

Lathyrane Diterpenoids from the Roots of *Euphorbia micractina*, and Their Biological Activities

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Table S1. Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters for the Oxygen and Carbon Atoms of **1**.

Atom	x	y	z	U(eq)
O(1)	-11854(2)	-10394(1)	-9074(1)	50(1)
O(2)	-12271(3)	-11212(2)	-10141(1)	95(1)
O(3)	-8796(2)	-10835(1)	-9633(1)	56(1)
O(4)	-9601(2)	-6847(1)	-8707(1)	66(1)
O(5)	-10259(1)	-9188(1)	-7722(1)	43(1)
O(6)	-10569(2)	-7672(1)	-7103(1)	69(1)
C(1)	-11690(2)	-8203(2)	-8564(1)	54(1)
C(2)	-12006(2)	-8516(2)	-9360(1)	55(1)
C(3)	-11228(2)	-9523(2)	-9464(1)	47(1)
C(4)	-9922(2)	-9299(2)	-9080(1)	42(1)
C(5)	-9089(2)	-10270(2)	-8952(1)	44(1)
C(6)	-7717(2)	-10392(2)	-9201(1)	49(1)
C(7)	-6890(3)	-11228(2)	-8826(1)	60(1)
C(8)	-6557(2)	-11036(2)	-8006(1)	52(1)
C(9)	-5637(2)	-10134(2)	-7829(1)	48(1)
C(10)	-5610(2)	-9626(2)	-7078(1)	48(1)
C(11)	-6097(2)	-8985(2)	-7746(1)	46(1)
C(12)	-7470(2)	-8722(2)	-7877(1)	41(1)
C(13)	-7929(2)	-7795(2)	-8123(1)	47(1)
C(14)	-9283(2)	-7662(2)	-8391(1)	47(1)
C(15)	-10273(2)	-8571(2)	-8405(1)	42(1)
C(16)	-13470(3)	-8587(3)	-9525(2)	76(1)
C(17)	-6990(3)	-9539(2)	-9606(1)	63(1)
C(18)	-4311(3)	-9258(2)	-6772(2)	68(1)
C(19)	-6560(3)	-9994(2)	-6488(1)	63(1)
C(20)	-7070(3)	-6829(2)	-8222(2)	84(1)
C(1')	-12282(3)	-11212(2)	-9477(2)	62(1)
C(2')	-12811(4)	-12078(2)	-9007(2)	84(1)
C(1'')	-10428(2)	-8610(2)	-7092(1)	50(1)
-10405(3)	-9273(2)	-6418(1)	66(1)	
H(1A)	-12297	-8539	-8224	64
H(1B)	-11759	-7443	-8505	64
H(2A)	-11631	-7978	-9689	66
H(3A)	-11104	-9686	-9990	57
H(4A)	-9424	-8855	-9425	51
H(5A)	-9348	-10712	-8530	52
H(7A)	-6075	-11296	-9099	72
H(7B)	-7347	-11898	-8863	72
H(8A)	-7372	-10914	-7741	62
H(8B)	-6177	-11679	-7808	62
H(9A)	-4769	-10205	-8057	58
H(11A)	-5472	-8458	-7929	55
H(12A)	-8084	-9247	-7781	50

H(16A)	-13597	-8787	-10033	93
H(16B)	-13871	-7912	-9437	93
H(16C)	-13863	-9106	-9207	93
H(17A)	-7606	-9054	-9821	94
H(17B)	-6466	-9849	-9991	94
H(17C)	-6433	-9168	-9265	94
H(18A)	-4069	-9693	-6358	92
H(18B)	-4385	-8537	-6613	92
H(18C)	-3652	-9311	-7151	92
H(19B)	-6092	-10381	-6114	94
H(19C)	-7211	-10443	-6710	94
H(19D)	-6979	-9393	-6267	94
H(20A)	-6207	-6975	-8035	96
H(20B)	-7442	-6246	-7954	96
H(20C)	-7017	-6654	-8739	96
H(2'A)	-13105	-12646	-9317	97
H(2'B)	-13533	-11817	-8718	97
H(2'C)	-12135	-12329	-8680	97
H(2'D)	-10526	-8834	-5989	90
H(2'E)	-9576	-9629	-6383	90
H(2'F)	-11097	-9785	-6443	90

Table S2. Bond Lengths for **1**.

Bond	Length (Å)	Bond	Length (Å)
O(1)-C(1')	1.339(3)	C(2)-H(2A)	0.9800
O(1)-C(3)	1.454(3)	C(3)-C(4)	1.526(3)
O(2)-C(1')	1.197(3)	C(3)-H(3A)	0.9800
O(3)-C(5)	1.451(3)	C(4)-C(5)	1.512(3)
O(3)-C(6)	1.459(3)	C(4)-C(15)	1.569(3)
O(4)-C(14)	1.222(3)	C(4)-H(4A)	0.9800
O(5)-C(1'')	1.361(3)	C(5)-C(6)	1.477(3)
O(5)-C(15)	1.458(2)	C(5)-H(5A)	0.9800
O(6)-C(1'')	1.197(3)	C(6)-C(17)	1.499(4)
C(1)-C(2)	1.524(4)	C(6)-C(7)	1.513(4)
C(1)-C(15)	1.545(3)	C(7)-C(8)	1.536(3)
C(1)-H(1A)	0.9700	C(7)-H(7A)	0.9700
C(1)-H(1B)	0.9700	C(7)-H(7B)	0.9700
C(2)-C(3)	1.512(4)	C(8)-C(9)	1.511(3)
C(2)-C(16)	1.524(4)	C(8)-H(8A)	0.9700
C(8)-H(8B)	0.9700	C(17)-H(17C)	0.9600
C(9)-C(10)	1.498(3)	C(18)-H(18A)	0.9600
C(9)-C(11)	1.535(3)	C(18)-H(18B)	0.9600
C(9)-H(9A)	0.9800	C(18)-H(18C)	0.9600
C(10)-C(18)	1.509(4)	C(19)-H(19B)	0.9600
C(10)-C(19)	1.511(4)	C(19)-H(19C)	0.9600
C(10)-C(11)	1.535(3)	C(19)-H(19D)	0.9600

C(11)-C(12)	1.459(3)	C(20)-H(20A)	0.9600
C(11)-H(11A)	0.9800	C(20)-H(20B)	0.9600
C(12)-C(13)	1.339(3)	C(20)-H(20C)	0.9600
C(12)-H(12A)	0.9300	C(1')-C(2')	1.487(4)
C(13)-C(14)	1.472(3)	C(2')-H(2'A)	0.9600
C(13)-C(20)	1.514(3)	C(2')-H(2'B)	0.9600
C(14)-C(15)	1.531(3)	C(2')-H(2'C)	0.9600
C(16)-H(16A)	0.9600	C(1'')-C(2'')	1.477(3)
C(16)-H(16B)	0.9600	C(2'')-H(2'D)	0.9600
C(16)-H(16C)	0.9600	C(2'')-H(2'E)	0.9600
C(17)-H(17A)	0.9600	C(2'')-H(2'F)	0.9600
C(17)-H(17B)	0.9600		

Table S3. Bond Angles for **1**.

Bond	Angle (°)	Bond	Angle (°)
C(1')-O(1)-C(3)	117.92(18)	C(3)-C(4)-C(15)	105.14(17)
C(5)-O(3)-C(6)	60.99(14)	C(5)-C(4)-H(4A)	105.8
C(1'')-O(5)-C(15)	114.53(15)	C(3)-C(4)-H(4A)	105.8
C(2)-C(1)-C(15)	107.1(2)	C(15)-C(4)-H(4A)	105.8
C(2)-C(1)-H(1A)	110.3	O(3)-C(5)-C(6)	59.80(14)
C(15)-C(1)-H(1A)	110.3	O(3)-C(5)-C(4)	112.76(18)
C(2)-C(1)-H(1B)	110.3	C(6)-C(5)-C(4)	124.8(2)
C(15)-C(1)-H(1B)	110.3	O(3)-C(5)-H(5A)	115.5
H(1A)-C(1)-H(1B)	108.5	C(6)-C(5)-H(5A)	115.5
C(3)-C(2)-C(1)	102.95(19)	C(4)-C(5)-H(5A)	115.5
C(3)-C(2)-C(16)	116.1(2)	O(3)-C(6)-C(5)	59.21(14)
C(1)-C(2)-C(16)	113.9(2)	O(3)-C(6)-C(17)	112.9(2)
C(3)-C(2)-H(2A)	107.8	C(5)-C(6)-C(17)	122.8(2)
C(1)-C(2)-H(2A)	107.8	O(3)-C(6)-C(7)	112.9(2)
C(16)-C(2)-H(2A)	107.8	C(5)-C(6)-C(7)	117.7(2)
O(1)-C(3)-C(2)	110.45(18)	C(17)-C(6)-C(7)	116.5(2)
O(1)-C(3)-C(4)	107.74(17)	C(6)-C(7)-C(8)	116.25(19)
C(2)-C(3)-C(4)	104.23(19)	C(6)-C(7)-H(7A)	108.2
O(1)-C(3)-H(3A)	111.4	C(8)-C(7)-H(7A)	108.2
C(2)-C(3)-H(3A)	111.4	C(6)-C(7)-H(7B)	108.2
C(4)-C(3)-H(3A)	111.4	C(8)-C(7)-H(7B)	108.2
C(5)-C(4)-C(3)	114.14(18)	H(7A)-C(7)-H(7B)	107.4
C(5)-C(4)-C(15)	119.17(17)	C(9)-C(8)-C(7)	117.4(2)
C(9)-C(8)-H(8A)	107.9	H(16B)-C(16)-H(16C)	109.5
C(7)-C(8)-H(8A)	107.9	C(6)-C(17)-H(17A)	109.5
C(9)-C(8)-H(8B)	107.9	C(6)-C(17)-H(17B)	109.5
C(7)-C(8)-H(8B)	107.9	H(17A)-C(17)-H(17B)	109.5
H(8A)-C(8)-H(8B)	107.2	C(6)-C(17)-H(17C)	109.5
C(10)-C(9)-C(8)	121.7(2)	H(17A)-C(17)-H(17C)	109.5
C(10)-C(9)-C(11)	60.80(14)	H(17B)-C(17)-H(17C)	109.5
C(8)-C(9)-C(11)	123.07(19)	C(10)-C(18)-H(18A)	109.5

C(10)-C(9)-H(9A)	113.8	C(10)-C(18)-H(18B)	109.5
C(8)-C(9)-H(9A)	113.8	H(18A)-C(18)-H(18B)	109.5
C(11)-C(9)-H(9A)	113.8	C(10)-C(18)-H(18C)	109.5
C(9)-C(10)-C(18)	118.6(2)	H(18A)-C(18)-H(18C)	109.5
C(9)-C(10)-C(19)	119.4(2)	H(18B)-C(18)-H(18C)	109.5
C(18)-C(10)-C(19)	113.6(2)	C(10)-C(19)-H(19B)	109.5
C(9)-C(10)-C(11)	60.80(14)	C(10)-C(19)-H(19C)	109.5
C(18)-C(10)-C(11)	114.0(2)	H(19B)-C(19)-H(19C)	109.5
C(19)-C(10)-C(11)	120.5(2)	C(10)-C(19)-H(19D)	109.5
C(12)-C(11)-C(9)	119.62(19)	H(19B)-C(19)-H(19D)	109.5
C(12)-C(11)-C(10)	123.9(2)	H(19C)-C(19)-H(19D)	109.5
C(9)-C(11)-C(10)	58.41(14)	C(13)-C(20)-H(20A)	109.5
C(12)-C(11)-H(11A)	114.5	C(13)-C(20)-H(20B)	109.5
C(9)-C(11)-H(11A)	114.5	H(20A)-C(20)-H(20B)	109.5
C(10)-C(11)-H(11A)	114.5	C(13)-C(20)-H(20C)	109.5
C(13)-C(12)-C(11)	126.1(2)	H(20A)-C(20)-H(20C)	109.5
C(13)-C(12)-H(12A)	116.9	H(20B)-C(20)-H(20C)	109.5
C(11)-C(12)-H(12A)	116.9	O(2)-C(1')-O(1)	122.6(3)
C(12)-C(13)-C(14)	122.4(2)	O(2)-C(1')-C(2')	125.1(3)
C(12)-C(13)-C(20)	123.0(2)	O(1)-C(1')-C(2')	112.3(2)
C(14)-C(13)-C(20)	114.3(2)	C(1')-C(2')-H(2'A)	109.5
O(4)-C(14)-C(13)	119.9(2)	C(1')-C(2')-H(2'B)	109.5
O(4)-C(14)-C(15)	116.8(2)	H(2'A)-C(2')-H(2'B)	109.5
C(13)-C(14)-C(15)	122.57(18)	C(1')-C(2')-H(2'C)	109.5
O(5)-C(15)-C(14)	112.49(17)	H(2'A)-C(2')-H(2'C)	109.5
O(5)-C(15)-C(1)	109.13(18)	H(2'B)-C(2')-H(2'C)	109.5
C(14)-C(15)-C(1)	113.16(18)	O(6)-C(1'')-O(5)	122.3(2)
O(5)-C(15)-C(4)	109.76(15)	O(6)-C(1'')-C(2'')	125.3(2)
C(14)-C(15)-C(4)	107.68(17)	O(5)-C(1'')-C(2'')	112.3(2)
C(1)-C(15)-C(4)	104.26(18)	C(1'')-C(2'')-H(2'D)	109.5
C(2)-C(16)-H(16A)	109.5	C(1'')-C(2'')-H(2'E)	109.5
C(2)-C(16)-H(16B)	109.5	H(2'D)-C(2'')-H(2'E)	109.5
H(16A)-C(16)-H(16B)	109.5	C(1'')-C(2'')-H(2'F)	109.5
C(2)-C(16)-H(16C)	109.5	H(2'D)-C(2'')-H(2'F)	109.5
H(16A)-C(16)-H(16C)	109.5	H(2'E)-C(2'')-H(2'F)	109.5

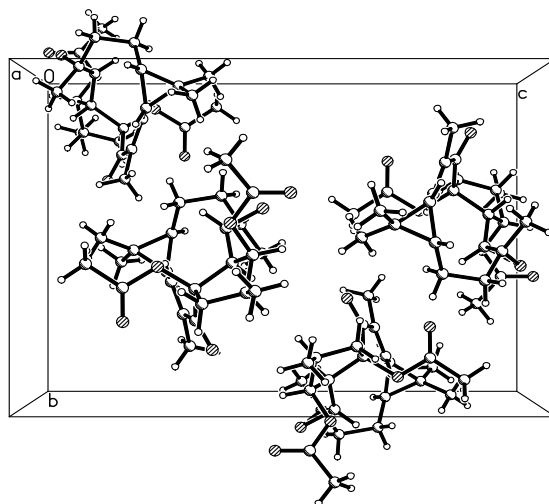


Figure S1. Crystal Cell Diagram for **1**.

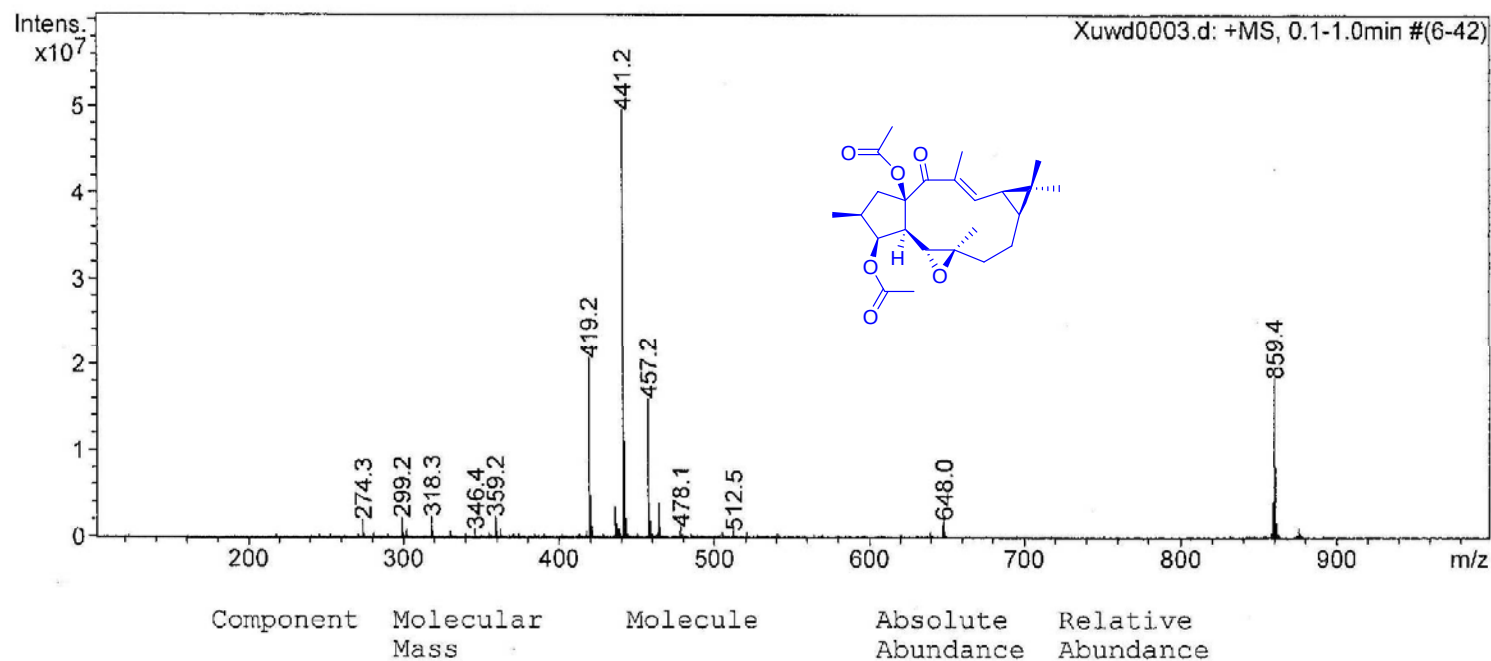


Figure S2. (+)-ESIMS Spectrum of 1.

Data:E_9_1

Sample Name:

Description:

Ionization Mode:ESI+

History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[];Smooth[3]];Correct Base[5.0%];Average(MS[...

Charge number:1

Tolerance:5.00(mmu)

Element:¹²C:0 .. 100, ¹H:0 .. 200, ²³Na:1 .. 1, ¹⁶O:0 .. 10

Acquired:12:00:00 AM

Operator:Accutof

Mass Calibration data:TFA100-2000-P-070410

Created:10/14/2008 11:33:08 AM

Created by:Accutof

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

Mass	Mass Difference (mmu)	Mass Difference (ppm)	¹² C	¹ H	²³ Na	¹⁶ O	Unsaturation Number
441.22740	2.09	4.73	24	34	1	6	7.5

(+)-HRESIMS Data of 1.

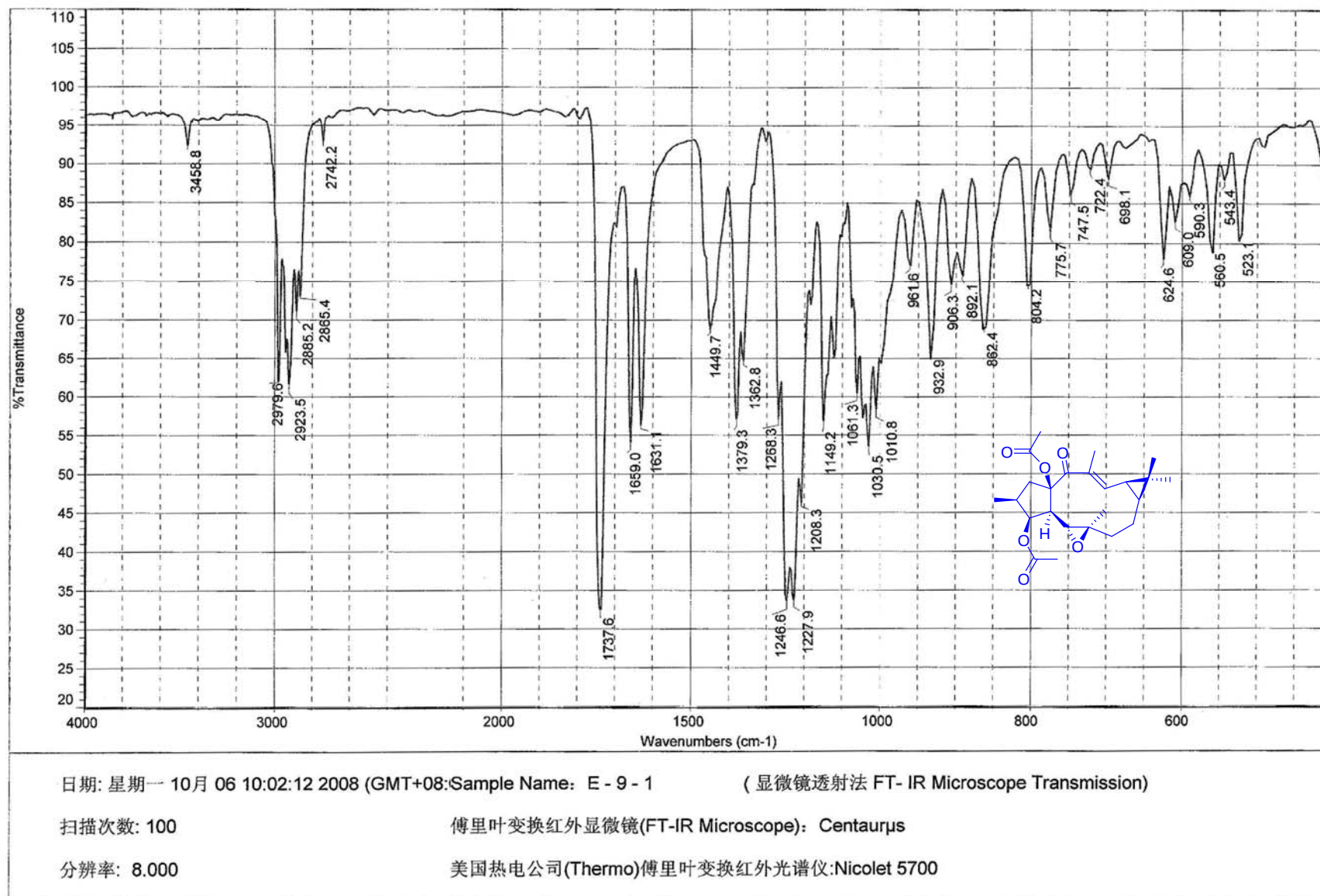


Figure S3. The IR Spectrum of 1.

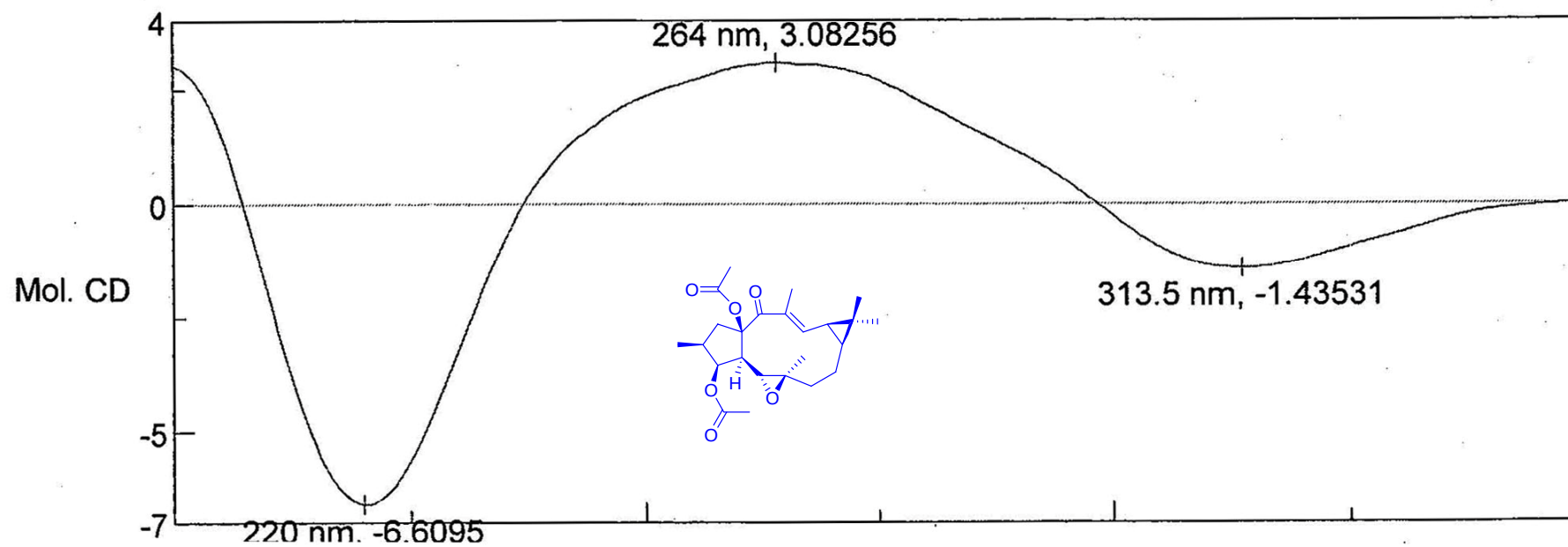


Figure S4. The CD Spectrum of 1.

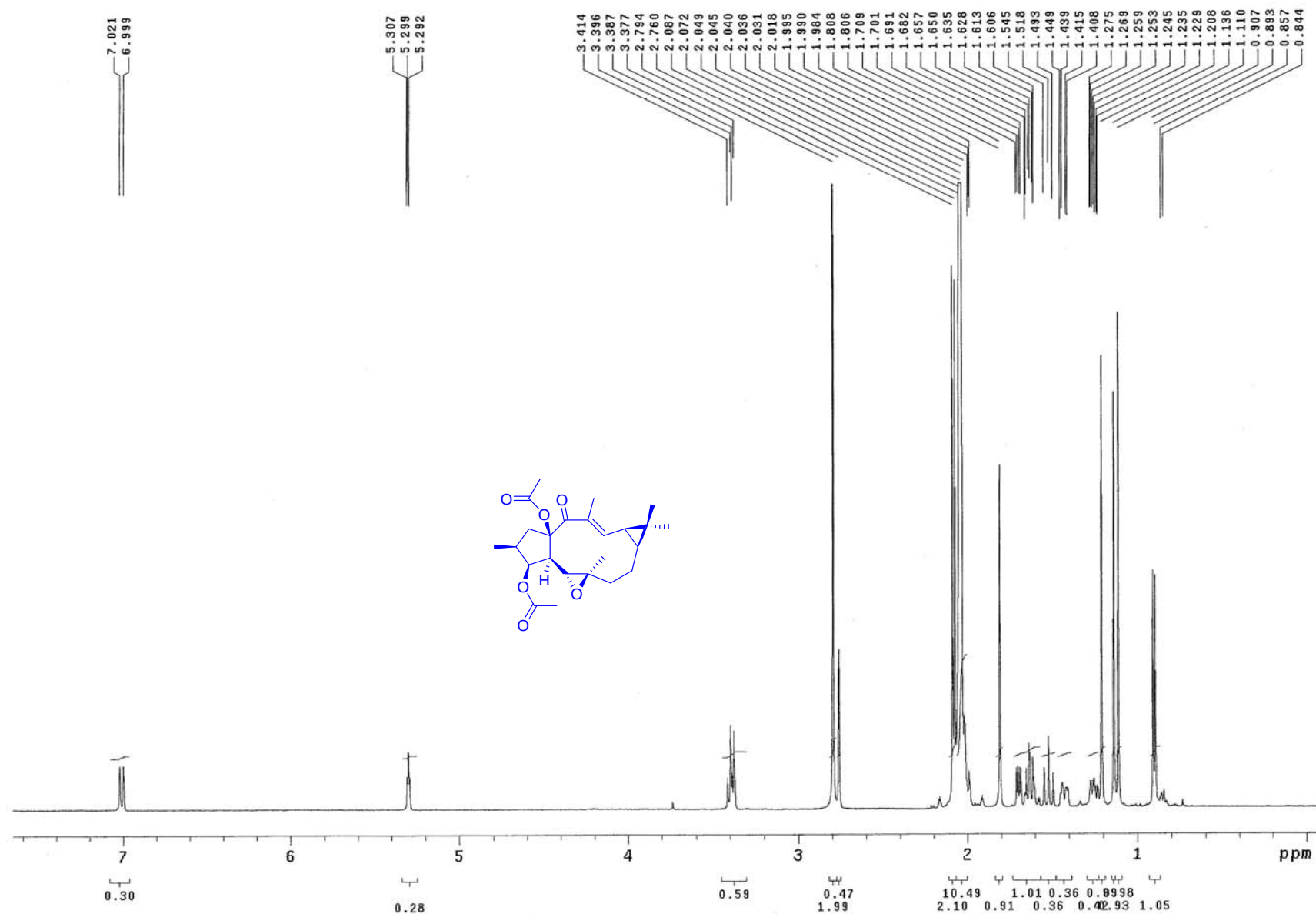


Figure S5. The ^1H NMR Spectrum of 1 in CD_3COCD_3 (500 MHz).

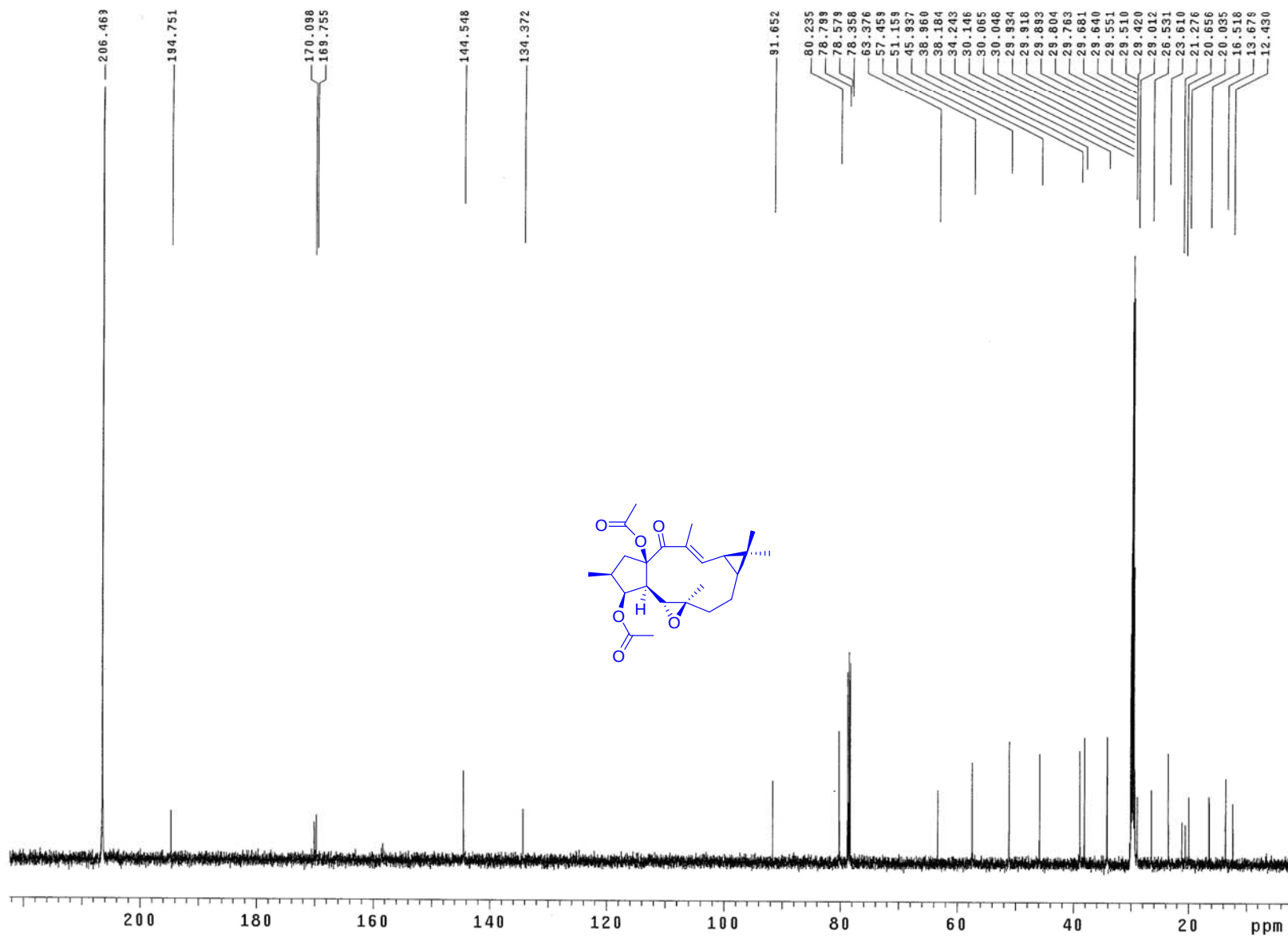


Figure S6. The ^{13}C NMR Spectrum of 1 in CD_3COCD_3 (150 MHz).

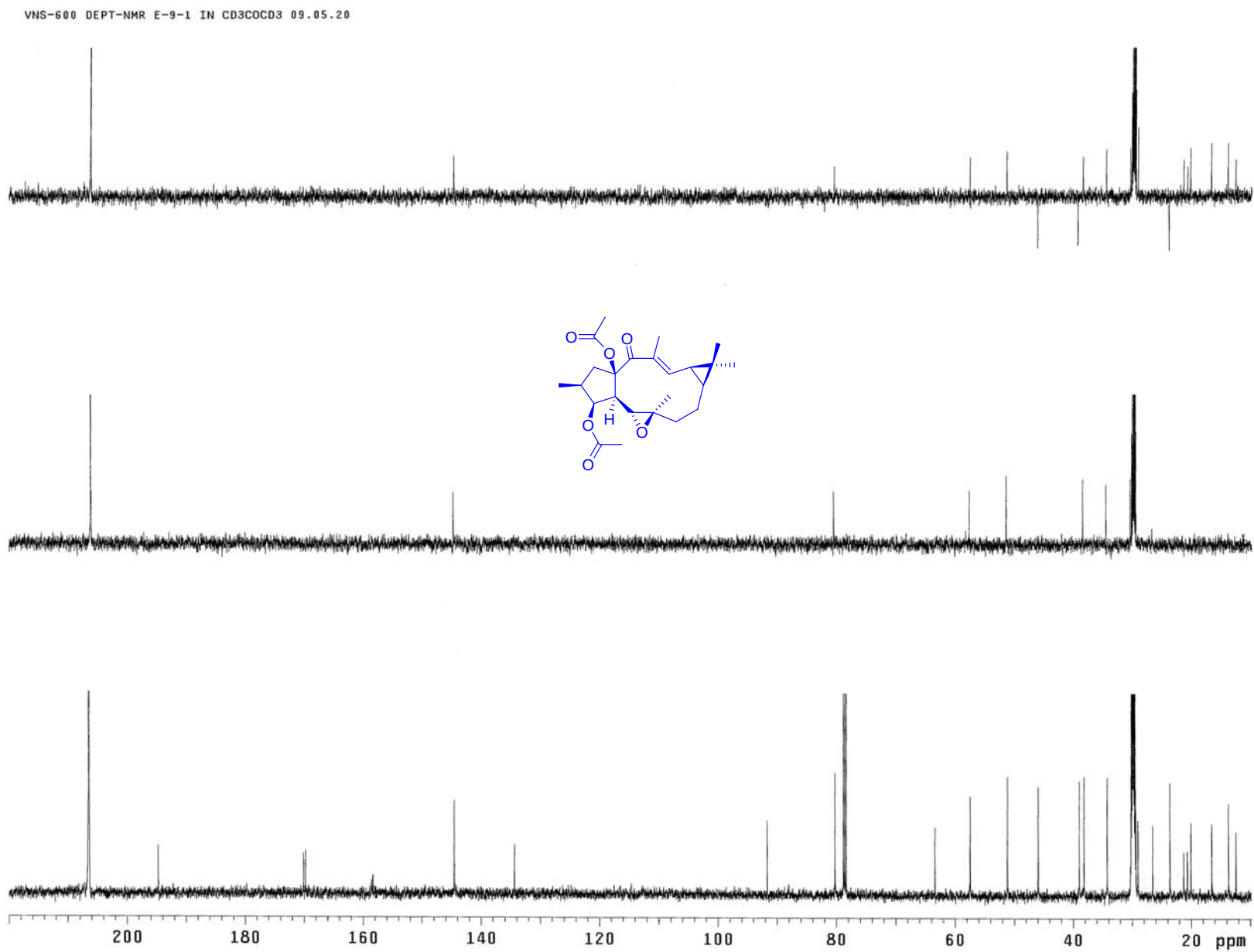


Figure S7. The DEPT Spectrum of 1 in CD₃COCD₃ (150 MHz).

SYS-600 gCOSY E-9-1 in CD3COCD3 08.01.15

Solvent: acetone
Ambient temperature
Operator: vnmr2
VNMR5-600 "wormhole"

Relax. delay 1.301 sec
Acq. time 0.189 sec
Width 5411.3 Hz
2D Width 5411.3 Hz
2 repetitions
256 increments
OBSERVE H1, 599.6981353 MHz
DATA PROCESSING
Sine bell 0.095 sec
F1 DATA PROCESSING
Sine bell 0.023 sec
FT size 2048 x 2048
Total time 13 min, 25 sec

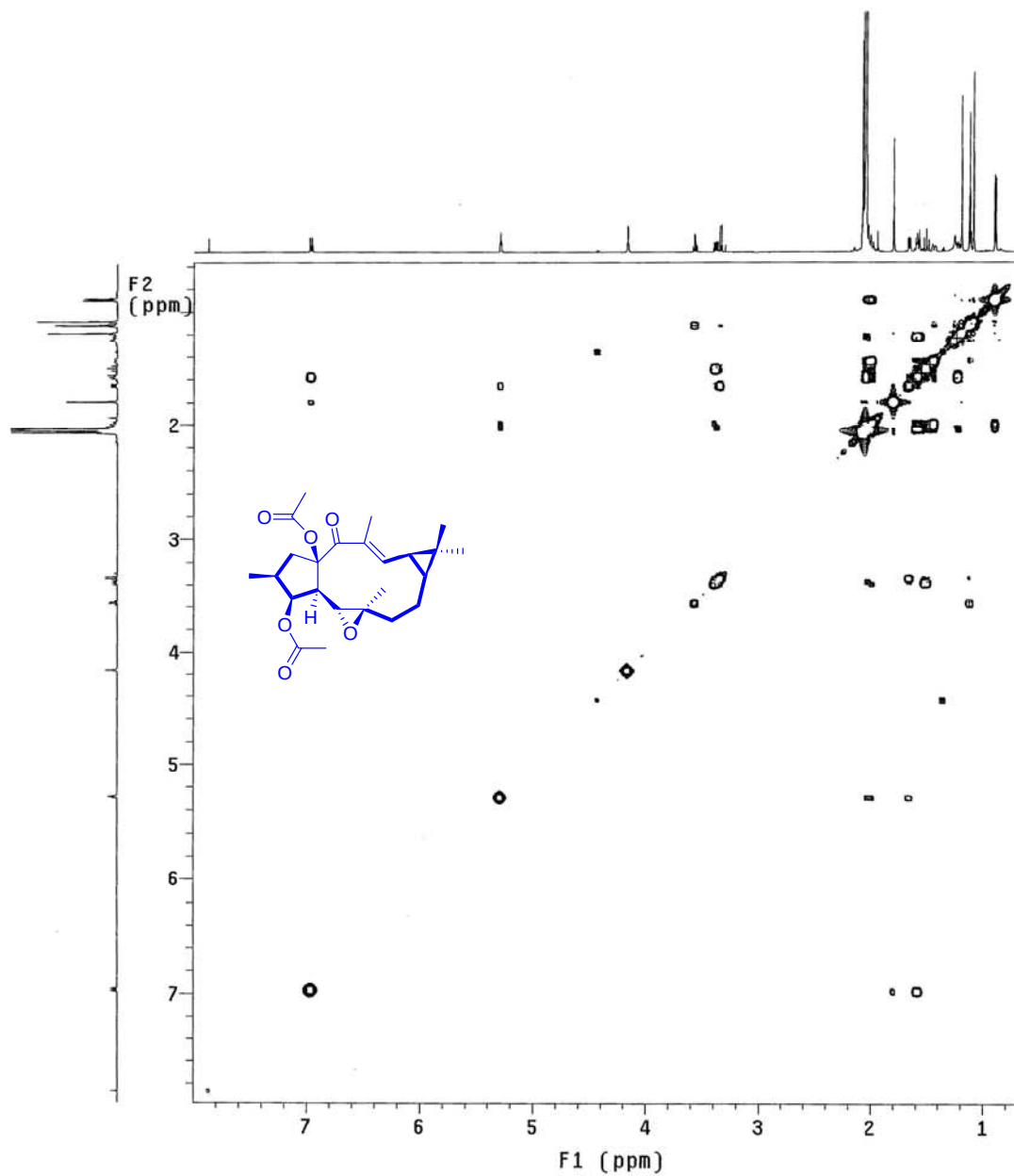


Figure S8. The ¹H-¹H gCOSY Spectrum of 1 in CD₃COCD₃ (600 MHz).

Solvent: acetone
Ambient temperature
Operator: vnmr2
VNMR5-600 "wormhole"

Relax. delay 1.000 sec
Acq. time 0.128 sec
Width 5208.3 Hz
2D Width 32894.7 Hz
16 repetitions
160 increments
OBSERVE H1, 599.6981335 MHz
DECOUPLE C13, 150.8110842 MHz
Power 42 dB
on during acquisition
off during delay
GARP-1 modulated
DATA PROCESSING
Sine bell 0.018 sec
F1 DATA PROCESSING
Sine bell 0.002 sec
FT size 2048 x 2048
Total time 51 min, 2 sec

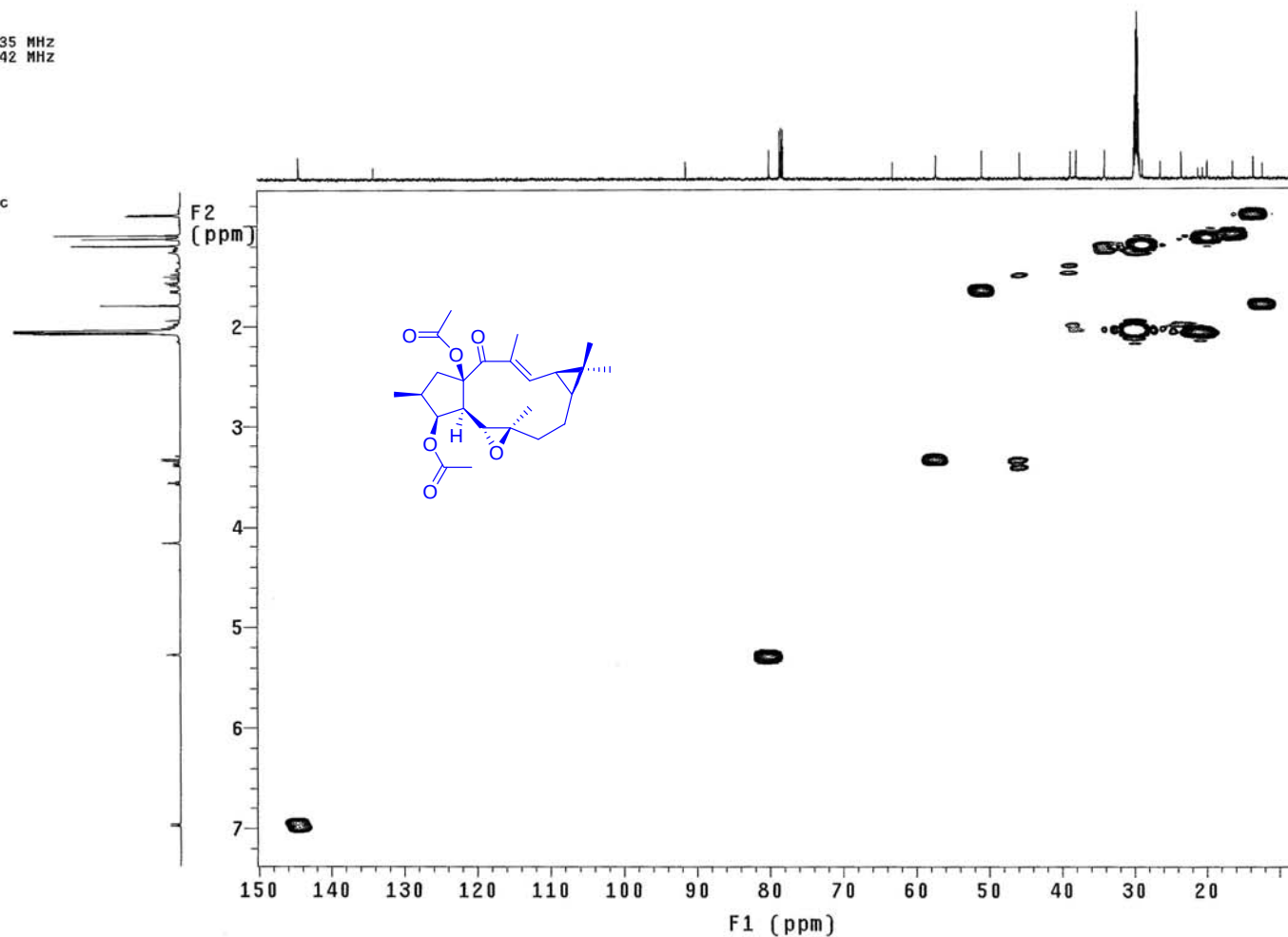


Figure S9. The gHSQC Spectrum of 1 in CD₃COCD₃ (600MHz for ¹H NMR).

SVC-600 gHMBC E-9-1 in CD3COCD3 08.01.15

Solvent: acetone
Ambient temperature
Operator: vnmr2
VNMR-600 "wormhole"

Relax. delay 1.000 sec
Mixing 0.080 sec
Acq. time 0.128 sec
Width 5319.1 Hz
2D Width 32894.7 Hz
32 repetitions
256 increments
OBSERVE H1, 599.6981375 MHz
DATA PROCESSING
Sine bell 0.043 sec
F1 DATA PROCESSING
Sine bell 0.003 sec
FT size 2048 x 2048
Total time 2 hr, 46 min, 19 sec

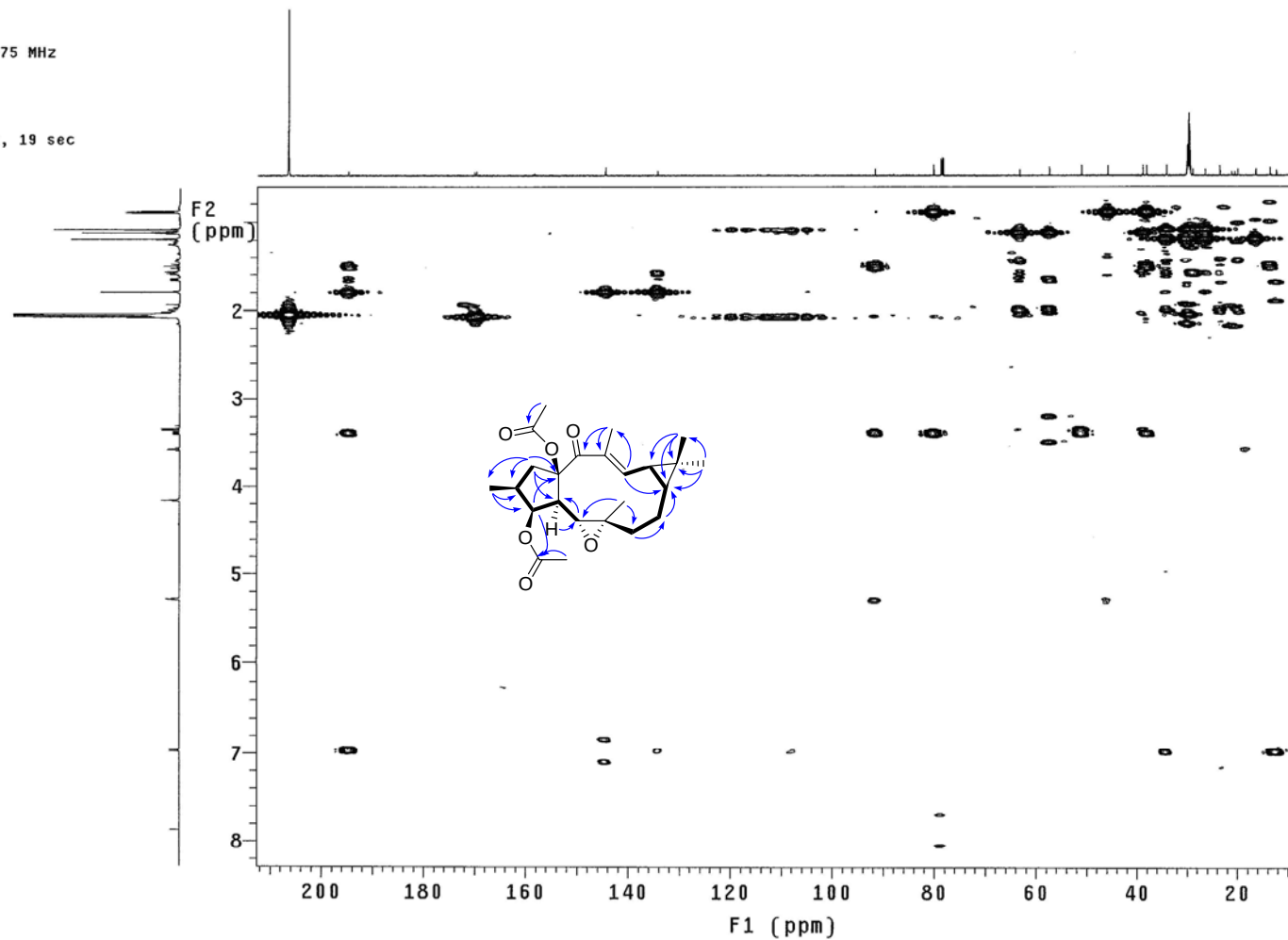


Figure S10. The gHMBC Spectrum of 1 in CD_3COCD_3 (600MHz for ^1H NMR).

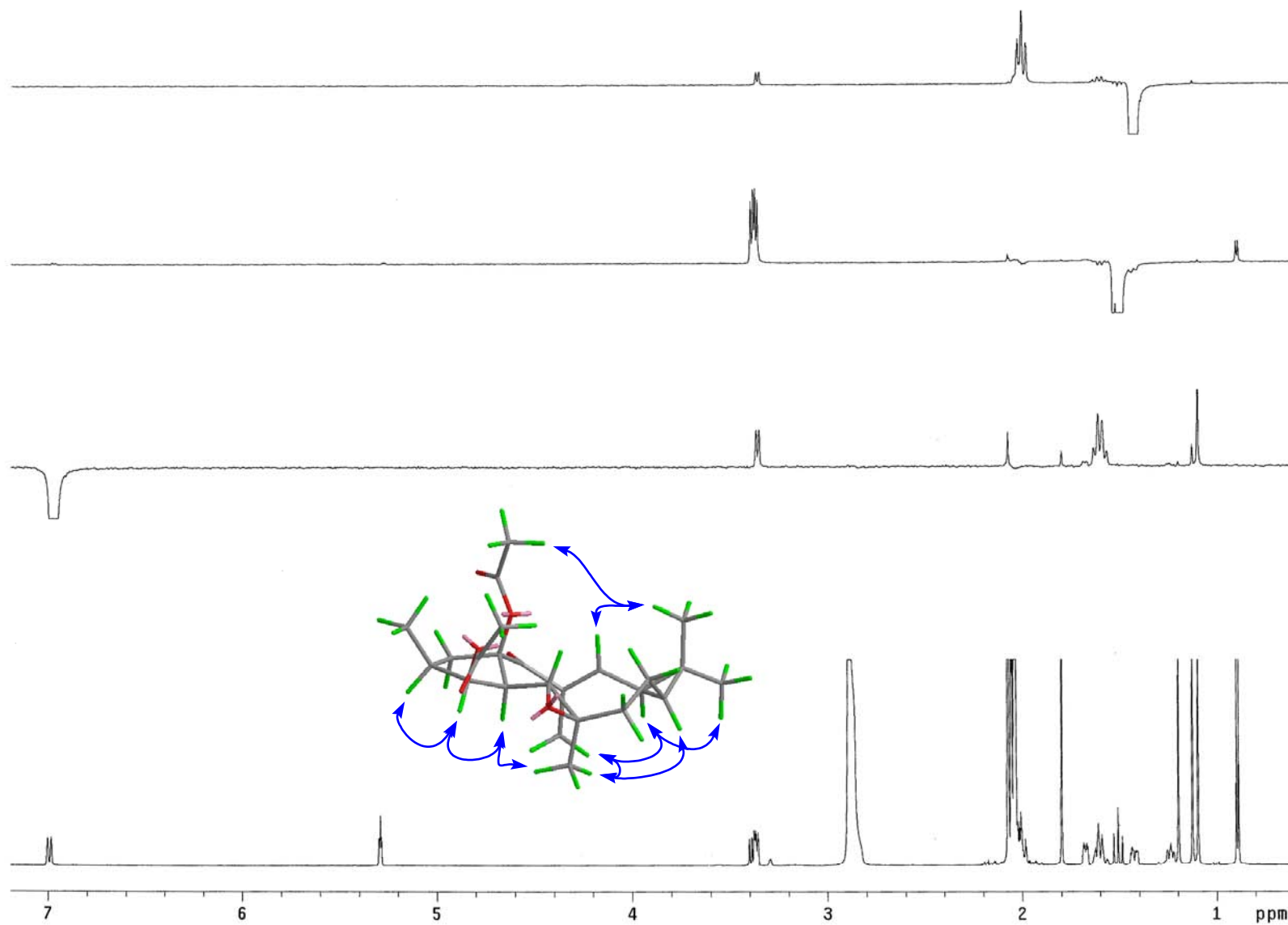


Figure S11. The NOE Difference Spectrum 1 of 1 in CD_3COCD_3 (600 MHz).

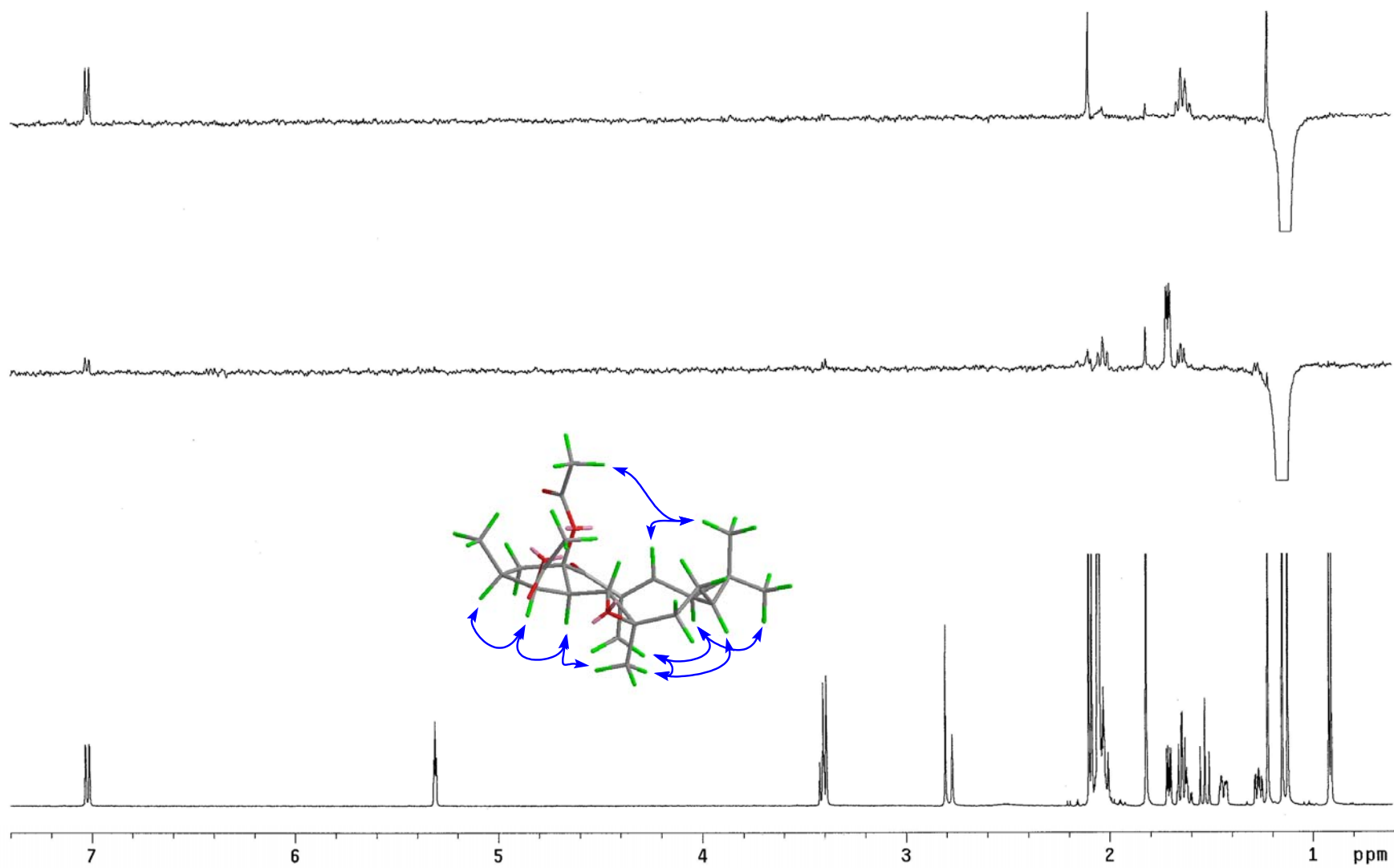


Figure S12. The NOE Difference Spectrum 2 of 1 in CD₃COCD₃ (600 MHz).

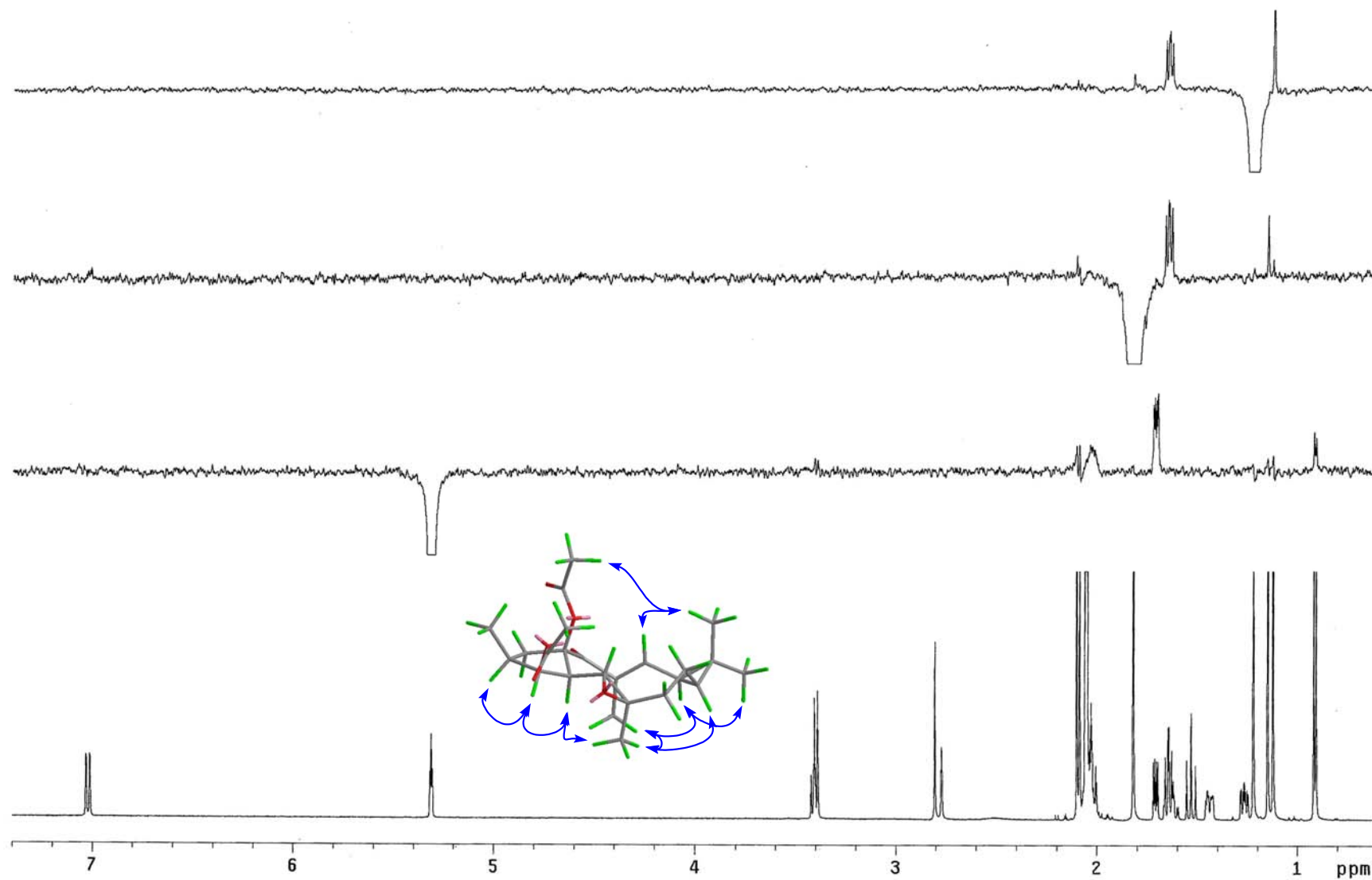


Figure S13. The NOE Difference Spectrum 3 of 1 in CD₃COCD₃ (600 MHz).

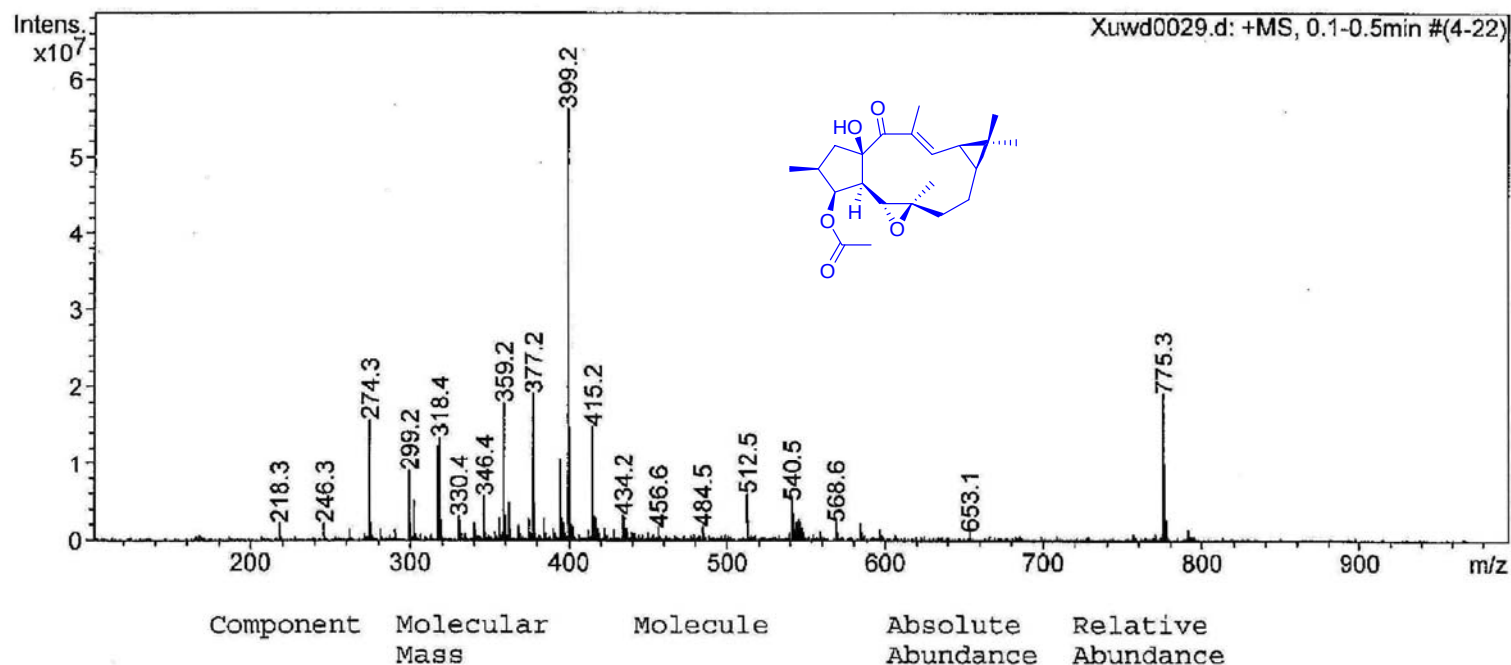


Figure S14. (+)-ESIMS Spectrum of 2.

Data:EM_E_10_16

Sample Name:

Description:

Ionization Mode:ESI+

History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[];Smooth[3]];Correct Base[5.0%];Average(MS[...

Acquired:12/9/2008 11:03:42 AM

Operator:Accutof

Mass Calibration data:TFA100-2000-P-070410

Created:12/9/2008 11:08:56 AM

Created by:Accutof

Charge number:1

Tolerance:5.00(mmu)

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

Element:¹²C:0 .. 100, ¹H:0 .. 200, ³⁹K:1 .. 1, ¹⁶O:0 .. 10

Mass	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	¹² C	¹ H	³⁹ K	¹⁶ O	Unsaturation Number
415.19331	415.18868	4.63	11.14	22	32	1	5	6.5

(+)-HRESIMS Data of 2.

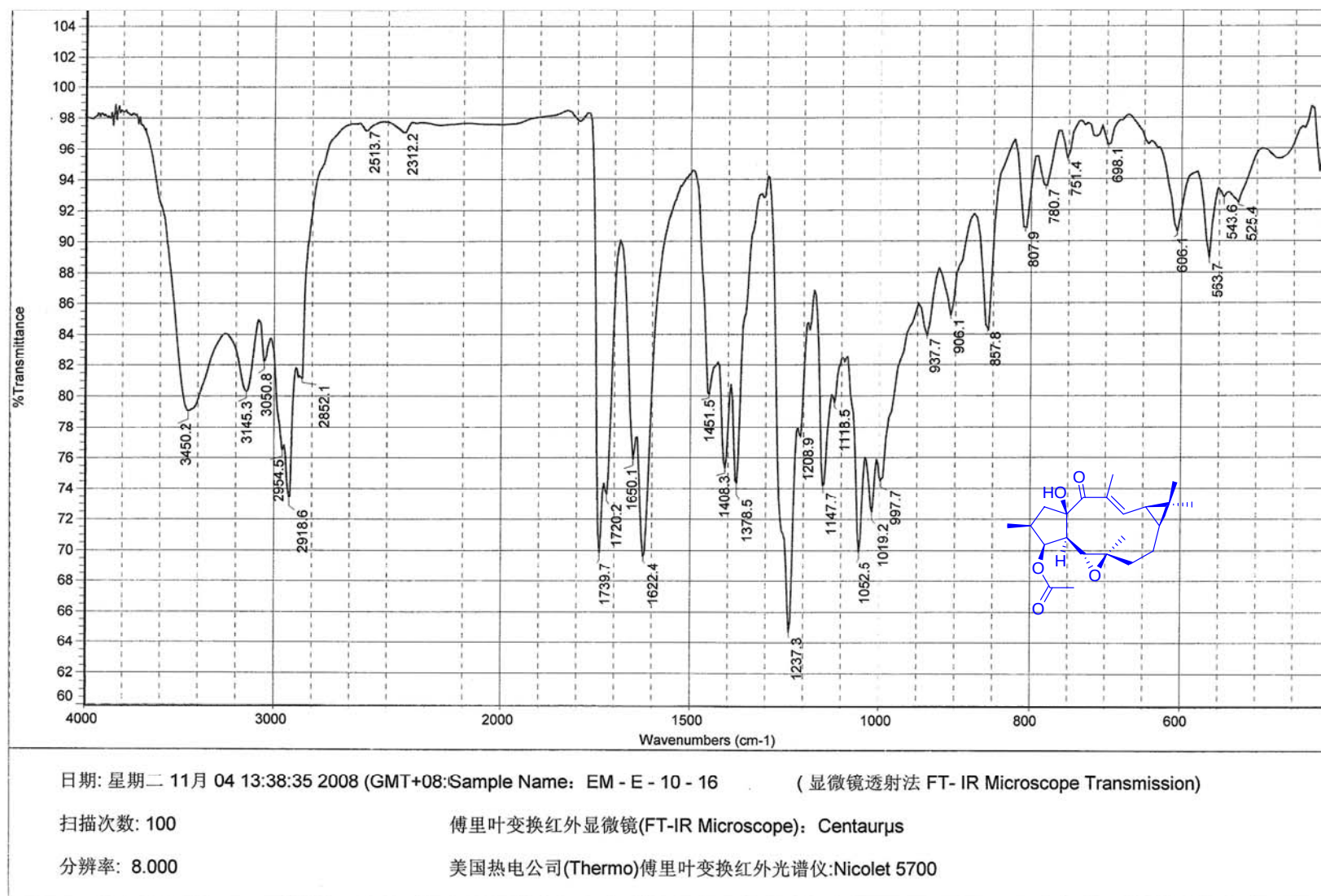


Figure S15. The IR Spectrum of 2.
S27

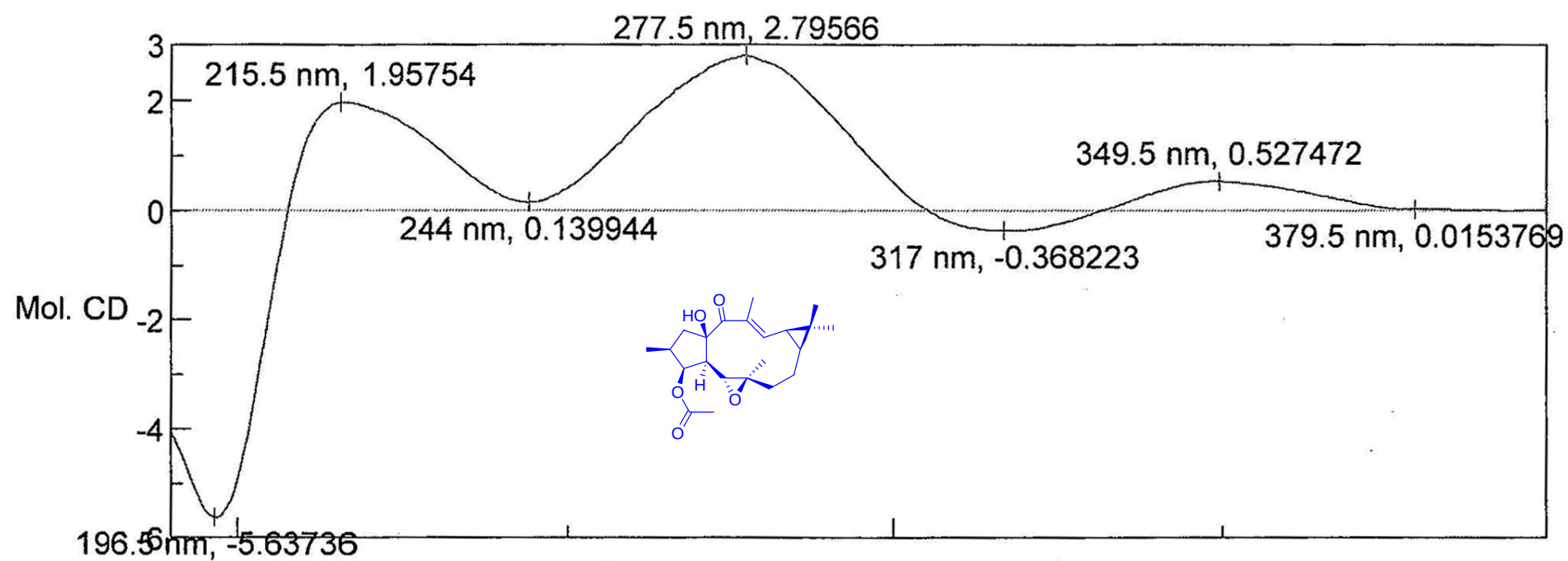


Figure S16. The CD Spectrum of 2.

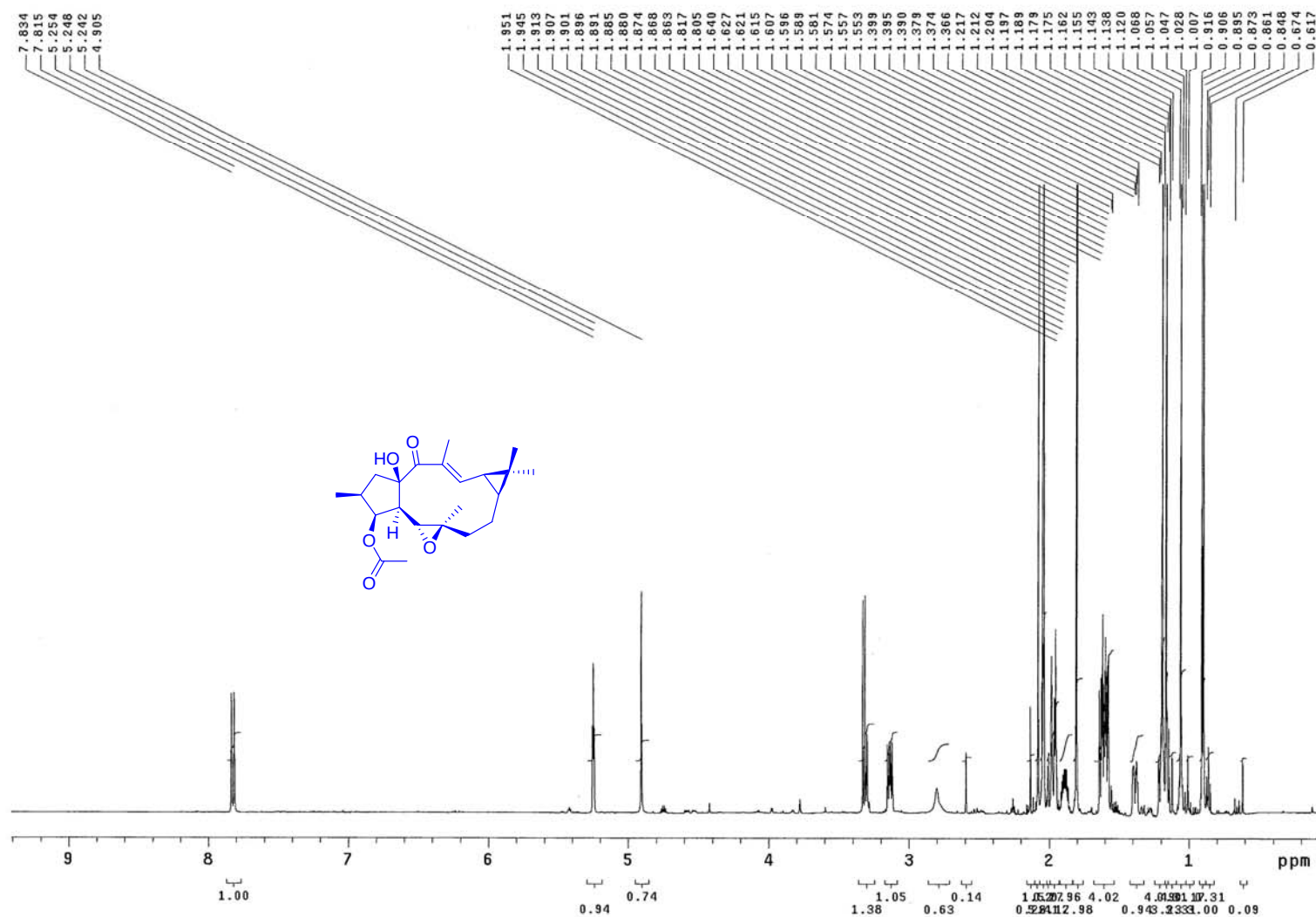


Figure S17. The ¹H NMR Spectrum of 2 in CD₃COCD₃ (600 MHz).

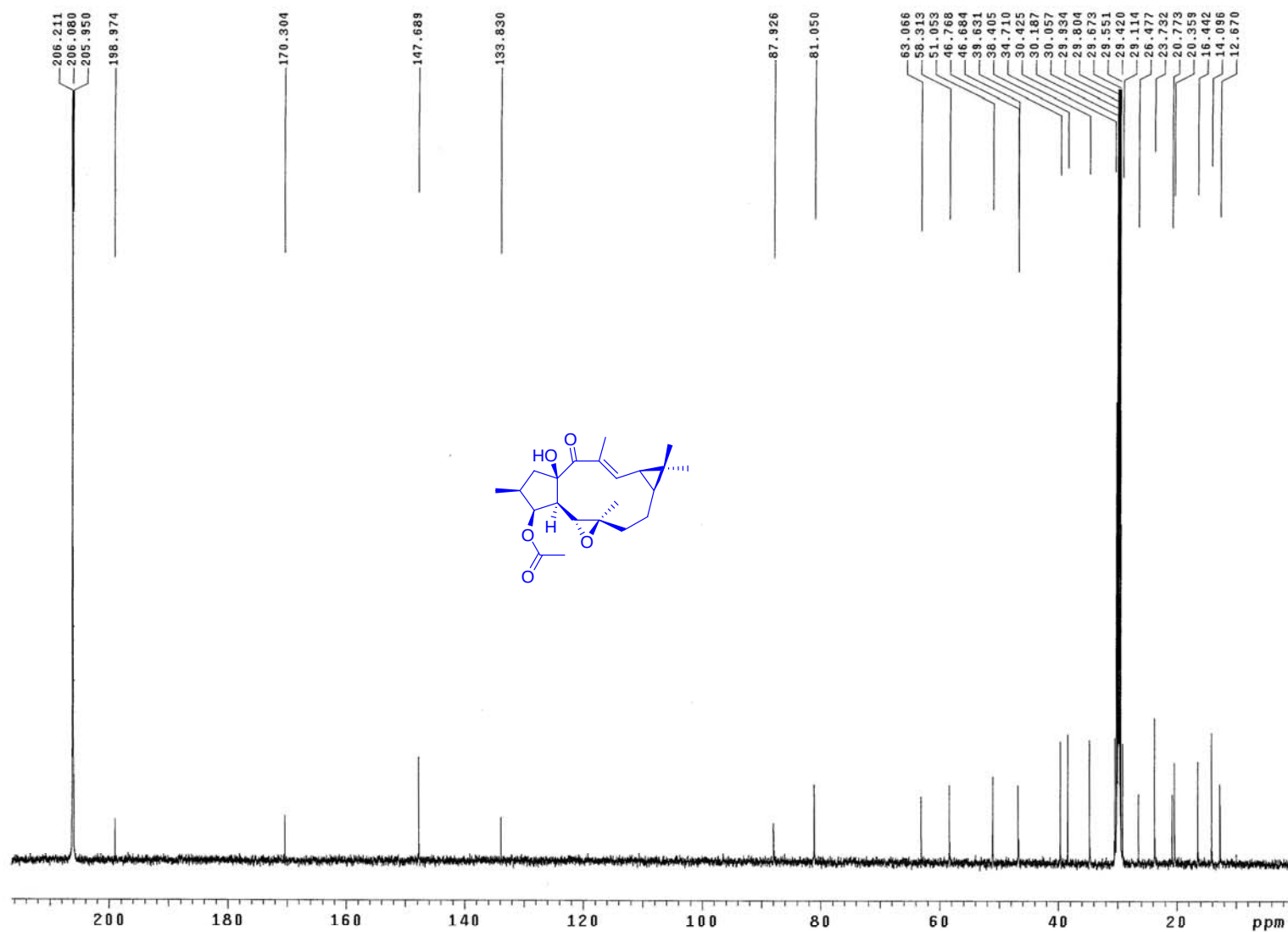


Figure S18. The ^{13}C NMR Spectrum of 2 in CD_3COCD_3 (150 MHz).

