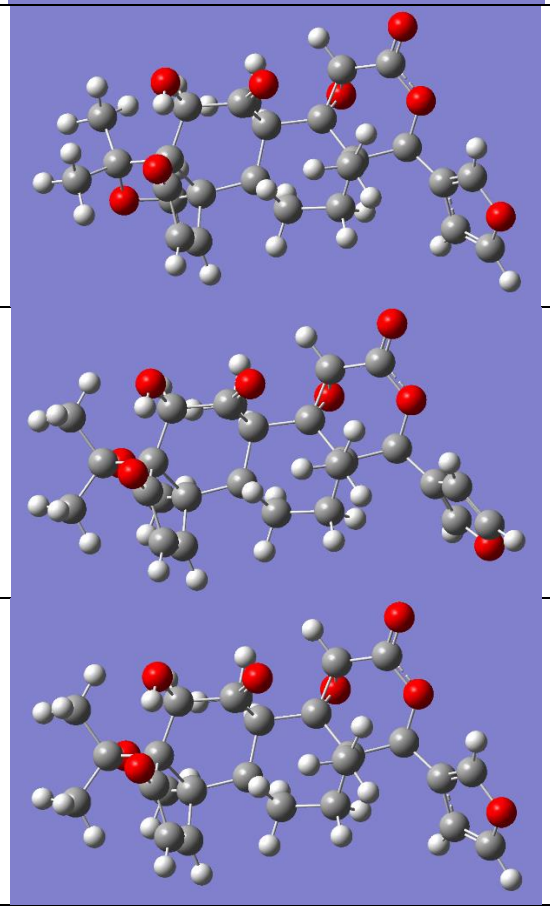
No.	Sample Name	Measurement Date	PMT Voltage[V]	Temperature[C]	Optical Rotation Monitor	Specific O.R.
1	8			24.00	0.0124	34.9097
2	8	2025/4/26 03.24 p.m	328	24.00	0.0091	34.2643
3	8	2025/4/26 03.24 p.m	344	24.00	0.0077	34.5217
4	8	2025/4/26 03.24 p.m	293	24.00	0.0074	34.6570
5	8	2025/4/26 03.24 p.m	393	24.00	0.0028	34.2718
6	8	2025/4/26 03.24 p.m	374	24.00	0.0088	34.4913

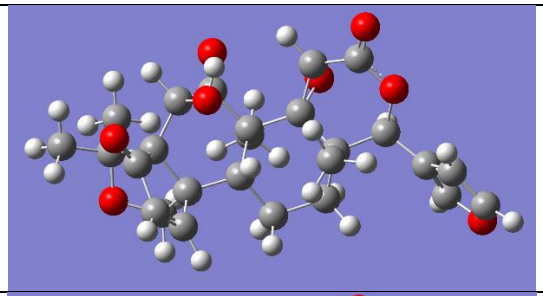
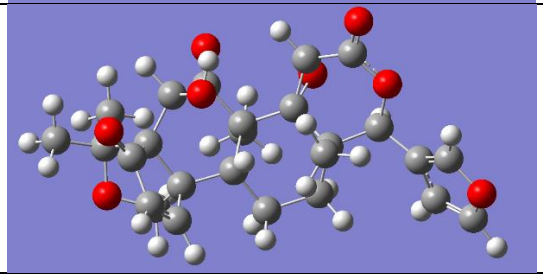
Table S 5. ECD calculation of compound **8**

A panel of relatively favored conformations in an energy range of 3 kcal/mol above the global minimum was obtained by performing the first conformational analysis of compound 8 using the GMMX fucntion searching algorithm via the MMFF94 molecular mechanics force field, obtained conformers were optimized using the Gaussian 16 software package's density functional theory (DFT) using the B3LYP/6-31G(d) level in gas phase. Time-dependent density functional theory (TDDFT) calculations at the M062X/def2TZVP//M062X/def2tzvp level in MeOH using the Polarizable Continuum Model (PCM) solvent model were used to theoretically calculate ECD for these dominating conformers. The Gaussian 16 software program was used to measure each conformer's energies, oscillator strengths, and rotational strengths. The oretical calculations of ECD spectra for each conformer were then approximated by the Gaussian distribution. The final ECD spectrum of the individual conformers was summed up because of Boltzmann-weighed population contribution by the Specdisc software.