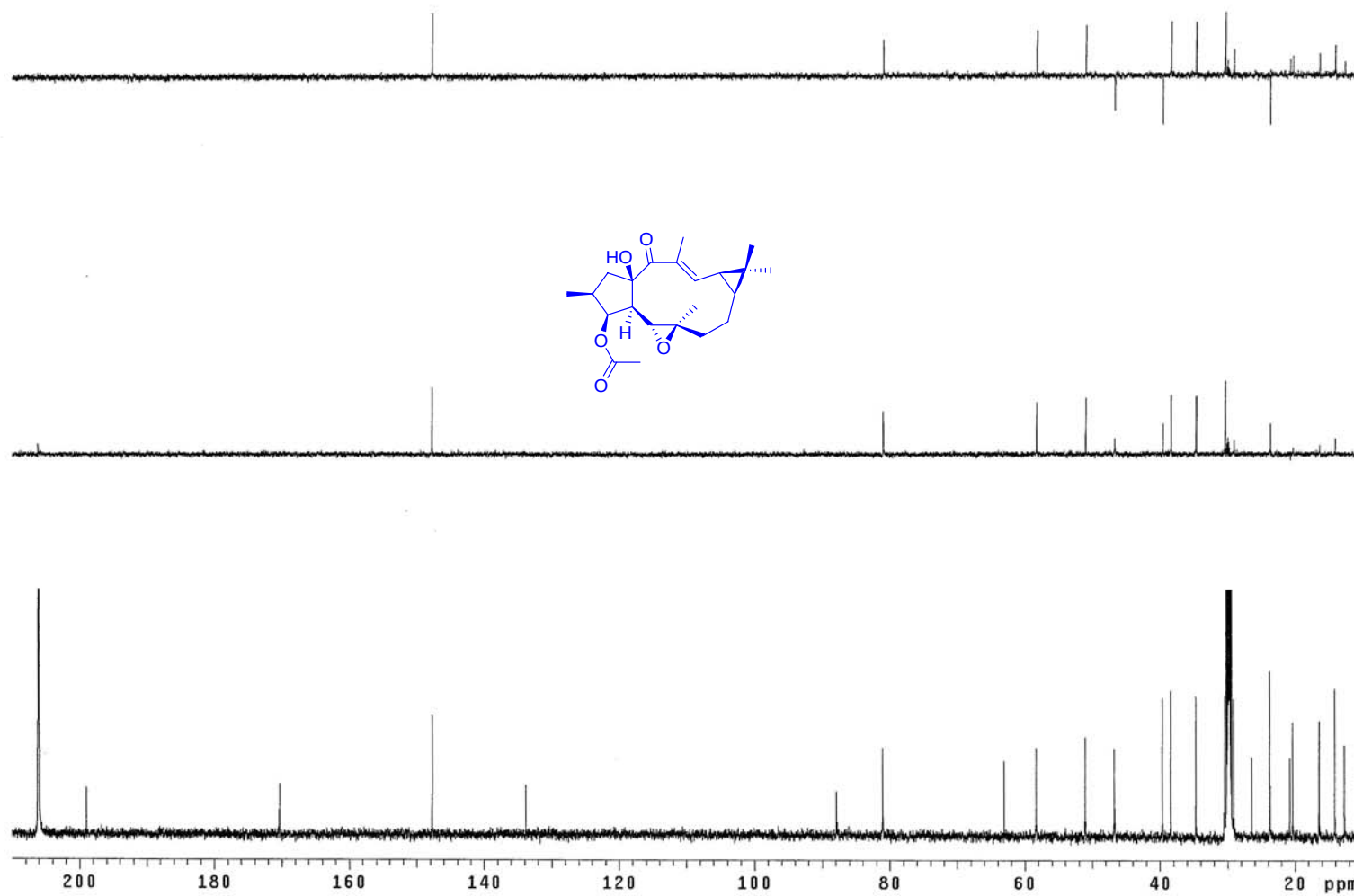


Figure S19. The DEPT Spectrum of 2 in CD₃COCD₃ (150 MHz).

VNS-600 gCOSY EM-E-10-16 IN CD3COCD3 2008.09.17

Solvent: acetone
Ambient temperature
Operator: vnmr2
VNMRS-600 "wormhole"

Relax. delay 1.000 sec
Acq. time 0.190 sec
Width 5387.9 Hz
2D Width 5387.9 Hz
4 repetitions
256 increments
OBSERVE H1, 599.6981281 MHz
DATA PROCESSING
Sq. sine bell 0.095 sec
F1 DATA PROCESSING
Sq. sine bell 0.024 sec
FT size 2048 x 2048
Total time 21 min, 15 sec

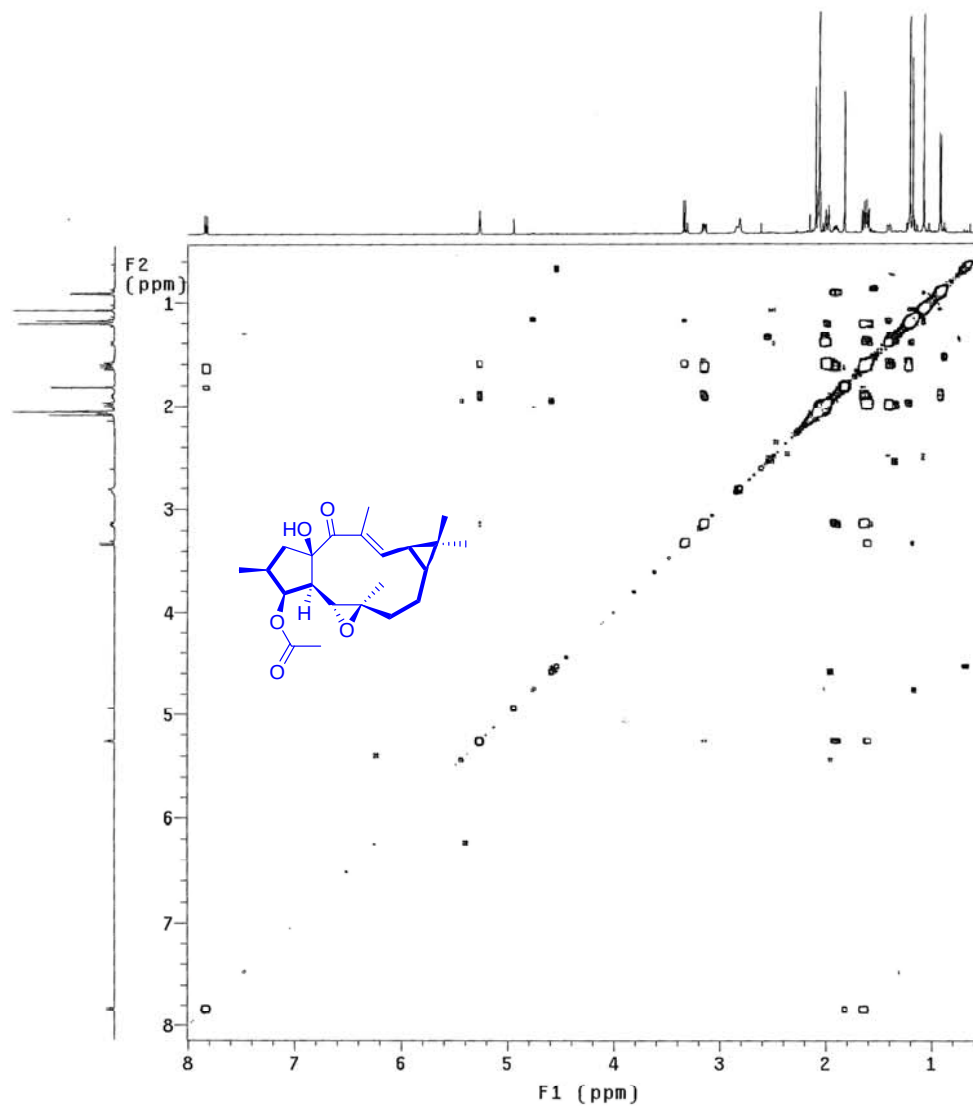


Figure S20. The ^1H - ^1H gCOSY Spectrum of 2 in CD_3COCD_3 (600 MHz).

VNS-600 gHSQC EM-E-10-16 IN CD3COCD3 2008.09.17

Solvent: acetone
Ambient temperature
Operator: vnmr2
VNMRS-600 "wormhole"

Relax. delay 1.000 sec
Acq. time 0.199 sec
Width 5656.1 Hz
2D Width 24509.8 Hz
64 repetitions
200 increments
OBSERVE H1, 599.6981281 MHz
DECOUPLE C13, 150.8061588 MHz
Power 42 dB
on during acquisition
off during delay
GARP-1 modulated
DATA PROCESSING
Sine bell 0.038 sec
F1 DATA PROCESSING
Sine bell 0.004 sec
FT size 2048 x 8192
Total time 4 hr, 28 min, 1 sec

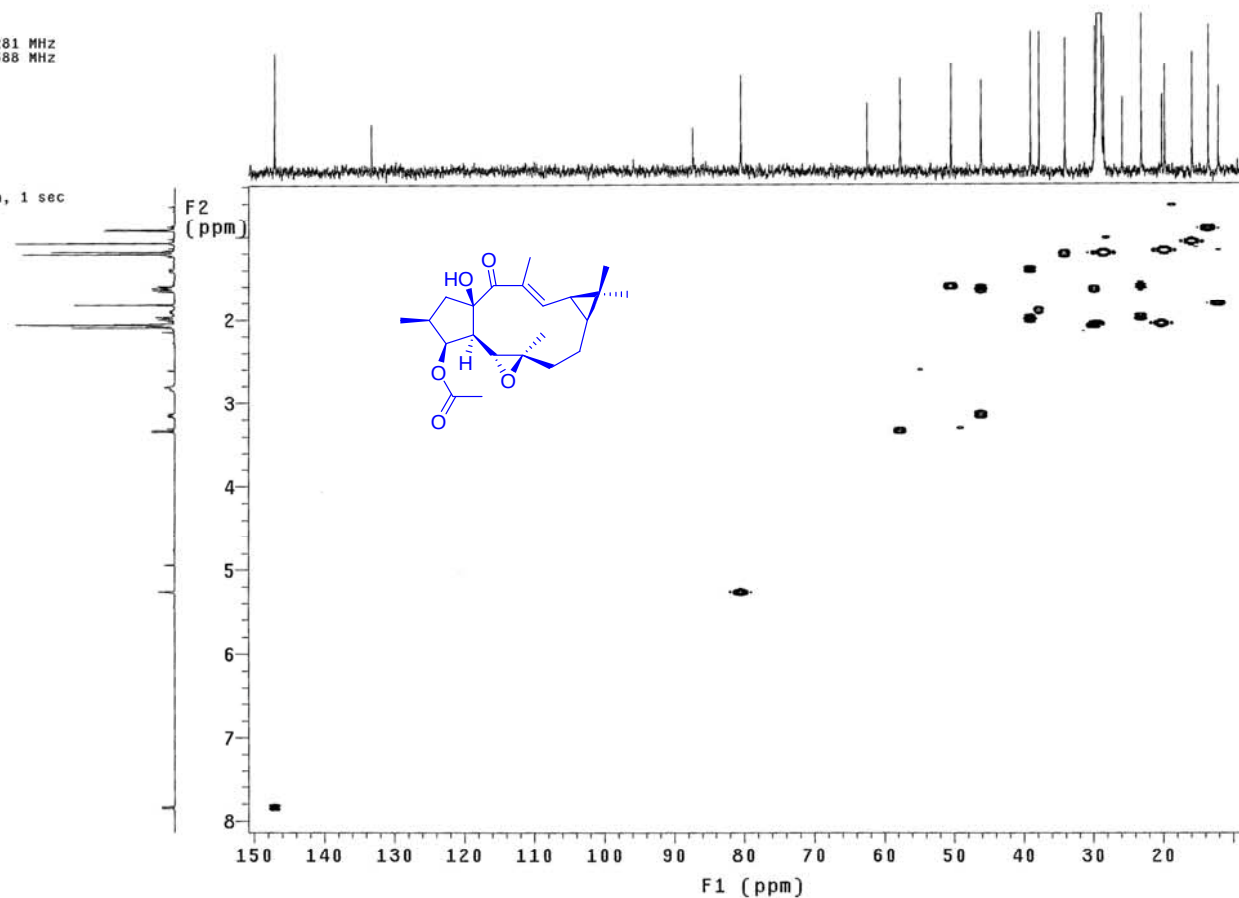


Figure S21. The gHSQC Spectrum of 2 in CD_3COCD_3 (600MHz for ^1H NMR).

VNS-600 gHMBC EM-E-10-16 IN CD3COCD3 2008.09.17

Solvent: acetone
Ambient temperature
Operator: vnmr2
VNMRS-600 "wormhole"

Relax. delay 1.000 sec
Mixing 0.080 sec
Acq. time 0.126 sec
Width 5760.4 Hz
2D Width 32894.7 Hz
128 repetitions
320 increments
OBSERVE H1, 599.6981281 MHz
DATA PROCESSING
Sine bell 0.029 sec
F1 DATA PROCESSING
Sine bell 0.003 sec
FT size 2048 x 8192
Total time 13 hr, 49 min, 46 sec

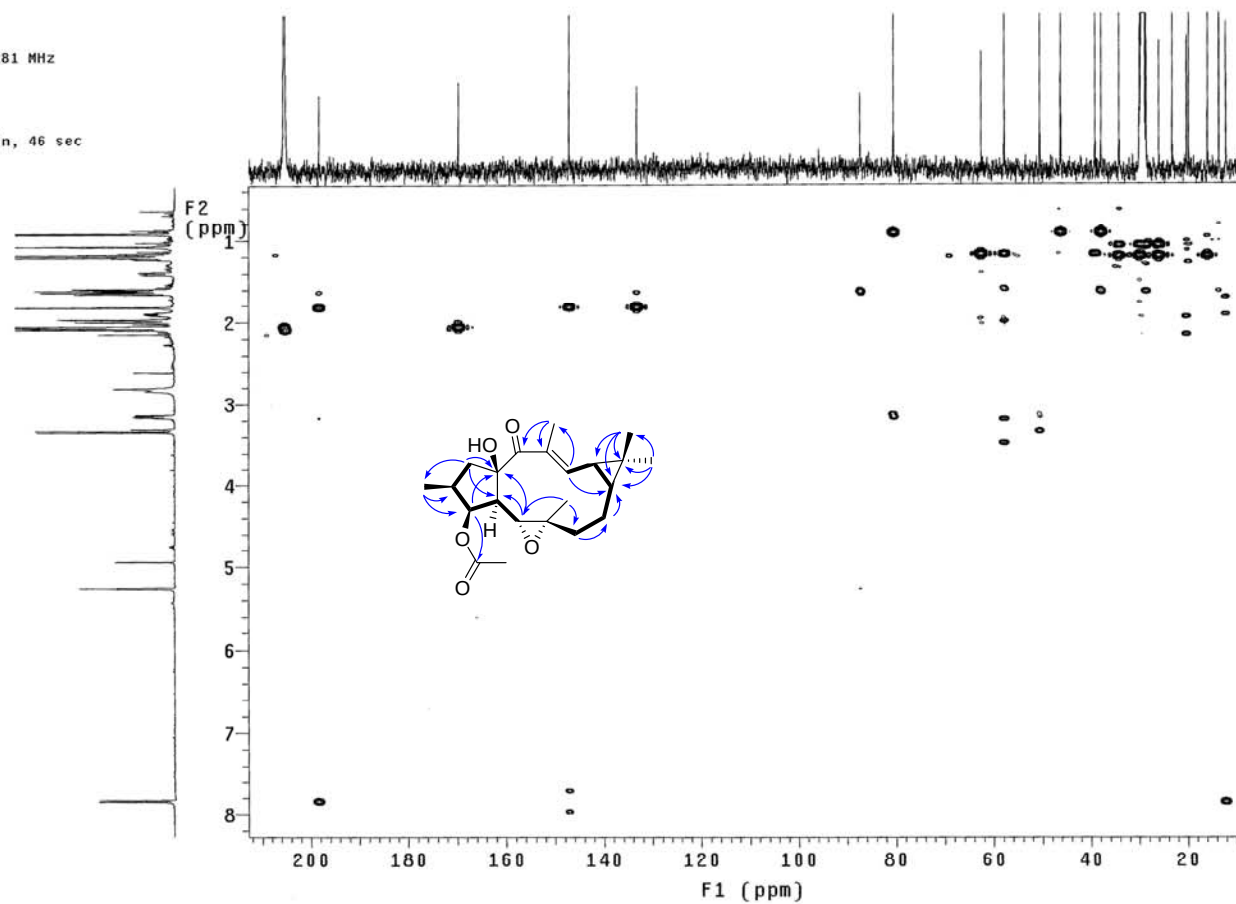


Figure S22. The gHMBC Spectrum of 2 in CD_3COCD_3 (600MHz for ^1H NMR).

VNS-600 NOESY1D EM-E-10-16 IN CD3COCD3 08.10.17

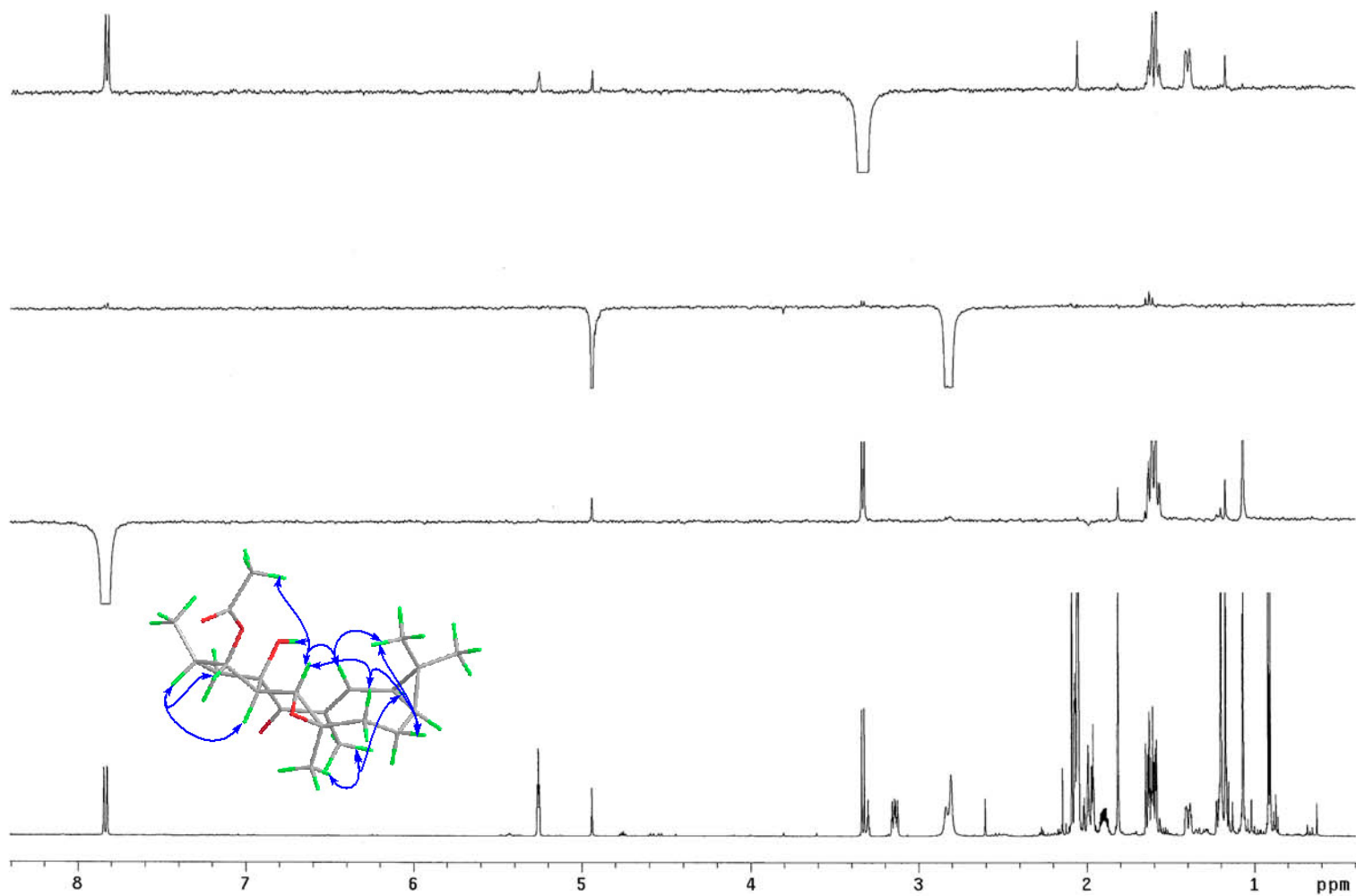


Figure S23. The NOE Difference Spectrum 1 of 2 in CD₃COCD₃ (600 MHz).

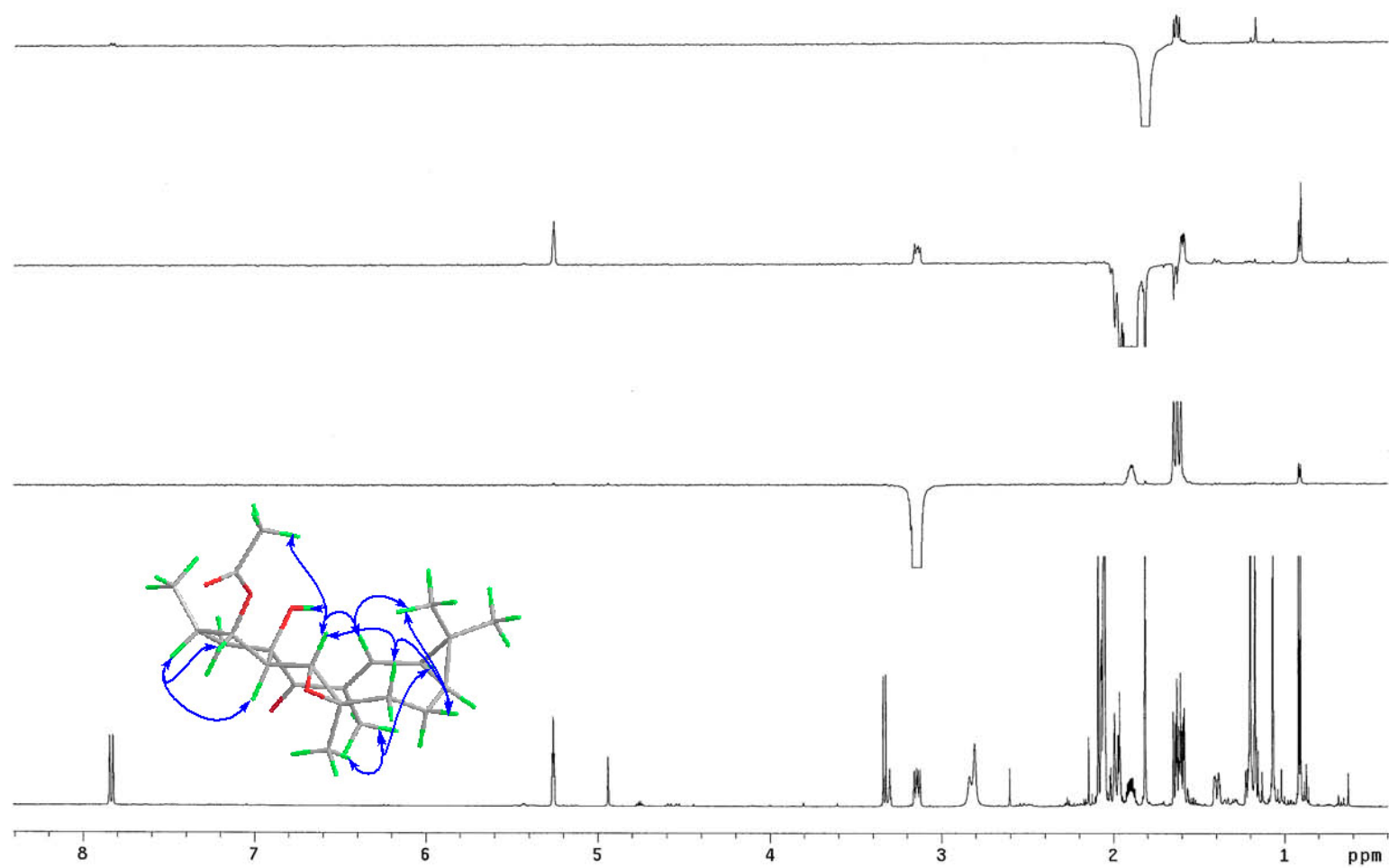


Figure S24. The NOE Difference Spectrum 2 of 2 in CD_3COCD_3 (600 MHz).
S36

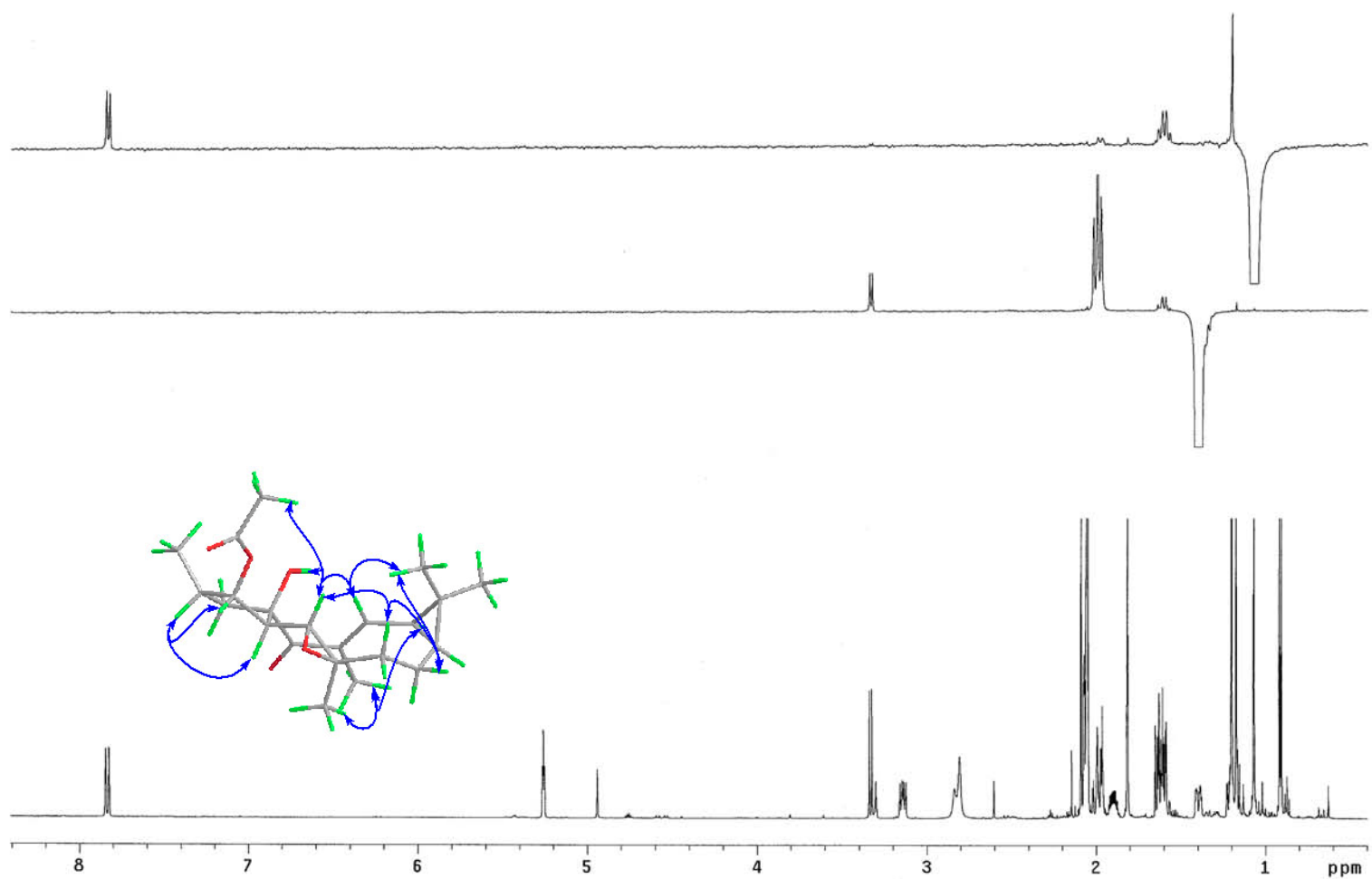


Figure S25. The NOE Difference Spectrum 3 of 2 in CD₃COCD₃ (600 MHz).

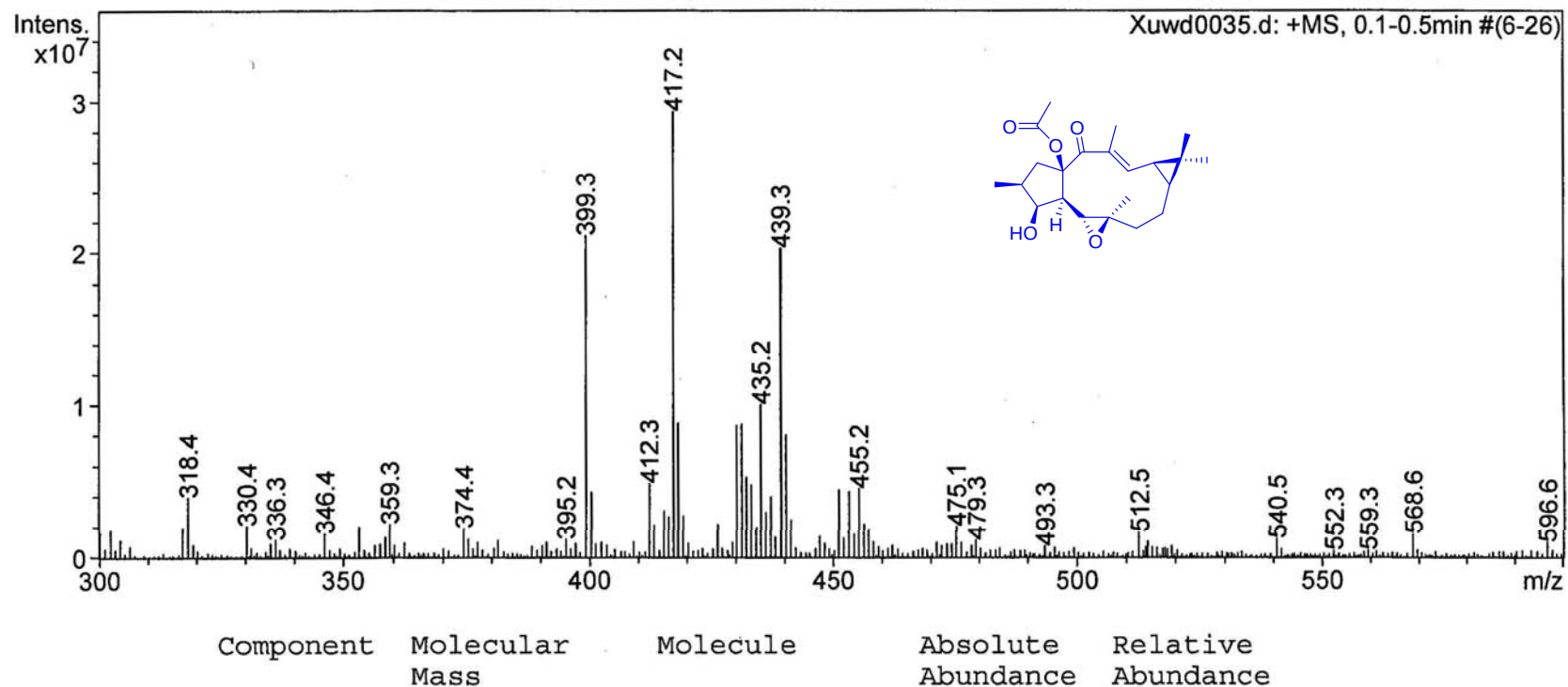
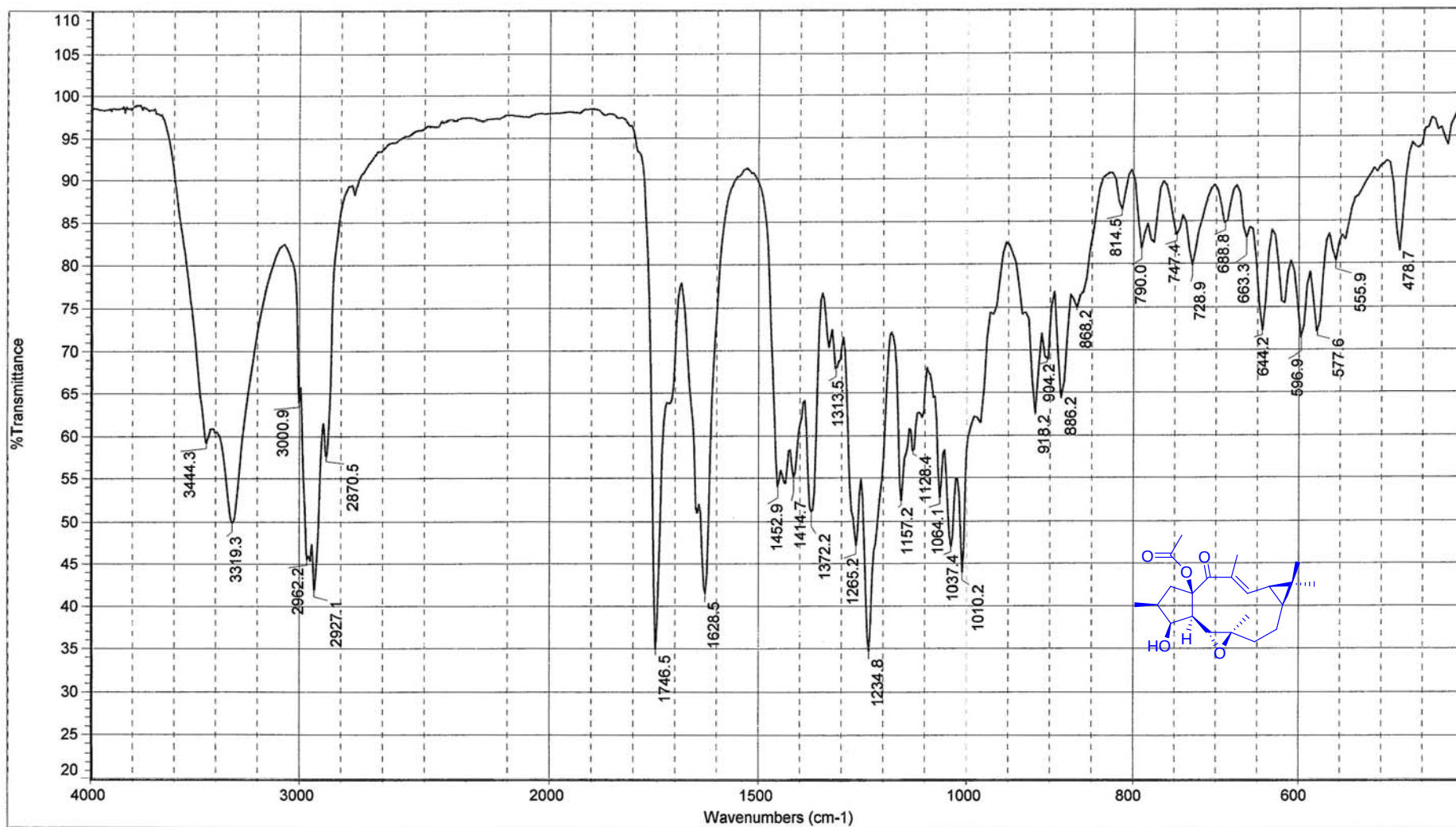


Figure S26. (+)-ESIMS Spectrum of 3.

Peak List

<i>m/z</i>	<i>z</i>	Abund	Formula	Ion
317.21096		28446		
377.23272		59921		
399.21513	1	280189	C ₂₂ H ₃₂ Na O ₅	(M+Na)+
400.21858	1	61003	C ₂₂ H ₃₂ Na O ₅	(M+Na)+
415.18890		51884		
481.21796		18752		
775.43996	1	103704		
776.44317	1	46486		

(+)-HRESIMS Data of 3.



日期: 星期二 10月 07 13:27:11 2008 (GMT+08: Sample Name: EM - E - 12 - 3

(显微镜透射法 FT- IR Microscope Transmission)

扫描次数: 100

傅里叶变换红外显微镜(FT-IR Microscope): Centaurus

分辨率: 8.000

美国热电公司(Thermo)傅里叶变换红外光谱仪:Nicolet 5700

Figure S27. The IR Spectrum of 3.

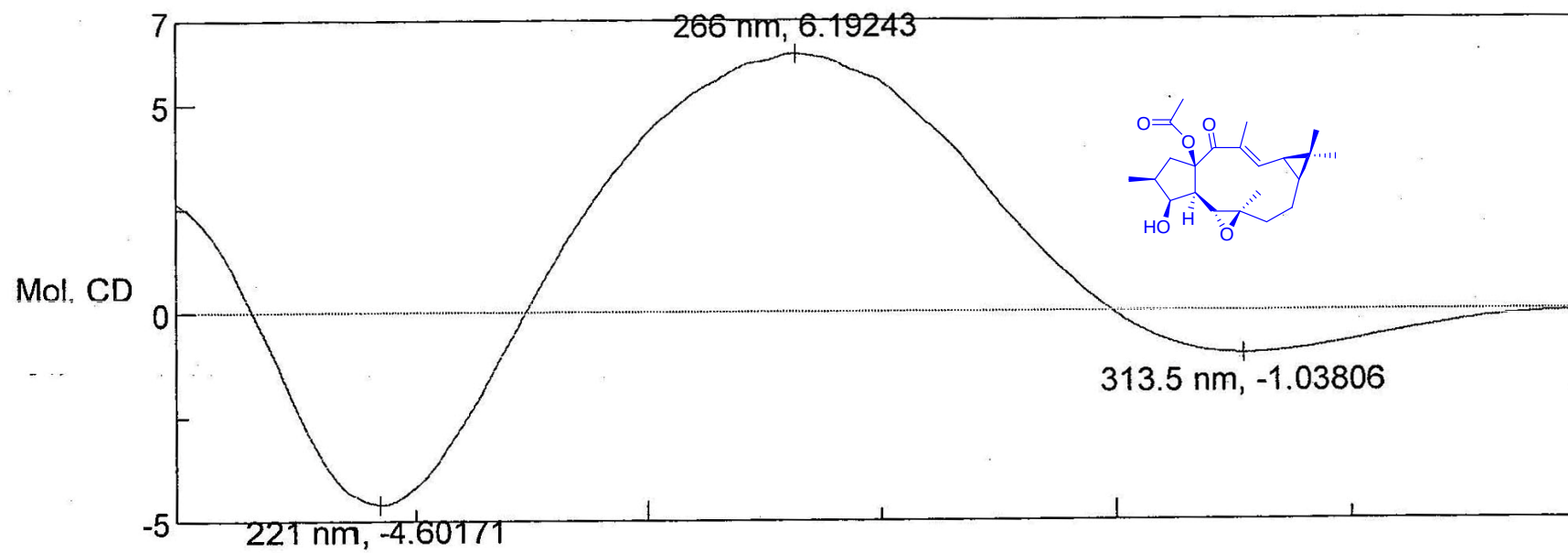


Figure S28. The CD Spectrum of 3.

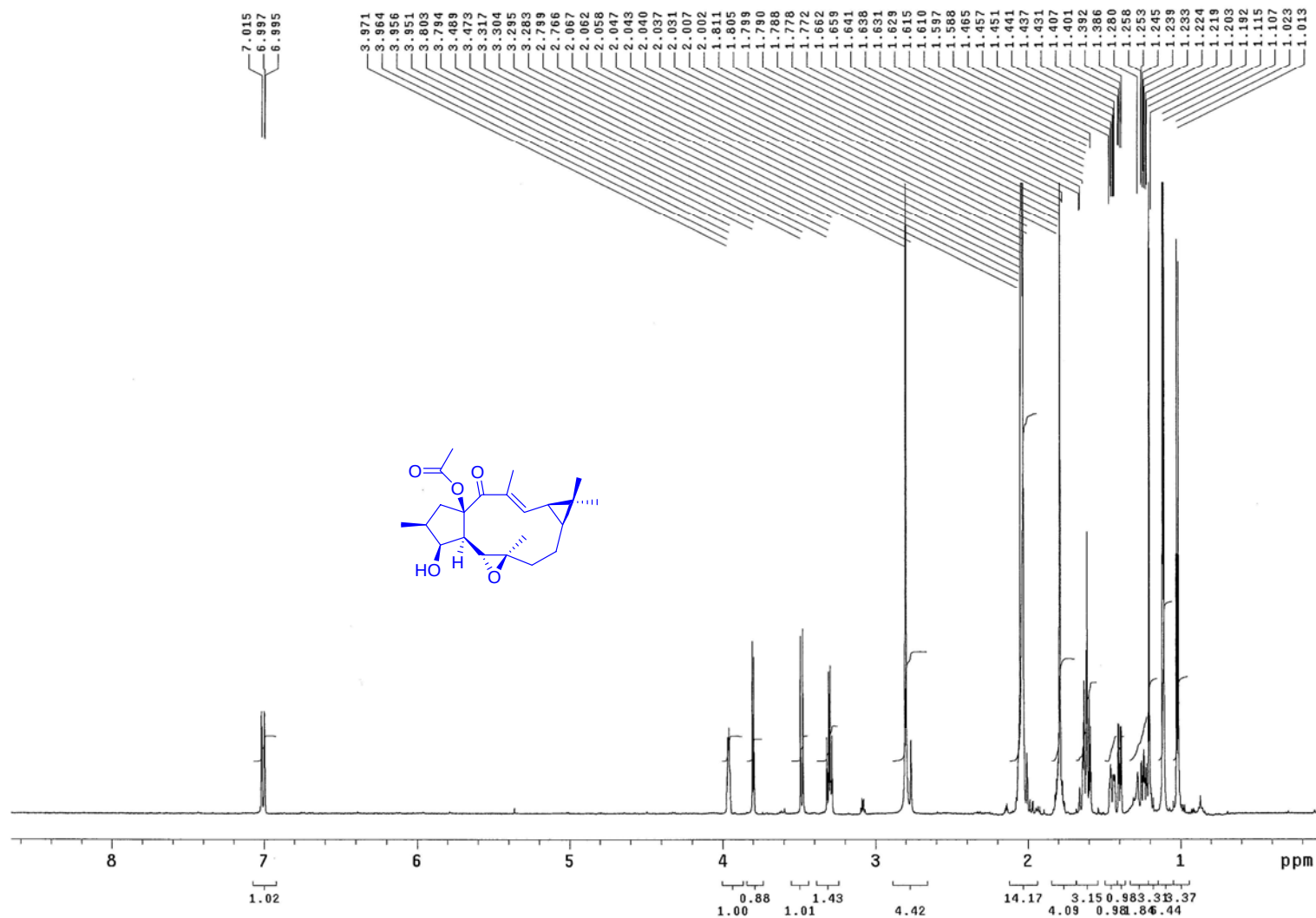


Figure S29. The ^1H NMR Spectrum of 3 in CD_3COCD_3 (600 MHz).

S42

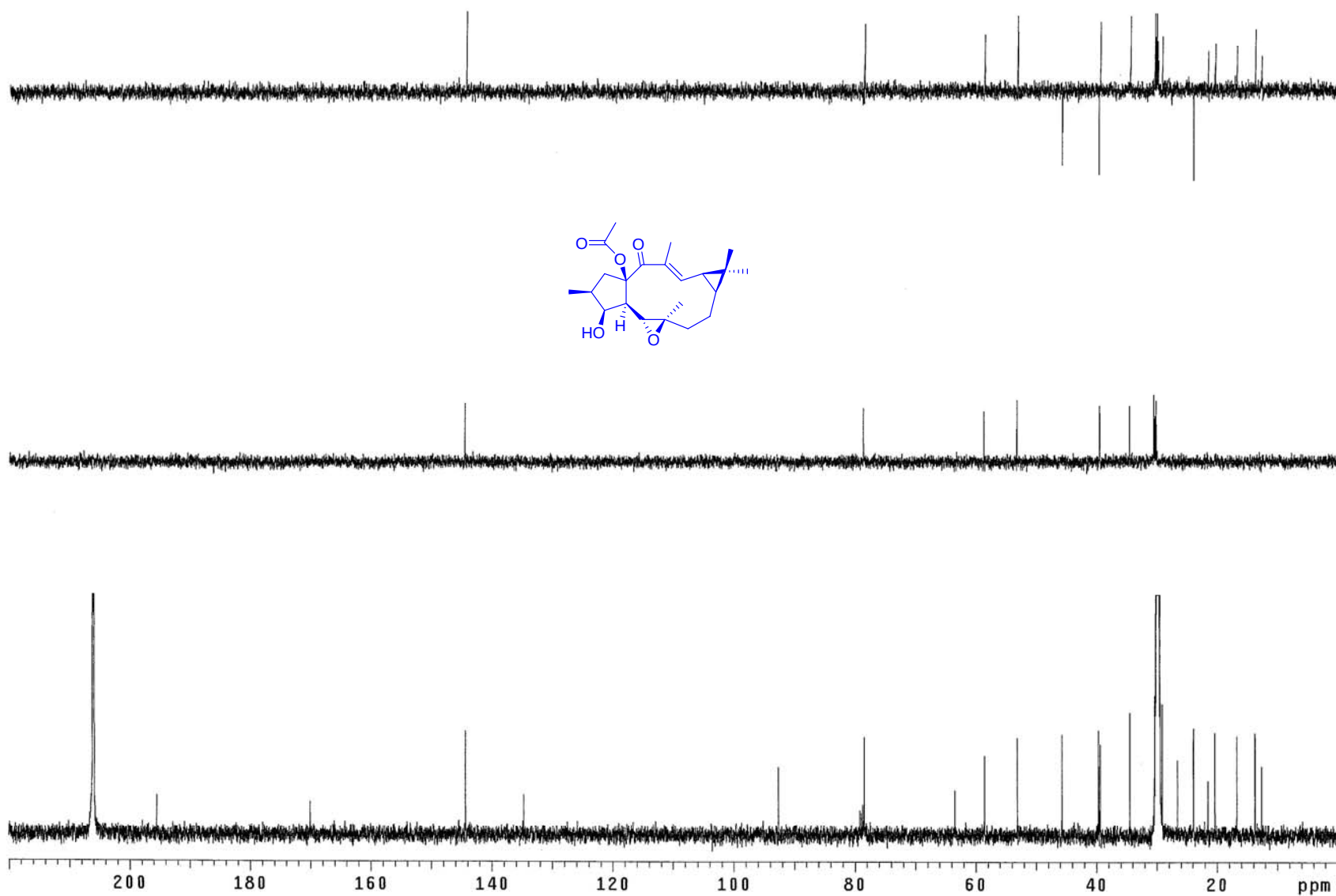


Figure S31. The DEPT Spectrum of 3 in CD₃COCD₃ (150 MHz).

VNS-600 gCOSY EM-E-12-3 IN CD3COCD3 09.04.08

Solvent: acetone
Temp. 25.0 C / 298.1 K
Operator: vnmr2
VNMR-600 "wormhole"

Relax. delay 1.301 sec
Acq. time 0.206 sec
Width 4960.3 Hz
2D Width 4960.3 Hz
4 repetitions
200 increments
OBSERVE H1, 599.6998264 MHz
DATA PROCESSING
Sq. sine bell 0.103 sec
F1 DATA PROCESSING
Sq. sine bell 0.018 sec
FT size 2048 x 2048
Total time 20 min, 56 sec

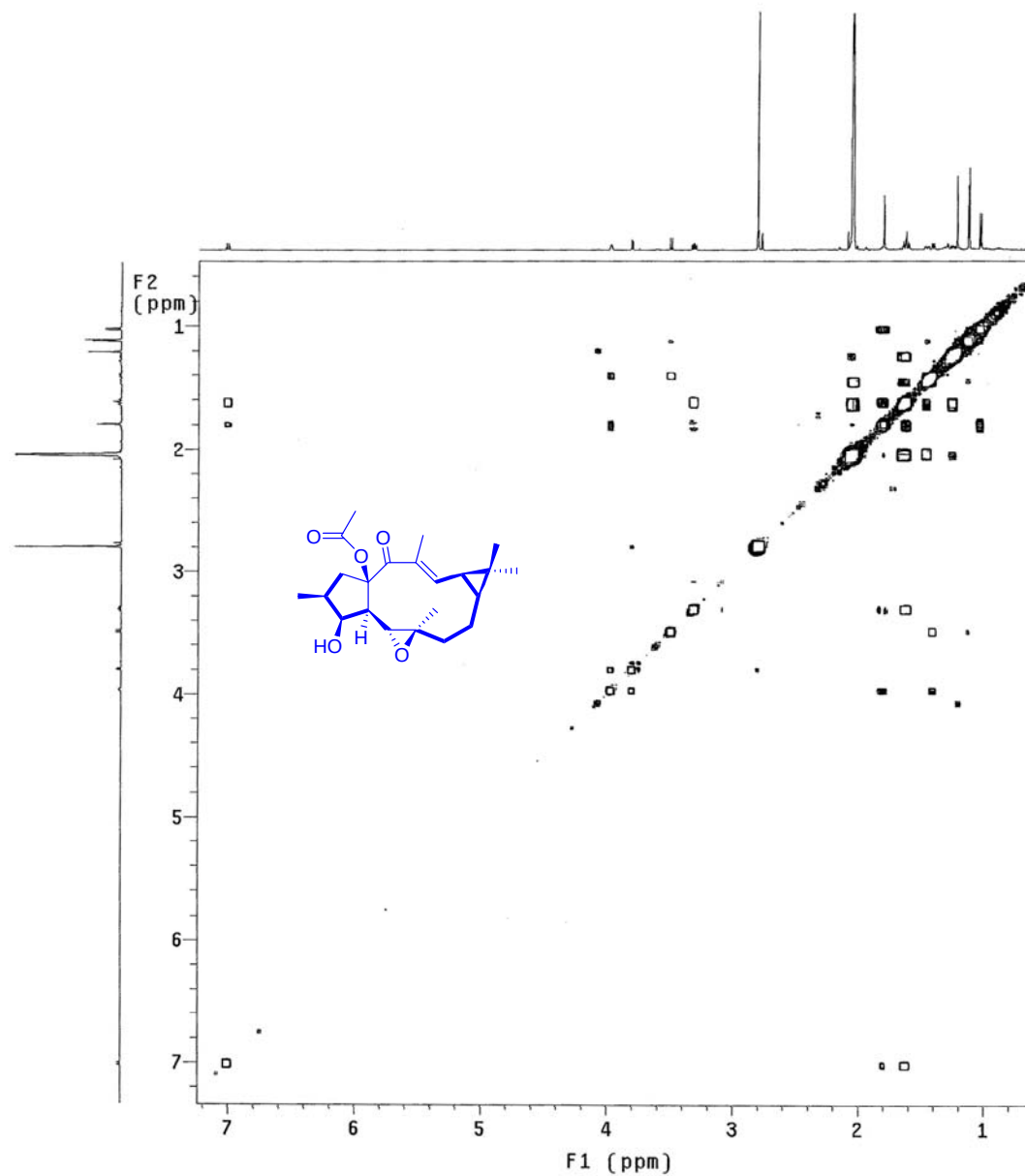


Figure S32. The ^1H - ^1H gCOSY Spectrum of 3 in CD_3COCD_3 (600 MHz).

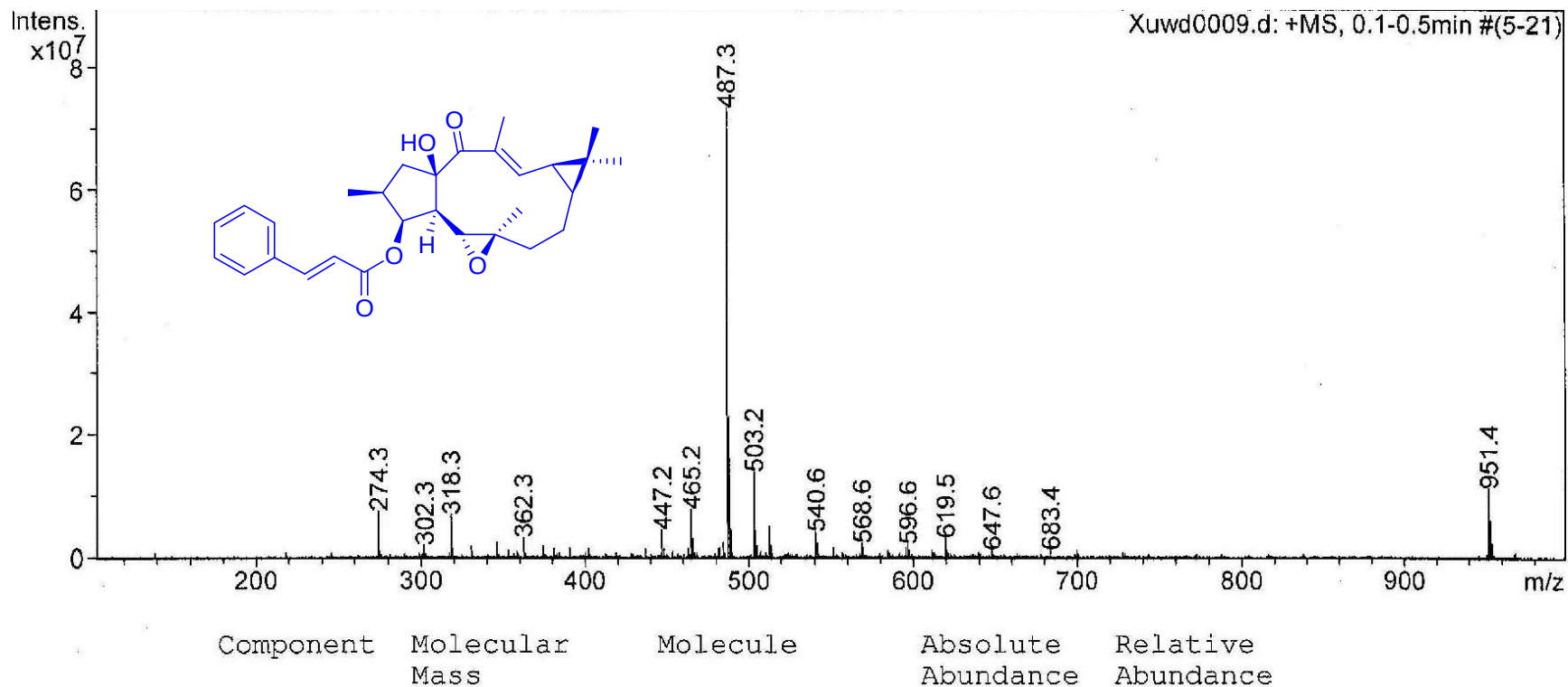


Figure S33. (+)-ESIMS Spectrum of 4.

Data:E_9_6

Sample Name:

Description:

Ionization Mode:ESI+

History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[];Smooth[3];Correct Base[5.0%];Average(MS[...

Acquired:12:00:00 AM

Operator:Accutof

Mass Calibration data:TFA100-2000-P-070410

Created:10/14/2008 10:57:37 AM

Created by:Accutof

Charge number:1

Tolerance:5.00(mmu)

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

Element:¹²C:0 .. 100, ¹H:0 .. 200, ²³Na:1 .. 1, ¹⁶O:0 .. 10

Mass	Mass Difference (mmu)	Mass Difference (ppm)	¹² C	¹ H	²³ Na	¹⁶ O	Unsaturation Number
487.24833	2.28	4.69	29	36	1	5	11.5
	-3.59	-7.37	22	40	1	10	2.5

(+)-HRESIMS Data of 4.

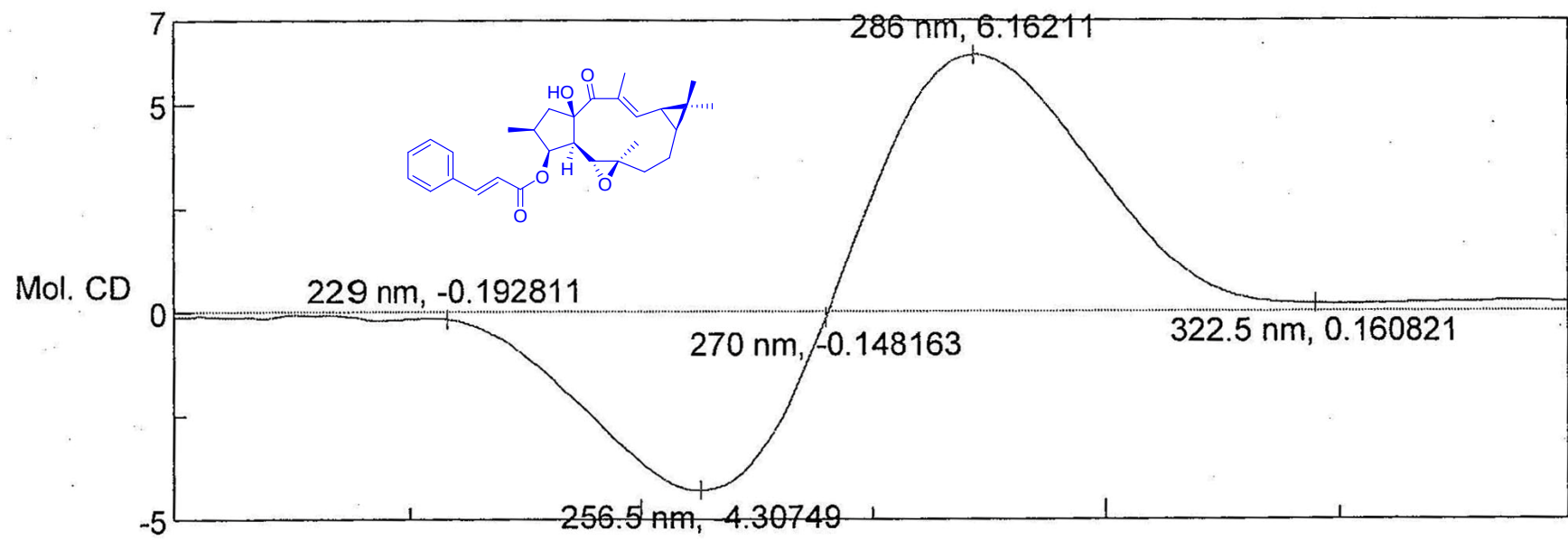
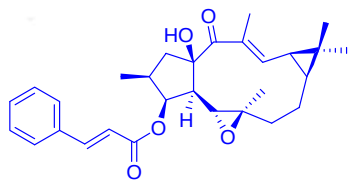


Figure S35 The CD Spectrum of 4.



S48

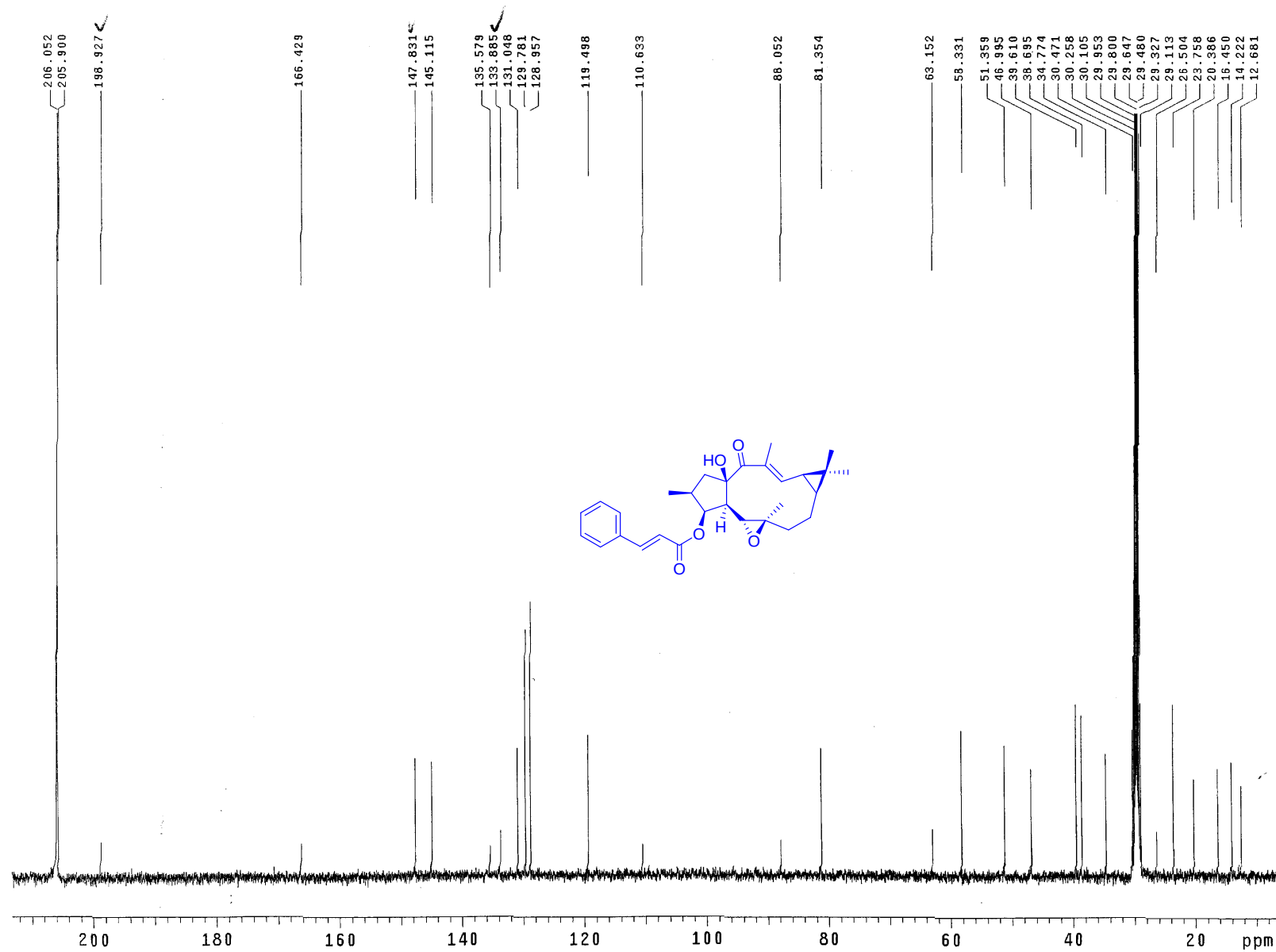


Figure S37. The ^{13}C NMR Spectrum of 4 in CD_3COCD_3 (125 MHz).

Solvent: Acetone
 Temp. 25.0 C / 298.1 K
 INOVA-500 "INM-501"

 Relax. delay 1.000 sec
 Acq. time 0.241 sec
 Width 4255.3 Hz
 2D Width 4255.3 Hz
 8 repetitions
 256 increments
 OBSERVE H1, 499.7728089 MHz
 DATA PROCESSING
 Sine bell 0.120 sec
 F1 DATA PROCESSING
 Sine bell 0.030 sec
 FT size 2048 x 2048
 Total time 44 min, 8 sec

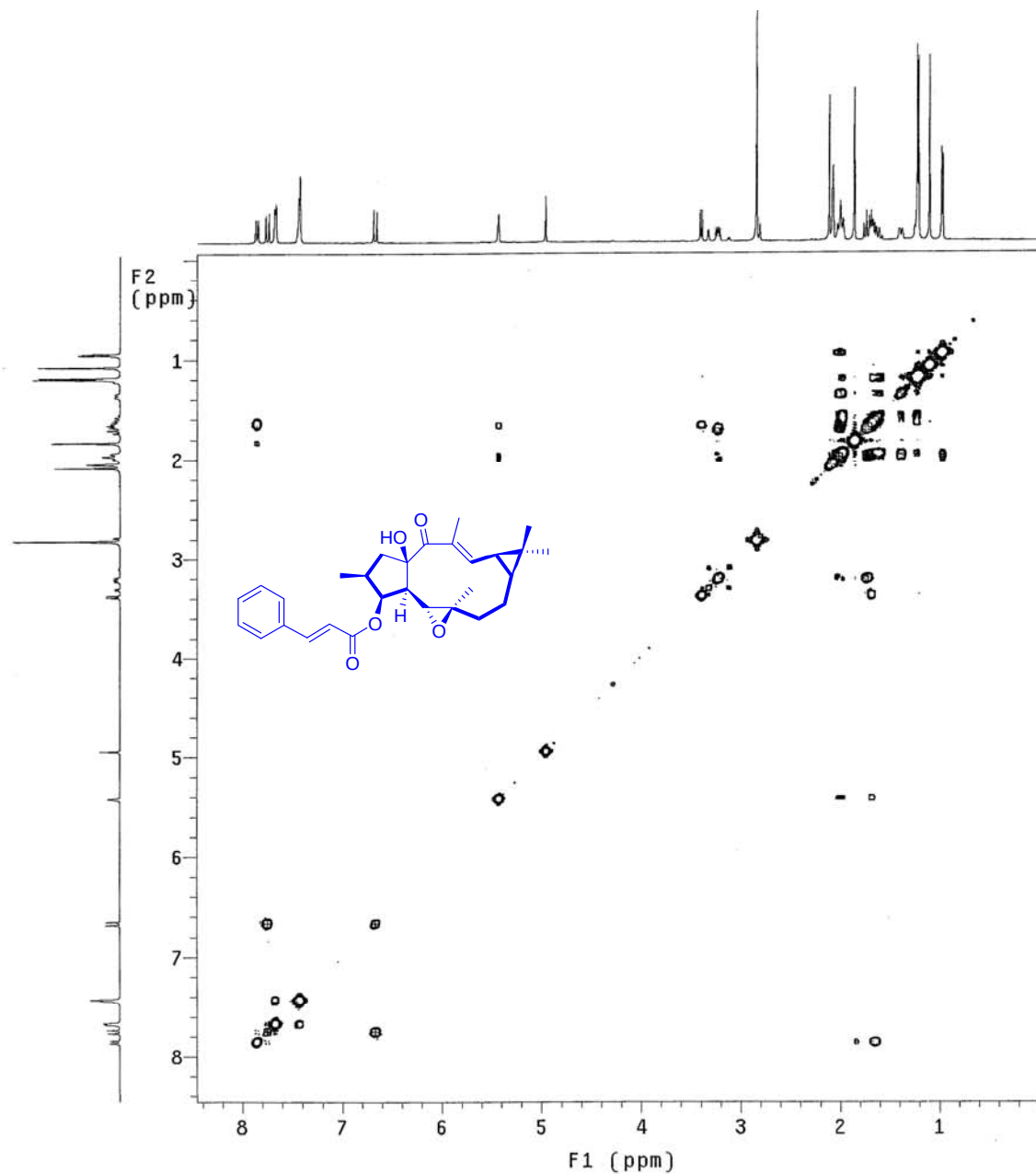


Figure S38. The ^1H - ^1H gCOSY Spectrum of 4 in CD_3COCD_3 (500 MHz).

Solvent: Acetone
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "IMM-501"

Relax. delay 1.000 sec
Acq. time 0.242 sec
Width 4228.8 Hz
2D Width 26586.9 Hz
32 repetitions
256 increments
OBSERVE H1, 499.7728089 MHz
DECOUPLE C13, 125.6813268 MHz
Power 48 dB
on during acquisition
off during delay
GARP-1 modulated
DATA PROCESSING
Sine bell 0.056 sec
F1 DATA PROCESSING
Sine bell 0.005 sec
FT size 2048 x 4096
Total time 3 hr, 17 sec

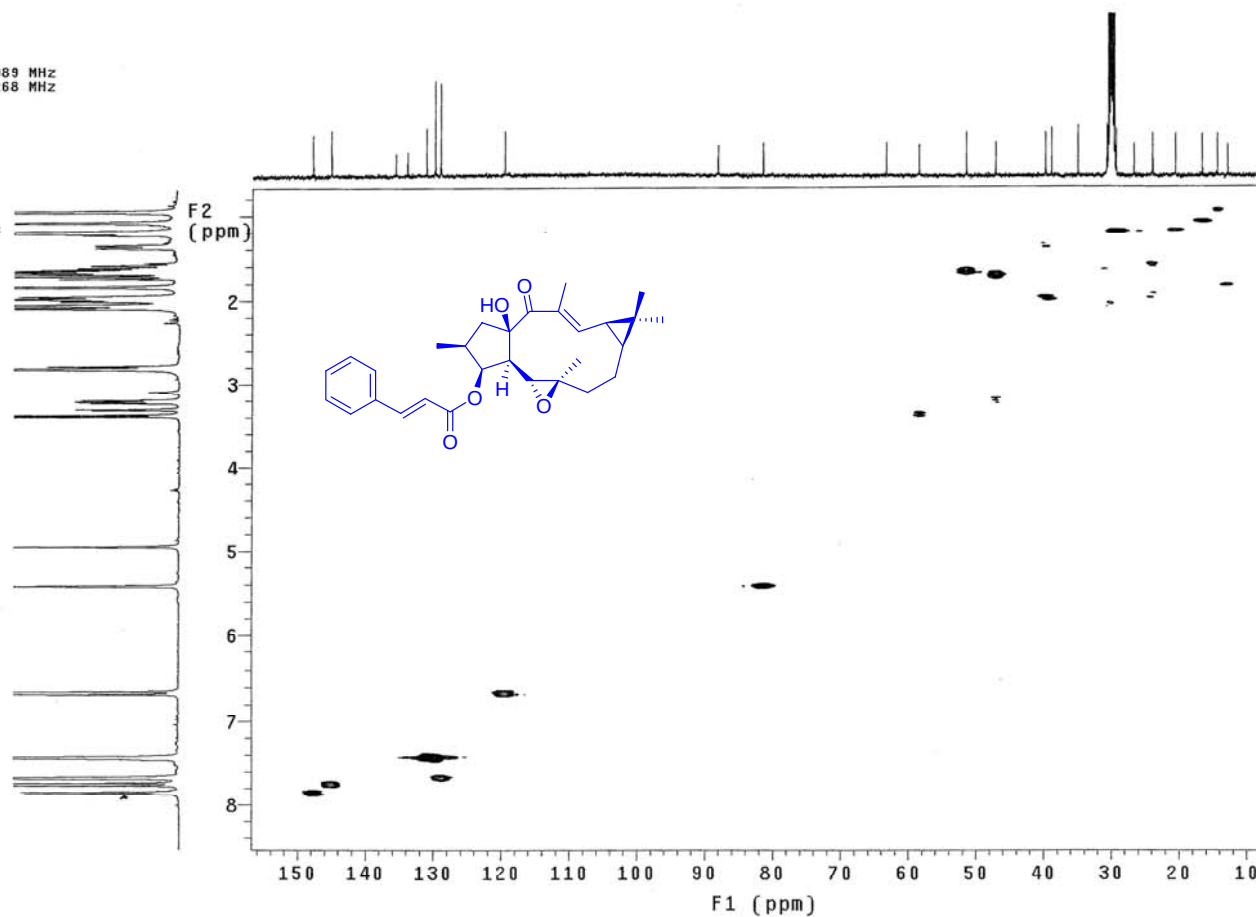


Figure S39. The gHSQC Spectrum of 4 in CD₃COCD₃ (500MHz for ¹H NMR).
S51

Solvent: Acetone
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "IMM-501"

Relax. delay 1.000 sec
Acq. time 0.237 sec
Width 4321.1 Hz
2D Width 27700.8 Hz
80 repetitions
320 increments
OBSERVE H1, 499.7728089 MHz
DATA PROCESSING
Sine bell 0.059 sec
F1 DATA PROCESSING
Sine bell 0.003 sec
FT size 2048 x 4096
Total time 9 hr, 25 min, 49 sec

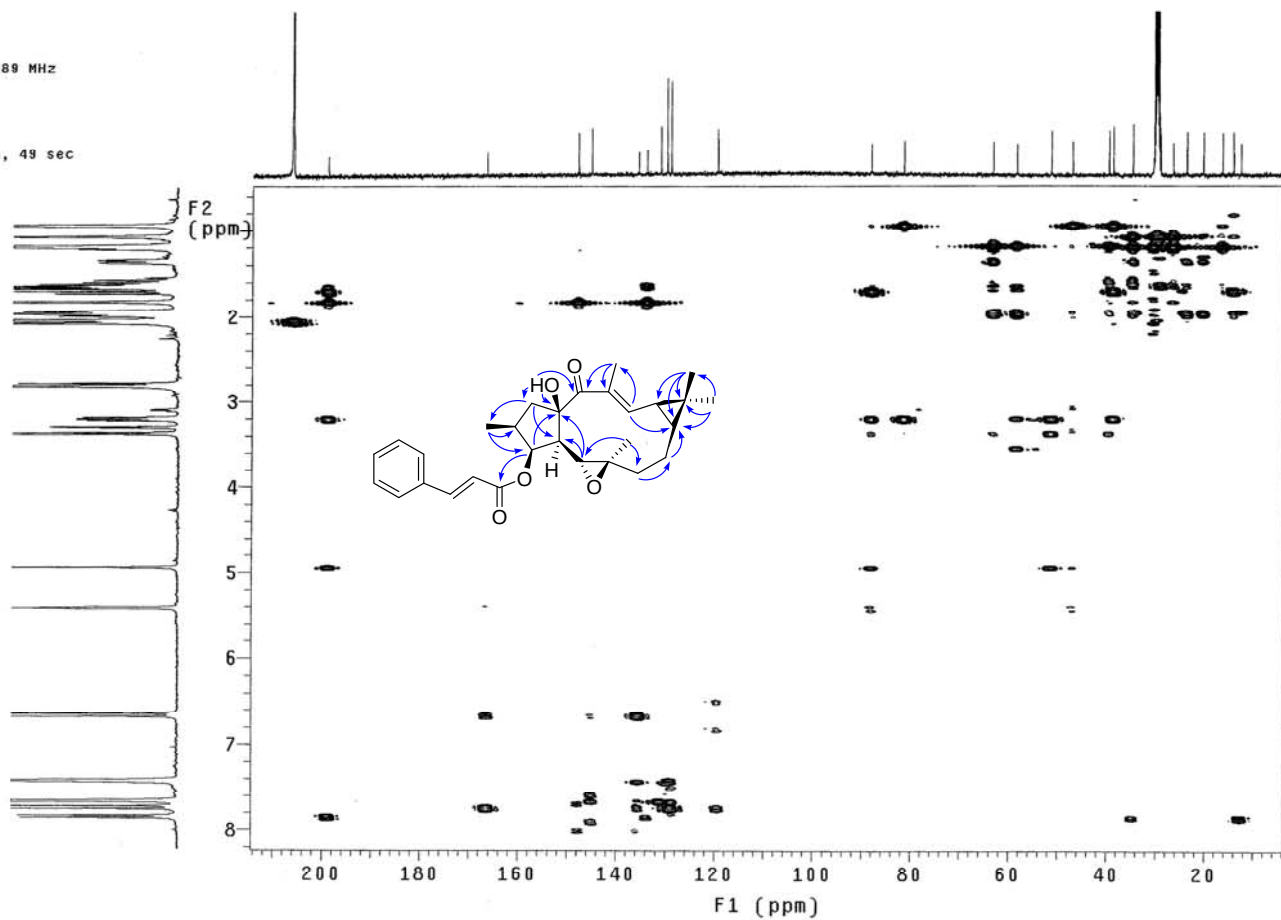


Figure S40. The gHMBC Spectrum of 4 in CD₃COCD₃ (500MHz for ¹H NMR).
S52

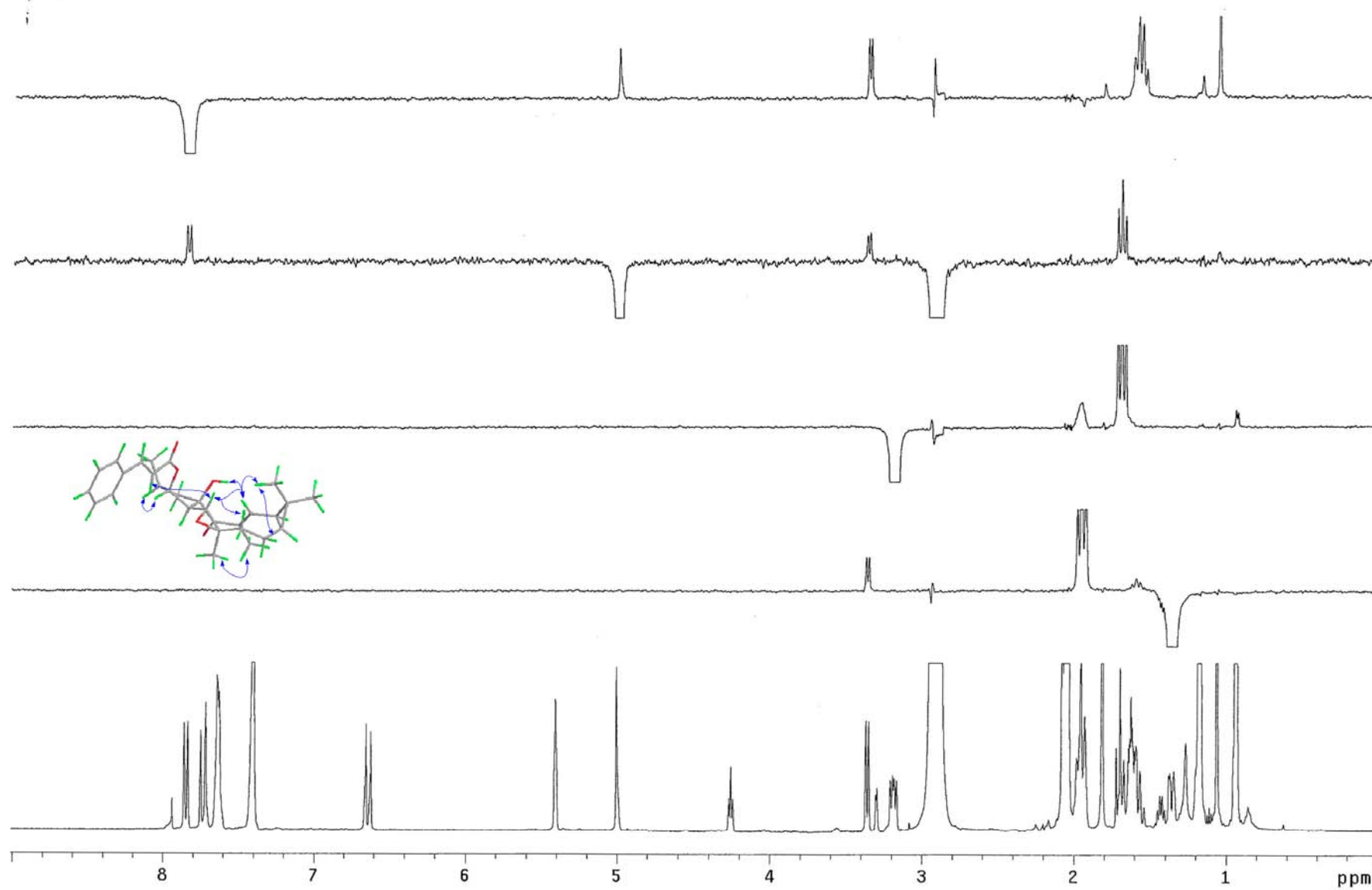


Figure S41. The NOE Difference Spectrum 1 of 4 in CD₃COCD₃ (500 MHz).
S53

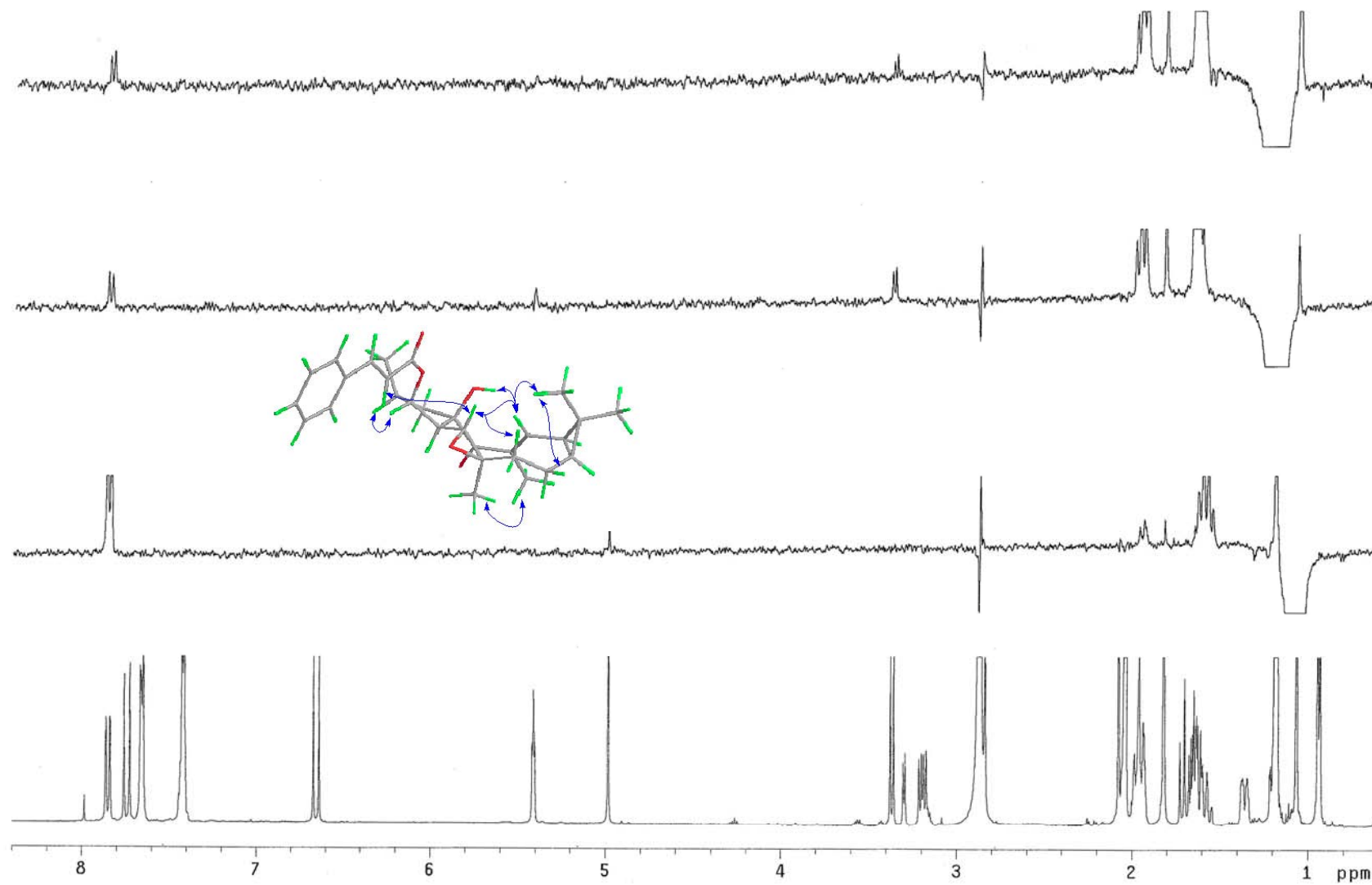


Figure S42. The NOE Difference Spectrum 2 of 4 in CD₃COCD₃ (500 MHz).