Energy analyses of conformers

No.	3D conformers	Free energy			
		Energy (KCal/Mol)	ΔE	Bolt. Factor	Bolt. Distr. (%)
1		111.818	0.000	1	36.77
2		112.149	0.331	0.571779046	21.03

3		112.328	0.510	0.42261099	15.54
4		112.451	0.633	0.343341663	12.63
5		113.168	1.350	0.102292374	3.76
6		113.273	1.455	0.085670454	3.15

7		113.558	1.740	0.052941712	1.95
8		113.695	1.877	0.042006394	1.54

ECD Spectrum

X-Axis: Wavelength (nm)

Y-Axis: Δε (L mol-1 cm-1)

Y-Axis2: Rvel (10-40 esu2 cm2)

Peak information

#	X	Y	Y2
#	320.8000000000	4.4485957400	34.6873391359
#	311.5900000000	4.3189683400	34.6720015718
#	226.5800000000	-7.1585421400	-79.0288055085
#	219.5400000000	9.8911296600	112.6975927409
#	211.9700000000	-8.3565648600	-98.6133682599

```
#    202.3900000000      -0.6035186200      -7.4590587474
#    199.3300000000      32.9488742200      413.4760112812
#    198.2000000000      -4.6591791200      -58.8014670164
#    192.6600000000      -3.2930251200      -42.7548997124
#    190.5100000000      -6.5689296400      -86.2500265678
#    190.1000000000       5.7645409600       75.8516472955
#    188.0600000000      -5.3366657200      -70.9832651918
#    186.6600000000       2.5821009400       34.6022515236
#    185.0700000000       4.7877932600       64.7115449475
#    182.6200000000       5.3197897000       72.8666041374
#    181.2100000000      -6.8989030000      -95.2314249523
#    177.5600000000      14.5785403000      205.3767654686
#    176.0700000000      -0.5978234000       -8.4931726069
#    175.4700000000      12.6032772800      179.6648087421
#    172.9100000000      -4.6398922400      -67.1228190581
#    171.6000000000     -10.0771502200     -146.8935929201
#    169.6700000000       8.1779865200      120.5656897074
#    167.5300000000       1.0201082400       15.2312684123
#    167.1400000000       2.5252885000       37.7931427215
#    165.9100000000      11.3890424000      171.7105782907
#    165.2800000000      -3.6442769400      -55.1535502287
#    164.6600000000     -15.2678016800     -231.9374101201
#    164.5000000000     -13.1731486800     -200.3115980388
```

```
#   163.6500000000    0.1601649600     2.4481267783
#   162.2100000000    6.1456664800    94.7706300459
#   320.8500000000    2.9081802000    22.6726181657
#   311.6200000000    2.6499305600    21.2711796140
#   226.9100000000   -4.5820439600   -50.5112388290
#   219.5500000000    6.0442843600    68.8642546005
#   212.3700000000   -5.6457182800   -66.4979780870
#   201.4400000000    2.0413821200    25.3490097356
#   198.2700000000    6.5930128800    83.1781624813
#   196.4900000000   -4.5374525200   -57.7635725228
#   195.1500000000   -2.6255781200   -33.6541629611
#   190.6000000000   -2.7492657600   -36.0808060681
#   190.1800000000    2.1547642800    28.3411408780
#   187.9400000000   -3.4251389600   -45.5870382783
#   186.4800000000    3.4060377200    45.6877317344
#   184.8300000000    3.5281281200    47.7479014188
#   182.2800000000    1.7873772000    24.5278565860
#   181.1400000000   -3.9471738800   -54.5072534756
#   177.1900000000   12.9336618400   182.5848327675
#   176.0500000000    3.4354444400    48.8123036507
#   175.1100000000    0.6700312400     9.5712025792
#   172.8300000000   -1.7156764400   -24.8312545478
#   171.6000000000   -5.9649912400   -86.9510700795
```