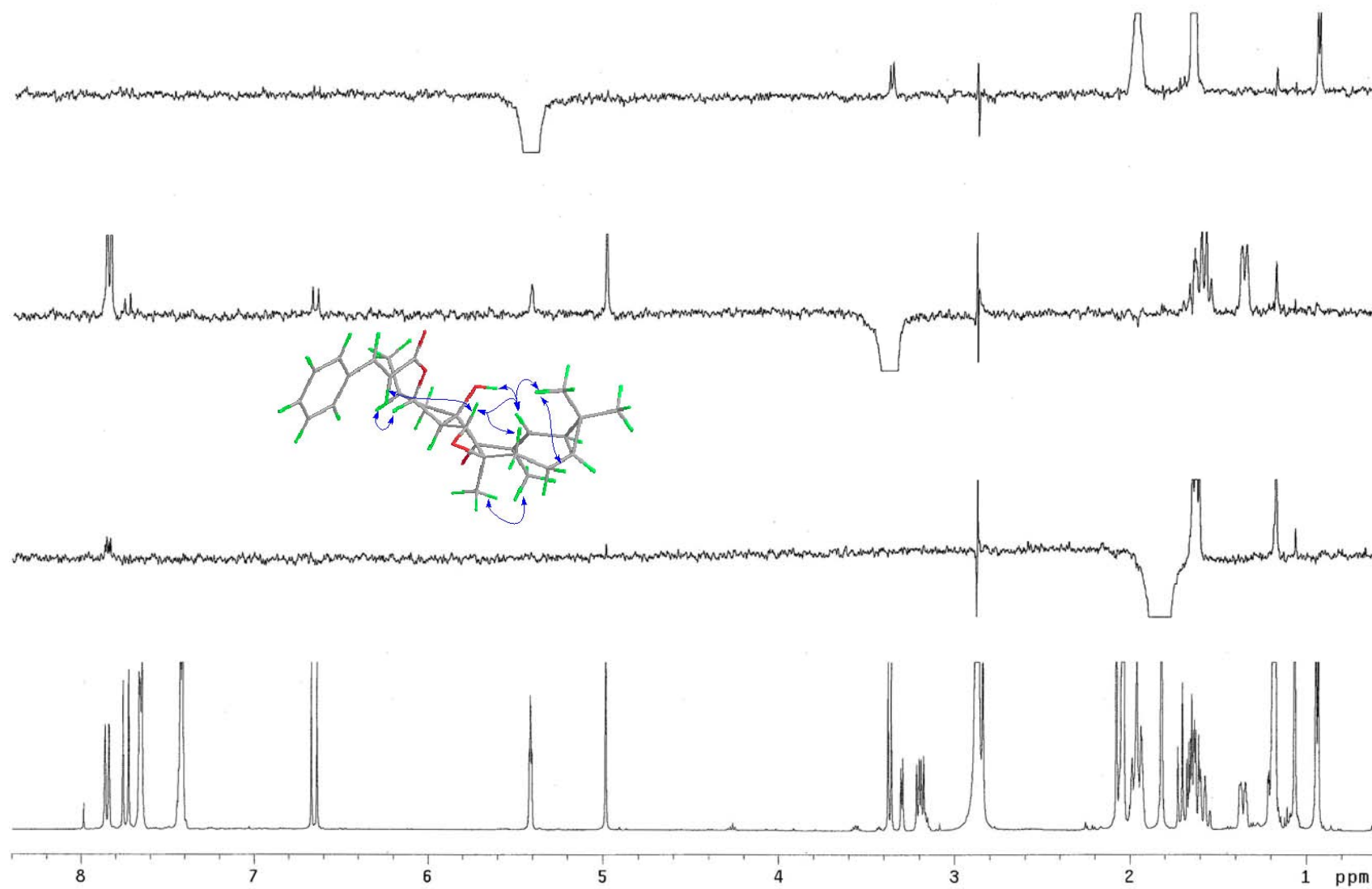
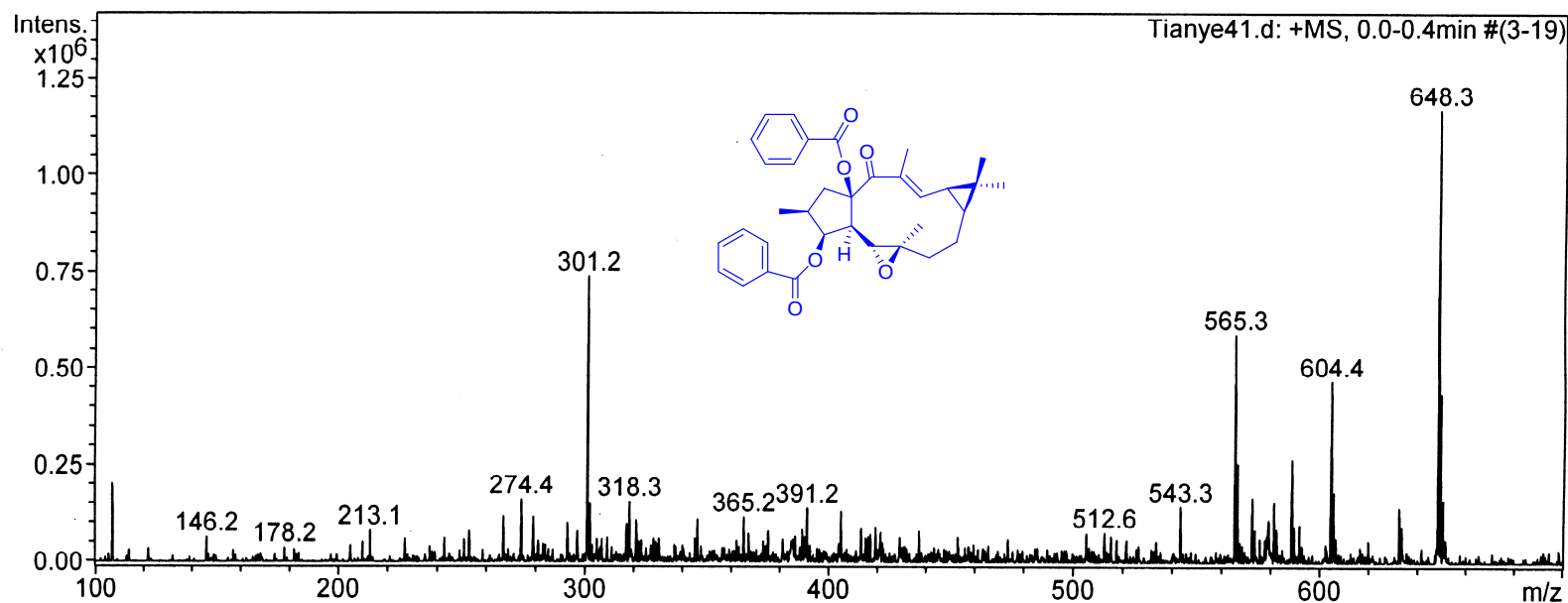


Figure S43. The NOE Difference Spectrum 3 of 4 in CD_3COCD_3 (500 MHz).



Component Molecular Mass Molecule Absolute Abundance Relative Abundance

Figure S44. The (+)-ESIMS Spectrum of 5.

MS Formula Results: + Scan (8.777 min) Sub (201011151.d)

m/z		Ion	Formula	Abundance											
543.2735		(M+H)+	C34 H39 O6	486963.9											
+	Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross S	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Mat	Mass Match	m/z	DBE
	☒	C34 H38 O6	C34 H39 O6	543.2741	99.95		542.2662	542.2668	1.26	1.26	99.94	99.97	99.94	543.2735	16
	☐	C29 H38 N2 O8	C29 H39 N2 O8	543.2701	99.1		542.2662	542.2628	-6.17	6.17	99.04	99.99	98.69	543.2735	12
	☐	C41 H34 O	C41 H35 O	543.2682	97.58		542.2662	542.261	-9.57	9.57	96.77	99.97	96.88	543.2735	25
	☐	C22 H42 N2 O13	C22 H43 N2 O13	543.276	97.16		542.2662	542.2687	4.66	4.66	91.33	99.98	99.25	543.2735	3
m/z		Ion	Formula	Abundance											
565.2546		(M+Na)+	C34 H38 Na O6	1461613.9											
+	Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross S	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Mat	Mass Match	m/z	DBE
	☒	C34 H38 O6	C34 H38 Na O6	565.2561	99.78		542.2655	542.2668	2.56	2.56	99.63	99.93	99.79	565.2546	16
	☐	C29 H38 N2 O8	C29 H38 N2 Na O8	565.252	98.76		542.2655	542.2628	-4.88	4.88	97.02	99.89	99.24	565.2546	12
	☐	C41 H34 O	C41 H34 Na O	565.2502	98.64		542.2655	542.261	-8.28	8.28	98.93	99.92	97.83	565.2546	25
	☐	C22 H42 N2 O13	C22 H42 N2 Na O13	565.2579	95.65		542.2655	542.2687	5.95	5.95	86.78	99.86	98.87	565.2546	3

(+)-HRESIMS Data of 5.

S56

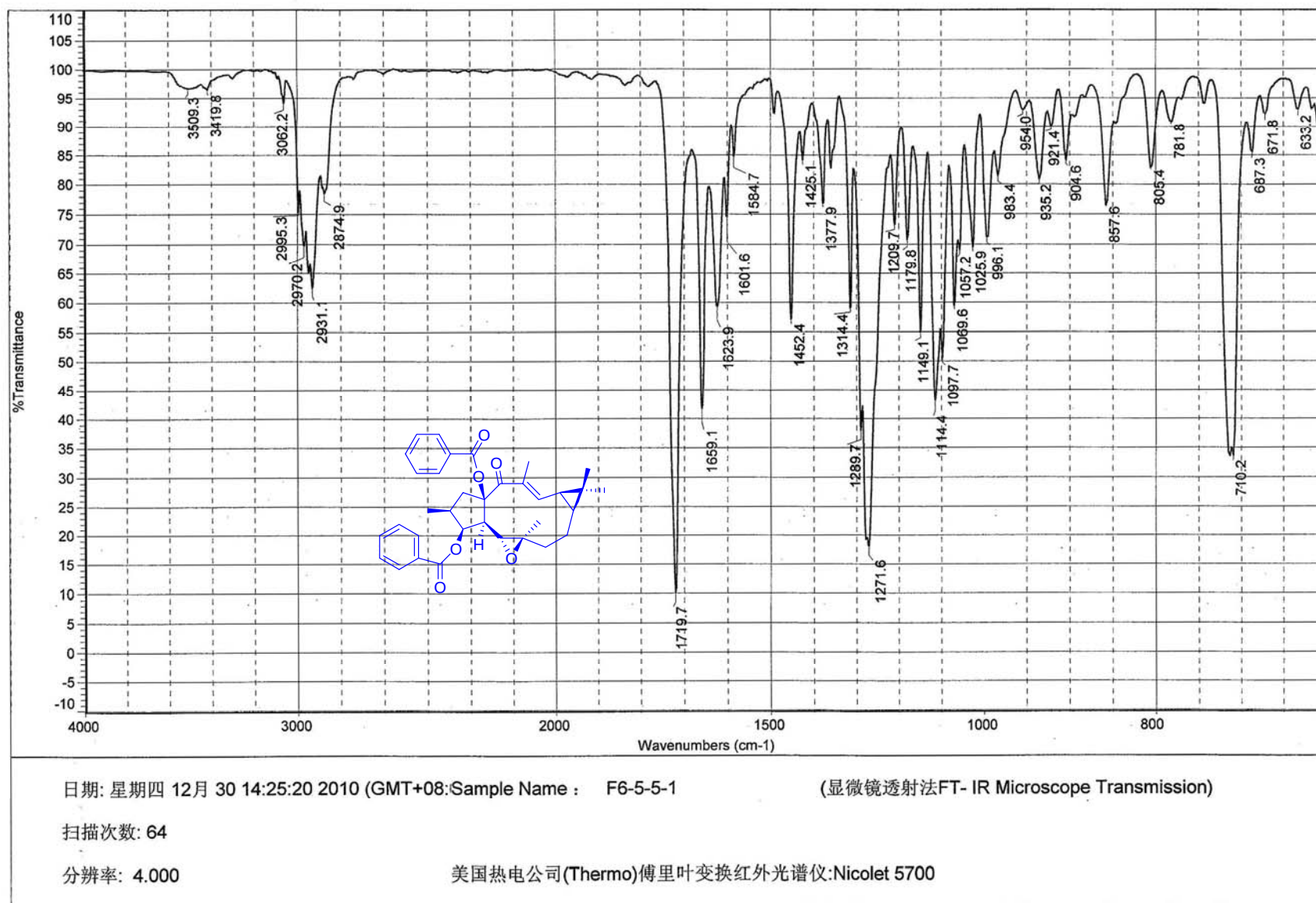


Figure S45. The IR Spectrum of 5.

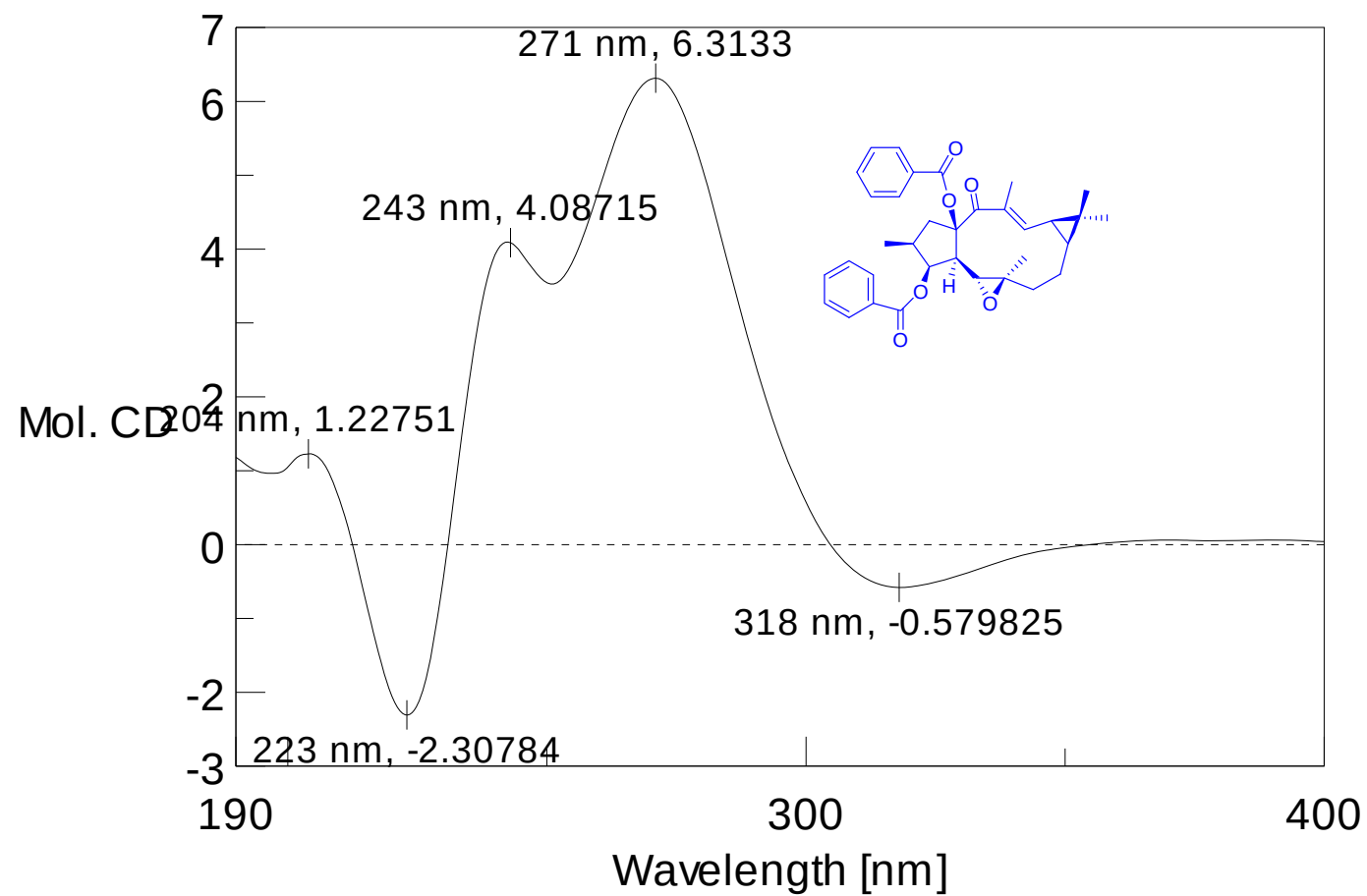


Figure S46. The CD Spectrum 5.

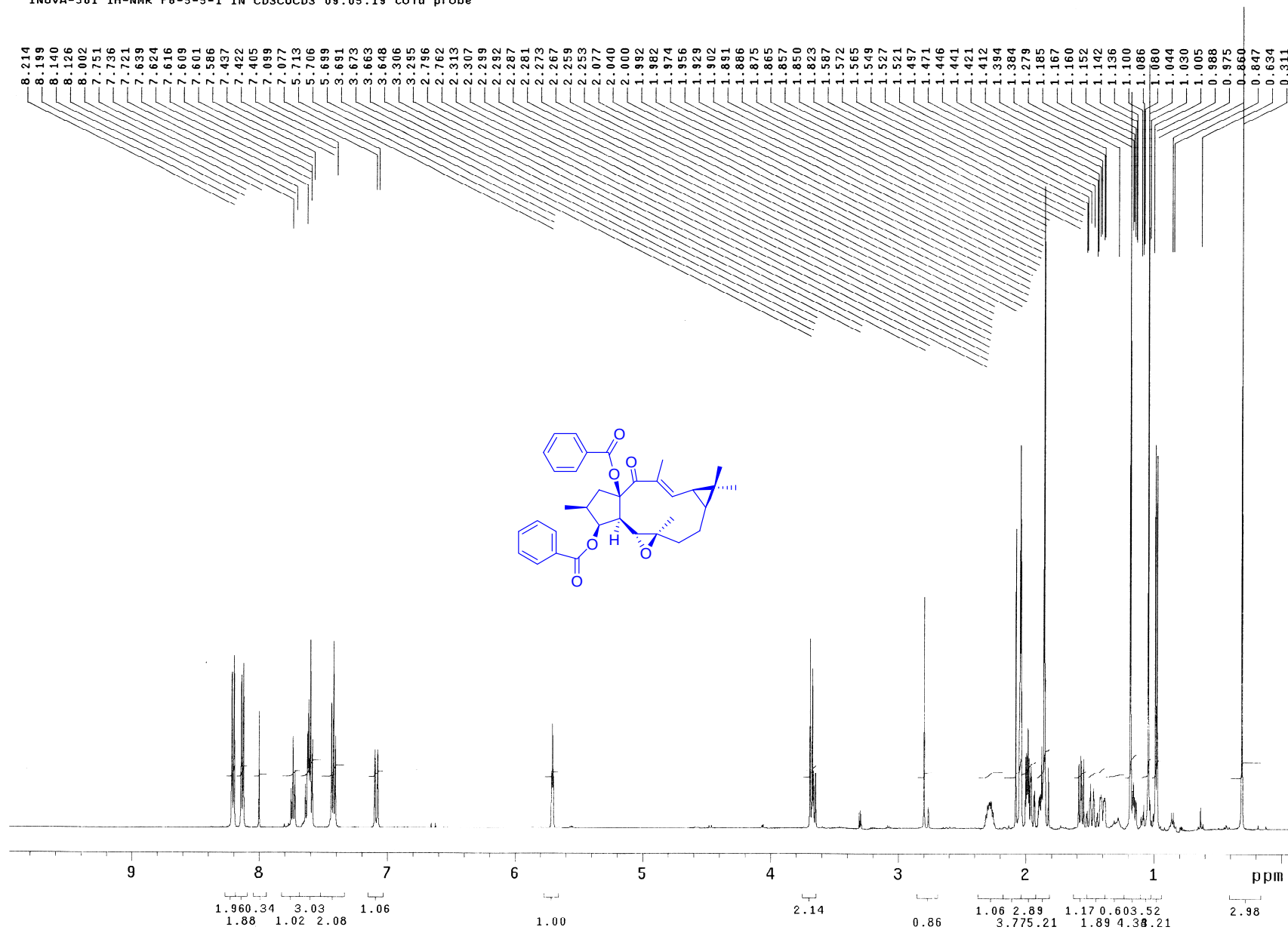


Figure S47. The ^1H NMR Spectrum of 5 in CD_3COCD_3 (500 MHz).

BRUKER AV500-III 13C-NMR F6-5-5-1 IN CD3COCD3 2010.12.10
C13CPD Acetone D:\\ shijiangong 47

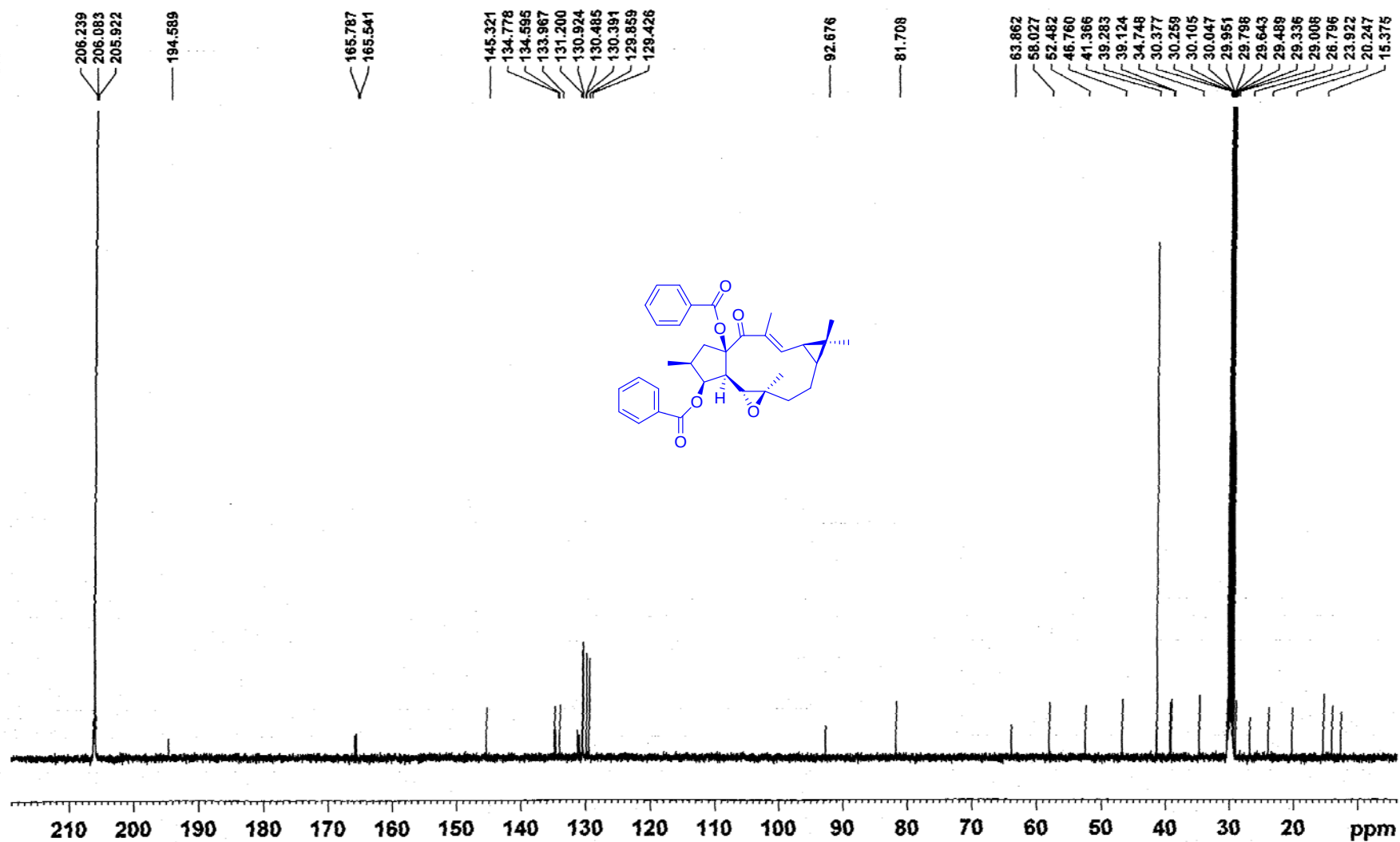
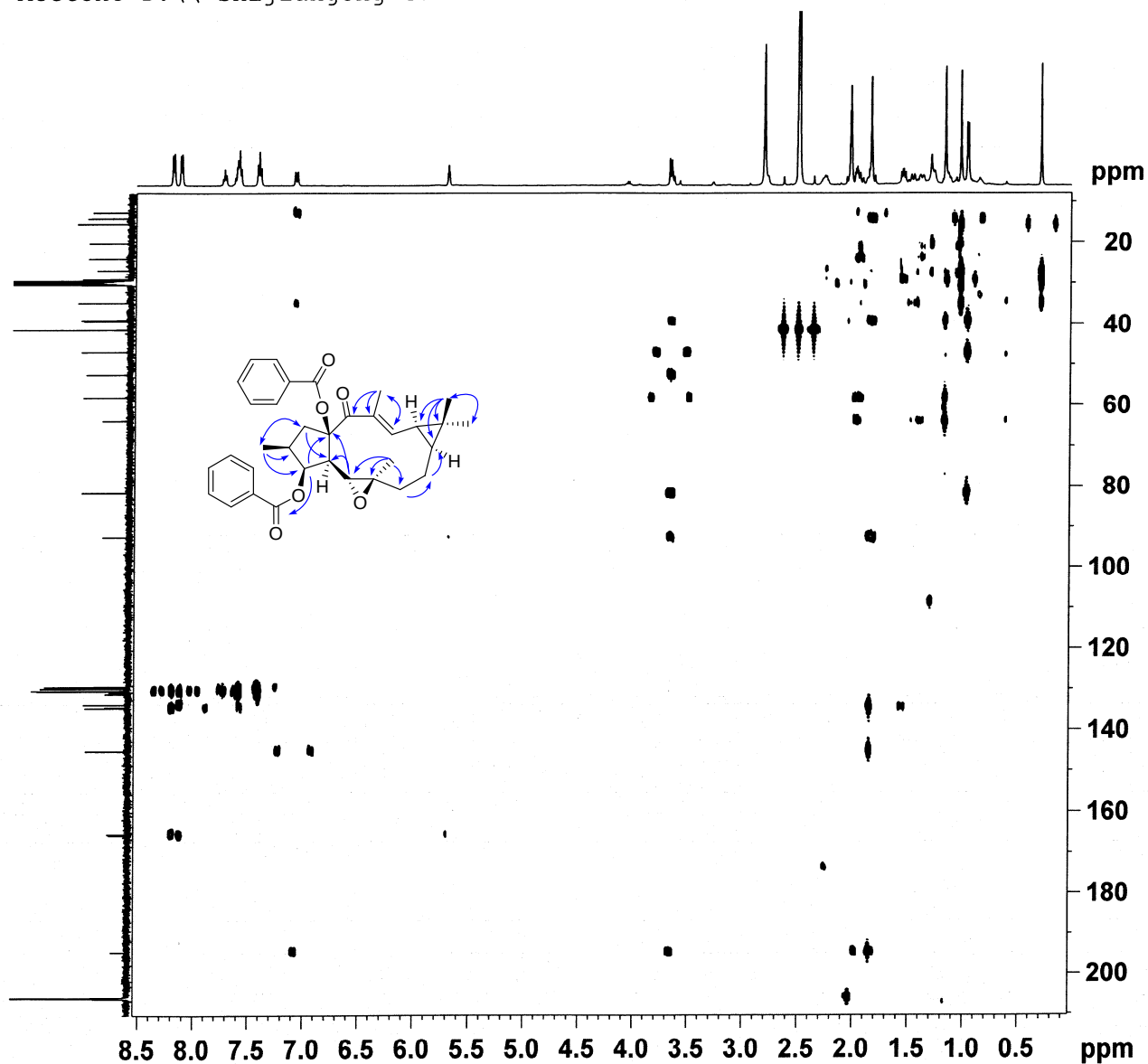


Figure S48. The ^{13}C NMR Spectrum of 5 in CD_3COCD_3 (125 MHz).

BRUKER AV500-III HMBC-NMR F6-5-5-1 IN CD₃COCD₃ 2010.12.10
 HMBCGPNP Acetone D:\\ shijiangong 47



```

NAME      20101210-F6-5-5-1
EXPNO     3
PROCNO    1
Date_     20101210
Time      23.01
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   hmbcgpndqf
TD        4096
SOLVENT   Acetone
NS        32
DS        16
SWH       4587.156 Hz
FIDRES    1.119911 Hz
AQ        0.4465140 sec
RG        203
DW        109.000 usec
DE        6.50 usec
TE        298.3 K
CNST13    8.0000000
D0        0.00000300 sec
D1        0.86073601 sec
D6        0.06250000 sec
D16       0.00020000 sec
IN0       0.00001655 sec

===== CHANNEL f1 =====
NUC1      1H
P1        14.60 usec
P2        29.20 usec
PL1       2.00 dB
PL1W      12.39386463 W
SFO1      500.0621246 MHz

===== CHANNEL f2 =====
NUC2      13C
P3        10.00 usec
PL2       0.90 dB
PL2W      73.29839325 W
SFO2      125.7552758 MHz

===== GRADIENT CHANNEL =====
GPNAM1    SINE.100
GPNAM2    SINE.100
GPNAM3    SINE.100
GPZ1      50.00 %
GPZ2      30.00 %
GPZ3      40.10 %
P16       1000.00 usec
ND0       2
TD        128
SFO1      125.7553 MHz
FIDRES    235.791138 Hz
SW        240.000 ppm
FnMODE    QF
SI        1024
SF        500.0600173 MHz
WDW       SINE
SSB       0
LB        0.00 Hz
GB        0
PC        1.40
SI        1024
MC2       QF
SF        125.7400808 MHz
WDW       SINE
SSB       0
LB        0.00 Hz
GB        0
  
```

Figure S49. The gHMBC Spectrum of **5** in CD₃COCD₃ (500 MHz for ¹H NMR).

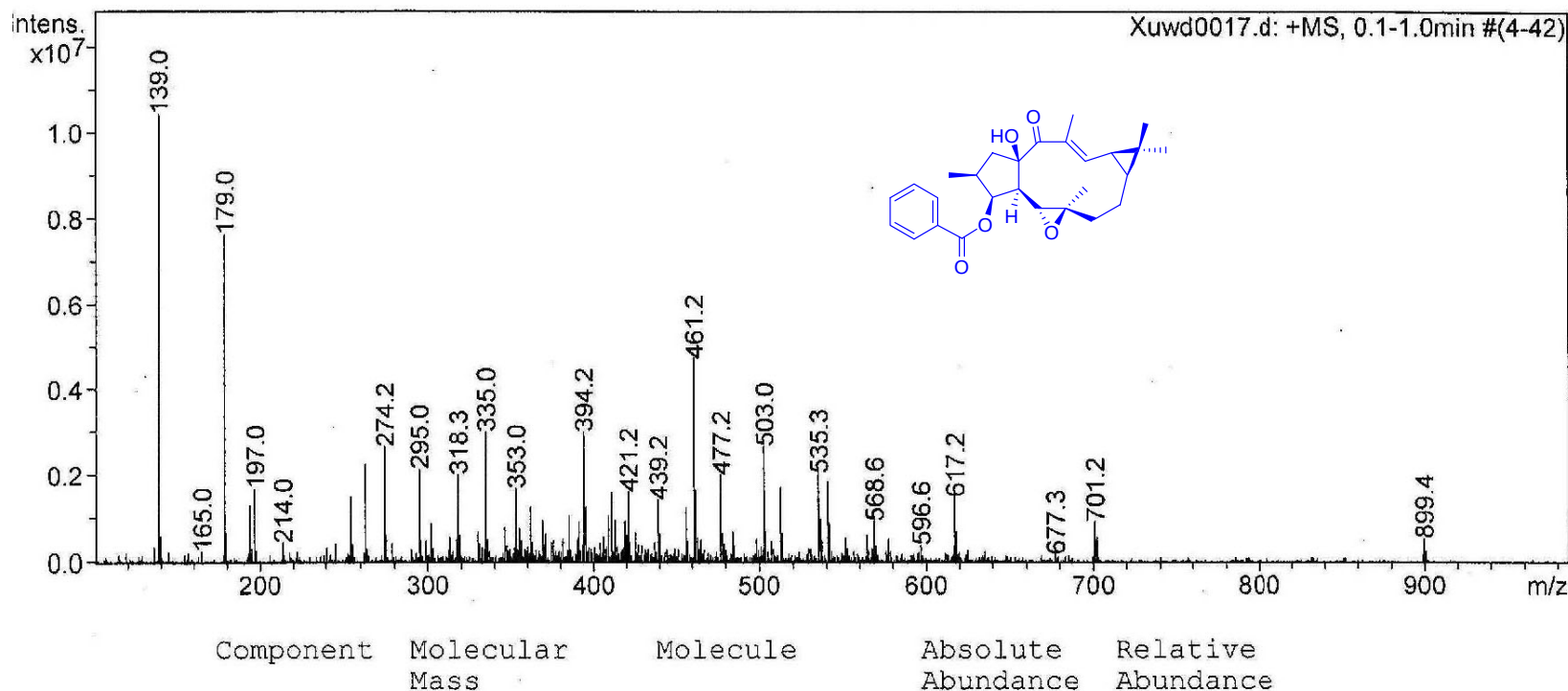


Figure S50. (+)-ESIMS Spectrum of 6.

Data:EM_9_23

Sample Name:

Description:

Ionization Mode:ESI+

History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[];Smooth[3];Correct Base[5.0%];Average(MS[...

Acquired:10/14/2008 11:13:47 AM

Operator:Accutof

Mass Calibration data:TFA100-2000-P-070410

Created:10/14/2008 11:28:36 AM

Created by:Accutof

Charge number:1

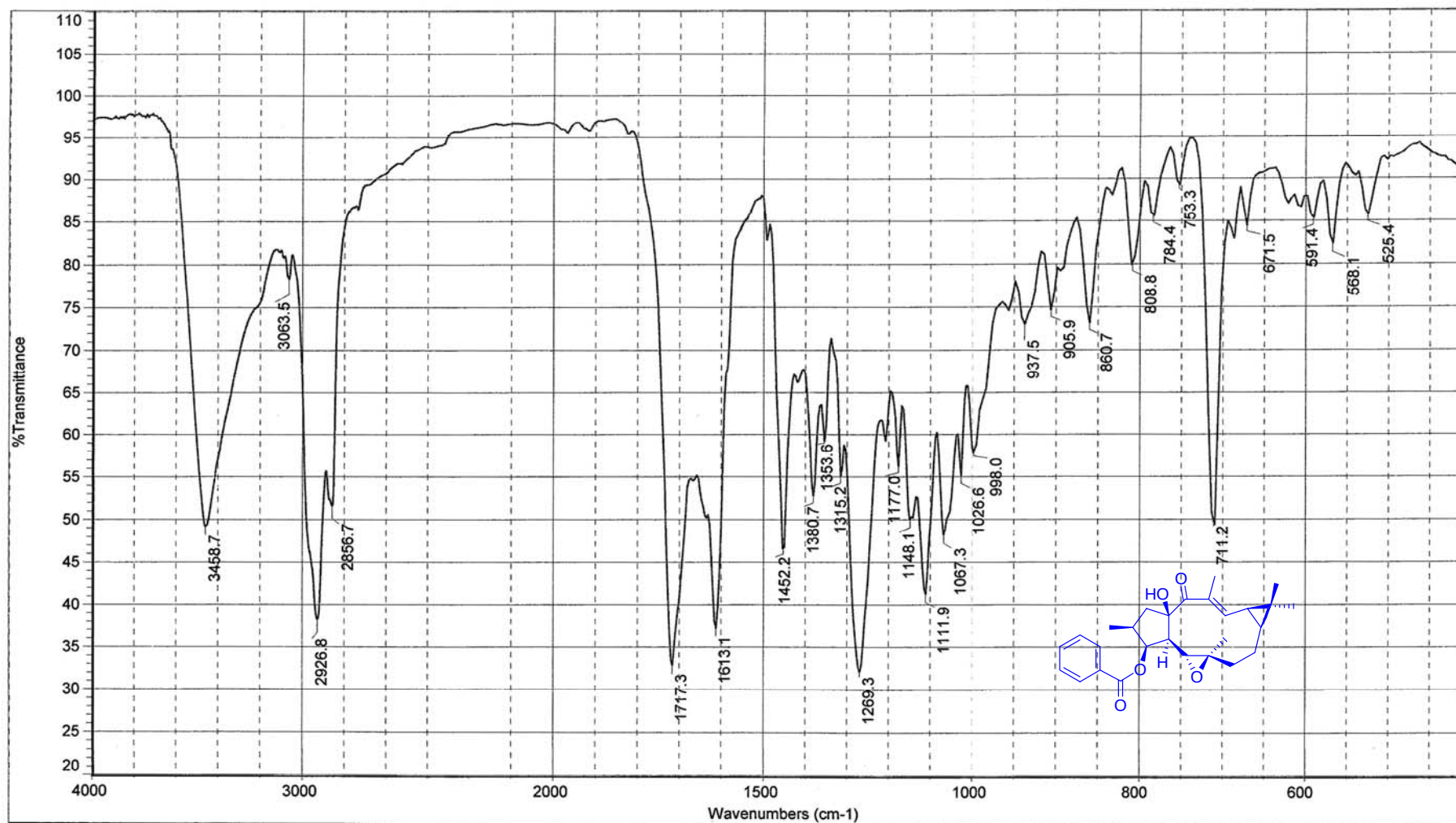
Tolerance:5.00(mmu)

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

Element:¹²C:0 .. 100, ¹H:0 .. 200, ²³Na:1 .. 1, ¹⁶O:0 .. 10

Mass	Mass Difference (mmu)	Mass Difference (ppm)	¹² C	¹ H	²³ Na	¹⁶ O	Unsaturation Number
461.23159	1.20	2.59	27	34	1	5	10.5
	-4.68	-10.14	20	38	1	10	1.5

(+)-HRESIMS Data of 6.



日期: 星期二 10月 07 14:01:44 2008 (GMT+08: Sample Name: EM - E - 9 - 23

(显微镜透射法 FT- IR Microscope Transmission)

扫描次数: 100

傅里叶变换红外显微镜(FT-IR Microscope): Centaur μ s

分辨率: 8.000

美国热电公司(Thermo)傅里叶变换红外光谱仪:Nicolet 5700

Figure S51. The IR Spectrum of 6.

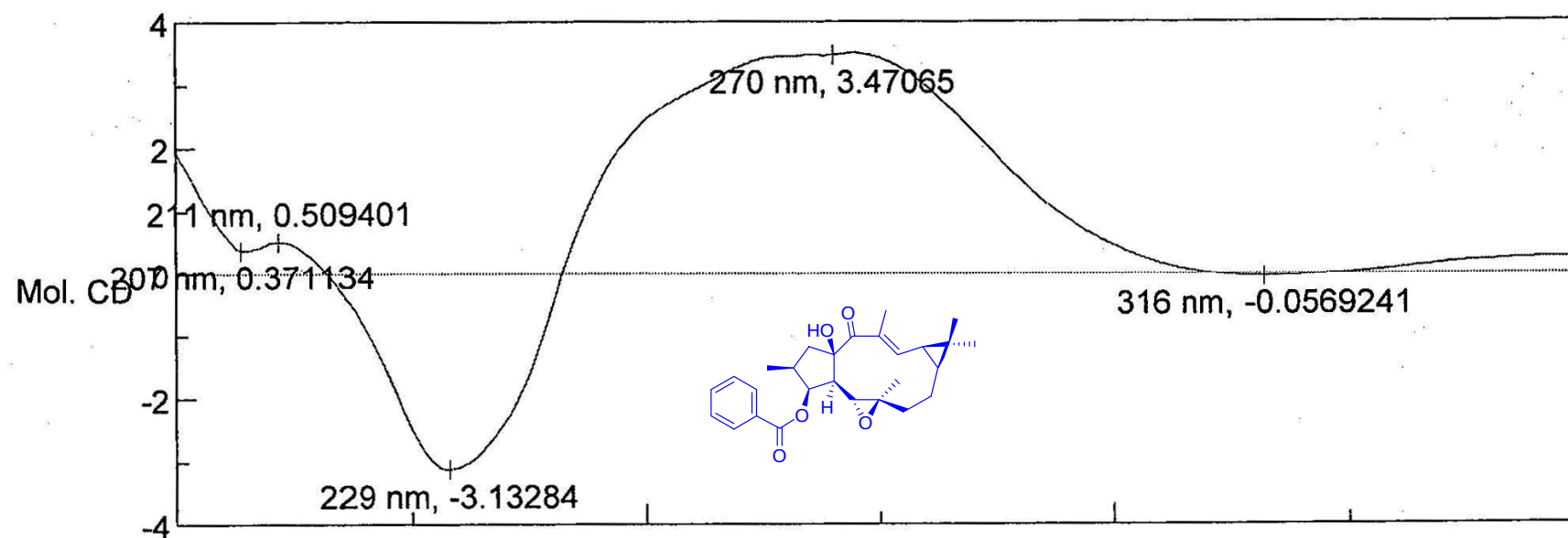


Figure S52. The CD Spectrum of 6.

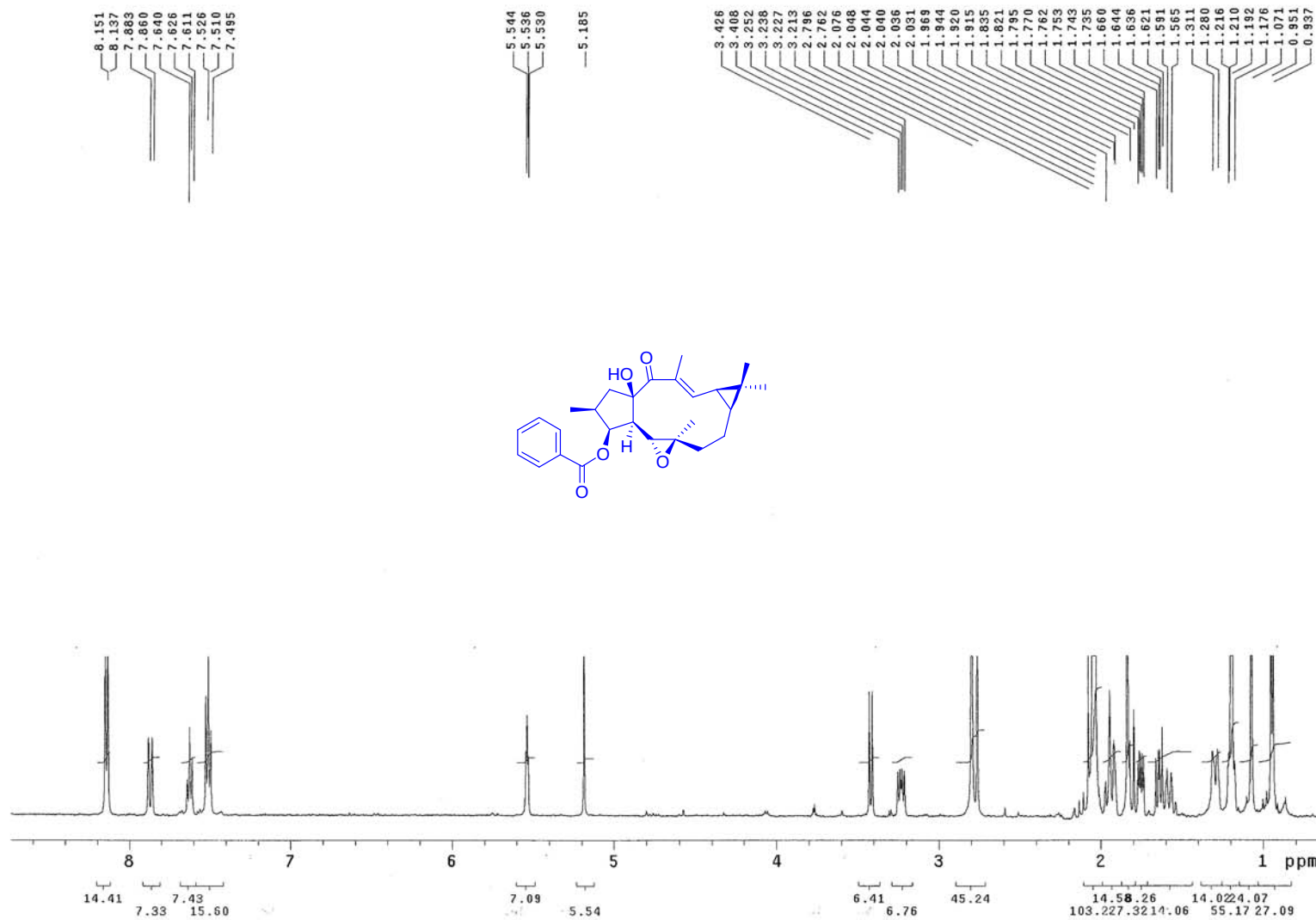


Figure S53. The ^1H NMR Spectrum of 6 in CD_3COCD_3 (500 MHz).

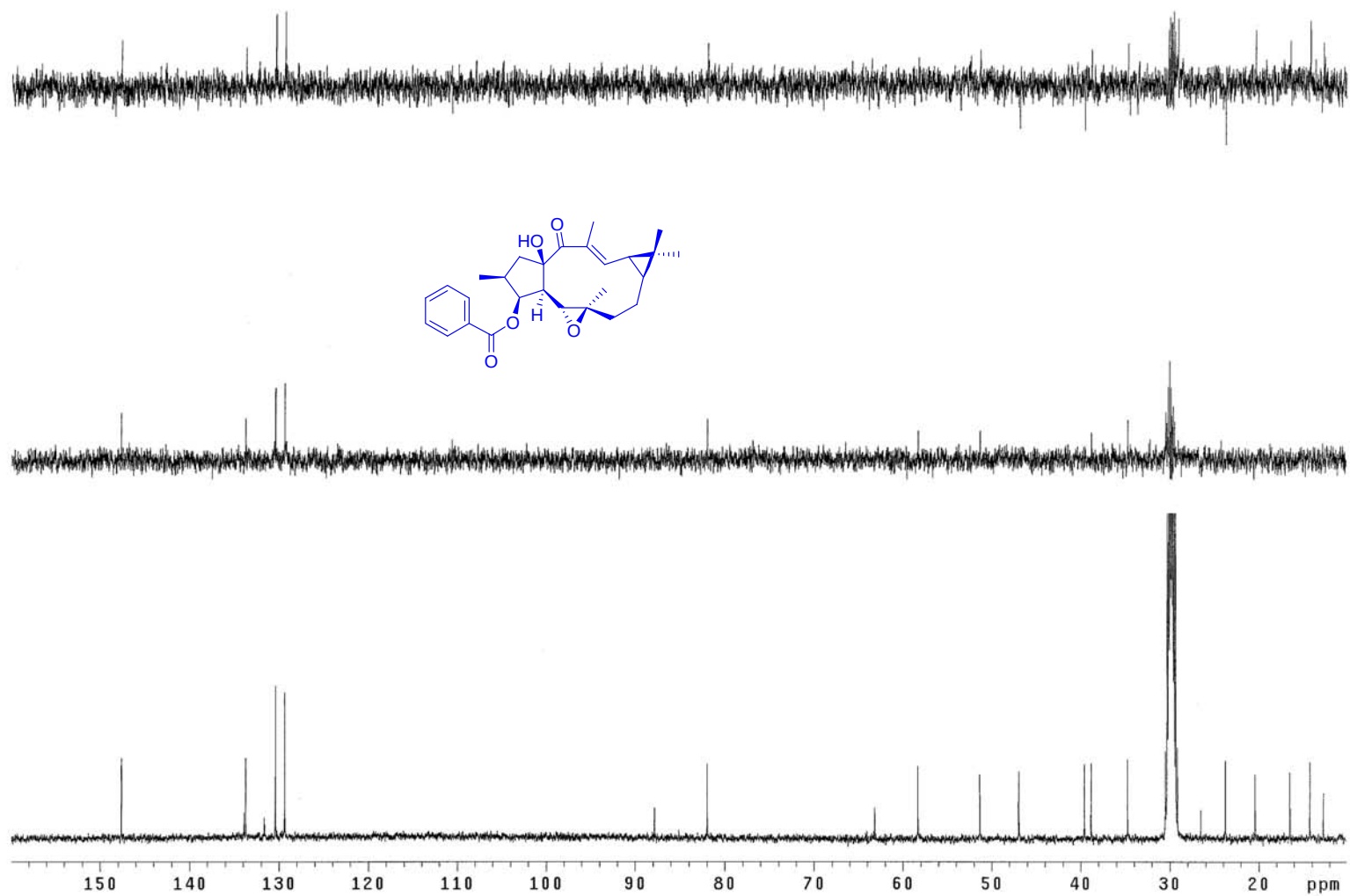


Figure S55. The DEPT Spectrum of 6 in CD₃COCD₃ (125 MHz).

INOVA-501 gCOSY EM-E-9-23 IN CD3COCD3 08.05.07

Solvent: Acetone
Temp. 25.0 C / 298.1 K
INOVA-500 "IMM-501"

Relax. delay 1.000 sec
Acq. time 0.234 sec
Width 4369.0 Hz
2D Width 4369.0 Hz
8 repetitions
256 increments
OBSERVE H1, 499.7728092 MHz
DATA PROCESSING
Sine bell 0.117 sec
F1 DATA PROCESSING
Sine bell 0.022 sec
FT size 2048 x 2048
Total time 43 min, 54 sec

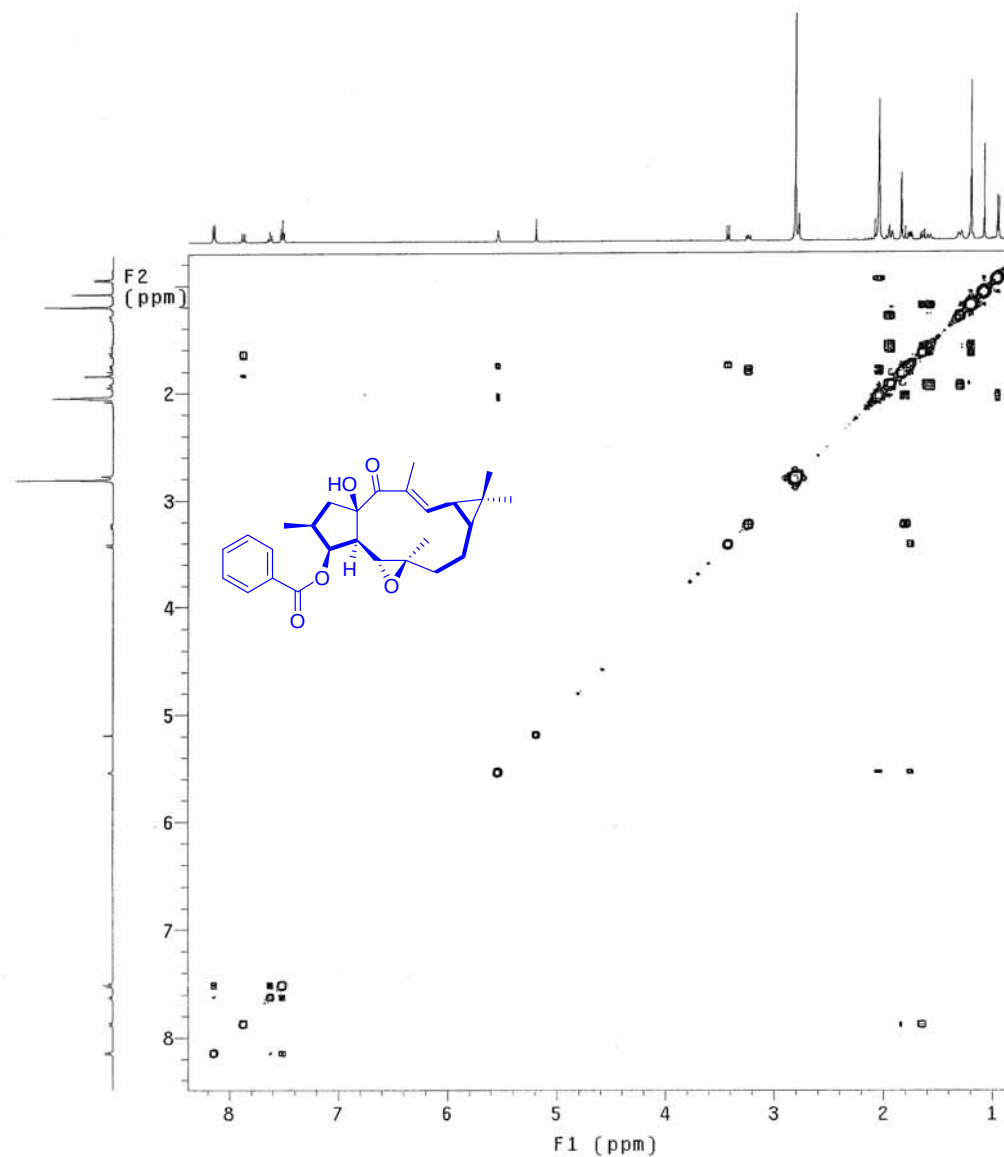


Figure S56. The ^1H - ^1H gCOSY Spectrum of 6 in CD_3COCD_3 (500 MHz).

INOVA-501 gHSQC EM-E-9-23 IN CD3COCD3 08.05.07

Solvent: Acetone
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "INM-501"

Relax. delay 1.000 sec
Acq. time 0.234 sec
Width 4369.0 Hz
2D Width 27137.0 Hz
96 repetitions
160 increments
OBSERVE H1, 499.7728092 MHz
DECOUPLE C13, 125.6818041 MHz
Power 48 dB
on during acquisition
off during delay
GARP-1 modulated
DATA PROCESSING
Sine bell 0.056 sec
F1 DATA PROCESSING
Sine bell 0.003 sec
FT size 2048 x 4096
Total time 5 hr, 34 min, 58 sec

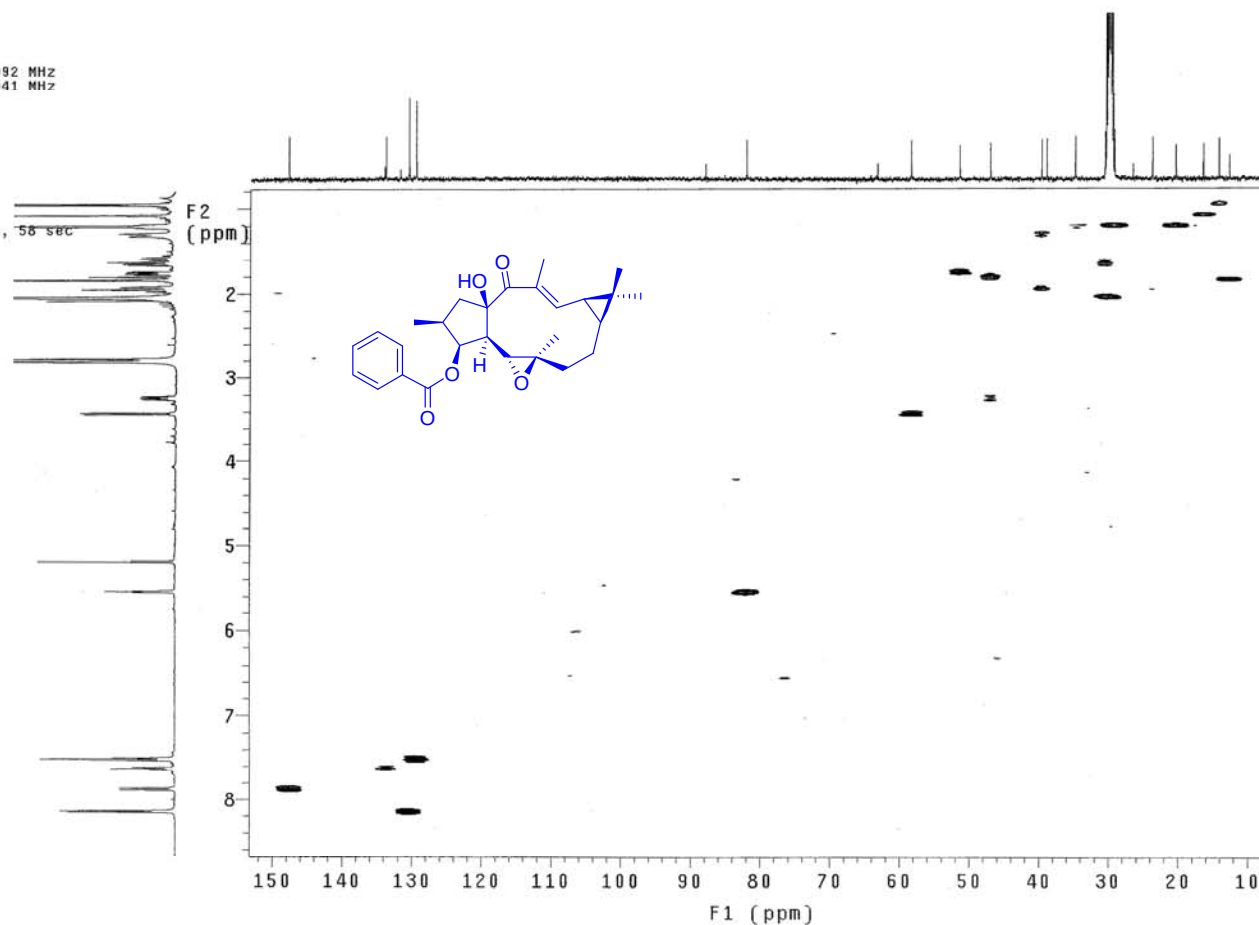


Figure S57. The gHSQC Spectrum of 6 in CD_3COCD_3 (500 MHz for ^1H NMR).

Solvent: Acetone
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "IMN-501"

Relax. delay 1.000 sec
Acq. time 0.228 sec
Width 4486.1 Hz
2D Width 27137.0 Hz
128 repetitions
180 increments
OBSERVE H1, 499.7728092 MHz
DATA PROCESSING
Sine bell 0.061 sec
F1 DATA PROCESSING
Sine bell 0.004 sec
FT size 2048 x 4096
Total time 8 hr, 25 min, 1 sec

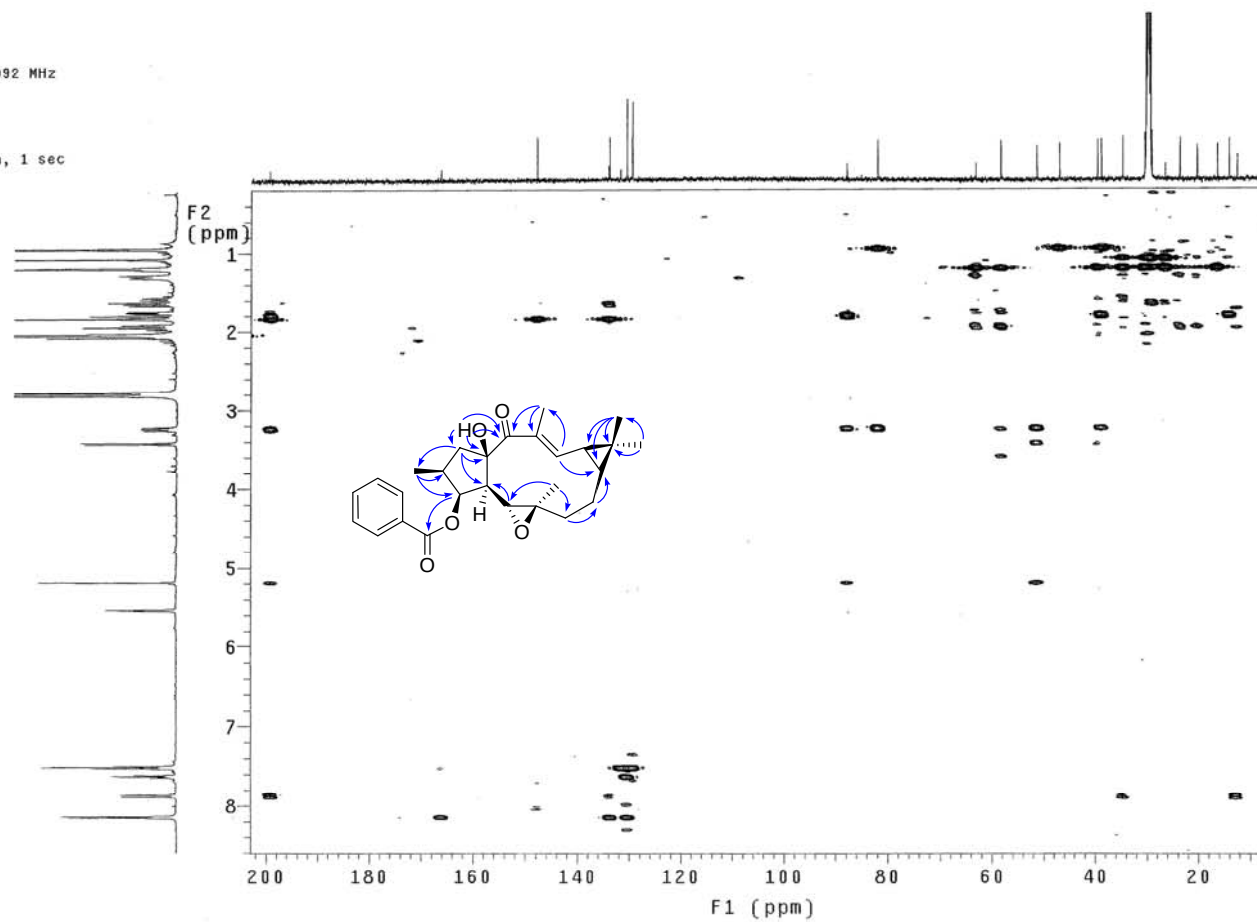


Figure S58. The gHMBC Spectrum of 6 in CD₃COCD₃ (500 MHz for ¹H NMR).

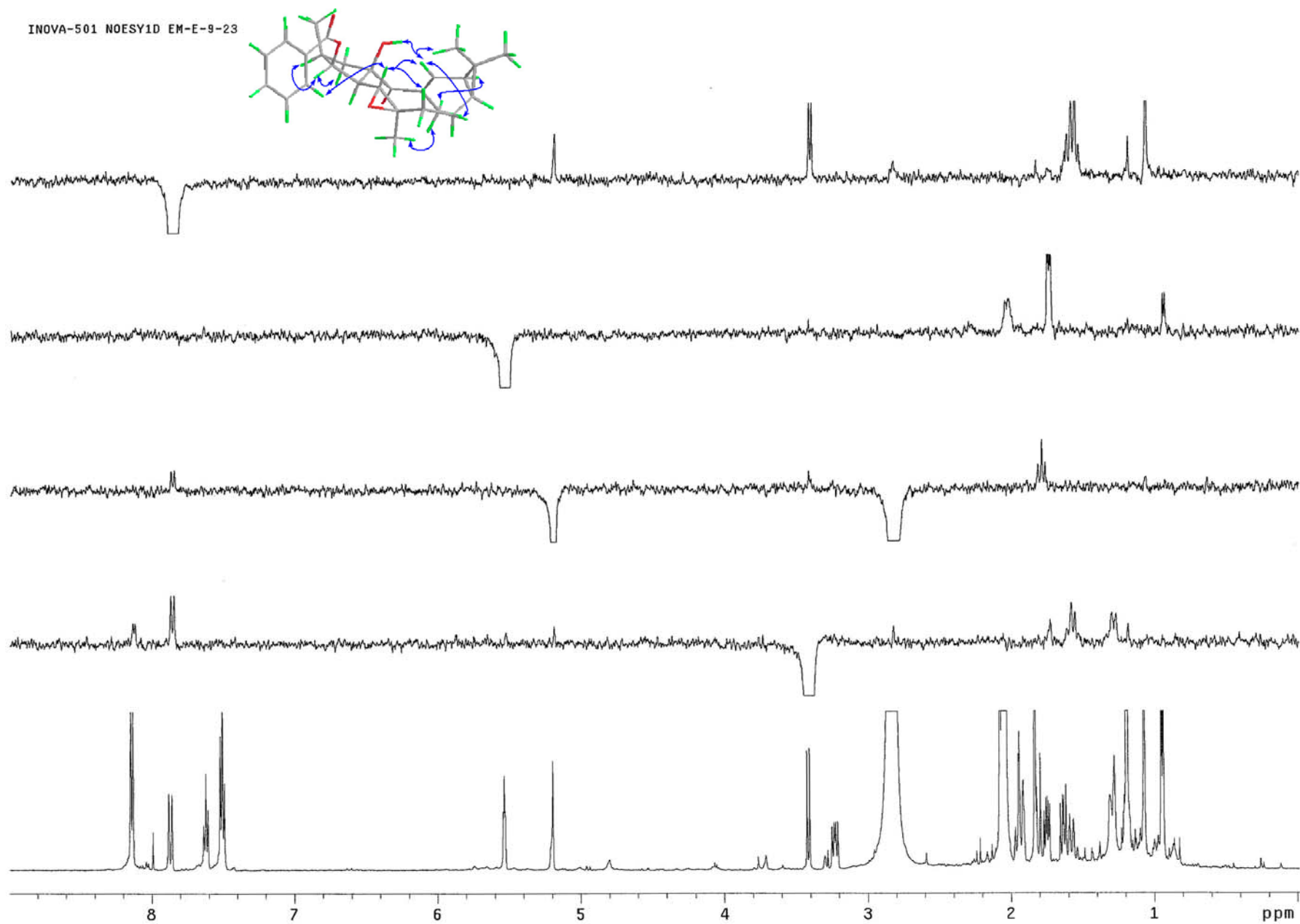


Figure S59. The NOE Difference Spectrum 1 of 6 in CD_3COCD_3 (500 MHz).

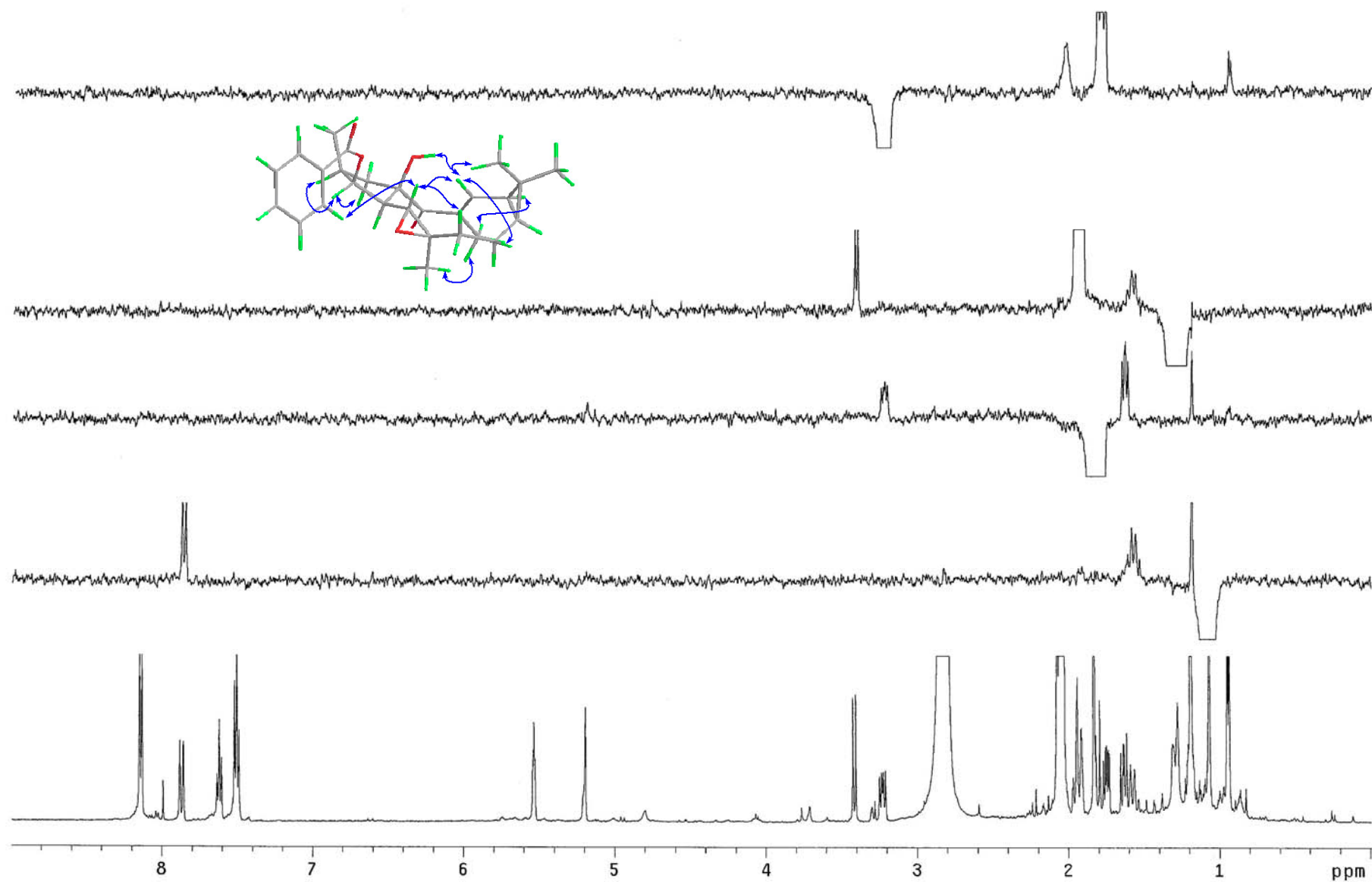


Figure S60. The NOE Difference Spectrum 2 of 6 in CD₃COCD₃ (500 MHz).

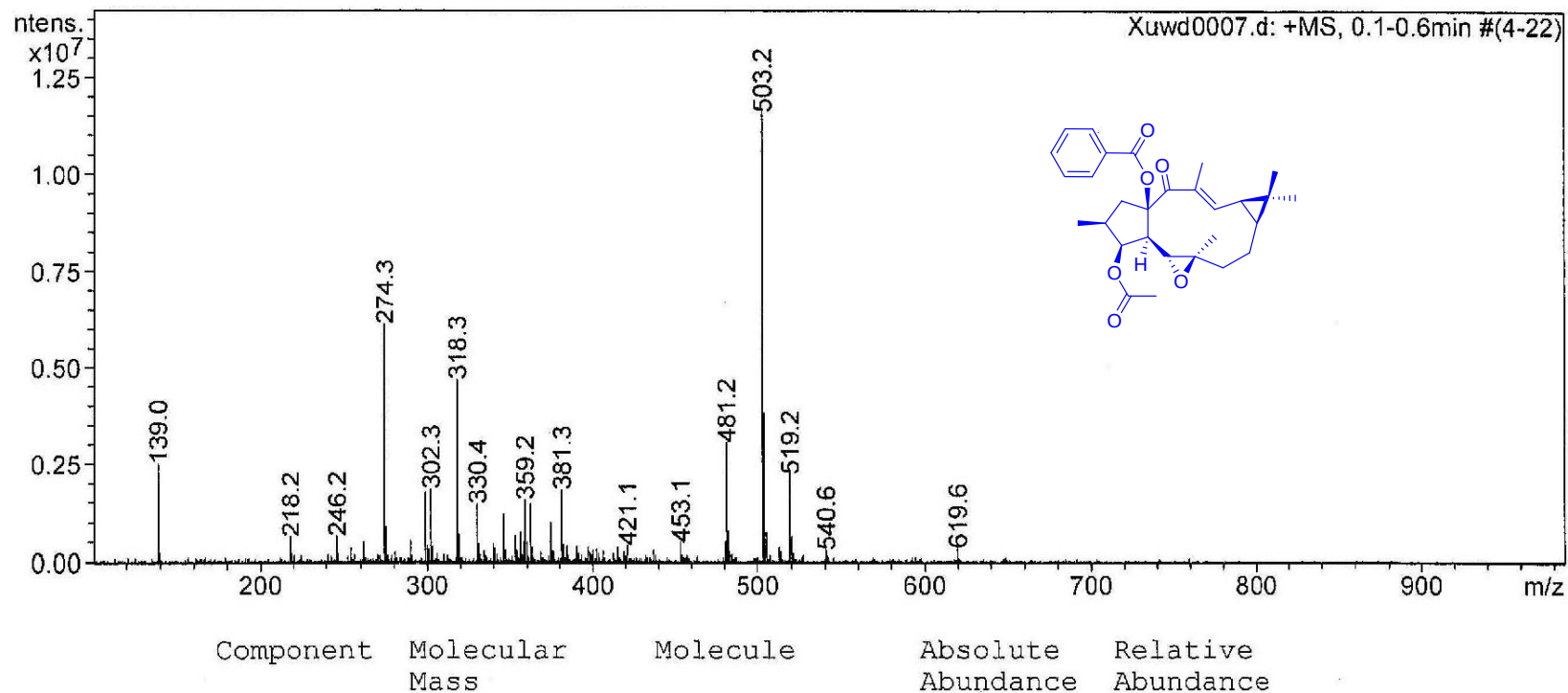
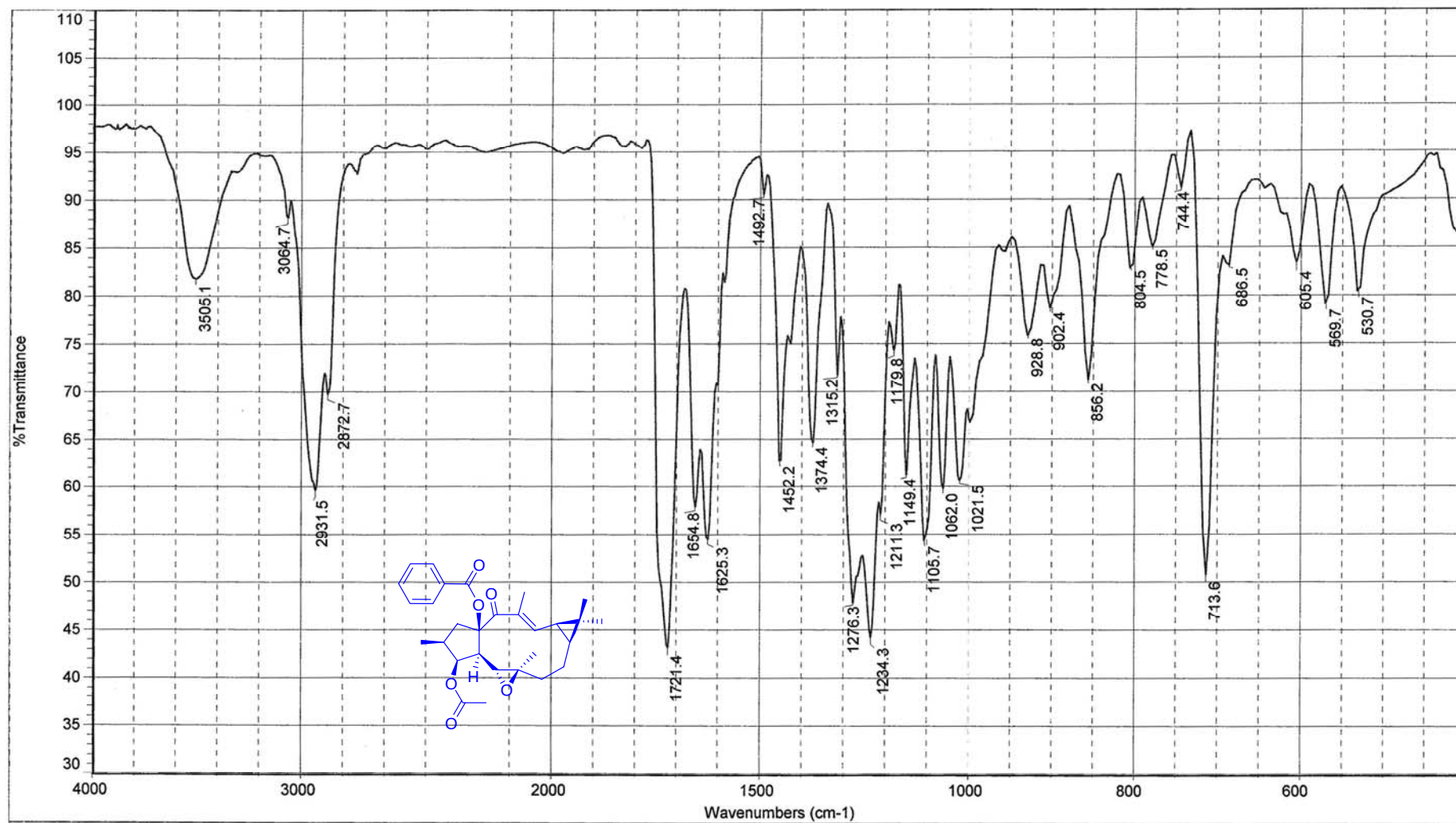


Figure S61. (+)-ESIMS Spectrum of 7.
MS Formula Results: + Scan (9.276 min) Sub (200905202.d)

m/z	Ion	Formula	Abundance							
481.25734	(M+H) ⁺	C ₂₉ H ₃₇ O ₆	222290.2							
Best	Formula (M)	Ion Formula	Score	Cr	Calc m/z	Diff (ppm)	Mass Ma	Abund M	Spacing	DBE
✓	C ₂₉ H ₃₆ O ₆	C ₂₉ H ₃₇ O ₆	96.4		481.25847	2.37	94.28	97.75	99.05	12
m/z	Ion	Formula	Abundance							
503.23957	(M+Na) ⁺	C ₂₉ H ₃₆ NaO ₆	531147.5							
Best	Formula (M)	Ion Formula	Score	Cr	Calc m/z	Diff (ppm)	Mass Ma	Abund M	Spacing	DBE
✓	C ₂₉ H ₃₆ O ₆	C ₂₉ H ₃₆ NaO ₆	97.69		503.24041	1.78	96.92	98.05	98.8	12

(+)-HRESIMS Data of 7.



日期: 星期一 10月 06 09:00:10 2008 (GMT+08: Sample Name: E - 9 - 4

(显微镜透射法 FT- IR Microscope Transmission)

扫描次数: 100

傅里叶变换红外显微镜(FT-IR Microscope): Centaurus

分辨率: 8.000

美国热电公司(Thermo)傅立叶变换红外光谱仪:Nicolet 5700

Figure S62. The IR Spectrum of 7.

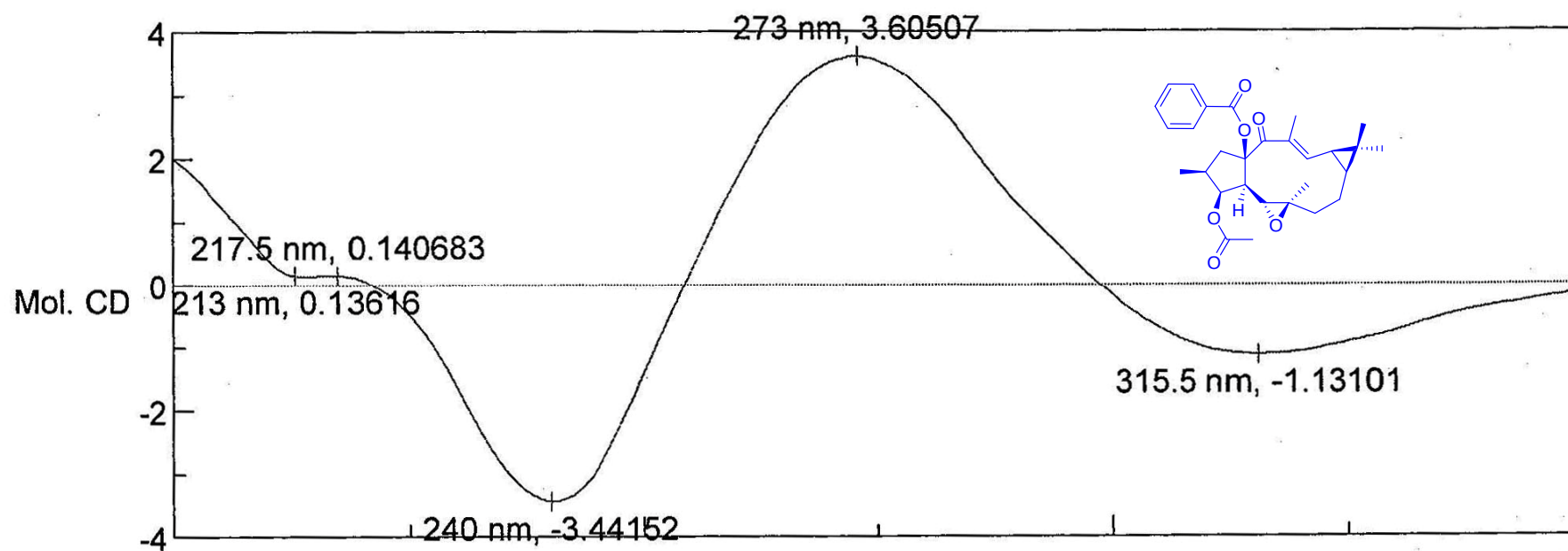


Figure S63. The CD Spectrum of 7.

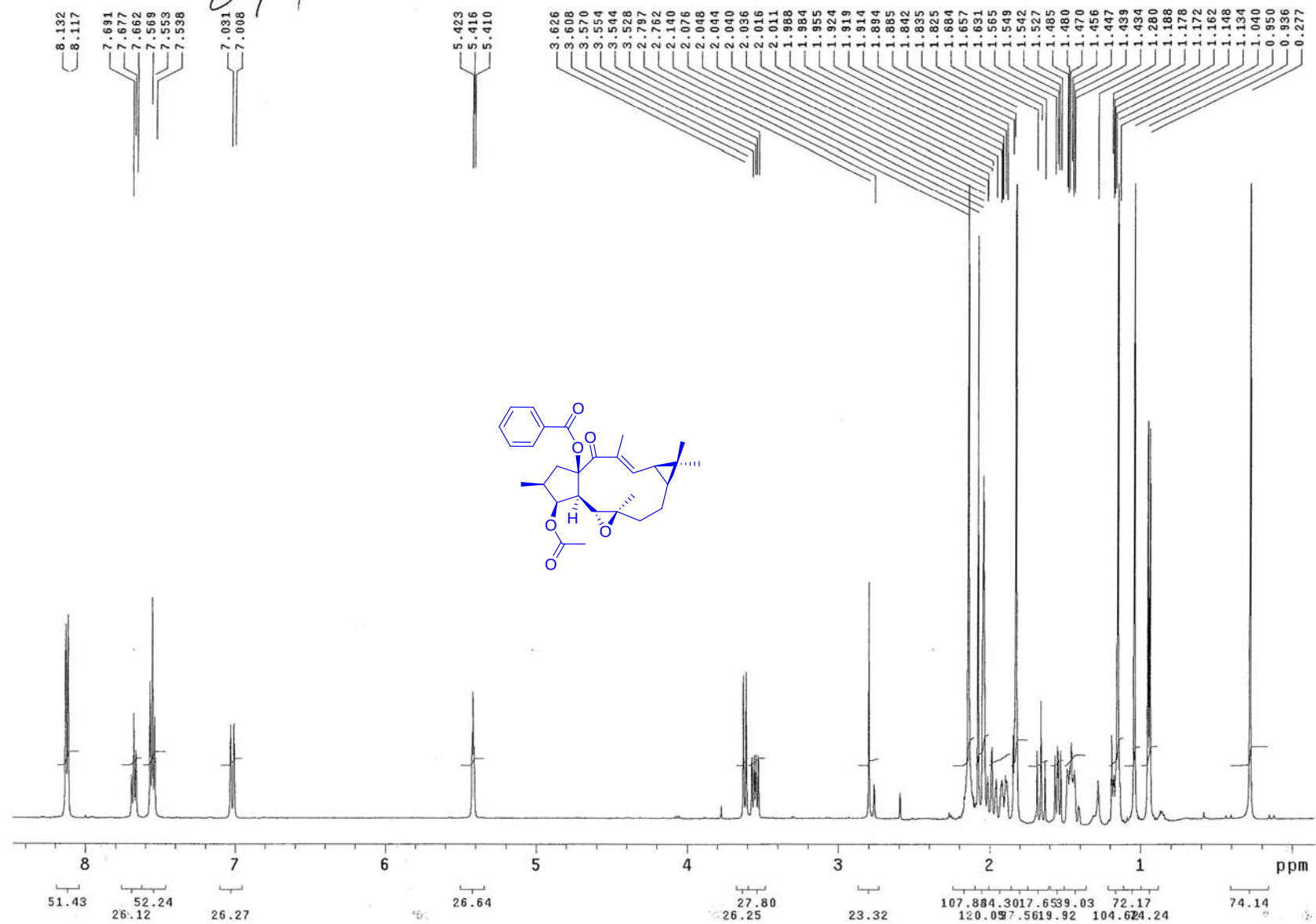


Figure S64. The ^1H NMR Spectrum of 7 in CD_3COCD_3 (500 MHz).

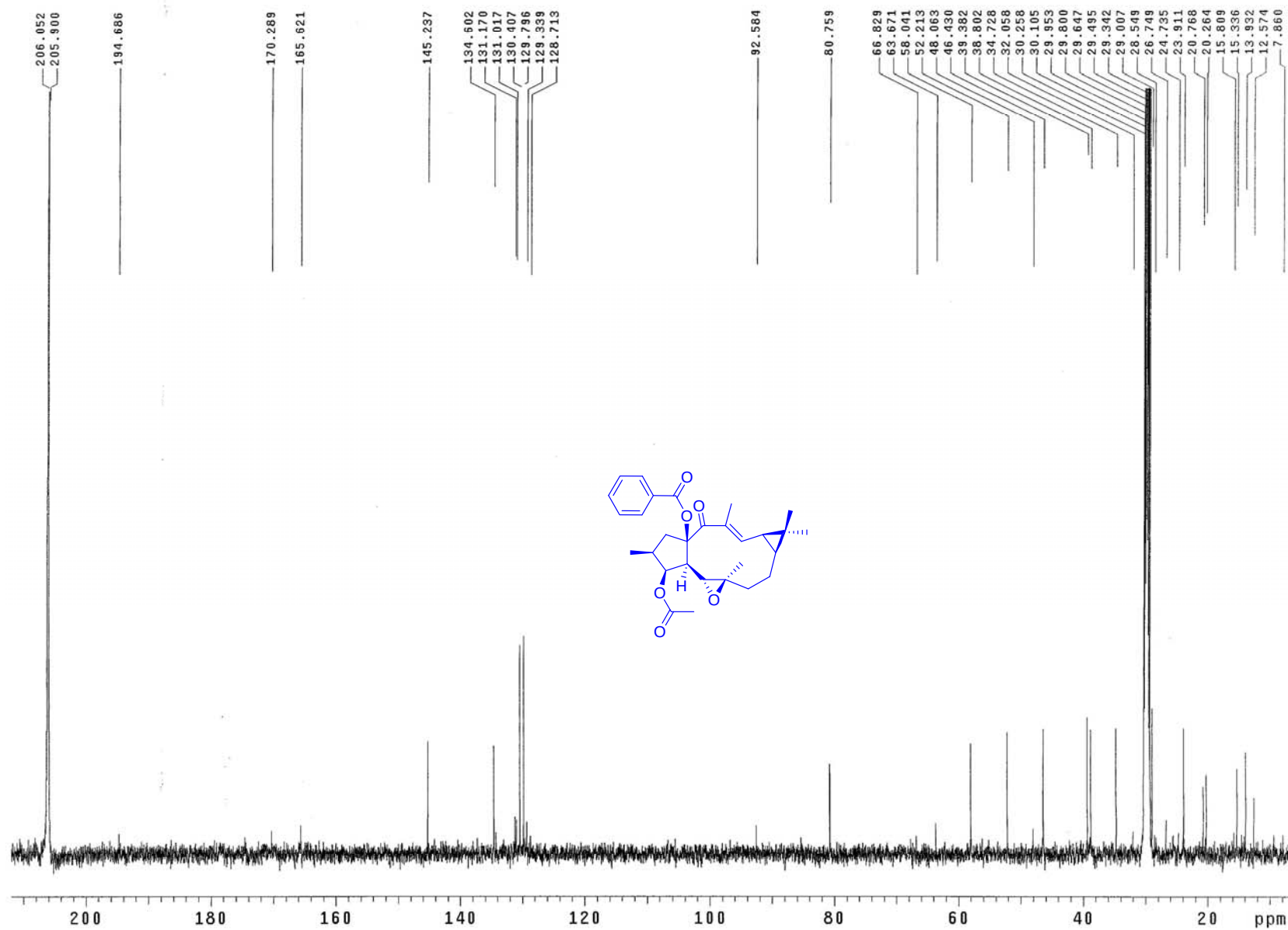


Figure S65. The ¹³C NMR Spectrum of 7 in CD₃COCD₃ (125 MHz).

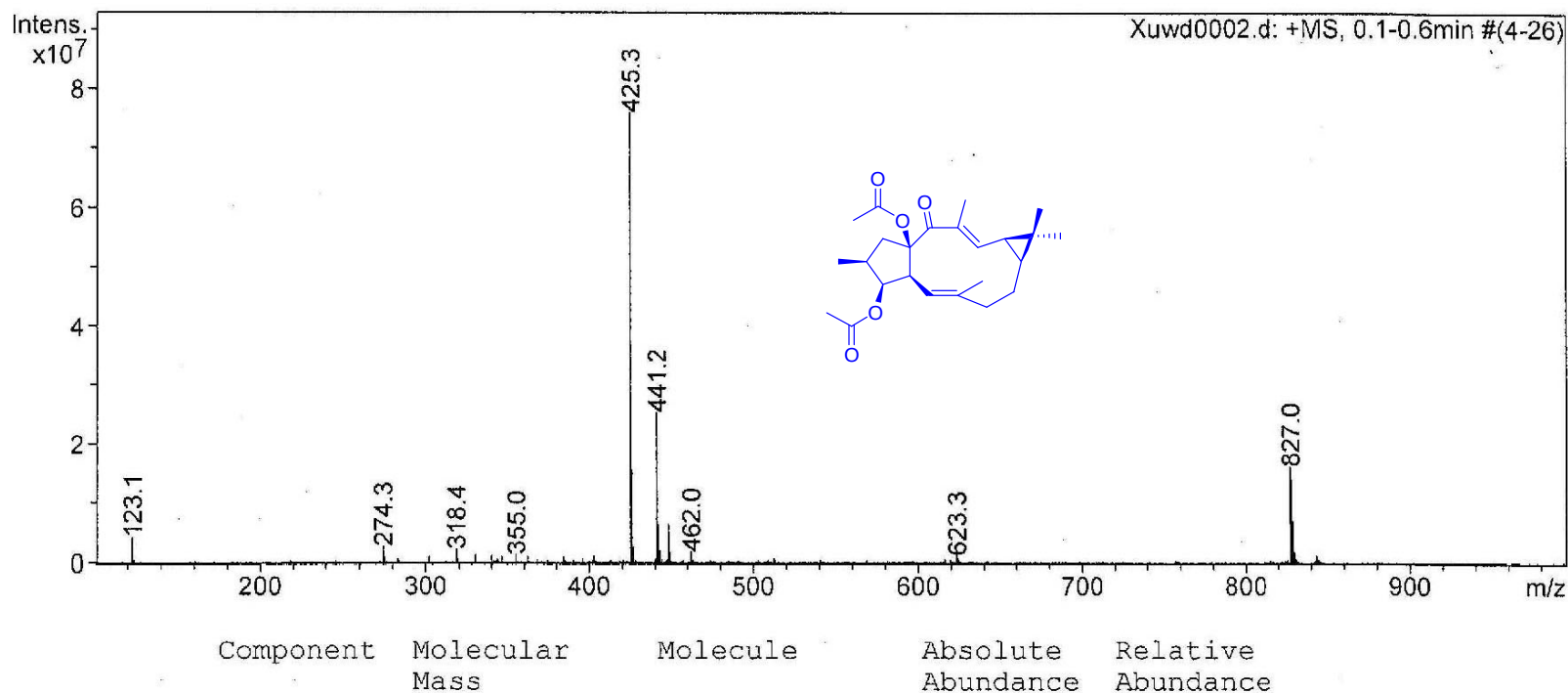


Figure S66. (+)-ESIMS Spectrum of 8.

Data:E_3_3_4

Sample Name:

Description:

Ionization Mode:ESI+

History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[];Smooth[3];Correct Base[5.0%];Average(MS[...

Acquired:12:00:00 AM

Operator:Accutof

Mass Calibration data:TFA100-2000-P-070410

Created:10/14/2008 11:02:34 AM

Created by:Accutof

Charge number:1

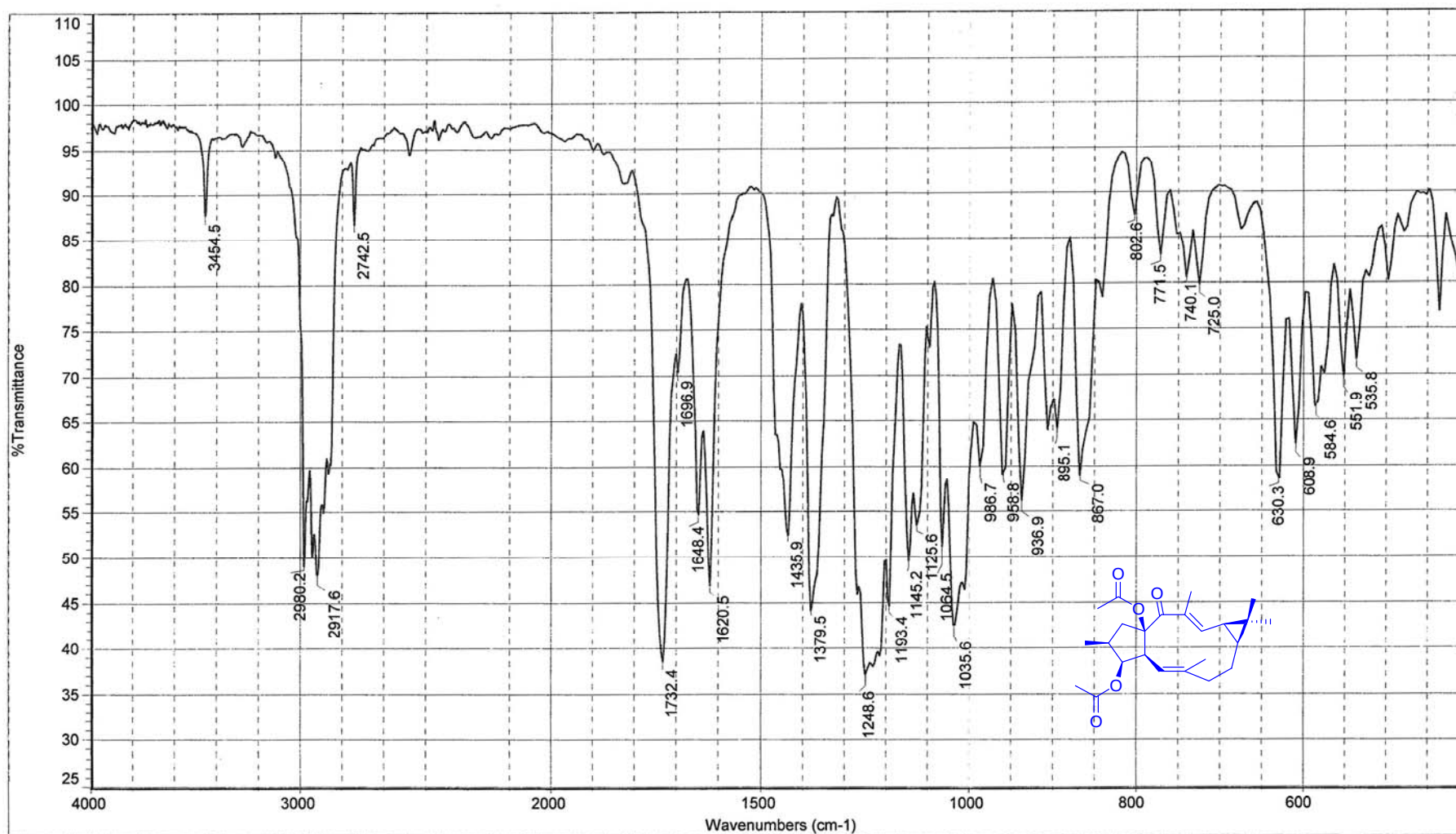
Tolerance:5.00(mmu)

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

Element:¹²C:0 .. 100, ¹H:0 .. 200, ²³Na:1 .. 1, ¹⁶O:0 .. 10

Mass	Mass Difference (mmu)	Mass Difference (ppm)	¹² C	¹ H	²³ Na	¹⁶ O	Unsaturation Number
425.23089	0.50	1.18	24	34	1	5	7.5

(+)-HRESIMS Data of 8.



日期: 星期四 9月 25 16:29:16 2008 (GMT+08:00) Sample Name: E - 3 - 3 - 4

(显微镜透射法 FT- IR Microscope Transmission)

扫描次数: 100

傅里叶变换红外显微镜(FT-IR Microscope): Centaurus

分辨率: 8.000

美国热电公司(Thermo)傅里叶变换红外光谱仪:Nicolet 5700

Figure S67. The IR Spectrum of 8.

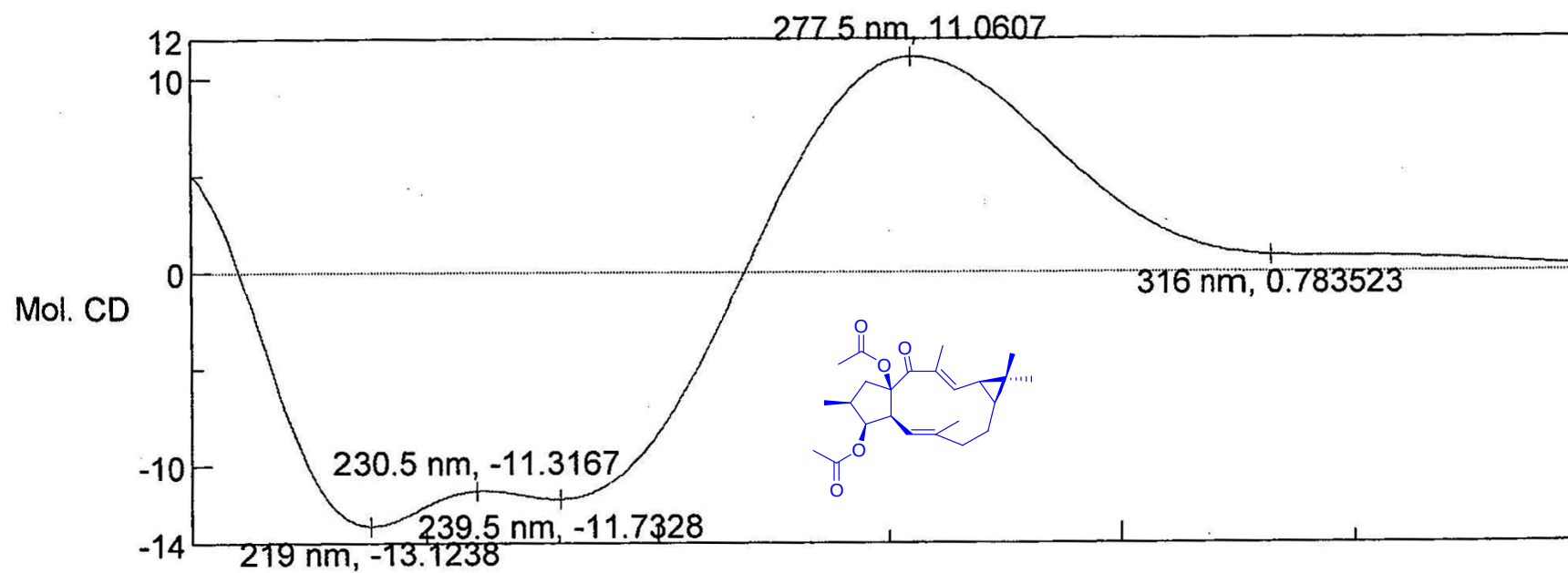


Figure S68. The CD Spectrum of 8.

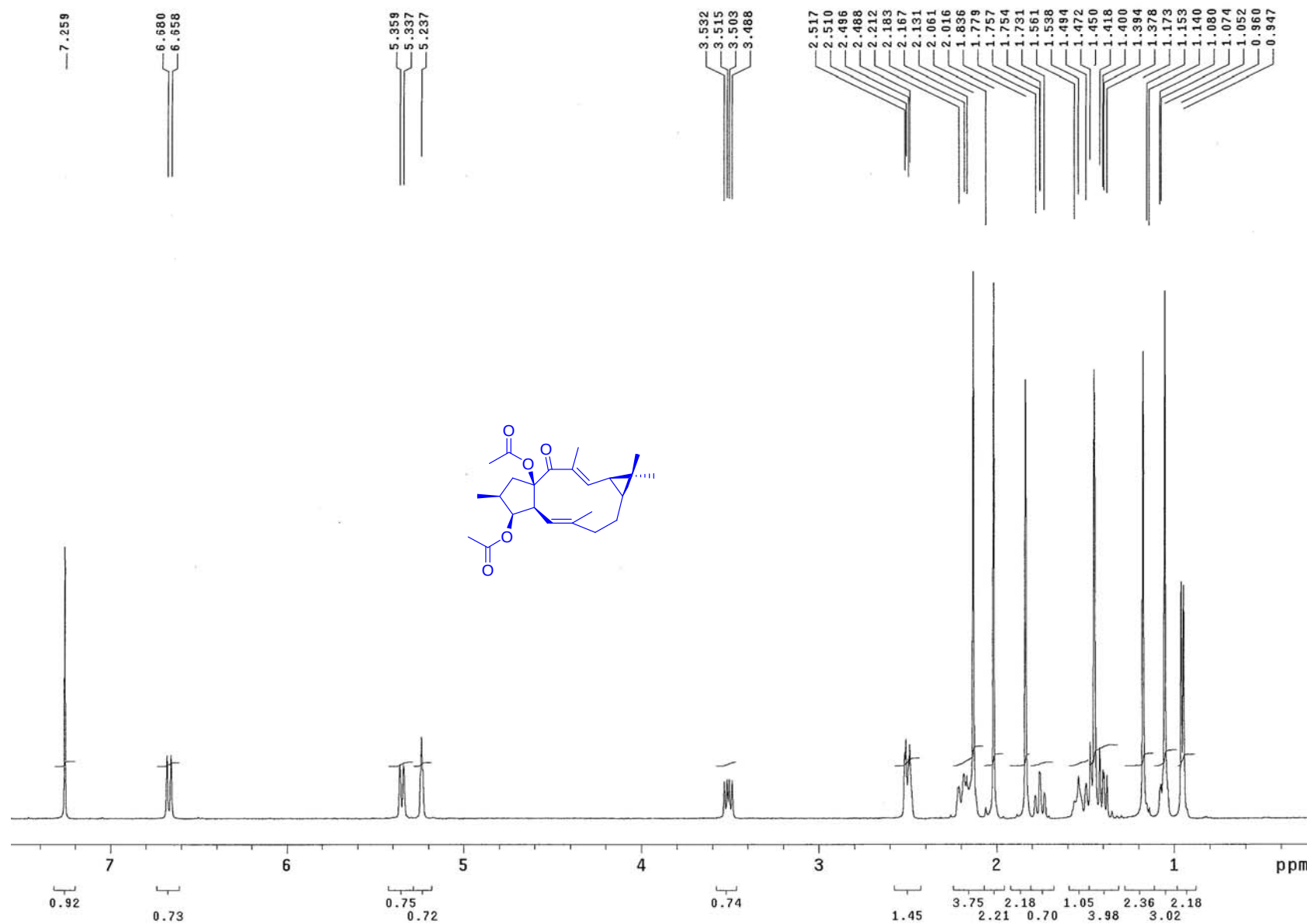


Figure S69. The ^1H NMR Spectrum of 8 in CDCl_3 (500 MHz).

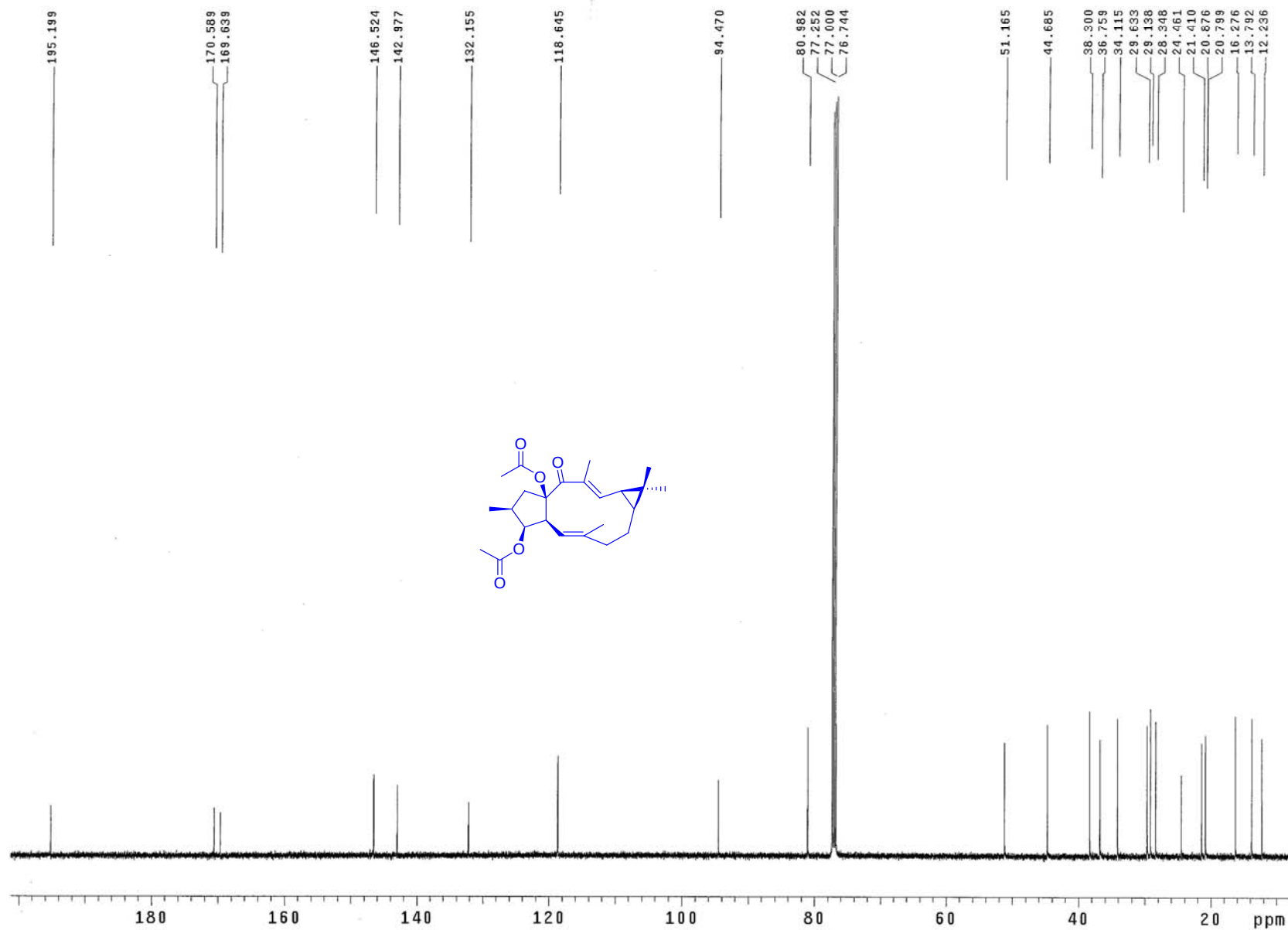


Figure S70. The ^{13}C NMR Spectrum of 8 in CDCl_3 (125 MHz).
S82

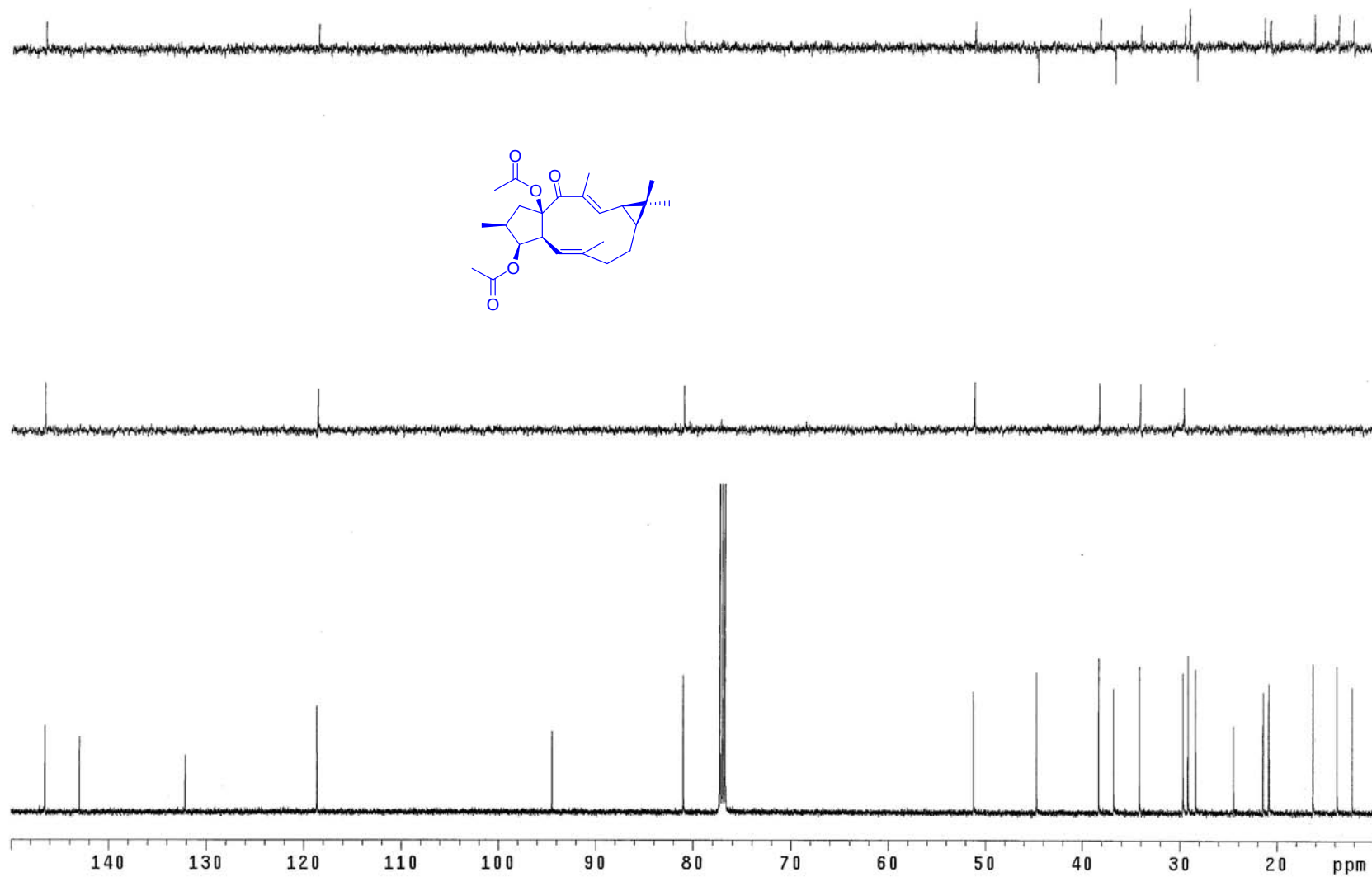


Figure S71. The DEPT Spectrum of 8 in CDCl₃ (125 MHz).

INOVA-501 gCOSY E-3-3-4 CDCL3 07.06.06

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "IMM-501"

Relax. delay 1.000 sec
Acq. time 0.134 sec
Width 3821.0 Hz
2D Width 3821.0 Hz
4 repetitions
128 increments
OBSERVE H1, 499.7702080 MHz
DATA PROCESSING
Sine bell 0.067 sec
F1 DATA PROCESSING
Sine bell 0.016 sec
FT size 1024 x 1024
Total time 10 min, 14 sec

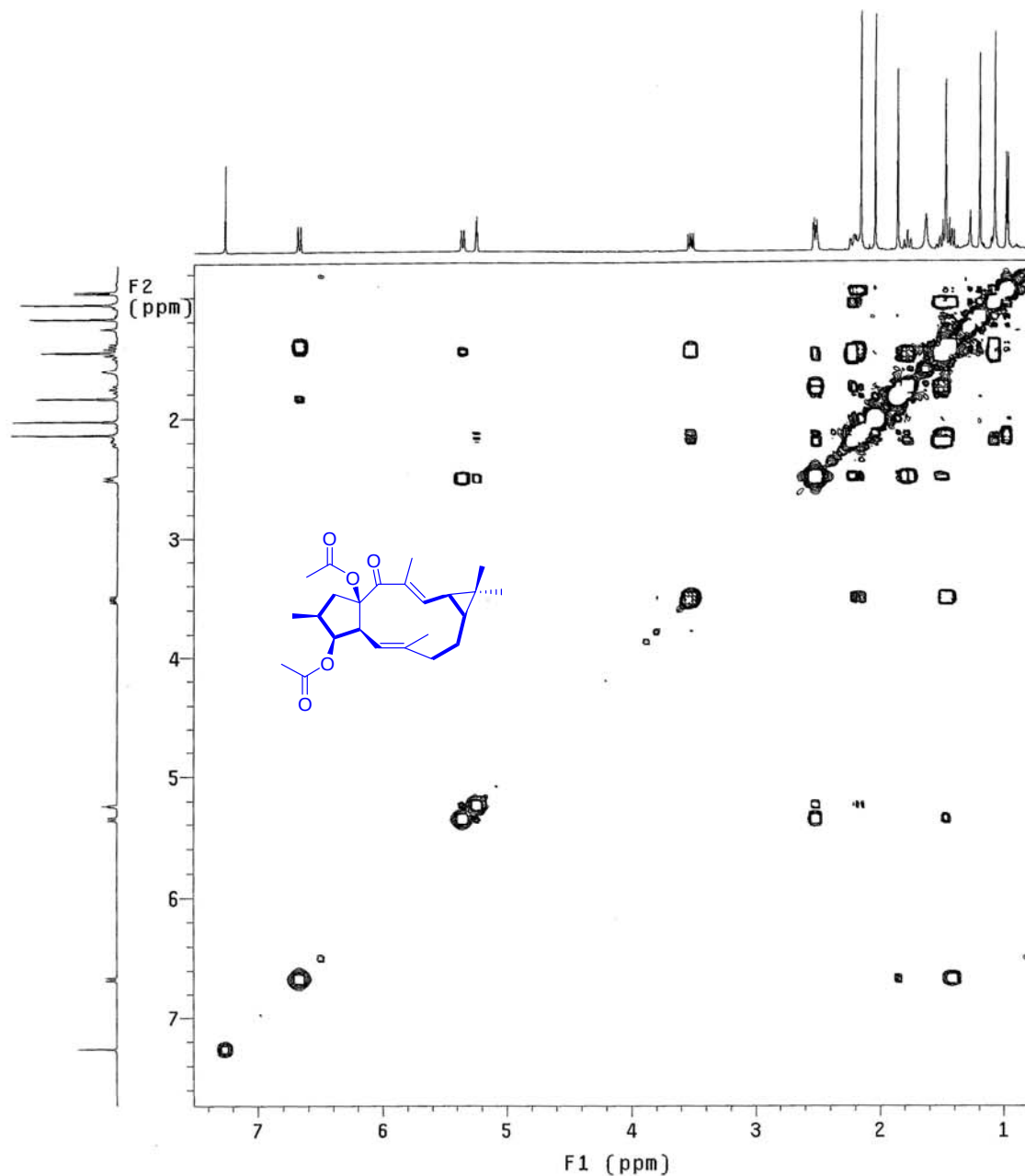


Figure S72. The ^1H - ^1H gCOSY Spectrum of 8 in CDCl_3 (500 MHz).
S84

Solvent: CDCl₃
 Temp. 25.0 C / 298.1 K
 User: 1-14-87
 INOVA-500 "IMM-501"

Relax. delay 1.000 sec
 Acq. time 0.142 sec
 Width 3616.5 Hz
 2D Width 25181.0 Hz
 64 repetitions
 256 increments
 OBSERVE H1, 499.7702080 MHz
 DECOUPLE C13, 125.6798469 MHz
 Power 48 dB
 on during acquisition
 off during delay
 GARP-1 modulated
 DATA PROCESSING
 Sine bell 0.033 sec
 F1 DATA PROCESSING
 Sine bell 0.005 sec
 FT size 1024 x 4096
 Total time 5 hr, 32 min, 27 sec

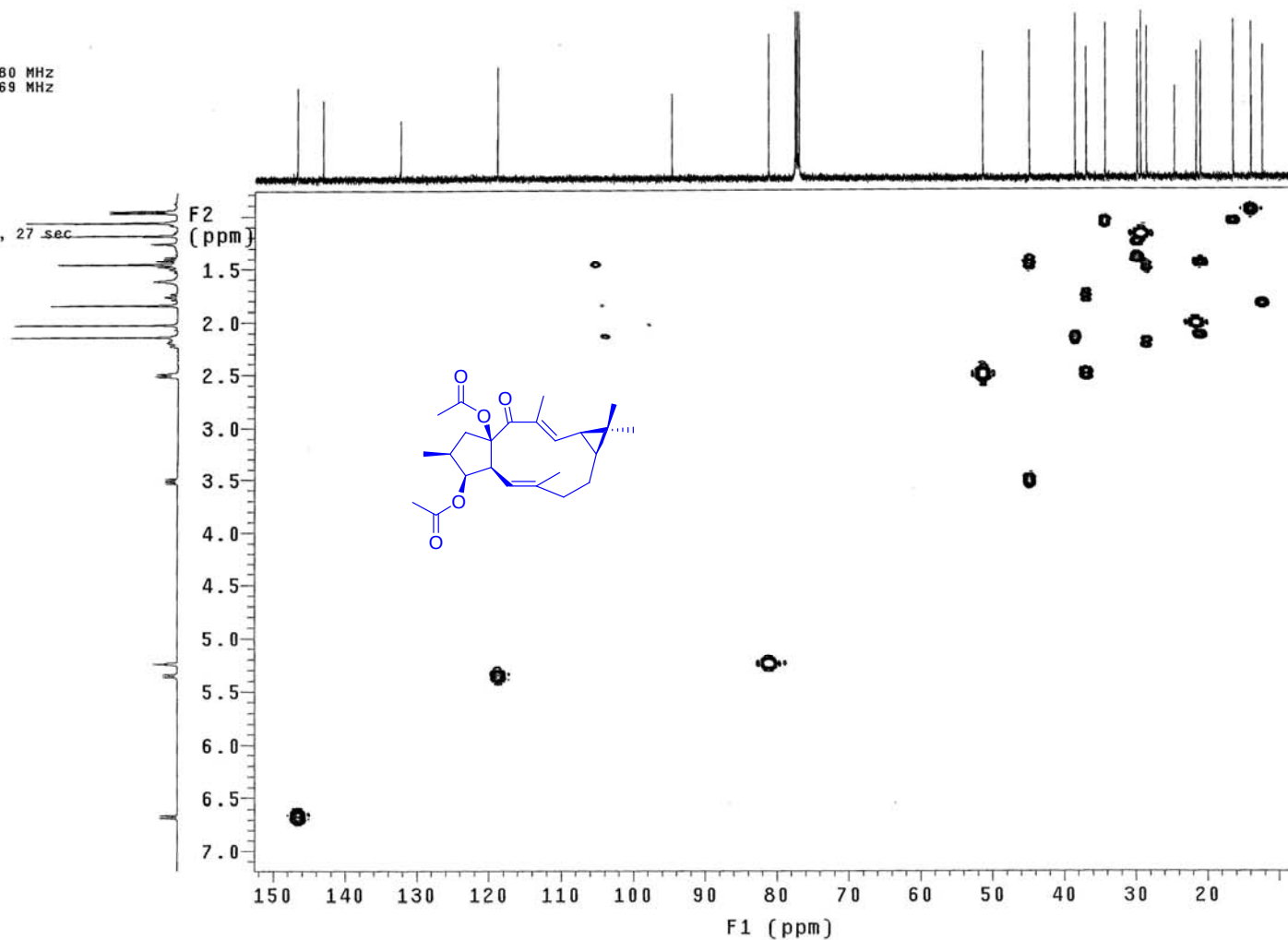


Figure S73. The gHSQC Spectrum of **8** in CDCl₃ (500MHz for ¹H NMR).

Solvent: CDCl₃
 Temp. 25.0 C / 298.1 K
 User: 1-14-87
 INOVA-500 "IMM-501"

Relax. delay 1.000 sec
 Acq. time 0.146 sec
 Width 3495.0 Hz
 2D Width 25181.0 Hz
 80 repetitions
 320 increments
 OBSERVE H1, 499.7702080 MHz
 DATA PROCESSING
 Sine bell 0.034 sec
 F1 DATA PROCESSING
 Sine bell 0.007 sec
 FT size 1024 x 8192
 Total time 8 hr, 47 min, 25 sec

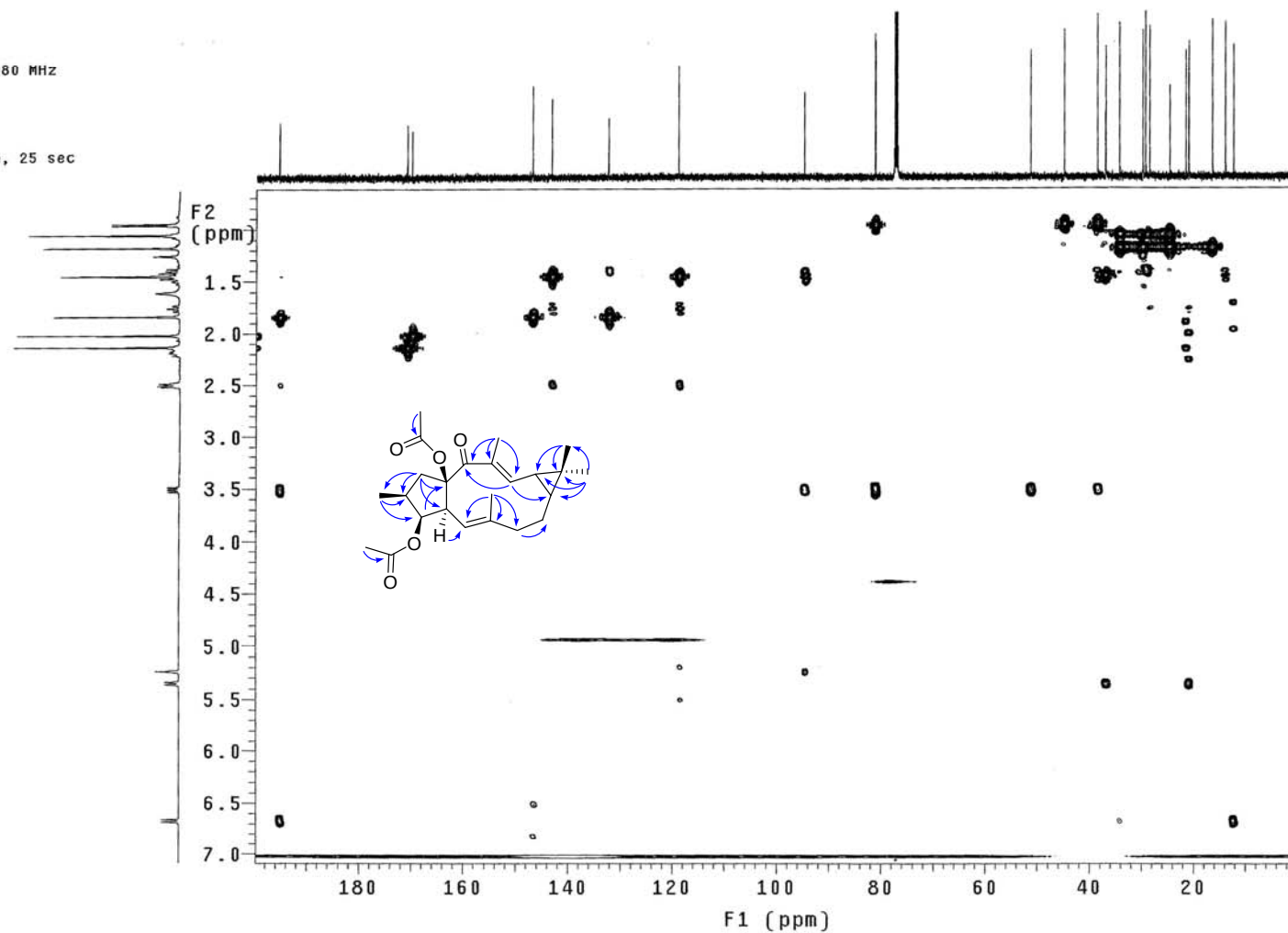


Figure S74. The gHMBC Spectrum of 8 in CDCl₃ (500MHz for ¹H NMR).

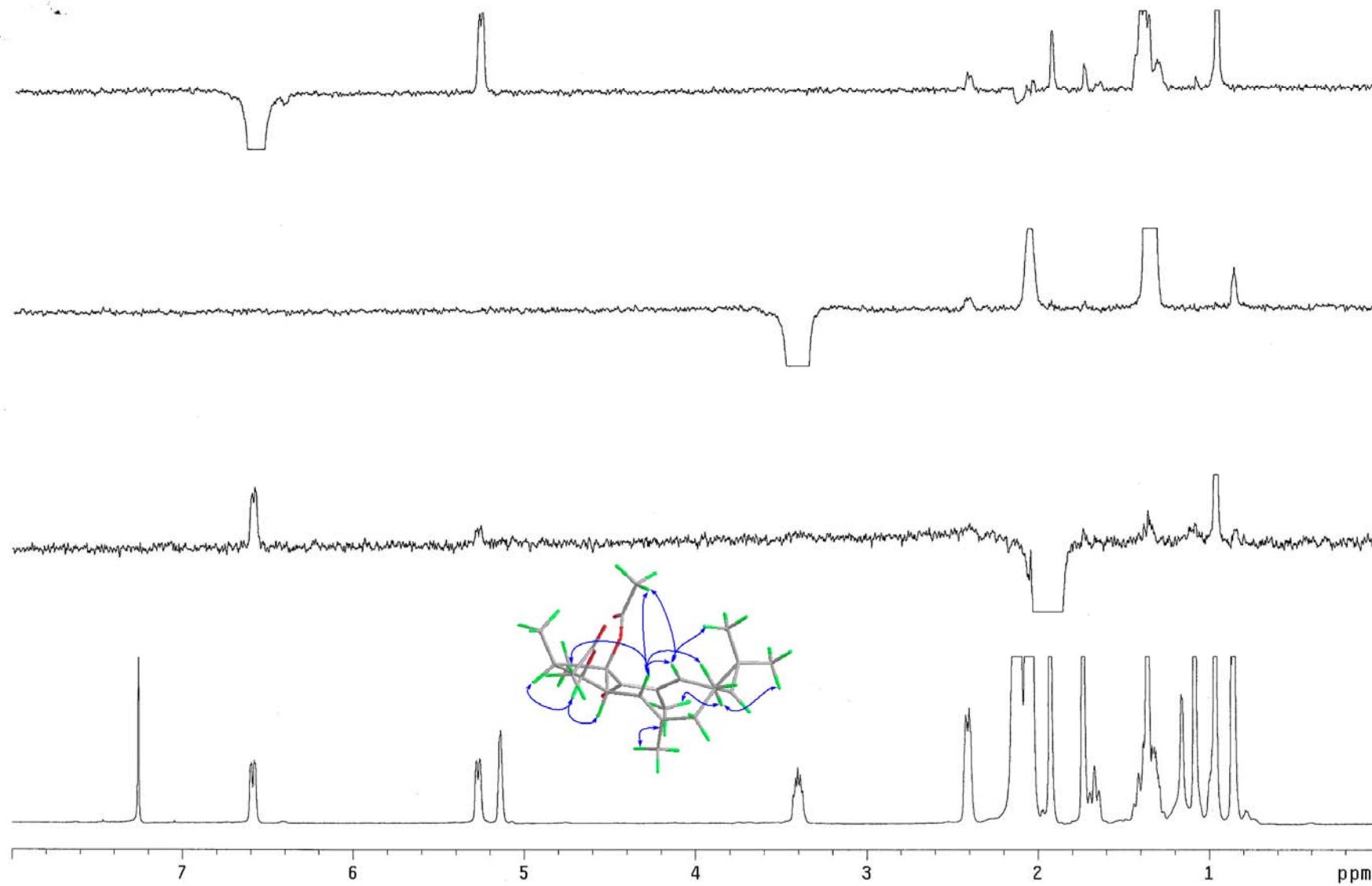


Figure S75. The NOE Difference Spectrum 1 of 8 in CDCl₃ (500 MHz).

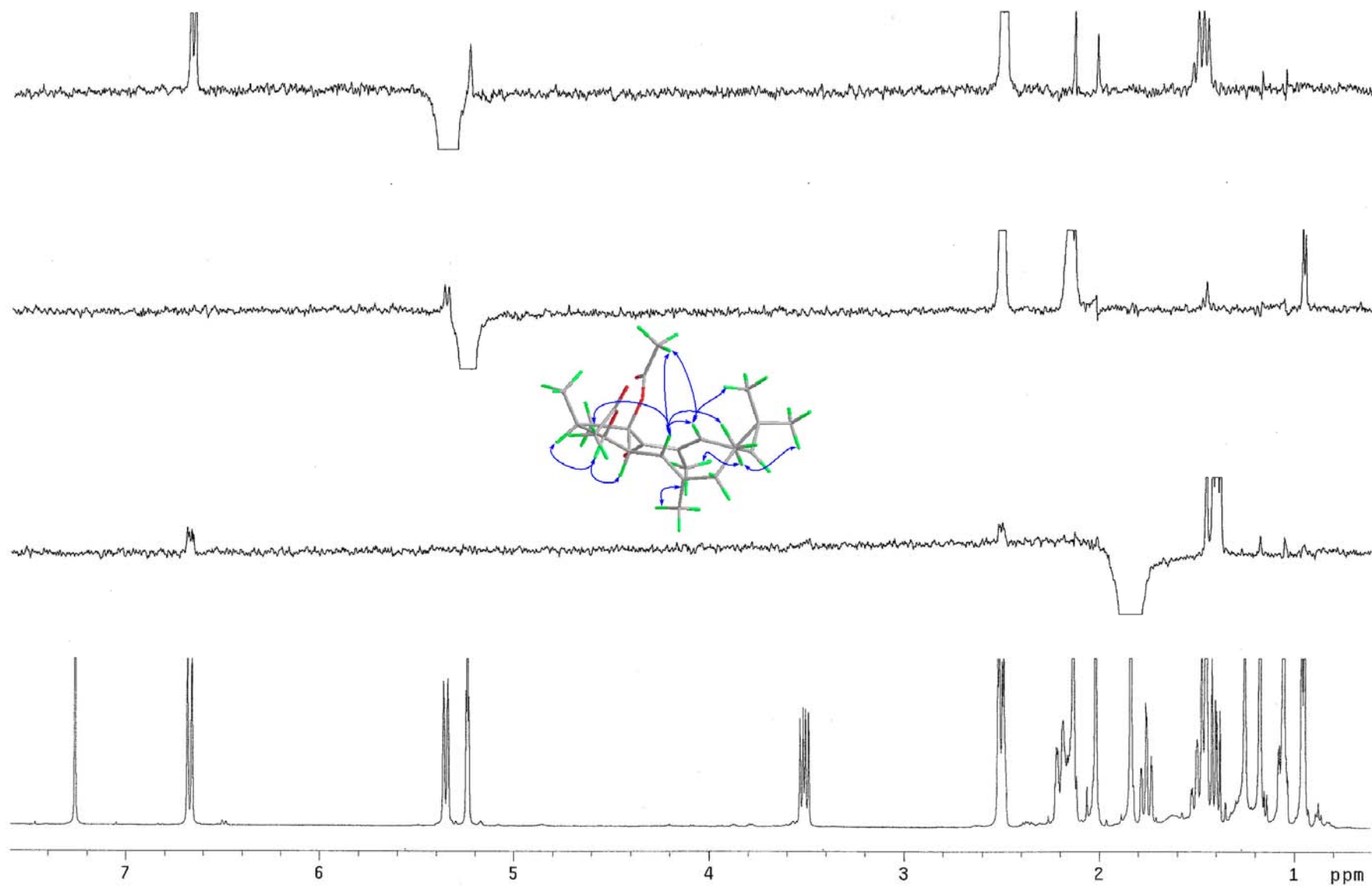


Figure S76. The NOE Difference Spectrum 2 of 8 in CDCl₃ (500 MHz).

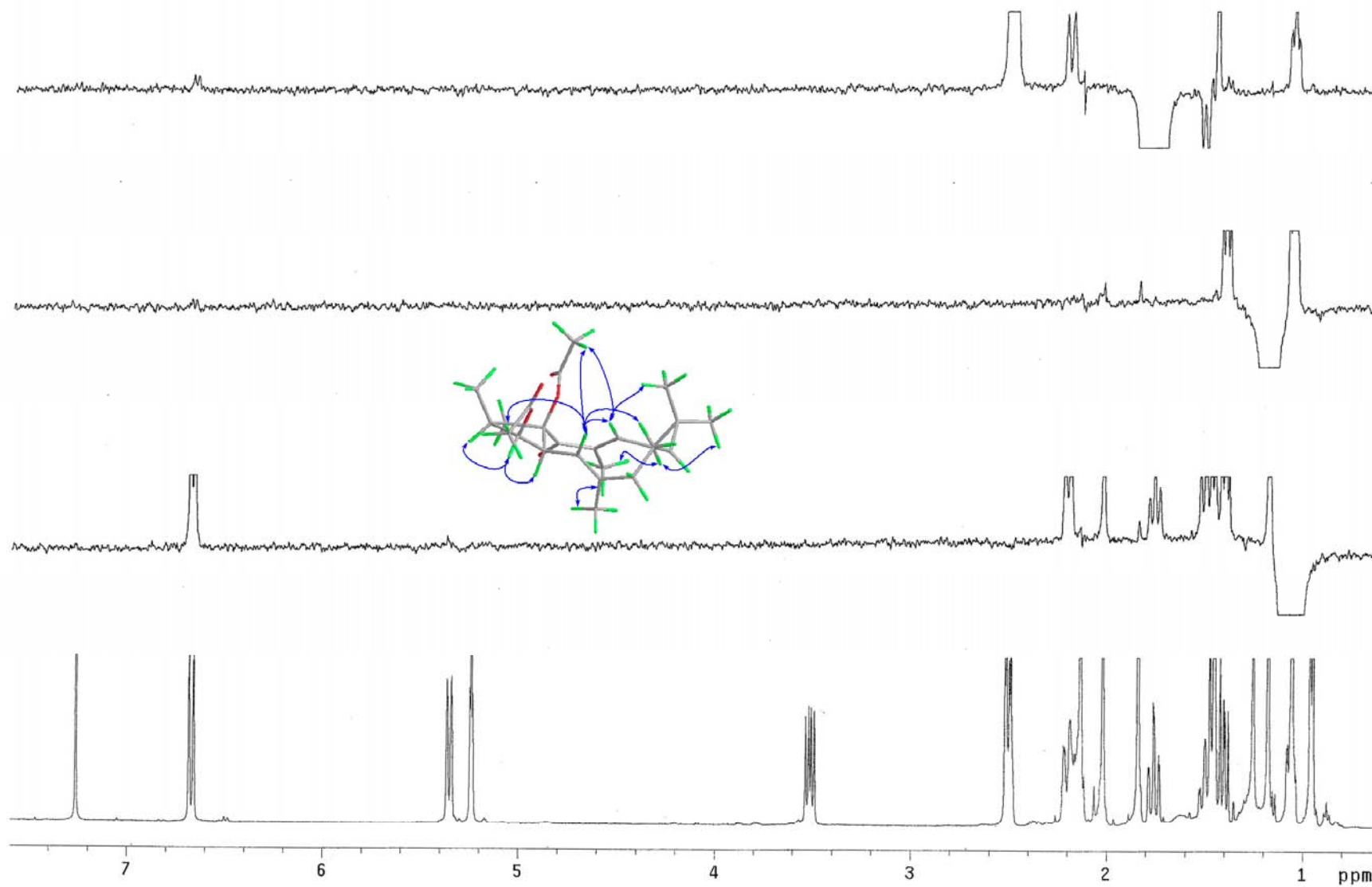


Figure S77. The NOE Difference Spectrum 3 of 8 in CDCl₃ (500 MHz).

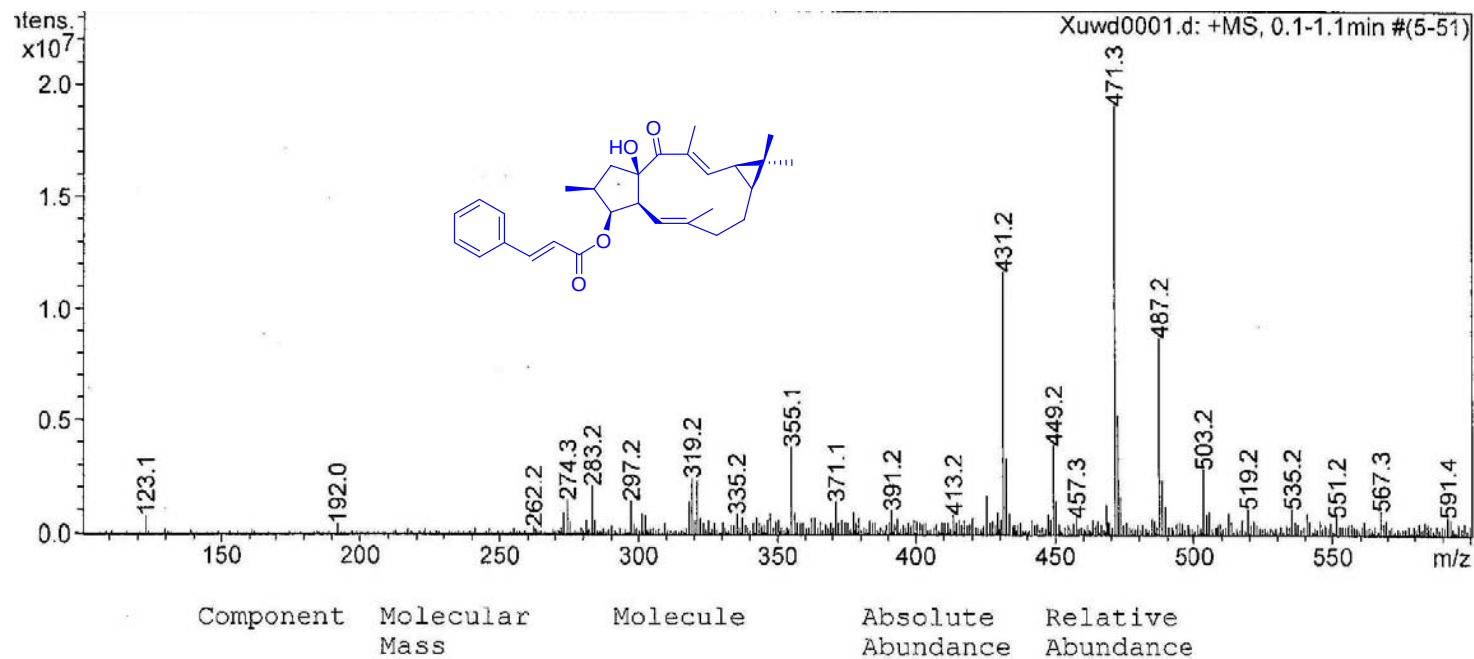


Figure S78. (+)-ESIMS Spectrum of 9.

Data:E_3_4

Sample Name:

Description:

Ionization Mode:ESI+

History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[];Smooth[3]];Add[Correct Base[5.0%];Average(...

Acquired:10/14/2008 10:26:54 AM

Operator:Accutof

Mass Calibration data:TFA100-2000-P-070410

Created:10/14/2008 10:37:10 AM

Created by:Accutof

Charge number:1

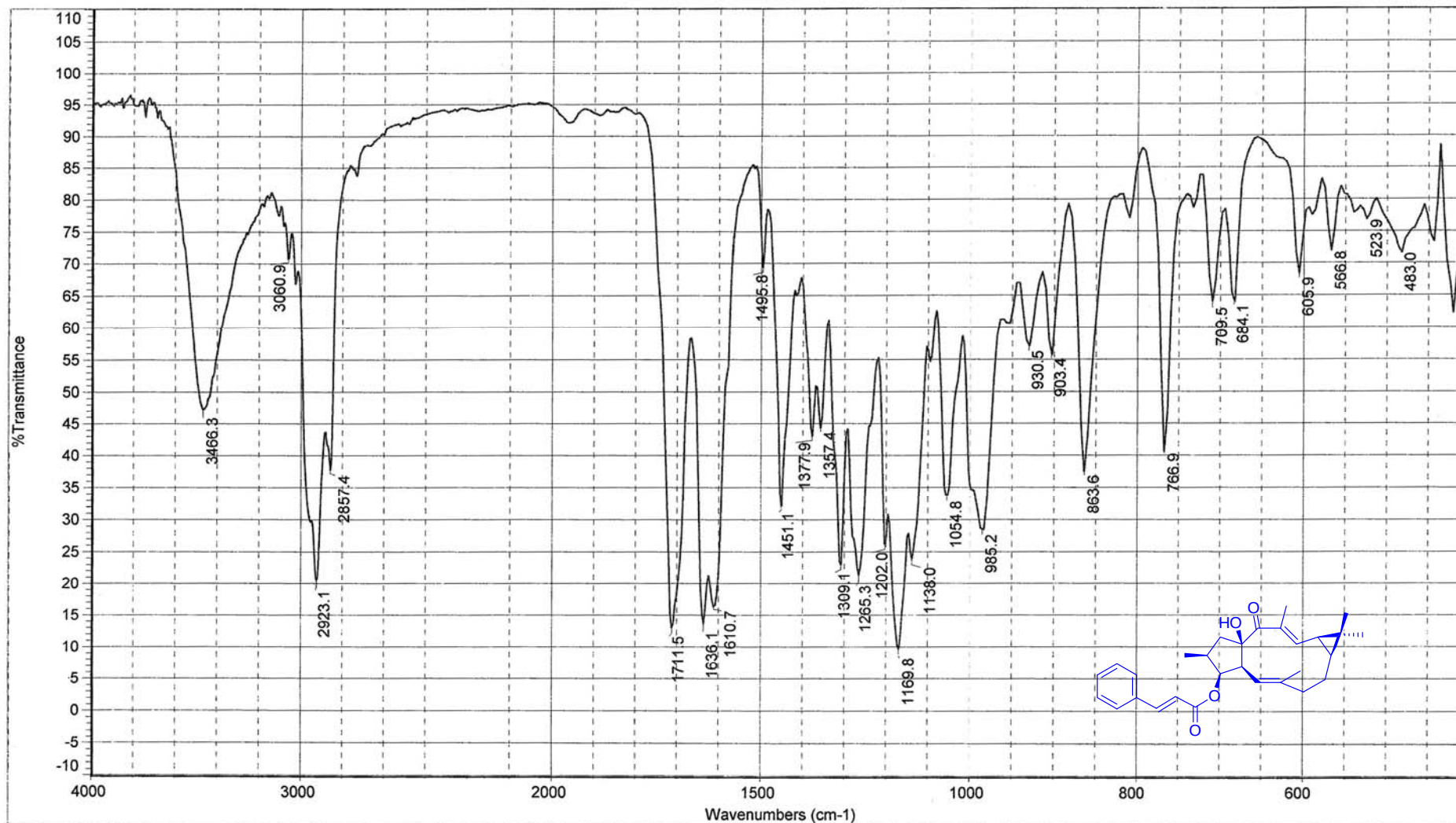
Tolerance:5.00(mmu)

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

Element:¹²C:0 .. 100, ¹H:0 .. 200, ²³Na:1 .. 1, ¹⁶O:0 .. 10

Mass	Mass Difference (mmu)	Mass Difference (ppm)	¹² C	¹ H	²³ Na	¹⁶ O	Unsaturation Number
471.25573	4.60	9.77	29	36	1	4	11.5
	-1.27	-2.70	22	40	1	9	2.5

(+)-HRESIMS Data of 9.



日期: 星期四 9月 25 16:47:30 2008 (GMT+08:00) Sample Name: E - 3 - 4

(显微镜透射法 FT- IR Microscope Transmission)

扫描次数: 100

傅里叶变换红外显微镜(FT-IR Microscope): Centaurus

分辨率: 8.000

美国热电公司(Thermo)傅里叶变换红外光谱仪:Nicolet 5700

Figure S79. The IR Spectrum of 9.
S91

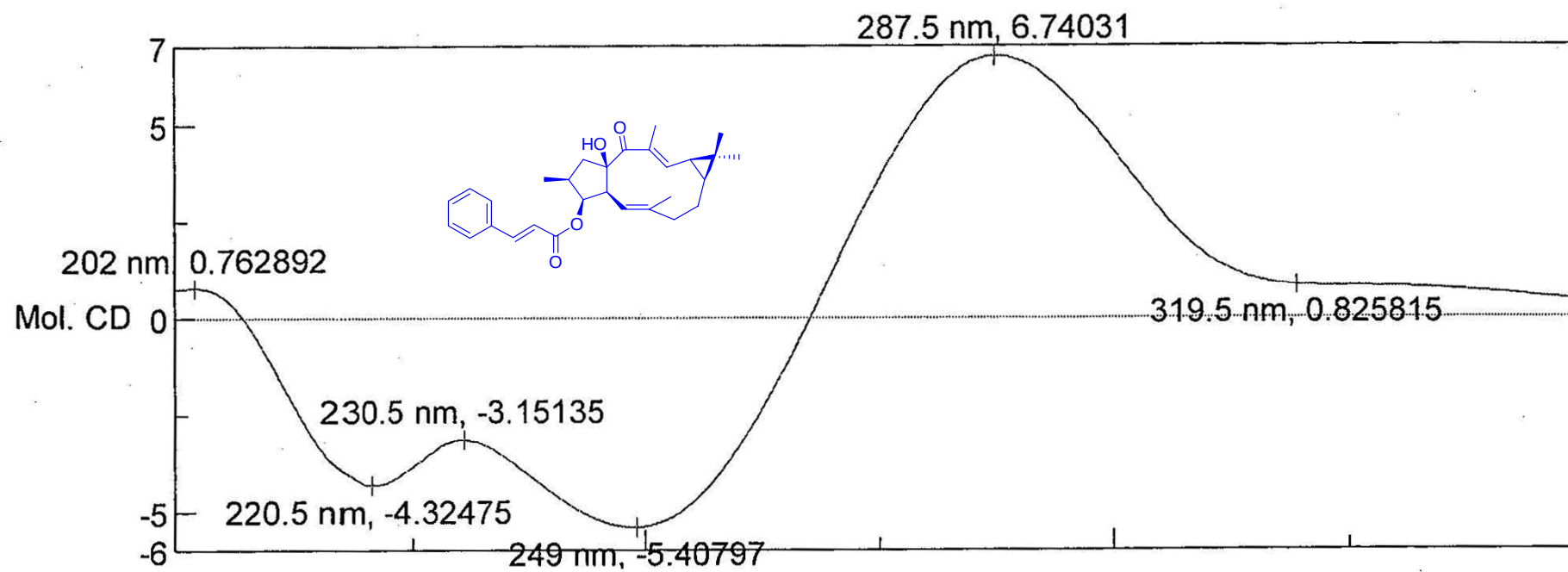


Figure S80. The CD Spectrum of 9.

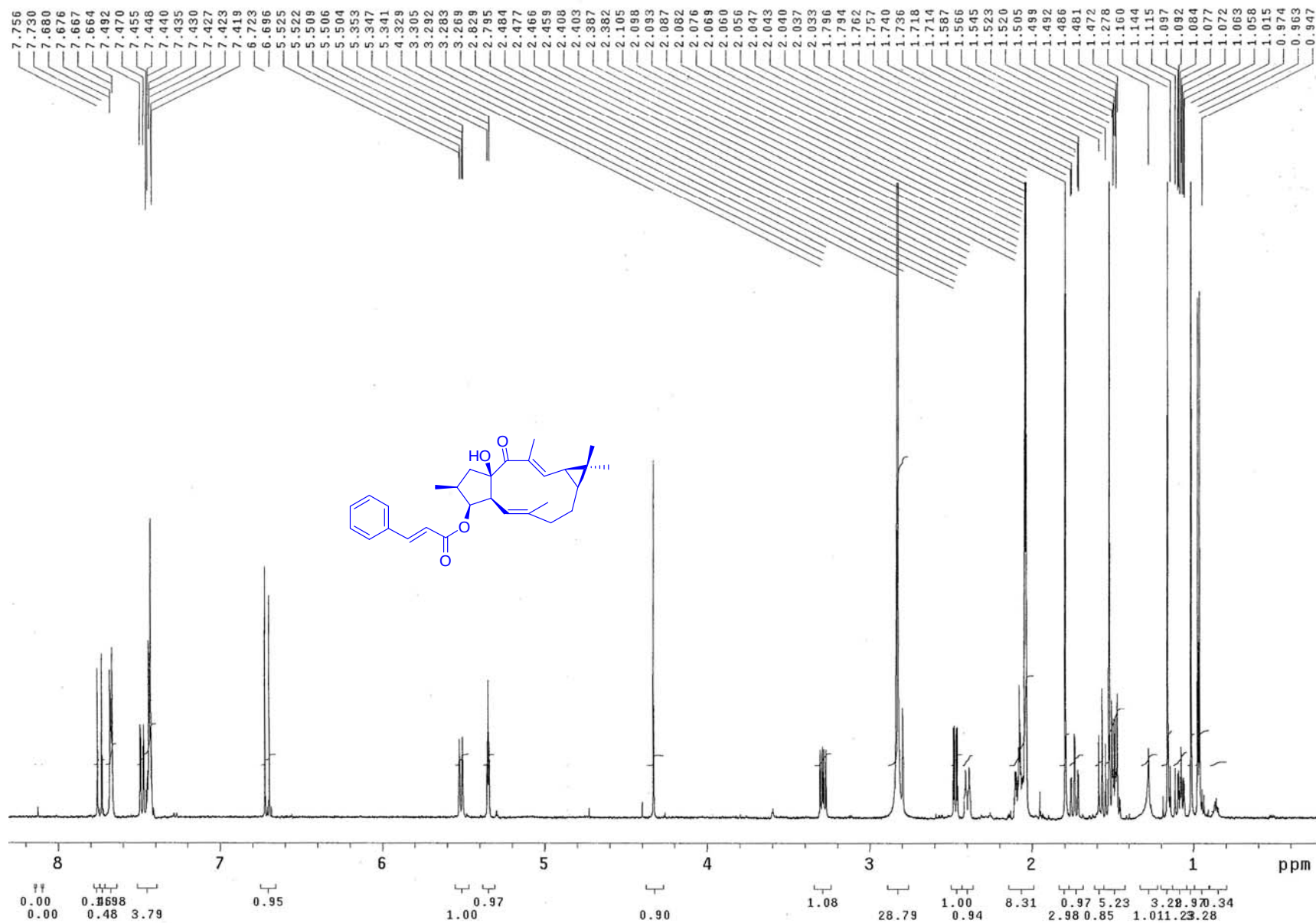


Figure S81. The ¹H NMR Spectrum of 9 in CD₃COCD₃ (600 MHz).

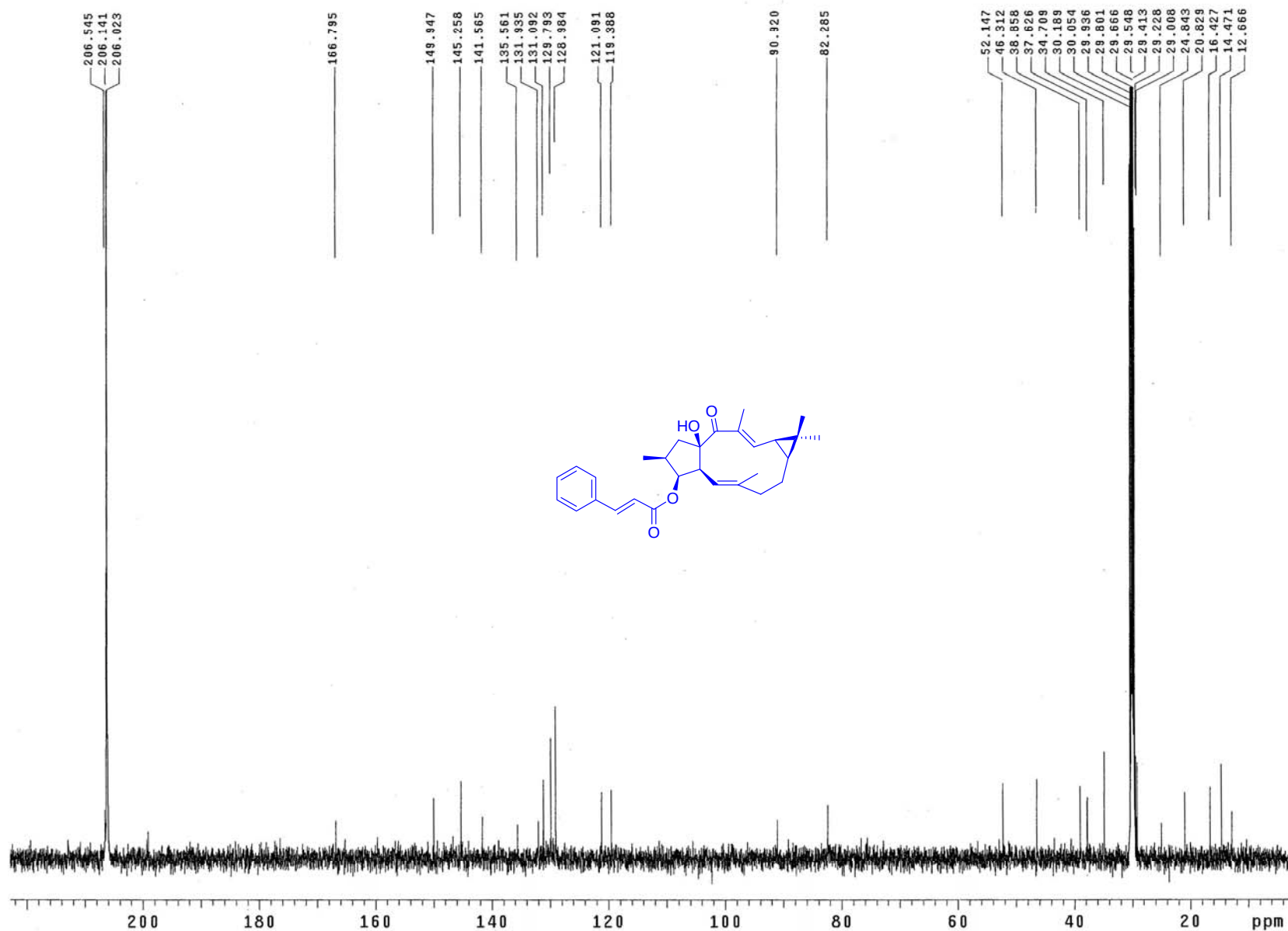


Figure S82. The ^{13}C NMR Spectrum of 9 in CD_3COCD_3 (150 MHz).