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#   169.3900000000    1.8054282000    26.6609031988
#   168.5100000000    1.2363294000    18.3523178671
#   167.5300000000    5.2974105600    79.0958047055
#   166.4900000000   10.9132188800   163.9634760188
#   165.9200000000   -1.1631845600   -17.5360709572
#   165.4700000000   -6.6772508800  -100.9394261726
#   163.9000000000   -5.5678692400   -84.9752553385
#   163.7500000000   -0.8380040000   -12.8010969680
#   162.0500000000   17.9396964400   276.9162610170
#   306.6000000000   -0.8705190000    -7.1021282150
#   288.9800000000   -1.1734222500   -10.1570814842
#   224.6300000000   -1.6753035000   -18.6555536826
#   217.8500000000    0.4200885000     4.8235372078
#   214.7400000000    8.5240935000    99.2927777547
#   207.9400000000   -1.1522745000   -13.8611835900
#   202.9800000000    0.0918937500     1.1324398167
#   196.1700000000    3.3674842500    42.9393420428
#   193.4800000000   -1.3599105000   -17.5815294594
#   187.9100000000   -1.0621845000   -14.1394485353
#   179.8000000000   -4.5193200000   -62.8732355777
#   178.9800000000   -1.1642182500   -16.2709272599
#   178.4600000000    1.0180852500    14.2700554666
#   178.2100000000    0.3441067500     4.8299599102
```

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#    177.9300000000     1.8784642500     26.4080394344
#    175.3700000000    -0.4381942500     -6.2501980184
#    174.0700000000     1.0783402500     15.4958102968
#    172.1300000000    -0.9568650000    -13.9051764744
#    169.6700000000     0.4415385000      6.5094743865
#    169.3700000000    -0.0605475000     -0.8942153749
#    167.2400000000    -0.6084487500     -9.1005208445
#    166.8600000000    -2.2822020000    -34.2124555976
#    166.5100000000    -0.3573960000     -5.3689798140
#    165.5900000000     3.8543505000     58.2236601731
#    165.0600000000    -4.6185945000    -69.9923213826
#    164.5100000000    -0.5711550000     -8.6844853138
#    164.1000000000     0.7965652500     12.1421384286
#    162.6400000000    -2.2367670000    -34.4013737454
#    158.6700000000    -1.6102807500    -25.3857023661
#    158.4500000000    -2.4230602500    -38.2520199830
#    306.6200000000    -0.4187183000     -3.4158899233
#    289.0300000000    -0.5738982000     -4.9667733721
#    224.6100000000    -0.9242691000    -10.2932317413
#    218.0400000000     0.0591495000      0.6785741461
#    214.7800000000     4.2132022000     49.0682838190
#    207.9900000000    -0.4709118000     -5.6634298110
#    204.2000000000    -0.4333071000     -5.3078968185
```

```
#    197.3200000000    -0.2673971000    -3.3897525062
#    193.5700000000    -0.6927659000    -8.9522222717
#    191.3000000000    -0.8466580000   -11.0707093945
#    179.6700000000    -2.2182120000   -30.8823177390
#    179.4700000000     0.0415104000     0.5785587417
#    178.7800000000    -0.6505740000    -9.1024892413
#    178.5200000000     0.7824983000    10.9642499857
#    177.6500000000     0.4582829000     6.4528392335
#    175.5900000000     0.0791386000     1.1273817201
#    174.7300000000     0.4168806000     5.9679697439
#    172.2000000000    -0.3129542000    -4.5460063880
#    169.9900000000     1.2487336000    18.3750626314
#    169.5400000000    -0.2404473000    -3.5475631111
#    168.6200000000    -0.5680138000    -8.4262086034
#    167.3200000000     1.1958962000    17.8783746706
#    166.6700000000    -2.5945269000   -38.9388522991
#    165.8900000000     0.4102113000     6.1854288673
#    165.4000000000     3.3672163000    50.9234611823
#    164.5800000000     0.3498539000     5.3173110468
#    164.3000000000    -1.7165528000   -26.1337665652
#    164.1700000000     1.2184327000    18.5647947542
#    158.7900000000     1.8954348000    29.8585082051
#    158.5300000000    -1.7810697000   -28.1029467288
```

```
#    310.6600000000      -0.3072969900      -2.4743171926
#    287.5400000000      -1.4581967400     -12.6852858767
#    224.9300000000      10.8427047300     120.5792705667
#    224.4500000000      -6.4500579000     -71.8830354128
#    221.6300000000       1.6215685200      18.3016043591
#    206.6600000000       0.2313639900       2.8004108051
#    200.5700000000      -2.2208858100     -27.6976331709
#    198.3100000000       0.4680947700       5.9043429962
#    196.1800000000       4.5770739300      58.3600427712
#    190.1500000000      -1.5200885700     -19.9965451505
#    187.8800000000      -1.0380813300     -13.8208016166
#    181.7900000000      -0.1563318900      -2.1510969928
#    179.3600000000      -0.3092661000      -4.3130960215
#    178.1000000000       1.6068838500      22.5685143361
#    175.4500000000      -0.9557133300     -13.6256326253
#    174.9800000000      -1.0635896700     -15.2043585582
#    173.8900000000       0.3585839400       5.1582053992
#    172.3600000000      -2.0093802300     -29.1613781046
#    170.2000000000       1.3113629100      19.2728412773
#    170.0200000000       0.3239636400       4.7662702401
#    169.3200000000       0.3223162800       4.7616381228
#    167.1500000000       5.1079871700      76.4409051938
#    166.3000000000      -1.4240783700     -21.4202258323
```

```
#    165.3200000000    -0.1221491700    -1.8481938812
#    165.1800000000    -4.2652595700    -64.5907620884
#    164.6000000000    -1.4142971700    -21.4928122964
#    162.6000000000     0.0497425500     0.7652263360
#    162.4500000000     1.3173989400     20.2852329029
#    162.0600000000     2.1663684900     33.4378927160
#    160.2300000000     0.5283778500     8.2486556735
#    310.7100000000    -0.2177069400    -1.7526671508
#    287.5900000000    -1.0302811200    -8.9611627516
#    224.9200000000     6.7864797000     75.4742635287
#    224.4200000000    -4.3660960200    -48.6647087931
#    221.8300000000     1.6160958000     18.2233923981
#    207.9500000000    -0.6288678000    -7.5645454703
#    200.4900000000    -1.2567733200    -15.6800210384
#    198.2800000000     1.1215195200     14.1484977810
#    197.3700000000    -1.7361847800    -22.0037756378
#    191.2800000000    -1.5825229200    -20.6948770229
#    190.2300000000    -0.8868924900    -11.6620358971
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