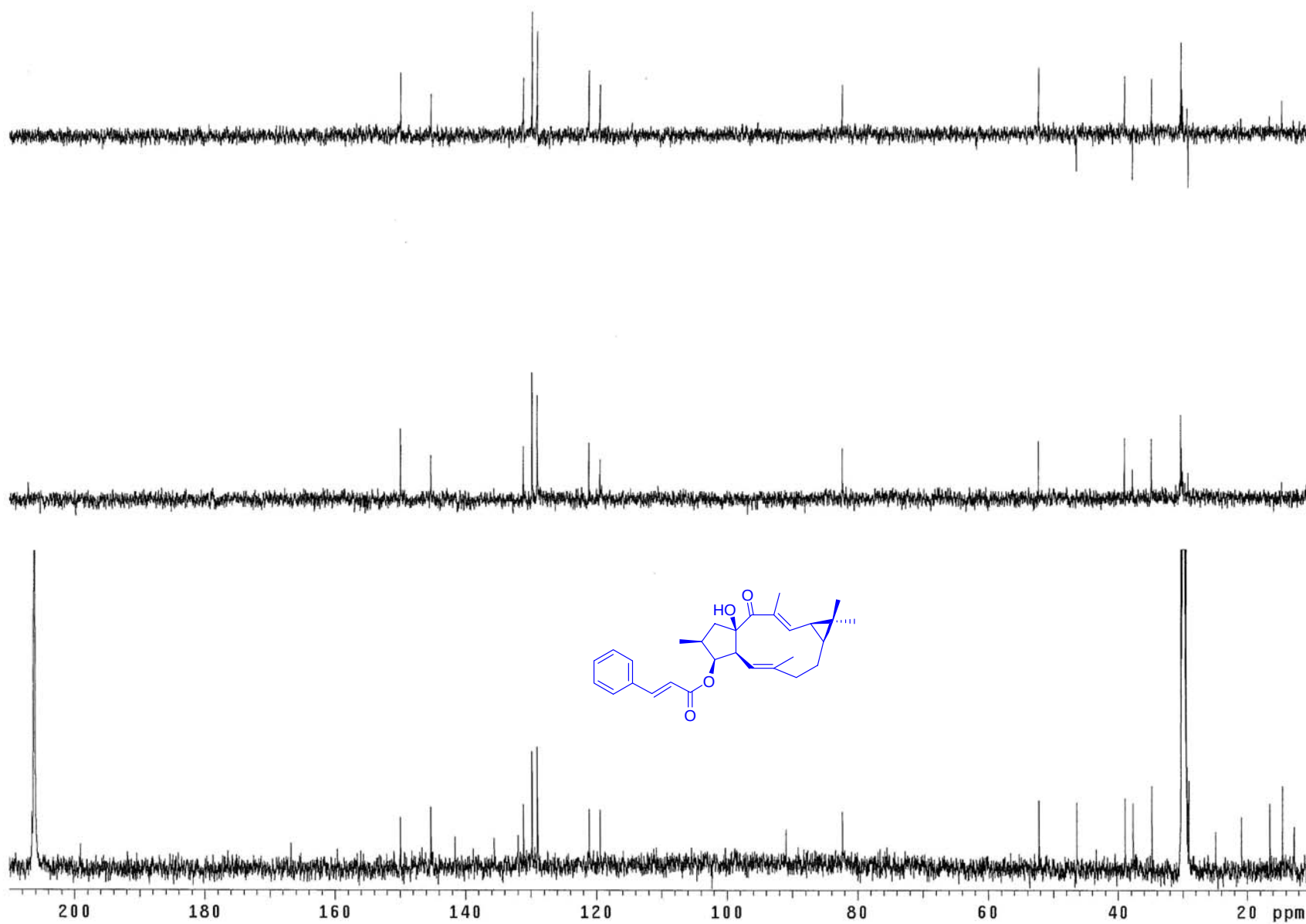


Figure S83. The DEPT Spectrum of 9 in CD₃COCD₃ (150 MHz).

SYS-600 gCOSY E-3-4 in CD3COCD3 08.01.29

Solvent: acetone
Ambient temperature
Operator: vnmr2
VNMRS-600 "wormhole"

Relax. delay 1.301 sec
Acq. time 0.215 sec
Width 4771.0 Hz
2D Width 4771.0 Hz
2 repetitions
256 increments
OBSERVE H1, 599.6981356 MHz
DATA PROCESSING
Sine bell 0.099 sec
F1 DATA PROCESSING
Sine bell 0.027 sec
FT size 2048 x 2048
Total time 13 min, 40 sec

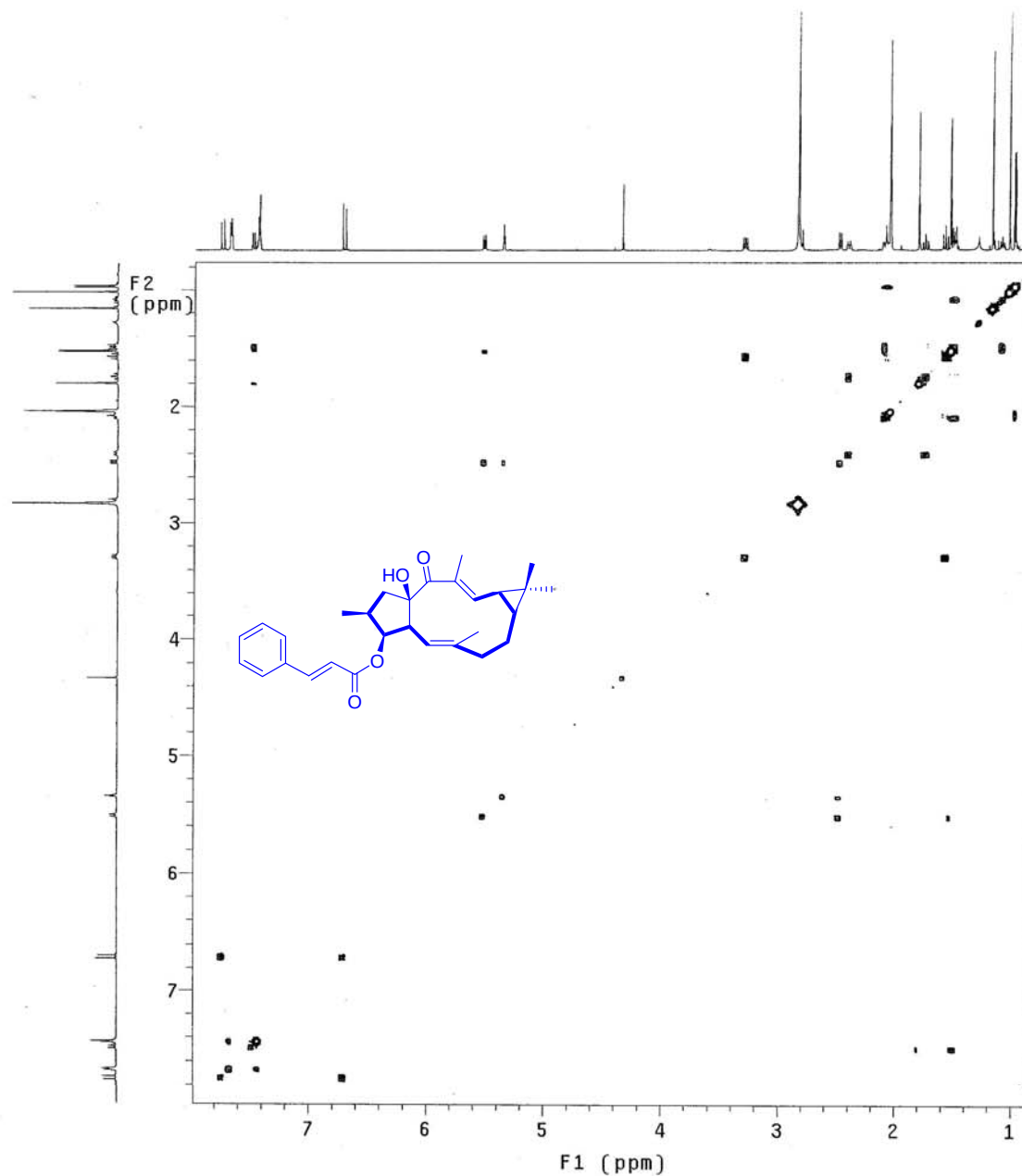


Figure S84. The ^1H - ^1H gCOSY Spectrum of 9 in CD_3COCD_3 (600 MHz).

Solvent: acetone
Ambient temperature
Operator: vnmr2
VNMR5-600 "wormhole"

Relax. delay 1.301 sec
Acq. time 0.199 sec
Width 5020.1 Hz
2D Width 25000.0 Hz
80 repetitions
160 increments
OBSERVE H1, 599.6981281 MHz
DECOUPLE C13, 150.8075646 MHz
Power 42 dB
on during acquisition
off during delay
GARP-1 modulated
DATA PROCESSING
Sine bell 0.041 sec
F1 DATA PROCESSING
Sine bell 0.003 sec
FT size 2048 x 8192
Total time 5 hr, 32 min, 10 sec

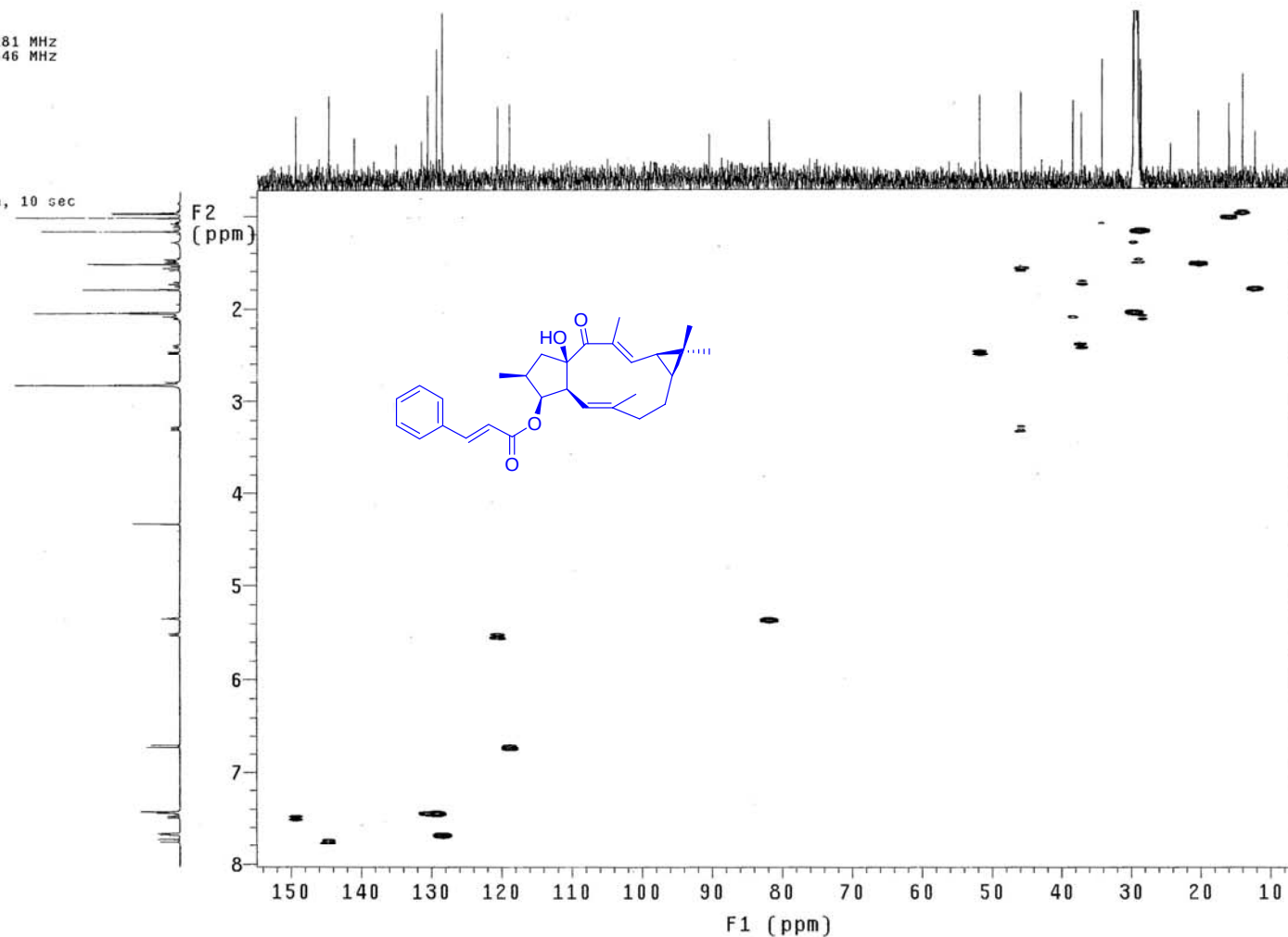


Figure S85. The gHSQC Spectrum of 9 in CD₃COCD₃ (600MHz for ¹H NMR).

SYS-600 gHMBC E-3-4 in CD3COCD3 08.01.29

Solvent: acetone
Ambient temperature
Operator: vnmr2
VNMRS-600 "wormhole"

Relax. delay 1.000 sec
Mixing 0.080 sec
Acq. time 0.128 sec
Width 4699.2 Hz
2D Width 32894.7 Hz
128 repetitions
256 increments
OBSERVE H1, 599.6981281 MHz
DATA PROCESSING
Sine bell 0.028 sec
F1 DATA PROCESSING
Sine bell 0.004 sec
FT size 2048 x 8192
Total time 11 hr, 3 min, 24 sec

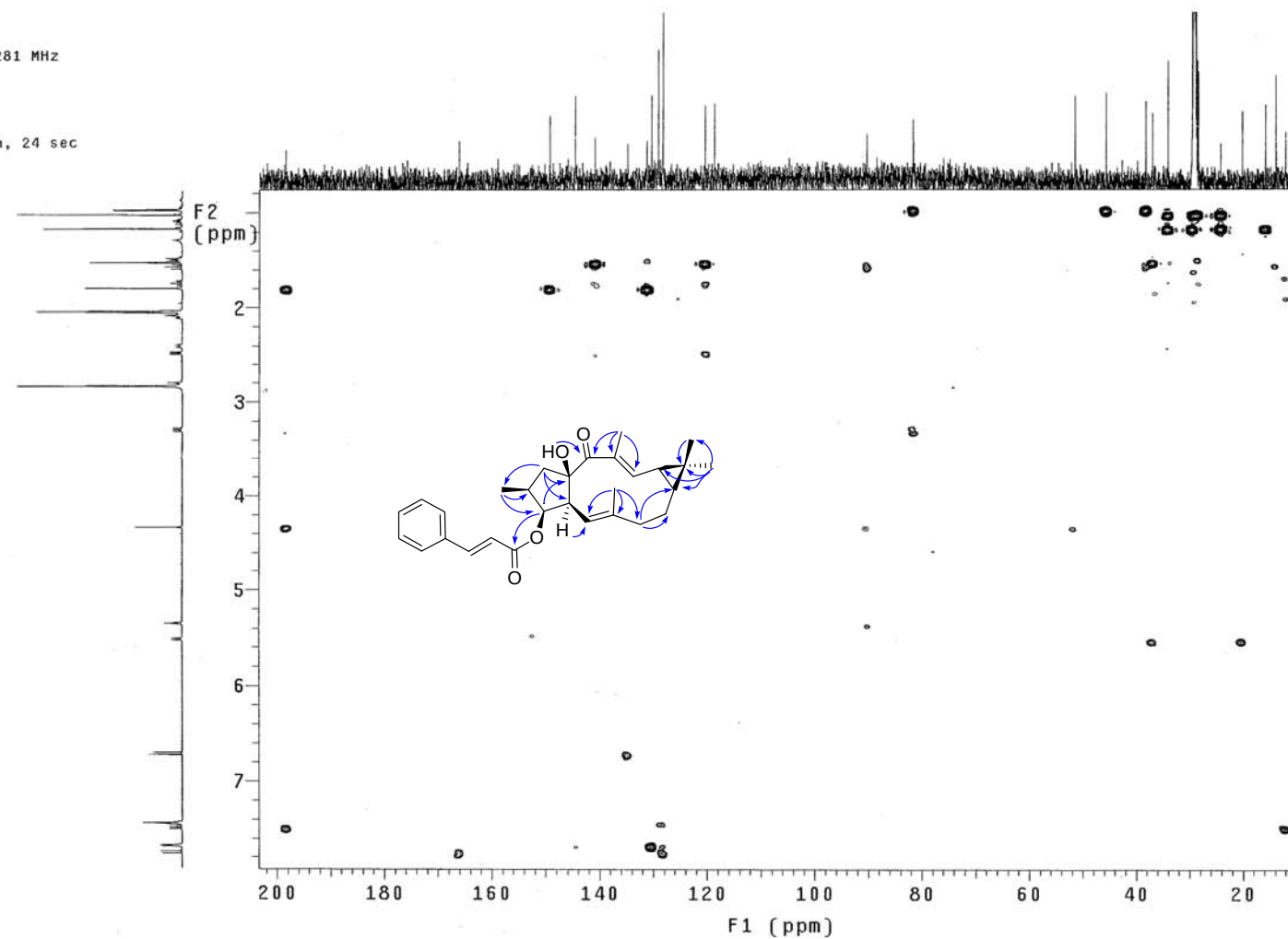


Figure S86. The gHMBC Spectrum of 9 in CD₃COCD₃ (600MHz for ¹H NMR).
S98

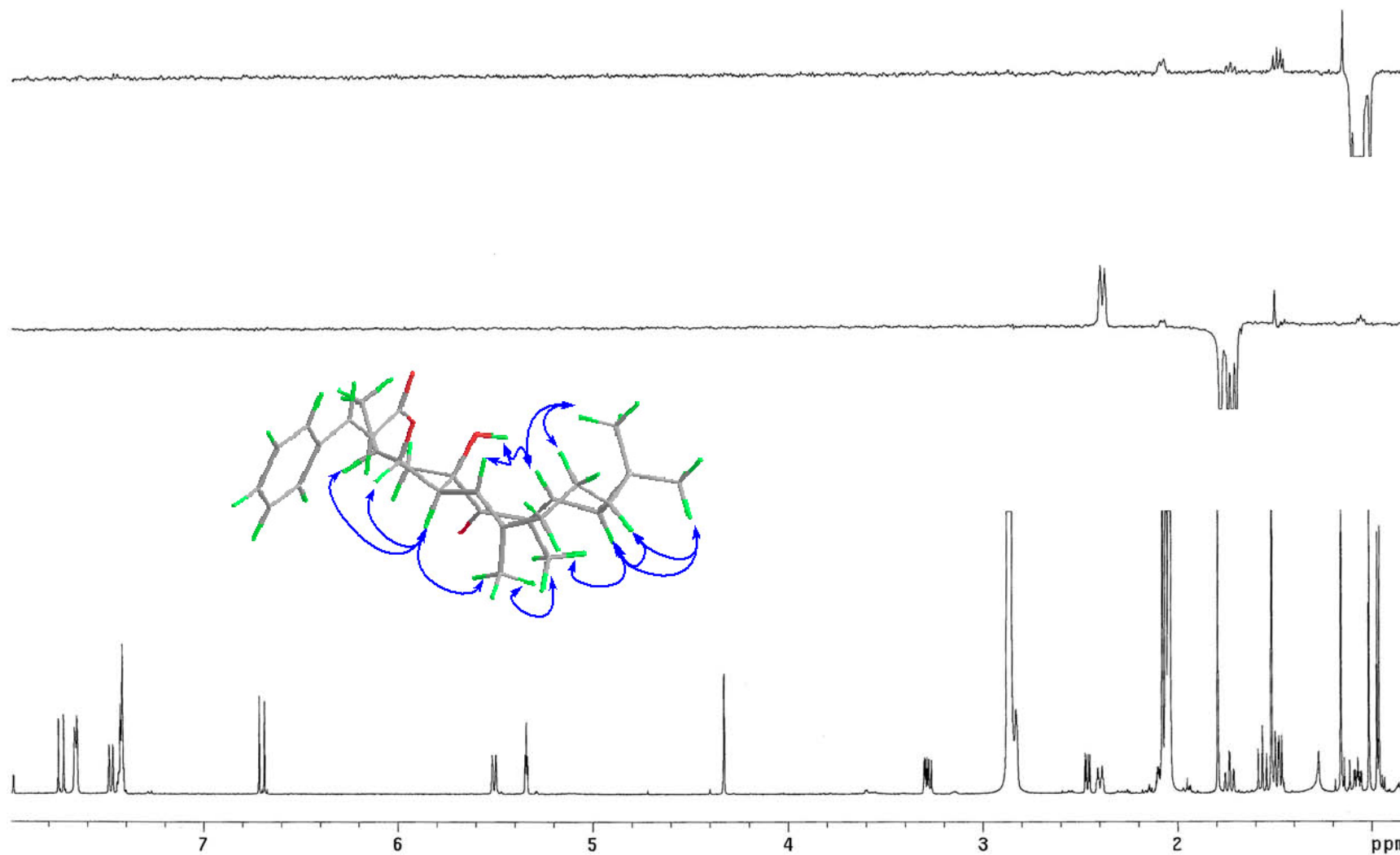


Figure S87. The NOE Difference Spectrum 1 of 9 in CD₃COCD₃ (600 MHz).

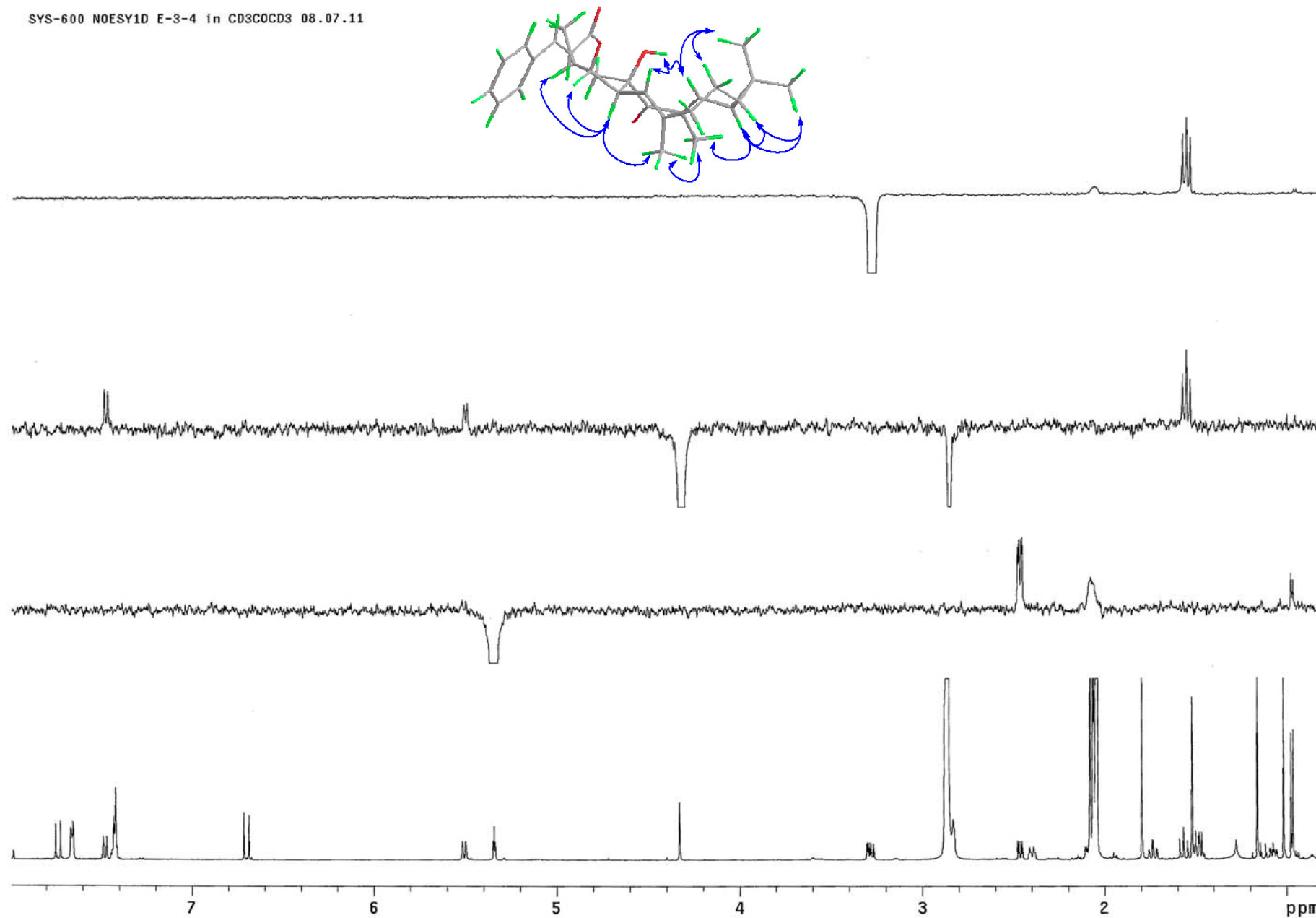


Figure S88. The NOE Difference Spectrum 2 of 9 in CD₃COCD₃ (600 MHz).

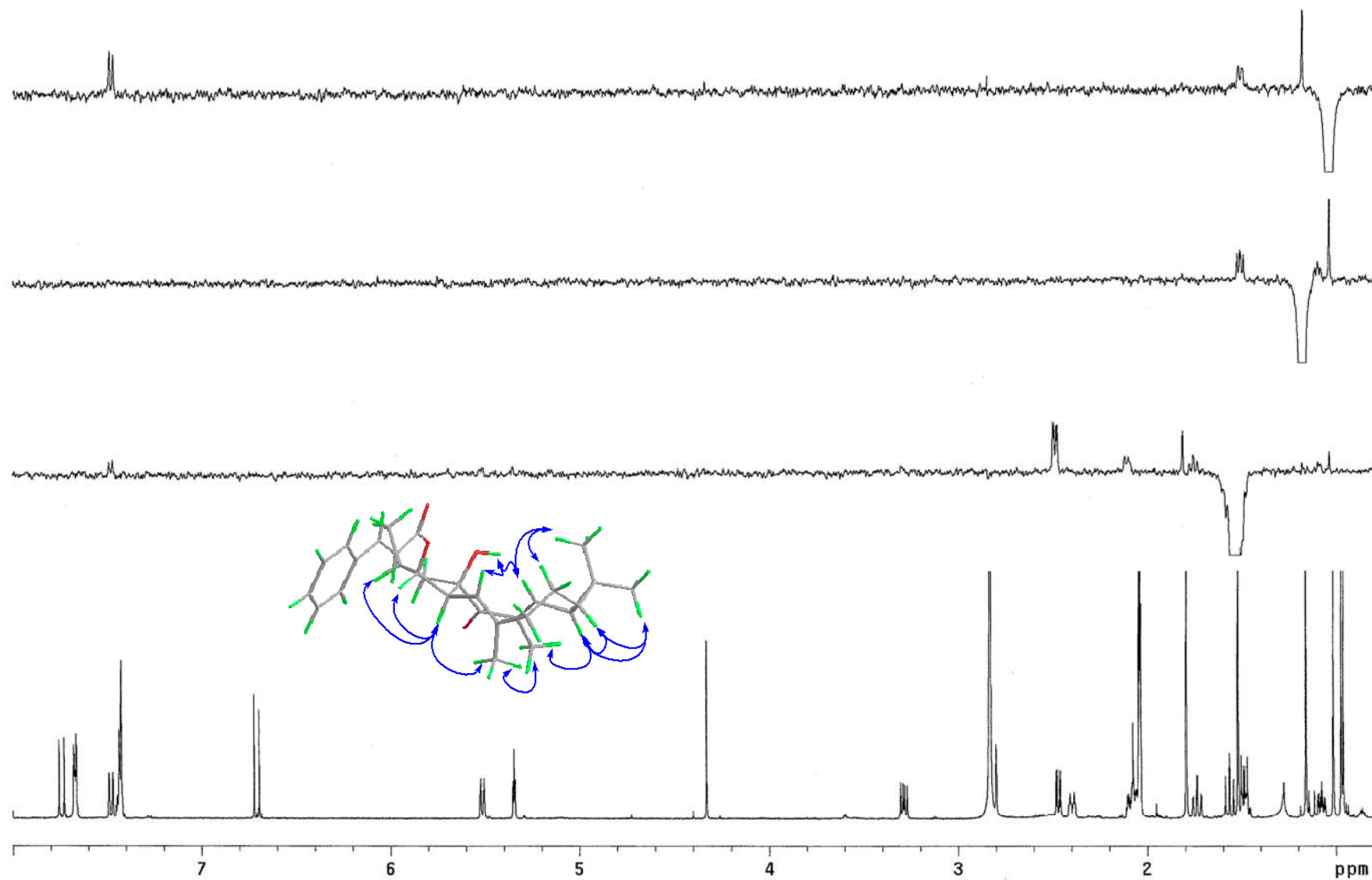


Figure S89. The NOE Difference Spectrum 3 of 9 in CD₃COCD₃ (600 MHz).

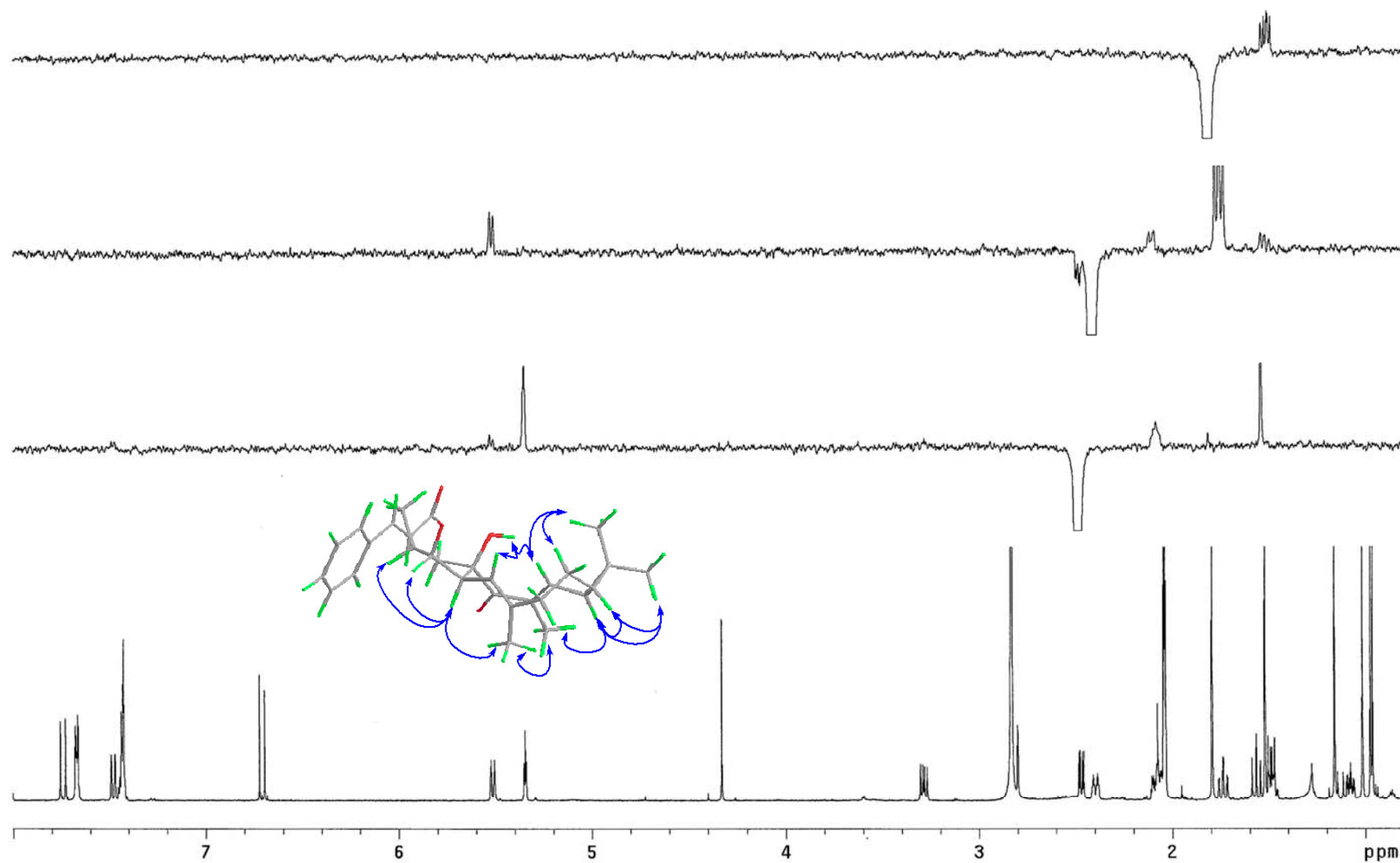


Figure S90. The NOE Difference Spectrum 4 of 9 in CD₃COCD₃ (600 MHz).
S102

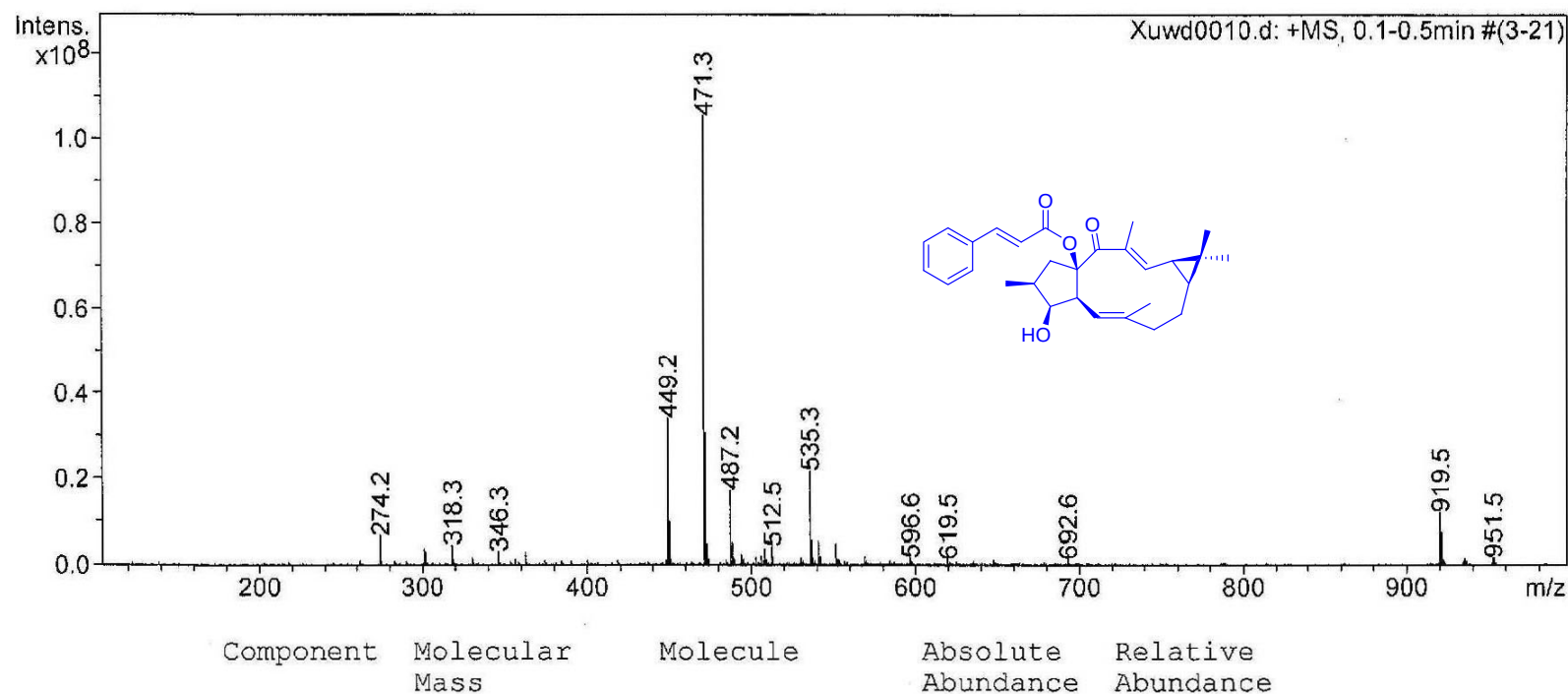


Figure S91. (+)-ESIMS Spectrum of 10.

MS Formula Results: + Scan (9.601 min) Sub (200905201.d)

m/z		Ion	Formula	Abundance							
449.26977		(M+H)+	C29 H37 O4	515146.4							
Best		Formula (M)	Ion Formula	Score	Cr	Calc m/z	Diff (ppm)	Mass Ma	Abund M	Spacing	DBE
☒		C29 H36 O4	C29 H37 O4	96.21		449.26864	-2.53	93.91	96.98	99.87	12
m/z		Ion	Formula	Abundance							
471.25179		(M+Na)+	C29 H36 Na O4	744389.3							
Best		Formula (M)	Ion Formula	Score	Cr	Calc m/z	Diff (ppm)	Mass Ma	Abund M	Spacing	DBE
☒		C29 H36 O4	C29 H36 Na O4	96.12		471.25058	-2.67	93.55	98.31	98.62	12

(+)-HRESIMS Data of 10.

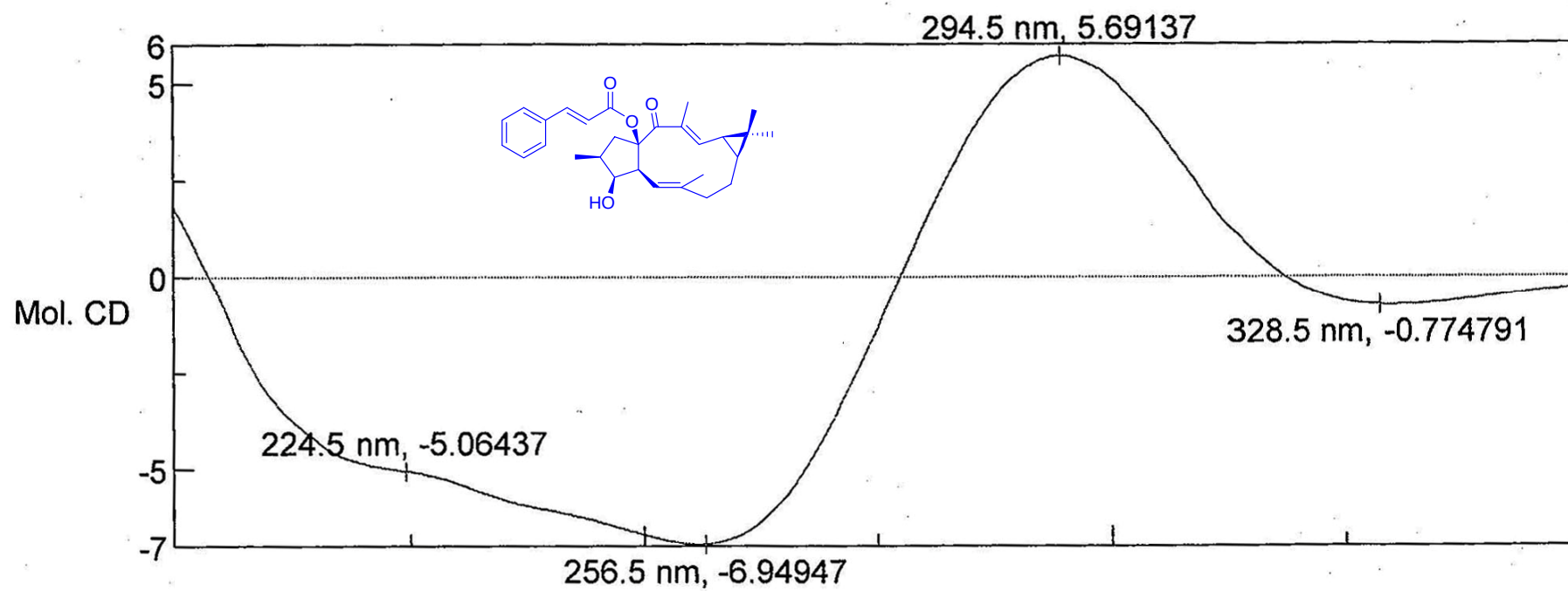


Figure S93. The CD Spectrum of 10.

S106

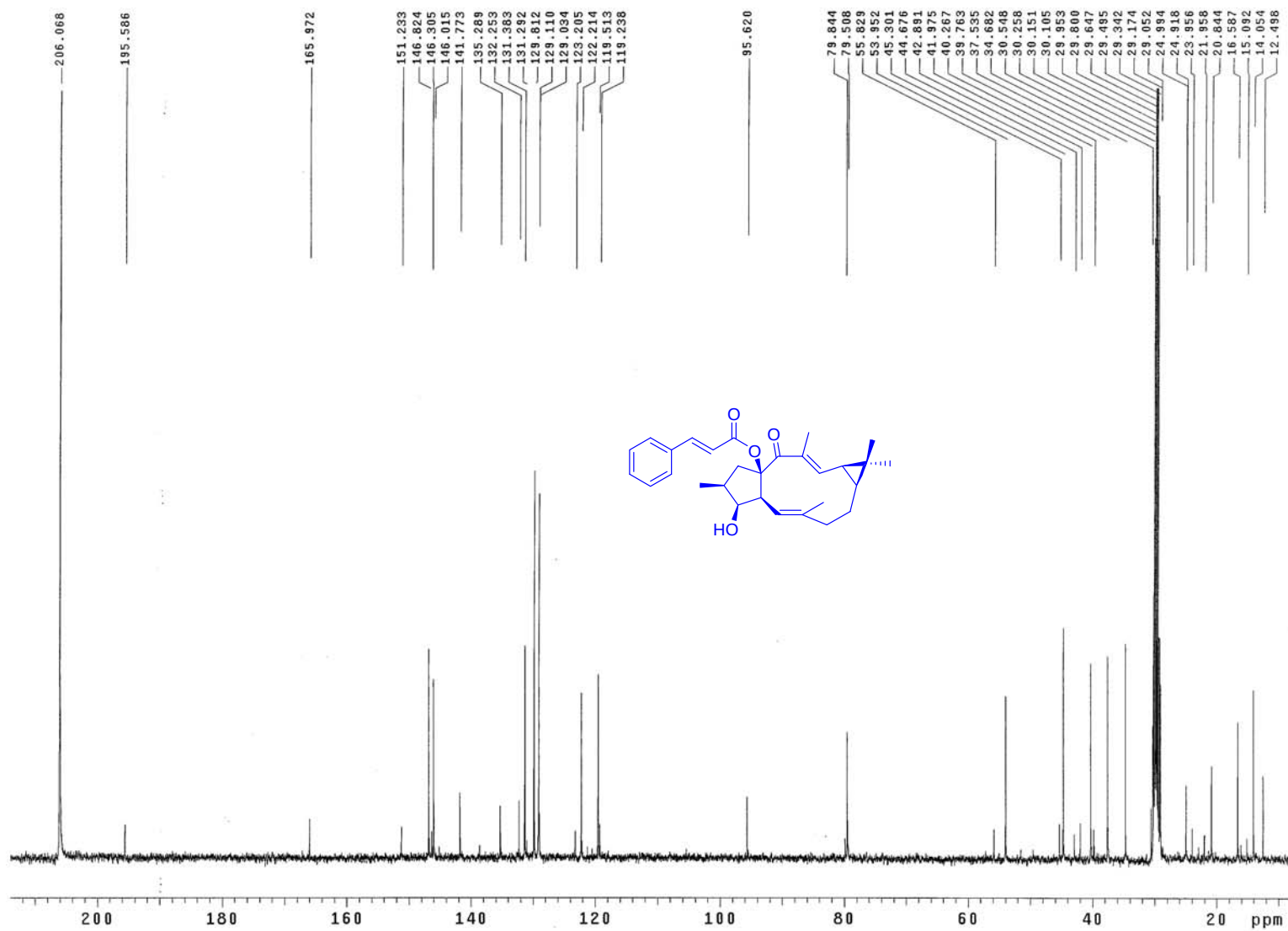


Figure S95. The ¹³C NMR Spectrum of 10 in CD₃COCD₃ (125 MHz).

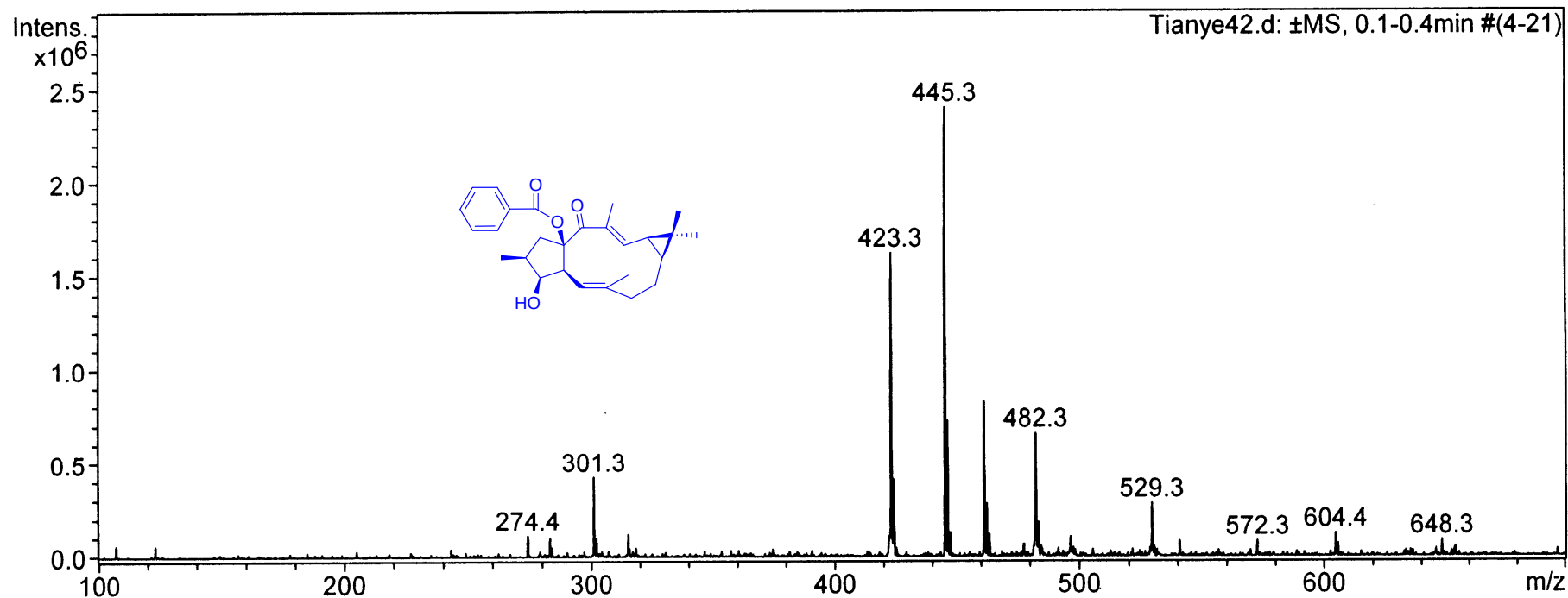


Figure S96. The (+)-ESIMS Spectrum of 11.

MS Formula Results: + Scan (8.263 min) Sub (201011152.d)

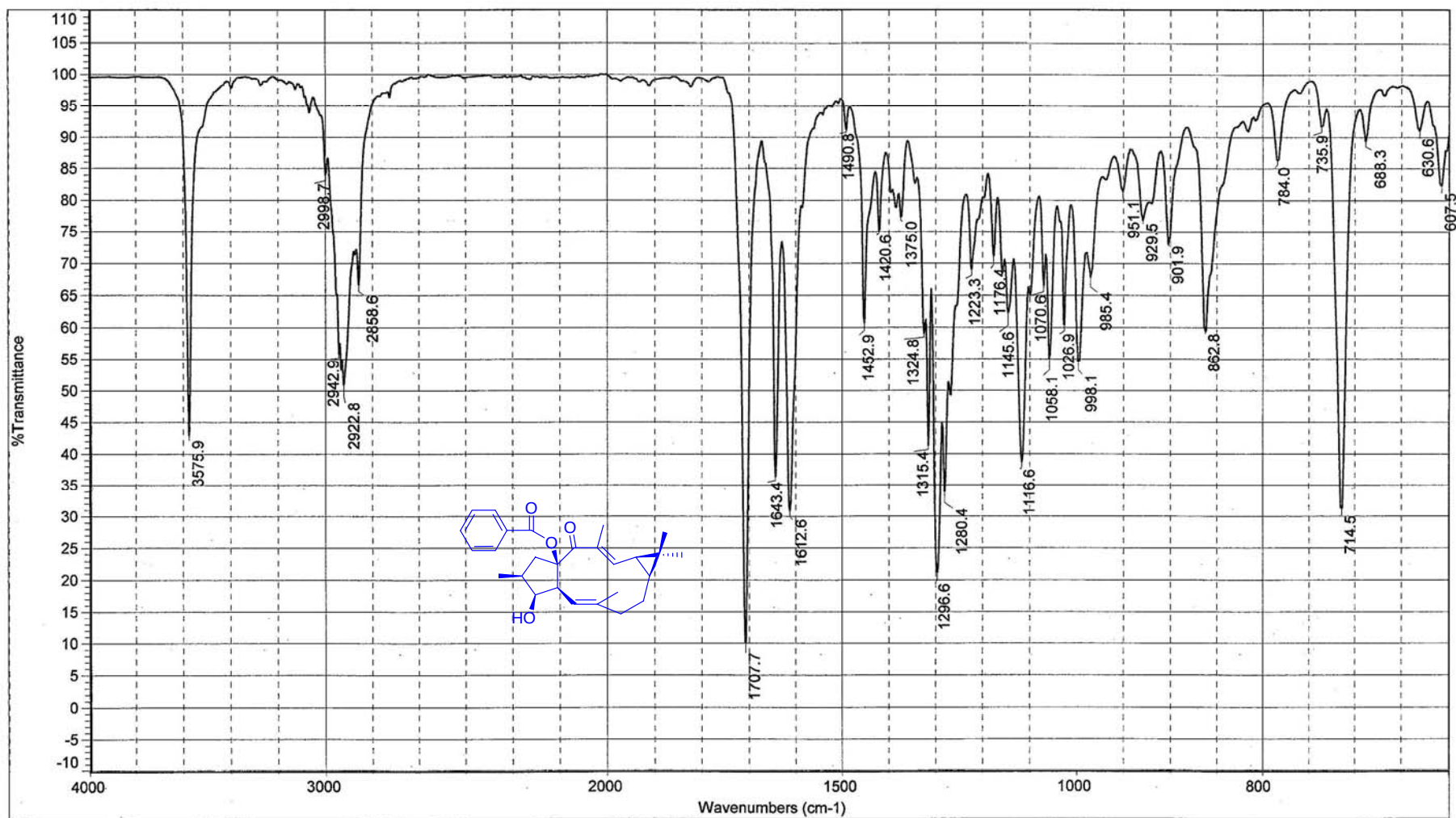
m/z	Ion	Formula	Abundance
423.2527	(M+H) ⁺	C ₂₇ H ₃₅ O ₄	959463.4

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross S	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Mat	Mass Match	m/z	DBE
☒	C ₂₇ H ₃₄ O ₄	C ₂₇ H ₃₅ O ₄	423.253	99.92		422.2454	422.2457	0.74	0.74	99.77	99.99	99.98	423.2527	11
☐	C ₂₂ H ₃₄ N ₂ O ₆	C ₂₂ H ₃₅ N ₂ O ₆	423.249	97.92		422.2454	422.2417	-8.8	8.8	96.97	100	97.46	423.2527	7

m/z	Ion	Formula	Abundance
445.234	(M+Na) ⁺	C ₂₇ H ₃₄ NaO ₄	1424797.1

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross S	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Mat	Mass Match	m/z	DBE
☒	C ₂₇ H ₃₄ O ₄	C ₂₇ H ₃₄ NaO ₄	445.2349	99.82		422.2448	422.2457	2.05	2.05	99.62	99.95	99.87	445.234	11
☐	C ₂₂ H ₃₄ N ₂ O ₆	C ₂₂ H ₃₄ N ₂ NaO ₆	445.2309	98.16		422.2449	422.2417	-7.49	7.49	96.44	99.91	98.31	445.234	7

(+)-HRESIMS Data of 11.



日期: 星期四 12月 30 15:23:36 2010 (GMT+08:Sample Name : F6-3-1-1

(显微镜透射法FT- IR Microscope Transmission)

扫描次数: 64

分辨率: 4.000

美国热电公司(Thermo)傅里叶变换红外光谱仪:Nicolet 5700

Figure S97. The IR Spectrum of 11.

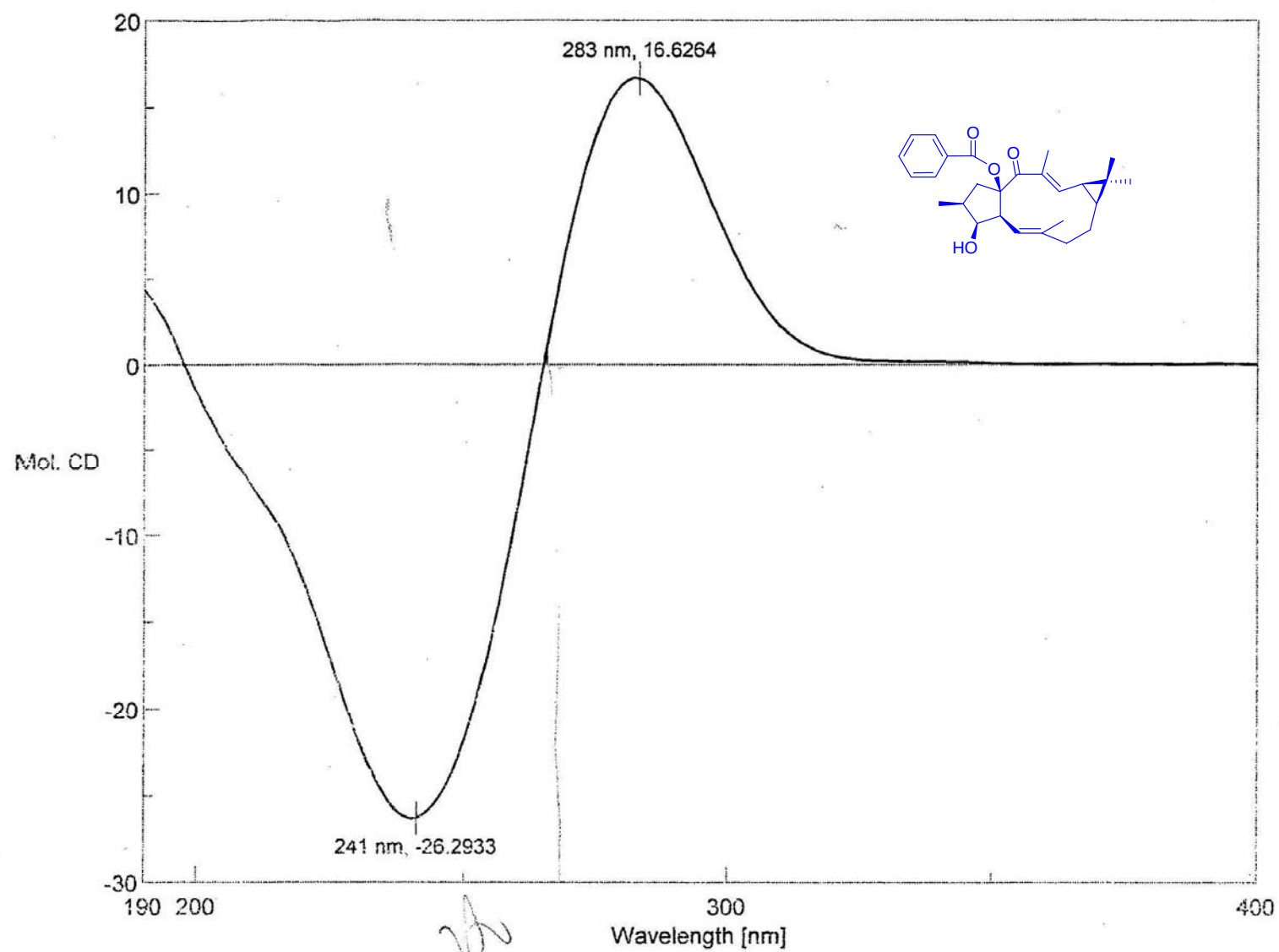


Figure S98. The CD Spectrum of 11.

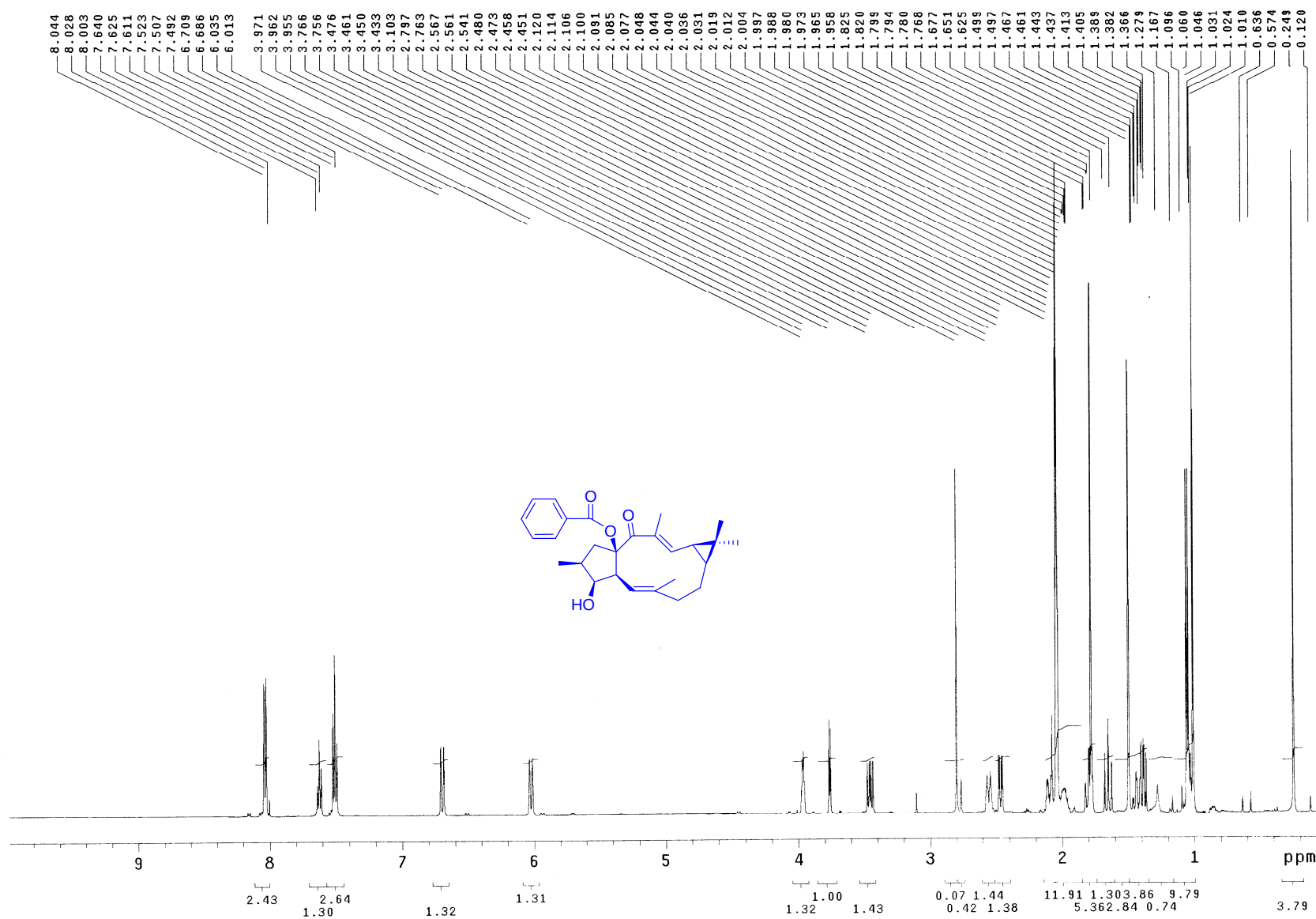


Figure S99. The ^1H NMR Spectrum of 11 in CD_3COCD_3 (500 MHz).

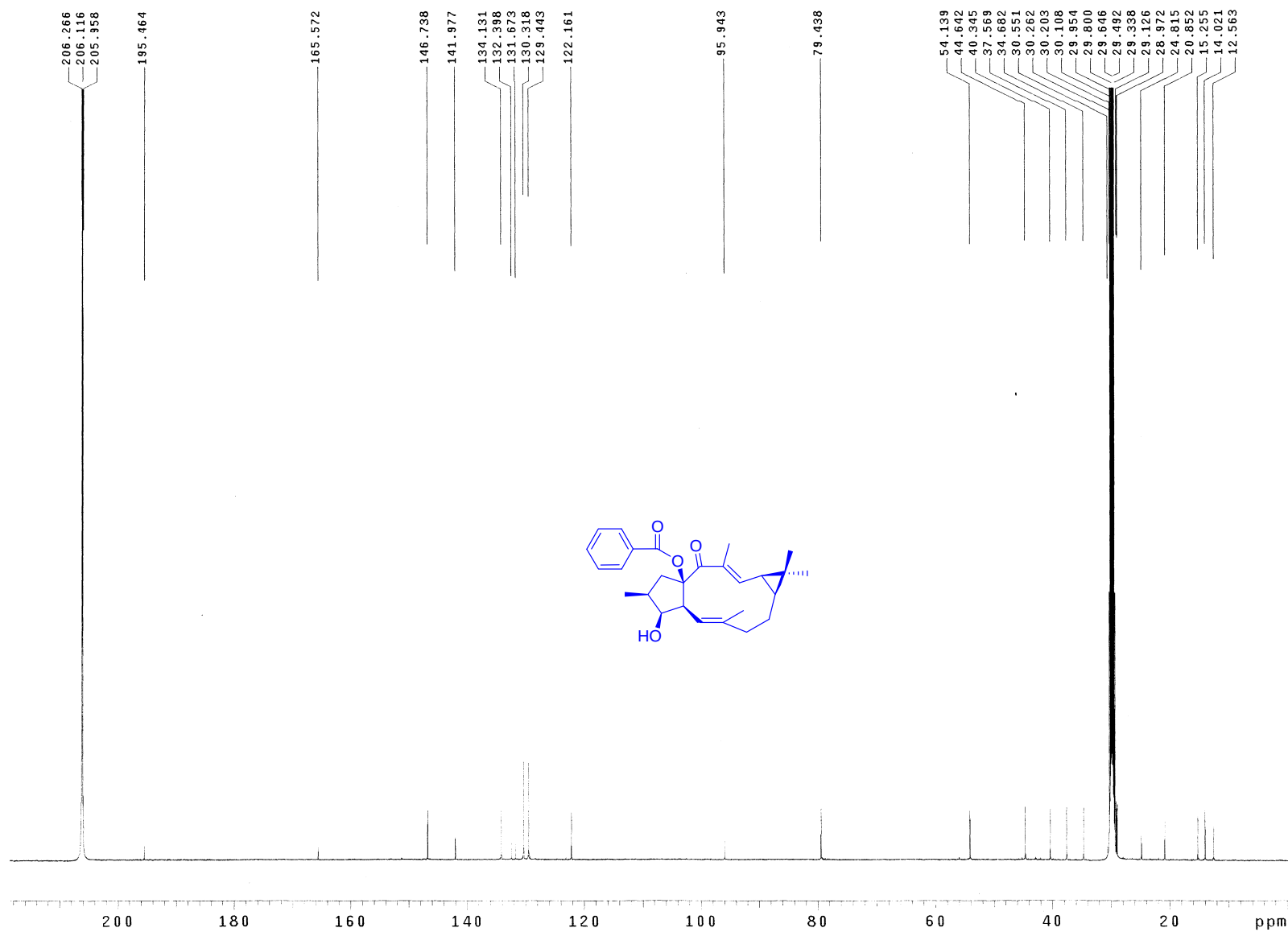


Figure S100. The ^{13}C NMR Spectrum of 11 in CD_3COCD_3 (125 MHz).
S112

INOVA-501 DEPT F6-3-1-1 IN CD3COCD3 09.06.04 cold probe

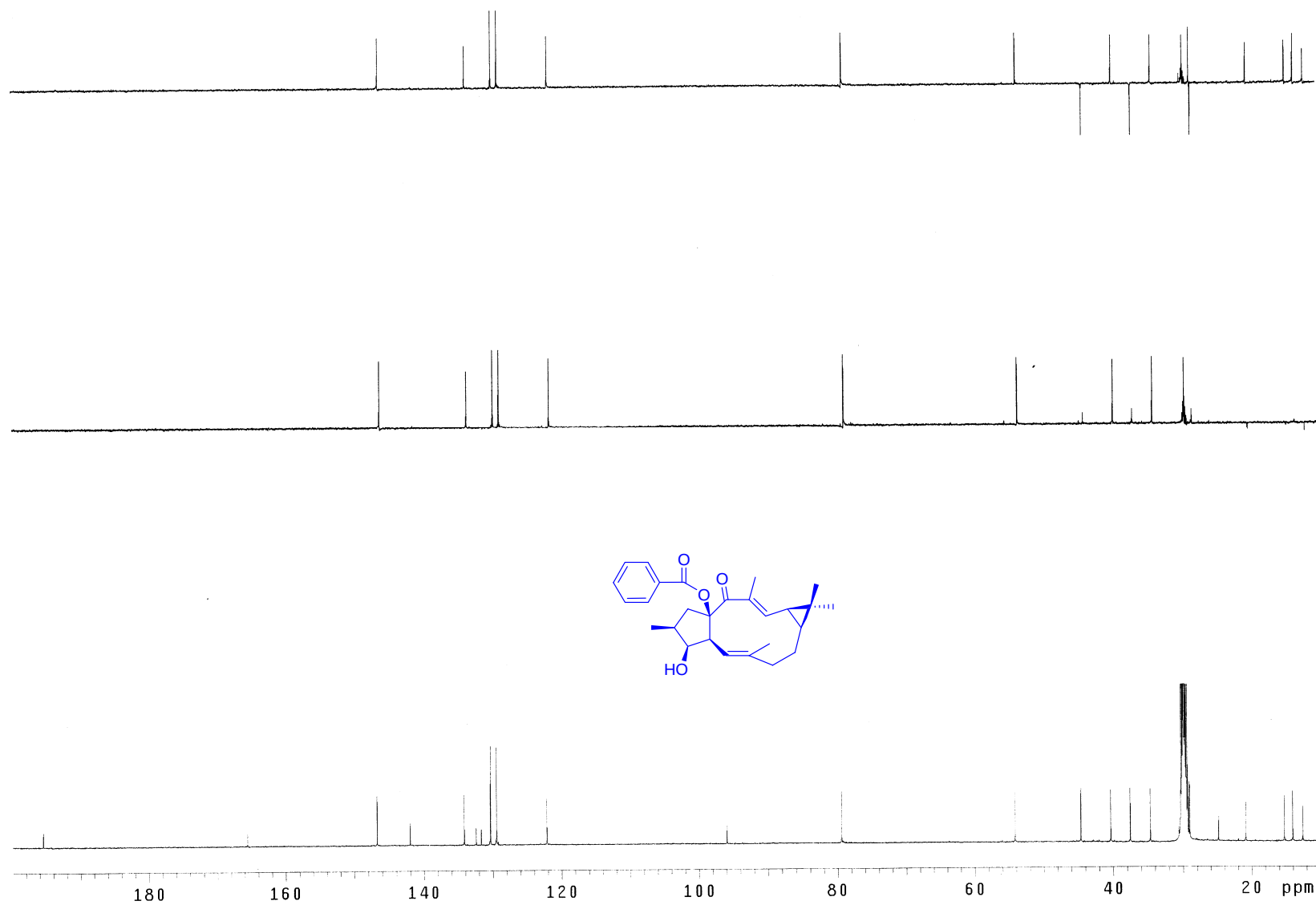


Figure S101. The DEPT Spectrum of 11 in CD₃COCD₃ (125 MHz).

S113

INOVA-501 gCOSY F6-3-1-1 IN CD3COCD3 09.06.04 cold probe

Solvent: acetone
Temp. 25.0 C / 298.1 K
Sample #6, Operator: walkup
File: Gcosy_01
INOVA-500 "IMM-501"

Relax. delay 1.301 sec
Acq. time 0.201 sec
Width 5102.0 Hz
2D Width 5102.0 Hz
2 repetitions
256 increments
OBSERVE H1, 499.7733193 MHz
DATA PROCESSING
Sine bell 0.100 sec
F1 DATA PROCESSING
Sine bell 0.026 sec
FT size 4096 x 4096
Total time 13 min, 32 sec

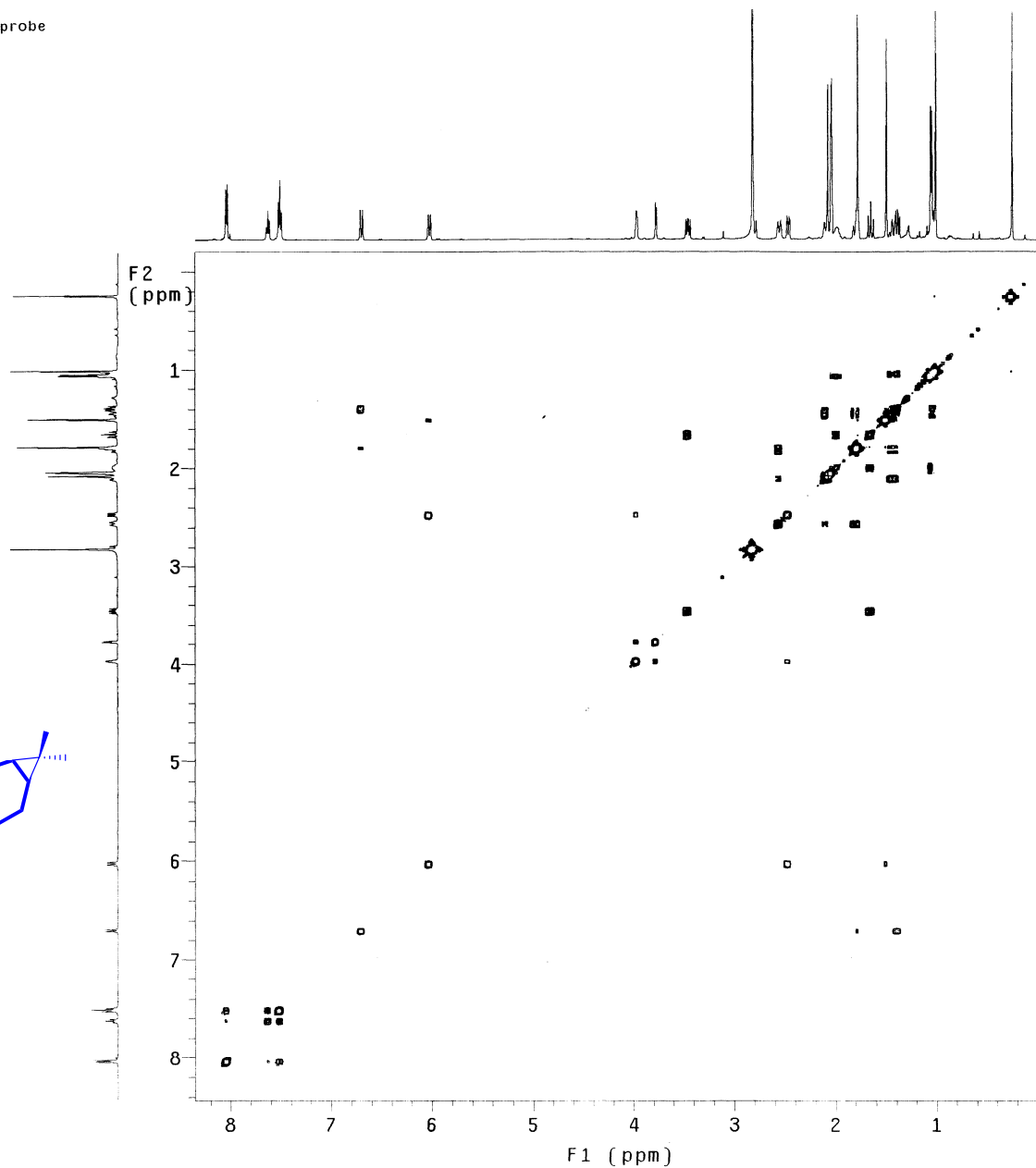
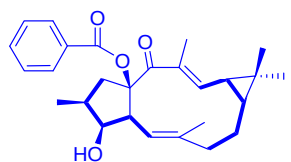


Figure S102. The ¹H-¹H gCOSY Spectrum of 11 in CD₃COCD₃ (500 MHz).

INOVA-501 gHSQC F6-3-1-1 IN CD3COCD3 09.06.04 cold probe

Solvent: acetone
Temp. 25.0 C / 298.1 K
Sample #6, Operator: walkup
File: Ghsqc_01
INOVA-500 "IMM-501"

Relax. delay 1.301 sec
Acq. time 0.199 sec
Width 5102.0 Hz
2D Width 25133.5 Hz
32 repetitions
2 x 128 increments
OBSERVE H1, 499.7733181 MHz
DECOUPLE C13, 125.6793772 MHz
Power 33 dB
on during acquisition
off during delay
W40_cold modulated
DATA PROCESSING
Sine bell 0.053 sec
F1 DATA PROCESSING
Sine bell 0.003 sec
FT size 4096 x 2048
Total time 3 hr, 32 min, 39 sec

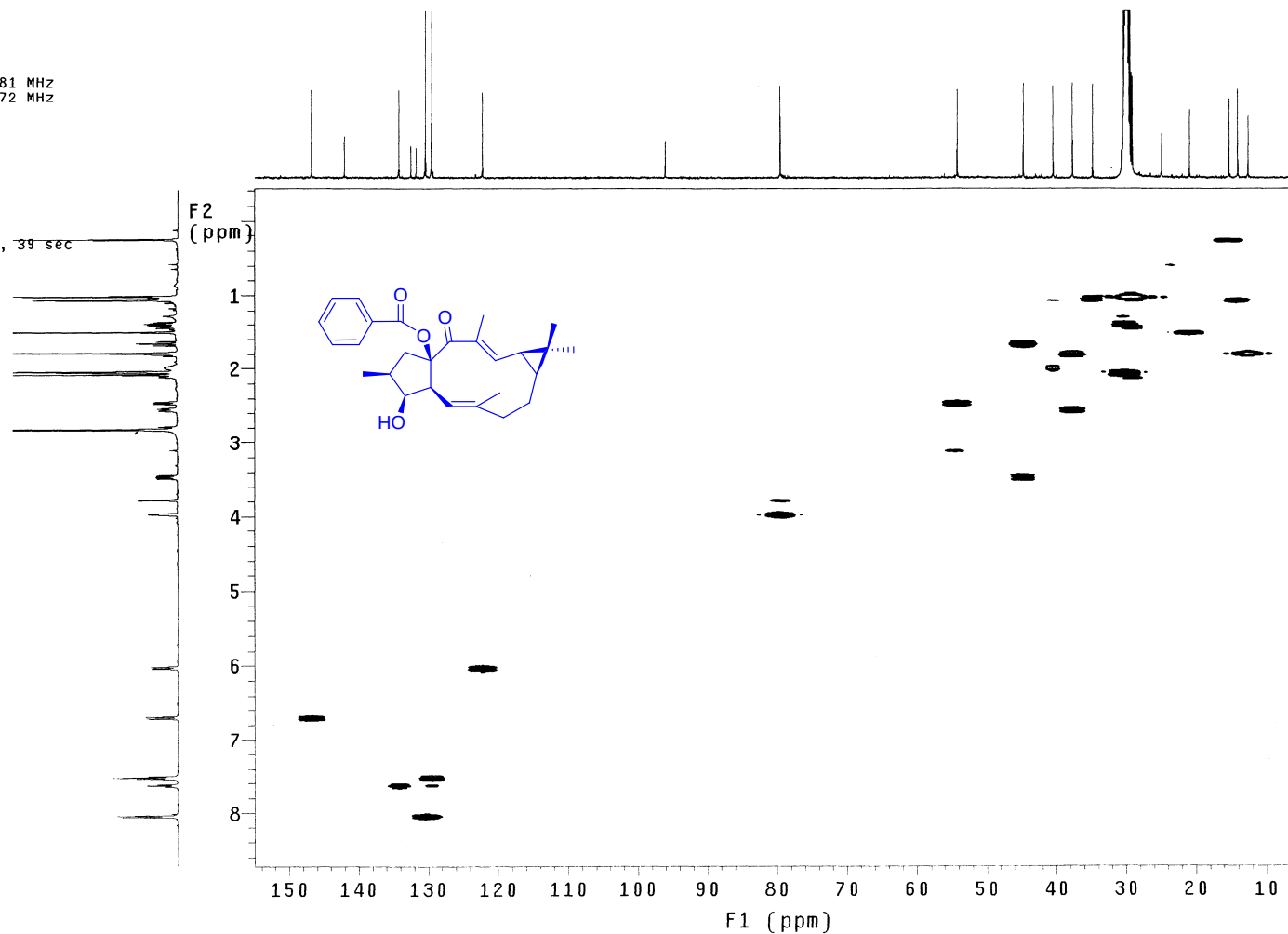


Figure S103. The gHSQC Spectrum of 11 in CD_3COCD_3 (500 MHz for ^1H NMR).

S115

Solvent: acetone
Temp. 25.0 C / 298.1 K
Sample #6, Operator: walkup
File: Ghmbc_01
INOVA-500 "1H-501"

Relax. delay 1.000 sec
Mixing 0.080 sec
Acq. time 0.128 sec
Width 5102.0 Hz
2D Width 30165.9 Hz
32 repetitions
256 increments
OBSERVE H1, 499.7733266 MHz
DATA PROCESSING
Sine bell 0.042 sec
F1 DATA PROCESSING
Sine bell 0.004 sec
FT size 2048 x 2048
Total time 2 hr, 46 min, 22 sec

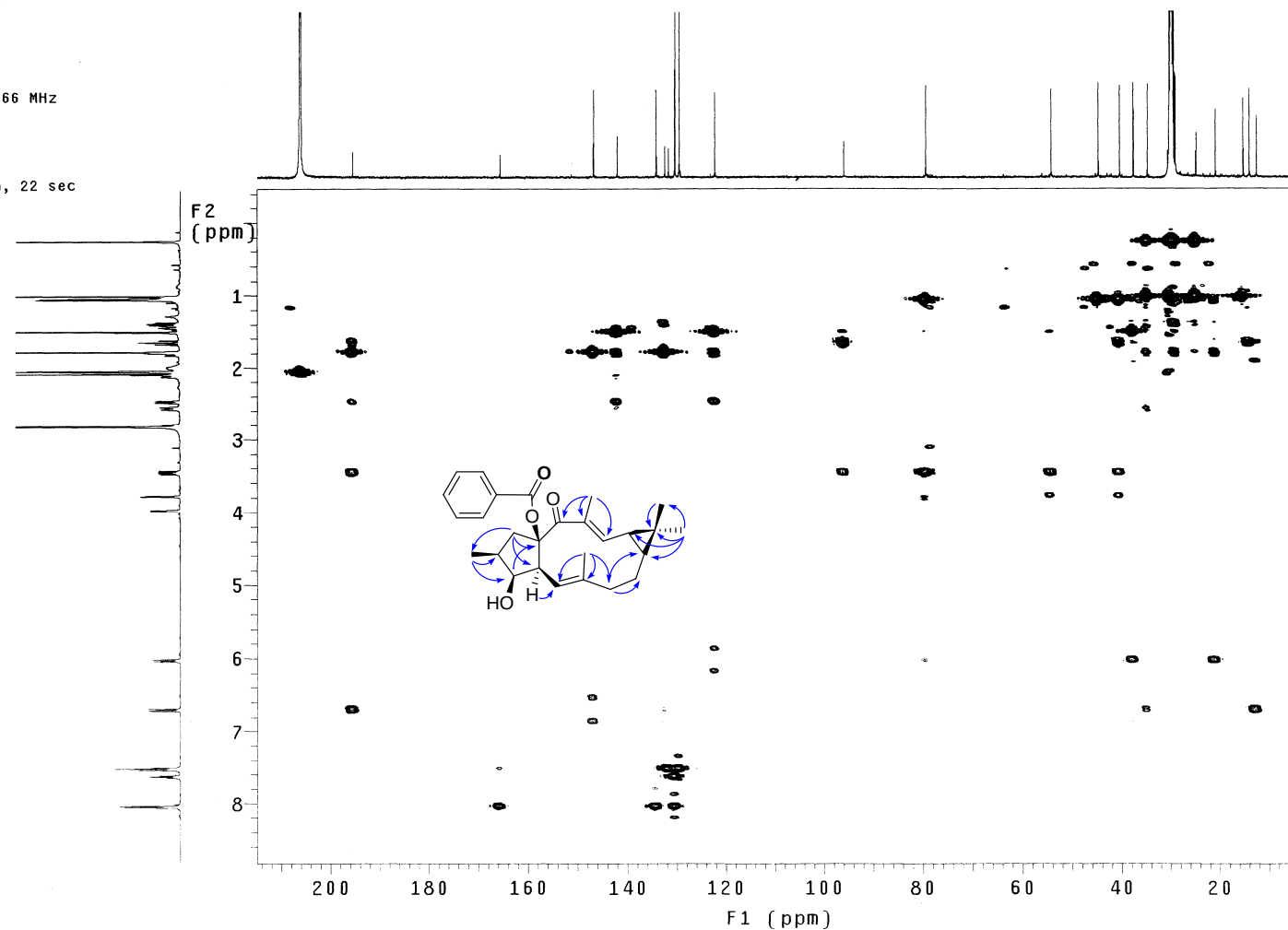


Figure S104. The gHMBC Spectrum of 11 in CD_3COCD_3 (500 MHz for ^1H NMR).

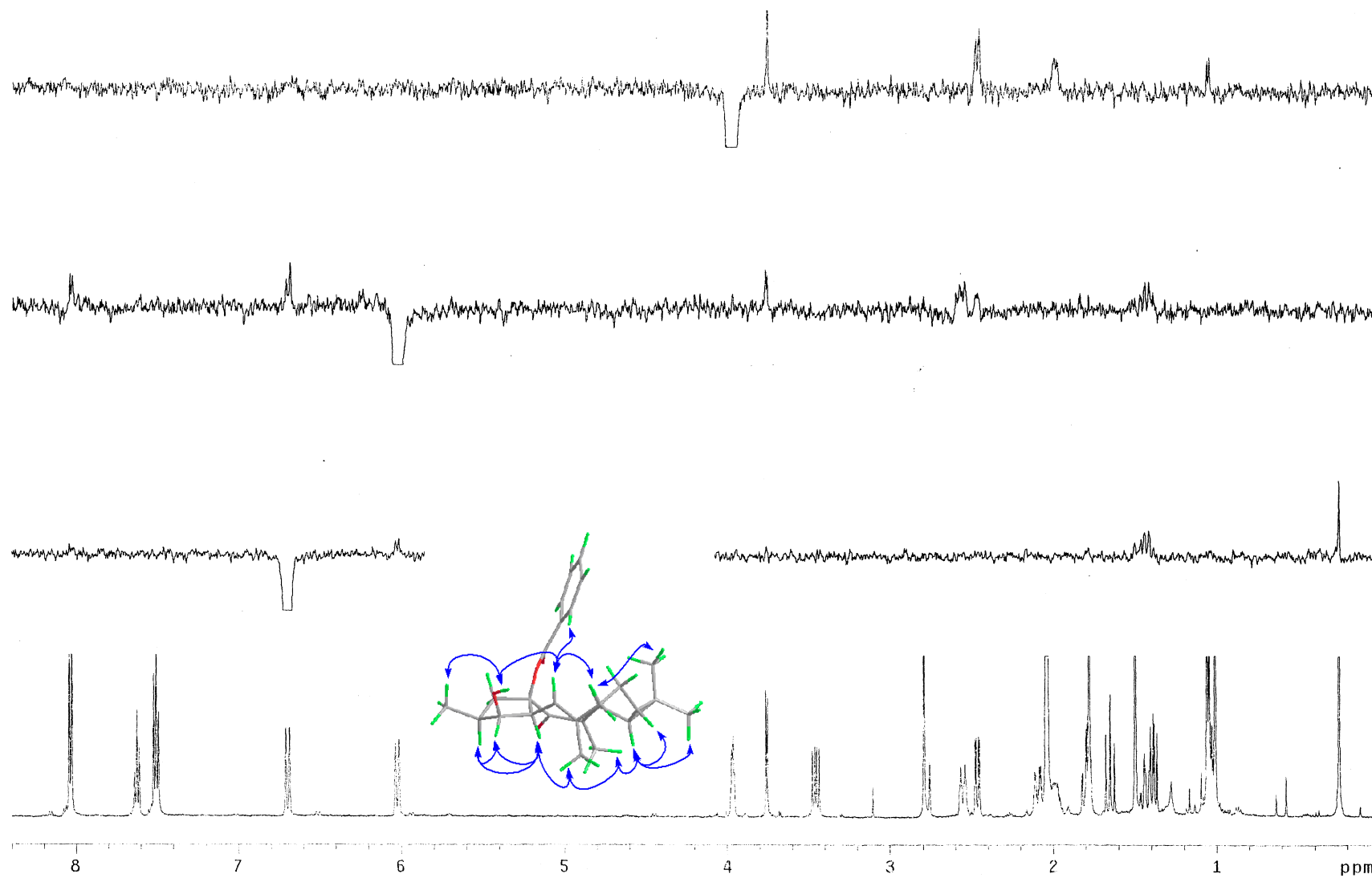


Figure S105. The NOE Difference Spectrum 1 of 11 in CD₃COCD₃ (500 MHz).

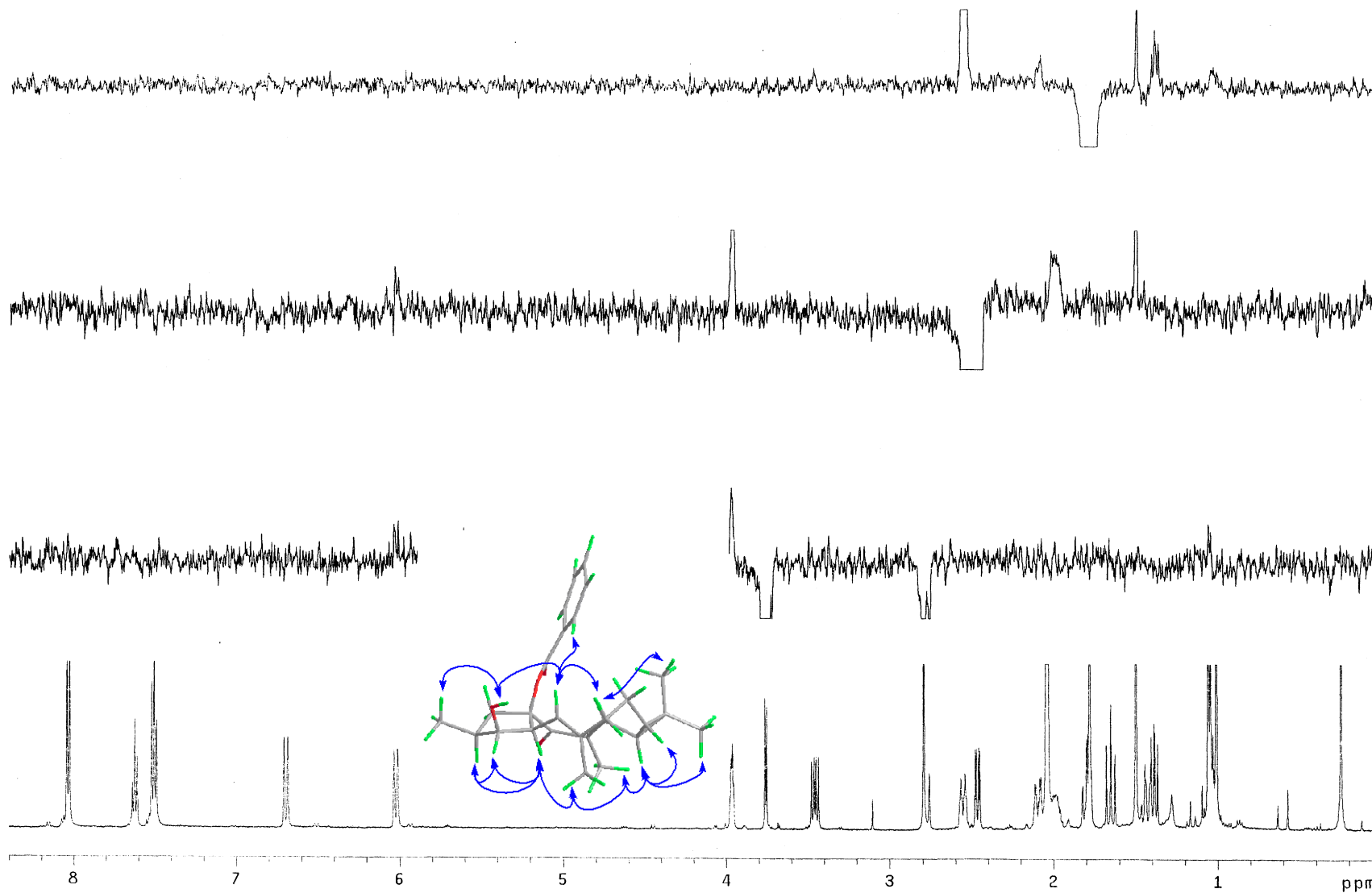


Figure S106. The NOE Difference Spectrum 2 of 11 in CD₃COCD₃ (500 MHz).

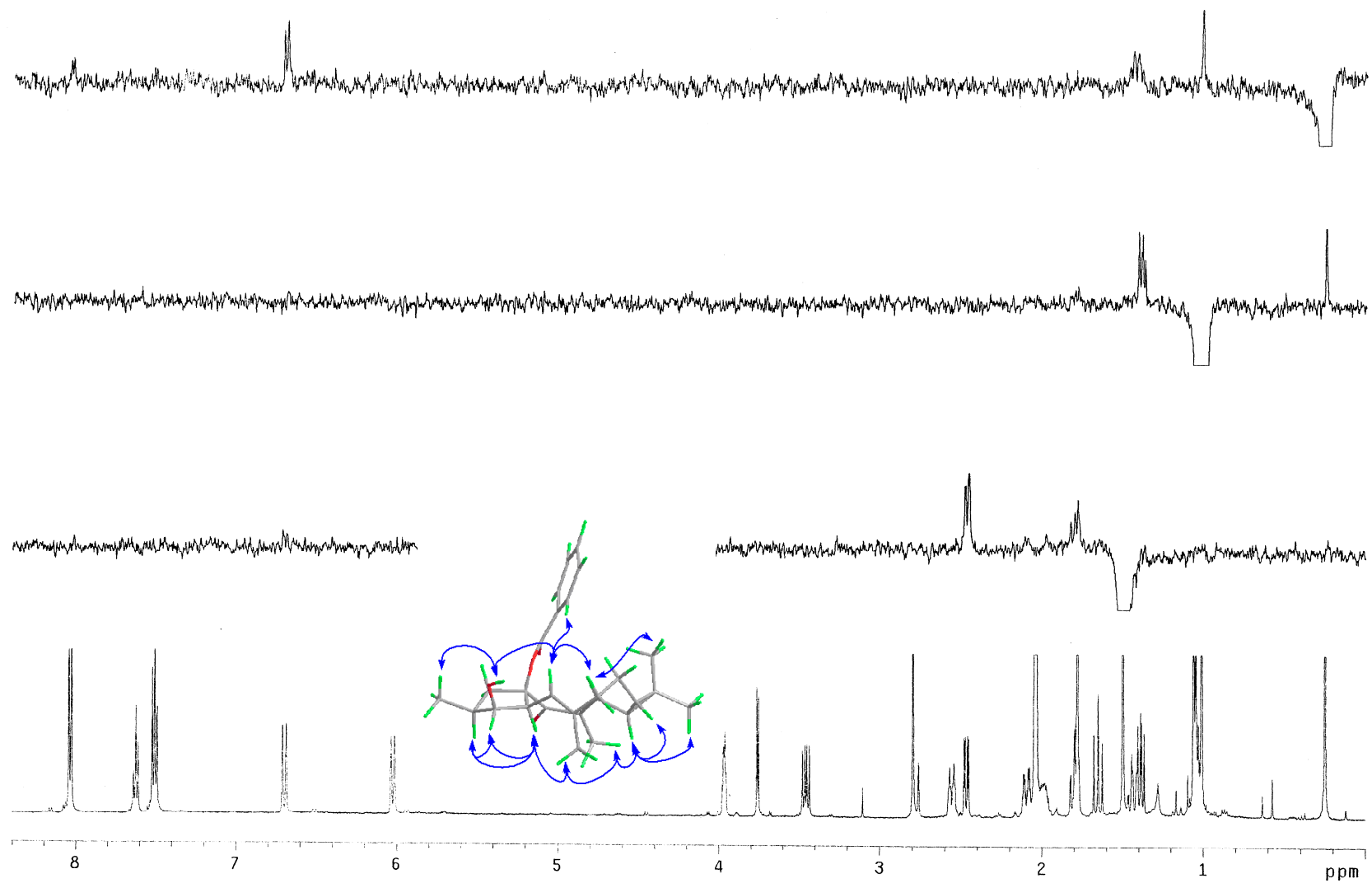


Figure S107. The NOE Difference Spectrum 3 of 11 in CD₃COCD₃ (500 MHz).

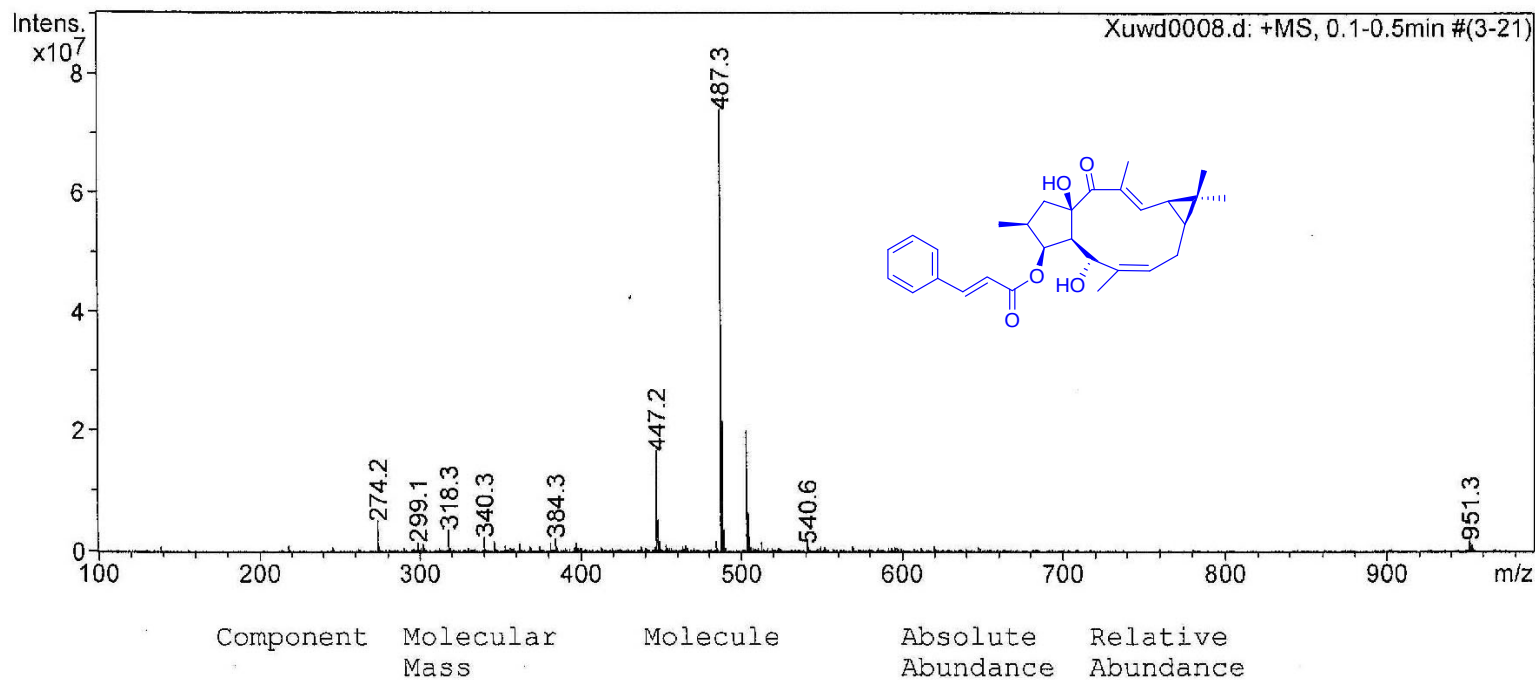


Figure S108. (+)-ESIMS Spectrum of 12.

Data:E_9_5

Sample Name:

Description:

Ionization Mode:ESI+

History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[];Smooth[3]];Correct Base[5.0%];Average(MS[...

Acquired:10/14/2008 10:47:56 AM

Operator:Accutof

Mass Calibration data:TFA100-2000-P-070410

Created:10/14/2008 10:52:30 AM

Created by:Accutof

Charge number:1

Tolerance:5.00(mmu)

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

Element:¹²C:0 .. 100, ¹H:0 .. 200, ²³Na:1 .. 1, ¹⁶O:0 .. 10

Mass	Mass Difference (mmu)	Mass Difference (ppm)	¹² C	¹ H	²³ Na	¹⁶ O	Unsaturation Number
487.24905	-2.87	-5.89	22	40	1	10	2.5
	3.00	6.16	29	36	1	5	11.5

(+)-HRESIMS Data of 12.

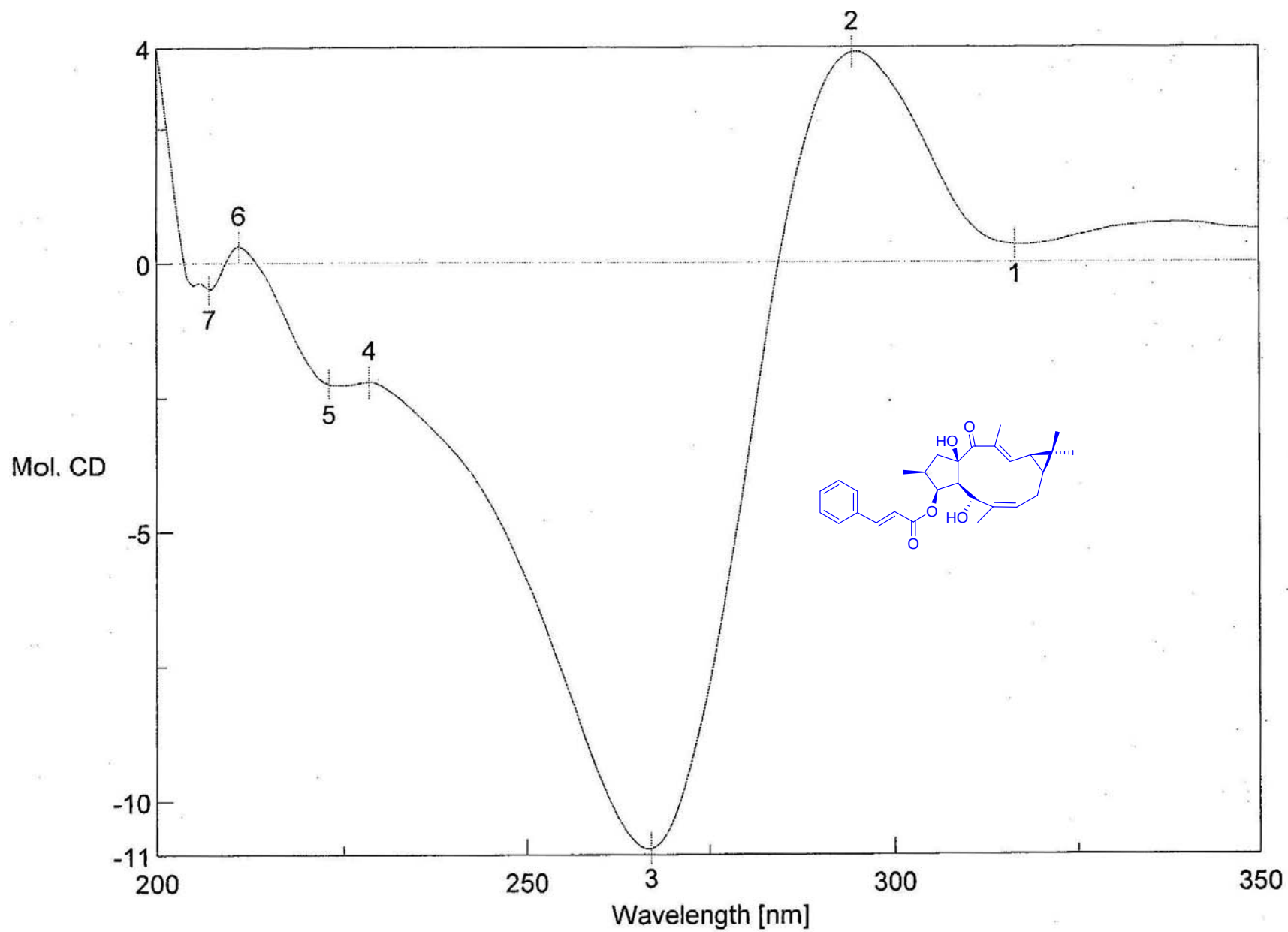


Figure S110. The CD Spectrum of 12.

Figure S111. The ^1H NMR Spectrum of 12 in CD_3COCD_3 (500 MHz).
S123

S124

INOVA-501 gCOSY E-9-5 IN CD₃COCD₃ 08.01.03

Solvent: Acetone
Temp. 25.0 C / 298.1 K
INOVA-500 "IMM-501"

Relax. delay 1.000 sec
Acq. time 0.202 sec
Width 5062.7 Hz
2D Width 5062.7 Hz
2 repetitions
256 increments
OBSERVE H1, 499.7728092 MHz
DATA PROCESSING
Sine bell 0.101 sec
F1 DATA PROCESSING
Sine bell 0.025 sec
FT size 2048 x 2048
Total time 10 min, 54 sec

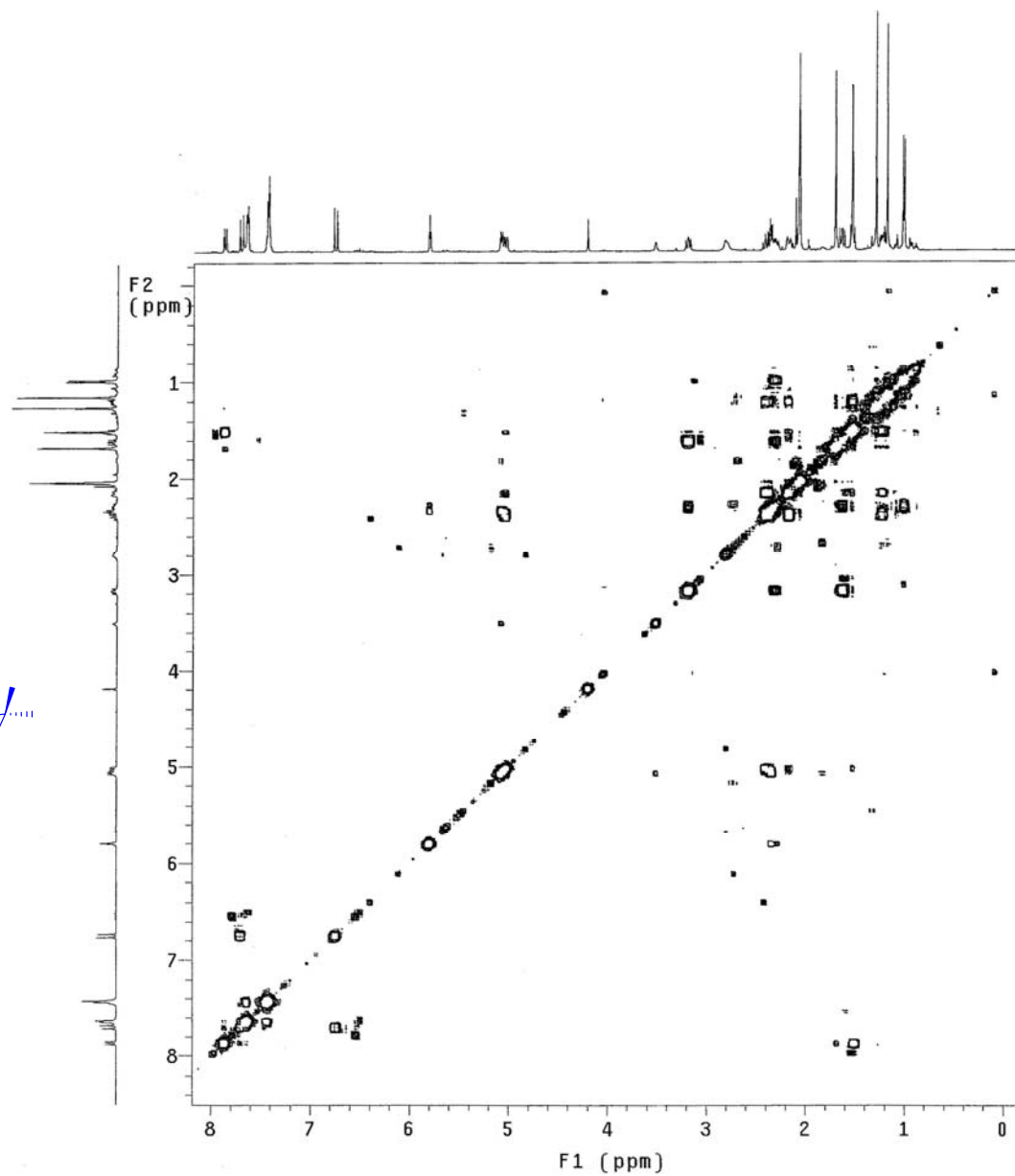
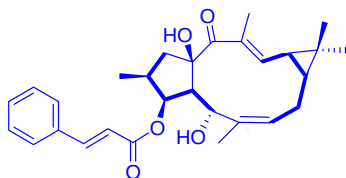


Figure S113. The ¹H-¹H gCOSY Spectrum of 12 in CD₃COCD₃ (500 MHz).

Solvent: Acetone
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "IMM-501"

Relax. delay 1.000 sec
Acq. time 0.202 sec
Width 5062.7 Hz
2D Width 27472.5 Hz
64 repetitions
256 increments
OBSERVE H1, 499.7728092 MHz
DECOUPLE C13, 125.6816388 MHz
Power 48 dB
on during acquisition
off during delay
GARP-1 modulated
DATA PROCESSING
Sine bell 0.049 sec
F1 DATA PROCESSING
Sine bell 0.005 sec
FT size 2048 x 4096
Total time 5 hr, 48 min, 56 sec

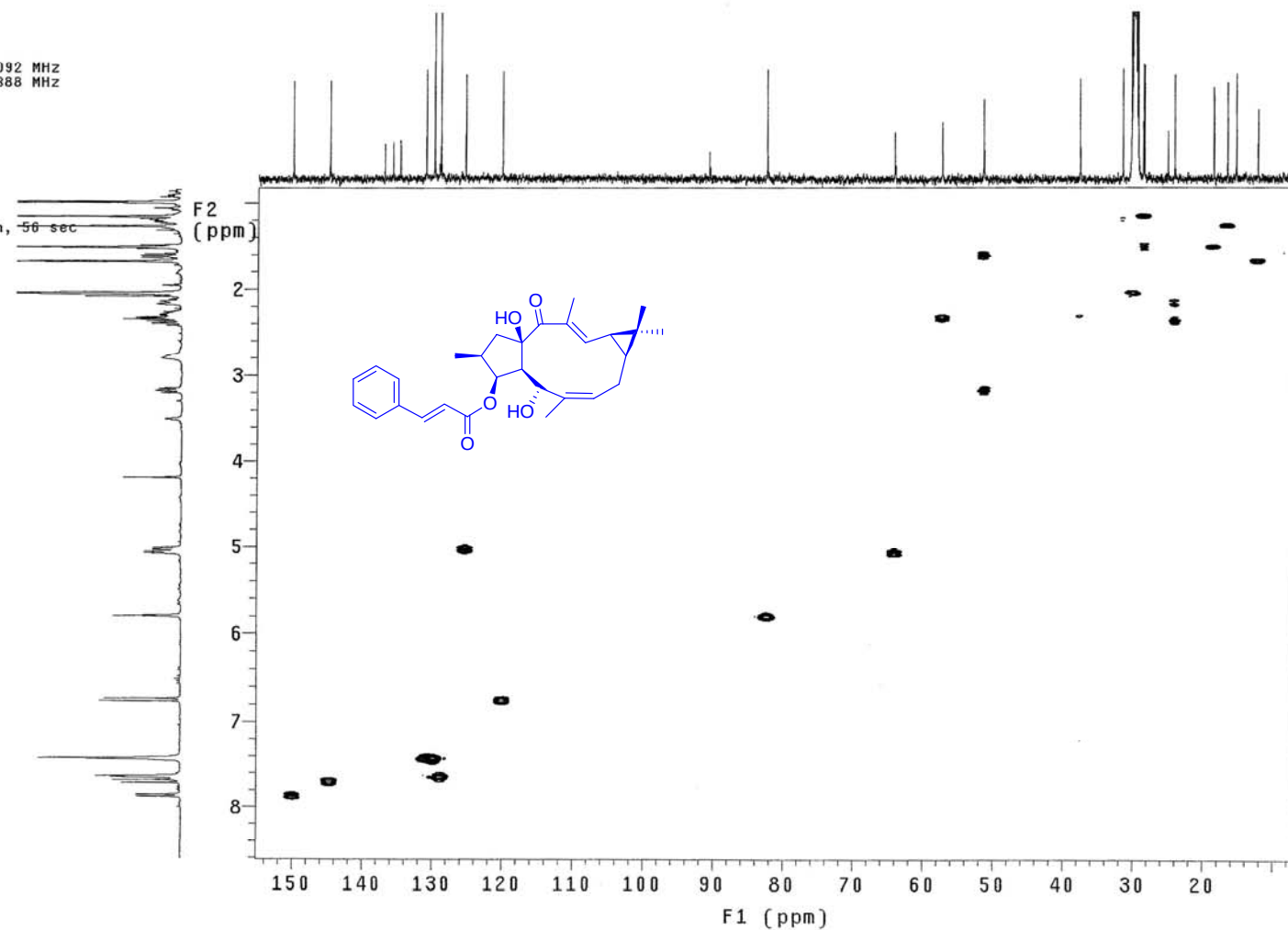


Figure S114. The gHSQC Spectrum of 12 in CD_3COCD_3 (500MHz for ^1H NMR).

Solvent: Acetone
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "IMM-501"

Relax. delay 1.000 sec
Acq. time 0.202 sec
Width 5062.7 Hz
2D Width 27472.5 Hz
80 repetitions
320 increments
OBSERVE H1, 499.7728092 MHz
DATA PROCESSING
Sine bell 0.055 sec
F1 DATA PROCESSING
Sine bell 0.006 sec
F1 size 2048 x 4096
Total time 9 hr, 11 min, 1 sec

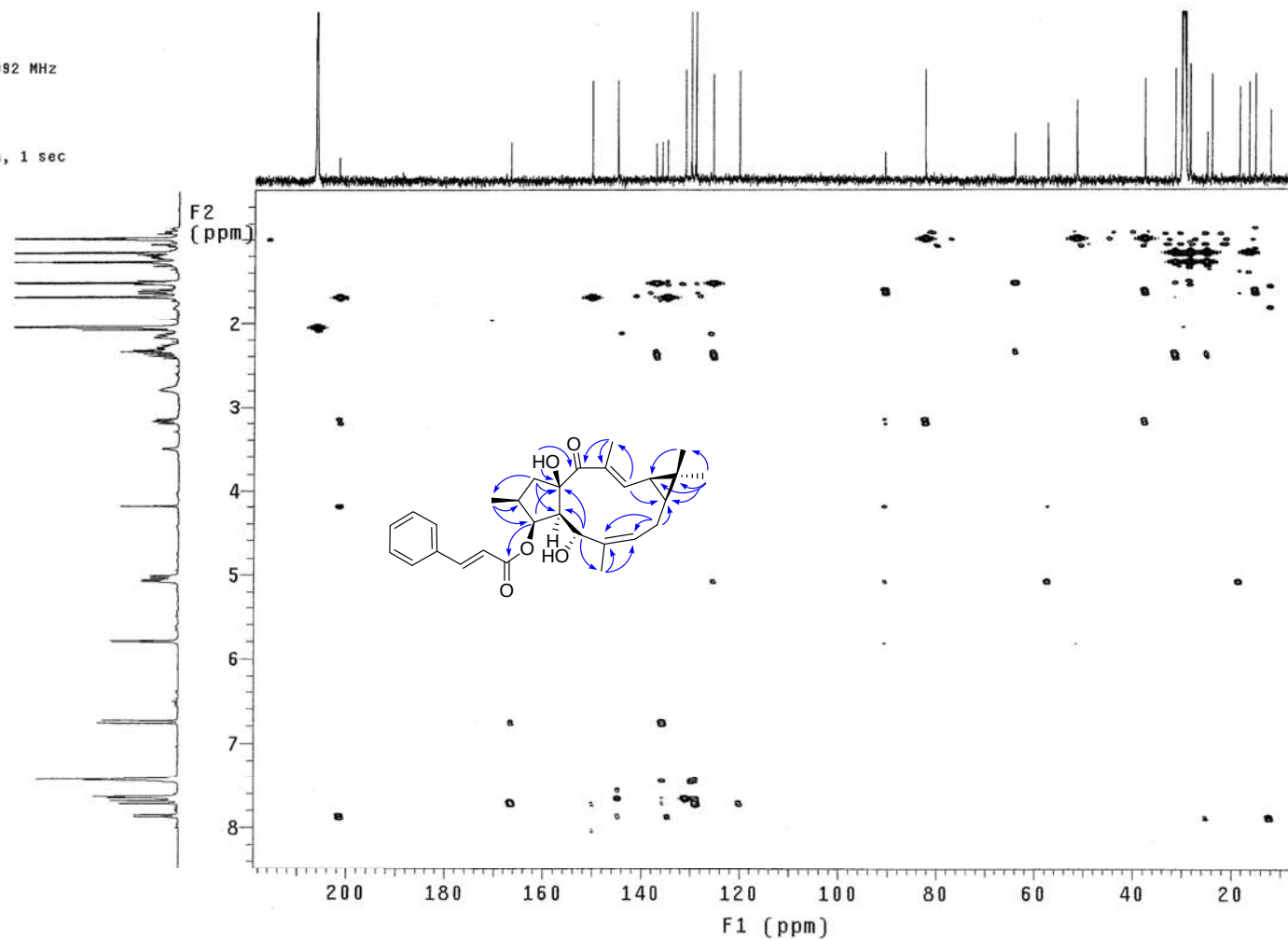


Figure S115. The gHMBC Spectrum of 12 in CD_3COCD_3 (500MHz for ^1H NMR).

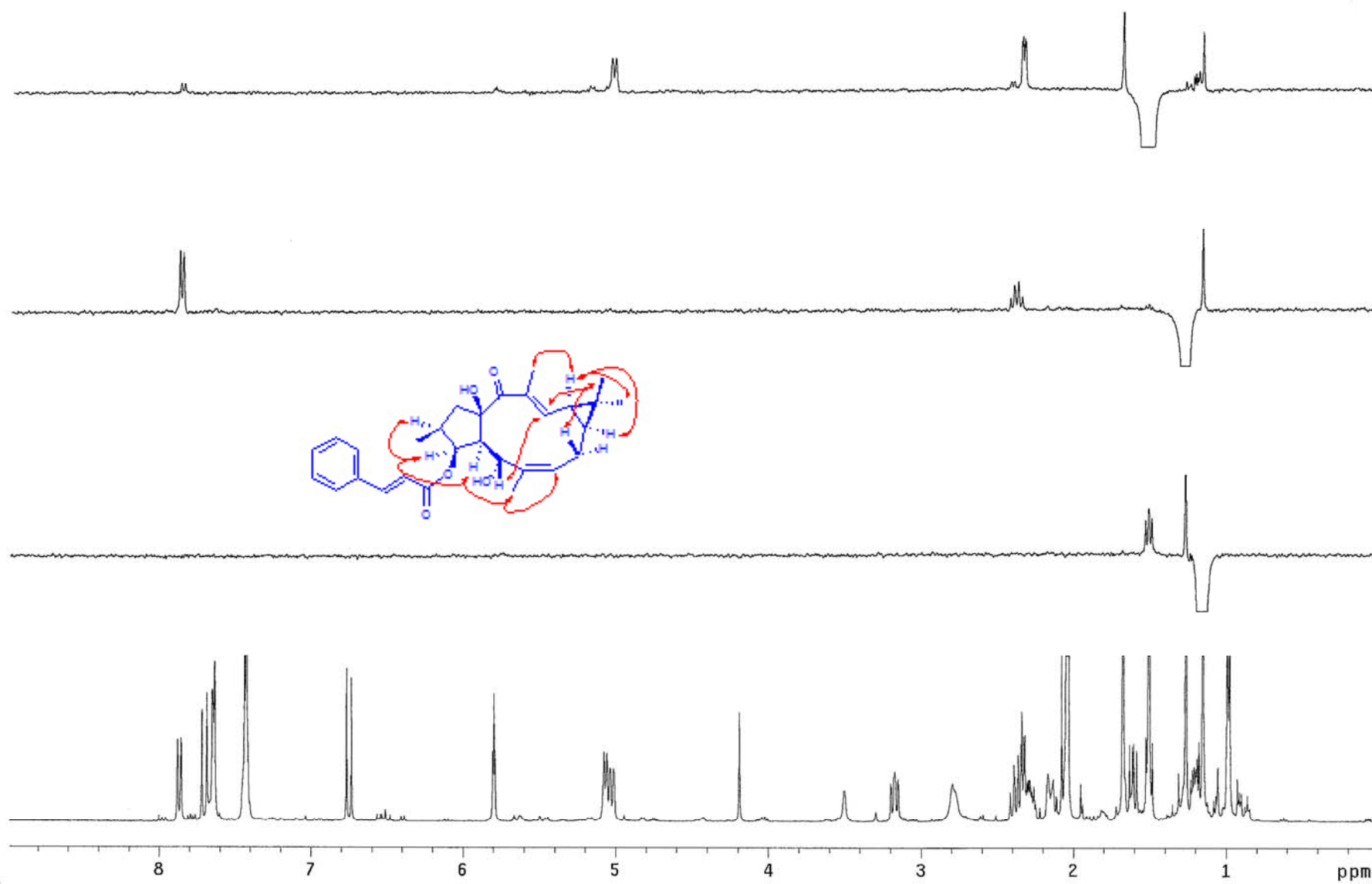


Figure S116. The NOE Difference Spectrum 1 of 12 in CD₃COCD₃ (500 MHz).

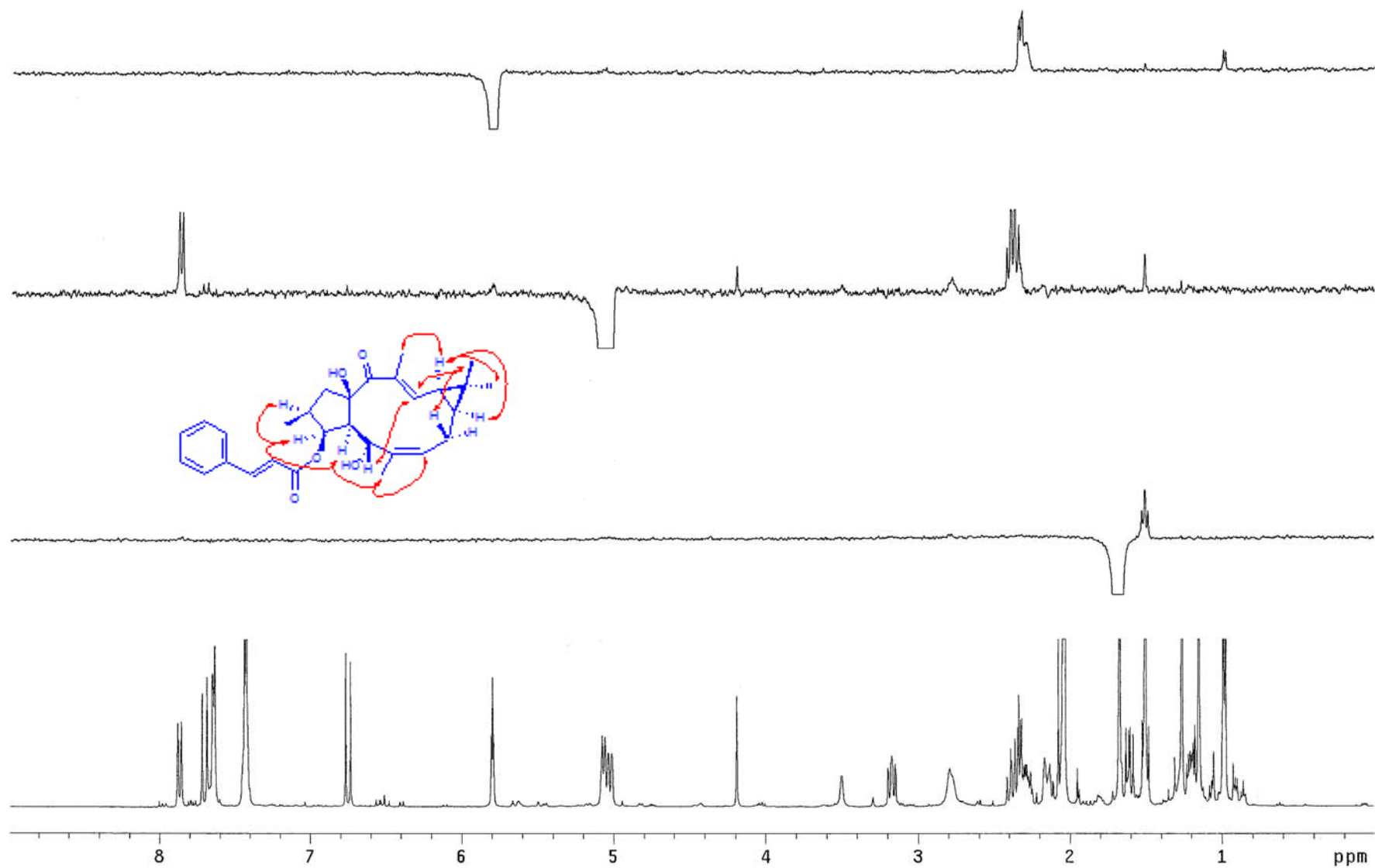


Figure S117. The NOE Difference Spectrum 2 of 12 in CD₃COCD₃ (500 MHz).

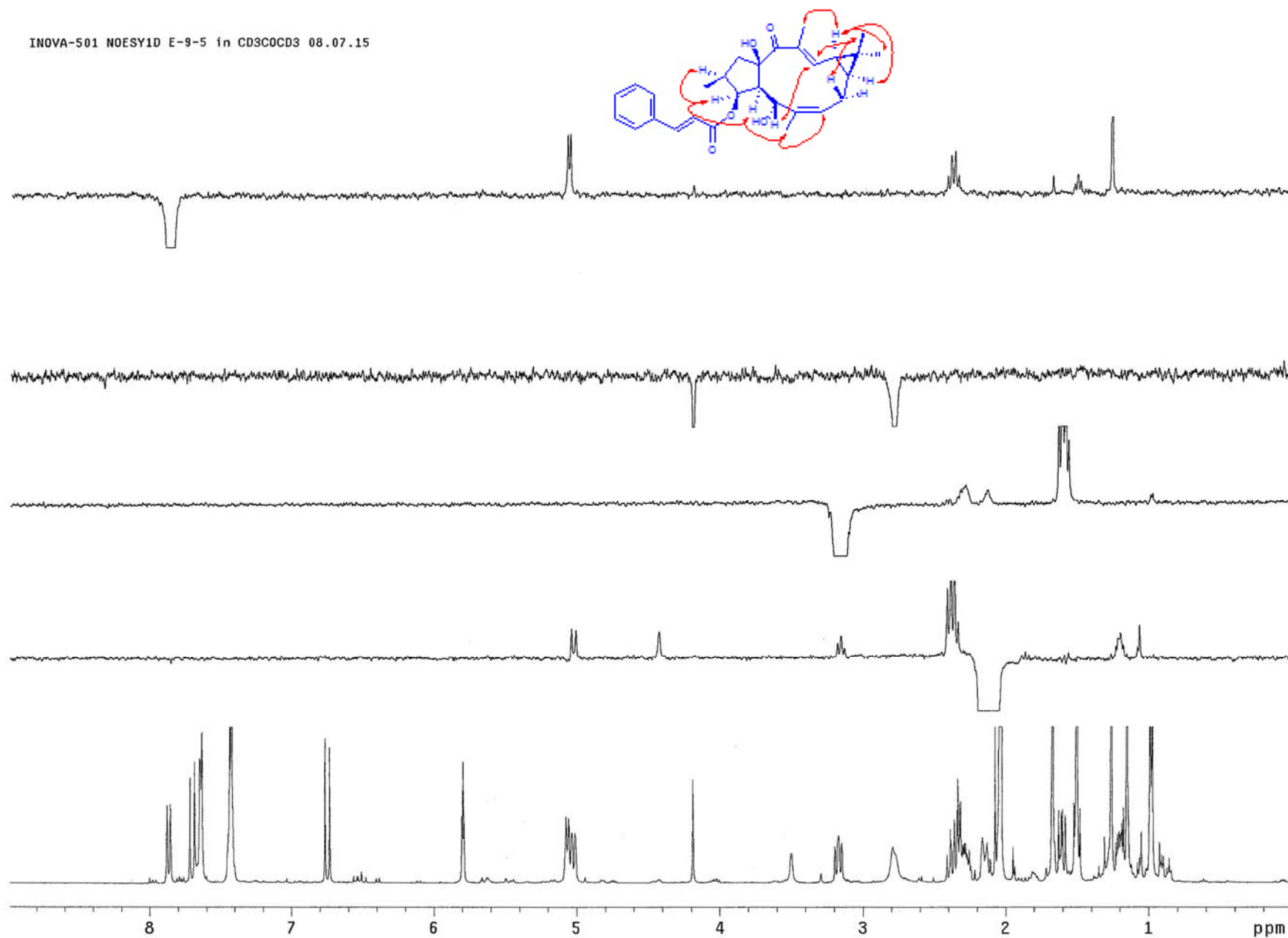


Figure S118. The NOE Difference Spectrum 3 of 12 in CD₃COCD₃ (500 MHz).

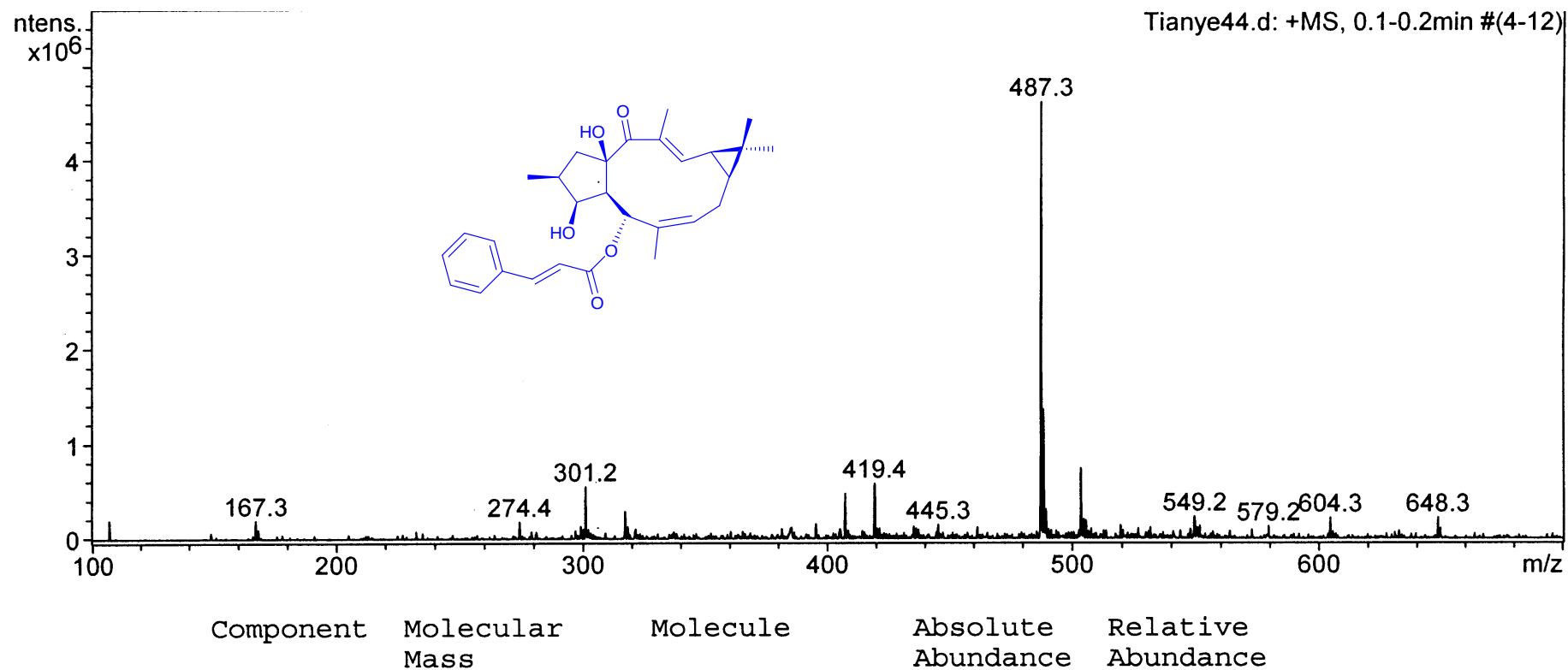
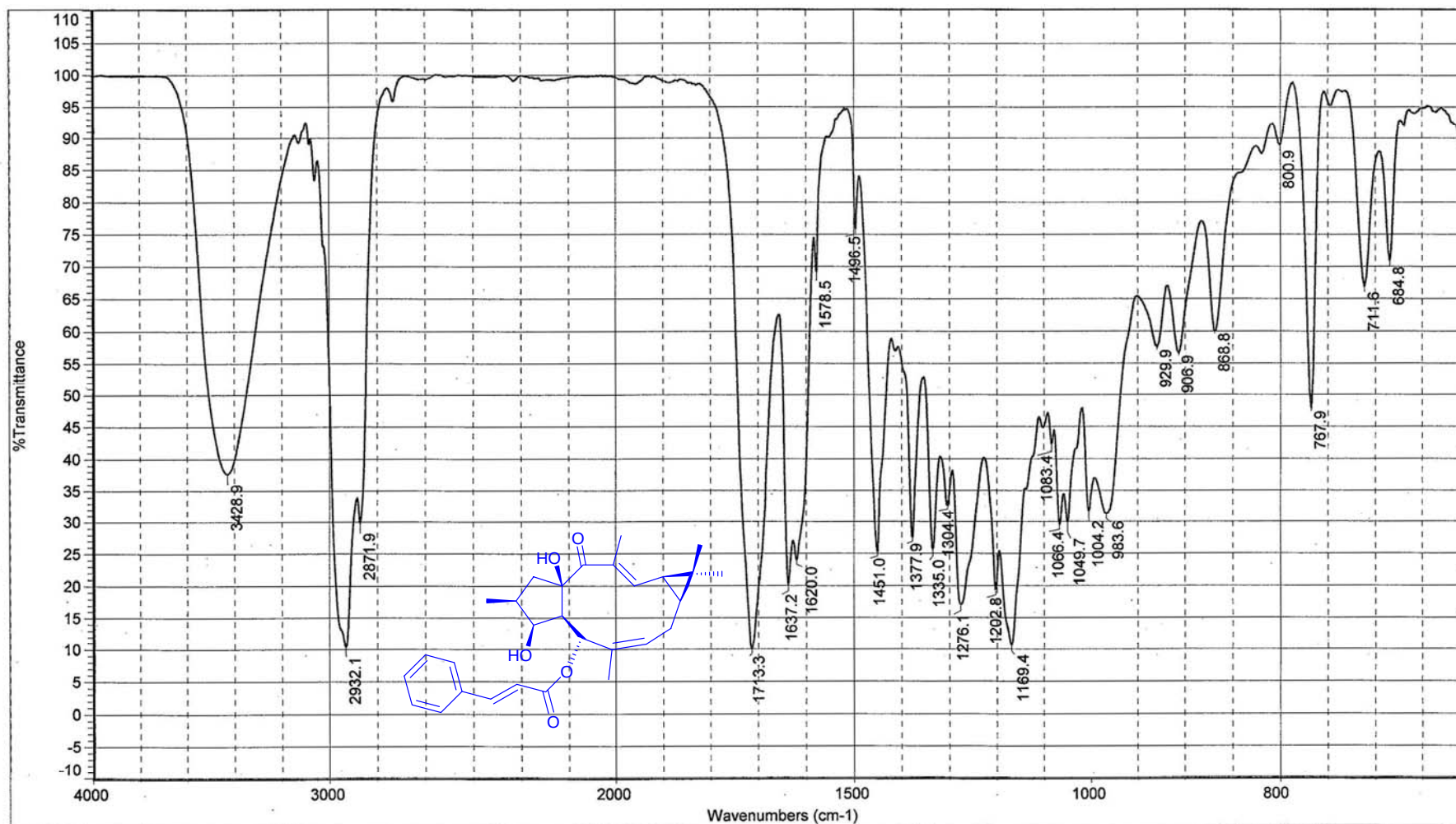


Figure S119. The (+)-ESIMS Spectrum of 13.

m/z	Ion	Formula	Abundance
487.2476	(M+Na)+	C29 H36 Na O5	1435287.8

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross S	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Mat	Mass Match	m/z	DBE
☒	C29 H36 O5	C29 H36 Na O5	487.2455	99.55		464.2584	464.2563	-4.64	4.64	99.56	99.96	99.33	487.2476	12
☐	C22 H40 O10	C22 H40 Na O10	487.2514	97.06		464.2584	464.2621	8.01	8.01	93.05	99.94	98.03	487.2476	3



日期: 星期四 12月 30 14:29:24 2010 (GMT+08:Sample Name : 10-A-2

(显微镜透射法FT- IR Microscope Transmission)

扫描次数: 64

分辨率: 4.000

美国热电公司(Thermo)傅里叶变换红外光谱仪:Nicolet 5700

Figure S120. The IR Spectrum of 13.

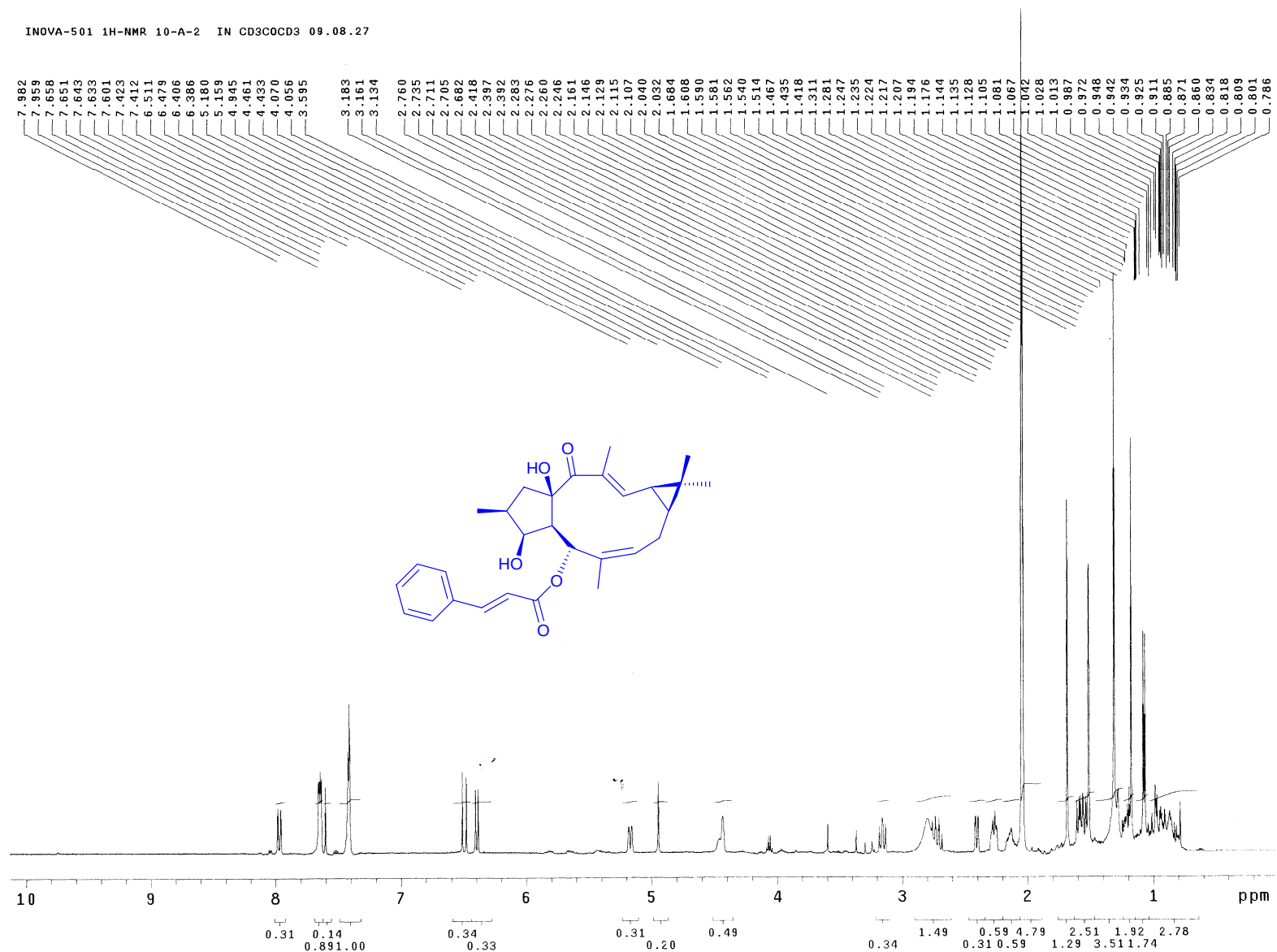


Figure S122. The ^1H NMR Spectrum of 13 in CD_3COCD_3 (500 MHz).

VNS-600 13C-NMR 10-A-2 IN CD3COCD3 09.09.18

Sample ID: 6001

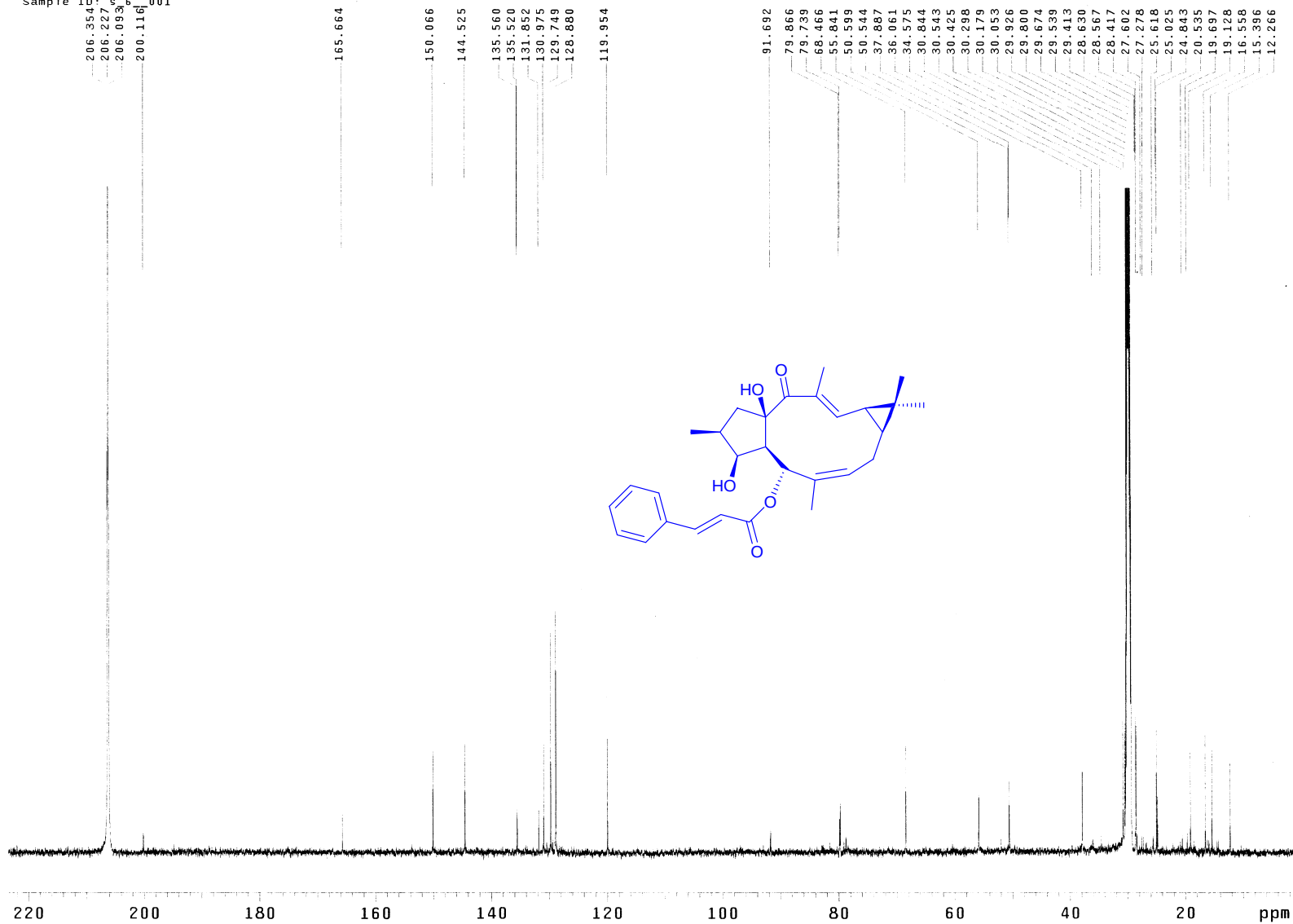


Figure S123. The ^{13}C NMR Spectrum of 13 in CD_3COCD_3 (150 MHz).

S135

S136

INOVA-501 gCOSY 10-A-2 IN CD3COCD3 09.12.01 cold probe

Solvent: acetone
Temp. 25.0 C / 298.1 K
Sample #4, Operator: walkup
File: Gcosy_01
INOVA-500 "IMM-501"

Relax. delay 1.301 sec
Acq. time 0.220 sec
Width 4658.2 Hz
2D Width 4658.2 Hz
2 repetitions
256 increments
OBSERVE H1, 499.7733213 MHz
DATA PROCESSING
Sine bell 0.110 sec
F1 DATA PROCESSING
Sine bell 0.027 sec
FT size 4096 x 4096
Total time 13 min, 43 sec

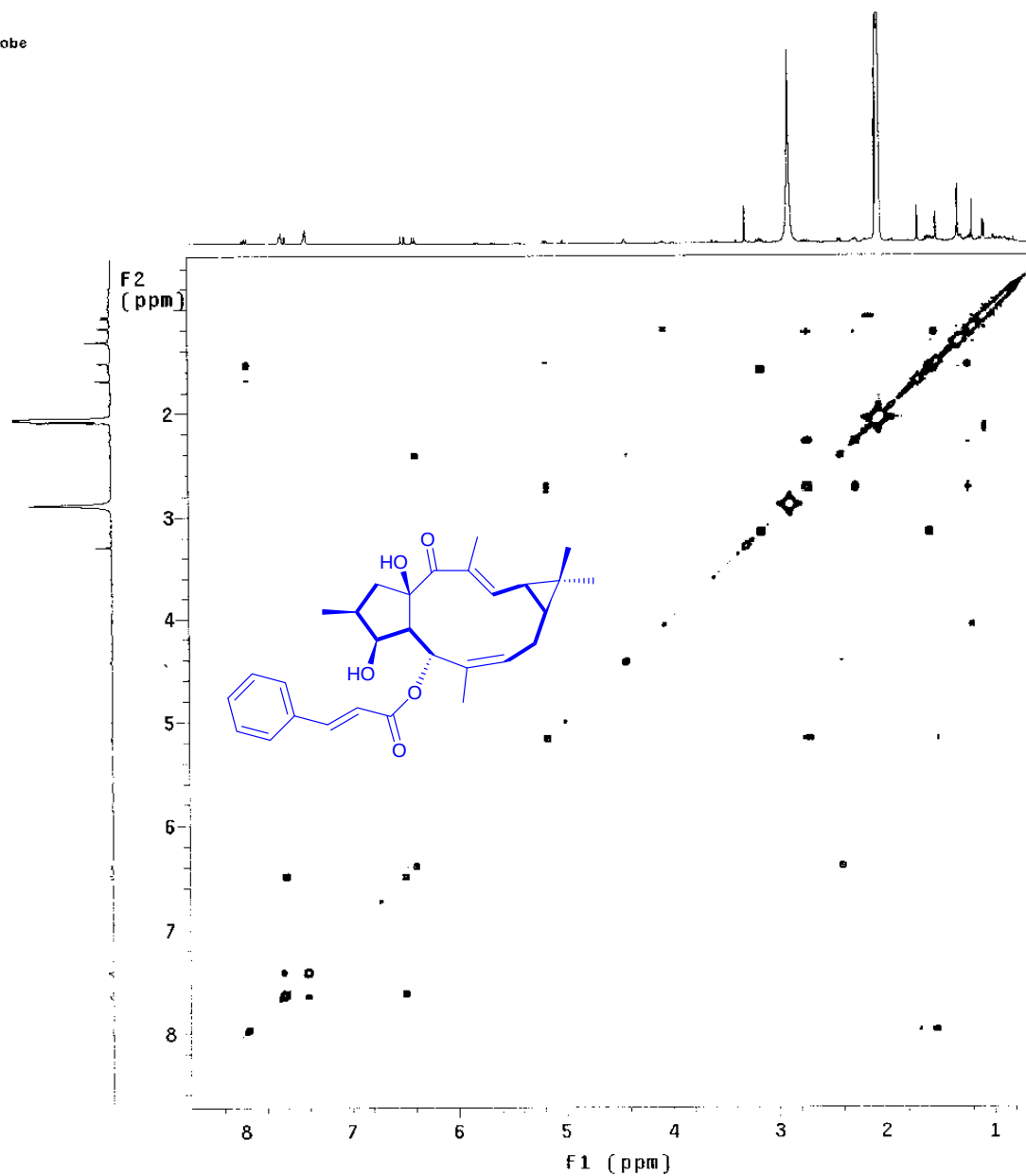


Figure S125. The ^1H - ^1H gCOSY Spectrum of 13 in CD_3COCD_3 (500 MHz).

S137

INOVA-501 gHMQC 10-A-2 IN CD3COCD3 09.12.01 cold probe

Solvent: acetone
Temp. 25.0 C / 298.1 K
Sample #4, Operator: walkup
File: Ghmqc_01
INOVA-500 "IMM-501"

Relax. delay 1.000 sec
Acq. time 0.128 sec
Width 4658.2 Hz
2D Width 25133.5 Hz
8 repetitions
2 x 256 increments
OBSERVE H1, 499.7733239 MHz
DECOUPLE C13, 125.6793772 MHz
Power 30 dB
on during acquisition
off during delay
W40_cold modulated
DATA PROCESSING
Sine bell 0.025 sec
F1 DATA PROCESSING
Sine bell 0.005 sec
FT size 2048 x 2048
Total time 1 hr, 21 min, 27 sec

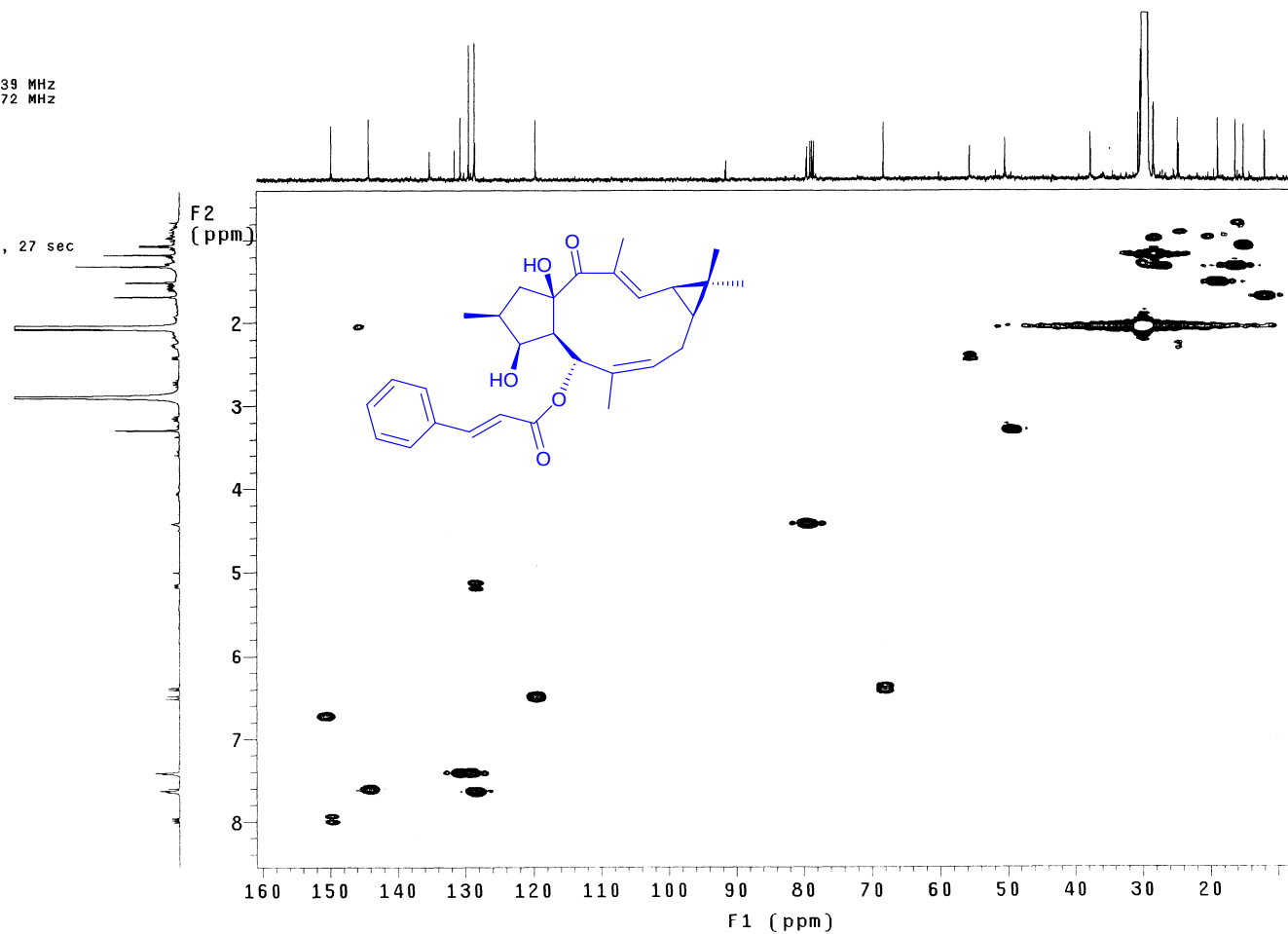


Figure S126. The gHSQC Spectrum of 13 in CD_3COCD_3 (500 MHz for ^1H NMR).

INOVA-501 gHMBC 10-A-2 IN CD3COCD3 09.12.01 cold probe

Solvent: acetone
Temp. 25.0 C / 298.1 K
Sample #4, Operator: walkup
File: HMBCCD3COCOD31201-10-A-2
INOVA-500 "IMM-501"

Relax. delay 1.000 sec
Mixing 0.080 sec
Acq. time 0.128 sec
Width 4658.2 Hz
2D Width 30165.9 Hz
32 repetitions
256 increments
OBSERVE H1, 499.7733238 MHz
DATA PROCESSING
Sine bell 0.054 sec
F1 DATA PROCESSING
Sine bell 0.003 sec
FT size 2048 x 2048
Total time 2 hr, 46 min, 21 sec

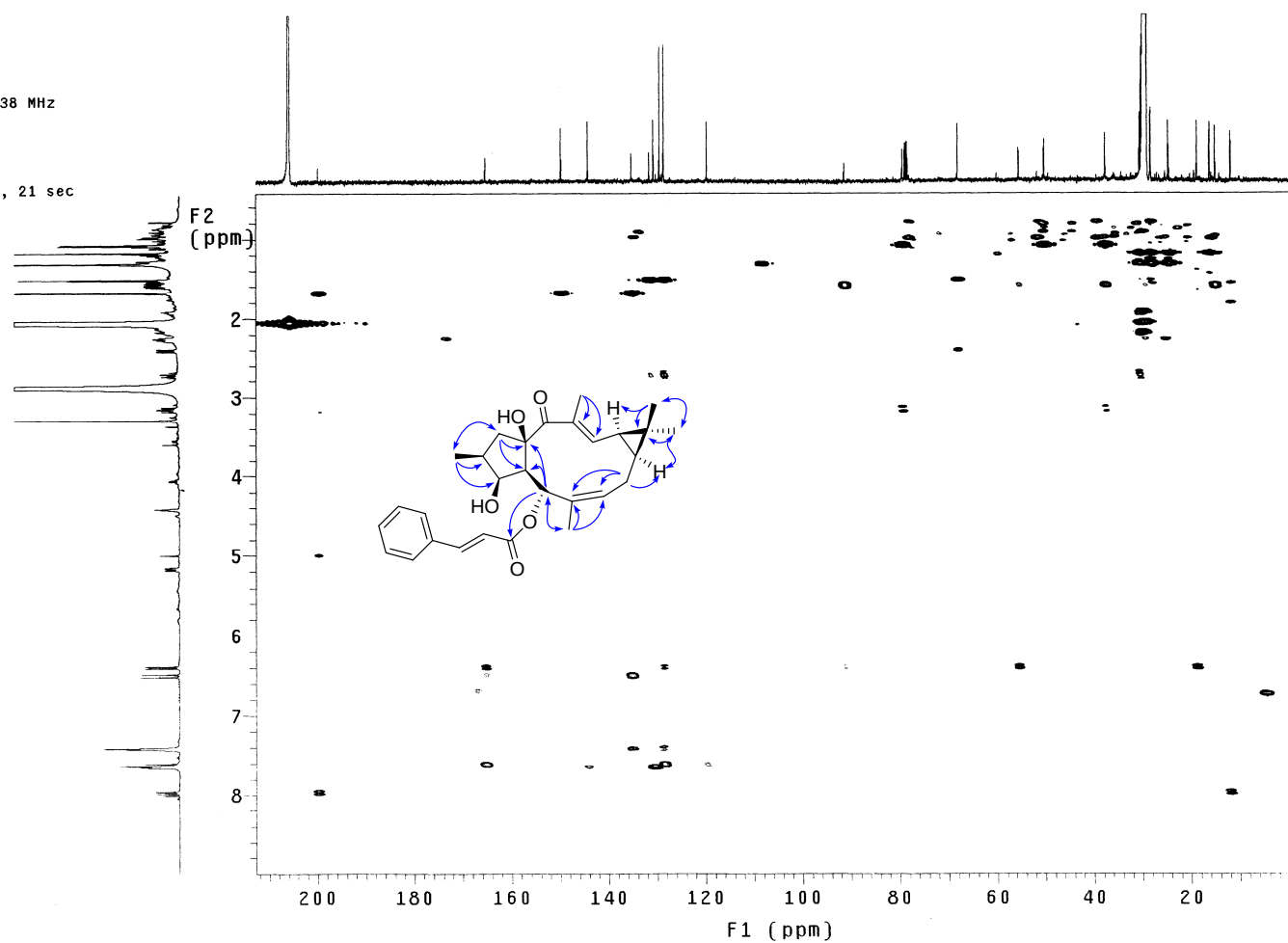


Figure S127. The gHMBC Spectrum of 13 in CD₃COCD₃ (500 MHz for ¹H NMR).
S139

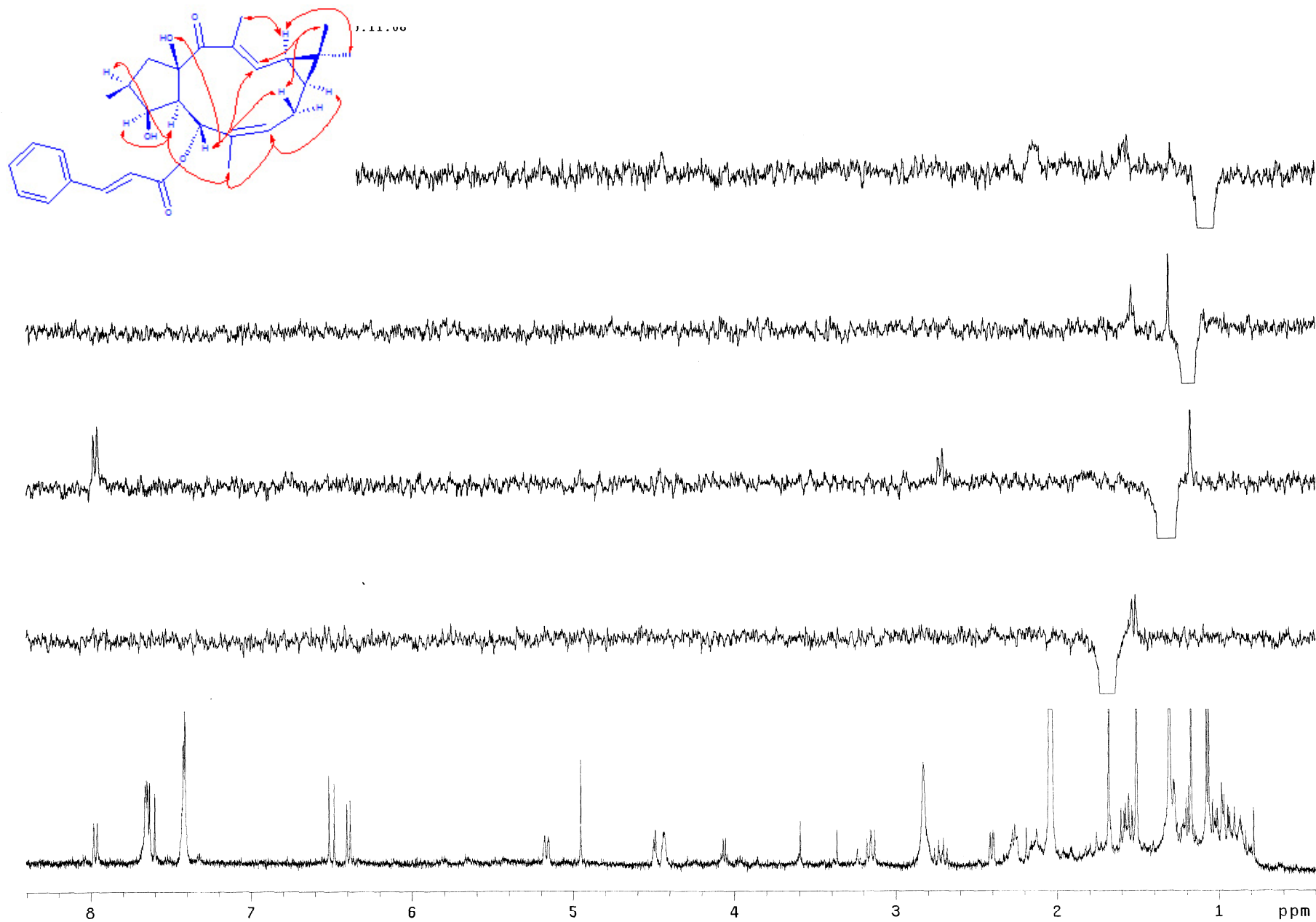


Figure S128. The NOE Difference Spectrum 1 of 13 in CD_3COCD_3 (500 MHz).

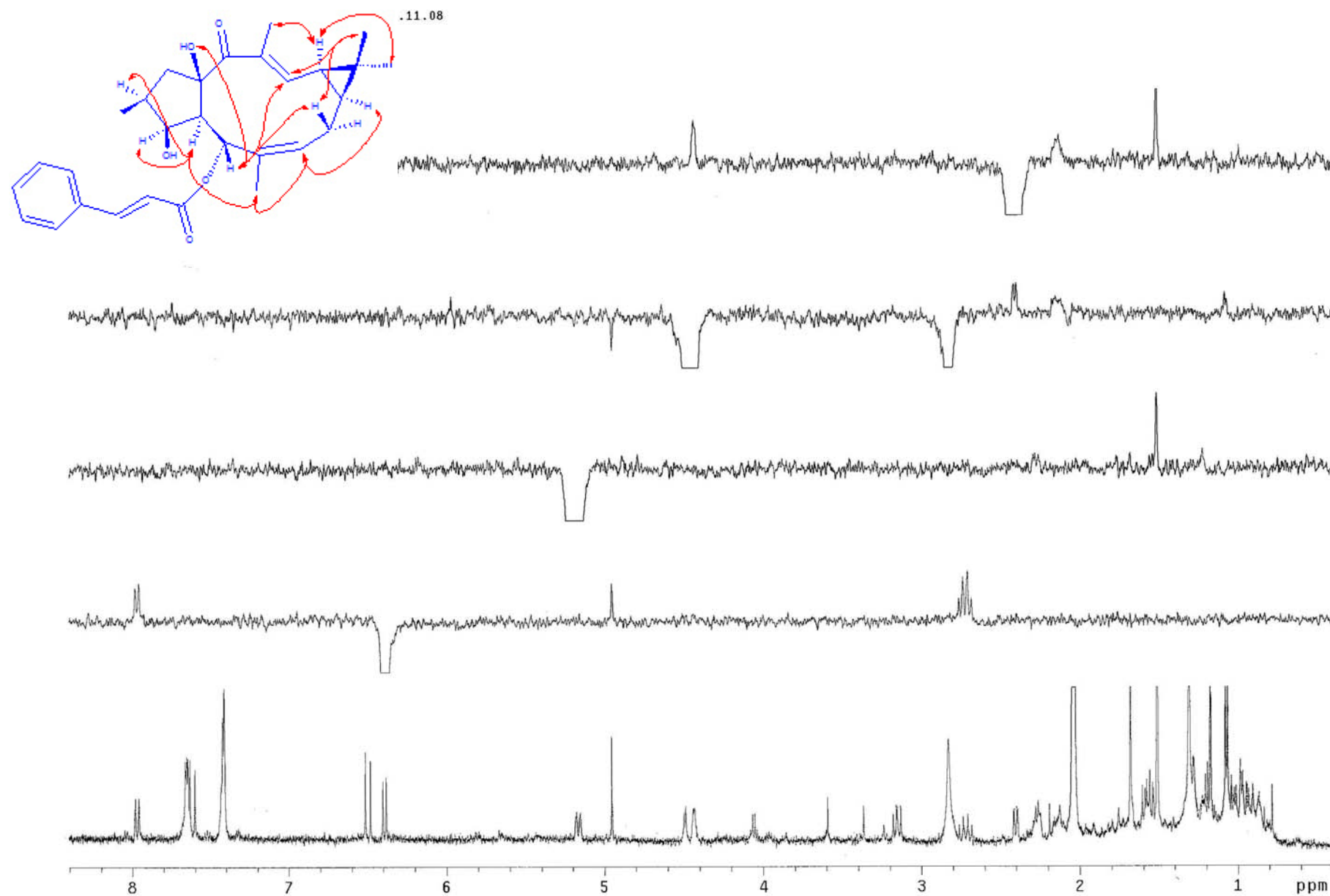


Figure S129. The NOE Difference Spectrum 2 of 13 in CD_3COCD_3 (500 MHz).

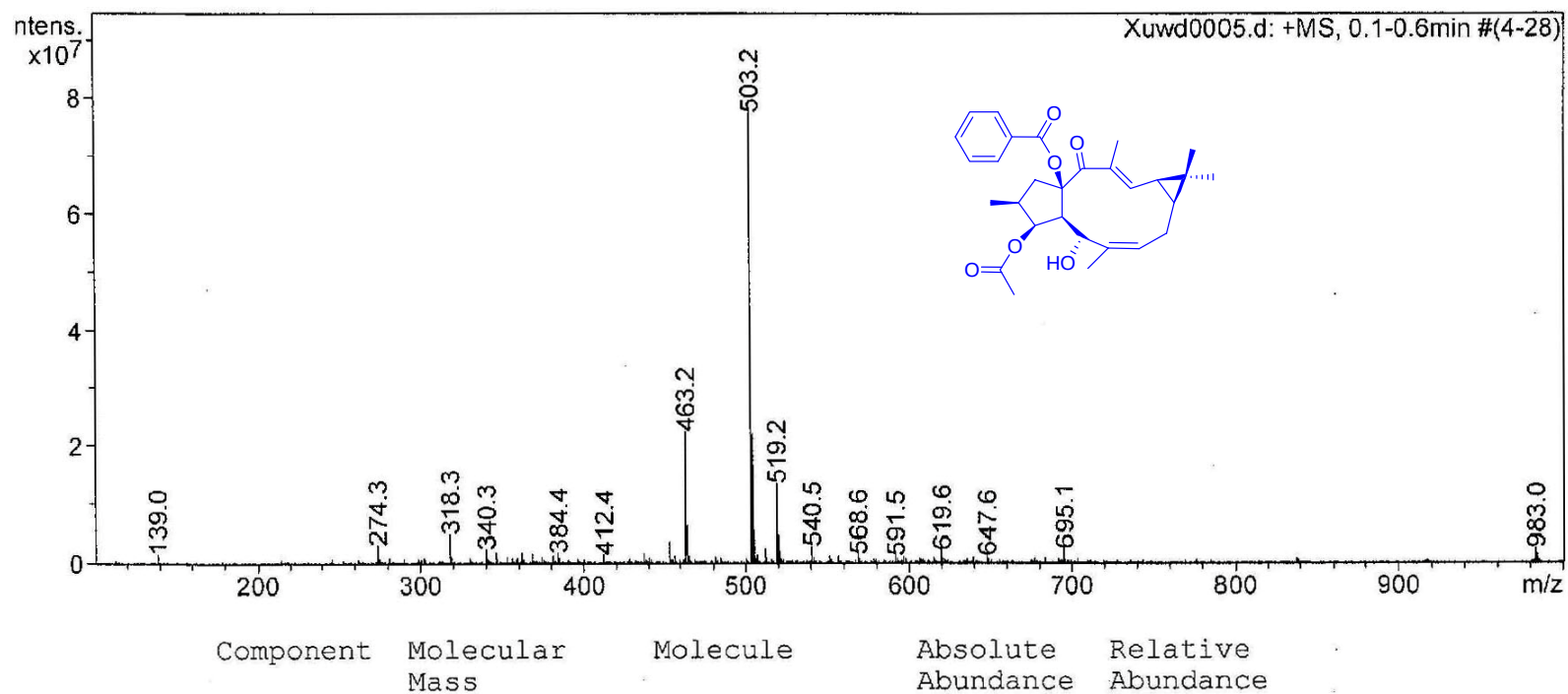


Figure S130. (+)-ESIMS Spectrum of 14.

Data:E_9_2_1

Sample Name:

Description:

Ionization Mode:ESI+

History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[];Smooth[3]];Correct Base[5.0%];Average(MS[...

Acquired:10/14/2008 11:04:13 AM

Operator:Accutof

Mass Calibration data:TFA100-2000-P-070410

Created:10/14/2008 11:09:36 AM

Created by:Accutof

Charge number:1

Tolerance:5.00(mmu)

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

Element:¹²C:0 .. 100, ¹H:0 .. 200, ²³Na:1 .. 1, ¹⁶O:0 .. 10

Mass	Mass Difference (mmu)	Mass Difference (ppm)	¹² C	¹ H	²³ Na	¹⁶ O	Unsaturation Number
503.24136	0.40	0.80	29	36	1	6	11.5

(+)-HRESIMS Data of 14.

S142

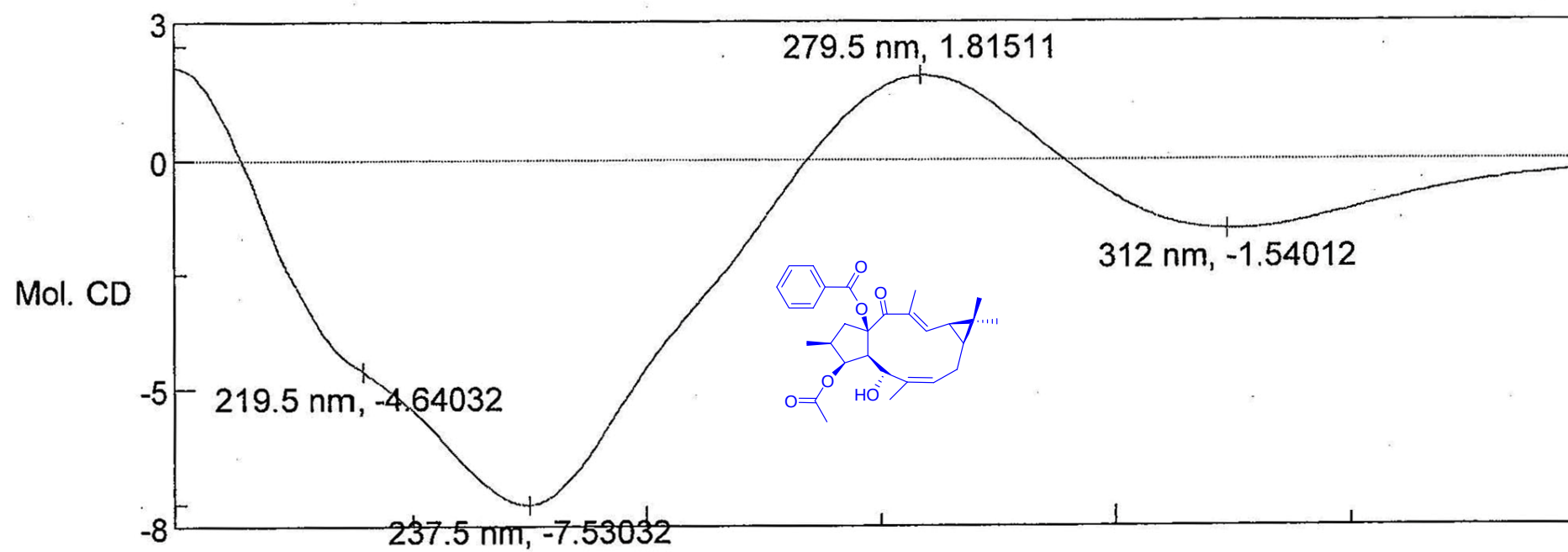


Figure S132. The CD Spectrum of 14.

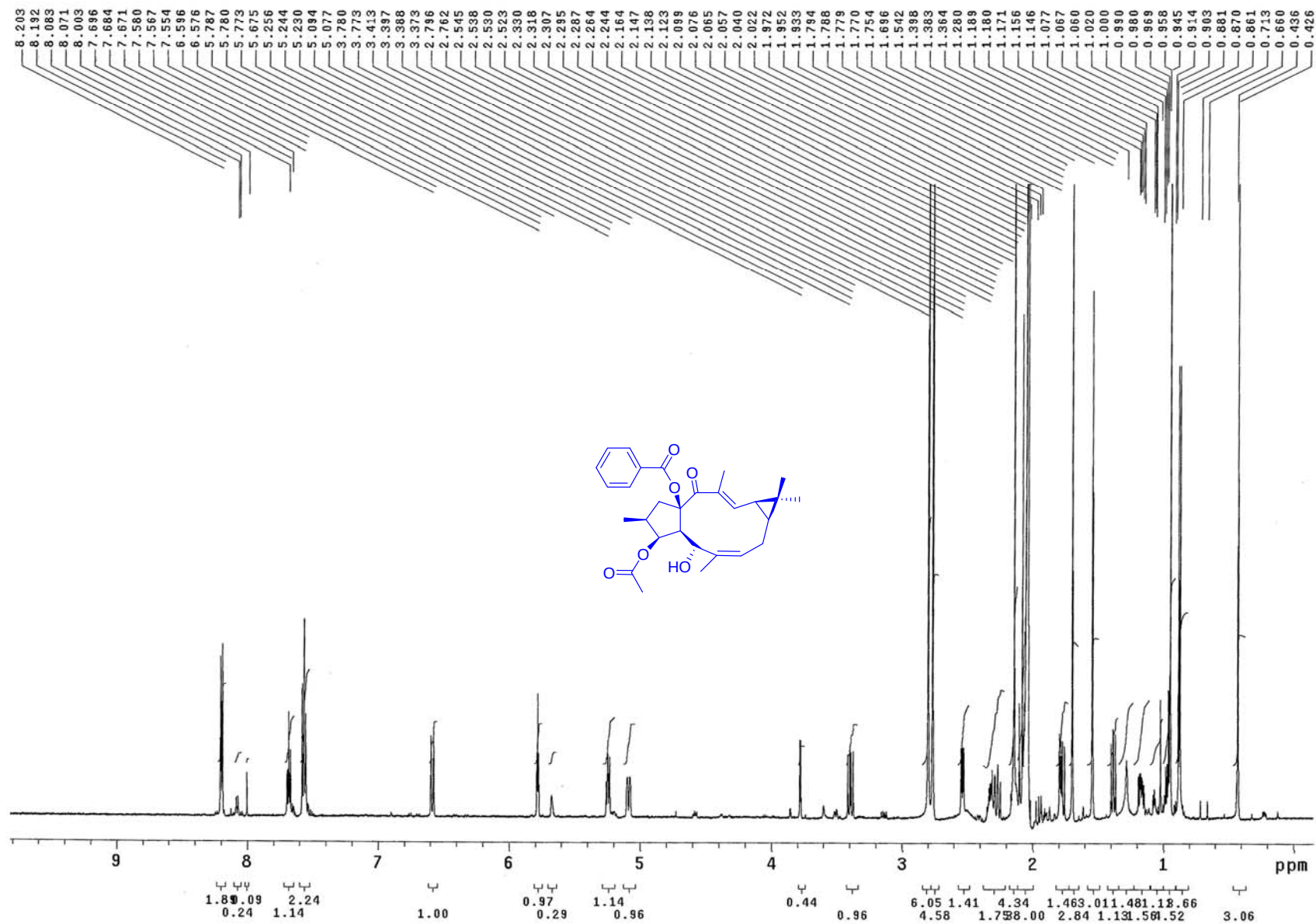


Figure S133. The ¹H NMR Spectrum of 14 in CD₃COCD₃ (600 MHz).

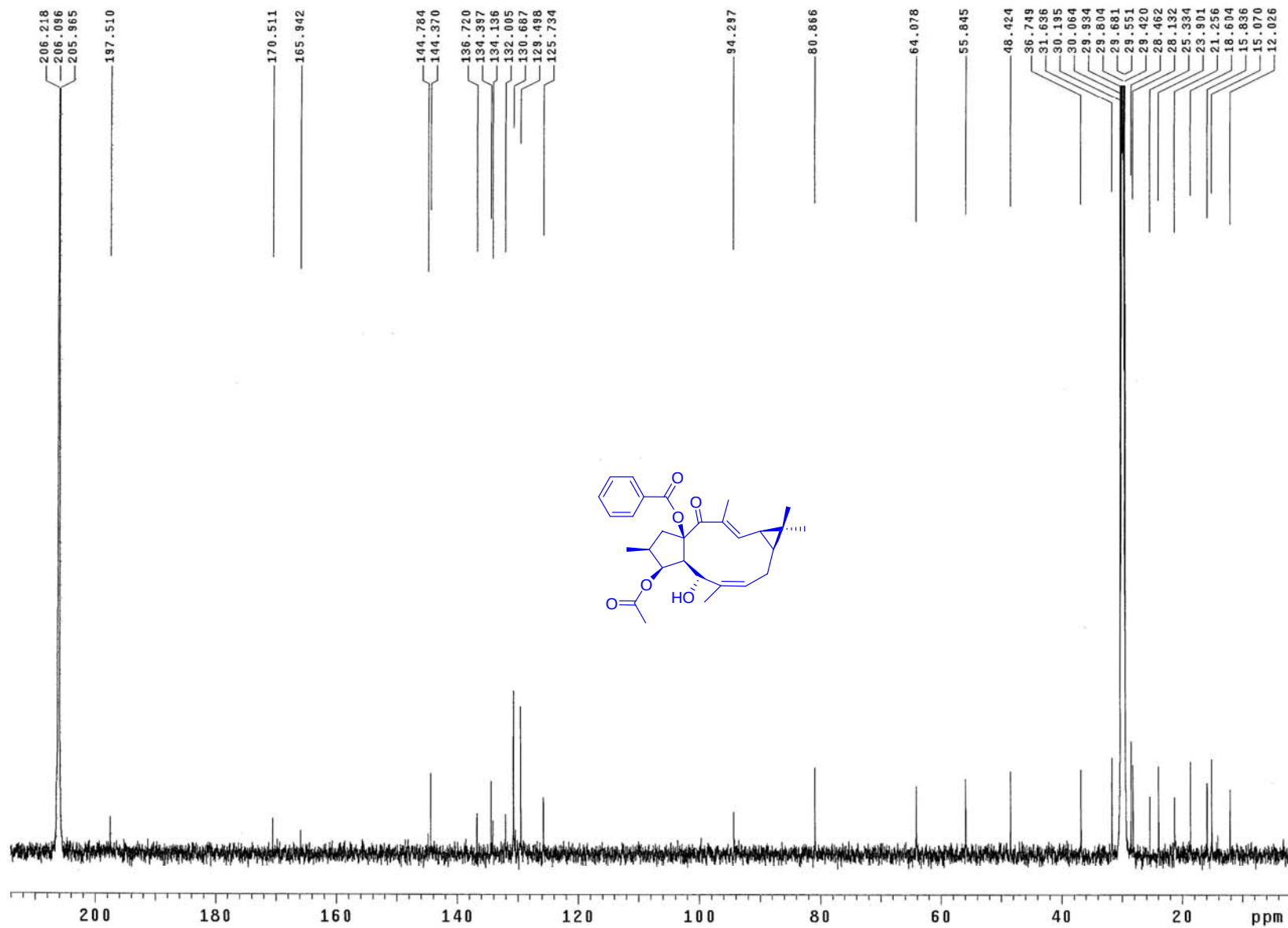


Figure S134. The ^{13}C NMR Spectrum of 14 in CD_3COCD_3 (150 MHz).

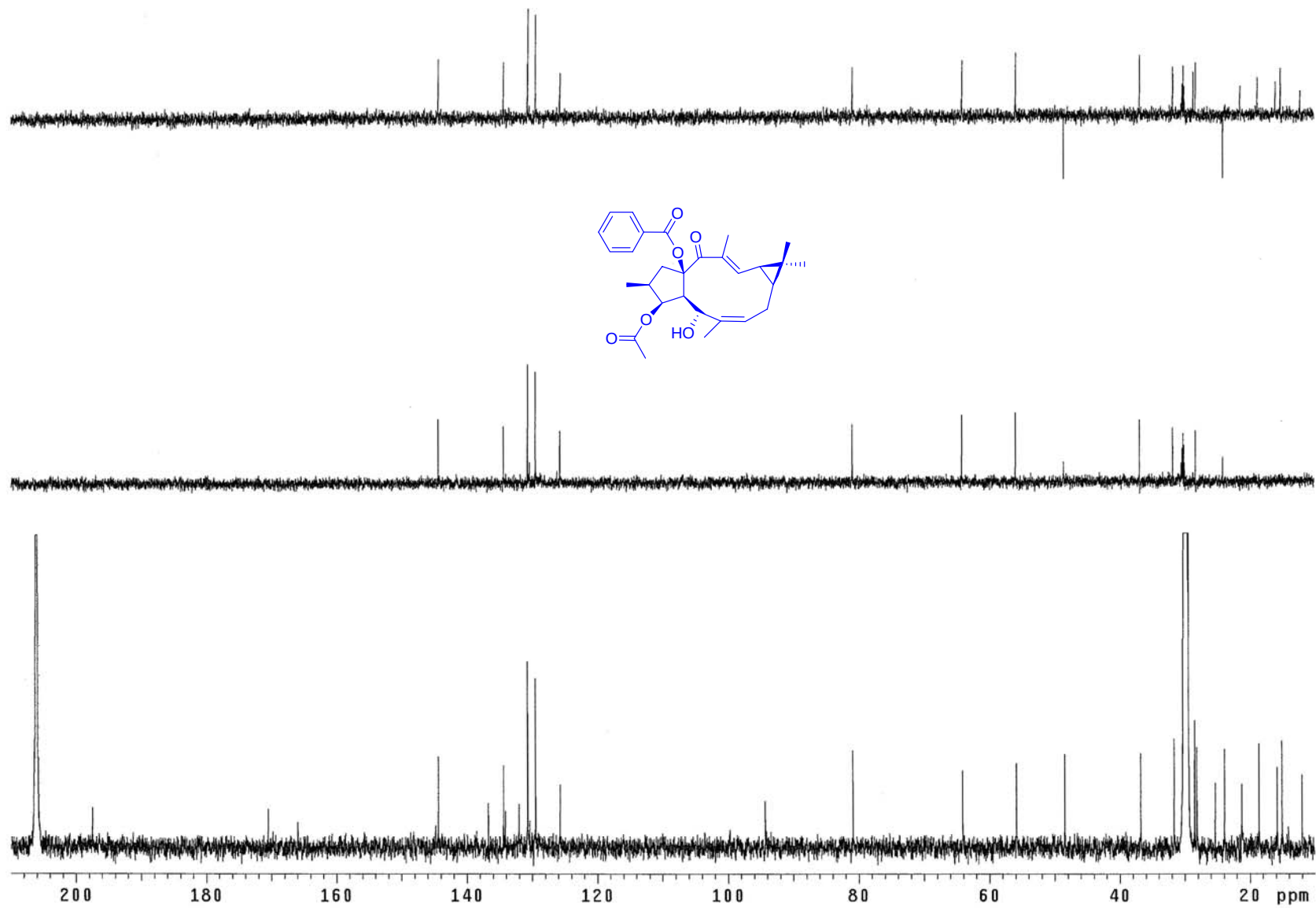


Figure S135. The DEPT Spectrum of 14 in CD₃COCD₃ (150 MHz).

SYS-600 gCOSY E-9-2-1 in CD3COCD3 08.06.06

Solvent: acetone
Ambient temperature
Operator: vnmr2
VNMR-600 "wormhole"

Relax. delay 1.301 sec
Acq. time 0.178 sec
Width 5760.4 Hz
2D Width 5760.4 Hz
4 repetitions
256 increments
OBSERVE H1, 599.6981349 MHz
DATA PROCESSING
Sine bell 0.089 sec
F1 DATA PROCESSING
Sine bell 0.022 sec
FT size 2048 x 2048
Total time 26 min, 13 sec

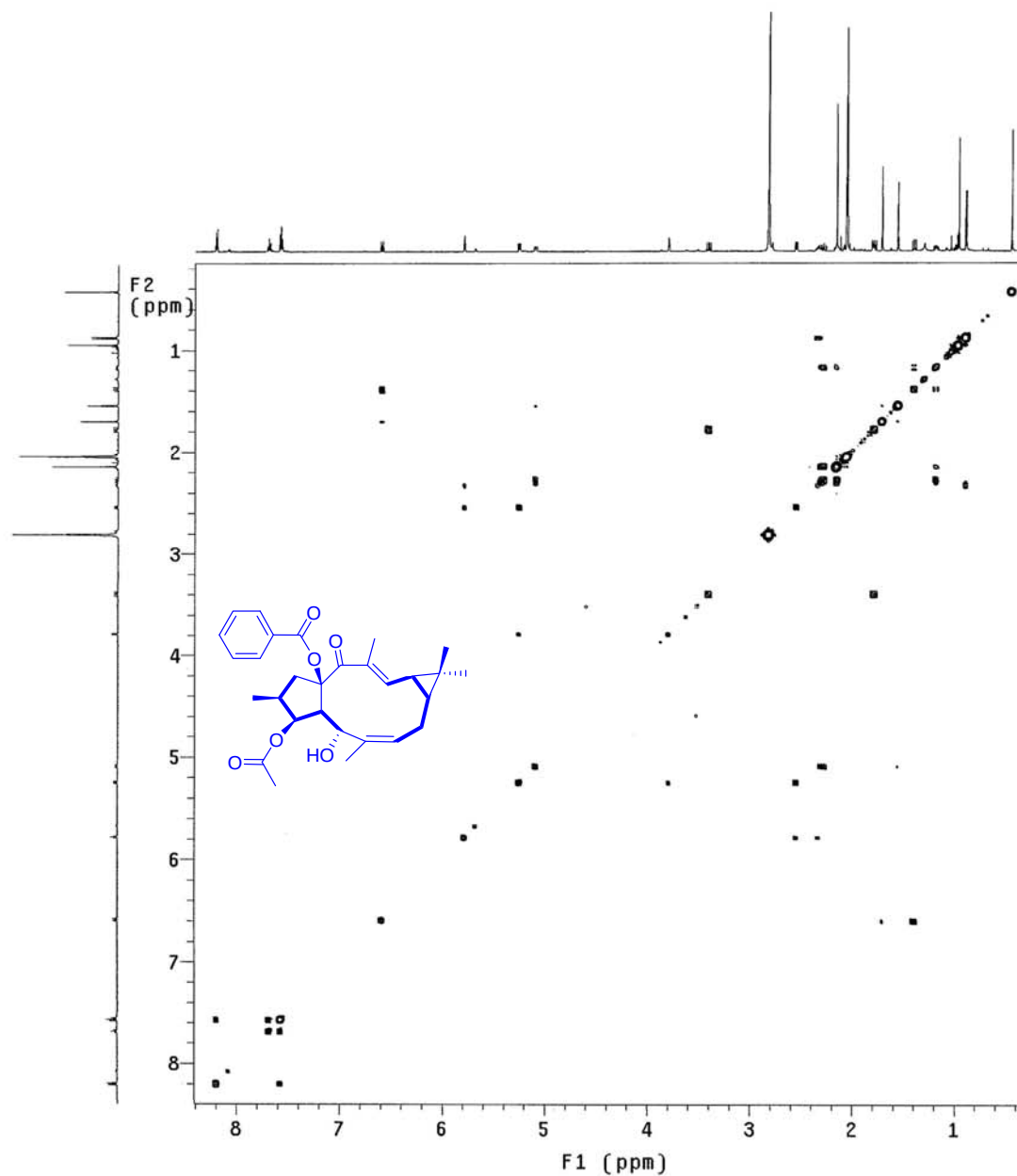


Figure S136. The ^1H - ^1H gCOSY Spectrum of 14 in CD_3COCD_3 (600 MHz).

S148

Solvent: acetone
Ambient temperature
Operator: vnmr2
VNMR-600 "wormhole"

Relax. delay 1.301 sec
Acq. time 0.199 sec
Width 5630.6 Hz
2D Width 33783.8 Hz
256 repetitions
160 increments
OBSERVE H1, 599.6981281 MHz
DECOUPLE C13, 150.8105411 MHz
Power 42 dB
on during acquisition
off during delay
GARP-1 modulated
DATA PROCESSING
Sine bell 0.038 sec
F1 DATA PROCESSING
Sine bell 0.003 sec
FT size 2048 x 8192
Total time 17 hr, 40 min, 28 sec

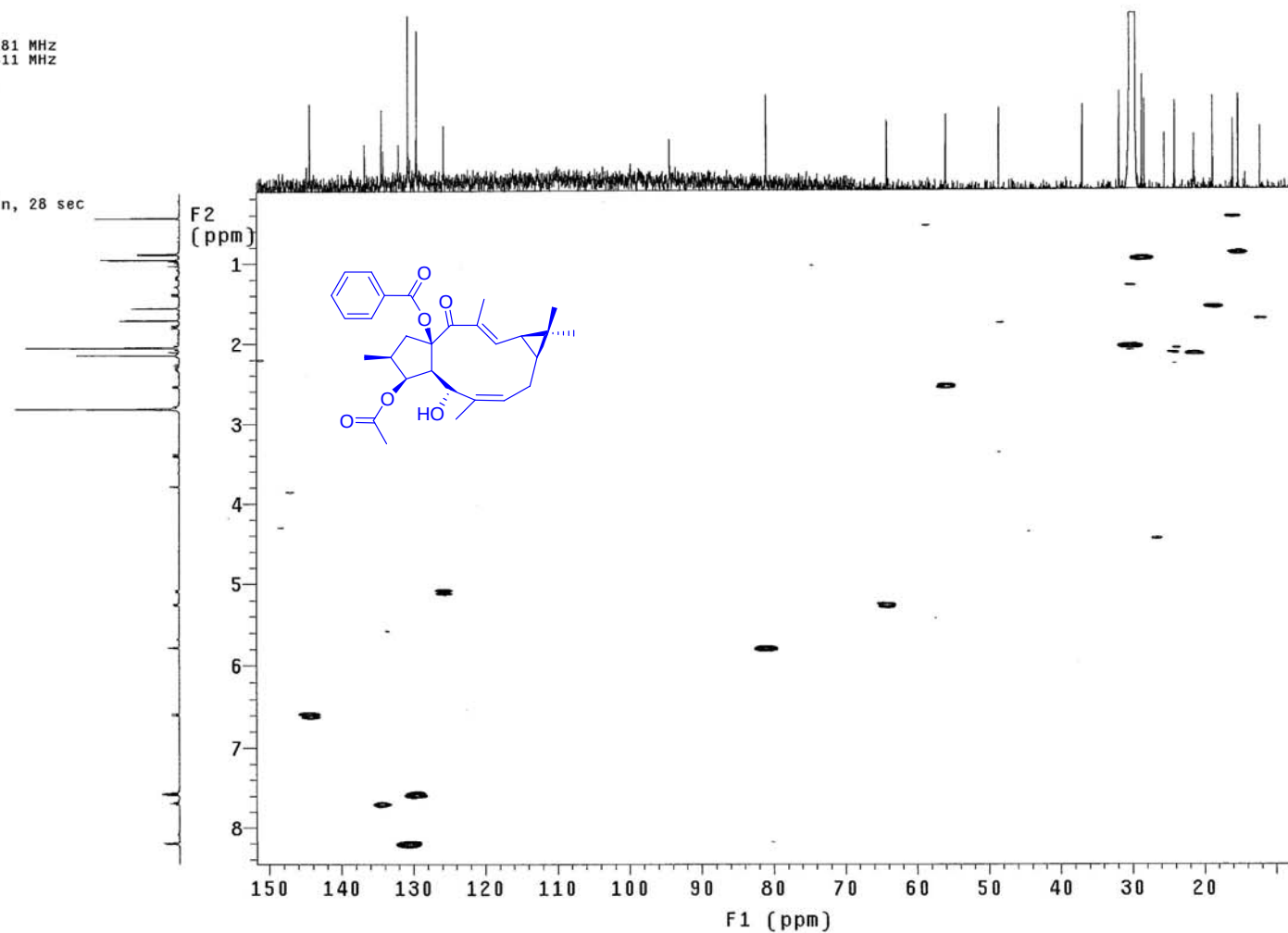


Figure S137. The gHSQC Spectrum of 14 in CD_3COCD_3 (600MHz for ^1H NMR).

SYS-600 gHMBC E-9-2-1 in CD3COCD3 08.06.06

Solvent: acetone
Ambient temperature
Operator: vnmr2
VNMRS-600 "wormhole"

Relax. delay 1.000 sec
Mixing 0.080 sec
Acq. time 0.128 sec
Width 5506.6 Hz
2D Width 33783.8 Hz
256 repetitions
256 increments
OBSERVE H1, 599.6981354 MHz
DATA PROCESSING
Sine bell 0.025 sec
F1 DATA PROCESSING
Sine bell 0.004 sec
FT size 2048 x 8192
Total time 22 hr, 5 min, 59 sec

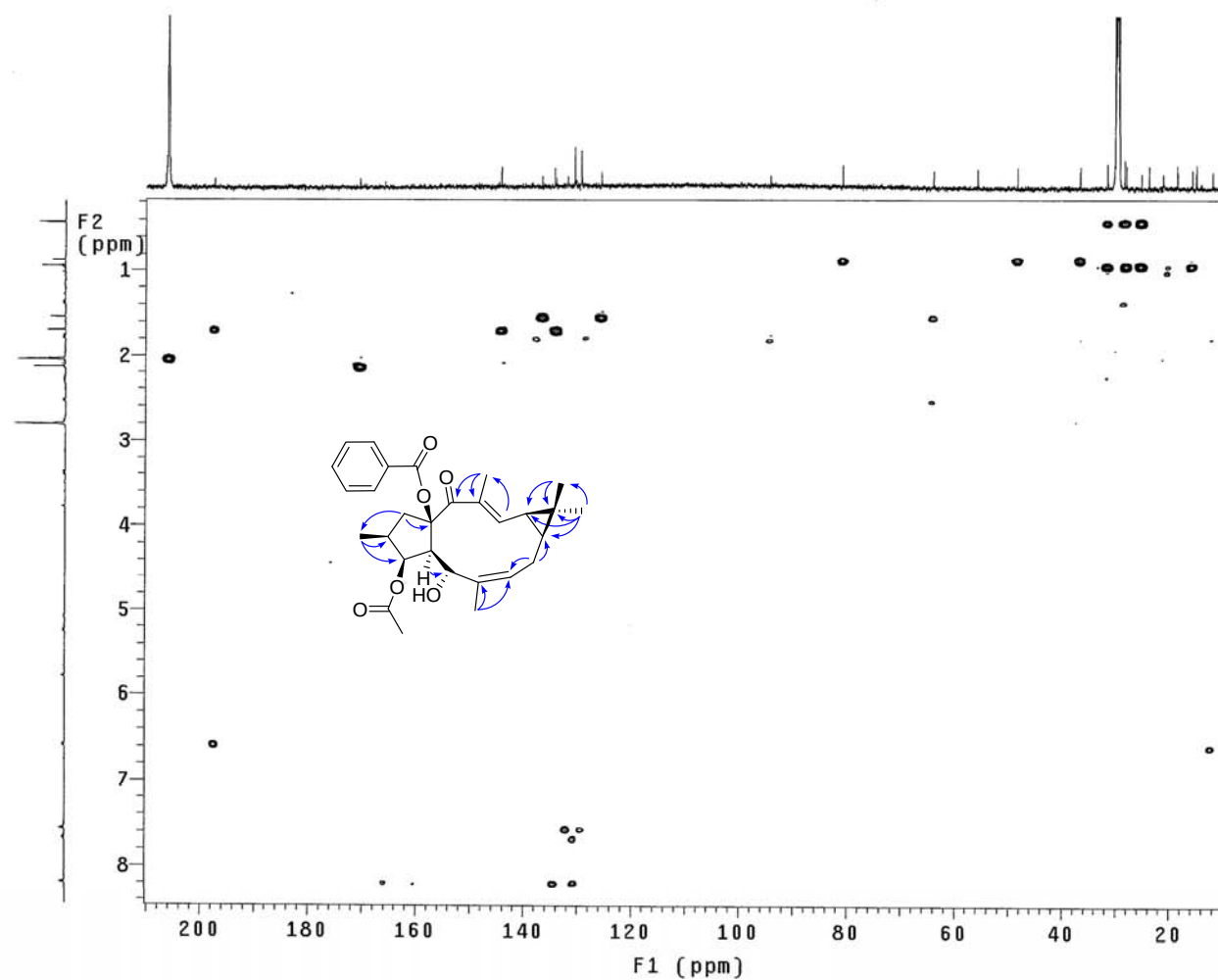


Figure S138. The gHMBC Spectrum of 14 in CD₃COCD₃ (600MHz for ¹H NMR).
S150

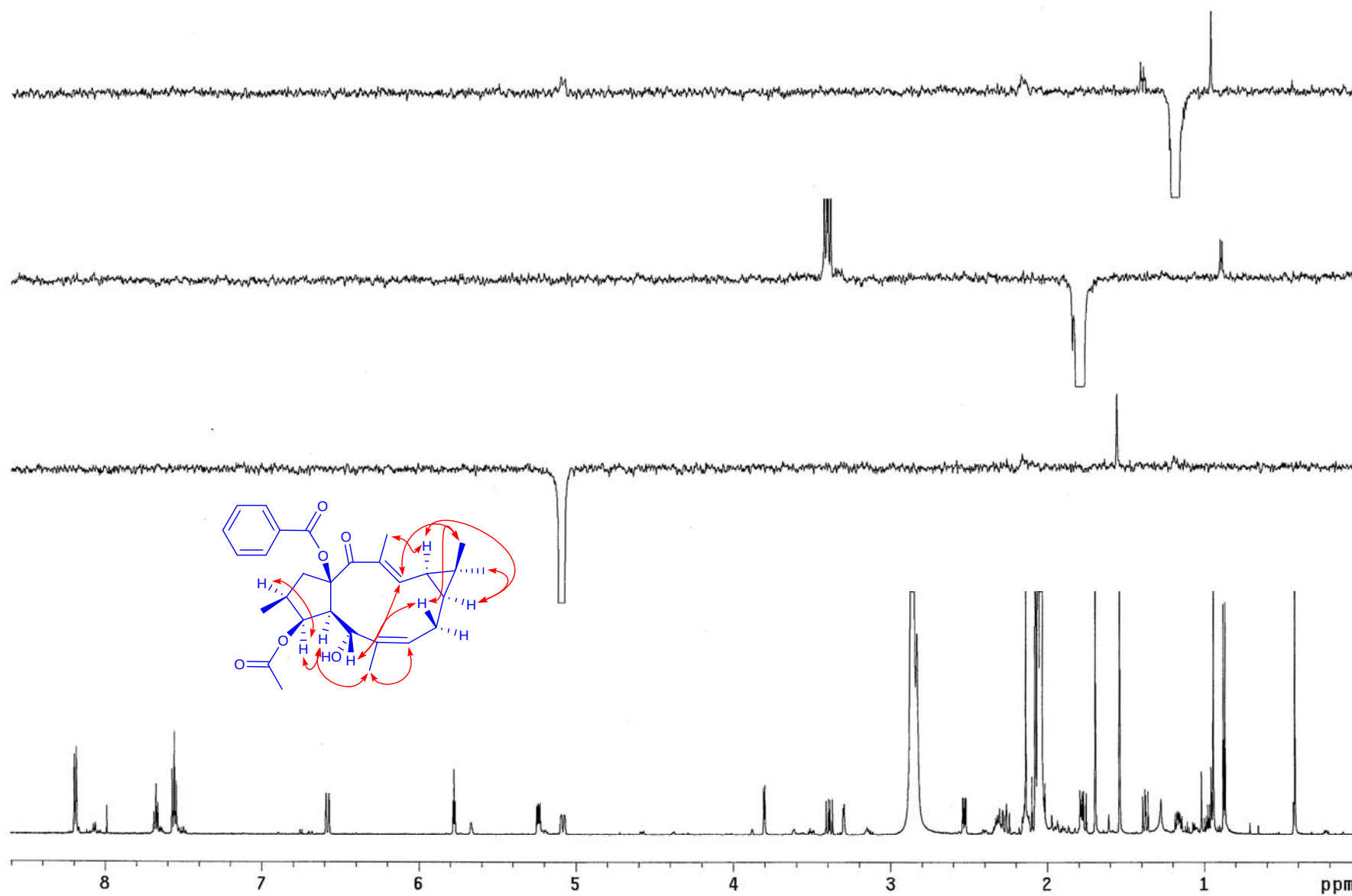


Figure S139. The NOE Difference Spectrum 1 of 14 in CD₃COCD₃ (600 MHz).

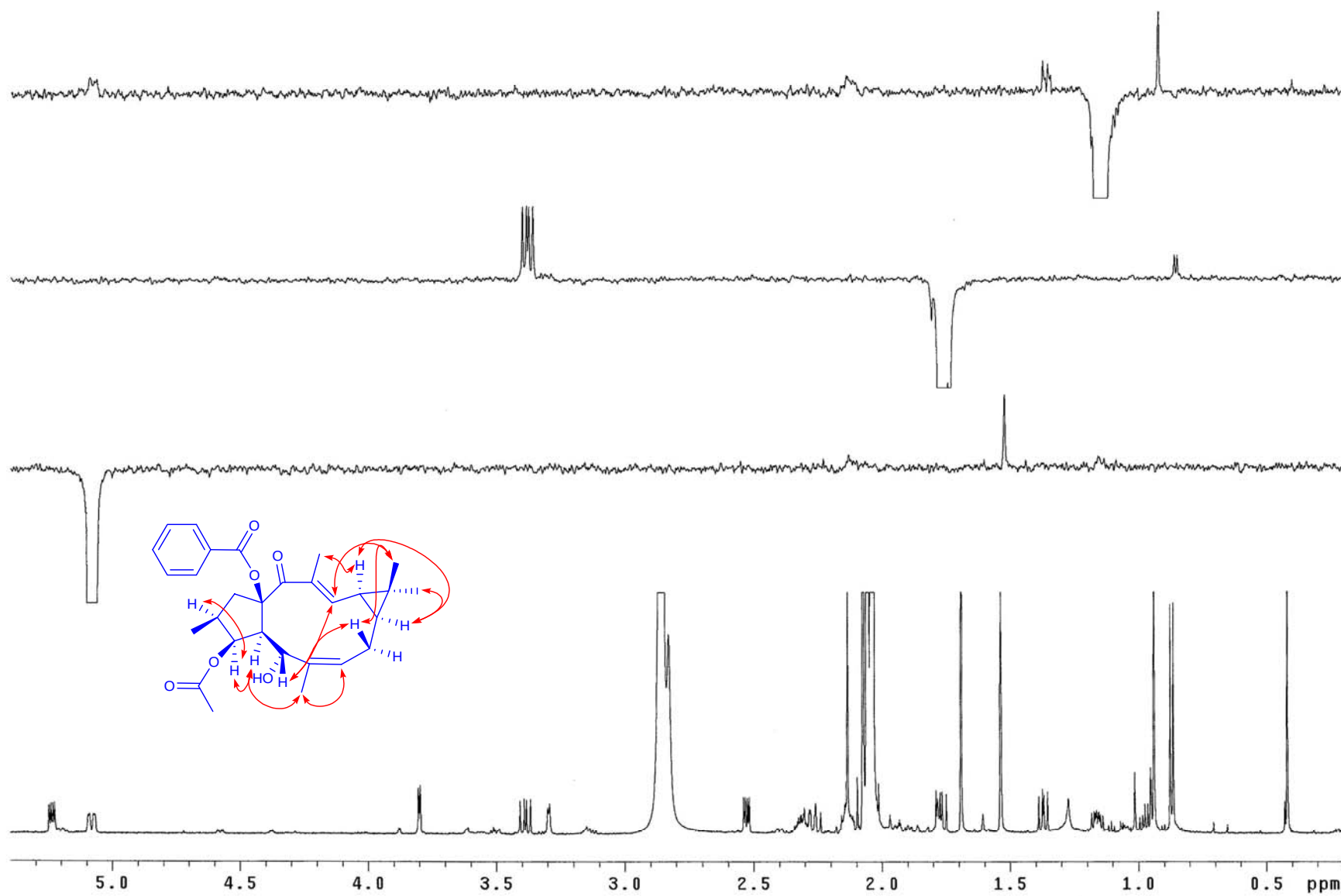


Figure S140. The NOE Difference Spectrum 2 of 14 in CD₃COCD₃ (600 MHz).
S152

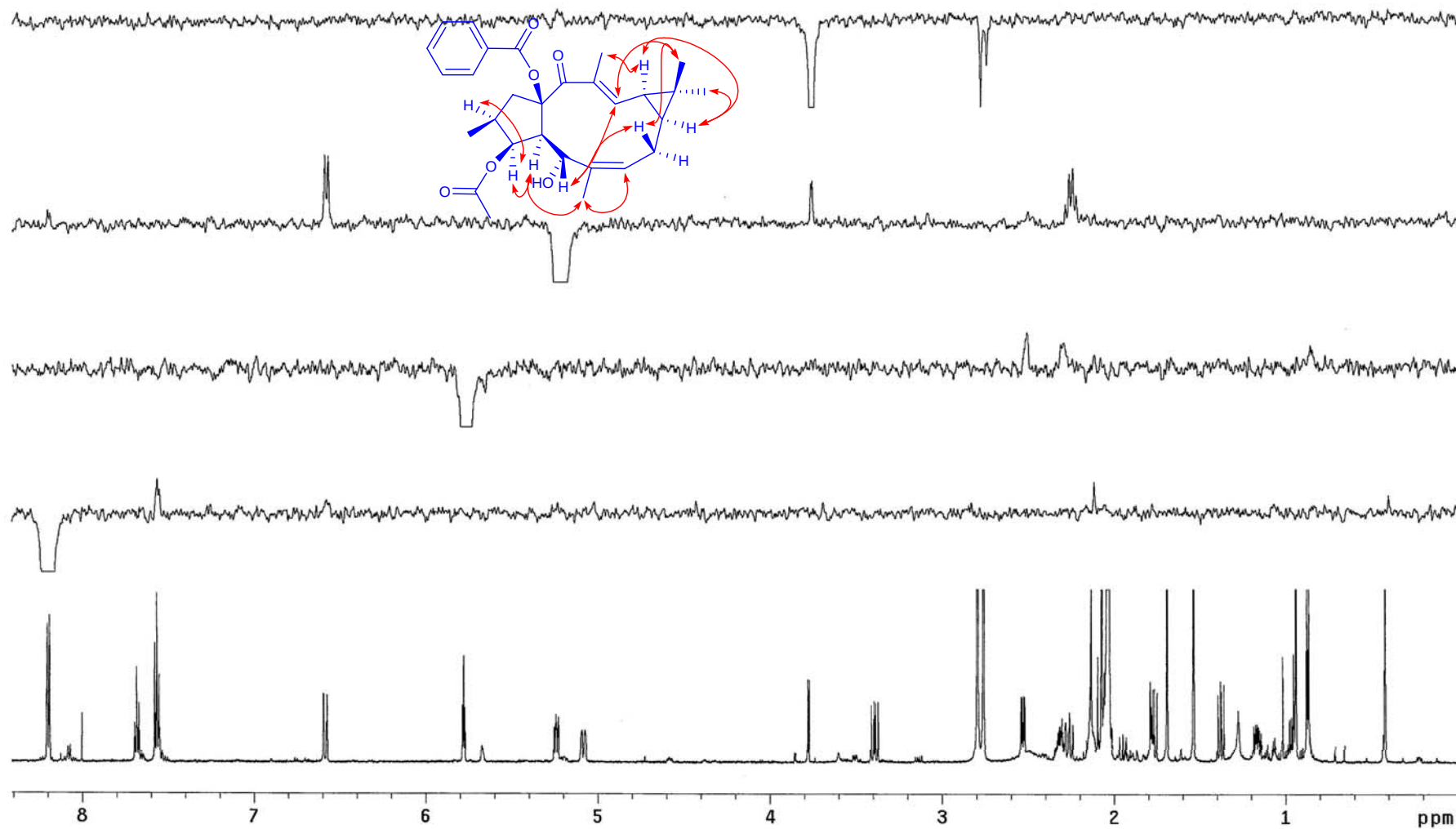


Figure S141. The NOE Difference Spectrum 3 of 14 in CD₃COCD₃ (600 MHz).

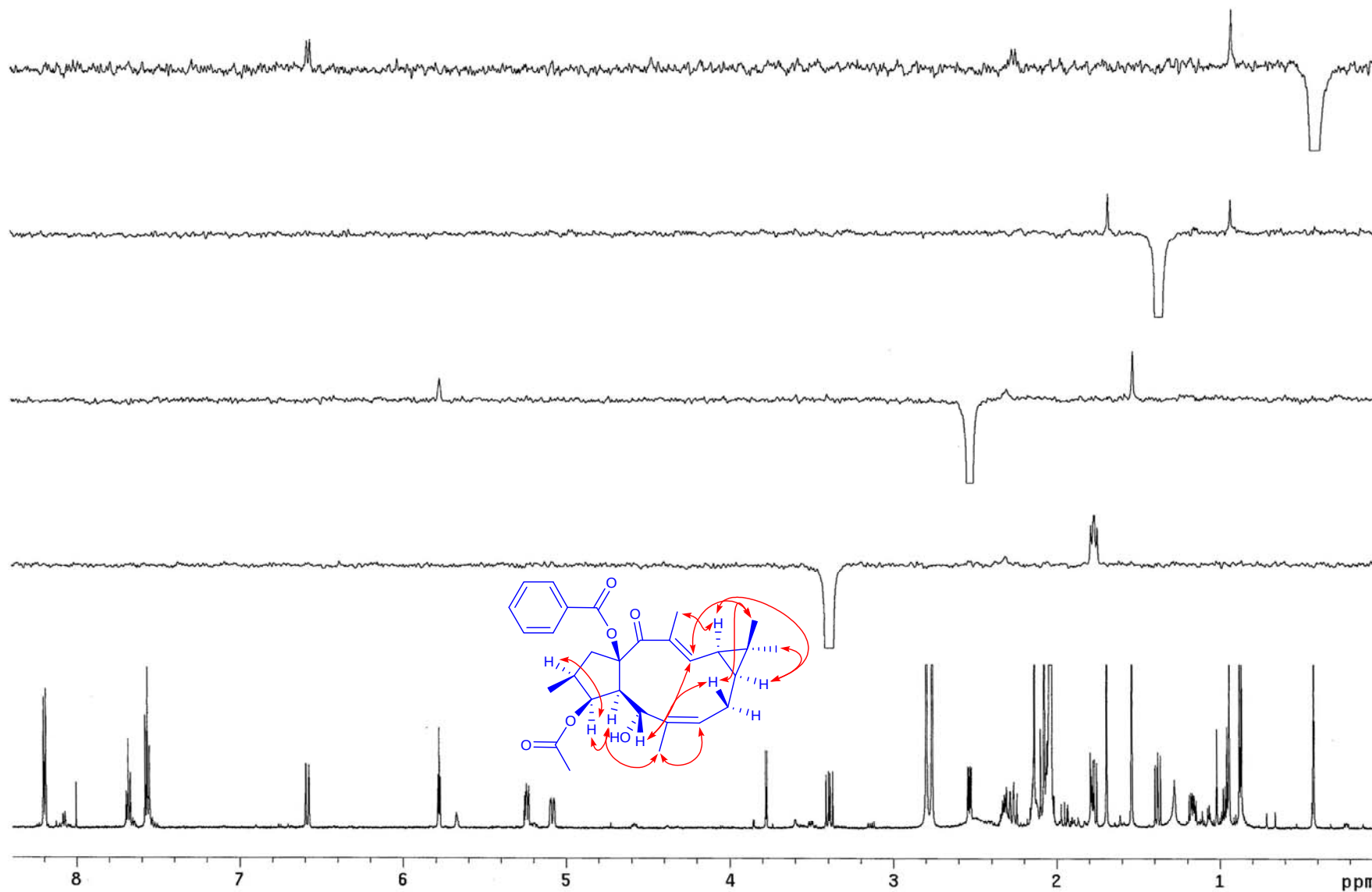


Figure S142. The NOE Difference Spectrum 4 of 14 in CD₃COCD₃ (600 MHz).

S154

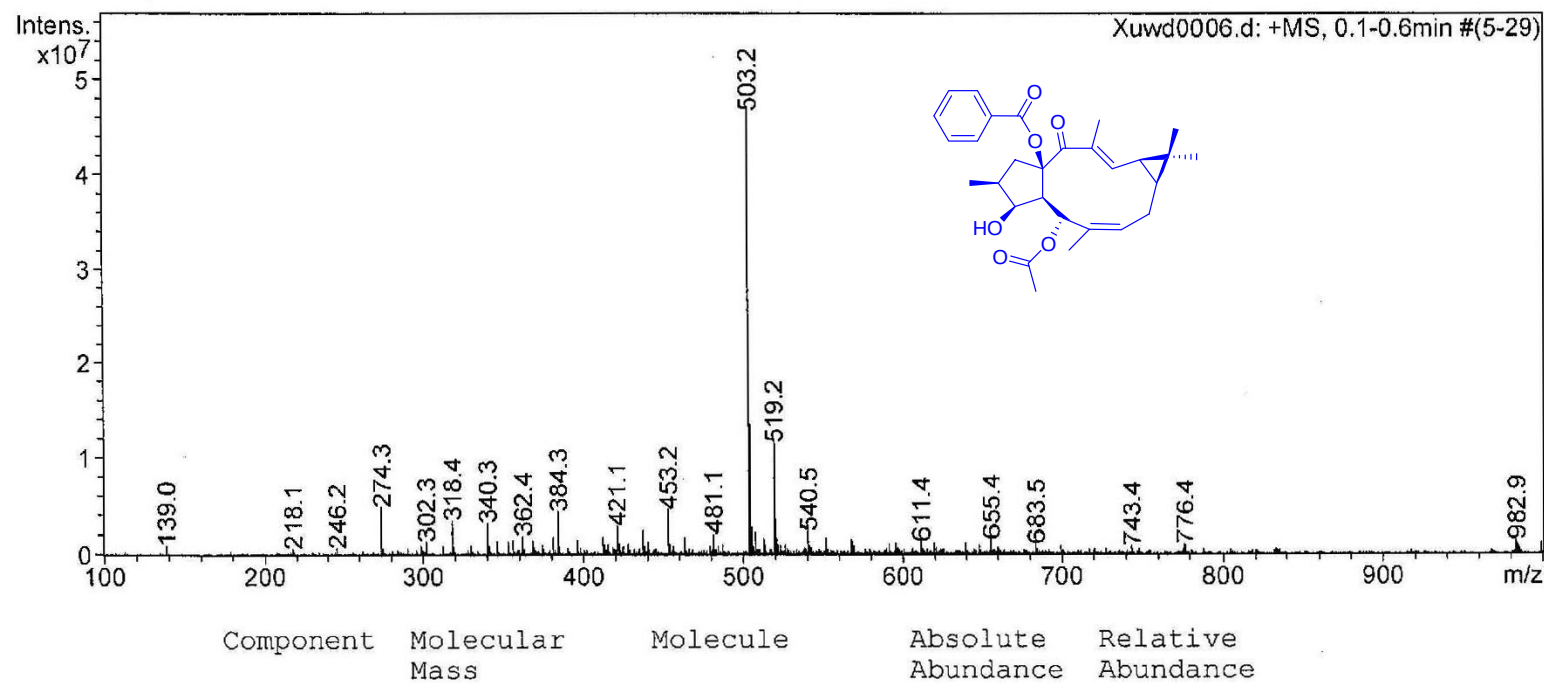


Figure S143. (+)-ESIMS Spectrum of 15.

Data:E_9_3

Sample Name:

Description:

Ionization Mode:ESI+

History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[];Smooth[3];Correct Base[5.0%];Average(MS[...

Acquired:12:00:00 AM

Operator:Accutof

Mass Calibration data:TFA100-2000-P-070410

Created:10/14/2008 10:46:01 AM

Created by:Accutof

Charge number:1

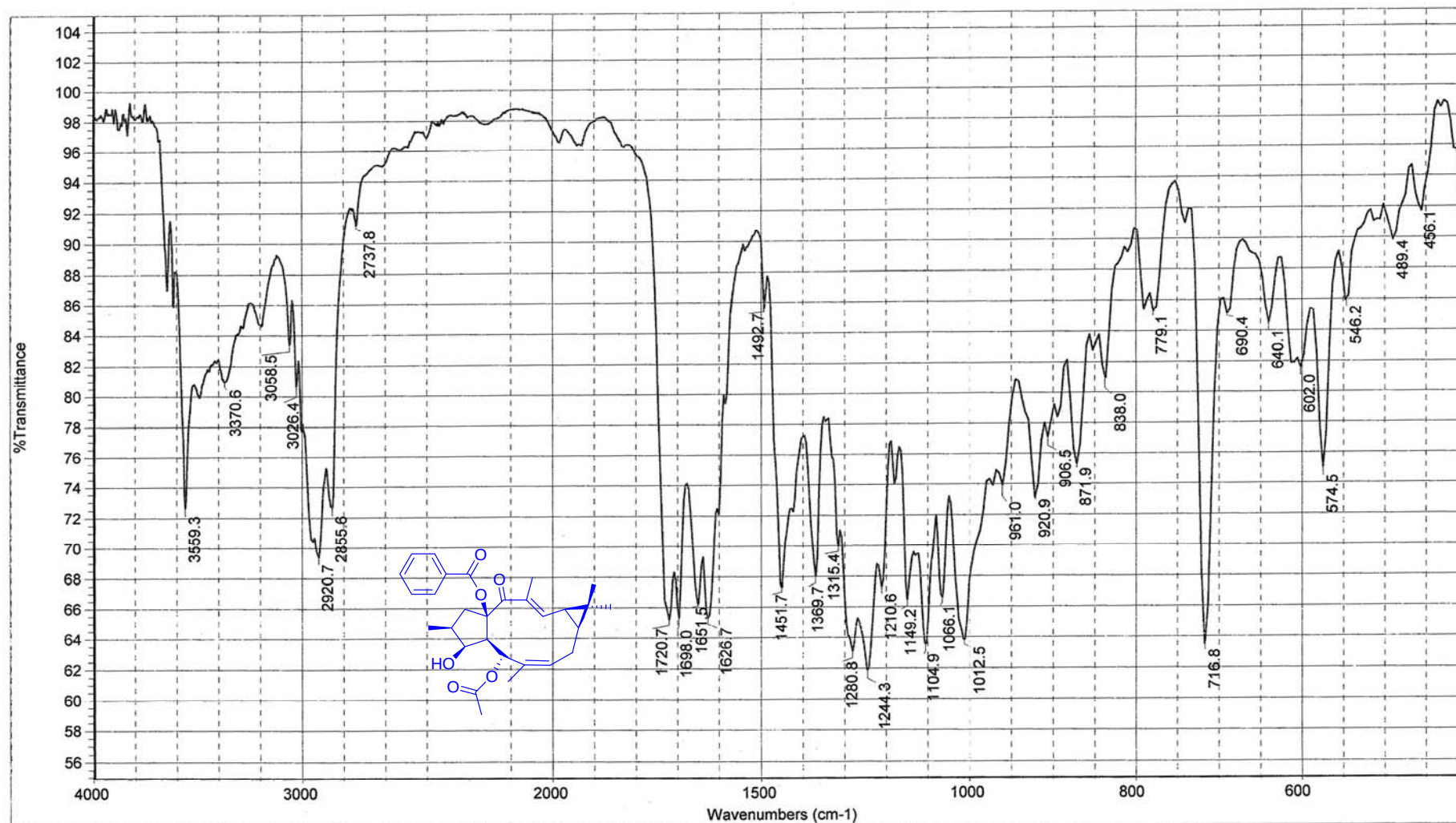
Tolerance:5.00(mmu)

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

Element:¹²C:0 .. 100, ¹H:0 .. 200, ³⁹K:1 .. 1, ¹⁶O:0 .. 10

Mass	Mass Difference (mmu)	Mass Difference (ppm)	¹² C	¹ H	³⁹ K	¹⁶ O	Unsaturation Number
519.21887	3.98	7.66	29	36	1	6	11.5

(+)-HRESIMS Data of 15.



日期: 星期一 10月 06 09:12:43 2008 (GMT+08: Sample Name: E - 9 - 3

(显微镜透射法 FT- IR Microscope Transmission)

扫描次数: 100

傅里叶变换红外显微镜(FT-IR Microscope): Centaurus

分辨率: 8.000

美国热电公司(Thermo)傅立叶变换红外光谱仪:Nicolet 5700

Figure S144. The IR Spectrum of 15.

S156

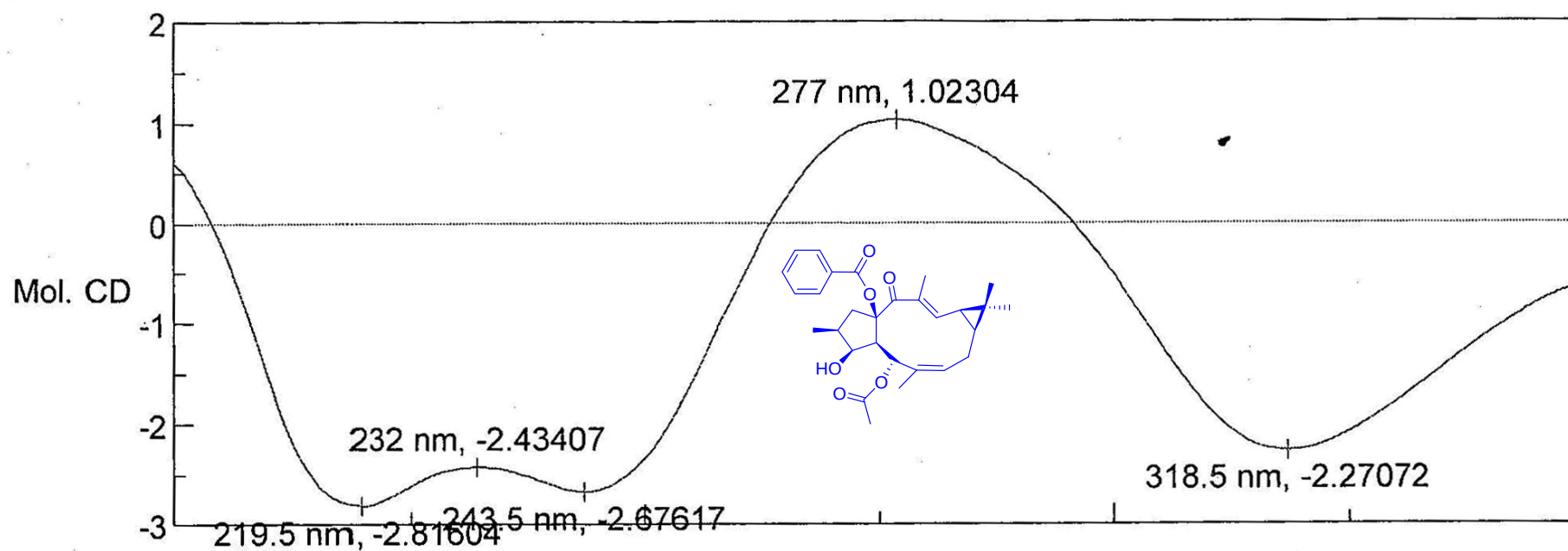


Figure S145. The CD Spectrum of 15.

S158

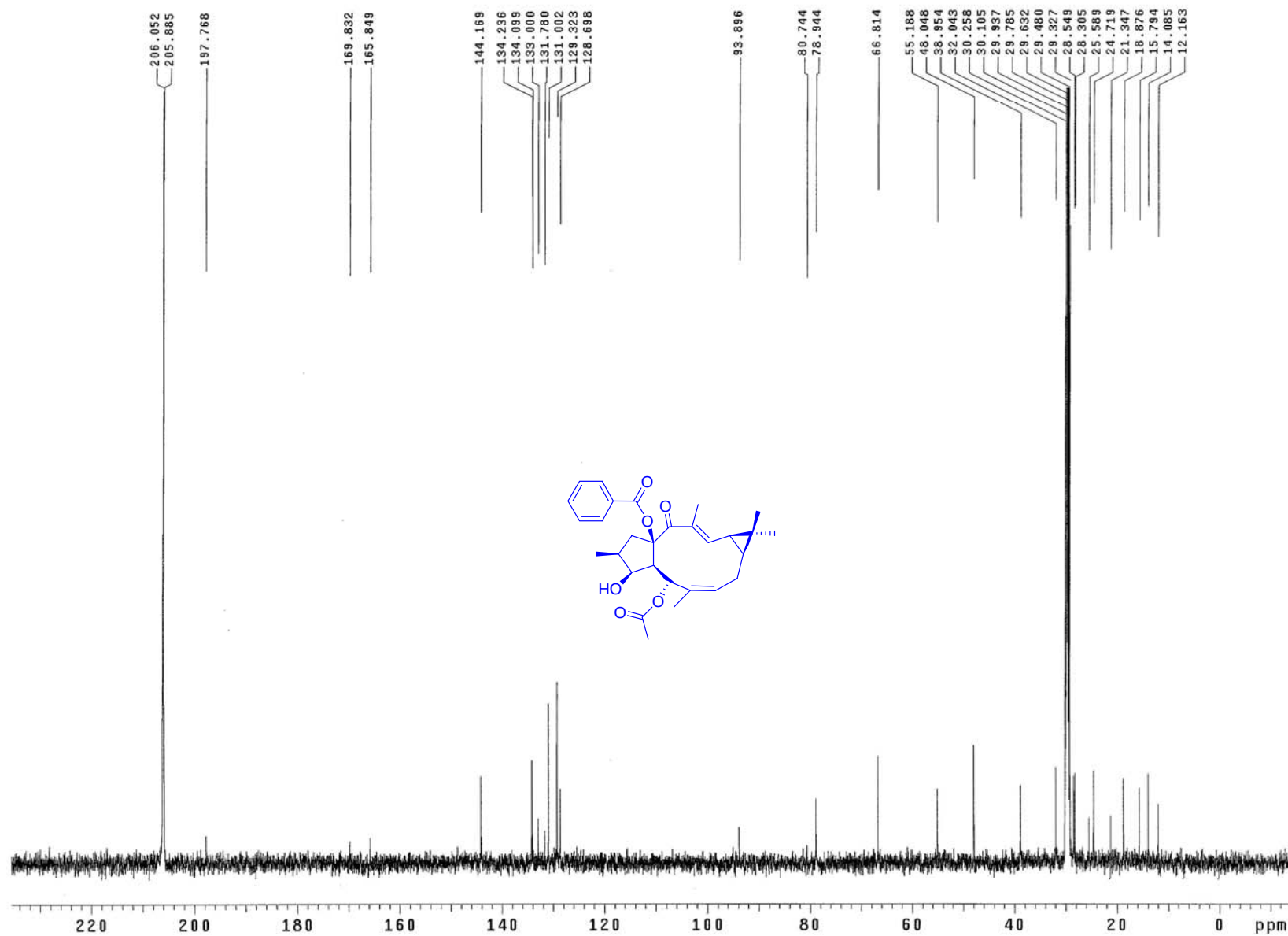


Figure S147. The ^{13}C NMR Spectrum of 15 in CD_3COCD_3 (125 MHz).

INOVA-501 gCOSY E-9-3 IN CD3COCD3 08.01.14

Solvent: Acetone
Temp. 25.0 C / 298.1 K
INOVA-500 "IMM-501"

Relax. delay 1.000 sec
Acq. time 0.222 sec
Width 4609.6 Hz
2D Width 4609.6 Hz
8 repetitions
200 increments
OBSERVE H1, 499.7728092 MHz
DATA PROCESSING
Sine bell 0.111 sec
F1 DATA PROCESSING
Sine bell 0.023 sec
FT size 2048 x 2048
Total time 33 min, 50 sec

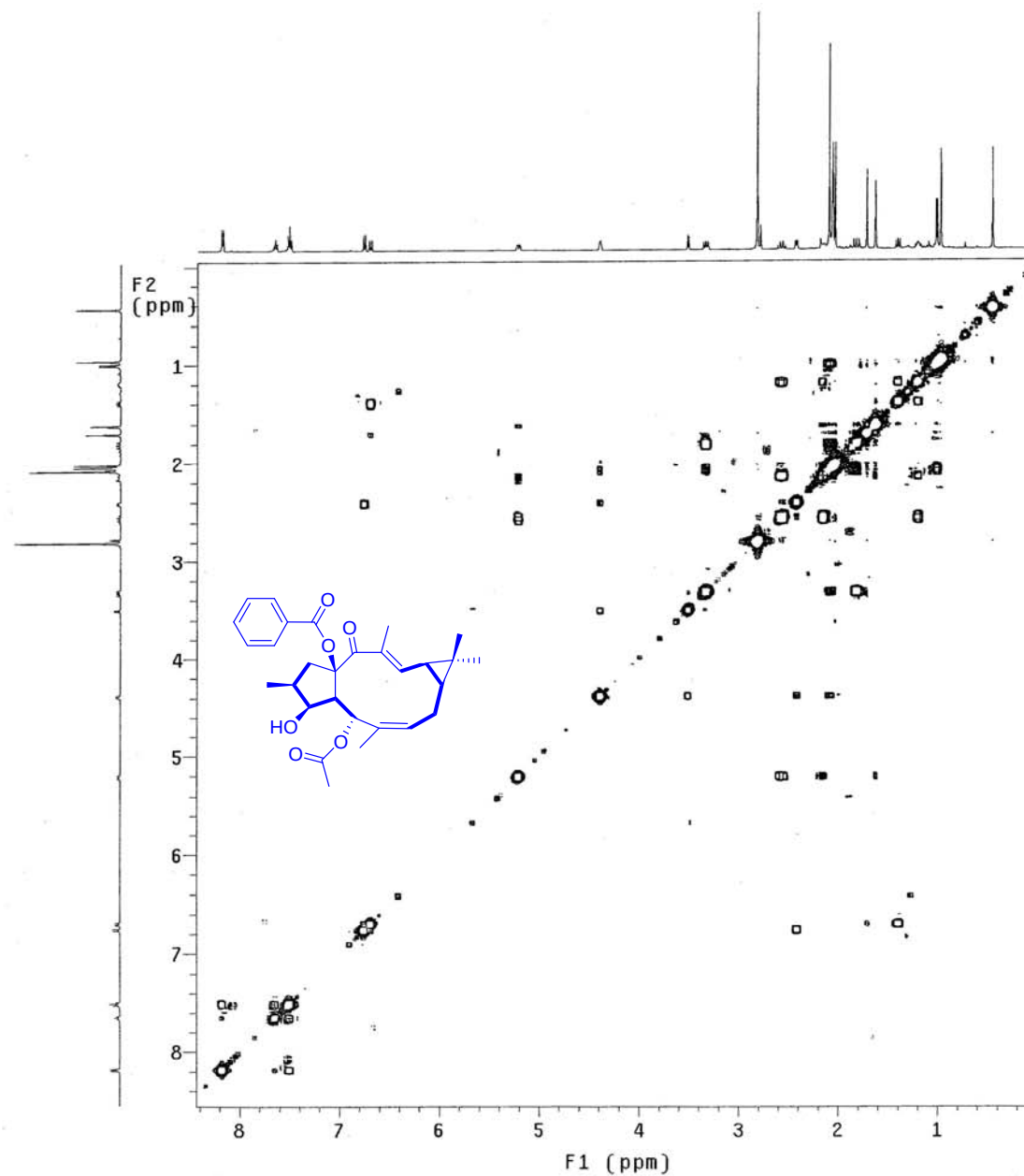


Figure S148. The ^1H - ^1H gCOSY Spectrum of 15 in CD_3COCD_3 (500 MHz).
S160

Solvent: Acetone
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "IMM-501"

Relax. delay 1.000 sec
Acq. time 0.222 sec
Width 4609.6 Hz
2D Width 27962.3 Hz
64 repetitions
256 increments
OBSERVE H1, 499.7728092 MHz
DECOUPLE C13, 125.6815149 MHz
Power 48 dB
on during acquisition
off during delay
GARP-1 modulated
DATA PROCESSING
Sine bell 0.052 sec
F1 DATA PROCESSING
Sine bell 0.005 sec
FT size 2048 x 4096
Total time 5 hr, 54 min, 21 sec

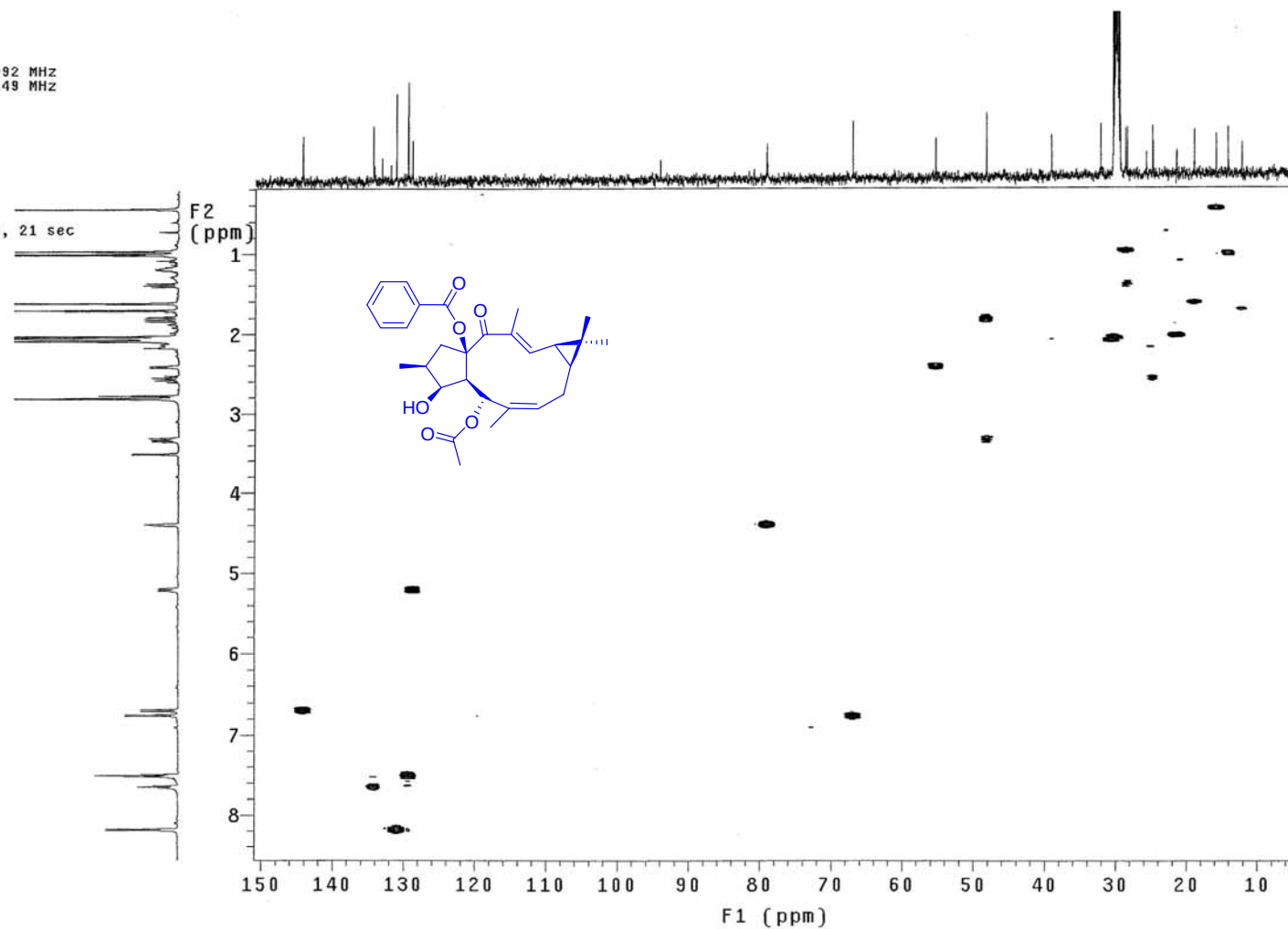


Figure S149. The gHSQC Spectrum of 15 in CD_3COCD_3 (500MHz for ^1H NMR).

Solvent: Acetone
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "IMM-501"

Relax. delay 1.000 sec
Acq. time 0.219 sec
Width 4668.8 Hz
2D Width 27962.3 Hz
80 repetitions
320 increments
OBSERVE H1, 499.7728092 MHz
DATA PROCESSING
Sine bell 0.055 sec
F1 DATA PROCESSING
Sine bell 0.004 sec
FT size 2048 x 4096
Total time 9 hr, 18 min, 15 sec

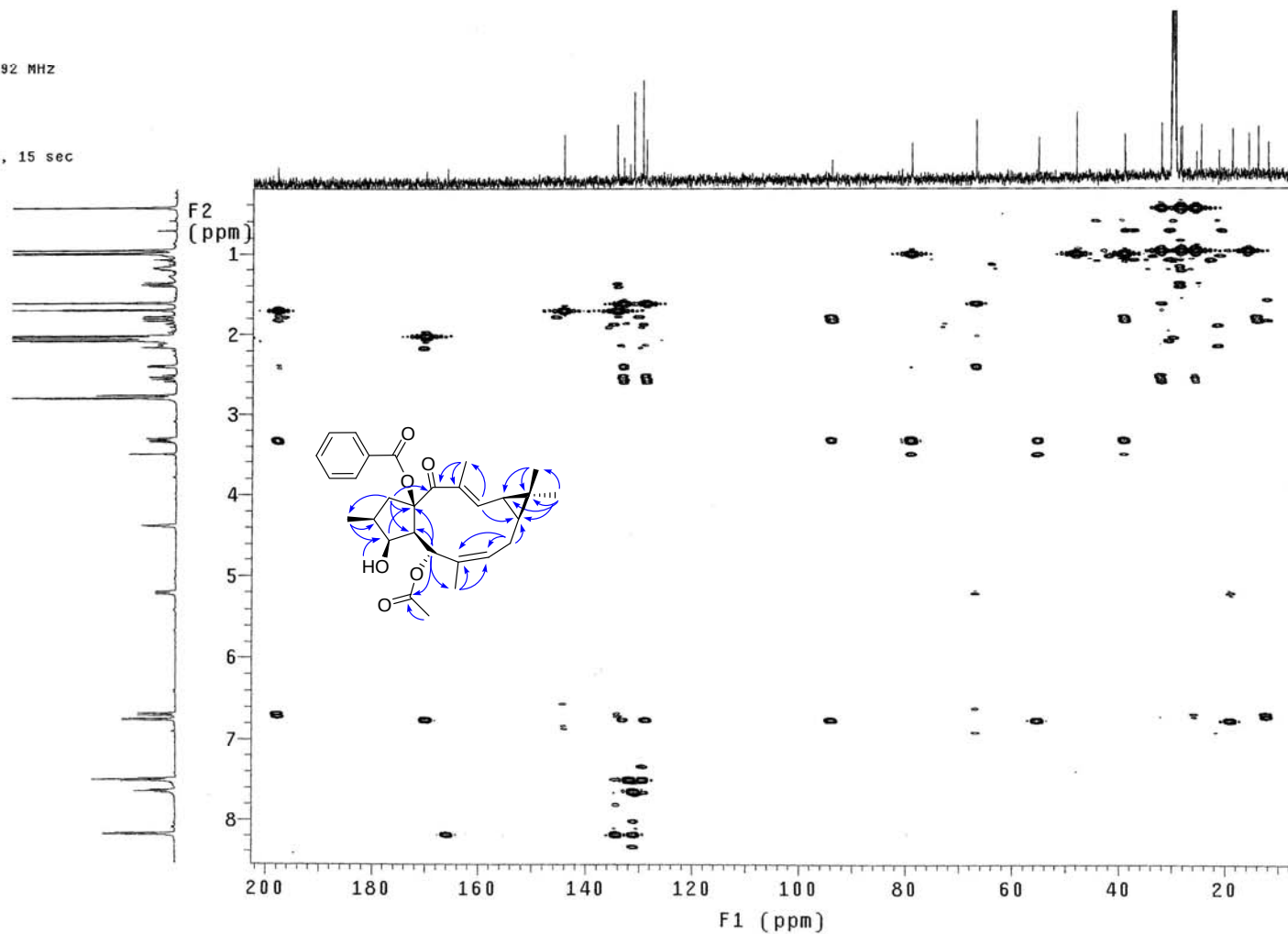


Figure S150. The gHMBC Spectrum of 15 in CD₃COCD₃ (500MHz for ¹H NMR).

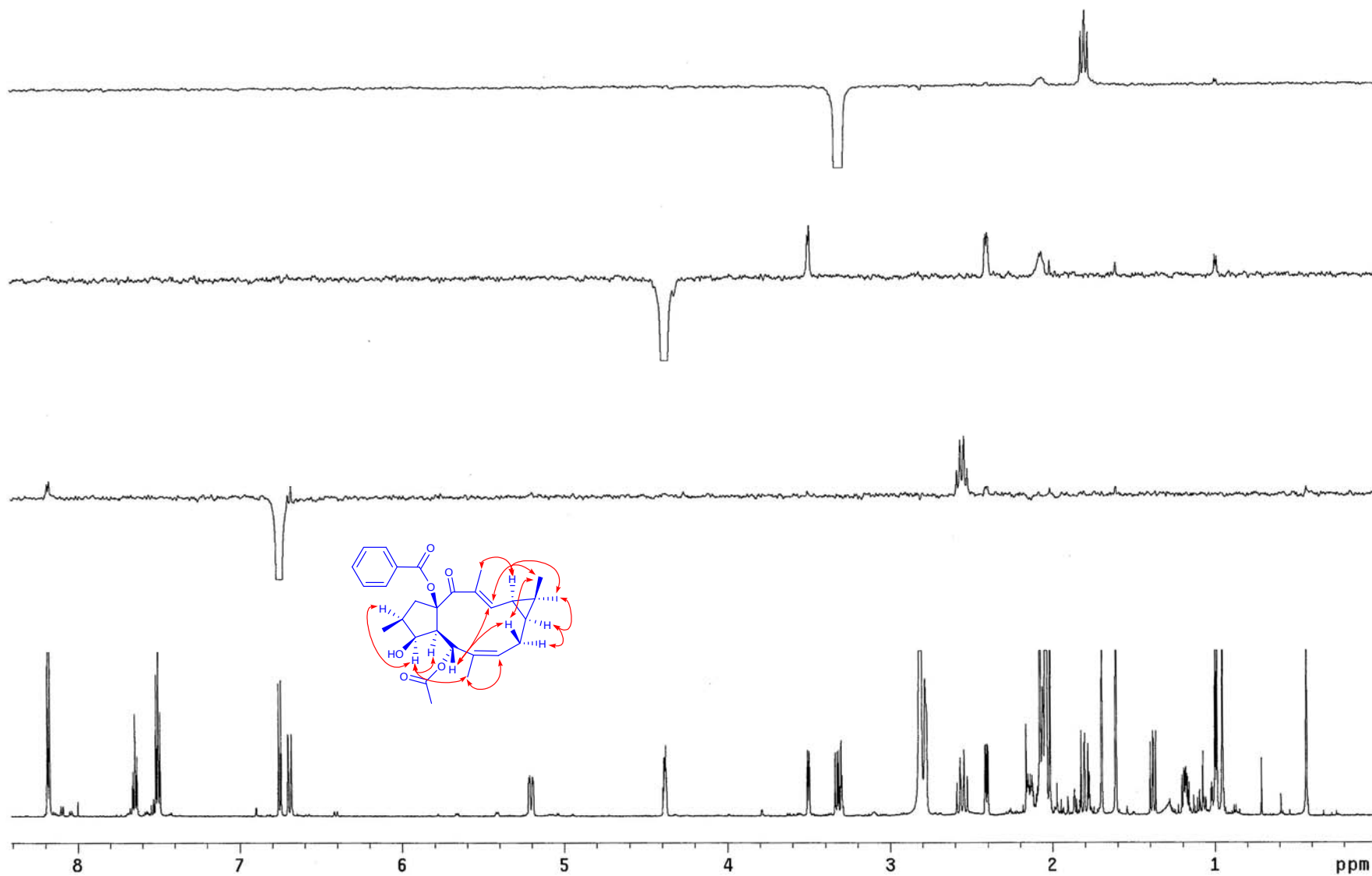


Figure S151. The NOE Difference Spectrum 1 of 15 in CD₃COCD₃ (600 MHz).

S163

Solvent: Acetone
Temp. 25.0 C / 298.1 K
INOVA-500 "IMM-501"

Relax. delay 1.600 sec
Mixing 0.800 sec
Acq. time 0.227 sec
Width 4513.1 Hz
2D Width 4513.1 Hz
8 repetitions
2 x 200 increments
OBSERVE H1, 499.7728092 MHz
DATA PROCESSING
Gauss apodization 0.044 sec
F1 DATA PROCESSING
Gauss apodization 0.017 sec
FT size 2048 x 2048
Total time 2 hr, 23 min, 25 sec

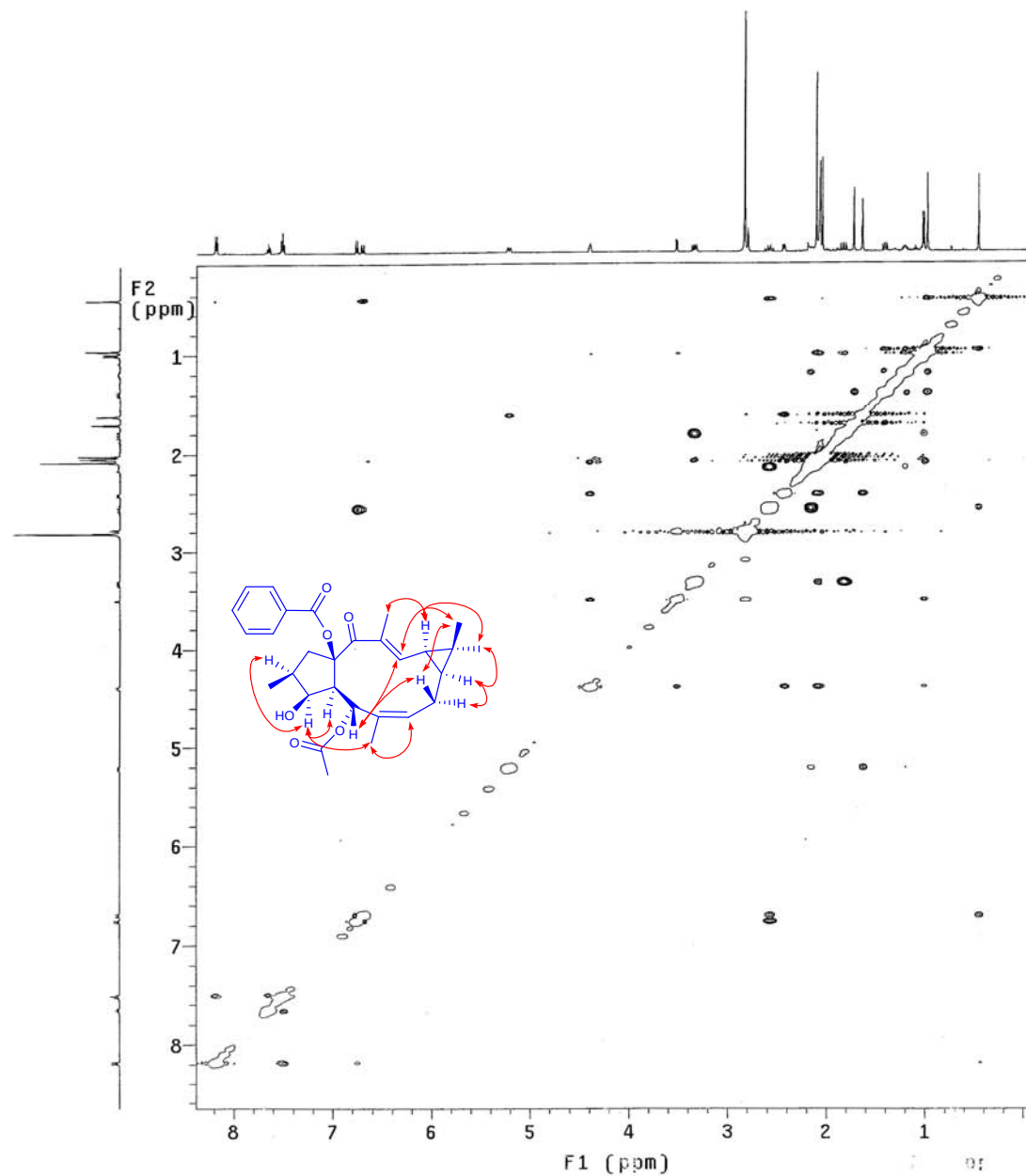


Figure S152. The NOESY Spectrum of 15 in CD₃COCD₃ (500 MHz).

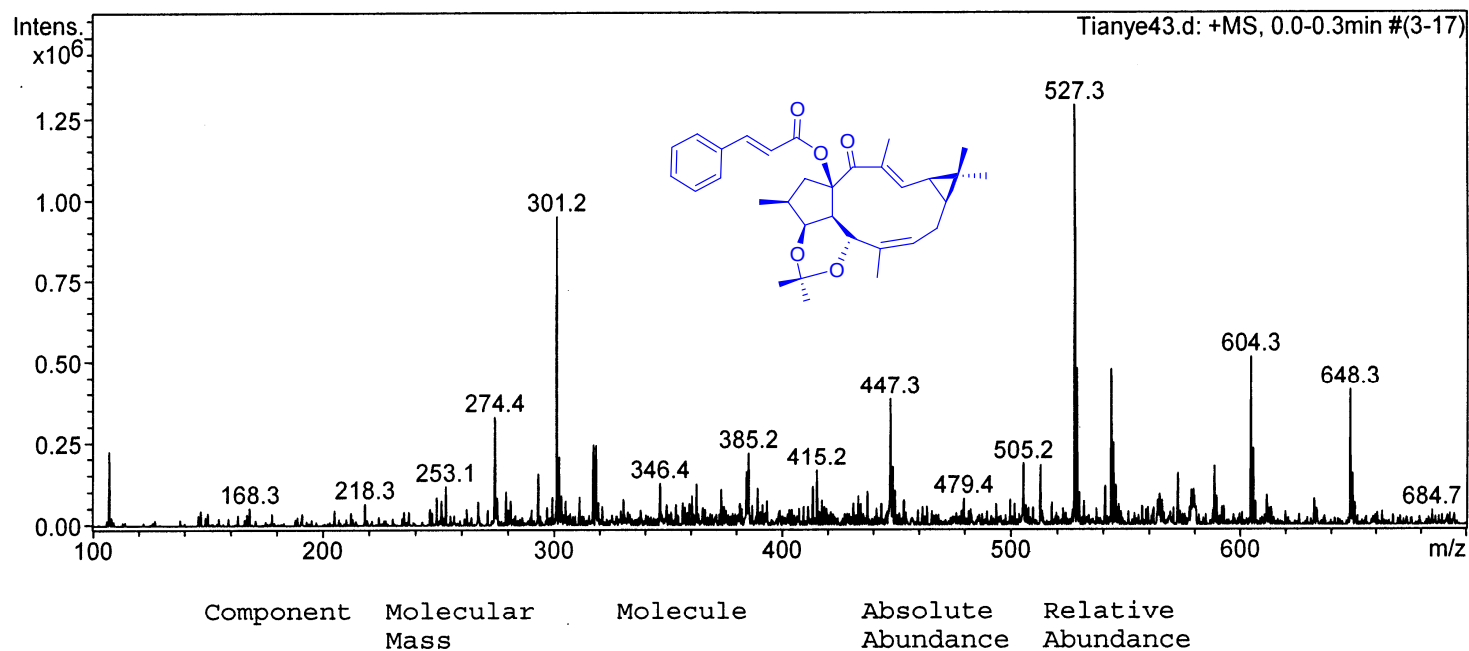


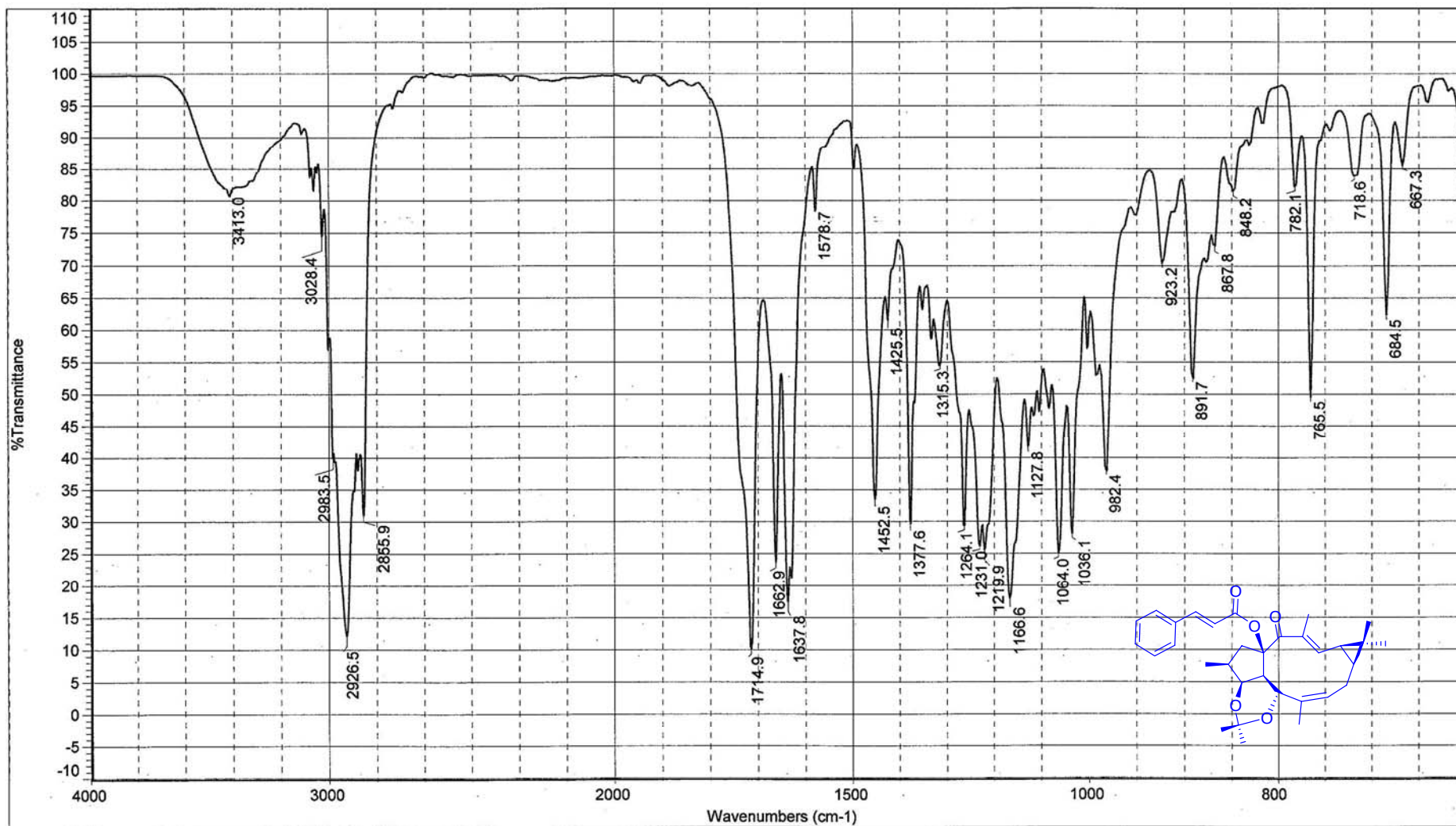
Figure S153. The (+)-ESIMS Spectrum of 16.

MS Formula Results: + Scan (9.205 min) Sub (201011153.d)

m/z	Ion	Formula	Abundance
527.2772	(M+Na)+	C32 H40 Na O5	513089.5

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross S	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Mat	Mass Match	m/z	DBE
☒	C32 H40 O5	C32 H40 Na O5	527.2768	99.98		504.288	504.2876	-0.77	0.77	99.97	99.97	99.98	527.2772	13
☐	C27 H40 N2 O7	C27 H40 N2 Na O7	527.2728	98.55		504.288	504.2836	-8.76	8.76	98.92	99.99	97.6	527.2772	9
☐	C20 H44 N2 O12	C20 H44 N2 Na O12	527.2786	97.16		504.288	504.2894	2.89	2.89	90.52	100	99.74	527.2772	0

(+)-HRESIMS Data of 16.



日期: 星期四 12月 30 17:04:53 2010 (GMT+08: Sample Name : F4-1-1-C

(显微镜透射法FT- IR Microscope Transmission)

扫描次数: 64

分辨率: 4.000

美国热电公司(Thermo)傅里叶变换红外光谱仪:Nicolet 5700

Figure S154. The IR Spectrum of 16.
S166

INOVA-501 1H-NMR F4-1-1-C IN CD3C0CD3 09.06.21 cold probe

Chemical structure of the compound (1) is shown above the spectrum. The structure is a complex polycyclic molecule with a benzylidene group, a lactone, and a bicyclic system.

1H-NMR spectrum (400 MHz, CDCl₃) of compound 1. The spectrum shows peaks from 0.7 to 7.7 ppm. The following table lists the chemical shifts (ppm) and integration values for the peaks:

Chemical Shift (ppm)	Integration
7.713	0.38
7.690	0.37
7.681	
7.444	
7.440	
7.433	
6.796	
6.763	
6.578	
6.556	
5.422	
5.411	
5.283	
5.264	
5.259	
4.030	
4.024	
4.017	
3.590	
3.360	
3.345	
3.334	
3.320	
2.794	
2.484	
2.456	
2.432	
2.317	
2.286	
2.123	
2.116	
2.106	
2.049	
2.044	
2.040	
2.036	
2.032	
1.999	
1.992	
1.986	
1.706	
1.698	
1.645	
1.620	
1.595	
1.529	
1.452	
1.436	
1.430	
1.413	
1.368	
1.357	
1.341	
1.334	
1.328	
1.318	
1.294	
1.282	
1.226	
1.209	
1.195	
1.093	
1.074	
1.038	
1.015	
1.001	
0.972	
0.959	
0.948	
0.868	
0.855	
0.839	
0.834	
0.820	
0.718	

Figure S155. The ^1H NMR Spectrum of 16 in CD_3COCD_3 (500 MHz).

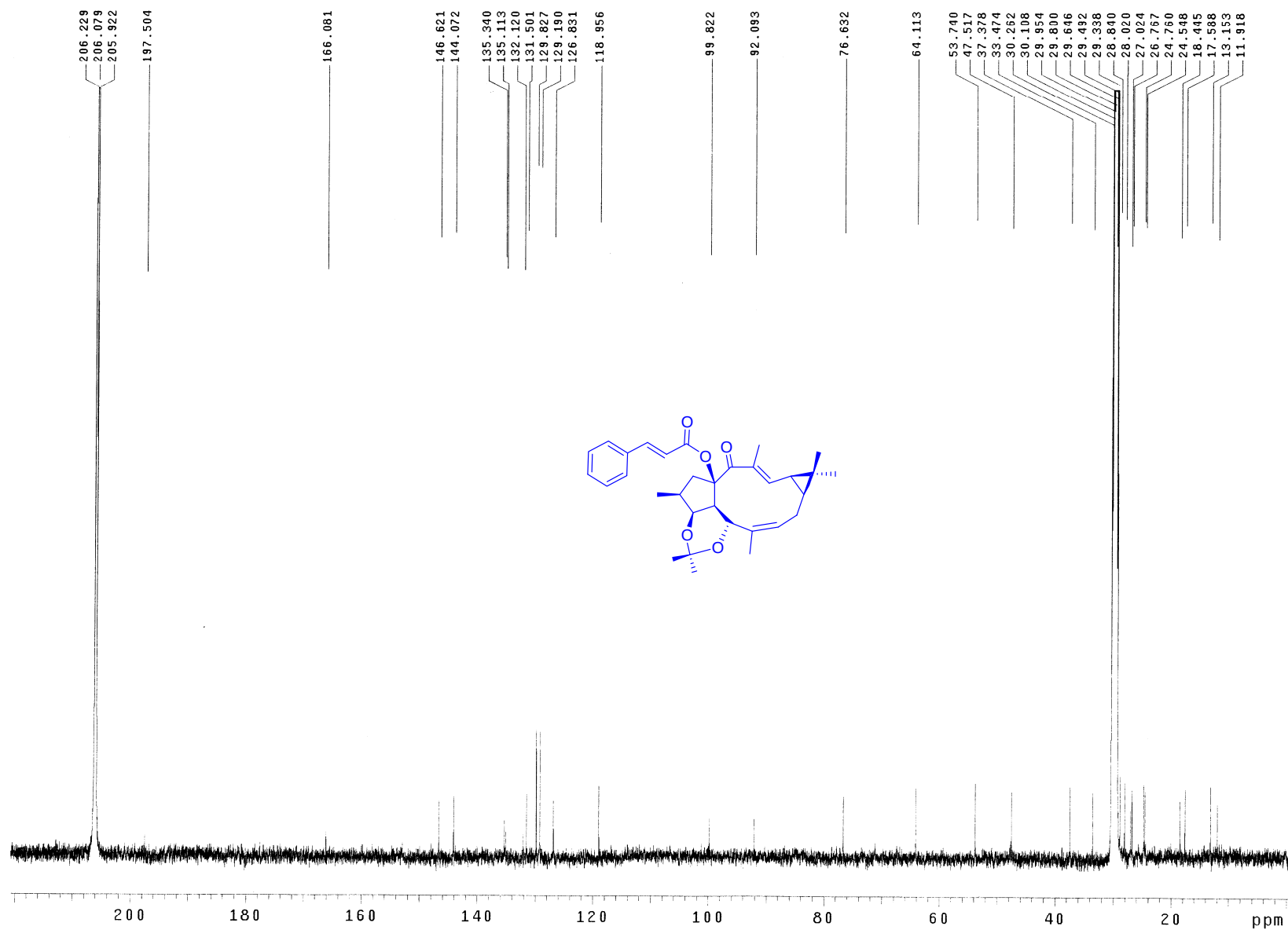


Figure S156. The ^{13}C NMR Spectrum of 16 in CD_3COCD_3 (125 MHz).

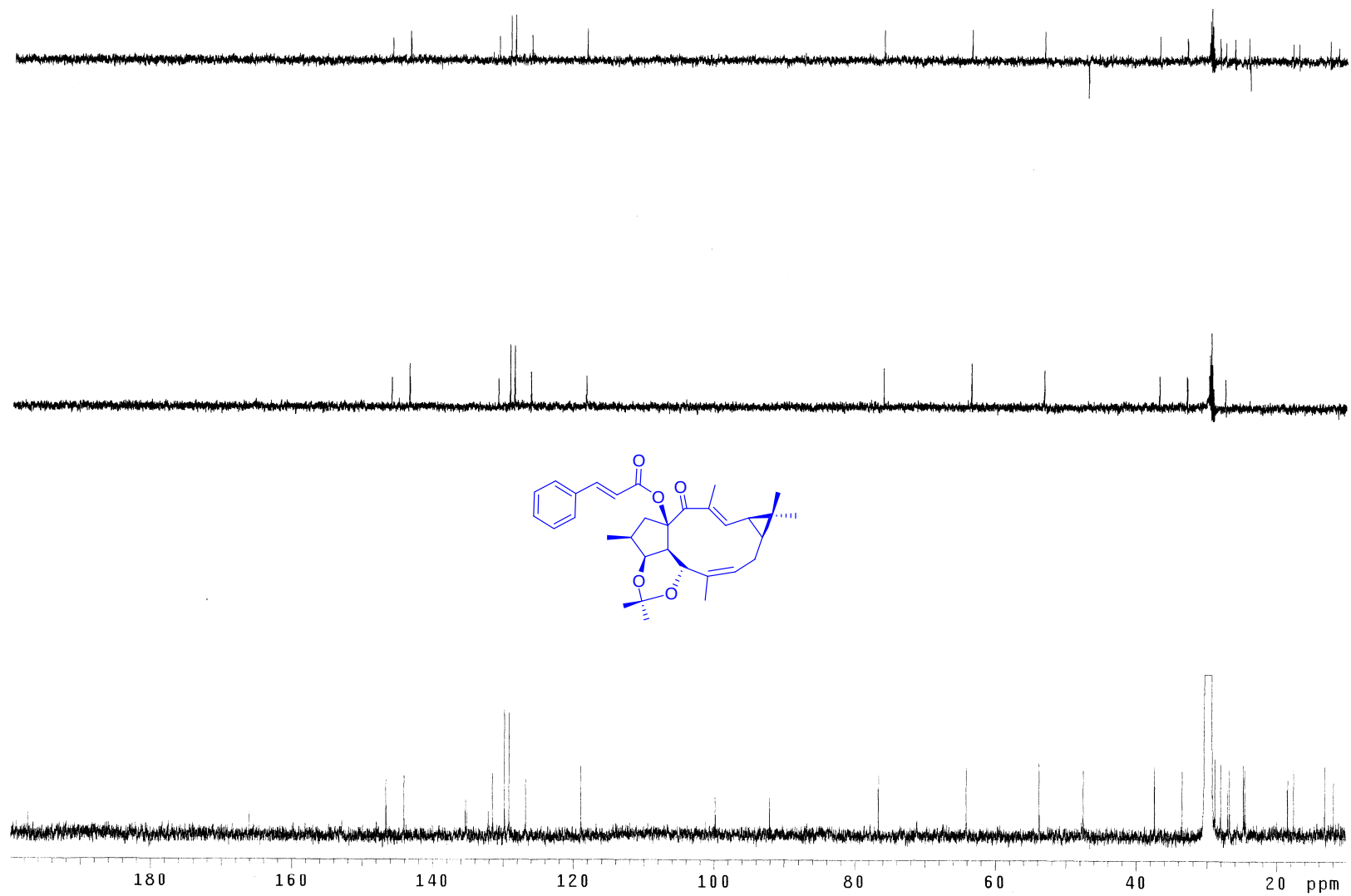


Figure S157. The DEPT Spectrum of 16 in CD_3COCD_3 (125 MHz).
S169

INOVA-501 gCOSY F4-1-1-C IN CD3COCD3 09.07.06 cold probe

Solvent: acetone
Temp. 25.0 C / 298.1 K
Sample #8, Operator: walkup
File: Gcosy_01
INOVA-500 "1HM-501"

Relax. delay 1.301 sec
Acq. time 0.229 sec
Width 4473.8 Hz
2D Width 4473.8 Hz
2 repetitions
256 increments
OBSERVE H1, 499.7733218 MHz
DATA PROCESSING
Sine bell 0.114 sec
F1 DATA PROCESSING
Sine bell 0.029 sec
FT size 4096 x 4096
Total time 13 min, 49 sec

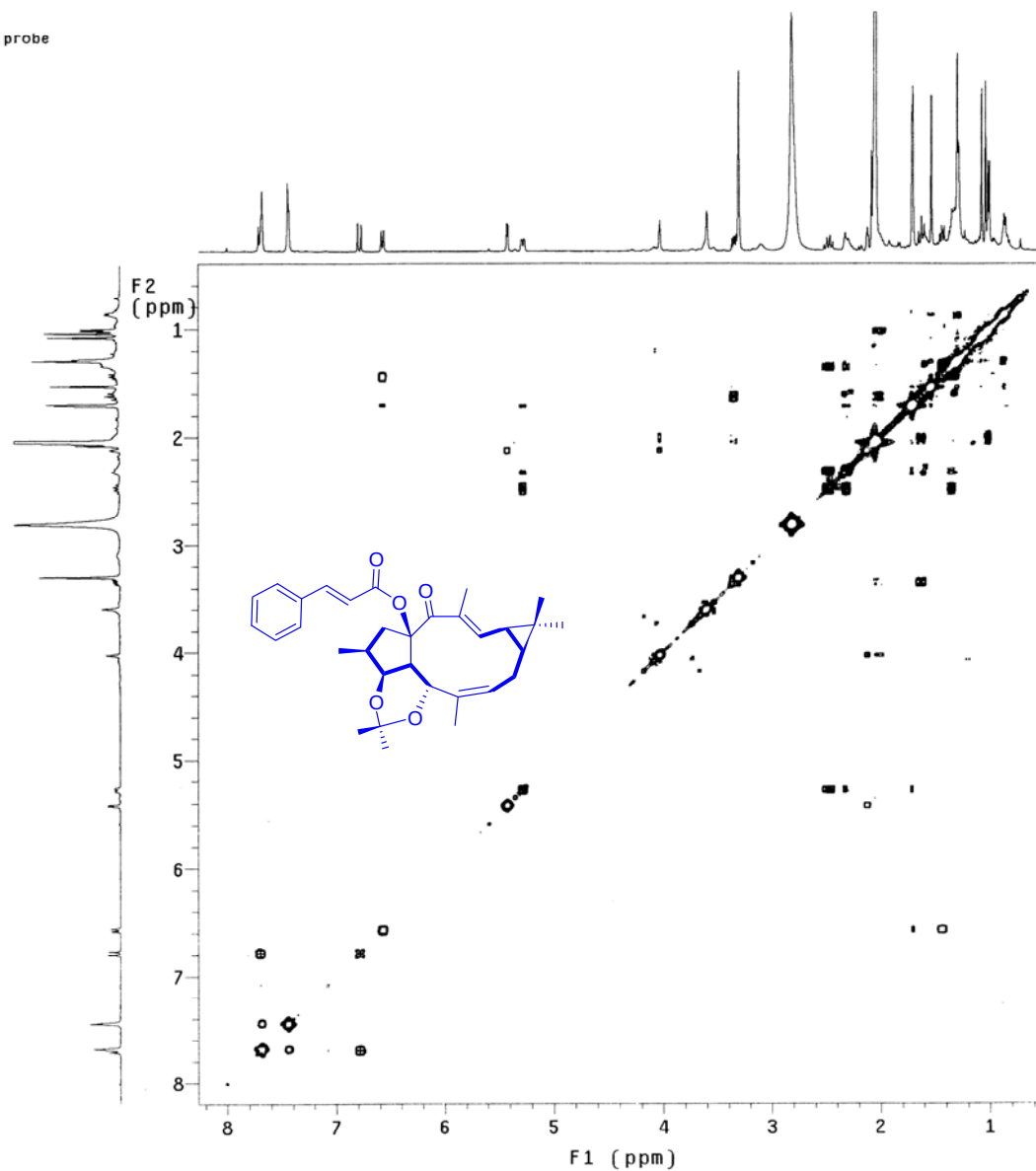


Figure S158. The ^1H - ^1H gCOSY Spectrum of 16 in CD_3COCD_3 (500 MHz).

S170

INOVA-501 gHSQC F4-1-1-C IN CD3COCD3 09.07.06 cold probe

Solvent: acetone
Temp. 25.0 C / 298.1 K
Sample #9, Operator: walkup
File: Ghsqc_01
INOVA-500 "IMM-501"

Relax. delay 1.301 sec
Acq. time 0.199 sec
Width 4473.8 Hz
2D Width 25133.5 Hz
8 repetitions
2 x 160 increments
OBSERVE H1, 499.7733203 MHz
DECOUPLE C13, 125.6793772 MHz
Power 33 dB
on during acquisition
off during delay
W40_cold modulated
DATA PROCESSING
Sine bell 0.056 sec
F1 DATA PROCESSING
Sine bell 0.003 sec
FT size 4096 x 2048
Total time 1 hr, 7 min, 3 sec

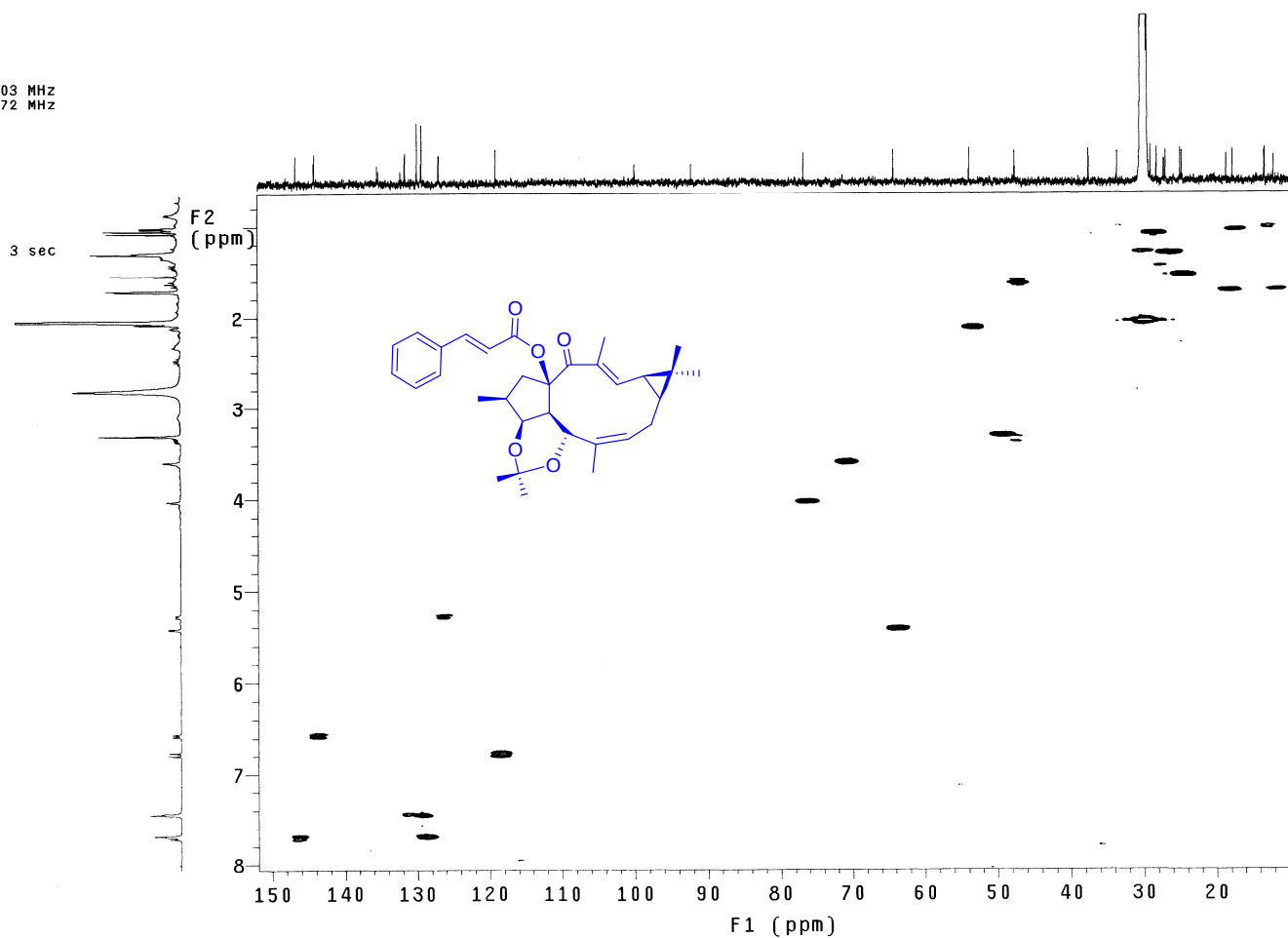


Figure S159. The gHSQC Spectrum of 16 in CD_3COCD_3 (500 MHz for ^1H NMR).

INOVA-501 gHMBC F4-1-1-C IN CD3COCD3 09.07.06 cold probe

Solvent: acetone
Temp. 25.0 C / 298.1 K
Sample #9, Operator: walkup
File: HMBCCD3C0CD30706-F4-1-1-C
INOVA-500 "IMM-501"

Relax. delay 1.000 sec
Mixing 0.080 sec
Acq. time 0.128 sec
Width 4473.8 Hz
2D Width 30165.9 Hz
32 repetitions
256 increments
OBSERVE H1, 499.7733233 MHz
DATA PROCESSING
Sine bell 0.044 sec
F1 DATA PROCESSING
Sine bell 0.004 sec
FT size 2048 x 2048
Total time 2 hr, 46 min, 22 sec

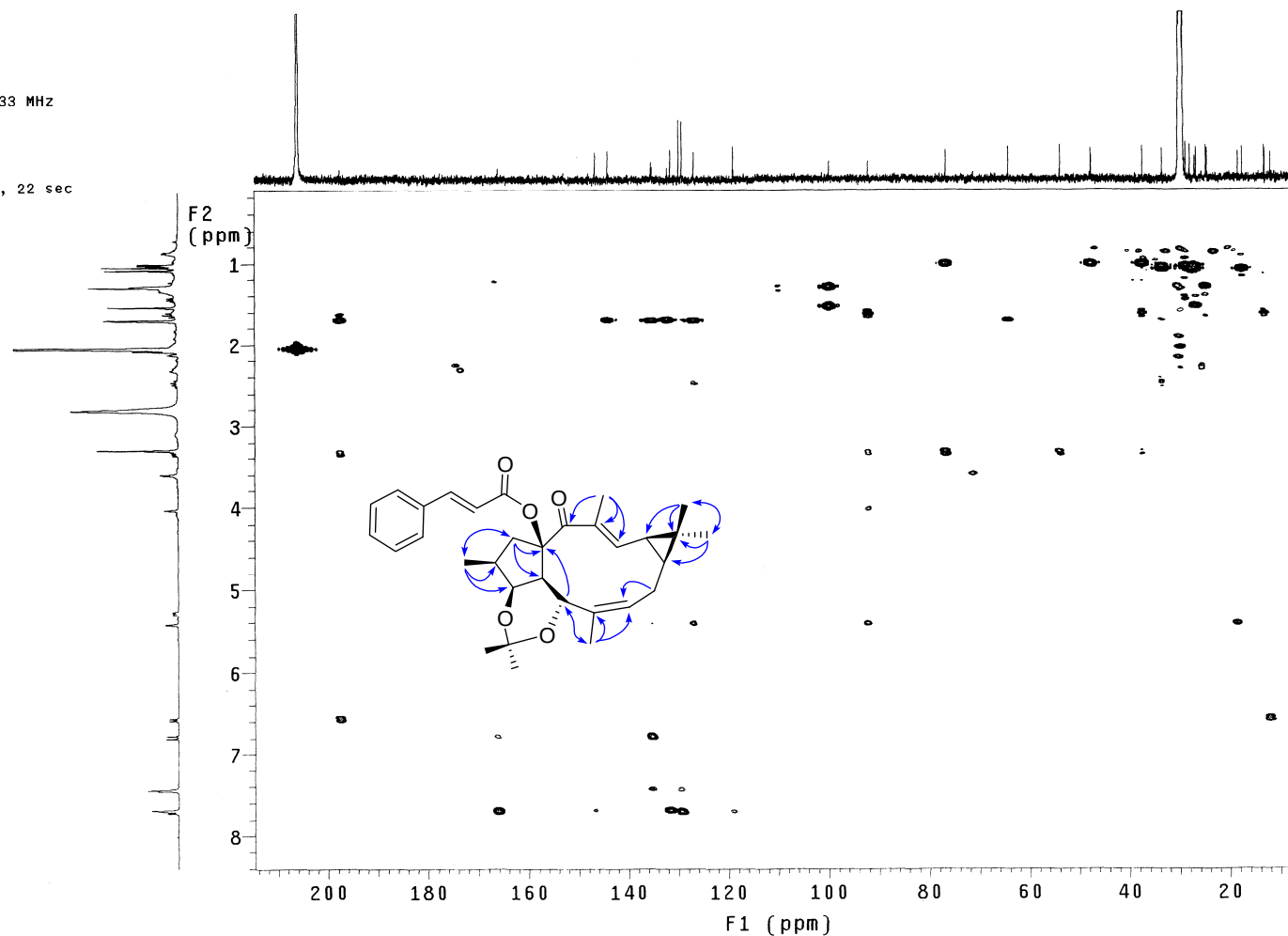


Figure S160. The gHMBC Spectrum of 16 in CD₃COCD₃ (500 MHz for ¹H NMR).

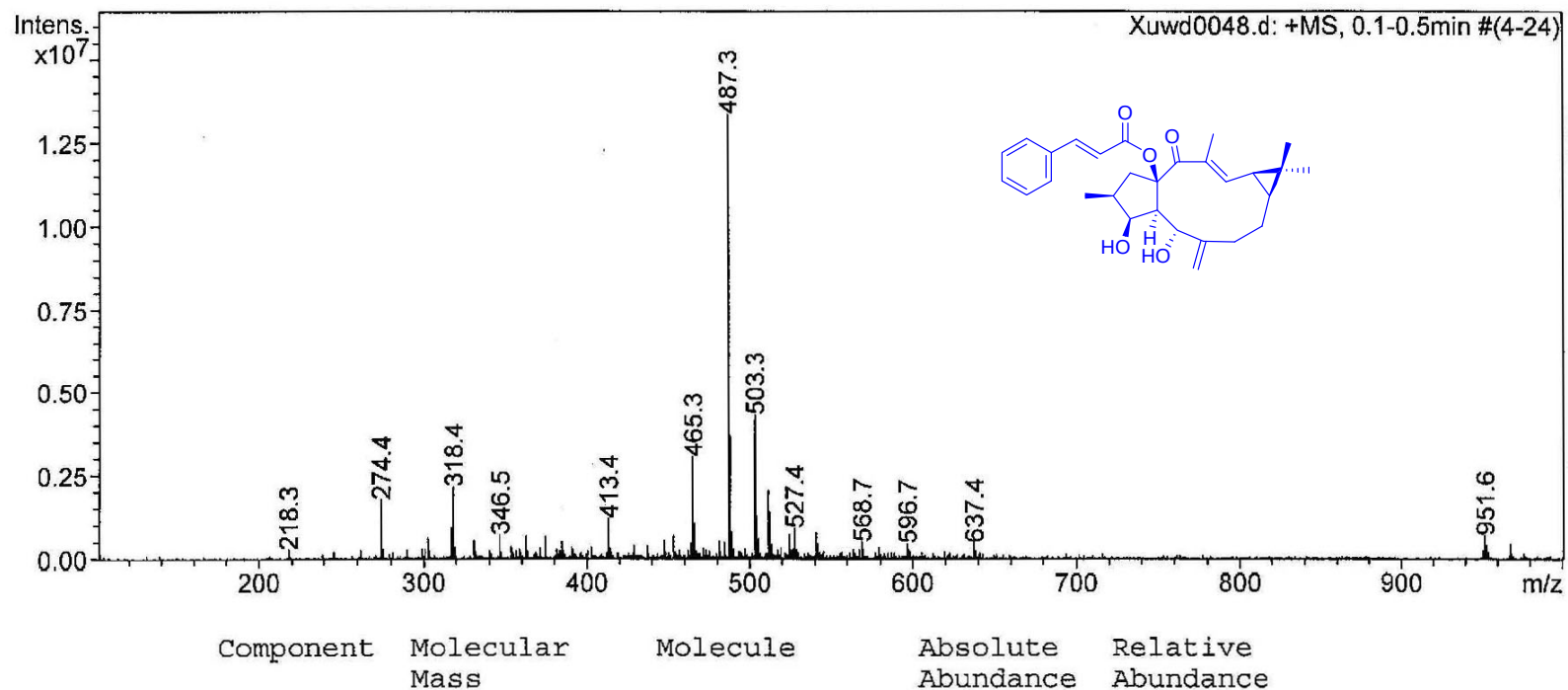


Figure S161. (+)-ESIMS Spectrum of 17.
 MS Formula Results: + Scan (9.180 min) Sub (200904164.d)

m/z	Ion	Formula	Abundance
465.26535	(M+H) ⁺	C ₂₉ H ₃₇ O ₅	568767

Best	Formula (M)	Ion Formula	Score	Cr	Calc m/z	Diff (ppm)	Mass Ma	Abund M	Spacing	DBE
☐	C ₂₂ H ₄₀ O ₁₀	C ₂₂ H ₄₁ O ₁₀	67.88		465.26942	8.8	45.56	78.91	99.29	3
☒	C ₂₉ H ₃₆ O ₅	C ₂₉ H ₃₇ O ₅	92.71		465.26355	-3.86	85.97	98.43	99.3	12

m/z	Ion	Formula	Abundance
487.24806	(M+Na) ⁺	C ₂₉ H ₃₆ NaO ₅	1622477.5

Best	Formula (M)	Ion Formula	Score	Cr	Calc m/z	Diff (ppm)	Mass Ma	Abund M	Spacing	DBE
☐	C ₂₂ H ₄₀ O ₁₀	C ₂₂ H ₄₀ NaO ₁₀	71.3		487.25137	7.17	60.91	65.74	98.76	3
☒	C ₂₉ H ₃₆ O ₅	C ₂₉ H ₃₆ NaO ₅	87.2		487.2455	-5.48	74.86	98.5	98.32	12

(+)-HRESIMS Data of 17.

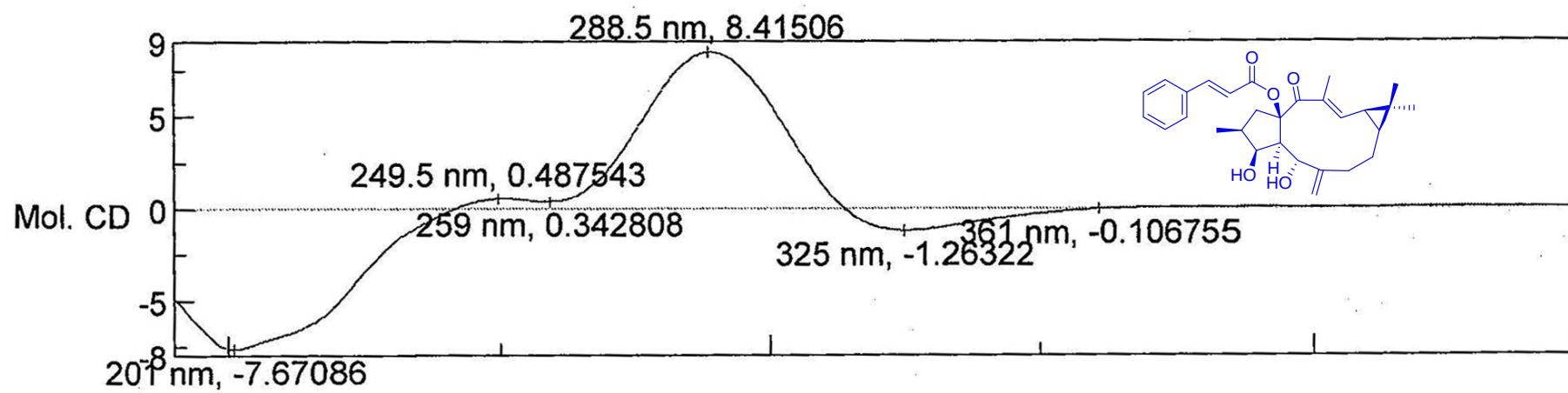


Figure S163. The CD Spectrum of 17.

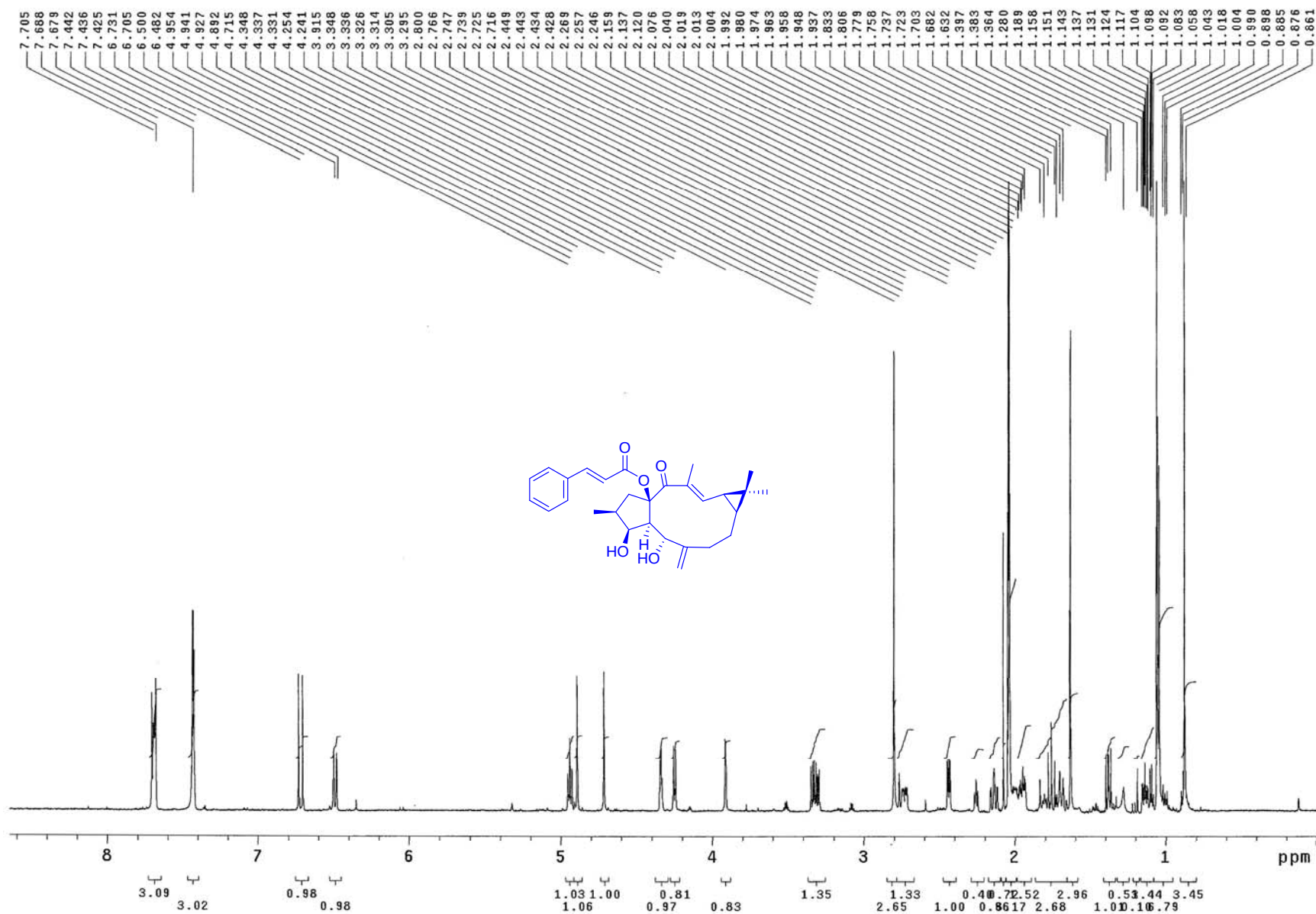
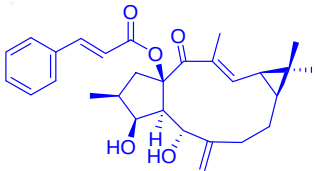
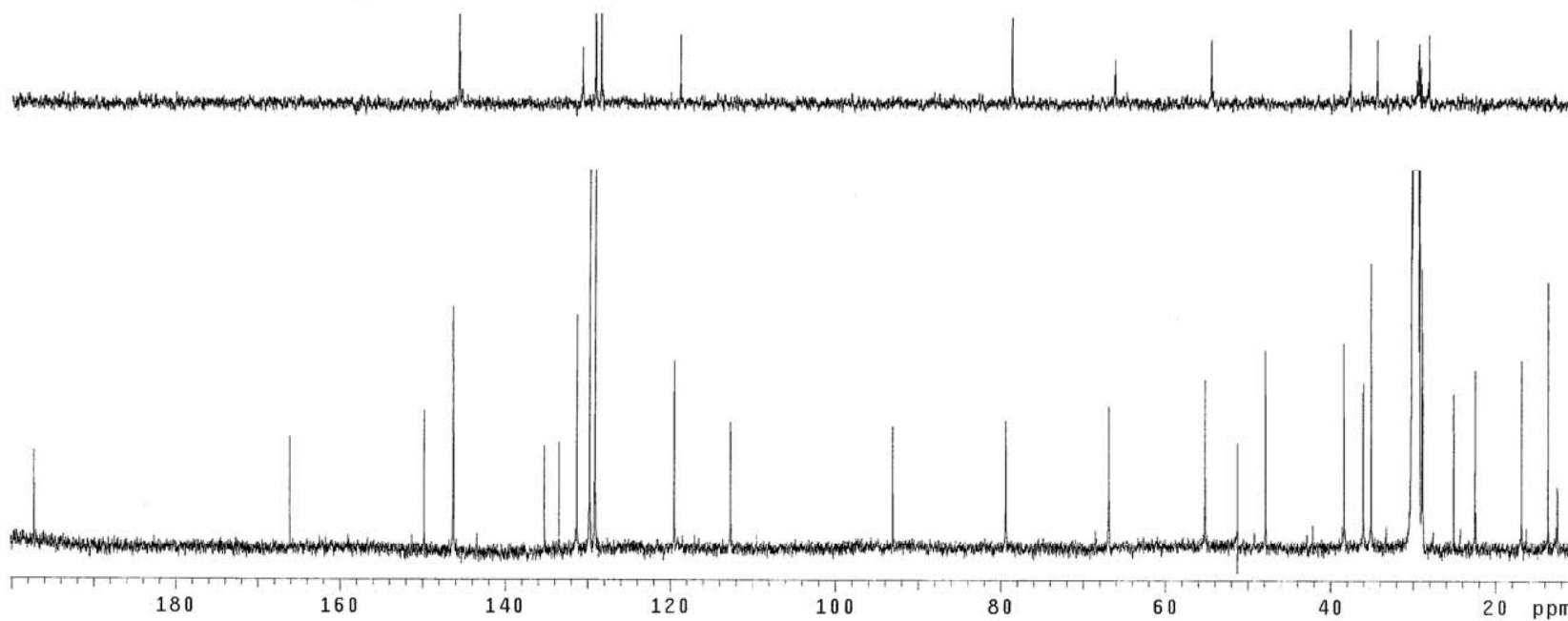
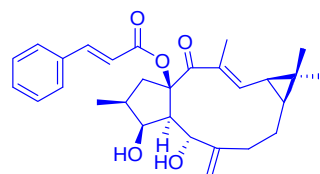


Figure S164. The ^1H NMR Spectrum of 17 in CD_3COCD_3 (600 MHz).



S177



S178

INOVA-500 gCOSY EM-E-13-13 IN CD3COCD3 09.03.09 COLD PROBE

Solvent: acetone
Temp. 25.0 C / 298.1 K
Operator: walkup
INOVA-500 "IMM-501"

Relax. delay 1.301 sec
Acq. time 0.133 sec
Width 3860.8 Hz
2D Width 3860.8 Hz
8 repetitions
256 increments
OBSERVE H1, 499.7733235 MHz
DATA PROCESSING
Sine bell 0.066 sec
F1 DATA PROCESSING
Sine bell 0.033 sec
FT size 1024 x 1024
Total time 50 min, 53 sec

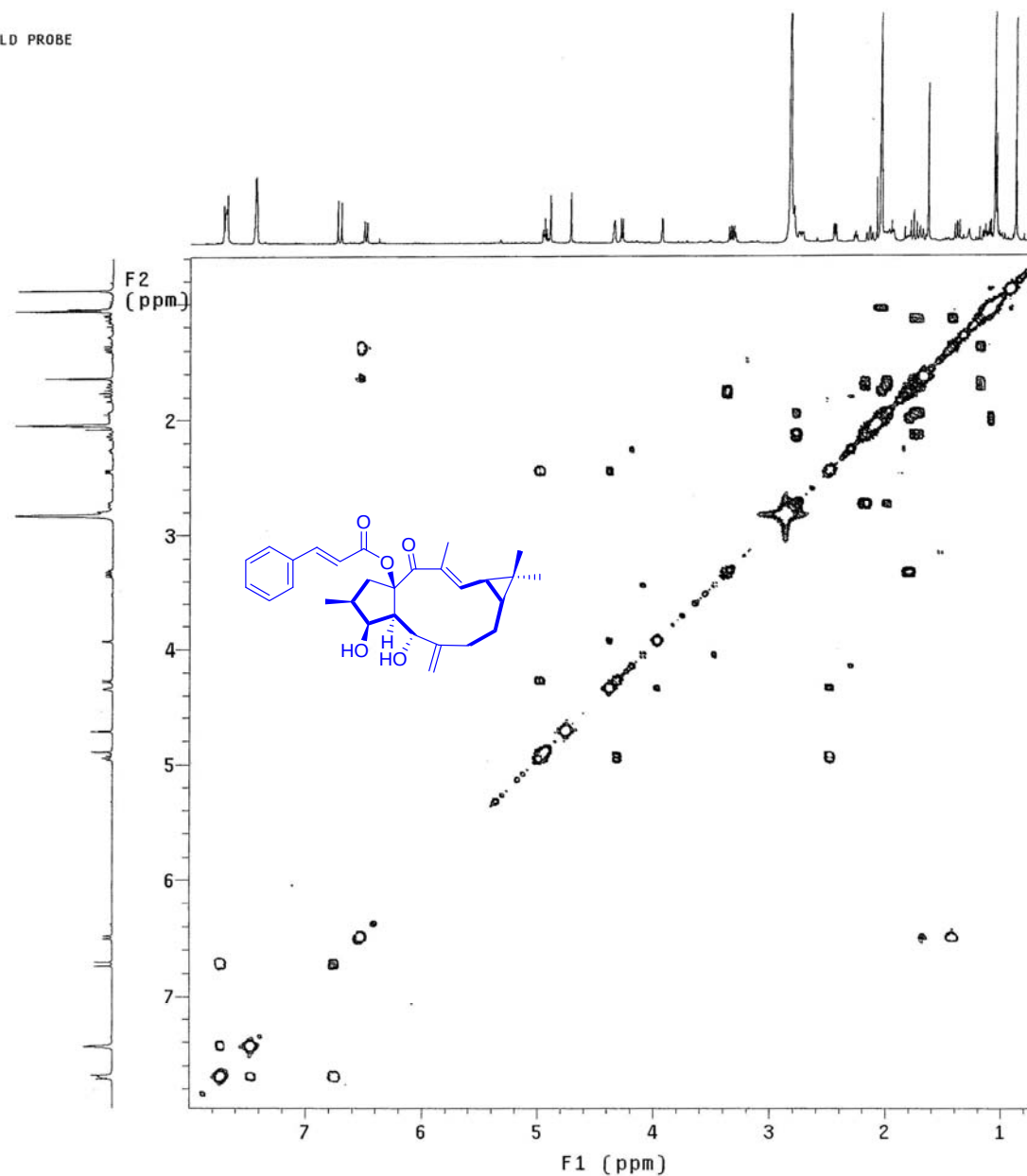


Figure S167. The ^1H - ^1H gCOSY Spectrum of 17 in CD_3COCD_3 (500 MHz).

S179

Solvent: acetone
Temp. 25.0 C / 298.1 K
Operator: walkup
INOVA-500 "IMM-501"

Relax. delay 1.301 sec
Acq. time 0.199 sec
Width 4055.2 Hz
2D Width 28040.7 Hz
32 repetitions
2 x 160 increments
OBSERVE H1, 499.7733233 MHz
DECOUPLE C13, 125.6825344 MHz
Power 33 dB
on during acquisition
off during delay
W40_cold modulated
DATA PROCESSING
Gauss apodization 0.044 sec
F1 DATA PROCESSING
Gauss apodization 0.003 sec
FT size 4096 x 2048
Total time 4 hr, 25 min, 39 sec

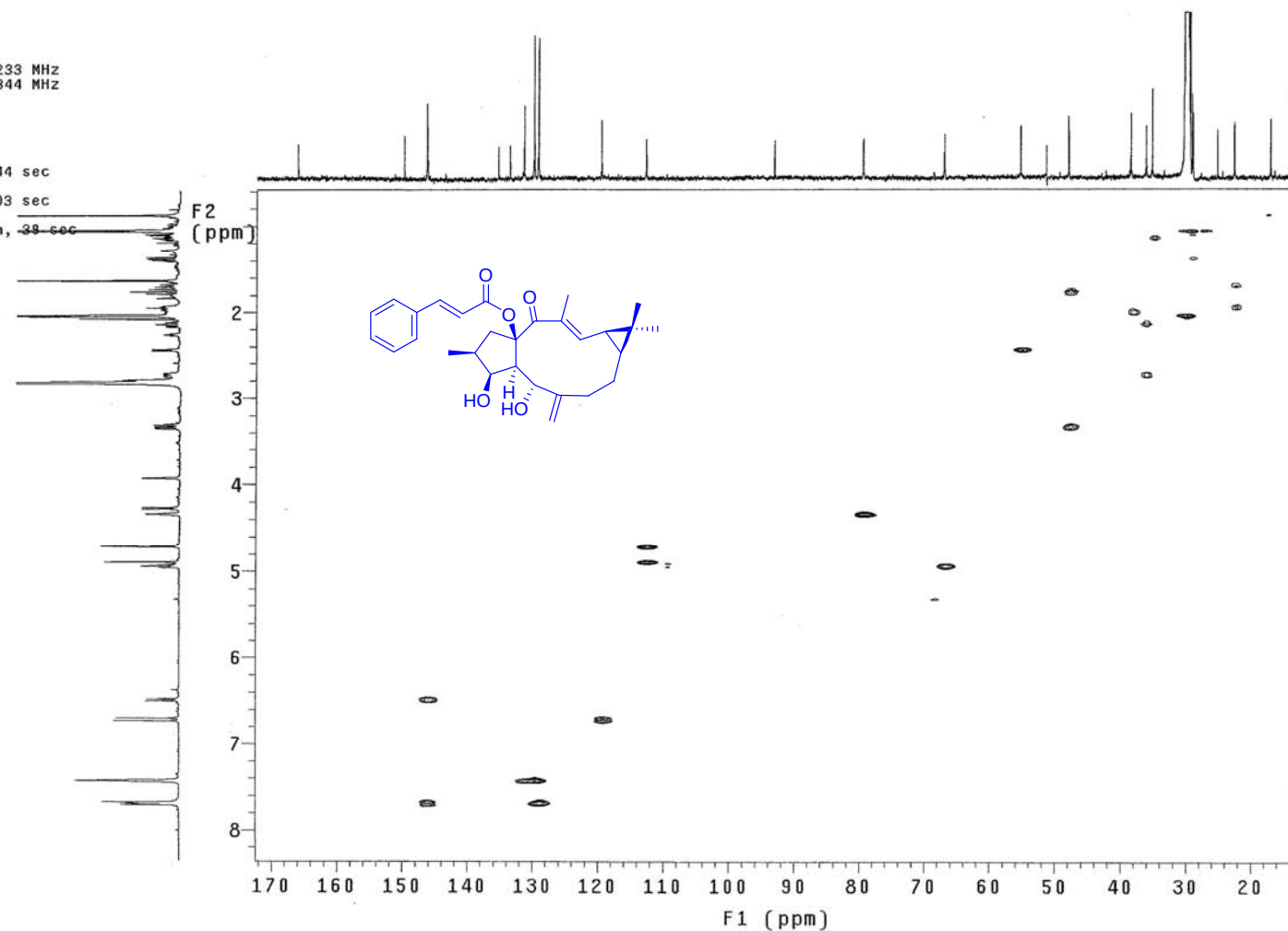


Figure S168. The gHSQC Spectrum of 17 in CD_3COCD_3 (500MHz for ^1H NMR).

Solvent: acetone
Temp, 25.0 C / 298.1 K
Operator: walkup
INOVA-500 "IMM-501"

Relax. delay 1.000 sec
Mixing 0.080 sec
Acq. time 0.128 sec
Width 3984.7 Hz
2D Width 28040.7 Hz
128 repetitions
256 increments
OBSERVE H1, 499.7733212 MHz
DATA PROCESSING
Sine bell 0.034 sec
F1 DATA PROCESSING
Sine bell 0.004 sec
FT size 2048 x 2048
Total time 11 hr, 3 min, 42 sec

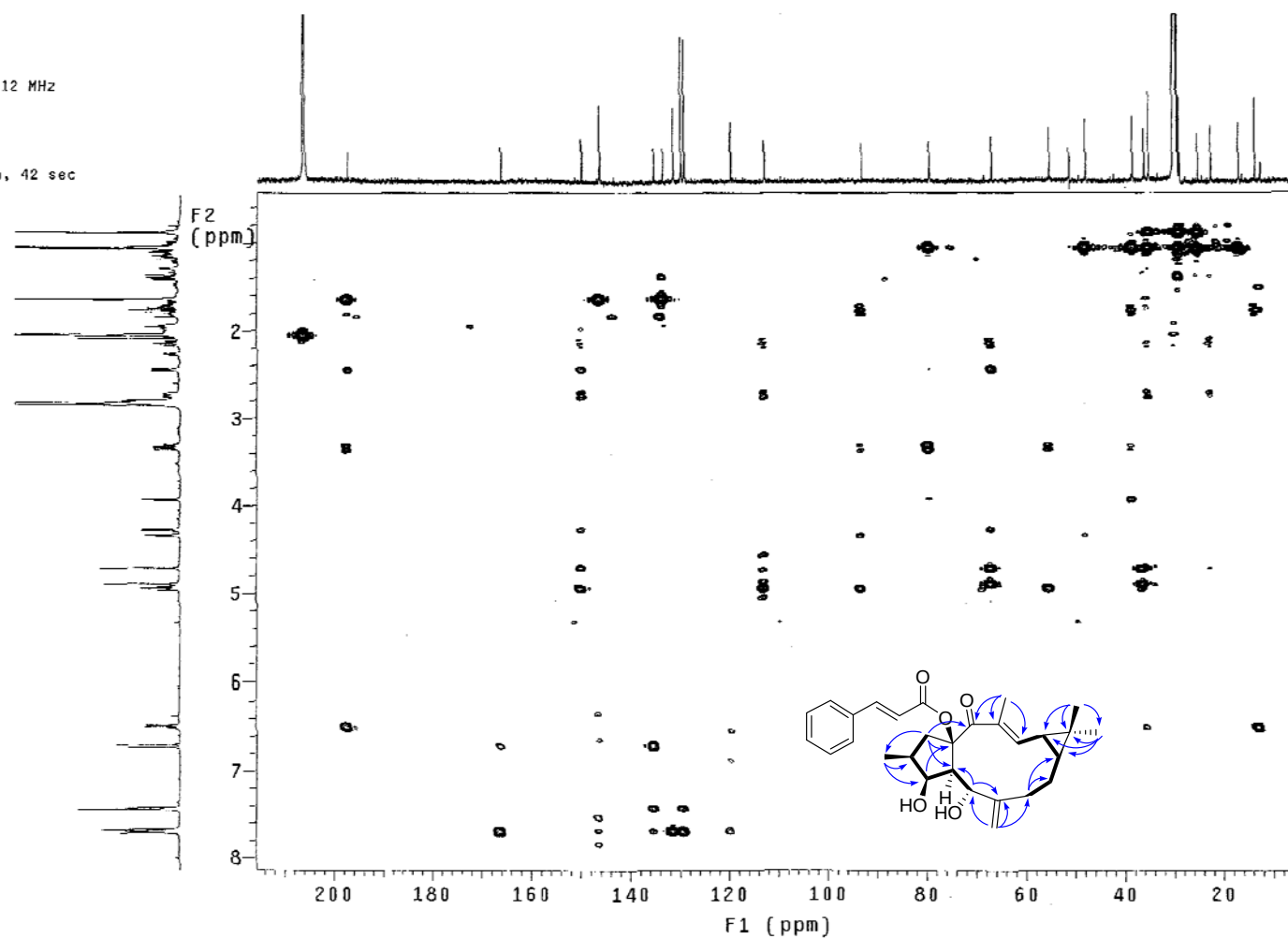


Figure S169. The gHMBC Spectrum of 17 in CD₃COCD₃ (500MHz for ¹H NMR).

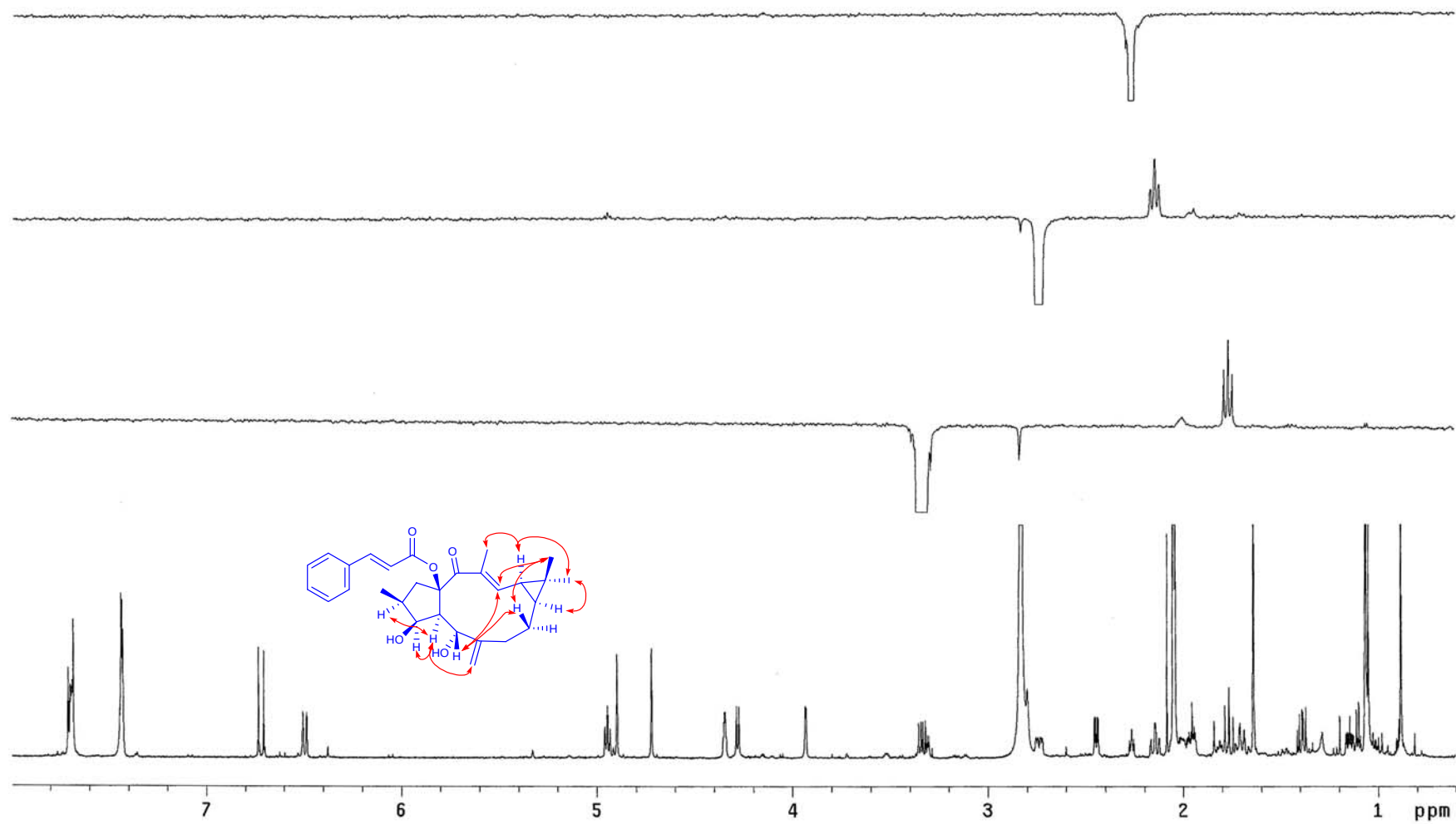


Figure S170. The NOE Difference Spectrum 1 of 17 in CD_3COCD_3 (600 MHz).

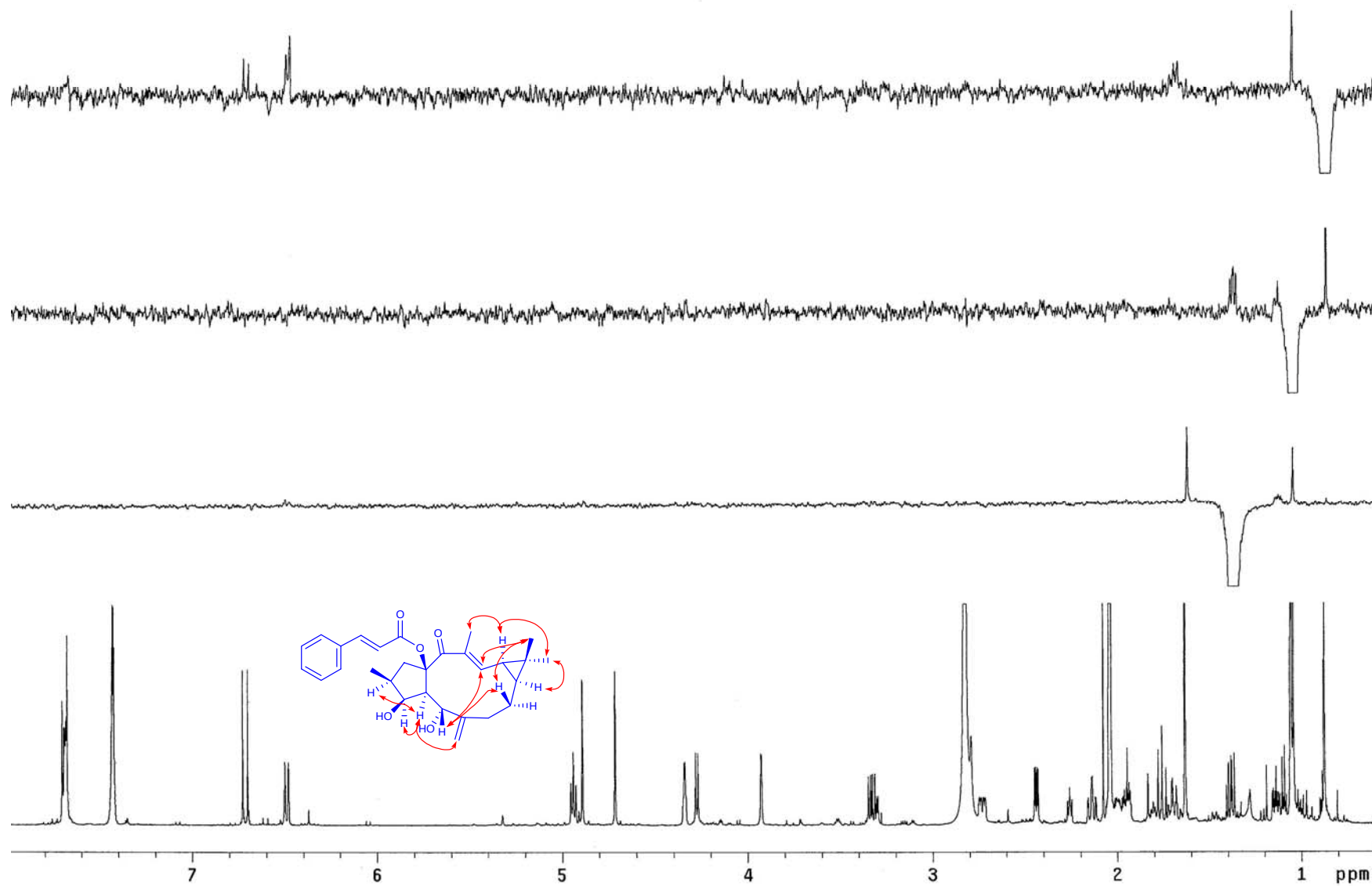


Figure S171. The NOE Difference Spectrum 2 of 17 in CD₃COCD₃ (600 MHz).

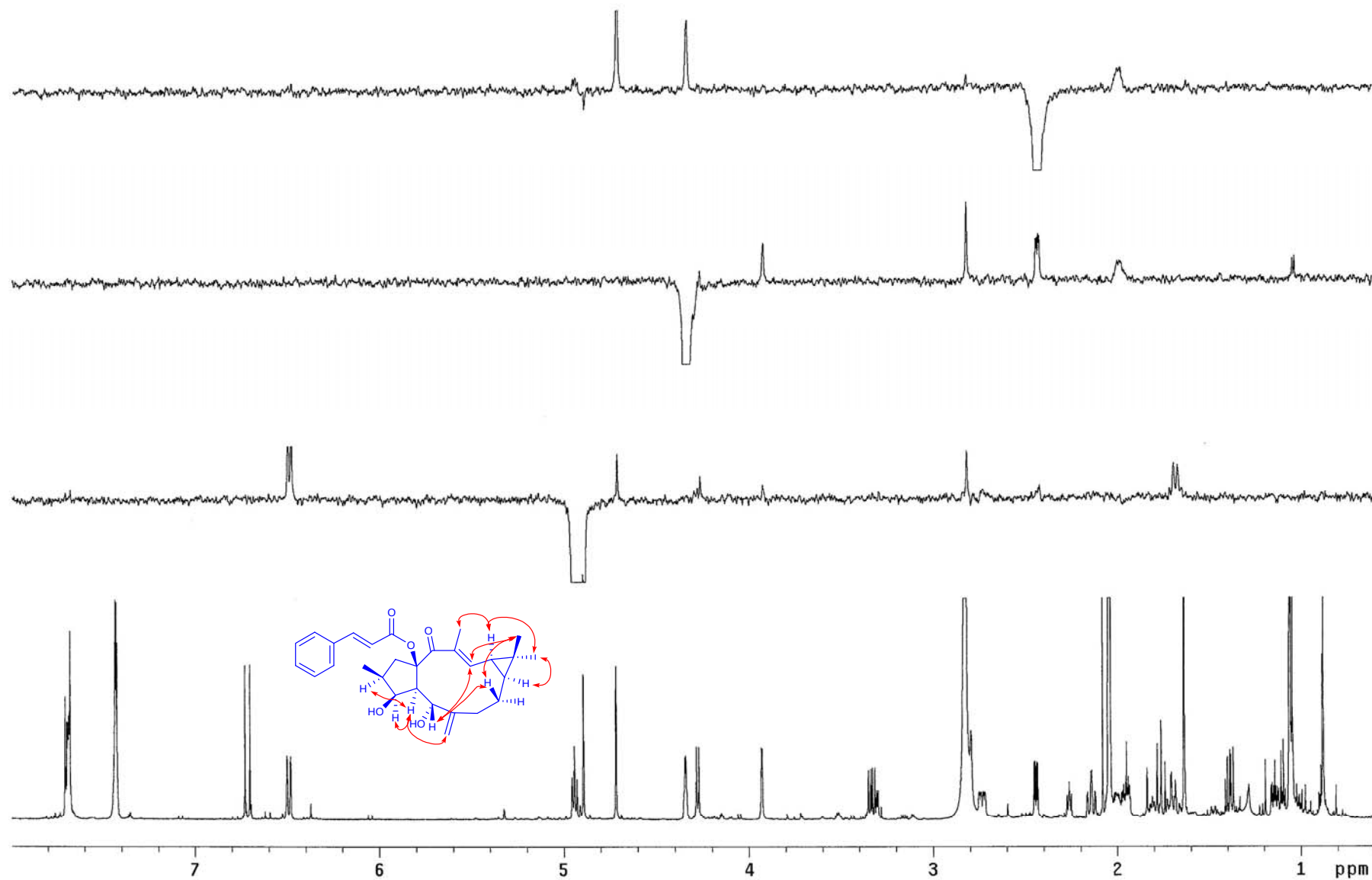


Figure S172. The NOE Difference Spectrum 3 of 17 in CD₃COCD₃ (600 MHz).

S184